Full wwPDB EM Validation Report (i)

Apr 22, 2024 – 08:51 pm BST

PDB ID	:	7A4I
EMDB ID	:	EMD-11634
Title	:	Aquifex aeolicus lumazine synthase-derived nucleocapsid variant NC-3
Authors	:	Tetter, S.; Hilvert, D.
Deposited on	:	2020-08-19
Resolution	:	7.04 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

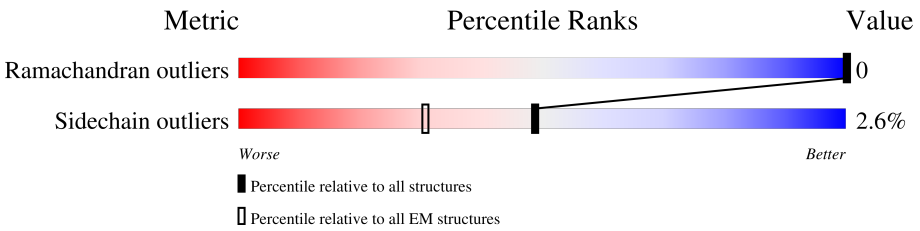
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 7.04 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	0A	197	14% 78% • 20%
1	0B	197	16% 79% • 20%
1	0C	197	23% 77% • 20%
1	0D	197	15% 80% • 19%
1	1A	197	16% 78% • 20%
1	1B	197	16% 79% • 20%
1	1C	197	26% 77% • 20%
1	1D	197	17% 80% • 19%
1	2A	197	14% 78% • 20%

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Mol	Chain	Length	Quality of chain
1	2B	197	14% 79% 20%
1	2C	197	23% 77% 20%
1	2D	197	17% 80% 19%
1	3A	197	14% 78% 20%
1	3B	197	15% 79% 20%
1	3C	197	22% 77% 20%
1	3D	197	17% 80% 19%
1	4A	197	14% 78% 20%
1	4B	197	16% 79% 20%
1	4C	197	25% 77% 20%
1	4D	197	16% 80% 19%
1	5A	197	14% 78% 20%
1	5B	197	16% 79% 20%
1	5C	197	24% 77% 20%
1	5D	197	16% 80% 19%
1	6A	197	14% 78% 20%
1	6B	197	15% 79% 20%
1	6C	197	23% 77% 20%
1	6D	197	17% 80% 19%
1	7A	197	14% 78% 20%
1	7B	197	14% 79% 20%
1	7C	197	23% 77% 20%
1	7D	197	17% 80% 19%
1	AA	197	14% 78% 20%
1	AB	197	15% 79% 20%

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Mol	Chain	Length	Quality of chain
1	AC	197	22% 77% 20%
1	AD	197	17% 80% 19%
1	BA	197	12% 78% 20%
1	BB	197	15% 79% 20%
1	BC	197	23% 77% 20%
1	BD	197	16% 80% 19%
1	CA	197	14% 78% 20%
1	CB	197	16% 79% 20%
1	CC	197	23% 77% 20%
1	CD	197	15% 80% 19%
1	DA	197	13% 78% 20%
1	DB	197	15% 79% 20%
1	DC	197	22% 77% 20%
1	DD	197	17% 80% 19%
1	EA	197	14% 78% 20%
1	EB	197	14% 79% 20%
1	EC	197	23% 77% 20%
1	ED	197	17% 80% 19%
1	FA	197	14% 78% 20%
1	FB	197	14% 79% 20%
1	FC	197	23% 77% 20%
1	FD	197	17% 80% 19%
1	GA	197	14% 78% 20%
1	GB	197	14% 79% 20%
1	GC	197	24% 77% 20%

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Mol	Chain	Length	Quality of chain
1	GD	197	17% 80% 19%
1	HA	197	12% 78% 20%
1	HB	197	15% 79% 20%
1	HC	197	23% 77% 20%
1	HD	197	16% 80% 19%
1	IA	197	14% 78% 20%
1	IB	197	16% 79% 20%
1	IC	197	23% 77% 20%
1	ID	197	15% 80% 19%
1	JA	197	14% 78% 20%
1	JB	197	16% 79% 20%
1	JC	197	23% 77% 20%
1	JD	197	15% 80% 19%
1	KA	197	13% 78% 20%
1	KB	197	15% 79% 20%
1	KC	197	22% 77% 20%
1	KD	197	17% 80% 19%
1	LA	197	14% 78% 20%
1	LB	197	14% 79% 20%
1	LC	197	23% 77% 20%
1	LD	197	17% 80% 19%
1	MA	197	14% 78% 20%
1	MB	197	15% 79% 20%
1	MC	197	22% 77% 20%
1	MD	197	17% 80% 19%

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Mol	Chain	Length	Quality of chain
1	NA	197	12% 78% 20%
1	NB	197	15% 79% 20%
1	NC	197	23% 77% 20%
1	ND	197	16% 80% 19%
1	OA	197	14% 78% 20%
1	OB	197	16% 79% 20%
1	OC	197	24% 77% 20%
1	OD	197	17% 80% 19%
1	PA	197	14% 78% 20%
1	PB	197	16% 79% 20%
1	PC	197	23% 77% 20%
1	PD	197	15% 80% 19%
1	QA	197	14% 78% 20%
1	QB	197	14% 79% 20%
1	QC	197	23% 77% 20%
1	QD	197	17% 80% 19%
1	RA	197	14% 78% 20%
1	RB	197	15% 79% 20%
1	RC	197	22% 77% 20%
1	RD	197	17% 80% 19%
1	SA	197	14% 78% 20%
1	SB	197	16% 79% 20%
1	SC	197	23% 77% 20%
1	SD	197	17% 80% 19%
1	TA	197	15% 78% 20%

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Mol	Chain	Length	Quality of chain
1	TB	197	16% 79% 20%
1	TC	197	23% 77% 20%
1	TD	197	17% 80% 19%
1	UA	197	13% 78% 20%
1	UB	197	15% 79% 20%
1	UC	197	22% 77% 20%
1	UD	197	17% 80% 19%
1	VA	197	13% 78% 20%
1	VB	197	15% 79% 20%
1	VC	197	22% 77% 20%
1	VD	197	17% 80% 19%
1	WA	197	14% 78% 20%
1	WB	197	14% 79% 20%
1	WC	197	23% 77% 20%
1	WD	197	17% 80% 19%
1	XA	197	16% 78% 20%
1	XB	197	15% 79% 20%
1	XC	197	25% 77% 20%
1	XD	197	16% 80% 19%
1	YA	197	12% 78% 20%
1	YB	197	15% 79% 20%
1	YC	197	23% 77% 20%
1	YD	197	16% 80% 19%
1	ZA	197	12% 78% 20%
1	ZB	197	15% 79% 20%

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Mol	Chain	Length	Quality of chain
1	ZC	197	23% 77% • 20%
1	ZD	197	16% 80% • 19%
1	aA	197	14% 78% • 20%
1	aB	197	16% 79% • 20%
1	aC	197	23% 77% • 20%
1	aD	197	15% 80% • 19%
1	bA	197	13% 78% • 20%
1	bB	197	15% 79% • 20%
1	bC	197	22% 77% • 20%
1	bD	197	17% 80% • 19%
1	cA	197	14% 78% • 20%
1	cB	197	14% 79% • 20%
1	cC	197	24% 77% • 20%
1	cD	197	17% 80% • 19%
1	dA	197	13% 78% • 20%
1	dB	197	16% 79% • 20%
1	dC	197	24% 77% • 20%
1	dD	197	17% 80% • 19%
1	eA	197	14% 78% • 20%
1	eB	197	15% 79% • 20%
1	eC	197	22% 77% • 20%
1	eD	197	17% 80% • 19%
1	fA	197	12% 78% • 20%
1	fB	197	15% 79% • 20%
1	fC	197	23% 77% • 20%

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Mol	Chain	Length	Quality of chain
1	fD	197	16% 80% 19%
1	gA	197	14% 78% 20%
1	gB	197	16% 79% 20%
1	gC	197	23% 77% 20%
1	gD	197	15% 80% 19%
1	hA	197	13% 78% 20%
1	hB	197	15% 79% 20%
1	hC	197	22% 77% 20%
1	hD	197	17% 80% 19%
1	iA	197	15% 78% 20%
1	iB	197	15% 79% 20%
1	iC	197	24% 77% 20%
1	iD	197	17% 80% 19%
1	jA	197	14% 78% 20%
1	jB	197	14% 79% 20%
1	jC	197	23% 77% 20%
1	jD	197	17% 80% 19%
1	kA	197	15% 78% 20%
1	kB	197	14% 79% 20%
1	kC	197	24% 77% 20%
1	kD	197	17% 80% 19%
1	lA	197	12% 78% 20%
1	lB	197	15% 79% 20%
1	lC	197	23% 77% 20%
1	lD	197	16% 80% 19%

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Mol	Chain	Length	Quality of chain
1	mA	197	14% 78% 20%
1	mB	197	16% 79% 20%
1	mC	197	23% 77% 20%
1	mD	197	16% 80% 19%
1	nA	197	15% 78% 20%
1	nB	197	16% 79% 20%
1	nC	197	22% 77% 20%
1	nD	197	17% 80% 19%
1	oA	197	16% 78% 20%
1	oB	197	15% 79% 20%
1	oC	197	25% 77% 20%
1	oD	197	17% 80% 19%
1	pA	197	14% 78% 20%
1	pB	197	14% 79% 20%
1	pC	197	23% 77% 20%
1	pD	197	17% 80% 19%
1	qA	197	14% 78% 20%
1	qB	197	14% 79% 20%
1	qC	197	24% 77% 20%
1	qD	197	16% 80% 19%
1	rA	197	13% 78% 20%
1	rB	197	15% 79% 20%
1	rC	197	23% 77% 20%
1	rD	197	16% 80% 19%
1	sA	197	12% 78% 20%

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Mol	Chain	Length	Quality of chain
1	sB	197	15% 79% 20%
1	sC	197	23% 77% 20%
1	sD	197	16% 80% 19%
1	tA	197	15% 78% 20%
1	tB	197	14% 79% 20%
1	tC	197	23% 77% 20%
1	tD	197	16% 80% 19%
1	uA	197	14% 78% 20%
1	uB	197	15% 79% 20%
1	uC	197	25% 77% 20%
1	uD	197	17% 80% 19%
1	vA	197	14% 78% 20%
1	vB	197	15% 79% 20%
1	vC	197	24% 77% 20%
1	vD	197	17% 80% 19%
1	wA	197	14% 78% 20%
1	wB	197	14% 79% 20%
1	wC	197	23% 77% 20%
1	wD	197	17% 80% 19%
1	xA	197	14% 78% 20%
1	xB	197	15% 79% 20%
1	xC	197	22% 77% 20%
1	xD	197	17% 80% 19%
1	yA	197	12% 78% 20%
1	yB	197	15% 79% 20%

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Mol	Chain	Length	Quality of chain
1	yC	197	23% 77% • 20%
1	yD	197	16% 80% • 19%
1	zA	197	14% 78% • 20%
1	zB	197	16% 79% • 20%
1	zC	197	23% 77% • 20%
1	zD	197	15% 80% • 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 290520 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 Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	157	1205	755	220	228	2	0	0
1	AB	158	1210	758	221	229	2	0	0
1	AC	157	1205	755	220	228	2	0	0
1	AD	159	1222	765	222	233	2	0	0
1	BA	157	1205	755	220	228	2	0	0
1	BB	158	1210	758	221	229	2	0	0
1	BC	157	1205	755	220	228	2	0	0
1	BD	159	1222	765	222	233	2	0	0
1	CA	157	1205	755	220	228	2	0	0
1	CB	158	1210	758	221	229	2	0	0
1	CC	157	1205	755	220	228	2	0	0
1	CD	159	1222	765	222	233	2	0	0
1	DA	157	1205	755	220	228	2	0	0
1	DB	158	1210	758	221	229	2	0	0
1	DC	157	1205	755	220	228	2	0	0
1	DD	159	1222	765	222	233	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	EA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	EB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	EC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	ED	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	FA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	FB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	FC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	FD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	GA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	GB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	GC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	GD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	HA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	HB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	HC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	HD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	IA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	IB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	IC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	ID	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	5A	157	1205	755	220	228	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	5B	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	5C	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	5D	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	JA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	JB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	JC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	JD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	KA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	KB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	KC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	KD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	LA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	LB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	LC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	LD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	MA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	MB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	MC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	MD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	NA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	NB	158	1210	758	221	229	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	NC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	ND	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	OA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	OB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	OC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	OD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	PA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	PB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	PC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	PD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	6A	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	6B	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	6C	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	6D	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	7A	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	7B	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	7C	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	7D	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	QA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	QB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	QC	157	1205	755	220	228	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	QD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	RA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	RB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	RC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	RD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	SA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	SB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	SC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	SD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	TA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	TB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	TC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	TD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	UA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	UB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	UC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	UD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	VA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	VB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	VC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	VD	159	1222	765	222	233	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	WA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	WB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	WC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	WD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	XA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	XB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	XC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	XD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	YA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	YB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	YC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	YD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	ZA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	ZB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	ZC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	ZD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	aA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	aB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	aC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	aD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	bA	157	1205	755	220	228	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	bB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	bC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	bD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	cA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	cB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	cC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	cD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	dA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	dB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	dC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	dD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	eA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	eB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	eC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	eD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	fA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	fB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	fC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	fD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	gA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	gB	158	1210	758	221	229	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	gC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	gD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	hA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	hB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	hC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	hD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	iA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	iB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	iC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	iD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	jA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	jB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	jC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	jD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	kA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	kB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	kC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	kD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	lA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	lB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	lC	157	1205	755	220	228	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	lD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	mA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	mB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	mC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	mD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	nA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	nB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	nC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	nD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	oA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	oB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	oC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	oD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	pA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	pB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	pC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	pD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	qA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	qB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	qC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	qD	159	1222	765	222	233	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	rA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	rB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	rC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	rD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	sA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	sB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	sC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	sD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	tA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	tB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	tC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	tD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	uA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	uB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	uC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	uD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	vA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	vB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	vC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	vD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	wA	157	1205	755	220	228	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	wB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	wC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	wD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	xA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	xB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	xC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	xD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	yA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	yB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	yC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	yD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	zA	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	zB	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	zC	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	zD	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	0A	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	0B	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	0C	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	0D	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	1A	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	1B	158	1210	758	221	229	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1C	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	1D	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	2A	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	2B	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	2C	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	2D	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	3A	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	3B	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	3C	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	3D	159	1222	765	222	233	2	0	0
			Total	C	N	O	S		
1	4A	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	4B	158	1210	758	221	229	2	0	0
			Total	C	N	O	S		
1	4C	157	1205	755	220	228	2	0	0
			Total	C	N	O	S		
1	4D	159	1222	765	222	233	2	0	0

There are 9120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1	MET	-	cloning artifact	UNP P03045
AA	2	GLY	-	cloning artifact	UNP P03045
AA	3	ASN	-	cloning artifact	UNP P03045
AA	4	ALA	-	cloning artifact	UNP P03045
AA	5	LYS	-	cloning artifact	UNP P03045
AA	6	THR	-	cloning artifact	UNP P03045
AA	24	ALA	-	linker	UNP P03045
AA	25	GLY	-	linker	UNP P03045
AA	26	ALA	-	linker	UNP P03045
AA	27	GLY	-	linker	UNP P03045
AA	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
AA	29	GLY	-	linker	UNP P03045
AA	30	ALA	-	linker	UNP P03045
AA	31	MET	-	linker	UNP P03045
AA	39	ASN	ILE	engineered mutation	UNP O66529
AA	42	VAL	GLU	engineered mutation	UNP O66529
AA	58	VAL	ILE	engineered mutation	UNP O66529
AA	61	ASP	GLY	engineered mutation	UNP O66529
AA	62	ILE	VAL	engineered mutation	UNP O66529
AA	97	TYR	PHE	engineered mutation	UNP O66529
AA	102	GLY	-	linker	UNP O66529
AA	103	THR	-	linker	UNP O66529
AA	104	GLY	-	linker	UNP O66529
AA	105	HIS	-	linker	UNP O66529
AA	106	HIS	-	linker	UNP O66529
AA	107	HIS	-	linker	UNP O66529
AA	108	HIS	-	linker	UNP O66529
AA	109	HIS	-	linker	UNP O66529
AA	110	HIS	-	linker	UNP O66529
AA	111	GLY	-	linker	UNP O66529
AA	112	SER	-	linker	UNP O66529
AA	113	SER	-	linker	UNP O66529
AA	114	ILE	MET	engineered mutation	UNP O66529
AA	115	GLU	GLN	engineered mutation	UNP O66529
AA	138	THR	ALA	engineered mutation	UNP O66529
AA	177	ASP	GLY	engineered mutation	UNP O66529
AA	191	PHE	ILE	engineered mutation	UNP O66529
AA	193	ASP	VAL	engineered mutation	UNP O66529
AB	1	MET	-	cloning artifact	UNP P03045
AB	2	GLY	-	cloning artifact	UNP P03045
AB	3	ASN	-	cloning artifact	UNP P03045
AB	4	ALA	-	cloning artifact	UNP P03045
AB	5	LYS	-	cloning artifact	UNP P03045
AB	6	THR	-	cloning artifact	UNP P03045
AB	24	ALA	-	linker	UNP P03045
AB	25	GLY	-	linker	UNP P03045
AB	26	ALA	-	linker	UNP P03045
AB	27	GLY	-	linker	UNP P03045
AB	28	ALA	-	linker	UNP P03045
AB	29	GLY	-	linker	UNP P03045
AB	30	ALA	-	linker	UNP P03045
AB	31	MET	-	linker	UNP P03045
AB	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
AB	42	VAL	GLU	engineered mutation	UNP O66529
AB	58	VAL	ILE	engineered mutation	UNP O66529
AB	61	ASP	GLY	engineered mutation	UNP O66529
AB	62	ILE	VAL	engineered mutation	UNP O66529
AB	97	TYR	PHE	engineered mutation	UNP O66529
AB	102	GLY	-	linker	UNP O66529
AB	103	THR	-	linker	UNP O66529
AB	104	GLY	-	linker	UNP O66529
AB	105	HIS	-	linker	UNP O66529
AB	106	HIS	-	linker	UNP O66529
AB	107	HIS	-	linker	UNP O66529
AB	108	HIS	-	linker	UNP O66529
AB	109	HIS	-	linker	UNP O66529
AB	110	HIS	-	linker	UNP O66529
AB	111	GLY	-	linker	UNP O66529
AB	112	SER	-	linker	UNP O66529
AB	113	SER	-	linker	UNP O66529
AB	114	ILE	MET	engineered mutation	UNP O66529
AB	115	GLU	GLN	engineered mutation	UNP O66529
AB	138	THR	ALA	engineered mutation	UNP O66529
AB	177	ASP	GLY	engineered mutation	UNP O66529
AB	191	PHE	ILE	engineered mutation	UNP O66529
AB	193	ASP	VAL	engineered mutation	UNP O66529
AC	1	MET	-	cloning artifact	UNP P03045
AC	2	GLY	-	cloning artifact	UNP P03045
AC	3	ASN	-	cloning artifact	UNP P03045
AC	4	ALA	-	cloning artifact	UNP P03045
AC	5	LYS	-	cloning artifact	UNP P03045
AC	6	THR	-	cloning artifact	UNP P03045
AC	24	ALA	-	linker	UNP P03045
AC	25	GLY	-	linker	UNP P03045
AC	26	ALA	-	linker	UNP P03045
AC	27	GLY	-	linker	UNP P03045
AC	28	ALA	-	linker	UNP P03045
AC	29	GLY	-	linker	UNP P03045
AC	30	ALA	-	linker	UNP P03045
AC	31	MET	-	linker	UNP P03045
AC	39	ASN	ILE	engineered mutation	UNP O66529
AC	42	VAL	GLU	engineered mutation	UNP O66529
AC	58	VAL	ILE	engineered mutation	UNP O66529
AC	61	ASP	GLY	engineered mutation	UNP O66529
AC	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
AC	97	TYR	PHE	engineered mutation	UNP O66529
AC	102	GLY	-	linker	UNP O66529
AC	103	THR	-	linker	UNP O66529
AC	104	GLY	-	linker	UNP O66529
AC	105	HIS	-	linker	UNP O66529
AC	106	HIS	-	linker	UNP O66529
AC	107	HIS	-	linker	UNP O66529
AC	108	HIS	-	linker	UNP O66529
AC	109	HIS	-	linker	UNP O66529
AC	110	HIS	-	linker	UNP O66529
AC	111	GLY	-	linker	UNP O66529
AC	112	SER	-	linker	UNP O66529
AC	113	SER	-	linker	UNP O66529
AC	114	ILE	MET	engineered mutation	UNP O66529
AC	115	GLU	GLN	engineered mutation	UNP O66529
AC	138	THR	ALA	engineered mutation	UNP O66529
AC	177	ASP	GLY	engineered mutation	UNP O66529
AC	191	PHE	ILE	engineered mutation	UNP O66529
AC	193	ASP	VAL	engineered mutation	UNP O66529
AD	1	MET	-	cloning artifact	UNP P03045
AD	2	GLY	-	cloning artifact	UNP P03045
AD	3	ASN	-	cloning artifact	UNP P03045
AD	4	ALA	-	cloning artifact	UNP P03045
AD	5	LYS	-	cloning artifact	UNP P03045
AD	6	THR	-	cloning artifact	UNP P03045
AD	24	ALA	-	linker	UNP P03045
AD	25	GLY	-	linker	UNP P03045
AD	26	ALA	-	linker	UNP P03045
AD	27	GLY	-	linker	UNP P03045
AD	28	ALA	-	linker	UNP P03045
AD	29	GLY	-	linker	UNP P03045
AD	30	ALA	-	linker	UNP P03045
AD	31	MET	-	linker	UNP P03045
AD	39	ASN	ILE	engineered mutation	UNP O66529
AD	42	VAL	GLU	engineered mutation	UNP O66529
AD	58	VAL	ILE	engineered mutation	UNP O66529
AD	61	ASP	GLY	engineered mutation	UNP O66529
AD	62	ILE	VAL	engineered mutation	UNP O66529
AD	97	TYR	PHE	engineered mutation	UNP O66529
AD	102	GLY	-	linker	UNP O66529
AD	103	THR	-	linker	UNP O66529
AD	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
AD	105	HIS	-	linker	UNP O66529
AD	106	HIS	-	linker	UNP O66529
AD	107	HIS	-	linker	UNP O66529
AD	108	HIS	-	linker	UNP O66529
AD	109	HIS	-	linker	UNP O66529
AD	110	HIS	-	linker	UNP O66529
AD	111	GLY	-	linker	UNP O66529
AD	112	SER	-	linker	UNP O66529
AD	113	SER	-	linker	UNP O66529
AD	114	ILE	MET	engineered mutation	UNP O66529
AD	115	GLU	GLN	engineered mutation	UNP O66529
AD	138	THR	ALA	engineered mutation	UNP O66529
AD	177	ASP	GLY	engineered mutation	UNP O66529
AD	191	PHE	ILE	engineered mutation	UNP O66529
AD	193	ASP	VAL	engineered mutation	UNP O66529
BA	1	MET	-	cloning artifact	UNP P03045
BA	2	GLY	-	cloning artifact	UNP P03045
BA	3	ASN	-	cloning artifact	UNP P03045
BA	4	ALA	-	cloning artifact	UNP P03045
BA	5	LYS	-	cloning artifact	UNP P03045
BA	6	THR	-	cloning artifact	UNP P03045
BA	24	ALA	-	linker	UNP P03045
BA	25	GLY	-	linker	UNP P03045
BA	26	ALA	-	linker	UNP P03045
BA	27	GLY	-	linker	UNP P03045
BA	28	ALA	-	linker	UNP P03045
BA	29	GLY	-	linker	UNP P03045
BA	30	ALA	-	linker	UNP P03045
BA	31	MET	-	linker	UNP P03045
BA	39	ASN	ILE	engineered mutation	UNP O66529
BA	42	VAL	GLU	engineered mutation	UNP O66529
BA	58	VAL	ILE	engineered mutation	UNP O66529
BA	61	ASP	GLY	engineered mutation	UNP O66529
BA	62	ILE	VAL	engineered mutation	UNP O66529
BA	97	TYR	PHE	engineered mutation	UNP O66529
BA	102	GLY	-	linker	UNP O66529
BA	103	THR	-	linker	UNP O66529
BA	104	GLY	-	linker	UNP O66529
BA	105	HIS	-	linker	UNP O66529
BA	106	HIS	-	linker	UNP O66529
BA	107	HIS	-	linker	UNP O66529
BA	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
BA	109	HIS	-	linker	UNP O66529
BA	110	HIS	-	linker	UNP O66529
BA	111	GLY	-	linker	UNP O66529
BA	112	SER	-	linker	UNP O66529
BA	113	SER	-	linker	UNP O66529
BA	114	ILE	MET	engineered mutation	UNP O66529
BA	115	GLU	GLN	engineered mutation	UNP O66529
BA	138	THR	ALA	engineered mutation	UNP O66529
BA	177	ASP	GLY	engineered mutation	UNP O66529
BA	191	PHE	ILE	engineered mutation	UNP O66529
BA	193	ASP	VAL	engineered mutation	UNP O66529
BB	1	MET	-	cloning artifact	UNP P03045
BB	2	GLY	-	cloning artifact	UNP P03045
BB	3	ASN	-	cloning artifact	UNP P03045
BB	4	ALA	-	cloning artifact	UNP P03045
BB	5	LYS	-	cloning artifact	UNP P03045
BB	6	THR	-	cloning artifact	UNP P03045
BB	24	ALA	-	linker	UNP P03045
BB	25	GLY	-	linker	UNP P03045
BB	26	ALA	-	linker	UNP P03045
BB	27	GLY	-	linker	UNP P03045
BB	28	ALA	-	linker	UNP P03045
BB	29	GLY	-	linker	UNP P03045
BB	30	ALA	-	linker	UNP P03045
BB	31	MET	-	linker	UNP P03045
BB	39	ASN	ILE	engineered mutation	UNP O66529
BB	42	VAL	GLU	engineered mutation	UNP O66529
BB	58	VAL	ILE	engineered mutation	UNP O66529
BB	61	ASP	GLY	engineered mutation	UNP O66529
BB	62	ILE	VAL	engineered mutation	UNP O66529
BB	97	TYR	PHE	engineered mutation	UNP O66529
BB	102	GLY	-	linker	UNP O66529
BB	103	THR	-	linker	UNP O66529
BB	104	GLY	-	linker	UNP O66529
BB	105	HIS	-	linker	UNP O66529
BB	106	HIS	-	linker	UNP O66529
BB	107	HIS	-	linker	UNP O66529
BB	108	HIS	-	linker	UNP O66529
BB	109	HIS	-	linker	UNP O66529
BB	110	HIS	-	linker	UNP O66529
BB	111	GLY	-	linker	UNP O66529
BB	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
BB	113	SER	-	linker	UNP O66529
BB	114	ILE	MET	engineered mutation	UNP O66529
BB	115	GLU	GLN	engineered mutation	UNP O66529
BB	138	THR	ALA	engineered mutation	UNP O66529
BB	177	ASP	GLY	engineered mutation	UNP O66529
BB	191	PHE	ILE	engineered mutation	UNP O66529
BB	193	ASP	VAL	engineered mutation	UNP O66529
BC	1	MET	-	cloning artifact	UNP P03045
BC	2	GLY	-	cloning artifact	UNP P03045
BC	3	ASN	-	cloning artifact	UNP P03045
BC	4	ALA	-	cloning artifact	UNP P03045
BC	5	LYS	-	cloning artifact	UNP P03045
BC	6	THR	-	cloning artifact	UNP P03045
BC	24	ALA	-	linker	UNP P03045
BC	25	GLY	-	linker	UNP P03045
BC	26	ALA	-	linker	UNP P03045
BC	27	GLY	-	linker	UNP P03045
BC	28	ALA	-	linker	UNP P03045
BC	29	GLY	-	linker	UNP P03045
BC	30	ALA	-	linker	UNP P03045
BC	31	MET	-	linker	UNP P03045
BC	39	ASN	ILE	engineered mutation	UNP O66529
BC	42	VAL	GLU	engineered mutation	UNP O66529
BC	58	VAL	ILE	engineered mutation	UNP O66529
BC	61	ASP	GLY	engineered mutation	UNP O66529
BC	62	ILE	VAL	engineered mutation	UNP O66529
BC	97	TYR	PHE	engineered mutation	UNP O66529
BC	102	GLY	-	linker	UNP O66529
BC	103	THR	-	linker	UNP O66529
BC	104	GLY	-	linker	UNP O66529
BC	105	HIS	-	linker	UNP O66529
BC	106	HIS	-	linker	UNP O66529
BC	107	HIS	-	linker	UNP O66529
BC	108	HIS	-	linker	UNP O66529
BC	109	HIS	-	linker	UNP O66529
BC	110	HIS	-	linker	UNP O66529
BC	111	GLY	-	linker	UNP O66529
BC	112	SER	-	linker	UNP O66529
BC	113	SER	-	linker	UNP O66529
BC	114	ILE	MET	engineered mutation	UNP O66529
BC	115	GLU	GLN	engineered mutation	UNP O66529
BC	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
BC	177	ASP	GLY	engineered mutation	UNP O66529
BC	191	PHE	ILE	engineered mutation	UNP O66529
BC	193	ASP	VAL	engineered mutation	UNP O66529
BD	1	MET	-	cloning artifact	UNP P03045
BD	2	GLY	-	cloning artifact	UNP P03045
BD	3	ASN	-	cloning artifact	UNP P03045
BD	4	ALA	-	cloning artifact	UNP P03045
BD	5	LYS	-	cloning artifact	UNP P03045
BD	6	THR	-	cloning artifact	UNP P03045
BD	24	ALA	-	linker	UNP P03045
BD	25	GLY	-	linker	UNP P03045
BD	26	ALA	-	linker	UNP P03045
BD	27	GLY	-	linker	UNP P03045
BD	28	ALA	-	linker	UNP P03045
BD	29	GLY	-	linker	UNP P03045
BD	30	ALA	-	linker	UNP P03045
BD	31	MET	-	linker	UNP P03045
BD	39	ASN	ILE	engineered mutation	UNP O66529
BD	42	VAL	GLU	engineered mutation	UNP O66529
BD	58	VAL	ILE	engineered mutation	UNP O66529
BD	61	ASP	GLY	engineered mutation	UNP O66529
BD	62	ILE	VAL	engineered mutation	UNP O66529
BD	97	TYR	PHE	engineered mutation	UNP O66529
BD	102	GLY	-	linker	UNP O66529
BD	103	THR	-	linker	UNP O66529
BD	104	GLY	-	linker	UNP O66529
BD	105	HIS	-	linker	UNP O66529
BD	106	HIS	-	linker	UNP O66529
BD	107	HIS	-	linker	UNP O66529
BD	108	HIS	-	linker	UNP O66529
BD	109	HIS	-	linker	UNP O66529
BD	110	HIS	-	linker	UNP O66529
BD	111	GLY	-	linker	UNP O66529
BD	112	SER	-	linker	UNP O66529
BD	113	SER	-	linker	UNP O66529
BD	114	ILE	MET	engineered mutation	UNP O66529
BD	115	GLU	GLN	engineered mutation	UNP O66529
BD	138	THR	ALA	engineered mutation	UNP O66529
BD	177	ASP	GLY	engineered mutation	UNP O66529
BD	191	PHE	ILE	engineered mutation	UNP O66529
BD	193	ASP	VAL	engineered mutation	UNP O66529
CA	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
CA	2	GLY	-	cloning artifact	UNP P03045
CA	3	ASN	-	cloning artifact	UNP P03045
CA	4	ALA	-	cloning artifact	UNP P03045
CA	5	LYS	-	cloning artifact	UNP P03045
CA	6	THR	-	cloning artifact	UNP P03045
CA	24	ALA	-	linker	UNP P03045
CA	25	GLY	-	linker	UNP P03045
CA	26	ALA	-	linker	UNP P03045
CA	27	GLY	-	linker	UNP P03045
CA	28	ALA	-	linker	UNP P03045
CA	29	GLY	-	linker	UNP P03045
CA	30	ALA	-	linker	UNP P03045
CA	31	MET	-	linker	UNP P03045
CA	39	ASN	ILE	engineered mutation	UNP O66529
CA	42	VAL	GLU	engineered mutation	UNP O66529
CA	58	VAL	ILE	engineered mutation	UNP O66529
CA	61	ASP	GLY	engineered mutation	UNP O66529
CA	62	ILE	VAL	engineered mutation	UNP O66529
CA	97	TYR	PHE	engineered mutation	UNP O66529
CA	102	GLY	-	linker	UNP O66529
CA	103	THR	-	linker	UNP O66529
CA	104	GLY	-	linker	UNP O66529
CA	105	HIS	-	linker	UNP O66529
CA	106	HIS	-	linker	UNP O66529
CA	107	HIS	-	linker	UNP O66529
CA	108	HIS	-	linker	UNP O66529
CA	109	HIS	-	linker	UNP O66529
CA	110	HIS	-	linker	UNP O66529
CA	111	GLY	-	linker	UNP O66529
CA	112	SER	-	linker	UNP O66529
CA	113	SER	-	linker	UNP O66529
CA	114	ILE	MET	engineered mutation	UNP O66529
CA	115	GLU	GLN	engineered mutation	UNP O66529
CA	138	THR	ALA	engineered mutation	UNP O66529
CA	177	ASP	GLY	engineered mutation	UNP O66529
CA	191	PHE	ILE	engineered mutation	UNP O66529
CA	193	ASP	VAL	engineered mutation	UNP O66529
CB	1	MET	-	cloning artifact	UNP P03045
CB	2	GLY	-	cloning artifact	UNP P03045
CB	3	ASN	-	cloning artifact	UNP P03045
CB	4	ALA	-	cloning artifact	UNP P03045
CB	5	LYS	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
CB	6	THR	-	cloning artifact	UNP P03045
CB	24	ALA	-	linker	UNP P03045
CB	25	GLY	-	linker	UNP P03045
CB	26	ALA	-	linker	UNP P03045
CB	27	GLY	-	linker	UNP P03045
CB	28	ALA	-	linker	UNP P03045
CB	29	GLY	-	linker	UNP P03045
CB	30	ALA	-	linker	UNP P03045
CB	31	MET	-	linker	UNP P03045
CB	39	ASN	ILE	engineered mutation	UNP O66529
CB	42	VAL	GLU	engineered mutation	UNP O66529
CB	58	VAL	ILE	engineered mutation	UNP O66529
CB	61	ASP	GLY	engineered mutation	UNP O66529
CB	62	ILE	VAL	engineered mutation	UNP O66529
CB	97	TYR	PHE	engineered mutation	UNP O66529
CB	102	GLY	-	linker	UNP O66529
CB	103	THR	-	linker	UNP O66529
CB	104	GLY	-	linker	UNP O66529
CB	105	HIS	-	linker	UNP O66529
CB	106	HIS	-	linker	UNP O66529
CB	107	HIS	-	linker	UNP O66529
CB	108	HIS	-	linker	UNP O66529
CB	109	HIS	-	linker	UNP O66529
CB	110	HIS	-	linker	UNP O66529
CB	111	GLY	-	linker	UNP O66529
CB	112	SER	-	linker	UNP O66529
CB	113	SER	-	linker	UNP O66529
CB	114	ILE	MET	engineered mutation	UNP O66529
CB	115	GLU	GLN	engineered mutation	UNP O66529
CB	138	THR	ALA	engineered mutation	UNP O66529
CB	177	ASP	GLY	engineered mutation	UNP O66529
CB	191	PHE	ILE	engineered mutation	UNP O66529
CB	193	ASP	VAL	engineered mutation	UNP O66529
CC	1	MET	-	cloning artifact	UNP P03045
CC	2	GLY	-	cloning artifact	UNP P03045
CC	3	ASN	-	cloning artifact	UNP P03045
CC	4	ALA	-	cloning artifact	UNP P03045
CC	5	LYS	-	cloning artifact	UNP P03045
CC	6	THR	-	cloning artifact	UNP P03045
CC	24	ALA	-	linker	UNP P03045
CC	25	GLY	-	linker	UNP P03045
CC	26	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
CC	27	GLY	-	linker	UNP P03045
CC	28	ALA	-	linker	UNP P03045
CC	29	GLY	-	linker	UNP P03045
CC	30	ALA	-	linker	UNP P03045
CC	31	MET	-	linker	UNP P03045
CC	39	ASN	ILE	engineered mutation	UNP O66529
CC	42	VAL	GLU	engineered mutation	UNP O66529
CC	58	VAL	ILE	engineered mutation	UNP O66529
CC	61	ASP	GLY	engineered mutation	UNP O66529
CC	62	ILE	VAL	engineered mutation	UNP O66529
CC	97	TYR	PHE	engineered mutation	UNP O66529
CC	102	GLY	-	linker	UNP O66529
CC	103	THR	-	linker	UNP O66529
CC	104	GLY	-	linker	UNP O66529
CC	105	HIS	-	linker	UNP O66529
CC	106	HIS	-	linker	UNP O66529
CC	107	HIS	-	linker	UNP O66529
CC	108	HIS	-	linker	UNP O66529
CC	109	HIS	-	linker	UNP O66529
CC	110	HIS	-	linker	UNP O66529
CC	111	GLY	-	linker	UNP O66529
CC	112	SER	-	linker	UNP O66529
CC	113	SER	-	linker	UNP O66529
CC	114	ILE	MET	engineered mutation	UNP O66529
CC	115	GLU	GLN	engineered mutation	UNP O66529
CC	138	THR	ALA	engineered mutation	UNP O66529
CC	177	ASP	GLY	engineered mutation	UNP O66529
CC	191	PHE	ILE	engineered mutation	UNP O66529
CC	193	ASP	VAL	engineered mutation	UNP O66529
CD	1	MET	-	cloning artifact	UNP P03045
CD	2	GLY	-	cloning artifact	UNP P03045
CD	3	ASN	-	cloning artifact	UNP P03045
CD	4	ALA	-	cloning artifact	UNP P03045
CD	5	LYS	-	cloning artifact	UNP P03045
CD	6	THR	-	cloning artifact	UNP P03045
CD	24	ALA	-	linker	UNP P03045
CD	25	GLY	-	linker	UNP P03045
CD	26	ALA	-	linker	UNP P03045
CD	27	GLY	-	linker	UNP P03045
CD	28	ALA	-	linker	UNP P03045
CD	29	GLY	-	linker	UNP P03045
CD	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
CD	31	MET	-	linker	UNP P03045
CD	39	ASN	ILE	engineered mutation	UNP O66529
CD	42	VAL	GLU	engineered mutation	UNP O66529
CD	58	VAL	ILE	engineered mutation	UNP O66529
CD	61	ASP	GLY	engineered mutation	UNP O66529
CD	62	ILE	VAL	engineered mutation	UNP O66529
CD	97	TYR	PHE	engineered mutation	UNP O66529
CD	102	GLY	-	linker	UNP O66529
CD	103	THR	-	linker	UNP O66529
CD	104	GLY	-	linker	UNP O66529
CD	105	HIS	-	linker	UNP O66529
CD	106	HIS	-	linker	UNP O66529
CD	107	HIS	-	linker	UNP O66529
CD	108	HIS	-	linker	UNP O66529
CD	109	HIS	-	linker	UNP O66529
CD	110	HIS	-	linker	UNP O66529
CD	111	GLY	-	linker	UNP O66529
CD	112	SER	-	linker	UNP O66529
CD	113	SER	-	linker	UNP O66529
CD	114	ILE	MET	engineered mutation	UNP O66529
CD	115	GLU	GLN	engineered mutation	UNP O66529
CD	138	THR	ALA	engineered mutation	UNP O66529
CD	177	ASP	GLY	engineered mutation	UNP O66529
CD	191	PHE	ILE	engineered mutation	UNP O66529
CD	193	ASP	VAL	engineered mutation	UNP O66529
DA	1	MET	-	cloning artifact	UNP P03045
DA	2	GLY	-	cloning artifact	UNP P03045
DA	3	ASN	-	cloning artifact	UNP P03045
DA	4	ALA	-	cloning artifact	UNP P03045
DA	5	LYS	-	cloning artifact	UNP P03045
DA	6	THR	-	cloning artifact	UNP P03045
DA	24	ALA	-	linker	UNP P03045
DA	25	GLY	-	linker	UNP P03045
DA	26	ALA	-	linker	UNP P03045
DA	27	GLY	-	linker	UNP P03045
DA	28	ALA	-	linker	UNP P03045
DA	29	GLY	-	linker	UNP P03045
DA	30	ALA	-	linker	UNP P03045
DA	31	MET	-	linker	UNP P03045
DA	39	ASN	ILE	engineered mutation	UNP O66529
DA	42	VAL	GLU	engineered mutation	UNP O66529
DA	58	VAL	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
DA	61	ASP	GLY	engineered mutation	UNP O66529
DA	62	ILE	VAL	engineered mutation	UNP O66529
DA	97	TYR	PHE	engineered mutation	UNP O66529
DA	102	GLY	-	linker	UNP O66529
DA	103	THR	-	linker	UNP O66529
DA	104	GLY	-	linker	UNP O66529
DA	105	HIS	-	linker	UNP O66529
DA	106	HIS	-	linker	UNP O66529
DA	107	HIS	-	linker	UNP O66529
DA	108	HIS	-	linker	UNP O66529
DA	109	HIS	-	linker	UNP O66529
DA	110	HIS	-	linker	UNP O66529
DA	111	GLY	-	linker	UNP O66529
DA	112	SER	-	linker	UNP O66529
DA	113	SER	-	linker	UNP O66529
DA	114	ILE	MET	engineered mutation	UNP O66529
DA	115	GLU	GLN	engineered mutation	UNP O66529
DA	138	THR	ALA	engineered mutation	UNP O66529
DA	177	ASP	GLY	engineered mutation	UNP O66529
DA	191	PHE	ILE	engineered mutation	UNP O66529
DA	193	ASP	VAL	engineered mutation	UNP O66529
DB	1	MET	-	cloning artifact	UNP P03045
DB	2	GLY	-	cloning artifact	UNP P03045
DB	3	ASN	-	cloning artifact	UNP P03045
DB	4	ALA	-	cloning artifact	UNP P03045
DB	5	LYS	-	cloning artifact	UNP P03045
DB	6	THR	-	cloning artifact	UNP P03045
DB	24	ALA	-	linker	UNP P03045
DB	25	GLY	-	linker	UNP P03045
DB	26	ALA	-	linker	UNP P03045
DB	27	GLY	-	linker	UNP P03045
DB	28	ALA	-	linker	UNP P03045
DB	29	GLY	-	linker	UNP P03045
DB	30	ALA	-	linker	UNP P03045
DB	31	MET	-	linker	UNP P03045
DB	39	ASN	ILE	engineered mutation	UNP O66529
DB	42	VAL	GLU	engineered mutation	UNP O66529
DB	58	VAL	ILE	engineered mutation	UNP O66529
DB	61	ASP	GLY	engineered mutation	UNP O66529
DB	62	ILE	VAL	engineered mutation	UNP O66529
DB	97	TYR	PHE	engineered mutation	UNP O66529
DB	102	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
DB	103	THR	-	linker	UNP O66529
DB	104	GLY	-	linker	UNP O66529
DB	105	HIS	-	linker	UNP O66529
DB	106	HIS	-	linker	UNP O66529
DB	107	HIS	-	linker	UNP O66529
DB	108	HIS	-	linker	UNP O66529
DB	109	HIS	-	linker	UNP O66529
DB	110	HIS	-	linker	UNP O66529
DB	111	GLY	-	linker	UNP O66529
DB	112	SER	-	linker	UNP O66529
DB	113	SER	-	linker	UNP O66529
DB	114	ILE	MET	engineered mutation	UNP O66529
DB	115	GLU	GLN	engineered mutation	UNP O66529
DB	138	THR	ALA	engineered mutation	UNP O66529
DB	177	ASP	GLY	engineered mutation	UNP O66529
DB	191	PHE	ILE	engineered mutation	UNP O66529
DB	193	ASP	VAL	engineered mutation	UNP O66529
DC	1	MET	-	cloning artifact	UNP P03045
DC	2	GLY	-	cloning artifact	UNP P03045
DC	3	ASN	-	cloning artifact	UNP P03045
DC	4	ALA	-	cloning artifact	UNP P03045
DC	5	LYS	-	cloning artifact	UNP P03045
DC	6	THR	-	cloning artifact	UNP P03045
DC	24	ALA	-	linker	UNP P03045
DC	25	GLY	-	linker	UNP P03045
DC	26	ALA	-	linker	UNP P03045
DC	27	GLY	-	linker	UNP P03045
DC	28	ALA	-	linker	UNP P03045
DC	29	GLY	-	linker	UNP P03045
DC	30	ALA	-	linker	UNP P03045
DC	31	MET	-	linker	UNP P03045
DC	39	ASN	ILE	engineered mutation	UNP O66529
DC	42	VAL	GLU	engineered mutation	UNP O66529
DC	58	VAL	ILE	engineered mutation	UNP O66529
DC	61	ASP	GLY	engineered mutation	UNP O66529
DC	62	ILE	VAL	engineered mutation	UNP O66529
DC	97	TYR	PHE	engineered mutation	UNP O66529
DC	102	GLY	-	linker	UNP O66529
DC	103	THR	-	linker	UNP O66529
DC	104	GLY	-	linker	UNP O66529
DC	105	HIS	-	linker	UNP O66529
DC	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
DC	107	HIS	-	linker	UNP O66529
DC	108	HIS	-	linker	UNP O66529
DC	109	HIS	-	linker	UNP O66529
DC	110	HIS	-	linker	UNP O66529
DC	111	GLY	-	linker	UNP O66529
DC	112	SER	-	linker	UNP O66529
DC	113	SER	-	linker	UNP O66529
DC	114	ILE	MET	engineered mutation	UNP O66529
DC	115	GLU	GLN	engineered mutation	UNP O66529
DC	138	THR	ALA	engineered mutation	UNP O66529
DC	177	ASP	GLY	engineered mutation	UNP O66529
DC	191	PHE	ILE	engineered mutation	UNP O66529
DC	193	ASP	VAL	engineered mutation	UNP O66529
DD	1	MET	-	cloning artifact	UNP P03045
DD	2	GLY	-	cloning artifact	UNP P03045
DD	3	ASN	-	cloning artifact	UNP P03045
DD	4	ALA	-	cloning artifact	UNP P03045
DD	5	LYS	-	cloning artifact	UNP P03045
DD	6	THR	-	cloning artifact	UNP P03045
DD	24	ALA	-	linker	UNP P03045
DD	25	GLY	-	linker	UNP P03045
DD	26	ALA	-	linker	UNP P03045
DD	27	GLY	-	linker	UNP P03045
DD	28	ALA	-	linker	UNP P03045
DD	29	GLY	-	linker	UNP P03045
DD	30	ALA	-	linker	UNP P03045
DD	31	MET	-	linker	UNP P03045
DD	39	ASN	ILE	engineered mutation	UNP O66529
DD	42	VAL	GLU	engineered mutation	UNP O66529
DD	58	VAL	ILE	engineered mutation	UNP O66529
DD	61	ASP	GLY	engineered mutation	UNP O66529
DD	62	ILE	VAL	engineered mutation	UNP O66529
DD	97	TYR	PHE	engineered mutation	UNP O66529
DD	102	GLY	-	linker	UNP O66529
DD	103	THR	-	linker	UNP O66529
DD	104	GLY	-	linker	UNP O66529
DD	105	HIS	-	linker	UNP O66529
DD	106	HIS	-	linker	UNP O66529
DD	107	HIS	-	linker	UNP O66529
DD	108	HIS	-	linker	UNP O66529
DD	109	HIS	-	linker	UNP O66529
DD	110	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
DD	111	GLY	-	linker	UNP O66529
DD	112	SER	-	linker	UNP O66529
DD	113	SER	-	linker	UNP O66529
DD	114	ILE	MET	engineered mutation	UNP O66529
DD	115	GLU	GLN	engineered mutation	UNP O66529
DD	138	THR	ALA	engineered mutation	UNP O66529
DD	177	ASP	GLY	engineered mutation	UNP O66529
DD	191	PHE	ILE	engineered mutation	UNP O66529
DD	193	ASP	VAL	engineered mutation	UNP O66529
EA	1	MET	-	cloning artifact	UNP P03045
EA	2	GLY	-	cloning artifact	UNP P03045
EA	3	ASN	-	cloning artifact	UNP P03045
EA	4	ALA	-	cloning artifact	UNP P03045
EA	5	LYS	-	cloning artifact	UNP P03045
EA	6	THR	-	cloning artifact	UNP P03045
EA	24	ALA	-	linker	UNP P03045
EA	25	GLY	-	linker	UNP P03045
EA	26	ALA	-	linker	UNP P03045
EA	27	GLY	-	linker	UNP P03045
EA	28	ALA	-	linker	UNP P03045
EA	29	GLY	-	linker	UNP P03045
EA	30	ALA	-	linker	UNP P03045
EA	31	MET	-	linker	UNP P03045
EA	39	ASN	ILE	engineered mutation	UNP O66529
EA	42	VAL	GLU	engineered mutation	UNP O66529
EA	58	VAL	ILE	engineered mutation	UNP O66529
EA	61	ASP	GLY	engineered mutation	UNP O66529
EA	62	ILE	VAL	engineered mutation	UNP O66529
EA	97	TYR	PHE	engineered mutation	UNP O66529
EA	102	GLY	-	linker	UNP O66529
EA	103	THR	-	linker	UNP O66529
EA	104	GLY	-	linker	UNP O66529
EA	105	HIS	-	linker	UNP O66529
EA	106	HIS	-	linker	UNP O66529
EA	107	HIS	-	linker	UNP O66529
EA	108	HIS	-	linker	UNP O66529
EA	109	HIS	-	linker	UNP O66529
EA	110	HIS	-	linker	UNP O66529
EA	111	GLY	-	linker	UNP O66529
EA	112	SER	-	linker	UNP O66529
EA	113	SER	-	linker	UNP O66529
EA	114	ILE	MET	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
EA	115	GLU	GLN	engineered mutation	UNP O66529
EA	138	THR	ALA	engineered mutation	UNP O66529
EA	177	ASP	GLY	engineered mutation	UNP O66529
EA	191	PHE	ILE	engineered mutation	UNP O66529
EA	193	ASP	VAL	engineered mutation	UNP O66529
EB	1	MET	-	cloning artifact	UNP P03045
EB	2	GLY	-	cloning artifact	UNP P03045
EB	3	ASN	-	cloning artifact	UNP P03045
EB	4	ALA	-	cloning artifact	UNP P03045
EB	5	LYS	-	cloning artifact	UNP P03045
EB	6	THR	-	cloning artifact	UNP P03045
EB	24	ALA	-	linker	UNP P03045
EB	25	GLY	-	linker	UNP P03045
EB	26	ALA	-	linker	UNP P03045
EB	27	GLY	-	linker	UNP P03045
EB	28	ALA	-	linker	UNP P03045
EB	29	GLY	-	linker	UNP P03045
EB	30	ALA	-	linker	UNP P03045
EB	31	MET	-	linker	UNP P03045
EB	39	ASN	ILE	engineered mutation	UNP O66529
EB	42	VAL	GLU	engineered mutation	UNP O66529
EB	58	VAL	ILE	engineered mutation	UNP O66529
EB	61	ASP	GLY	engineered mutation	UNP O66529
EB	62	ILE	VAL	engineered mutation	UNP O66529
EB	97	TYR	PHE	engineered mutation	UNP O66529
EB	102	GLY	-	linker	UNP O66529
EB	103	THR	-	linker	UNP O66529
EB	104	GLY	-	linker	UNP O66529
EB	105	HIS	-	linker	UNP O66529
EB	106	HIS	-	linker	UNP O66529
EB	107	HIS	-	linker	UNP O66529
EB	108	HIS	-	linker	UNP O66529
EB	109	HIS	-	linker	UNP O66529
EB	110	HIS	-	linker	UNP O66529
EB	111	GLY	-	linker	UNP O66529
EB	112	SER	-	linker	UNP O66529
EB	113	SER	-	linker	UNP O66529
EB	114	ILE	MET	engineered mutation	UNP O66529
EB	115	GLU	GLN	engineered mutation	UNP O66529
EB	138	THR	ALA	engineered mutation	UNP O66529
EB	177	ASP	GLY	engineered mutation	UNP O66529
EB	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
EB	193	ASP	VAL	engineered mutation	UNP O66529
EC	1	MET	-	cloning artifact	UNP P03045
EC	2	GLY	-	cloning artifact	UNP P03045
EC	3	ASN	-	cloning artifact	UNP P03045
EC	4	ALA	-	cloning artifact	UNP P03045
EC	5	LYS	-	cloning artifact	UNP P03045
EC	6	THR	-	cloning artifact	UNP P03045
EC	24	ALA	-	linker	UNP P03045
EC	25	GLY	-	linker	UNP P03045
EC	26	ALA	-	linker	UNP P03045
EC	27	GLY	-	linker	UNP P03045
EC	28	ALA	-	linker	UNP P03045
EC	29	GLY	-	linker	UNP P03045
EC	30	ALA	-	linker	UNP P03045
EC	31	MET	-	linker	UNP P03045
EC	39	ASN	ILE	engineered mutation	UNP O66529
EC	42	VAL	GLU	engineered mutation	UNP O66529
EC	58	VAL	ILE	engineered mutation	UNP O66529
EC	61	ASP	GLY	engineered mutation	UNP O66529
EC	62	ILE	VAL	engineered mutation	UNP O66529
EC	97	TYR	PHE	engineered mutation	UNP O66529
EC	102	GLY	-	linker	UNP O66529
EC	103	THR	-	linker	UNP O66529
EC	104	GLY	-	linker	UNP O66529
EC	105	HIS	-	linker	UNP O66529
EC	106	HIS	-	linker	UNP O66529
EC	107	HIS	-	linker	UNP O66529
EC	108	HIS	-	linker	UNP O66529
EC	109	HIS	-	linker	UNP O66529
EC	110	HIS	-	linker	UNP O66529
EC	111	GLY	-	linker	UNP O66529
EC	112	SER	-	linker	UNP O66529
EC	113	SER	-	linker	UNP O66529
EC	114	ILE	MET	engineered mutation	UNP O66529
EC	115	GLU	GLN	engineered mutation	UNP O66529
EC	138	THR	ALA	engineered mutation	UNP O66529
EC	177	ASP	GLY	engineered mutation	UNP O66529
EC	191	PHE	ILE	engineered mutation	UNP O66529
EC	193	ASP	VAL	engineered mutation	UNP O66529
ED	1	MET	-	cloning artifact	UNP P03045
ED	2	GLY	-	cloning artifact	UNP P03045
ED	3	ASN	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
ED	4	ALA	-	cloning artifact	UNP P03045
ED	5	LYS	-	cloning artifact	UNP P03045
ED	6	THR	-	cloning artifact	UNP P03045
ED	24	ALA	-	linker	UNP P03045
ED	25	GLY	-	linker	UNP P03045
ED	26	ALA	-	linker	UNP P03045
ED	27	GLY	-	linker	UNP P03045
ED	28	ALA	-	linker	UNP P03045
ED	29	GLY	-	linker	UNP P03045
ED	30	ALA	-	linker	UNP P03045
ED	31	MET	-	linker	UNP P03045
ED	39	ASN	ILE	engineered mutation	UNP O66529
ED	42	VAL	GLU	engineered mutation	UNP O66529
ED	58	VAL	ILE	engineered mutation	UNP O66529
ED	61	ASP	GLY	engineered mutation	UNP O66529
ED	62	ILE	VAL	engineered mutation	UNP O66529
ED	97	TYR	PHE	engineered mutation	UNP O66529
ED	102	GLY	-	linker	UNP O66529
ED	103	THR	-	linker	UNP O66529
ED	104	GLY	-	linker	UNP O66529
ED	105	HIS	-	linker	UNP O66529
ED	106	HIS	-	linker	UNP O66529
ED	107	HIS	-	linker	UNP O66529
ED	108	HIS	-	linker	UNP O66529
ED	109	HIS	-	linker	UNP O66529
ED	110	HIS	-	linker	UNP O66529
ED	111	GLY	-	linker	UNP O66529
ED	112	SER	-	linker	UNP O66529
ED	113	SER	-	linker	UNP O66529
ED	114	ILE	MET	engineered mutation	UNP O66529
ED	115	GLU	GLN	engineered mutation	UNP O66529
ED	138	THR	ALA	engineered mutation	UNP O66529
ED	177	ASP	GLY	engineered mutation	UNP O66529
ED	191	PHE	ILE	engineered mutation	UNP O66529
ED	193	ASP	VAL	engineered mutation	UNP O66529
FA	1	MET	-	cloning artifact	UNP P03045
FA	2	GLY	-	cloning artifact	UNP P03045
FA	3	ASN	-	cloning artifact	UNP P03045
FA	4	ALA	-	cloning artifact	UNP P03045
FA	5	LYS	-	cloning artifact	UNP P03045
FA	6	THR	-	cloning artifact	UNP P03045
FA	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
FA	25	GLY	-	linker	UNP P03045
FA	26	ALA	-	linker	UNP P03045
FA	27	GLY	-	linker	UNP P03045
FA	28	ALA	-	linker	UNP P03045
FA	29	GLY	-	linker	UNP P03045
FA	30	ALA	-	linker	UNP P03045
FA	31	MET	-	linker	UNP P03045
FA	39	ASN	ILE	engineered mutation	UNP O66529
FA	42	VAL	GLU	engineered mutation	UNP O66529
FA	58	VAL	ILE	engineered mutation	UNP O66529
FA	61	ASP	GLY	engineered mutation	UNP O66529
FA	62	ILE	VAL	engineered mutation	UNP O66529
FA	97	TYR	PHE	engineered mutation	UNP O66529
FA	102	GLY	-	linker	UNP O66529
FA	103	THR	-	linker	UNP O66529
FA	104	GLY	-	linker	UNP O66529
FA	105	HIS	-	linker	UNP O66529
FA	106	HIS	-	linker	UNP O66529
FA	107	HIS	-	linker	UNP O66529
FA	108	HIS	-	linker	UNP O66529
FA	109	HIS	-	linker	UNP O66529
FA	110	HIS	-	linker	UNP O66529
FA	111	GLY	-	linker	UNP O66529
FA	112	SER	-	linker	UNP O66529
FA	113	SER	-	linker	UNP O66529
FA	114	ILE	MET	engineered mutation	UNP O66529
FA	115	GLU	GLN	engineered mutation	UNP O66529
FA	138	THR	ALA	engineered mutation	UNP O66529
FA	177	ASP	GLY	engineered mutation	UNP O66529
FA	191	PHE	ILE	engineered mutation	UNP O66529
FA	193	ASP	VAL	engineered mutation	UNP O66529
FB	1	MET	-	cloning artifact	UNP P03045
FB	2	GLY	-	cloning artifact	UNP P03045
FB	3	ASN	-	cloning artifact	UNP P03045
FB	4	ALA	-	cloning artifact	UNP P03045
FB	5	LYS	-	cloning artifact	UNP P03045
FB	6	THR	-	cloning artifact	UNP P03045
FB	24	ALA	-	linker	UNP P03045
FB	25	GLY	-	linker	UNP P03045
FB	26	ALA	-	linker	UNP P03045
FB	27	GLY	-	linker	UNP P03045
FB	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
FB	29	GLY	-	linker	UNP P03045
FB	30	ALA	-	linker	UNP P03045
FB	31	MET	-	linker	UNP P03045
FB	39	ASN	ILE	engineered mutation	UNP O66529
FB	42	VAL	GLU	engineered mutation	UNP O66529
FB	58	VAL	ILE	engineered mutation	UNP O66529
FB	61	ASP	GLY	engineered mutation	UNP O66529
FB	62	ILE	VAL	engineered mutation	UNP O66529
FB	97	TYR	PHE	engineered mutation	UNP O66529
FB	102	GLY	-	linker	UNP O66529
FB	103	THR	-	linker	UNP O66529
FB	104	GLY	-	linker	UNP O66529
FB	105	HIS	-	linker	UNP O66529
FB	106	HIS	-	linker	UNP O66529
FB	107	HIS	-	linker	UNP O66529
FB	108	HIS	-	linker	UNP O66529
FB	109	HIS	-	linker	UNP O66529
FB	110	HIS	-	linker	UNP O66529
FB	111	GLY	-	linker	UNP O66529
FB	112	SER	-	linker	UNP O66529
FB	113	SER	-	linker	UNP O66529
FB	114	ILE	MET	engineered mutation	UNP O66529
FB	115	GLU	GLN	engineered mutation	UNP O66529
FB	138	THR	ALA	engineered mutation	UNP O66529
FB	177	ASP	GLY	engineered mutation	UNP O66529
FB	191	PHE	ILE	engineered mutation	UNP O66529
FB	193	ASP	VAL	engineered mutation	UNP O66529
FC	1	MET	-	cloning artifact	UNP P03045
FC	2	GLY	-	cloning artifact	UNP P03045
FC	3	ASN	-	cloning artifact	UNP P03045
FC	4	ALA	-	cloning artifact	UNP P03045
FC	5	LYS	-	cloning artifact	UNP P03045
FC	6	THR	-	cloning artifact	UNP P03045
FC	24	ALA	-	linker	UNP P03045
FC	25	GLY	-	linker	UNP P03045
FC	26	ALA	-	linker	UNP P03045
FC	27	GLY	-	linker	UNP P03045
FC	28	ALA	-	linker	UNP P03045
FC	29	GLY	-	linker	UNP P03045
FC	30	ALA	-	linker	UNP P03045
FC	31	MET	-	linker	UNP P03045
FC	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
FC	42	VAL	GLU	engineered mutation	UNP O66529
FC	58	VAL	ILE	engineered mutation	UNP O66529
FC	61	ASP	GLY	engineered mutation	UNP O66529
FC	62	ILE	VAL	engineered mutation	UNP O66529
FC	97	TYR	PHE	engineered mutation	UNP O66529
FC	102	GLY	-	linker	UNP O66529
FC	103	THR	-	linker	UNP O66529
FC	104	GLY	-	linker	UNP O66529
FC	105	HIS	-	linker	UNP O66529
FC	106	HIS	-	linker	UNP O66529
FC	107	HIS	-	linker	UNP O66529
FC	108	HIS	-	linker	UNP O66529
FC	109	HIS	-	linker	UNP O66529
FC	110	HIS	-	linker	UNP O66529
FC	111	GLY	-	linker	UNP O66529
FC	112	SER	-	linker	UNP O66529
FC	113	SER	-	linker	UNP O66529
FC	114	ILE	MET	engineered mutation	UNP O66529
FC	115	GLU	GLN	engineered mutation	UNP O66529
FC	138	THR	ALA	engineered mutation	UNP O66529
FC	177	ASP	GLY	engineered mutation	UNP O66529
FC	191	PHE	ILE	engineered mutation	UNP O66529
FC	193	ASP	VAL	engineered mutation	UNP O66529
FD	1	MET	-	cloning artifact	UNP P03045
FD	2	GLY	-	cloning artifact	UNP P03045
FD	3	ASN	-	cloning artifact	UNP P03045
FD	4	ALA	-	cloning artifact	UNP P03045
FD	5	LYS	-	cloning artifact	UNP P03045
FD	6	THR	-	cloning artifact	UNP P03045
FD	24	ALA	-	linker	UNP P03045
FD	25	GLY	-	linker	UNP P03045
FD	26	ALA	-	linker	UNP P03045
FD	27	GLY	-	linker	UNP P03045
FD	28	ALA	-	linker	UNP P03045
FD	29	GLY	-	linker	UNP P03045
FD	30	ALA	-	linker	UNP P03045
FD	31	MET	-	linker	UNP P03045
FD	39	ASN	ILE	engineered mutation	UNP O66529
FD	42	VAL	GLU	engineered mutation	UNP O66529
FD	58	VAL	ILE	engineered mutation	UNP O66529
FD	61	ASP	GLY	engineered mutation	UNP O66529
FD	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
FD	97	TYR	PHE	engineered mutation	UNP O66529
FD	102	GLY	-	linker	UNP O66529
FD	103	THR	-	linker	UNP O66529
FD	104	GLY	-	linker	UNP O66529
FD	105	HIS	-	linker	UNP O66529
FD	106	HIS	-	linker	UNP O66529
FD	107	HIS	-	linker	UNP O66529
FD	108	HIS	-	linker	UNP O66529
FD	109	HIS	-	linker	UNP O66529
FD	110	HIS	-	linker	UNP O66529
FD	111	GLY	-	linker	UNP O66529
FD	112	SER	-	linker	UNP O66529
FD	113	SER	-	linker	UNP O66529
FD	114	ILE	MET	engineered mutation	UNP O66529
FD	115	GLU	GLN	engineered mutation	UNP O66529
FD	138	THR	ALA	engineered mutation	UNP O66529
FD	177	ASP	GLY	engineered mutation	UNP O66529
FD	191	PHE	ILE	engineered mutation	UNP O66529
FD	193	ASP	VAL	engineered mutation	UNP O66529
GA	1	MET	-	cloning artifact	UNP P03045
GA	2	GLY	-	cloning artifact	UNP P03045
GA	3	ASN	-	cloning artifact	UNP P03045
GA	4	ALA	-	cloning artifact	UNP P03045
GA	5	LYS	-	cloning artifact	UNP P03045
GA	6	THR	-	cloning artifact	UNP P03045
GA	24	ALA	-	linker	UNP P03045
GA	25	GLY	-	linker	UNP P03045
GA	26	ALA	-	linker	UNP P03045
GA	27	GLY	-	linker	UNP P03045
GA	28	ALA	-	linker	UNP P03045
GA	29	GLY	-	linker	UNP P03045
GA	30	ALA	-	linker	UNP P03045
GA	31	MET	-	linker	UNP P03045
GA	39	ASN	ILE	engineered mutation	UNP O66529
GA	42	VAL	GLU	engineered mutation	UNP O66529
GA	58	VAL	ILE	engineered mutation	UNP O66529
GA	61	ASP	GLY	engineered mutation	UNP O66529
GA	62	ILE	VAL	engineered mutation	UNP O66529
GA	97	TYR	PHE	engineered mutation	UNP O66529
GA	102	GLY	-	linker	UNP O66529
GA	103	THR	-	linker	UNP O66529
GA	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
GA	105	HIS	-	linker	UNP O66529
GA	106	HIS	-	linker	UNP O66529
GA	107	HIS	-	linker	UNP O66529
GA	108	HIS	-	linker	UNP O66529
GA	109	HIS	-	linker	UNP O66529
GA	110	HIS	-	linker	UNP O66529
GA	111	GLY	-	linker	UNP O66529
GA	112	SER	-	linker	UNP O66529
GA	113	SER	-	linker	UNP O66529
GA	114	ILE	MET	engineered mutation	UNP O66529
GA	115	GLU	GLN	engineered mutation	UNP O66529
GA	138	THR	ALA	engineered mutation	UNP O66529
GA	177	ASP	GLY	engineered mutation	UNP O66529
GA	191	PHE	ILE	engineered mutation	UNP O66529
GA	193	ASP	VAL	engineered mutation	UNP O66529
GB	1	MET	-	cloning artifact	UNP P03045
GB	2	GLY	-	cloning artifact	UNP P03045
GB	3	ASN	-	cloning artifact	UNP P03045
GB	4	ALA	-	cloning artifact	UNP P03045
GB	5	LYS	-	cloning artifact	UNP P03045
GB	6	THR	-	cloning artifact	UNP P03045
GB	24	ALA	-	linker	UNP P03045
GB	25	GLY	-	linker	UNP P03045
GB	26	ALA	-	linker	UNP P03045
GB	27	GLY	-	linker	UNP P03045
GB	28	ALA	-	linker	UNP P03045
GB	29	GLY	-	linker	UNP P03045
GB	30	ALA	-	linker	UNP P03045
GB	31	MET	-	linker	UNP P03045
GB	39	ASN	ILE	engineered mutation	UNP O66529
GB	42	VAL	GLU	engineered mutation	UNP O66529
GB	58	VAL	ILE	engineered mutation	UNP O66529
GB	61	ASP	GLY	engineered mutation	UNP O66529
GB	62	ILE	VAL	engineered mutation	UNP O66529
GB	97	TYR	PHE	engineered mutation	UNP O66529
GB	102	GLY	-	linker	UNP O66529
GB	103	THR	-	linker	UNP O66529
GB	104	GLY	-	linker	UNP O66529
GB	105	HIS	-	linker	UNP O66529
GB	106	HIS	-	linker	UNP O66529
GB	107	HIS	-	linker	UNP O66529
GB	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
GB	109	HIS	-	linker	UNP O66529
GB	110	HIS	-	linker	UNP O66529
GB	111	GLY	-	linker	UNP O66529
GB	112	SER	-	linker	UNP O66529
GB	113	SER	-	linker	UNP O66529
GB	114	ILE	MET	engineered mutation	UNP O66529
GB	115	GLU	GLN	engineered mutation	UNP O66529
GB	138	THR	ALA	engineered mutation	UNP O66529
GB	177	ASP	GLY	engineered mutation	UNP O66529
GB	191	PHE	ILE	engineered mutation	UNP O66529
GB	193	ASP	VAL	engineered mutation	UNP O66529
GC	1	MET	-	cloning artifact	UNP P03045
GC	2	GLY	-	cloning artifact	UNP P03045
GC	3	ASN	-	cloning artifact	UNP P03045
GC	4	ALA	-	cloning artifact	UNP P03045
GC	5	LYS	-	cloning artifact	UNP P03045
GC	6	THR	-	cloning artifact	UNP P03045
GC	24	ALA	-	linker	UNP P03045
GC	25	GLY	-	linker	UNP P03045
GC	26	ALA	-	linker	UNP P03045
GC	27	GLY	-	linker	UNP P03045
GC	28	ALA	-	linker	UNP P03045
GC	29	GLY	-	linker	UNP P03045
GC	30	ALA	-	linker	UNP P03045
GC	31	MET	-	linker	UNP P03045
GC	39	ASN	ILE	engineered mutation	UNP O66529
GC	42	VAL	GLU	engineered mutation	UNP O66529
GC	58	VAL	ILE	engineered mutation	UNP O66529
GC	61	ASP	GLY	engineered mutation	UNP O66529
GC	62	ILE	VAL	engineered mutation	UNP O66529
GC	97	TYR	PHE	engineered mutation	UNP O66529
GC	102	GLY	-	linker	UNP O66529
GC	103	THR	-	linker	UNP O66529
GC	104	GLY	-	linker	UNP O66529
GC	105	HIS	-	linker	UNP O66529
GC	106	HIS	-	linker	UNP O66529
GC	107	HIS	-	linker	UNP O66529
GC	108	HIS	-	linker	UNP O66529
GC	109	HIS	-	linker	UNP O66529
GC	110	HIS	-	linker	UNP O66529
GC	111	GLY	-	linker	UNP O66529
GC	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
GC	113	SER	-	linker	UNP O66529
GC	114	ILE	MET	engineered mutation	UNP O66529
GC	115	GLU	GLN	engineered mutation	UNP O66529
GC	138	THR	ALA	engineered mutation	UNP O66529
GC	177	ASP	GLY	engineered mutation	UNP O66529
GC	191	PHE	ILE	engineered mutation	UNP O66529
GC	193	ASP	VAL	engineered mutation	UNP O66529
GD	1	MET	-	cloning artifact	UNP P03045
GD	2	GLY	-	cloning artifact	UNP P03045
GD	3	ASN	-	cloning artifact	UNP P03045
GD	4	ALA	-	cloning artifact	UNP P03045
GD	5	LYS	-	cloning artifact	UNP P03045
GD	6	THR	-	cloning artifact	UNP P03045
GD	24	ALA	-	linker	UNP P03045
GD	25	GLY	-	linker	UNP P03045
GD	26	ALA	-	linker	UNP P03045
GD	27	GLY	-	linker	UNP P03045
GD	28	ALA	-	linker	UNP P03045
GD	29	GLY	-	linker	UNP P03045
GD	30	ALA	-	linker	UNP P03045
GD	31	MET	-	linker	UNP P03045
GD	39	ASN	ILE	engineered mutation	UNP O66529
GD	42	VAL	GLU	engineered mutation	UNP O66529
GD	58	VAL	ILE	engineered mutation	UNP O66529
GD	61	ASP	GLY	engineered mutation	UNP O66529
GD	62	ILE	VAL	engineered mutation	UNP O66529
GD	97	TYR	PHE	engineered mutation	UNP O66529
GD	102	GLY	-	linker	UNP O66529
GD	103	THR	-	linker	UNP O66529
GD	104	GLY	-	linker	UNP O66529
GD	105	HIS	-	linker	UNP O66529
GD	106	HIS	-	linker	UNP O66529
GD	107	HIS	-	linker	UNP O66529
GD	108	HIS	-	linker	UNP O66529
GD	109	HIS	-	linker	UNP O66529
GD	110	HIS	-	linker	UNP O66529
GD	111	GLY	-	linker	UNP O66529
GD	112	SER	-	linker	UNP O66529
GD	113	SER	-	linker	UNP O66529
GD	114	ILE	MET	engineered mutation	UNP O66529
GD	115	GLU	GLN	engineered mutation	UNP O66529
GD	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
GD	177	ASP	GLY	engineered mutation	UNP O66529
GD	191	PHE	ILE	engineered mutation	UNP O66529
GD	193	ASP	VAL	engineered mutation	UNP O66529
HA	1	MET	-	cloning artifact	UNP P03045
HA	2	GLY	-	cloning artifact	UNP P03045
HA	3	ASN	-	cloning artifact	UNP P03045
HA	4	ALA	-	cloning artifact	UNP P03045
HA	5	LYS	-	cloning artifact	UNP P03045
HA	6	THR	-	cloning artifact	UNP P03045
HA	24	ALA	-	linker	UNP P03045
HA	25	GLY	-	linker	UNP P03045
HA	26	ALA	-	linker	UNP P03045
HA	27	GLY	-	linker	UNP P03045
HA	28	ALA	-	linker	UNP P03045
HA	29	GLY	-	linker	UNP P03045
HA	30	ALA	-	linker	UNP P03045
HA	31	MET	-	linker	UNP P03045
HA	39	ASN	ILE	engineered mutation	UNP O66529
HA	42	VAL	GLU	engineered mutation	UNP O66529
HA	58	VAL	ILE	engineered mutation	UNP O66529
HA	61	ASP	GLY	engineered mutation	UNP O66529
HA	62	ILE	VAL	engineered mutation	UNP O66529
HA	97	TYR	PHE	engineered mutation	UNP O66529
HA	102	GLY	-	linker	UNP O66529
HA	103	THR	-	linker	UNP O66529
HA	104	GLY	-	linker	UNP O66529
HA	105	HIS	-	linker	UNP O66529
HA	106	HIS	-	linker	UNP O66529
HA	107	HIS	-	linker	UNP O66529
HA	108	HIS	-	linker	UNP O66529
HA	109	HIS	-	linker	UNP O66529
HA	110	HIS	-	linker	UNP O66529
HA	111	GLY	-	linker	UNP O66529
HA	112	SER	-	linker	UNP O66529
HA	113	SER	-	linker	UNP O66529
HA	114	ILE	MET	engineered mutation	UNP O66529
HA	115	GLU	GLN	engineered mutation	UNP O66529
HA	138	THR	ALA	engineered mutation	UNP O66529
HA	177	ASP	GLY	engineered mutation	UNP O66529
HA	191	PHE	ILE	engineered mutation	UNP O66529
HA	193	ASP	VAL	engineered mutation	UNP O66529
HB	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
HB	2	GLY	-	cloning artifact	UNP P03045
HB	3	ASN	-	cloning artifact	UNP P03045
HB	4	ALA	-	cloning artifact	UNP P03045
HB	5	LYS	-	cloning artifact	UNP P03045
HB	6	THR	-	cloning artifact	UNP P03045
HB	24	ALA	-	linker	UNP P03045
HB	25	GLY	-	linker	UNP P03045
HB	26	ALA	-	linker	UNP P03045
HB	27	GLY	-	linker	UNP P03045
HB	28	ALA	-	linker	UNP P03045
HB	29	GLY	-	linker	UNP P03045
HB	30	ALA	-	linker	UNP P03045
HB	31	MET	-	linker	UNP P03045
HB	39	ASN	ILE	engineered mutation	UNP O66529
HB	42	VAL	GLU	engineered mutation	UNP O66529
HB	58	VAL	ILE	engineered mutation	UNP O66529
HB	61	ASP	GLY	engineered mutation	UNP O66529
HB	62	ILE	VAL	engineered mutation	UNP O66529
HB	97	TYR	PHE	engineered mutation	UNP O66529
HB	102	GLY	-	linker	UNP O66529
HB	103	THR	-	linker	UNP O66529
HB	104	GLY	-	linker	UNP O66529
HB	105	HIS	-	linker	UNP O66529
HB	106	HIS	-	linker	UNP O66529
HB	107	HIS	-	linker	UNP O66529
HB	108	HIS	-	linker	UNP O66529
HB	109	HIS	-	linker	UNP O66529
HB	110	HIS	-	linker	UNP O66529
HB	111	GLY	-	linker	UNP O66529
HB	112	SER	-	linker	UNP O66529
HB	113	SER	-	linker	UNP O66529
HB	114	ILE	MET	engineered mutation	UNP O66529
HB	115	GLU	GLN	engineered mutation	UNP O66529
HB	138	THR	ALA	engineered mutation	UNP O66529
HB	177	ASP	GLY	engineered mutation	UNP O66529
HB	191	PHE	ILE	engineered mutation	UNP O66529
HB	193	ASP	VAL	engineered mutation	UNP O66529
HC	1	MET	-	cloning artifact	UNP P03045
HC	2	GLY	-	cloning artifact	UNP P03045
HC	3	ASN	-	cloning artifact	UNP P03045
HC	4	ALA	-	cloning artifact	UNP P03045
HC	5	LYS	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
HC	6	THR	-	cloning artifact	UNP P03045
HC	24	ALA	-	linker	UNP P03045
HC	25	GLY	-	linker	UNP P03045
HC	26	ALA	-	linker	UNP P03045
HC	27	GLY	-	linker	UNP P03045
HC	28	ALA	-	linker	UNP P03045
HC	29	GLY	-	linker	UNP P03045
HC	30	ALA	-	linker	UNP P03045
HC	31	MET	-	linker	UNP P03045
HC	39	ASN	ILE	engineered mutation	UNP O66529
HC	42	VAL	GLU	engineered mutation	UNP O66529
HC	58	VAL	ILE	engineered mutation	UNP O66529
HC	61	ASP	GLY	engineered mutation	UNP O66529
HC	62	ILE	VAL	engineered mutation	UNP O66529
HC	97	TYR	PHE	engineered mutation	UNP O66529
HC	102	GLY	-	linker	UNP O66529
HC	103	THR	-	linker	UNP O66529
HC	104	GLY	-	linker	UNP O66529
HC	105	HIS	-	linker	UNP O66529
HC	106	HIS	-	linker	UNP O66529
HC	107	HIS	-	linker	UNP O66529
HC	108	HIS	-	linker	UNP O66529
HC	109	HIS	-	linker	UNP O66529
HC	110	HIS	-	linker	UNP O66529
HC	111	GLY	-	linker	UNP O66529
HC	112	SER	-	linker	UNP O66529
HC	113	SER	-	linker	UNP O66529
HC	114	ILE	MET	engineered mutation	UNP O66529
HC	115	GLU	GLN	engineered mutation	UNP O66529
HC	138	THR	ALA	engineered mutation	UNP O66529
HC	177	ASP	GLY	engineered mutation	UNP O66529
HC	191	PHE	ILE	engineered mutation	UNP O66529
HC	193	ASP	VAL	engineered mutation	UNP O66529
HD	1	MET	-	cloning artifact	UNP P03045
HD	2	GLY	-	cloning artifact	UNP P03045
HD	3	ASN	-	cloning artifact	UNP P03045
HD	4	ALA	-	cloning artifact	UNP P03045
HD	5	LYS	-	cloning artifact	UNP P03045
HD	6	THR	-	cloning artifact	UNP P03045
HD	24	ALA	-	linker	UNP P03045
HD	25	GLY	-	linker	UNP P03045
HD	26	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
HD	27	GLY	-	linker	UNP P03045
HD	28	ALA	-	linker	UNP P03045
HD	29	GLY	-	linker	UNP P03045
HD	30	ALA	-	linker	UNP P03045
HD	31	MET	-	linker	UNP P03045
HD	39	ASN	ILE	engineered mutation	UNP O66529
HD	42	VAL	GLU	engineered mutation	UNP O66529
HD	58	VAL	ILE	engineered mutation	UNP O66529
HD	61	ASP	GLY	engineered mutation	UNP O66529
HD	62	ILE	VAL	engineered mutation	UNP O66529
HD	97	TYR	PHE	engineered mutation	UNP O66529
HD	102	GLY	-	linker	UNP O66529
HD	103	THR	-	linker	UNP O66529
HD	104	GLY	-	linker	UNP O66529
HD	105	HIS	-	linker	UNP O66529
HD	106	HIS	-	linker	UNP O66529
HD	107	HIS	-	linker	UNP O66529
HD	108	HIS	-	linker	UNP O66529
HD	109	HIS	-	linker	UNP O66529
HD	110	HIS	-	linker	UNP O66529
HD	111	GLY	-	linker	UNP O66529
HD	112	SER	-	linker	UNP O66529
HD	113	SER	-	linker	UNP O66529
HD	114	ILE	MET	engineered mutation	UNP O66529
HD	115	GLU	GLN	engineered mutation	UNP O66529
HD	138	THR	ALA	engineered mutation	UNP O66529
HD	177	ASP	GLY	engineered mutation	UNP O66529
HD	191	PHE	ILE	engineered mutation	UNP O66529
HD	193	ASP	VAL	engineered mutation	UNP O66529
IA	1	MET	-	cloning artifact	UNP P03045
IA	2	GLY	-	cloning artifact	UNP P03045
IA	3	ASN	-	cloning artifact	UNP P03045
IA	4	ALA	-	cloning artifact	UNP P03045
IA	5	LYS	-	cloning artifact	UNP P03045
IA	6	THR	-	cloning artifact	UNP P03045
IA	24	ALA	-	linker	UNP P03045
IA	25	GLY	-	linker	UNP P03045
IA	26	ALA	-	linker	UNP P03045
IA	27	GLY	-	linker	UNP P03045
IA	28	ALA	-	linker	UNP P03045
IA	29	GLY	-	linker	UNP P03045
IA	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
IA	31	MET	-	linker	UNP P03045
IA	39	ASN	ILE	engineered mutation	UNP O66529
IA	42	VAL	GLU	engineered mutation	UNP O66529
IA	58	VAL	ILE	engineered mutation	UNP O66529
IA	61	ASP	GLY	engineered mutation	UNP O66529
IA	62	ILE	VAL	engineered mutation	UNP O66529
IA	97	TYR	PHE	engineered mutation	UNP O66529
IA	102	GLY	-	linker	UNP O66529
IA	103	THR	-	linker	UNP O66529
IA	104	GLY	-	linker	UNP O66529
IA	105	HIS	-	linker	UNP O66529
IA	106	HIS	-	linker	UNP O66529
IA	107	HIS	-	linker	UNP O66529
IA	108	HIS	-	linker	UNP O66529
IA	109	HIS	-	linker	UNP O66529
IA	110	HIS	-	linker	UNP O66529
IA	111	GLY	-	linker	UNP O66529
IA	112	SER	-	linker	UNP O66529
IA	113	SER	-	linker	UNP O66529
IA	114	ILE	MET	engineered mutation	UNP O66529
IA	115	GLU	GLN	engineered mutation	UNP O66529
IA	138	THR	ALA	engineered mutation	UNP O66529
IA	177	ASP	GLY	engineered mutation	UNP O66529
IA	191	PHE	ILE	engineered mutation	UNP O66529
IA	193	ASP	VAL	engineered mutation	UNP O66529
IB	1	MET	-	cloning artifact	UNP P03045
IB	2	GLY	-	cloning artifact	UNP P03045
IB	3	ASN	-	cloning artifact	UNP P03045
IB	4	ALA	-	cloning artifact	UNP P03045
IB	5	LYS	-	cloning artifact	UNP P03045
IB	6	THR	-	cloning artifact	UNP P03045
IB	24	ALA	-	linker	UNP P03045
IB	25	GLY	-	linker	UNP P03045
IB	26	ALA	-	linker	UNP P03045
IB	27	GLY	-	linker	UNP P03045
IB	28	ALA	-	linker	UNP P03045
IB	29	GLY	-	linker	UNP P03045
IB	30	ALA	-	linker	UNP P03045
IB	31	MET	-	linker	UNP P03045
IB	39	ASN	ILE	engineered mutation	UNP O66529
IB	42	VAL	GLU	engineered mutation	UNP O66529
IB	58	VAL	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
IB	61	ASP	GLY	engineered mutation	UNP O66529
IB	62	ILE	VAL	engineered mutation	UNP O66529
IB	97	TYR	PHE	engineered mutation	UNP O66529
IB	102	GLY	-	linker	UNP O66529
IB	103	THR	-	linker	UNP O66529
IB	104	GLY	-	linker	UNP O66529
IB	105	HIS	-	linker	UNP O66529
IB	106	HIS	-	linker	UNP O66529
IB	107	HIS	-	linker	UNP O66529
IB	108	HIS	-	linker	UNP O66529
IB	109	HIS	-	linker	UNP O66529
IB	110	HIS	-	linker	UNP O66529
IB	111	GLY	-	linker	UNP O66529
IB	112	SER	-	linker	UNP O66529
IB	113	SER	-	linker	UNP O66529
IB	114	ILE	MET	engineered mutation	UNP O66529
IB	115	GLU	GLN	engineered mutation	UNP O66529
IB	138	THR	ALA	engineered mutation	UNP O66529
IB	177	ASP	GLY	engineered mutation	UNP O66529
IB	191	PHE	ILE	engineered mutation	UNP O66529
IB	193	ASP	VAL	engineered mutation	UNP O66529
IC	1	MET	-	cloning artifact	UNP P03045
IC	2	GLY	-	cloning artifact	UNP P03045
IC	3	ASN	-	cloning artifact	UNP P03045
IC	4	ALA	-	cloning artifact	UNP P03045
IC	5	LYS	-	cloning artifact	UNP P03045
IC	6	THR	-	cloning artifact	UNP P03045
IC	24	ALA	-	linker	UNP P03045
IC	25	GLY	-	linker	UNP P03045
IC	26	ALA	-	linker	UNP P03045
IC	27	GLY	-	linker	UNP P03045
IC	28	ALA	-	linker	UNP P03045
IC	29	GLY	-	linker	UNP P03045
IC	30	ALA	-	linker	UNP P03045
IC	31	MET	-	linker	UNP P03045
IC	39	ASN	ILE	engineered mutation	UNP O66529
IC	42	VAL	GLU	engineered mutation	UNP O66529
IC	58	VAL	ILE	engineered mutation	UNP O66529
IC	61	ASP	GLY	engineered mutation	UNP O66529
IC	62	ILE	VAL	engineered mutation	UNP O66529
IC	97	TYR	PHE	engineered mutation	UNP O66529
IC	102	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
IC	103	THR	-	linker	UNP O66529
IC	104	GLY	-	linker	UNP O66529
IC	105	HIS	-	linker	UNP O66529
IC	106	HIS	-	linker	UNP O66529
IC	107	HIS	-	linker	UNP O66529
IC	108	HIS	-	linker	UNP O66529
IC	109	HIS	-	linker	UNP O66529
IC	110	HIS	-	linker	UNP O66529
IC	111	GLY	-	linker	UNP O66529
IC	112	SER	-	linker	UNP O66529
IC	113	SER	-	linker	UNP O66529
IC	114	ILE	MET	engineered mutation	UNP O66529
IC	115	GLU	GLN	engineered mutation	UNP O66529
IC	138	THR	ALA	engineered mutation	UNP O66529
IC	177	ASP	GLY	engineered mutation	UNP O66529
IC	191	PHE	ILE	engineered mutation	UNP O66529
IC	193	ASP	VAL	engineered mutation	UNP O66529
ID	1	MET	-	cloning artifact	UNP P03045
ID	2	GLY	-	cloning artifact	UNP P03045
ID	3	ASN	-	cloning artifact	UNP P03045
ID	4	ALA	-	cloning artifact	UNP P03045
ID	5	LYS	-	cloning artifact	UNP P03045
ID	6	THR	-	cloning artifact	UNP P03045
ID	24	ALA	-	linker	UNP P03045
ID	25	GLY	-	linker	UNP P03045
ID	26	ALA	-	linker	UNP P03045
ID	27	GLY	-	linker	UNP P03045
ID	28	ALA	-	linker	UNP P03045
ID	29	GLY	-	linker	UNP P03045
ID	30	ALA	-	linker	UNP P03045
ID	31	MET	-	linker	UNP P03045
ID	39	ASN	ILE	engineered mutation	UNP O66529
ID	42	VAL	GLU	engineered mutation	UNP O66529
ID	58	VAL	ILE	engineered mutation	UNP O66529
ID	61	ASP	GLY	engineered mutation	UNP O66529
ID	62	ILE	VAL	engineered mutation	UNP O66529
ID	97	TYR	PHE	engineered mutation	UNP O66529
ID	102	GLY	-	linker	UNP O66529
ID	103	THR	-	linker	UNP O66529
ID	104	GLY	-	linker	UNP O66529
ID	105	HIS	-	linker	UNP O66529
ID	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
ID	107	HIS	-	linker	UNP O66529
ID	108	HIS	-	linker	UNP O66529
ID	109	HIS	-	linker	UNP O66529
ID	110	HIS	-	linker	UNP O66529
ID	111	GLY	-	linker	UNP O66529
ID	112	SER	-	linker	UNP O66529
ID	113	SER	-	linker	UNP O66529
ID	114	ILE	MET	engineered mutation	UNP O66529
ID	115	GLU	GLN	engineered mutation	UNP O66529
ID	138	THR	ALA	engineered mutation	UNP O66529
ID	177	ASP	GLY	engineered mutation	UNP O66529
ID	191	PHE	ILE	engineered mutation	UNP O66529
ID	193	ASP	VAL	engineered mutation	UNP O66529
5A	1	MET	-	cloning artifact	UNP P03045
5A	2	GLY	-	cloning artifact	UNP P03045
5A	3	ASN	-	cloning artifact	UNP P03045
5A	4	ALA	-	cloning artifact	UNP P03045
5A	5	LYS	-	cloning artifact	UNP P03045
5A	6	THR	-	cloning artifact	UNP P03045
5A	24	ALA	-	linker	UNP P03045
5A	25	GLY	-	linker	UNP P03045
5A	26	ALA	-	linker	UNP P03045
5A	27	GLY	-	linker	UNP P03045
5A	28	ALA	-	linker	UNP P03045
5A	29	GLY	-	linker	UNP P03045
5A	30	ALA	-	linker	UNP P03045
5A	31	MET	-	linker	UNP P03045
5A	39	ASN	ILE	engineered mutation	UNP O66529
5A	42	VAL	GLU	engineered mutation	UNP O66529
5A	58	VAL	ILE	engineered mutation	UNP O66529
5A	61	ASP	GLY	engineered mutation	UNP O66529
5A	62	ILE	VAL	engineered mutation	UNP O66529
5A	97	TYR	PHE	engineered mutation	UNP O66529
5A	102	GLY	-	linker	UNP O66529
5A	103	THR	-	linker	UNP O66529
5A	104	GLY	-	linker	UNP O66529
5A	105	HIS	-	linker	UNP O66529
5A	106	HIS	-	linker	UNP O66529
5A	107	HIS	-	linker	UNP O66529
5A	108	HIS	-	linker	UNP O66529
5A	109	HIS	-	linker	UNP O66529
5A	110	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
5A	111	GLY	-	linker	UNP O66529
5A	112	SER	-	linker	UNP O66529
5A	113	SER	-	linker	UNP O66529
5A	114	ILE	MET	engineered mutation	UNP O66529
5A	115	GLU	GLN	engineered mutation	UNP O66529
5A	138	THR	ALA	engineered mutation	UNP O66529
5A	177	ASP	GLY	engineered mutation	UNP O66529
5A	191	PHE	ILE	engineered mutation	UNP O66529
5A	193	ASP	VAL	engineered mutation	UNP O66529
5B	1	MET	-	cloning artifact	UNP P03045
5B	2	GLY	-	cloning artifact	UNP P03045
5B	3	ASN	-	cloning artifact	UNP P03045
5B	4	ALA	-	cloning artifact	UNP P03045
5B	5	LYS	-	cloning artifact	UNP P03045
5B	6	THR	-	cloning artifact	UNP P03045
5B	24	ALA	-	linker	UNP P03045
5B	25	GLY	-	linker	UNP P03045
5B	26	ALA	-	linker	UNP P03045
5B	27	GLY	-	linker	UNP P03045
5B	28	ALA	-	linker	UNP P03045
5B	29	GLY	-	linker	UNP P03045
5B	30	ALA	-	linker	UNP P03045
5B	31	MET	-	linker	UNP P03045
5B	39	ASN	ILE	engineered mutation	UNP O66529
5B	42	VAL	GLU	engineered mutation	UNP O66529
5B	58	VAL	ILE	engineered mutation	UNP O66529
5B	61	ASP	GLY	engineered mutation	UNP O66529
5B	62	ILE	VAL	engineered mutation	UNP O66529
5B	97	TYR	PHE	engineered mutation	UNP O66529
5B	102	GLY	-	linker	UNP O66529
5B	103	THR	-	linker	UNP O66529
5B	104	GLY	-	linker	UNP O66529
5B	105	HIS	-	linker	UNP O66529
5B	106	HIS	-	linker	UNP O66529
5B	107	HIS	-	linker	UNP O66529
5B	108	HIS	-	linker	UNP O66529
5B	109	HIS	-	linker	UNP O66529
5B	110	HIS	-	linker	UNP O66529
5B	111	GLY	-	linker	UNP O66529
5B	112	SER	-	linker	UNP O66529
5B	113	SER	-	linker	UNP O66529
5B	114	ILE	MET	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
5B	115	GLU	GLN	engineered mutation	UNP O66529
5B	138	THR	ALA	engineered mutation	UNP O66529
5B	177	ASP	GLY	engineered mutation	UNP O66529
5B	191	PHE	ILE	engineered mutation	UNP O66529
5B	193	ASP	VAL	engineered mutation	UNP O66529
5C	1	MET	-	cloning artifact	UNP P03045
5C	2	GLY	-	cloning artifact	UNP P03045
5C	3	ASN	-	cloning artifact	UNP P03045
5C	4	ALA	-	cloning artifact	UNP P03045
5C	5	LYS	-	cloning artifact	UNP P03045
5C	6	THR	-	cloning artifact	UNP P03045
5C	24	ALA	-	linker	UNP P03045
5C	25	GLY	-	linker	UNP P03045
5C	26	ALA	-	linker	UNP P03045
5C	27	GLY	-	linker	UNP P03045
5C	28	ALA	-	linker	UNP P03045
5C	29	GLY	-	linker	UNP P03045
5C	30	ALA	-	linker	UNP P03045
5C	31	MET	-	linker	UNP P03045
5C	39	ASN	ILE	engineered mutation	UNP O66529
5C	42	VAL	GLU	engineered mutation	UNP O66529
5C	58	VAL	ILE	engineered mutation	UNP O66529
5C	61	ASP	GLY	engineered mutation	UNP O66529
5C	62	ILE	VAL	engineered mutation	UNP O66529
5C	97	TYR	PHE	engineered mutation	UNP O66529
5C	102	GLY	-	linker	UNP O66529
5C	103	THR	-	linker	UNP O66529
5C	104	GLY	-	linker	UNP O66529
5C	105	HIS	-	linker	UNP O66529
5C	106	HIS	-	linker	UNP O66529
5C	107	HIS	-	linker	UNP O66529
5C	108	HIS	-	linker	UNP O66529
5C	109	HIS	-	linker	UNP O66529
5C	110	HIS	-	linker	UNP O66529
5C	111	GLY	-	linker	UNP O66529
5C	112	SER	-	linker	UNP O66529
5C	113	SER	-	linker	UNP O66529
5C	114	ILE	MET	engineered mutation	UNP O66529
5C	115	GLU	GLN	engineered mutation	UNP O66529
5C	138	THR	ALA	engineered mutation	UNP O66529
5C	177	ASP	GLY	engineered mutation	UNP O66529
5C	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
5C	193	ASP	VAL	engineered mutation	UNP O66529
5D	1	MET	-	cloning artifact	UNP P03045
5D	2	GLY	-	cloning artifact	UNP P03045
5D	3	ASN	-	cloning artifact	UNP P03045
5D	4	ALA	-	cloning artifact	UNP P03045
5D	5	LYS	-	cloning artifact	UNP P03045
5D	6	THR	-	cloning artifact	UNP P03045
5D	24	ALA	-	linker	UNP P03045
5D	25	GLY	-	linker	UNP P03045
5D	26	ALA	-	linker	UNP P03045
5D	27	GLY	-	linker	UNP P03045
5D	28	ALA	-	linker	UNP P03045
5D	29	GLY	-	linker	UNP P03045
5D	30	ALA	-	linker	UNP P03045
5D	31	MET	-	linker	UNP P03045
5D	39	ASN	ILE	engineered mutation	UNP O66529
5D	42	VAL	GLU	engineered mutation	UNP O66529
5D	58	VAL	ILE	engineered mutation	UNP O66529
5D	61	ASP	GLY	engineered mutation	UNP O66529
5D	62	ILE	VAL	engineered mutation	UNP O66529
5D	97	TYR	PHE	engineered mutation	UNP O66529
5D	102	GLY	-	linker	UNP O66529
5D	103	THR	-	linker	UNP O66529
5D	104	GLY	-	linker	UNP O66529
5D	105	HIS	-	linker	UNP O66529
5D	106	HIS	-	linker	UNP O66529
5D	107	HIS	-	linker	UNP O66529
5D	108	HIS	-	linker	UNP O66529
5D	109	HIS	-	linker	UNP O66529
5D	110	HIS	-	linker	UNP O66529
5D	111	GLY	-	linker	UNP O66529
5D	112	SER	-	linker	UNP O66529
5D	113	SER	-	linker	UNP O66529
5D	114	ILE	MET	engineered mutation	UNP O66529
5D	115	GLU	GLN	engineered mutation	UNP O66529
5D	138	THR	ALA	engineered mutation	UNP O66529
5D	177	ASP	GLY	engineered mutation	UNP O66529
5D	191	PHE	ILE	engineered mutation	UNP O66529
5D	193	ASP	VAL	engineered mutation	UNP O66529
JA	1	MET	-	cloning artifact	UNP P03045
JA	2	GLY	-	cloning artifact	UNP P03045
JA	3	ASN	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
JA	4	ALA	-	cloning artifact	UNP P03045
JA	5	LYS	-	cloning artifact	UNP P03045
JA	6	THR	-	cloning artifact	UNP P03045
JA	24	ALA	-	linker	UNP P03045
JA	25	GLY	-	linker	UNP P03045
JA	26	ALA	-	linker	UNP P03045
JA	27	GLY	-	linker	UNP P03045
JA	28	ALA	-	linker	UNP P03045
JA	29	GLY	-	linker	UNP P03045
JA	30	ALA	-	linker	UNP P03045
JA	31	MET	-	linker	UNP P03045
JA	39	ASN	ILE	engineered mutation	UNP O66529
JA	42	VAL	GLU	engineered mutation	UNP O66529
JA	58	VAL	ILE	engineered mutation	UNP O66529
JA	61	ASP	GLY	engineered mutation	UNP O66529
JA	62	ILE	VAL	engineered mutation	UNP O66529
JA	97	TYR	PHE	engineered mutation	UNP O66529
JA	102	GLY	-	linker	UNP O66529
JA	103	THR	-	linker	UNP O66529
JA	104	GLY	-	linker	UNP O66529
JA	105	HIS	-	linker	UNP O66529
JA	106	HIS	-	linker	UNP O66529
JA	107	HIS	-	linker	UNP O66529
JA	108	HIS	-	linker	UNP O66529
JA	109	HIS	-	linker	UNP O66529
JA	110	HIS	-	linker	UNP O66529
JA	111	GLY	-	linker	UNP O66529
JA	112	SER	-	linker	UNP O66529
JA	113	SER	-	linker	UNP O66529
JA	114	ILE	MET	engineered mutation	UNP O66529
JA	115	GLU	GLN	engineered mutation	UNP O66529
JA	138	THR	ALA	engineered mutation	UNP O66529
JA	177	ASP	GLY	engineered mutation	UNP O66529
JA	191	PHE	ILE	engineered mutation	UNP O66529
JA	193	ASP	VAL	engineered mutation	UNP O66529
JB	1	MET	-	cloning artifact	UNP P03045
JB	2	GLY	-	cloning artifact	UNP P03045
JB	3	ASN	-	cloning artifact	UNP P03045
JB	4	ALA	-	cloning artifact	UNP P03045
JB	5	LYS	-	cloning artifact	UNP P03045
JB	6	THR	-	cloning artifact	UNP P03045
JB	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
JB	25	GLY	-	linker	UNP P03045
JB	26	ALA	-	linker	UNP P03045
JB	27	GLY	-	linker	UNP P03045
JB	28	ALA	-	linker	UNP P03045
JB	29	GLY	-	linker	UNP P03045
JB	30	ALA	-	linker	UNP P03045
JB	31	MET	-	linker	UNP P03045
JB	39	ASN	ILE	engineered mutation	UNP O66529
JB	42	VAL	GLU	engineered mutation	UNP O66529
JB	58	VAL	ILE	engineered mutation	UNP O66529
JB	61	ASP	GLY	engineered mutation	UNP O66529
JB	62	ILE	VAL	engineered mutation	UNP O66529
JB	97	TYR	PHE	engineered mutation	UNP O66529
JB	102	GLY	-	linker	UNP O66529
JB	103	THR	-	linker	UNP O66529
JB	104	GLY	-	linker	UNP O66529
JB	105	HIS	-	linker	UNP O66529
JB	106	HIS	-	linker	UNP O66529
JB	107	HIS	-	linker	UNP O66529
JB	108	HIS	-	linker	UNP O66529
JB	109	HIS	-	linker	UNP O66529
JB	110	HIS	-	linker	UNP O66529
JB	111	GLY	-	linker	UNP O66529
JB	112	SER	-	linker	UNP O66529
JB	113	SER	-	linker	UNP O66529
JB	114	ILE	MET	engineered mutation	UNP O66529
JB	115	GLU	GLN	engineered mutation	UNP O66529
JB	138	THR	ALA	engineered mutation	UNP O66529
JB	177	ASP	GLY	engineered mutation	UNP O66529
JB	191	PHE	ILE	engineered mutation	UNP O66529
JB	193	ASP	VAL	engineered mutation	UNP O66529
JC	1	MET	-	cloning artifact	UNP P03045
JC	2	GLY	-	cloning artifact	UNP P03045
JC	3	ASN	-	cloning artifact	UNP P03045
JC	4	ALA	-	cloning artifact	UNP P03045
JC	5	LYS	-	cloning artifact	UNP P03045
JC	6	THR	-	cloning artifact	UNP P03045
JC	24	ALA	-	linker	UNP P03045
JC	25	GLY	-	linker	UNP P03045
JC	26	ALA	-	linker	UNP P03045
JC	27	GLY	-	linker	UNP P03045
JC	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
JC	29	GLY	-	linker	UNP P03045
JC	30	ALA	-	linker	UNP P03045
JC	31	MET	-	linker	UNP P03045
JC	39	ASN	ILE	engineered mutation	UNP O66529
JC	42	VAL	GLU	engineered mutation	UNP O66529
JC	58	VAL	ILE	engineered mutation	UNP O66529
JC	61	ASP	GLY	engineered mutation	UNP O66529
JC	62	ILE	VAL	engineered mutation	UNP O66529
JC	97	TYR	PHE	engineered mutation	UNP O66529
JC	102	GLY	-	linker	UNP O66529
JC	103	THR	-	linker	UNP O66529
JC	104	GLY	-	linker	UNP O66529
JC	105	HIS	-	linker	UNP O66529
JC	106	HIS	-	linker	UNP O66529
JC	107	HIS	-	linker	UNP O66529
JC	108	HIS	-	linker	UNP O66529
JC	109	HIS	-	linker	UNP O66529
JC	110	HIS	-	linker	UNP O66529
JC	111	GLY	-	linker	UNP O66529
JC	112	SER	-	linker	UNP O66529
JC	113	SER	-	linker	UNP O66529
JC	114	ILE	MET	engineered mutation	UNP O66529
JC	115	GLU	GLN	engineered mutation	UNP O66529
JC	138	THR	ALA	engineered mutation	UNP O66529
JC	177	ASP	GLY	engineered mutation	UNP O66529
JC	191	PHE	ILE	engineered mutation	UNP O66529
JC	193	ASP	VAL	engineered mutation	UNP O66529
JD	1	MET	-	cloning artifact	UNP P03045
JD	2	GLY	-	cloning artifact	UNP P03045
JD	3	ASN	-	cloning artifact	UNP P03045
JD	4	ALA	-	cloning artifact	UNP P03045
JD	5	LYS	-	cloning artifact	UNP P03045
JD	6	THR	-	cloning artifact	UNP P03045
JD	24	ALA	-	linker	UNP P03045
JD	25	GLY	-	linker	UNP P03045
JD	26	ALA	-	linker	UNP P03045
JD	27	GLY	-	linker	UNP P03045
JD	28	ALA	-	linker	UNP P03045
JD	29	GLY	-	linker	UNP P03045
JD	30	ALA	-	linker	UNP P03045
JD	31	MET	-	linker	UNP P03045
JD	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
JD	42	VAL	GLU	engineered mutation	UNP O66529
JD	58	VAL	ILE	engineered mutation	UNP O66529
JD	61	ASP	GLY	engineered mutation	UNP O66529
JD	62	ILE	VAL	engineered mutation	UNP O66529
JD	97	TYR	PHE	engineered mutation	UNP O66529
JD	102	GLY	-	linker	UNP O66529
JD	103	THR	-	linker	UNP O66529
JD	104	GLY	-	linker	UNP O66529
JD	105	HIS	-	linker	UNP O66529
JD	106	HIS	-	linker	UNP O66529
JD	107	HIS	-	linker	UNP O66529
JD	108	HIS	-	linker	UNP O66529
JD	109	HIS	-	linker	UNP O66529
JD	110	HIS	-	linker	UNP O66529
JD	111	GLY	-	linker	UNP O66529
JD	112	SER	-	linker	UNP O66529
JD	113	SER	-	linker	UNP O66529
JD	114	ILE	MET	engineered mutation	UNP O66529
JD	115	GLU	GLN	engineered mutation	UNP O66529
JD	138	THR	ALA	engineered mutation	UNP O66529
JD	177	ASP	GLY	engineered mutation	UNP O66529
JD	191	PHE	ILE	engineered mutation	UNP O66529
JD	193	ASP	VAL	engineered mutation	UNP O66529
KA	1	MET	-	cloning artifact	UNP P03045
KA	2	GLY	-	cloning artifact	UNP P03045
KA	3	ASN	-	cloning artifact	UNP P03045
KA	4	ALA	-	cloning artifact	UNP P03045
KA	5	LYS	-	cloning artifact	UNP P03045
KA	6	THR	-	cloning artifact	UNP P03045
KA	24	ALA	-	linker	UNP P03045
KA	25	GLY	-	linker	UNP P03045
KA	26	ALA	-	linker	UNP P03045
KA	27	GLY	-	linker	UNP P03045
KA	28	ALA	-	linker	UNP P03045
KA	29	GLY	-	linker	UNP P03045
KA	30	ALA	-	linker	UNP P03045
KA	31	MET	-	linker	UNP P03045
KA	39	ASN	ILE	engineered mutation	UNP O66529
KA	42	VAL	GLU	engineered mutation	UNP O66529
KA	58	VAL	ILE	engineered mutation	UNP O66529
KA	61	ASP	GLY	engineered mutation	UNP O66529
KA	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
KA	97	TYR	PHE	engineered mutation	UNP O66529
KA	102	GLY	-	linker	UNP O66529
KA	103	THR	-	linker	UNP O66529
KA	104	GLY	-	linker	UNP O66529
KA	105	HIS	-	linker	UNP O66529
KA	106	HIS	-	linker	UNP O66529
KA	107	HIS	-	linker	UNP O66529
KA	108	HIS	-	linker	UNP O66529
KA	109	HIS	-	linker	UNP O66529
KA	110	HIS	-	linker	UNP O66529
KA	111	GLY	-	linker	UNP O66529
KA	112	SER	-	linker	UNP O66529
KA	113	SER	-	linker	UNP O66529
KA	114	ILE	MET	engineered mutation	UNP O66529
KA	115	GLU	GLN	engineered mutation	UNP O66529
KA	138	THR	ALA	engineered mutation	UNP O66529
KA	177	ASP	GLY	engineered mutation	UNP O66529
KA	191	PHE	ILE	engineered mutation	UNP O66529
KA	193	ASP	VAL	engineered mutation	UNP O66529
KB	1	MET	-	cloning artifact	UNP P03045
KB	2	GLY	-	cloning artifact	UNP P03045
KB	3	ASN	-	cloning artifact	UNP P03045
KB	4	ALA	-	cloning artifact	UNP P03045
KB	5	LYS	-	cloning artifact	UNP P03045
KB	6	THR	-	cloning artifact	UNP P03045
KB	24	ALA	-	linker	UNP P03045
KB	25	GLY	-	linker	UNP P03045
KB	26	ALA	-	linker	UNP P03045
KB	27	GLY	-	linker	UNP P03045
KB	28	ALA	-	linker	UNP P03045
KB	29	GLY	-	linker	UNP P03045
KB	30	ALA	-	linker	UNP P03045
KB	31	MET	-	linker	UNP P03045
KB	39	ASN	ILE	engineered mutation	UNP O66529
KB	42	VAL	GLU	engineered mutation	UNP O66529
KB	58	VAL	ILE	engineered mutation	UNP O66529
KB	61	ASP	GLY	engineered mutation	UNP O66529
KB	62	ILE	VAL	engineered mutation	UNP O66529
KB	97	TYR	PHE	engineered mutation	UNP O66529
KB	102	GLY	-	linker	UNP O66529
KB	103	THR	-	linker	UNP O66529
KB	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
KB	105	HIS	-	linker	UNP O66529
KB	106	HIS	-	linker	UNP O66529
KB	107	HIS	-	linker	UNP O66529
KB	108	HIS	-	linker	UNP O66529
KB	109	HIS	-	linker	UNP O66529
KB	110	HIS	-	linker	UNP O66529
KB	111	GLY	-	linker	UNP O66529
KB	112	SER	-	linker	UNP O66529
KB	113	SER	-	linker	UNP O66529
KB	114	ILE	MET	engineered mutation	UNP O66529
KB	115	GLU	GLN	engineered mutation	UNP O66529
KB	138	THR	ALA	engineered mutation	UNP O66529
KB	177	ASP	GLY	engineered mutation	UNP O66529
KB	191	PHE	ILE	engineered mutation	UNP O66529
KB	193	ASP	VAL	engineered mutation	UNP O66529
KC	1	MET	-	cloning artifact	UNP P03045
KC	2	GLY	-	cloning artifact	UNP P03045
KC	3	ASN	-	cloning artifact	UNP P03045
KC	4	ALA	-	cloning artifact	UNP P03045
KC	5	LYS	-	cloning artifact	UNP P03045
KC	6	THR	-	cloning artifact	UNP P03045
KC	24	ALA	-	linker	UNP P03045
KC	25	GLY	-	linker	UNP P03045
KC	26	ALA	-	linker	UNP P03045
KC	27	GLY	-	linker	UNP P03045
KC	28	ALA	-	linker	UNP P03045
KC	29	GLY	-	linker	UNP P03045
KC	30	ALA	-	linker	UNP P03045
KC	31	MET	-	linker	UNP P03045
KC	39	ASN	ILE	engineered mutation	UNP O66529
KC	42	VAL	GLU	engineered mutation	UNP O66529
KC	58	VAL	ILE	engineered mutation	UNP O66529
KC	61	ASP	GLY	engineered mutation	UNP O66529
KC	62	ILE	VAL	engineered mutation	UNP O66529
KC	97	TYR	PHE	engineered mutation	UNP O66529
KC	102	GLY	-	linker	UNP O66529
KC	103	THR	-	linker	UNP O66529
KC	104	GLY	-	linker	UNP O66529
KC	105	HIS	-	linker	UNP O66529
KC	106	HIS	-	linker	UNP O66529
KC	107	HIS	-	linker	UNP O66529
KC	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
KC	109	HIS	-	linker	UNP O66529
KC	110	HIS	-	linker	UNP O66529
KC	111	GLY	-	linker	UNP O66529
KC	112	SER	-	linker	UNP O66529
KC	113	SER	-	linker	UNP O66529
KC	114	ILE	MET	engineered mutation	UNP O66529
KC	115	GLU	GLN	engineered mutation	UNP O66529
KC	138	THR	ALA	engineered mutation	UNP O66529
KC	177	ASP	GLY	engineered mutation	UNP O66529
KC	191	PHE	ILE	engineered mutation	UNP O66529
KC	193	ASP	VAL	engineered mutation	UNP O66529
KD	1	MET	-	cloning artifact	UNP P03045
KD	2	GLY	-	cloning artifact	UNP P03045
KD	3	ASN	-	cloning artifact	UNP P03045
KD	4	ALA	-	cloning artifact	UNP P03045
KD	5	LYS	-	cloning artifact	UNP P03045
KD	6	THR	-	cloning artifact	UNP P03045
KD	24	ALA	-	linker	UNP P03045
KD	25	GLY	-	linker	UNP P03045
KD	26	ALA	-	linker	UNP P03045
KD	27	GLY	-	linker	UNP P03045
KD	28	ALA	-	linker	UNP P03045
KD	29	GLY	-	linker	UNP P03045
KD	30	ALA	-	linker	UNP P03045
KD	31	MET	-	linker	UNP P03045
KD	39	ASN	ILE	engineered mutation	UNP O66529
KD	42	VAL	GLU	engineered mutation	UNP O66529
KD	58	VAL	ILE	engineered mutation	UNP O66529
KD	61	ASP	GLY	engineered mutation	UNP O66529
KD	62	ILE	VAL	engineered mutation	UNP O66529
KD	97	TYR	PHE	engineered mutation	UNP O66529
KD	102	GLY	-	linker	UNP O66529
KD	103	THR	-	linker	UNP O66529
KD	104	GLY	-	linker	UNP O66529
KD	105	HIS	-	linker	UNP O66529
KD	106	HIS	-	linker	UNP O66529
KD	107	HIS	-	linker	UNP O66529
KD	108	HIS	-	linker	UNP O66529
KD	109	HIS	-	linker	UNP O66529
KD	110	HIS	-	linker	UNP O66529
KD	111	GLY	-	linker	UNP O66529
KD	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
KD	113	SER	-	linker	UNP O66529
KD	114	ILE	MET	engineered mutation	UNP O66529
KD	115	GLU	GLN	engineered mutation	UNP O66529
KD	138	THR	ALA	engineered mutation	UNP O66529
KD	177	ASP	GLY	engineered mutation	UNP O66529
KD	191	PHE	ILE	engineered mutation	UNP O66529
KD	193	ASP	VAL	engineered mutation	UNP O66529
LA	1	MET	-	cloning artifact	UNP P03045
LA	2	GLY	-	cloning artifact	UNP P03045
LA	3	ASN	-	cloning artifact	UNP P03045
LA	4	ALA	-	cloning artifact	UNP P03045
LA	5	LYS	-	cloning artifact	UNP P03045
LA	6	THR	-	cloning artifact	UNP P03045
LA	24	ALA	-	linker	UNP P03045
LA	25	GLY	-	linker	UNP P03045
LA	26	ALA	-	linker	UNP P03045
LA	27	GLY	-	linker	UNP P03045
LA	28	ALA	-	linker	UNP P03045
LA	29	GLY	-	linker	UNP P03045
LA	30	ALA	-	linker	UNP P03045
LA	31	MET	-	linker	UNP P03045
LA	39	ASN	ILE	engineered mutation	UNP O66529
LA	42	VAL	GLU	engineered mutation	UNP O66529
LA	58	VAL	ILE	engineered mutation	UNP O66529
LA	61	ASP	GLY	engineered mutation	UNP O66529
LA	62	ILE	VAL	engineered mutation	UNP O66529
LA	97	TYR	PHE	engineered mutation	UNP O66529
LA	102	GLY	-	linker	UNP O66529
LA	103	THR	-	linker	UNP O66529
LA	104	GLY	-	linker	UNP O66529
LA	105	HIS	-	linker	UNP O66529
LA	106	HIS	-	linker	UNP O66529
LA	107	HIS	-	linker	UNP O66529
LA	108	HIS	-	linker	UNP O66529
LA	109	HIS	-	linker	UNP O66529
LA	110	HIS	-	linker	UNP O66529
LA	111	GLY	-	linker	UNP O66529
LA	112	SER	-	linker	UNP O66529
LA	113	SER	-	linker	UNP O66529
LA	114	ILE	MET	engineered mutation	UNP O66529
LA	115	GLU	GLN	engineered mutation	UNP O66529
LA	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
LA	177	ASP	GLY	engineered mutation	UNP O66529
LA	191	PHE	ILE	engineered mutation	UNP O66529
LA	193	ASP	VAL	engineered mutation	UNP O66529
LB	1	MET	-	cloning artifact	UNP P03045
LB	2	GLY	-	cloning artifact	UNP P03045
LB	3	ASN	-	cloning artifact	UNP P03045
LB	4	ALA	-	cloning artifact	UNP P03045
LB	5	LYS	-	cloning artifact	UNP P03045
LB	6	THR	-	cloning artifact	UNP P03045
LB	24	ALA	-	linker	UNP P03045
LB	25	GLY	-	linker	UNP P03045
LB	26	ALA	-	linker	UNP P03045
LB	27	GLY	-	linker	UNP P03045
LB	28	ALA	-	linker	UNP P03045
LB	29	GLY	-	linker	UNP P03045
LB	30	ALA	-	linker	UNP P03045
LB	31	MET	-	linker	UNP P03045
LB	39	ASN	ILE	engineered mutation	UNP O66529
LB	42	VAL	GLU	engineered mutation	UNP O66529
LB	58	VAL	ILE	engineered mutation	UNP O66529
LB	61	ASP	GLY	engineered mutation	UNP O66529
LB	62	ILE	VAL	engineered mutation	UNP O66529
LB	97	TYR	PHE	engineered mutation	UNP O66529
LB	102	GLY	-	linker	UNP O66529
LB	103	THR	-	linker	UNP O66529
LB	104	GLY	-	linker	UNP O66529
LB	105	HIS	-	linker	UNP O66529
LB	106	HIS	-	linker	UNP O66529
LB	107	HIS	-	linker	UNP O66529
LB	108	HIS	-	linker	UNP O66529
LB	109	HIS	-	linker	UNP O66529
LB	110	HIS	-	linker	UNP O66529
LB	111	GLY	-	linker	UNP O66529
LB	112	SER	-	linker	UNP O66529
LB	113	SER	-	linker	UNP O66529
LB	114	ILE	MET	engineered mutation	UNP O66529
LB	115	GLU	GLN	engineered mutation	UNP O66529
LB	138	THR	ALA	engineered mutation	UNP O66529
LB	177	ASP	GLY	engineered mutation	UNP O66529
LB	191	PHE	ILE	engineered mutation	UNP O66529
LB	193	ASP	VAL	engineered mutation	UNP O66529
LC	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
LC	2	GLY	-	cloning artifact	UNP P03045
LC	3	ASN	-	cloning artifact	UNP P03045
LC	4	ALA	-	cloning artifact	UNP P03045
LC	5	LYS	-	cloning artifact	UNP P03045
LC	6	THR	-	cloning artifact	UNP P03045
LC	24	ALA	-	linker	UNP P03045
LC	25	GLY	-	linker	UNP P03045
LC	26	ALA	-	linker	UNP P03045
LC	27	GLY	-	linker	UNP P03045
LC	28	ALA	-	linker	UNP P03045
LC	29	GLY	-	linker	UNP P03045
LC	30	ALA	-	linker	UNP P03045
LC	31	MET	-	linker	UNP P03045
LC	39	ASN	ILE	engineered mutation	UNP O66529
LC	42	VAL	GLU	engineered mutation	UNP O66529
LC	58	VAL	ILE	engineered mutation	UNP O66529
LC	61	ASP	GLY	engineered mutation	UNP O66529
LC	62	ILE	VAL	engineered mutation	UNP O66529
LC	97	TYR	PHE	engineered mutation	UNP O66529
LC	102	GLY	-	linker	UNP O66529
LC	103	THR	-	linker	UNP O66529
LC	104	GLY	-	linker	UNP O66529
LC	105	HIS	-	linker	UNP O66529
LC	106	HIS	-	linker	UNP O66529
LC	107	HIS	-	linker	UNP O66529
LC	108	HIS	-	linker	UNP O66529
LC	109	HIS	-	linker	UNP O66529
LC	110	HIS	-	linker	UNP O66529
LC	111	GLY	-	linker	UNP O66529
LC	112	SER	-	linker	UNP O66529
LC	113	SER	-	linker	UNP O66529
LC	114	ILE	MET	engineered mutation	UNP O66529
LC	115	GLU	GLN	engineered mutation	UNP O66529
LC	138	THR	ALA	engineered mutation	UNP O66529
LC	177	ASP	GLY	engineered mutation	UNP O66529
LC	191	PHE	ILE	engineered mutation	UNP O66529
LC	193	ASP	VAL	engineered mutation	UNP O66529
LD	1	MET	-	cloning artifact	UNP P03045
LD	2	GLY	-	cloning artifact	UNP P03045
LD	3	ASN	-	cloning artifact	UNP P03045
LD	4	ALA	-	cloning artifact	UNP P03045
LD	5	LYS	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
LD	6	THR	-	cloning artifact	UNP P03045
LD	24	ALA	-	linker	UNP P03045
LD	25	GLY	-	linker	UNP P03045
LD	26	ALA	-	linker	UNP P03045
LD	27	GLY	-	linker	UNP P03045
LD	28	ALA	-	linker	UNP P03045
LD	29	GLY	-	linker	UNP P03045
LD	30	ALA	-	linker	UNP P03045
LD	31	MET	-	linker	UNP P03045
LD	39	ASN	ILE	engineered mutation	UNP O66529
LD	42	VAL	GLU	engineered mutation	UNP O66529
LD	58	VAL	ILE	engineered mutation	UNP O66529
LD	61	ASP	GLY	engineered mutation	UNP O66529
LD	62	ILE	VAL	engineered mutation	UNP O66529
LD	97	TYR	PHE	engineered mutation	UNP O66529
LD	102	GLY	-	linker	UNP O66529
LD	103	THR	-	linker	UNP O66529
LD	104	GLY	-	linker	UNP O66529
LD	105	HIS	-	linker	UNP O66529
LD	106	HIS	-	linker	UNP O66529
LD	107	HIS	-	linker	UNP O66529
LD	108	HIS	-	linker	UNP O66529
LD	109	HIS	-	linker	UNP O66529
LD	110	HIS	-	linker	UNP O66529
LD	111	GLY	-	linker	UNP O66529
LD	112	SER	-	linker	UNP O66529
LD	113	SER	-	linker	UNP O66529
LD	114	ILE	MET	engineered mutation	UNP O66529
LD	115	GLU	GLN	engineered mutation	UNP O66529
LD	138	THR	ALA	engineered mutation	UNP O66529
LD	177	ASP	GLY	engineered mutation	UNP O66529
LD	191	PHE	ILE	engineered mutation	UNP O66529
LD	193	ASP	VAL	engineered mutation	UNP O66529
MA	1	MET	-	cloning artifact	UNP P03045
MA	2	GLY	-	cloning artifact	UNP P03045
MA	3	ASN	-	cloning artifact	UNP P03045
MA	4	ALA	-	cloning artifact	UNP P03045
MA	5	LYS	-	cloning artifact	UNP P03045
MA	6	THR	-	cloning artifact	UNP P03045
MA	24	ALA	-	linker	UNP P03045
MA	25	GLY	-	linker	UNP P03045
MA	26	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
MA	27	GLY	-	linker	UNP P03045
MA	28	ALA	-	linker	UNP P03045
MA	29	GLY	-	linker	UNP P03045
MA	30	ALA	-	linker	UNP P03045
MA	31	MET	-	linker	UNP P03045
MA	39	ASN	ILE	engineered mutation	UNP O66529
MA	42	VAL	GLU	engineered mutation	UNP O66529
MA	58	VAL	ILE	engineered mutation	UNP O66529
MA	61	ASP	GLY	engineered mutation	UNP O66529
MA	62	ILE	VAL	engineered mutation	UNP O66529
MA	97	TYR	PHE	engineered mutation	UNP O66529
MA	102	GLY	-	linker	UNP O66529
MA	103	THR	-	linker	UNP O66529
MA	104	GLY	-	linker	UNP O66529
MA	105	HIS	-	linker	UNP O66529
MA	106	HIS	-	linker	UNP O66529
MA	107	HIS	-	linker	UNP O66529
MA	108	HIS	-	linker	UNP O66529
MA	109	HIS	-	linker	UNP O66529
MA	110	HIS	-	linker	UNP O66529
MA	111	GLY	-	linker	UNP O66529
MA	112	SER	-	linker	UNP O66529
MA	113	SER	-	linker	UNP O66529
MA	114	ILE	MET	engineered mutation	UNP O66529
MA	115	GLU	GLN	engineered mutation	UNP O66529
MA	138	THR	ALA	engineered mutation	UNP O66529
MA	177	ASP	GLY	engineered mutation	UNP O66529
MA	191	PHE	ILE	engineered mutation	UNP O66529
MA	193	ASP	VAL	engineered mutation	UNP O66529
MB	1	MET	-	cloning artifact	UNP P03045
MB	2	GLY	-	cloning artifact	UNP P03045
MB	3	ASN	-	cloning artifact	UNP P03045
MB	4	ALA	-	cloning artifact	UNP P03045
MB	5	LYS	-	cloning artifact	UNP P03045
MB	6	THR	-	cloning artifact	UNP P03045
MB	24	ALA	-	linker	UNP P03045
MB	25	GLY	-	linker	UNP P03045
MB	26	ALA	-	linker	UNP P03045
MB	27	GLY	-	linker	UNP P03045
MB	28	ALA	-	linker	UNP P03045
MB	29	GLY	-	linker	UNP P03045
MB	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
MB	31	MET	-	linker	UNP P03045
MB	39	ASN	ILE	engineered mutation	UNP O66529
MB	42	VAL	GLU	engineered mutation	UNP O66529
MB	58	VAL	ILE	engineered mutation	UNP O66529
MB	61	ASP	GLY	engineered mutation	UNP O66529
MB	62	ILE	VAL	engineered mutation	UNP O66529
MB	97	TYR	PHE	engineered mutation	UNP O66529
MB	102	GLY	-	linker	UNP O66529
MB	103	THR	-	linker	UNP O66529
MB	104	GLY	-	linker	UNP O66529
MB	105	HIS	-	linker	UNP O66529
MB	106	HIS	-	linker	UNP O66529
MB	107	HIS	-	linker	UNP O66529
MB	108	HIS	-	linker	UNP O66529
MB	109	HIS	-	linker	UNP O66529
MB	110	HIS	-	linker	UNP O66529
MB	111	GLY	-	linker	UNP O66529
MB	112	SER	-	linker	UNP O66529
MB	113	SER	-	linker	UNP O66529
MB	114	ILE	MET	engineered mutation	UNP O66529
MB	115	GLU	GLN	engineered mutation	UNP O66529
MB	138	THR	ALA	engineered mutation	UNP O66529
MB	177	ASP	GLY	engineered mutation	UNP O66529
MB	191	PHE	ILE	engineered mutation	UNP O66529
MB	193	ASP	VAL	engineered mutation	UNP O66529
MC	1	MET	-	cloning artifact	UNP P03045
MC	2	GLY	-	cloning artifact	UNP P03045
MC	3	ASN	-	cloning artifact	UNP P03045
MC	4	ALA	-	cloning artifact	UNP P03045
MC	5	LYS	-	cloning artifact	UNP P03045
MC	6	THR	-	cloning artifact	UNP P03045
MC	24	ALA	-	linker	UNP P03045
MC	25	GLY	-	linker	UNP P03045
MC	26	ALA	-	linker	UNP P03045
MC	27	GLY	-	linker	UNP P03045
MC	28	ALA	-	linker	UNP P03045
MC	29	GLY	-	linker	UNP P03045
MC	30	ALA	-	linker	UNP P03045
MC	31	MET	-	linker	UNP P03045
MC	39	ASN	ILE	engineered mutation	UNP O66529
MC	42	VAL	GLU	engineered mutation	UNP O66529
MC	58	VAL	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
MC	61	ASP	GLY	engineered mutation	UNP O66529
MC	62	ILE	VAL	engineered mutation	UNP O66529
MC	97	TYR	PHE	engineered mutation	UNP O66529
MC	102	GLY	-	linker	UNP O66529
MC	103	THR	-	linker	UNP O66529
MC	104	GLY	-	linker	UNP O66529
MC	105	HIS	-	linker	UNP O66529
MC	106	HIS	-	linker	UNP O66529
MC	107	HIS	-	linker	UNP O66529
MC	108	HIS	-	linker	UNP O66529
MC	109	HIS	-	linker	UNP O66529
MC	110	HIS	-	linker	UNP O66529
MC	111	GLY	-	linker	UNP O66529
MC	112	SER	-	linker	UNP O66529
MC	113	SER	-	linker	UNP O66529
MC	114	ILE	MET	engineered mutation	UNP O66529
MC	115	GLU	GLN	engineered mutation	UNP O66529
MC	138	THR	ALA	engineered mutation	UNP O66529
MC	177	ASP	GLY	engineered mutation	UNP O66529
MC	191	PHE	ILE	engineered mutation	UNP O66529
MC	193	ASP	VAL	engineered mutation	UNP O66529
MD	1	MET	-	cloning artifact	UNP P03045
MD	2	GLY	-	cloning artifact	UNP P03045
MD	3	ASN	-	cloning artifact	UNP P03045
MD	4	ALA	-	cloning artifact	UNP P03045
MD	5	LYS	-	cloning artifact	UNP P03045
MD	6	THR	-	cloning artifact	UNP P03045
MD	24	ALA	-	linker	UNP P03045
MD	25	GLY	-	linker	UNP P03045
MD	26	ALA	-	linker	UNP P03045
MD	27	GLY	-	linker	UNP P03045
MD	28	ALA	-	linker	UNP P03045
MD	29	GLY	-	linker	UNP P03045
MD	30	ALA	-	linker	UNP P03045
MD	31	MET	-	linker	UNP P03045
MD	39	ASN	ILE	engineered mutation	UNP O66529
MD	42	VAL	GLU	engineered mutation	UNP O66529
MD	58	VAL	ILE	engineered mutation	UNP O66529
MD	61	ASP	GLY	engineered mutation	UNP O66529
MD	62	ILE	VAL	engineered mutation	UNP O66529
MD	97	TYR	PHE	engineered mutation	UNP O66529
MD	102	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
MD	103	THR	-	linker	UNP O66529
MD	104	GLY	-	linker	UNP O66529
MD	105	HIS	-	linker	UNP O66529
MD	106	HIS	-	linker	UNP O66529
MD	107	HIS	-	linker	UNP O66529
MD	108	HIS	-	linker	UNP O66529
MD	109	HIS	-	linker	UNP O66529
MD	110	HIS	-	linker	UNP O66529
MD	111	GLY	-	linker	UNP O66529
MD	112	SER	-	linker	UNP O66529
MD	113	SER	-	linker	UNP O66529
MD	114	ILE	MET	engineered mutation	UNP O66529
MD	115	GLU	GLN	engineered mutation	UNP O66529
MD	138	THR	ALA	engineered mutation	UNP O66529
MD	177	ASP	GLY	engineered mutation	UNP O66529
MD	191	PHE	ILE	engineered mutation	UNP O66529
MD	193	ASP	VAL	engineered mutation	UNP O66529
NA	1	MET	-	cloning artifact	UNP P03045
NA	2	GLY	-	cloning artifact	UNP P03045
NA	3	ASN	-	cloning artifact	UNP P03045
NA	4	ALA	-	cloning artifact	UNP P03045
NA	5	LYS	-	cloning artifact	UNP P03045
NA	6	THR	-	cloning artifact	UNP P03045
NA	24	ALA	-	linker	UNP P03045
NA	25	GLY	-	linker	UNP P03045
NA	26	ALA	-	linker	UNP P03045
NA	27	GLY	-	linker	UNP P03045
NA	28	ALA	-	linker	UNP P03045
NA	29	GLY	-	linker	UNP P03045
NA	30	ALA	-	linker	UNP P03045
NA	31	MET	-	linker	UNP P03045
NA	39	ASN	ILE	engineered mutation	UNP O66529
NA	42	VAL	GLU	engineered mutation	UNP O66529
NA	58	VAL	ILE	engineered mutation	UNP O66529
NA	61	ASP	GLY	engineered mutation	UNP O66529
NA	62	ILE	VAL	engineered mutation	UNP O66529
NA	97	TYR	PHE	engineered mutation	UNP O66529
NA	102	GLY	-	linker	UNP O66529
NA	103	THR	-	linker	UNP O66529
NA	104	GLY	-	linker	UNP O66529
NA	105	HIS	-	linker	UNP O66529
NA	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
NA	107	HIS	-	linker	UNP O66529
NA	108	HIS	-	linker	UNP O66529
NA	109	HIS	-	linker	UNP O66529
NA	110	HIS	-	linker	UNP O66529
NA	111	GLY	-	linker	UNP O66529
NA	112	SER	-	linker	UNP O66529
NA	113	SER	-	linker	UNP O66529
NA	114	ILE	MET	engineered mutation	UNP O66529
NA	115	GLU	GLN	engineered mutation	UNP O66529
NA	138	THR	ALA	engineered mutation	UNP O66529
NA	177	ASP	GLY	engineered mutation	UNP O66529
NA	191	PHE	ILE	engineered mutation	UNP O66529
NA	193	ASP	VAL	engineered mutation	UNP O66529
NB	1	MET	-	cloning artifact	UNP P03045
NB	2	GLY	-	cloning artifact	UNP P03045
NB	3	ASN	-	cloning artifact	UNP P03045
NB	4	ALA	-	cloning artifact	UNP P03045
NB	5	LYS	-	cloning artifact	UNP P03045
NB	6	THR	-	cloning artifact	UNP P03045
NB	24	ALA	-	linker	UNP P03045
NB	25	GLY	-	linker	UNP P03045
NB	26	ALA	-	linker	UNP P03045
NB	27	GLY	-	linker	UNP P03045
NB	28	ALA	-	linker	UNP P03045
NB	29	GLY	-	linker	UNP P03045
NB	30	ALA	-	linker	UNP P03045
NB	31	MET	-	linker	UNP P03045
NB	39	ASN	ILE	engineered mutation	UNP O66529
NB	42	VAL	GLU	engineered mutation	UNP O66529
NB	58	VAL	ILE	engineered mutation	UNP O66529
NB	61	ASP	GLY	engineered mutation	UNP O66529
NB	62	ILE	VAL	engineered mutation	UNP O66529
NB	97	TYR	PHE	engineered mutation	UNP O66529
NB	102	GLY	-	linker	UNP O66529
NB	103	THR	-	linker	UNP O66529
NB	104	GLY	-	linker	UNP O66529
NB	105	HIS	-	linker	UNP O66529
NB	106	HIS	-	linker	UNP O66529
NB	107	HIS	-	linker	UNP O66529
NB	108	HIS	-	linker	UNP O66529
NB	109	HIS	-	linker	UNP O66529
NB	110	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
NB	111	GLY	-	linker	UNP O66529
NB	112	SER	-	linker	UNP O66529
NB	113	SER	-	linker	UNP O66529
NB	114	ILE	MET	engineered mutation	UNP O66529
NB	115	GLU	GLN	engineered mutation	UNP O66529
NB	138	THR	ALA	engineered mutation	UNP O66529
NB	177	ASP	GLY	engineered mutation	UNP O66529
NB	191	PHE	ILE	engineered mutation	UNP O66529
NB	193	ASP	VAL	engineered mutation	UNP O66529
NC	1	MET	-	cloning artifact	UNP P03045
NC	2	GLY	-	cloning artifact	UNP P03045
NC	3	ASN	-	cloning artifact	UNP P03045
NC	4	ALA	-	cloning artifact	UNP P03045
NC	5	LYS	-	cloning artifact	UNP P03045
NC	6	THR	-	cloning artifact	UNP P03045
NC	24	ALA	-	linker	UNP P03045
NC	25	GLY	-	linker	UNP P03045
NC	26	ALA	-	linker	UNP P03045
NC	27	GLY	-	linker	UNP P03045
NC	28	ALA	-	linker	UNP P03045
NC	29	GLY	-	linker	UNP P03045
NC	30	ALA	-	linker	UNP P03045
NC	31	MET	-	linker	UNP P03045
NC	39	ASN	ILE	engineered mutation	UNP O66529
NC	42	VAL	GLU	engineered mutation	UNP O66529
NC	58	VAL	ILE	engineered mutation	UNP O66529
NC	61	ASP	GLY	engineered mutation	UNP O66529
NC	62	ILE	VAL	engineered mutation	UNP O66529
NC	97	TYR	PHE	engineered mutation	UNP O66529
NC	102	GLY	-	linker	UNP O66529
NC	103	THR	-	linker	UNP O66529
NC	104	GLY	-	linker	UNP O66529
NC	105	HIS	-	linker	UNP O66529
NC	106	HIS	-	linker	UNP O66529
NC	107	HIS	-	linker	UNP O66529
NC	108	HIS	-	linker	UNP O66529
NC	109	HIS	-	linker	UNP O66529
NC	110	HIS	-	linker	UNP O66529
NC	111	GLY	-	linker	UNP O66529
NC	112	SER	-	linker	UNP O66529
NC	113	SER	-	linker	UNP O66529
NC	114	ILE	MET	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
NC	115	GLU	GLN	engineered mutation	UNP O66529
NC	138	THR	ALA	engineered mutation	UNP O66529
NC	177	ASP	GLY	engineered mutation	UNP O66529
NC	191	PHE	ILE	engineered mutation	UNP O66529
NC	193	ASP	VAL	engineered mutation	UNP O66529
ND	1	MET	-	cloning artifact	UNP P03045
ND	2	GLY	-	cloning artifact	UNP P03045
ND	3	ASN	-	cloning artifact	UNP P03045
ND	4	ALA	-	cloning artifact	UNP P03045
ND	5	LYS	-	cloning artifact	UNP P03045
ND	6	THR	-	cloning artifact	UNP P03045
ND	24	ALA	-	linker	UNP P03045
ND	25	GLY	-	linker	UNP P03045
ND	26	ALA	-	linker	UNP P03045
ND	27	GLY	-	linker	UNP P03045
ND	28	ALA	-	linker	UNP P03045
ND	29	GLY	-	linker	UNP P03045
ND	30	ALA	-	linker	UNP P03045
ND	31	MET	-	linker	UNP P03045
ND	39	ASN	ILE	engineered mutation	UNP O66529
ND	42	VAL	GLU	engineered mutation	UNP O66529
ND	58	VAL	ILE	engineered mutation	UNP O66529
ND	61	ASP	GLY	engineered mutation	UNP O66529
ND	62	ILE	VAL	engineered mutation	UNP O66529
ND	97	TYR	PHE	engineered mutation	UNP O66529
ND	102	GLY	-	linker	UNP O66529
ND	103	THR	-	linker	UNP O66529
ND	104	GLY	-	linker	UNP O66529
ND	105	HIS	-	linker	UNP O66529
ND	106	HIS	-	linker	UNP O66529
ND	107	HIS	-	linker	UNP O66529
ND	108	HIS	-	linker	UNP O66529
ND	109	HIS	-	linker	UNP O66529
ND	110	HIS	-	linker	UNP O66529
ND	111	GLY	-	linker	UNP O66529
ND	112	SER	-	linker	UNP O66529
ND	113	SER	-	linker	UNP O66529
ND	114	ILE	MET	engineered mutation	UNP O66529
ND	115	GLU	GLN	engineered mutation	UNP O66529
ND	138	THR	ALA	engineered mutation	UNP O66529
ND	177	ASP	GLY	engineered mutation	UNP O66529
ND	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
ND	193	ASP	VAL	engineered mutation	UNP O66529
OA	1	MET	-	cloning artifact	UNP P03045
OA	2	GLY	-	cloning artifact	UNP P03045
OA	3	ASN	-	cloning artifact	UNP P03045
OA	4	ALA	-	cloning artifact	UNP P03045
OA	5	LYS	-	cloning artifact	UNP P03045
OA	6	THR	-	cloning artifact	UNP P03045
OA	24	ALA	-	linker	UNP P03045
OA	25	GLY	-	linker	UNP P03045
OA	26	ALA	-	linker	UNP P03045
OA	27	GLY	-	linker	UNP P03045
OA	28	ALA	-	linker	UNP P03045
OA	29	GLY	-	linker	UNP P03045
OA	30	ALA	-	linker	UNP P03045
OA	31	MET	-	linker	UNP P03045
OA	39	ASN	ILE	engineered mutation	UNP O66529
OA	42	VAL	GLU	engineered mutation	UNP O66529
OA	58	VAL	ILE	engineered mutation	UNP O66529
OA	61	ASP	GLY	engineered mutation	UNP O66529
OA	62	ILE	VAL	engineered mutation	UNP O66529
OA	97	TYR	PHE	engineered mutation	UNP O66529
OA	102	GLY	-	linker	UNP O66529
OA	103	THR	-	linker	UNP O66529
OA	104	GLY	-	linker	UNP O66529
OA	105	HIS	-	linker	UNP O66529
OA	106	HIS	-	linker	UNP O66529
OA	107	HIS	-	linker	UNP O66529
OA	108	HIS	-	linker	UNP O66529
OA	109	HIS	-	linker	UNP O66529
OA	110	HIS	-	linker	UNP O66529
OA	111	GLY	-	linker	UNP O66529
OA	112	SER	-	linker	UNP O66529
OA	113	SER	-	linker	UNP O66529
OA	114	ILE	MET	engineered mutation	UNP O66529
OA	115	GLU	GLN	engineered mutation	UNP O66529
OA	138	THR	ALA	engineered mutation	UNP O66529
OA	177	ASP	GLY	engineered mutation	UNP O66529
OA	191	PHE	ILE	engineered mutation	UNP O66529
OA	193	ASP	VAL	engineered mutation	UNP O66529
OB	1	MET	-	cloning artifact	UNP P03045
OB	2	GLY	-	cloning artifact	UNP P03045
OB	3	ASN	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
OB	4	ALA	-	cloning artifact	UNP P03045
OB	5	LYS	-	cloning artifact	UNP P03045
OB	6	THR	-	cloning artifact	UNP P03045
OB	24	ALA	-	linker	UNP P03045
OB	25	GLY	-	linker	UNP P03045
OB	26	ALA	-	linker	UNP P03045
OB	27	GLY	-	linker	UNP P03045
OB	28	ALA	-	linker	UNP P03045
OB	29	GLY	-	linker	UNP P03045
OB	30	ALA	-	linker	UNP P03045
OB	31	MET	-	linker	UNP P03045
OB	39	ASN	ILE	engineered mutation	UNP O66529
OB	42	VAL	GLU	engineered mutation	UNP O66529
OB	58	VAL	ILE	engineered mutation	UNP O66529
OB	61	ASP	GLY	engineered mutation	UNP O66529
OB	62	ILE	VAL	engineered mutation	UNP O66529
OB	97	TYR	PHE	engineered mutation	UNP O66529
OB	102	GLY	-	linker	UNP O66529
OB	103	THR	-	linker	UNP O66529
OB	104	GLY	-	linker	UNP O66529
OB	105	HIS	-	linker	UNP O66529
OB	106	HIS	-	linker	UNP O66529
OB	107	HIS	-	linker	UNP O66529
OB	108	HIS	-	linker	UNP O66529
OB	109	HIS	-	linker	UNP O66529
OB	110	HIS	-	linker	UNP O66529
OB	111	GLY	-	linker	UNP O66529
OB	112	SER	-	linker	UNP O66529
OB	113	SER	-	linker	UNP O66529
OB	114	ILE	MET	engineered mutation	UNP O66529
OB	115	GLU	GLN	engineered mutation	UNP O66529
OB	138	THR	ALA	engineered mutation	UNP O66529
OB	177	ASP	GLY	engineered mutation	UNP O66529
OB	191	PHE	ILE	engineered mutation	UNP O66529
OB	193	ASP	VAL	engineered mutation	UNP O66529
OC	1	MET	-	cloning artifact	UNP P03045
OC	2	GLY	-	cloning artifact	UNP P03045
OC	3	ASN	-	cloning artifact	UNP P03045
OC	4	ALA	-	cloning artifact	UNP P03045
OC	5	LYS	-	cloning artifact	UNP P03045
OC	6	THR	-	cloning artifact	UNP P03045
OC	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
OC	25	GLY	-	linker	UNP P03045
OC	26	ALA	-	linker	UNP P03045
OC	27	GLY	-	linker	UNP P03045
OC	28	ALA	-	linker	UNP P03045
OC	29	GLY	-	linker	UNP P03045
OC	30	ALA	-	linker	UNP P03045
OC	31	MET	-	linker	UNP P03045
OC	39	ASN	ILE	engineered mutation	UNP O66529
OC	42	VAL	GLU	engineered mutation	UNP O66529
OC	58	VAL	ILE	engineered mutation	UNP O66529
OC	61	ASP	GLY	engineered mutation	UNP O66529
OC	62	ILE	VAL	engineered mutation	UNP O66529
OC	97	TYR	PHE	engineered mutation	UNP O66529
OC	102	GLY	-	linker	UNP O66529
OC	103	THR	-	linker	UNP O66529
OC	104	GLY	-	linker	UNP O66529
OC	105	HIS	-	linker	UNP O66529
OC	106	HIS	-	linker	UNP O66529
OC	107	HIS	-	linker	UNP O66529
OC	108	HIS	-	linker	UNP O66529
OC	109	HIS	-	linker	UNP O66529
OC	110	HIS	-	linker	UNP O66529
OC	111	GLY	-	linker	UNP O66529
OC	112	SER	-	linker	UNP O66529
OC	113	SER	-	linker	UNP O66529
OC	114	ILE	MET	engineered mutation	UNP O66529
OC	115	GLU	GLN	engineered mutation	UNP O66529
OC	138	THR	ALA	engineered mutation	UNP O66529
OC	177	ASP	GLY	engineered mutation	UNP O66529
OC	191	PHE	ILE	engineered mutation	UNP O66529
OC	193	ASP	VAL	engineered mutation	UNP O66529
OD	1	MET	-	cloning artifact	UNP P03045
OD	2	GLY	-	cloning artifact	UNP P03045
OD	3	ASN	-	cloning artifact	UNP P03045
OD	4	ALA	-	cloning artifact	UNP P03045
OD	5	LYS	-	cloning artifact	UNP P03045
OD	6	THR	-	cloning artifact	UNP P03045
OD	24	ALA	-	linker	UNP P03045
OD	25	GLY	-	linker	UNP P03045
OD	26	ALA	-	linker	UNP P03045
OD	27	GLY	-	linker	UNP P03045
OD	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
OD	29	GLY	-	linker	UNP P03045
OD	30	ALA	-	linker	UNP P03045
OD	31	MET	-	linker	UNP P03045
OD	39	ASN	ILE	engineered mutation	UNP O66529
OD	42	VAL	GLU	engineered mutation	UNP O66529
OD	58	VAL	ILE	engineered mutation	UNP O66529
OD	61	ASP	GLY	engineered mutation	UNP O66529
OD	62	ILE	VAL	engineered mutation	UNP O66529
OD	97	TYR	PHE	engineered mutation	UNP O66529
OD	102	GLY	-	linker	UNP O66529
OD	103	THR	-	linker	UNP O66529
OD	104	GLY	-	linker	UNP O66529
OD	105	HIS	-	linker	UNP O66529
OD	106	HIS	-	linker	UNP O66529
OD	107	HIS	-	linker	UNP O66529
OD	108	HIS	-	linker	UNP O66529
OD	109	HIS	-	linker	UNP O66529
OD	110	HIS	-	linker	UNP O66529
OD	111	GLY	-	linker	UNP O66529
OD	112	SER	-	linker	UNP O66529
OD	113	SER	-	linker	UNP O66529
OD	114	ILE	MET	engineered mutation	UNP O66529
OD	115	GLU	GLN	engineered mutation	UNP O66529
OD	138	THR	ALA	engineered mutation	UNP O66529
OD	177	ASP	GLY	engineered mutation	UNP O66529
OD	191	PHE	ILE	engineered mutation	UNP O66529
OD	193	ASP	VAL	engineered mutation	UNP O66529
PA	1	MET	-	cloning artifact	UNP P03045
PA	2	GLY	-	cloning artifact	UNP P03045
PA	3	ASN	-	cloning artifact	UNP P03045
PA	4	ALA	-	cloning artifact	UNP P03045
PA	5	LYS	-	cloning artifact	UNP P03045
PA	6	THR	-	cloning artifact	UNP P03045
PA	24	ALA	-	linker	UNP P03045
PA	25	GLY	-	linker	UNP P03045
PA	26	ALA	-	linker	UNP P03045
PA	27	GLY	-	linker	UNP P03045
PA	28	ALA	-	linker	UNP P03045
PA	29	GLY	-	linker	UNP P03045
PA	30	ALA	-	linker	UNP P03045
PA	31	MET	-	linker	UNP P03045
PA	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
PA	42	VAL	GLU	engineered mutation	UNP O66529
PA	58	VAL	ILE	engineered mutation	UNP O66529
PA	61	ASP	GLY	engineered mutation	UNP O66529
PA	62	ILE	VAL	engineered mutation	UNP O66529
PA	97	TYR	PHE	engineered mutation	UNP O66529
PA	102	GLY	-	linker	UNP O66529
PA	103	THR	-	linker	UNP O66529
PA	104	GLY	-	linker	UNP O66529
PA	105	HIS	-	linker	UNP O66529
PA	106	HIS	-	linker	UNP O66529
PA	107	HIS	-	linker	UNP O66529
PA	108	HIS	-	linker	UNP O66529
PA	109	HIS	-	linker	UNP O66529
PA	110	HIS	-	linker	UNP O66529
PA	111	GLY	-	linker	UNP O66529
PA	112	SER	-	linker	UNP O66529
PA	113	SER	-	linker	UNP O66529
PA	114	ILE	MET	engineered mutation	UNP O66529
PA	115	GLU	GLN	engineered mutation	UNP O66529
PA	138	THR	ALA	engineered mutation	UNP O66529
PA	177	ASP	GLY	engineered mutation	UNP O66529
PA	191	PHE	ILE	engineered mutation	UNP O66529
PA	193	ASP	VAL	engineered mutation	UNP O66529
PB	1	MET	-	cloning artifact	UNP P03045
PB	2	GLY	-	cloning artifact	UNP P03045
PB	3	ASN	-	cloning artifact	UNP P03045
PB	4	ALA	-	cloning artifact	UNP P03045
PB	5	LYS	-	cloning artifact	UNP P03045
PB	6	THR	-	cloning artifact	UNP P03045
PB	24	ALA	-	linker	UNP P03045
PB	25	GLY	-	linker	UNP P03045
PB	26	ALA	-	linker	UNP P03045
PB	27	GLY	-	linker	UNP P03045
PB	28	ALA	-	linker	UNP P03045
PB	29	GLY	-	linker	UNP P03045
PB	30	ALA	-	linker	UNP P03045
PB	31	MET	-	linker	UNP P03045
PB	39	ASN	ILE	engineered mutation	UNP O66529
PB	42	VAL	GLU	engineered mutation	UNP O66529
PB	58	VAL	ILE	engineered mutation	UNP O66529
PB	61	ASP	GLY	engineered mutation	UNP O66529
PB	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
PB	97	TYR	PHE	engineered mutation	UNP O66529
PB	102	GLY	-	linker	UNP O66529
PB	103	THR	-	linker	UNP O66529
PB	104	GLY	-	linker	UNP O66529
PB	105	HIS	-	linker	UNP O66529
PB	106	HIS	-	linker	UNP O66529
PB	107	HIS	-	linker	UNP O66529
PB	108	HIS	-	linker	UNP O66529
PB	109	HIS	-	linker	UNP O66529
PB	110	HIS	-	linker	UNP O66529
PB	111	GLY	-	linker	UNP O66529
PB	112	SER	-	linker	UNP O66529
PB	113	SER	-	linker	UNP O66529
PB	114	ILE	MET	engineered mutation	UNP O66529
PB	115	GLU	GLN	engineered mutation	UNP O66529
PB	138	THR	ALA	engineered mutation	UNP O66529
PB	177	ASP	GLY	engineered mutation	UNP O66529
PB	191	PHE	ILE	engineered mutation	UNP O66529
PB	193	ASP	VAL	engineered mutation	UNP O66529
PC	1	MET	-	cloning artifact	UNP P03045
PC	2	GLY	-	cloning artifact	UNP P03045
PC	3	ASN	-	cloning artifact	UNP P03045
PC	4	ALA	-	cloning artifact	UNP P03045
PC	5	LYS	-	cloning artifact	UNP P03045
PC	6	THR	-	cloning artifact	UNP P03045
PC	24	ALA	-	linker	UNP P03045
PC	25	GLY	-	linker	UNP P03045
PC	26	ALA	-	linker	UNP P03045
PC	27	GLY	-	linker	UNP P03045
PC	28	ALA	-	linker	UNP P03045
PC	29	GLY	-	linker	UNP P03045
PC	30	ALA	-	linker	UNP P03045
PC	31	MET	-	linker	UNP P03045
PC	39	ASN	ILE	engineered mutation	UNP O66529
PC	42	VAL	GLU	engineered mutation	UNP O66529
PC	58	VAL	ILE	engineered mutation	UNP O66529
PC	61	ASP	GLY	engineered mutation	UNP O66529
PC	62	ILE	VAL	engineered mutation	UNP O66529
PC	97	TYR	PHE	engineered mutation	UNP O66529
PC	102	GLY	-	linker	UNP O66529
PC	103	THR	-	linker	UNP O66529
PC	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
PC	105	HIS	-	linker	UNP O66529
PC	106	HIS	-	linker	UNP O66529
PC	107	HIS	-	linker	UNP O66529
PC	108	HIS	-	linker	UNP O66529
PC	109	HIS	-	linker	UNP O66529
PC	110	HIS	-	linker	UNP O66529
PC	111	GLY	-	linker	UNP O66529
PC	112	SER	-	linker	UNP O66529
PC	113	SER	-	linker	UNP O66529
PC	114	ILE	MET	engineered mutation	UNP O66529
PC	115	GLU	GLN	engineered mutation	UNP O66529
PC	138	THR	ALA	engineered mutation	UNP O66529
PC	177	ASP	GLY	engineered mutation	UNP O66529
PC	191	PHE	ILE	engineered mutation	UNP O66529
PC	193	ASP	VAL	engineered mutation	UNP O66529
PD	1	MET	-	cloning artifact	UNP P03045
PD	2	GLY	-	cloning artifact	UNP P03045
PD	3	ASN	-	cloning artifact	UNP P03045
PD	4	ALA	-	cloning artifact	UNP P03045
PD	5	LYS	-	cloning artifact	UNP P03045
PD	6	THR	-	cloning artifact	UNP P03045
PD	24	ALA	-	linker	UNP P03045
PD	25	GLY	-	linker	UNP P03045
PD	26	ALA	-	linker	UNP P03045
PD	27	GLY	-	linker	UNP P03045
PD	28	ALA	-	linker	UNP P03045
PD	29	GLY	-	linker	UNP P03045
PD	30	ALA	-	linker	UNP P03045
PD	31	MET	-	linker	UNP P03045
PD	39	ASN	ILE	engineered mutation	UNP O66529
PD	42	VAL	GLU	engineered mutation	UNP O66529
PD	58	VAL	ILE	engineered mutation	UNP O66529
PD	61	ASP	GLY	engineered mutation	UNP O66529
PD	62	ILE	VAL	engineered mutation	UNP O66529
PD	97	TYR	PHE	engineered mutation	UNP O66529
PD	102	GLY	-	linker	UNP O66529
PD	103	THR	-	linker	UNP O66529
PD	104	GLY	-	linker	UNP O66529
PD	105	HIS	-	linker	UNP O66529
PD	106	HIS	-	linker	UNP O66529
PD	107	HIS	-	linker	UNP O66529
PD	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
PD	109	HIS	-	linker	UNP O66529
PD	110	HIS	-	linker	UNP O66529
PD	111	GLY	-	linker	UNP O66529
PD	112	SER	-	linker	UNP O66529
PD	113	SER	-	linker	UNP O66529
PD	114	ILE	MET	engineered mutation	UNP O66529
PD	115	GLU	GLN	engineered mutation	UNP O66529
PD	138	THR	ALA	engineered mutation	UNP O66529
PD	177	ASP	GLY	engineered mutation	UNP O66529
PD	191	PHE	ILE	engineered mutation	UNP O66529
PD	193	ASP	VAL	engineered mutation	UNP O66529
6A	1	MET	-	cloning artifact	UNP P03045
6A	2	GLY	-	cloning artifact	UNP P03045
6A	3	ASN	-	cloning artifact	UNP P03045
6A	4	ALA	-	cloning artifact	UNP P03045
6A	5	LYS	-	cloning artifact	UNP P03045
6A	6	THR	-	cloning artifact	UNP P03045
6A	24	ALA	-	linker	UNP P03045
6A	25	GLY	-	linker	UNP P03045
6A	26	ALA	-	linker	UNP P03045
6A	27	GLY	-	linker	UNP P03045
6A	28	ALA	-	linker	UNP P03045
6A	29	GLY	-	linker	UNP P03045
6A	30	ALA	-	linker	UNP P03045
6A	31	MET	-	linker	UNP P03045
6A	39	ASN	ILE	engineered mutation	UNP O66529
6A	42	VAL	GLU	engineered mutation	UNP O66529
6A	58	VAL	ILE	engineered mutation	UNP O66529
6A	61	ASP	GLY	engineered mutation	UNP O66529
6A	62	ILE	VAL	engineered mutation	UNP O66529
6A	97	TYR	PHE	engineered mutation	UNP O66529
6A	102	GLY	-	linker	UNP O66529
6A	103	THR	-	linker	UNP O66529
6A	104	GLY	-	linker	UNP O66529
6A	105	HIS	-	linker	UNP O66529
6A	106	HIS	-	linker	UNP O66529
6A	107	HIS	-	linker	UNP O66529
6A	108	HIS	-	linker	UNP O66529
6A	109	HIS	-	linker	UNP O66529
6A	110	HIS	-	linker	UNP O66529
6A	111	GLY	-	linker	UNP O66529
6A	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
6A	113	SER	-	linker	UNP O66529
6A	114	ILE	MET	engineered mutation	UNP O66529
6A	115	GLU	GLN	engineered mutation	UNP O66529
6A	138	THR	ALA	engineered mutation	UNP O66529
6A	177	ASP	GLY	engineered mutation	UNP O66529
6A	191	PHE	ILE	engineered mutation	UNP O66529
6A	193	ASP	VAL	engineered mutation	UNP O66529
6B	1	MET	-	cloning artifact	UNP P03045
6B	2	GLY	-	cloning artifact	UNP P03045
6B	3	ASN	-	cloning artifact	UNP P03045
6B	4	ALA	-	cloning artifact	UNP P03045
6B	5	LYS	-	cloning artifact	UNP P03045
6B	6	THR	-	cloning artifact	UNP P03045
6B	24	ALA	-	linker	UNP P03045
6B	25	GLY	-	linker	UNP P03045
6B	26	ALA	-	linker	UNP P03045
6B	27	GLY	-	linker	UNP P03045
6B	28	ALA	-	linker	UNP P03045
6B	29	GLY	-	linker	UNP P03045
6B	30	ALA	-	linker	UNP P03045
6B	31	MET	-	linker	UNP P03045
6B	39	ASN	ILE	engineered mutation	UNP O66529
6B	42	VAL	GLU	engineered mutation	UNP O66529
6B	58	VAL	ILE	engineered mutation	UNP O66529
6B	61	ASP	GLY	engineered mutation	UNP O66529
6B	62	ILE	VAL	engineered mutation	UNP O66529
6B	97	TYR	PHE	engineered mutation	UNP O66529
6B	102	GLY	-	linker	UNP O66529
6B	103	THR	-	linker	UNP O66529
6B	104	GLY	-	linker	UNP O66529
6B	105	HIS	-	linker	UNP O66529
6B	106	HIS	-	linker	UNP O66529
6B	107	HIS	-	linker	UNP O66529
6B	108	HIS	-	linker	UNP O66529
6B	109	HIS	-	linker	UNP O66529
6B	110	HIS	-	linker	UNP O66529
6B	111	GLY	-	linker	UNP O66529
6B	112	SER	-	linker	UNP O66529
6B	113	SER	-	linker	UNP O66529
6B	114	ILE	MET	engineered mutation	UNP O66529
6B	115	GLU	GLN	engineered mutation	UNP O66529
6B	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
6B	177	ASP	GLY	engineered mutation	UNP O66529
6B	191	PHE	ILE	engineered mutation	UNP O66529
6B	193	ASP	VAL	engineered mutation	UNP O66529
6C	1	MET	-	cloning artifact	UNP P03045
6C	2	GLY	-	cloning artifact	UNP P03045
6C	3	ASN	-	cloning artifact	UNP P03045
6C	4	ALA	-	cloning artifact	UNP P03045
6C	5	LYS	-	cloning artifact	UNP P03045
6C	6	THR	-	cloning artifact	UNP P03045
6C	24	ALA	-	linker	UNP P03045
6C	25	GLY	-	linker	UNP P03045
6C	26	ALA	-	linker	UNP P03045
6C	27	GLY	-	linker	UNP P03045
6C	28	ALA	-	linker	UNP P03045
6C	29	GLY	-	linker	UNP P03045
6C	30	ALA	-	linker	UNP P03045
6C	31	MET	-	linker	UNP P03045
6C	39	ASN	ILE	engineered mutation	UNP O66529
6C	42	VAL	GLU	engineered mutation	UNP O66529
6C	58	VAL	ILE	engineered mutation	UNP O66529
6C	61	ASP	GLY	engineered mutation	UNP O66529
6C	62	ILE	VAL	engineered mutation	UNP O66529
6C	97	TYR	PHE	engineered mutation	UNP O66529
6C	102	GLY	-	linker	UNP O66529
6C	103	THR	-	linker	UNP O66529
6C	104	GLY	-	linker	UNP O66529
6C	105	HIS	-	linker	UNP O66529
6C	106	HIS	-	linker	UNP O66529
6C	107	HIS	-	linker	UNP O66529
6C	108	HIS	-	linker	UNP O66529
6C	109	HIS	-	linker	UNP O66529
6C	110	HIS	-	linker	UNP O66529
6C	111	GLY	-	linker	UNP O66529
6C	112	SER	-	linker	UNP O66529
6C	113	SER	-	linker	UNP O66529
6C	114	ILE	MET	engineered mutation	UNP O66529
6C	115	GLU	GLN	engineered mutation	UNP O66529
6C	138	THR	ALA	engineered mutation	UNP O66529
6C	177	ASP	GLY	engineered mutation	UNP O66529
6C	191	PHE	ILE	engineered mutation	UNP O66529
6C	193	ASP	VAL	engineered mutation	UNP O66529
6D	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
6D	2	GLY	-	cloning artifact	UNP P03045
6D	3	ASN	-	cloning artifact	UNP P03045
6D	4	ALA	-	cloning artifact	UNP P03045
6D	5	LYS	-	cloning artifact	UNP P03045
6D	6	THR	-	cloning artifact	UNP P03045
6D	24	ALA	-	linker	UNP P03045
6D	25	GLY	-	linker	UNP P03045
6D	26	ALA	-	linker	UNP P03045
6D	27	GLY	-	linker	UNP P03045
6D	28	ALA	-	linker	UNP P03045
6D	29	GLY	-	linker	UNP P03045
6D	30	ALA	-	linker	UNP P03045
6D	31	MET	-	linker	UNP P03045
6D	39	ASN	ILE	engineered mutation	UNP O66529
6D	42	VAL	GLU	engineered mutation	UNP O66529
6D	58	VAL	ILE	engineered mutation	UNP O66529
6D	61	ASP	GLY	engineered mutation	UNP O66529
6D	62	ILE	VAL	engineered mutation	UNP O66529
6D	97	TYR	PHE	engineered mutation	UNP O66529
6D	102	GLY	-	linker	UNP O66529
6D	103	THR	-	linker	UNP O66529
6D	104	GLY	-	linker	UNP O66529
6D	105	HIS	-	linker	UNP O66529
6D	106	HIS	-	linker	UNP O66529
6D	107	HIS	-	linker	UNP O66529
6D	108	HIS	-	linker	UNP O66529
6D	109	HIS	-	linker	UNP O66529
6D	110	HIS	-	linker	UNP O66529
6D	111	GLY	-	linker	UNP O66529
6D	112	SER	-	linker	UNP O66529
6D	113	SER	-	linker	UNP O66529
6D	114	ILE	MET	engineered mutation	UNP O66529
6D	115	GLU	GLN	engineered mutation	UNP O66529
6D	138	THR	ALA	engineered mutation	UNP O66529
6D	177	ASP	GLY	engineered mutation	UNP O66529
6D	191	PHE	ILE	engineered mutation	UNP O66529
6D	193	ASP	VAL	engineered mutation	UNP O66529
7A	1	MET	-	cloning artifact	UNP P03045
7A	2	GLY	-	cloning artifact	UNP P03045
7A	3	ASN	-	cloning artifact	UNP P03045
7A	4	ALA	-	cloning artifact	UNP P03045
7A	5	LYS	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
7A	6	THR	-	cloning artifact	UNP P03045
7A	24	ALA	-	linker	UNP P03045
7A	25	GLY	-	linker	UNP P03045
7A	26	ALA	-	linker	UNP P03045
7A	27	GLY	-	linker	UNP P03045
7A	28	ALA	-	linker	UNP P03045
7A	29	GLY	-	linker	UNP P03045
7A	30	ALA	-	linker	UNP P03045
7A	31	MET	-	linker	UNP P03045
7A	39	ASN	ILE	engineered mutation	UNP O66529
7A	42	VAL	GLU	engineered mutation	UNP O66529
7A	58	VAL	ILE	engineered mutation	UNP O66529
7A	61	ASP	GLY	engineered mutation	UNP O66529
7A	62	ILE	VAL	engineered mutation	UNP O66529
7A	97	TYR	PHE	engineered mutation	UNP O66529
7A	102	GLY	-	linker	UNP O66529
7A	103	THR	-	linker	UNP O66529
7A	104	GLY	-	linker	UNP O66529
7A	105	HIS	-	linker	UNP O66529
7A	106	HIS	-	linker	UNP O66529
7A	107	HIS	-	linker	UNP O66529
7A	108	HIS	-	linker	UNP O66529
7A	109	HIS	-	linker	UNP O66529
7A	110	HIS	-	linker	UNP O66529
7A	111	GLY	-	linker	UNP O66529
7A	112	SER	-	linker	UNP O66529
7A	113	SER	-	linker	UNP O66529
7A	114	ILE	MET	engineered mutation	UNP O66529
7A	115	GLU	GLN	engineered mutation	UNP O66529
7A	138	THR	ALA	engineered mutation	UNP O66529
7A	177	ASP	GLY	engineered mutation	UNP O66529
7A	191	PHE	ILE	engineered mutation	UNP O66529
7A	193	ASP	VAL	engineered mutation	UNP O66529
7B	1	MET	-	cloning artifact	UNP P03045
7B	2	GLY	-	cloning artifact	UNP P03045
7B	3	ASN	-	cloning artifact	UNP P03045
7B	4	ALA	-	cloning artifact	UNP P03045
7B	5	LYS	-	cloning artifact	UNP P03045
7B	6	THR	-	cloning artifact	UNP P03045
7B	24	ALA	-	linker	UNP P03045
7B	25	GLY	-	linker	UNP P03045
7B	26	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
7B	27	GLY	-	linker	UNP P03045
7B	28	ALA	-	linker	UNP P03045
7B	29	GLY	-	linker	UNP P03045
7B	30	ALA	-	linker	UNP P03045
7B	31	MET	-	linker	UNP P03045
7B	39	ASN	ILE	engineered mutation	UNP O66529
7B	42	VAL	GLU	engineered mutation	UNP O66529
7B	58	VAL	ILE	engineered mutation	UNP O66529
7B	61	ASP	GLY	engineered mutation	UNP O66529
7B	62	ILE	VAL	engineered mutation	UNP O66529
7B	97	TYR	PHE	engineered mutation	UNP O66529
7B	102	GLY	-	linker	UNP O66529
7B	103	THR	-	linker	UNP O66529
7B	104	GLY	-	linker	UNP O66529
7B	105	HIS	-	linker	UNP O66529
7B	106	HIS	-	linker	UNP O66529
7B	107	HIS	-	linker	UNP O66529
7B	108	HIS	-	linker	UNP O66529
7B	109	HIS	-	linker	UNP O66529
7B	110	HIS	-	linker	UNP O66529
7B	111	GLY	-	linker	UNP O66529
7B	112	SER	-	linker	UNP O66529
7B	113	SER	-	linker	UNP O66529
7B	114	ILE	MET	engineered mutation	UNP O66529
7B	115	GLU	GLN	engineered mutation	UNP O66529
7B	138	THR	ALA	engineered mutation	UNP O66529
7B	177	ASP	GLY	engineered mutation	UNP O66529
7B	191	PHE	ILE	engineered mutation	UNP O66529
7B	193	ASP	VAL	engineered mutation	UNP O66529
7C	1	MET	-	cloning artifact	UNP P03045
7C	2	GLY	-	cloning artifact	UNP P03045
7C	3	ASN	-	cloning artifact	UNP P03045
7C	4	ALA	-	cloning artifact	UNP P03045
7C	5	LYS	-	cloning artifact	UNP P03045
7C	6	THR	-	cloning artifact	UNP P03045
7C	24	ALA	-	linker	UNP P03045
7C	25	GLY	-	linker	UNP P03045
7C	26	ALA	-	linker	UNP P03045
7C	27	GLY	-	linker	UNP P03045
7C	28	ALA	-	linker	UNP P03045
7C	29	GLY	-	linker	UNP P03045
7C	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
7C	31	MET	-	linker	UNP P03045
7C	39	ASN	ILE	engineered mutation	UNP O66529
7C	42	VAL	GLU	engineered mutation	UNP O66529
7C	58	VAL	ILE	engineered mutation	UNP O66529
7C	61	ASP	GLY	engineered mutation	UNP O66529
7C	62	ILE	VAL	engineered mutation	UNP O66529
7C	97	TYR	PHE	engineered mutation	UNP O66529
7C	102	GLY	-	linker	UNP O66529
7C	103	THR	-	linker	UNP O66529
7C	104	GLY	-	linker	UNP O66529
7C	105	HIS	-	linker	UNP O66529
7C	106	HIS	-	linker	UNP O66529
7C	107	HIS	-	linker	UNP O66529
7C	108	HIS	-	linker	UNP O66529
7C	109	HIS	-	linker	UNP O66529
7C	110	HIS	-	linker	UNP O66529
7C	111	GLY	-	linker	UNP O66529
7C	112	SER	-	linker	UNP O66529
7C	113	SER	-	linker	UNP O66529
7C	114	ILE	MET	engineered mutation	UNP O66529
7C	115	GLU	GLN	engineered mutation	UNP O66529
7C	138	THR	ALA	engineered mutation	UNP O66529
7C	177	ASP	GLY	engineered mutation	UNP O66529
7C	191	PHE	ILE	engineered mutation	UNP O66529
7C	193	ASP	VAL	engineered mutation	UNP O66529
7D	1	MET	-	cloning artifact	UNP P03045
7D	2	GLY	-	cloning artifact	UNP P03045
7D	3	ASN	-	cloning artifact	UNP P03045
7D	4	ALA	-	cloning artifact	UNP P03045
7D	5	LYS	-	cloning artifact	UNP P03045
7D	6	THR	-	cloning artifact	UNP P03045
7D	24	ALA	-	linker	UNP P03045
7D	25	GLY	-	linker	UNP P03045
7D	26	ALA	-	linker	UNP P03045
7D	27	GLY	-	linker	UNP P03045
7D	28	ALA	-	linker	UNP P03045
7D	29	GLY	-	linker	UNP P03045
7D	30	ALA	-	linker	UNP P03045
7D	31	MET	-	linker	UNP P03045
7D	39	ASN	ILE	engineered mutation	UNP O66529
7D	42	VAL	GLU	engineered mutation	UNP O66529
7D	58	VAL	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
7D	61	ASP	GLY	engineered mutation	UNP O66529
7D	62	ILE	VAL	engineered mutation	UNP O66529
7D	97	TYR	PHE	engineered mutation	UNP O66529
7D	102	GLY	-	linker	UNP O66529
7D	103	THR	-	linker	UNP O66529
7D	104	GLY	-	linker	UNP O66529
7D	105	HIS	-	linker	UNP O66529
7D	106	HIS	-	linker	UNP O66529
7D	107	HIS	-	linker	UNP O66529
7D	108	HIS	-	linker	UNP O66529
7D	109	HIS	-	linker	UNP O66529
7D	110	HIS	-	linker	UNP O66529
7D	111	GLY	-	linker	UNP O66529
7D	112	SER	-	linker	UNP O66529
7D	113	SER	-	linker	UNP O66529
7D	114	ILE	MET	engineered mutation	UNP O66529
7D	115	GLU	GLN	engineered mutation	UNP O66529
7D	138	THR	ALA	engineered mutation	UNP O66529
7D	177	ASP	GLY	engineered mutation	UNP O66529
7D	191	PHE	ILE	engineered mutation	UNP O66529
7D	193	ASP	VAL	engineered mutation	UNP O66529
QA	1	MET	-	cloning artifact	UNP P03045
QA	2	GLY	-	cloning artifact	UNP P03045
QA	3	ASN	-	cloning artifact	UNP P03045
QA	4	ALA	-	cloning artifact	UNP P03045
QA	5	LYS	-	cloning artifact	UNP P03045
QA	6	THR	-	cloning artifact	UNP P03045
QA	24	ALA	-	linker	UNP P03045
QA	25	GLY	-	linker	UNP P03045
QA	26	ALA	-	linker	UNP P03045
QA	27	GLY	-	linker	UNP P03045
QA	28	ALA	-	linker	UNP P03045
QA	29	GLY	-	linker	UNP P03045
QA	30	ALA	-	linker	UNP P03045
QA	31	MET	-	linker	UNP P03045
QA	39	ASN	ILE	engineered mutation	UNP O66529
QA	42	VAL	GLU	engineered mutation	UNP O66529
QA	58	VAL	ILE	engineered mutation	UNP O66529
QA	61	ASP	GLY	engineered mutation	UNP O66529
QA	62	ILE	VAL	engineered mutation	UNP O66529
QA	97	TYR	PHE	engineered mutation	UNP O66529
QA	102	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
QA	103	THR	-	linker	UNP O66529
QA	104	GLY	-	linker	UNP O66529
QA	105	HIS	-	linker	UNP O66529
QA	106	HIS	-	linker	UNP O66529
QA	107	HIS	-	linker	UNP O66529
QA	108	HIS	-	linker	UNP O66529
QA	109	HIS	-	linker	UNP O66529
QA	110	HIS	-	linker	UNP O66529
QA	111	GLY	-	linker	UNP O66529
QA	112	SER	-	linker	UNP O66529
QA	113	SER	-	linker	UNP O66529
QA	114	ILE	MET	engineered mutation	UNP O66529
QA	115	GLU	GLN	engineered mutation	UNP O66529
QA	138	THR	ALA	engineered mutation	UNP O66529
QA	177	ASP	GLY	engineered mutation	UNP O66529
QA	191	PHE	ILE	engineered mutation	UNP O66529
QA	193	ASP	VAL	engineered mutation	UNP O66529
QB	1	MET	-	cloning artifact	UNP P03045
QB	2	GLY	-	cloning artifact	UNP P03045
QB	3	ASN	-	cloning artifact	UNP P03045
QB	4	ALA	-	cloning artifact	UNP P03045
QB	5	LYS	-	cloning artifact	UNP P03045
QB	6	THR	-	cloning artifact	UNP P03045
QB	24	ALA	-	linker	UNP P03045
QB	25	GLY	-	linker	UNP P03045
QB	26	ALA	-	linker	UNP P03045
QB	27	GLY	-	linker	UNP P03045
QB	28	ALA	-	linker	UNP P03045
QB	29	GLY	-	linker	UNP P03045
QB	30	ALA	-	linker	UNP P03045
QB	31	MET	-	linker	UNP P03045
QB	39	ASN	ILE	engineered mutation	UNP O66529
QB	42	VAL	GLU	engineered mutation	UNP O66529
QB	58	VAL	ILE	engineered mutation	UNP O66529
QB	61	ASP	GLY	engineered mutation	UNP O66529
QB	62	ILE	VAL	engineered mutation	UNP O66529
QB	97	TYR	PHE	engineered mutation	UNP O66529
QB	102	GLY	-	linker	UNP O66529
QB	103	THR	-	linker	UNP O66529
QB	104	GLY	-	linker	UNP O66529
QB	105	HIS	-	linker	UNP O66529
QB	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
QB	107	HIS	-	linker	UNP O66529
QB	108	HIS	-	linker	UNP O66529
QB	109	HIS	-	linker	UNP O66529
QB	110	HIS	-	linker	UNP O66529
QB	111	GLY	-	linker	UNP O66529
QB	112	SER	-	linker	UNP O66529
QB	113	SER	-	linker	UNP O66529
QB	114	ILE	MET	engineered mutation	UNP O66529
QB	115	GLU	GLN	engineered mutation	UNP O66529
QB	138	THR	ALA	engineered mutation	UNP O66529
QB	177	ASP	GLY	engineered mutation	UNP O66529
QB	191	PHE	ILE	engineered mutation	UNP O66529
QB	193	ASP	VAL	engineered mutation	UNP O66529
QC	1	MET	-	cloning artifact	UNP P03045
QC	2	GLY	-	cloning artifact	UNP P03045
QC	3	ASN	-	cloning artifact	UNP P03045
QC	4	ALA	-	cloning artifact	UNP P03045
QC	5	LYS	-	cloning artifact	UNP P03045
QC	6	THR	-	cloning artifact	UNP P03045
QC	24	ALA	-	linker	UNP P03045
QC	25	GLY	-	linker	UNP P03045
QC	26	ALA	-	linker	UNP P03045
QC	27	GLY	-	linker	UNP P03045
QC	28	ALA	-	linker	UNP P03045
QC	29	GLY	-	linker	UNP P03045
QC	30	ALA	-	linker	UNP P03045
QC	31	MET	-	linker	UNP P03045
QC	39	ASN	ILE	engineered mutation	UNP O66529
QC	42	VAL	GLU	engineered mutation	UNP O66529
QC	58	VAL	ILE	engineered mutation	UNP O66529
QC	61	ASP	GLY	engineered mutation	UNP O66529
QC	62	ILE	VAL	engineered mutation	UNP O66529
QC	97	TYR	PHE	engineered mutation	UNP O66529
QC	102	GLY	-	linker	UNP O66529
QC	103	THR	-	linker	UNP O66529
QC	104	GLY	-	linker	UNP O66529
QC	105	HIS	-	linker	UNP O66529
QC	106	HIS	-	linker	UNP O66529
QC	107	HIS	-	linker	UNP O66529
QC	108	HIS	-	linker	UNP O66529
QC	109	HIS	-	linker	UNP O66529
QC	110	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
QC	111	GLY	-	linker	UNP O66529
QC	112	SER	-	linker	UNP O66529
QC	113	SER	-	linker	UNP O66529
QC	114	ILE	MET	engineered mutation	UNP O66529
QC	115	GLU	GLN	engineered mutation	UNP O66529
QC	138	THR	ALA	engineered mutation	UNP O66529
QC	177	ASP	GLY	engineered mutation	UNP O66529
QC	191	PHE	ILE	engineered mutation	UNP O66529
QC	193	ASP	VAL	engineered mutation	UNP O66529
QD	1	MET	-	cloning artifact	UNP P03045
QD	2	GLY	-	cloning artifact	UNP P03045
QD	3	ASN	-	cloning artifact	UNP P03045
QD	4	ALA	-	cloning artifact	UNP P03045
QD	5	LYS	-	cloning artifact	UNP P03045
QD	6	THR	-	cloning artifact	UNP P03045
QD	24	ALA	-	linker	UNP P03045
QD	25	GLY	-	linker	UNP P03045
QD	26	ALA	-	linker	UNP P03045
QD	27	GLY	-	linker	UNP P03045
QD	28	ALA	-	linker	UNP P03045
QD	29	GLY	-	linker	UNP P03045
QD	30	ALA	-	linker	UNP P03045
QD	31	MET	-	linker	UNP P03045
QD	39	ASN	ILE	engineered mutation	UNP O66529
QD	42	VAL	GLU	engineered mutation	UNP O66529
QD	58	VAL	ILE	engineered mutation	UNP O66529
QD	61	ASP	GLY	engineered mutation	UNP O66529
QD	62	ILE	VAL	engineered mutation	UNP O66529
QD	97	TYR	PHE	engineered mutation	UNP O66529
QD	102	GLY	-	linker	UNP O66529
QD	103	THR	-	linker	UNP O66529
QD	104	GLY	-	linker	UNP O66529
QD	105	HIS	-	linker	UNP O66529
QD	106	HIS	-	linker	UNP O66529
QD	107	HIS	-	linker	UNP O66529
QD	108	HIS	-	linker	UNP O66529
QD	109	HIS	-	linker	UNP O66529
QD	110	HIS	-	linker	UNP O66529
QD	111	GLY	-	linker	UNP O66529
QD	112	SER	-	linker	UNP O66529
QD	113	SER	-	linker	UNP O66529
QD	114	ILE	MET	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
QD	115	GLU	GLN	engineered mutation	UNP O66529
QD	138	THR	ALA	engineered mutation	UNP O66529
QD	177	ASP	GLY	engineered mutation	UNP O66529
QD	191	PHE	ILE	engineered mutation	UNP O66529
QD	193	ASP	VAL	engineered mutation	UNP O66529
RA	1	MET	-	cloning artifact	UNP P03045
RA	2	GLY	-	cloning artifact	UNP P03045
RA	3	ASN	-	cloning artifact	UNP P03045
RA	4	ALA	-	cloning artifact	UNP P03045
RA	5	LYS	-	cloning artifact	UNP P03045
RA	6	THR	-	cloning artifact	UNP P03045
RA	24	ALA	-	linker	UNP P03045
RA	25	GLY	-	linker	UNP P03045
RA	26	ALA	-	linker	UNP P03045
RA	27	GLY	-	linker	UNP P03045
RA	28	ALA	-	linker	UNP P03045
RA	29	GLY	-	linker	UNP P03045
RA	30	ALA	-	linker	UNP P03045
RA	31	MET	-	linker	UNP P03045
RA	39	ASN	ILE	engineered mutation	UNP O66529
RA	42	VAL	GLU	engineered mutation	UNP O66529
RA	58	VAL	ILE	engineered mutation	UNP O66529
RA	61	ASP	GLY	engineered mutation	UNP O66529
RA	62	ILE	VAL	engineered mutation	UNP O66529
RA	97	TYR	PHE	engineered mutation	UNP O66529
RA	102	GLY	-	linker	UNP O66529
RA	103	THR	-	linker	UNP O66529
RA	104	GLY	-	linker	UNP O66529
RA	105	HIS	-	linker	UNP O66529
RA	106	HIS	-	linker	UNP O66529
RA	107	HIS	-	linker	UNP O66529
RA	108	HIS	-	linker	UNP O66529
RA	109	HIS	-	linker	UNP O66529
RA	110	HIS	-	linker	UNP O66529
RA	111	GLY	-	linker	UNP O66529
RA	112	SER	-	linker	UNP O66529
RA	113	SER	-	linker	UNP O66529
RA	114	ILE	MET	engineered mutation	UNP O66529
RA	115	GLU	GLN	engineered mutation	UNP O66529
RA	138	THR	ALA	engineered mutation	UNP O66529
RA	177	ASP	GLY	engineered mutation	UNP O66529
RA	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
RA	193	ASP	VAL	engineered mutation	UNP O66529
RB	1	MET	-	cloning artifact	UNP P03045
RB	2	GLY	-	cloning artifact	UNP P03045
RB	3	ASN	-	cloning artifact	UNP P03045
RB	4	ALA	-	cloning artifact	UNP P03045
RB	5	LYS	-	cloning artifact	UNP P03045
RB	6	THR	-	cloning artifact	UNP P03045
RB	24	ALA	-	linker	UNP P03045
RB	25	GLY	-	linker	UNP P03045
RB	26	ALA	-	linker	UNP P03045
RB	27	GLY	-	linker	UNP P03045
RB	28	ALA	-	linker	UNP P03045
RB	29	GLY	-	linker	UNP P03045
RB	30	ALA	-	linker	UNP P03045
RB	31	MET	-	linker	UNP P03045
RB	39	ASN	ILE	engineered mutation	UNP O66529
RB	42	VAL	GLU	engineered mutation	UNP O66529
RB	58	VAL	ILE	engineered mutation	UNP O66529
RB	61	ASP	GLY	engineered mutation	UNP O66529
RB	62	ILE	VAL	engineered mutation	UNP O66529
RB	97	TYR	PHE	engineered mutation	UNP O66529
RB	102	GLY	-	linker	UNP O66529
RB	103	THR	-	linker	UNP O66529
RB	104	GLY	-	linker	UNP O66529
RB	105	HIS	-	linker	UNP O66529
RB	106	HIS	-	linker	UNP O66529
RB	107	HIS	-	linker	UNP O66529
RB	108	HIS	-	linker	UNP O66529
RB	109	HIS	-	linker	UNP O66529
RB	110	HIS	-	linker	UNP O66529
RB	111	GLY	-	linker	UNP O66529
RB	112	SER	-	linker	UNP O66529
RB	113	SER	-	linker	UNP O66529
RB	114	ILE	MET	engineered mutation	UNP O66529
RB	115	GLU	GLN	engineered mutation	UNP O66529
RB	138	THR	ALA	engineered mutation	UNP O66529
RB	177	ASP	GLY	engineered mutation	UNP O66529
RB	191	PHE	ILE	engineered mutation	UNP O66529
RB	193	ASP	VAL	engineered mutation	UNP O66529
RC	1	MET	-	cloning artifact	UNP P03045
RC	2	GLY	-	cloning artifact	UNP P03045
RC	3	ASN	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
RC	4	ALA	-	cloning artifact	UNP P03045
RC	5	LYS	-	cloning artifact	UNP P03045
RC	6	THR	-	cloning artifact	UNP P03045
RC	24	ALA	-	linker	UNP P03045
RC	25	GLY	-	linker	UNP P03045
RC	26	ALA	-	linker	UNP P03045
RC	27	GLY	-	linker	UNP P03045
RC	28	ALA	-	linker	UNP P03045
RC	29	GLY	-	linker	UNP P03045
RC	30	ALA	-	linker	UNP P03045
RC	31	MET	-	linker	UNP P03045
RC	39	ASN	ILE	engineered mutation	UNP O66529
RC	42	VAL	GLU	engineered mutation	UNP O66529
RC	58	VAL	ILE	engineered mutation	UNP O66529
RC	61	ASP	GLY	engineered mutation	UNP O66529
RC	62	ILE	VAL	engineered mutation	UNP O66529
RC	97	TYR	PHE	engineered mutation	UNP O66529
RC	102	GLY	-	linker	UNP O66529
RC	103	THR	-	linker	UNP O66529
RC	104	GLY	-	linker	UNP O66529
RC	105	HIS	-	linker	UNP O66529
RC	106	HIS	-	linker	UNP O66529
RC	107	HIS	-	linker	UNP O66529
RC	108	HIS	-	linker	UNP O66529
RC	109	HIS	-	linker	UNP O66529
RC	110	HIS	-	linker	UNP O66529
RC	111	GLY	-	linker	UNP O66529
RC	112	SER	-	linker	UNP O66529
RC	113	SER	-	linker	UNP O66529
RC	114	ILE	MET	engineered mutation	UNP O66529
RC	115	GLU	GLN	engineered mutation	UNP O66529
RC	138	THR	ALA	engineered mutation	UNP O66529
RC	177	ASP	GLY	engineered mutation	UNP O66529
RC	191	PHE	ILE	engineered mutation	UNP O66529
RC	193	ASP	VAL	engineered mutation	UNP O66529
RD	1	MET	-	cloning artifact	UNP P03045
RD	2	GLY	-	cloning artifact	UNP P03045
RD	3	ASN	-	cloning artifact	UNP P03045
RD	4	ALA	-	cloning artifact	UNP P03045
RD	5	LYS	-	cloning artifact	UNP P03045
RD	6	THR	-	cloning artifact	UNP P03045
RD	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
RD	25	GLY	-	linker	UNP P03045
RD	26	ALA	-	linker	UNP P03045
RD	27	GLY	-	linker	UNP P03045
RD	28	ALA	-	linker	UNP P03045
RD	29	GLY	-	linker	UNP P03045
RD	30	ALA	-	linker	UNP P03045
RD	31	MET	-	linker	UNP P03045
RD	39	ASN	ILE	engineered mutation	UNP O66529
RD	42	VAL	GLU	engineered mutation	UNP O66529
RD	58	VAL	ILE	engineered mutation	UNP O66529
RD	61	ASP	GLY	engineered mutation	UNP O66529
RD	62	ILE	VAL	engineered mutation	UNP O66529
RD	97	TYR	PHE	engineered mutation	UNP O66529
RD	102	GLY	-	linker	UNP O66529
RD	103	THR	-	linker	UNP O66529
RD	104	GLY	-	linker	UNP O66529
RD	105	HIS	-	linker	UNP O66529
RD	106	HIS	-	linker	UNP O66529
RD	107	HIS	-	linker	UNP O66529
RD	108	HIS	-	linker	UNP O66529
RD	109	HIS	-	linker	UNP O66529
RD	110	HIS	-	linker	UNP O66529
RD	111	GLY	-	linker	UNP O66529
RD	112	SER	-	linker	UNP O66529
RD	113	SER	-	linker	UNP O66529
RD	114	ILE	MET	engineered mutation	UNP O66529
RD	115	GLU	GLN	engineered mutation	UNP O66529
RD	138	THR	ALA	engineered mutation	UNP O66529
RD	177	ASP	GLY	engineered mutation	UNP O66529
RD	191	PHE	ILE	engineered mutation	UNP O66529
RD	193	ASP	VAL	engineered mutation	UNP O66529
SA	1	MET	-	cloning artifact	UNP P03045
SA	2	GLY	-	cloning artifact	UNP P03045
SA	3	ASN	-	cloning artifact	UNP P03045
SA	4	ALA	-	cloning artifact	UNP P03045
SA	5	LYS	-	cloning artifact	UNP P03045
SA	6	THR	-	cloning artifact	UNP P03045
SA	24	ALA	-	linker	UNP P03045
SA	25	GLY	-	linker	UNP P03045
SA	26	ALA	-	linker	UNP P03045
SA	27	GLY	-	linker	UNP P03045
SA	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
SA	29	GLY	-	linker	UNP P03045
SA	30	ALA	-	linker	UNP P03045
SA	31	MET	-	linker	UNP P03045
SA	39	ASN	ILE	engineered mutation	UNP O66529
SA	42	VAL	GLU	engineered mutation	UNP O66529
SA	58	VAL	ILE	engineered mutation	UNP O66529
SA	61	ASP	GLY	engineered mutation	UNP O66529
SA	62	ILE	VAL	engineered mutation	UNP O66529
SA	97	TYR	PHE	engineered mutation	UNP O66529
SA	102	GLY	-	linker	UNP O66529
SA	103	THR	-	linker	UNP O66529
SA	104	GLY	-	linker	UNP O66529
SA	105	HIS	-	linker	UNP O66529
SA	106	HIS	-	linker	UNP O66529
SA	107	HIS	-	linker	UNP O66529
SA	108	HIS	-	linker	UNP O66529
SA	109	HIS	-	linker	UNP O66529
SA	110	HIS	-	linker	UNP O66529
SA	111	GLY	-	linker	UNP O66529
SA	112	SER	-	linker	UNP O66529
SA	113	SER	-	linker	UNP O66529
SA	114	ILE	MET	engineered mutation	UNP O66529
SA	115	GLU	GLN	engineered mutation	UNP O66529
SA	138	THR	ALA	engineered mutation	UNP O66529
SA	177	ASP	GLY	engineered mutation	UNP O66529
SA	191	PHE	ILE	engineered mutation	UNP O66529
SA	193	ASP	VAL	engineered mutation	UNP O66529
SB	1	MET	-	cloning artifact	UNP P03045
SB	2	GLY	-	cloning artifact	UNP P03045
SB	3	ASN	-	cloning artifact	UNP P03045
SB	4	ALA	-	cloning artifact	UNP P03045
SB	5	LYS	-	cloning artifact	UNP P03045
SB	6	THR	-	cloning artifact	UNP P03045
SB	24	ALA	-	linker	UNP P03045
SB	25	GLY	-	linker	UNP P03045
SB	26	ALA	-	linker	UNP P03045
SB	27	GLY	-	linker	UNP P03045
SB	28	ALA	-	linker	UNP P03045
SB	29	GLY	-	linker	UNP P03045
SB	30	ALA	-	linker	UNP P03045
SB	31	MET	-	linker	UNP P03045
SB	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
SB	42	VAL	GLU	engineered mutation	UNP O66529
SB	58	VAL	ILE	engineered mutation	UNP O66529
SB	61	ASP	GLY	engineered mutation	UNP O66529
SB	62	ILE	VAL	engineered mutation	UNP O66529
SB	97	TYR	PHE	engineered mutation	UNP O66529
SB	102	GLY	-	linker	UNP O66529
SB	103	THR	-	linker	UNP O66529
SB	104	GLY	-	linker	UNP O66529
SB	105	HIS	-	linker	UNP O66529
SB	106	HIS	-	linker	UNP O66529
SB	107	HIS	-	linker	UNP O66529
SB	108	HIS	-	linker	UNP O66529
SB	109	HIS	-	linker	UNP O66529
SB	110	HIS	-	linker	UNP O66529
SB	111	GLY	-	linker	UNP O66529
SB	112	SER	-	linker	UNP O66529
SB	113	SER	-	linker	UNP O66529
SB	114	ILE	MET	engineered mutation	UNP O66529
SB	115	GLU	GLN	engineered mutation	UNP O66529
SB	138	THR	ALA	engineered mutation	UNP O66529
SB	177	ASP	GLY	engineered mutation	UNP O66529
SB	191	PHE	ILE	engineered mutation	UNP O66529
SB	193	ASP	VAL	engineered mutation	UNP O66529
SC	1	MET	-	cloning artifact	UNP P03045
SC	2	GLY	-	cloning artifact	UNP P03045
SC	3	ASN	-	cloning artifact	UNP P03045
SC	4	ALA	-	cloning artifact	UNP P03045
SC	5	LYS	-	cloning artifact	UNP P03045
SC	6	THR	-	cloning artifact	UNP P03045
SC	24	ALA	-	linker	UNP P03045
SC	25	GLY	-	linker	UNP P03045
SC	26	ALA	-	linker	UNP P03045
SC	27	GLY	-	linker	UNP P03045
SC	28	ALA	-	linker	UNP P03045
SC	29	GLY	-	linker	UNP P03045
SC	30	ALA	-	linker	UNP P03045
SC	31	MET	-	linker	UNP P03045
SC	39	ASN	ILE	engineered mutation	UNP O66529
SC	42	VAL	GLU	engineered mutation	UNP O66529
SC	58	VAL	ILE	engineered mutation	UNP O66529
SC	61	ASP	GLY	engineered mutation	UNP O66529
SC	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
SC	97	TYR	PHE	engineered mutation	UNP O66529
SC	102	GLY	-	linker	UNP O66529
SC	103	THR	-	linker	UNP O66529
SC	104	GLY	-	linker	UNP O66529
SC	105	HIS	-	linker	UNP O66529
SC	106	HIS	-	linker	UNP O66529
SC	107	HIS	-	linker	UNP O66529
SC	108	HIS	-	linker	UNP O66529
SC	109	HIS	-	linker	UNP O66529
SC	110	HIS	-	linker	UNP O66529
SC	111	GLY	-	linker	UNP O66529
SC	112	SER	-	linker	UNP O66529
SC	113	SER	-	linker	UNP O66529
SC	114	ILE	MET	engineered mutation	UNP O66529
SC	115	GLU	GLN	engineered mutation	UNP O66529
SC	138	THR	ALA	engineered mutation	UNP O66529
SC	177	ASP	GLY	engineered mutation	UNP O66529
SC	191	PHE	ILE	engineered mutation	UNP O66529
SC	193	ASP	VAL	engineered mutation	UNP O66529
SD	1	MET	-	cloning artifact	UNP P03045
SD	2	GLY	-	cloning artifact	UNP P03045
SD	3	ASN	-	cloning artifact	UNP P03045
SD	4	ALA	-	cloning artifact	UNP P03045
SD	5	LYS	-	cloning artifact	UNP P03045
SD	6	THR	-	cloning artifact	UNP P03045
SD	24	ALA	-	linker	UNP P03045
SD	25	GLY	-	linker	UNP P03045
SD	26	ALA	-	linker	UNP P03045
SD	27	GLY	-	linker	UNP P03045
SD	28	ALA	-	linker	UNP P03045
SD	29	GLY	-	linker	UNP P03045
SD	30	ALA	-	linker	UNP P03045
SD	31	MET	-	linker	UNP P03045
SD	39	ASN	ILE	engineered mutation	UNP O66529
SD	42	VAL	GLU	engineered mutation	UNP O66529
SD	58	VAL	ILE	engineered mutation	UNP O66529
SD	61	ASP	GLY	engineered mutation	UNP O66529
SD	62	ILE	VAL	engineered mutation	UNP O66529
SD	97	TYR	PHE	engineered mutation	UNP O66529
SD	102	GLY	-	linker	UNP O66529
SD	103	THR	-	linker	UNP O66529
SD	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
SD	105	HIS	-	linker	UNP O66529
SD	106	HIS	-	linker	UNP O66529
SD	107	HIS	-	linker	UNP O66529
SD	108	HIS	-	linker	UNP O66529
SD	109	HIS	-	linker	UNP O66529
SD	110	HIS	-	linker	UNP O66529
SD	111	GLY	-	linker	UNP O66529
SD	112	SER	-	linker	UNP O66529
SD	113	SER	-	linker	UNP O66529
SD	114	ILE	MET	engineered mutation	UNP O66529
SD	115	GLU	GLN	engineered mutation	UNP O66529
SD	138	THR	ALA	engineered mutation	UNP O66529
SD	177	ASP	GLY	engineered mutation	UNP O66529
SD	191	PHE	ILE	engineered mutation	UNP O66529
SD	193	ASP	VAL	engineered mutation	UNP O66529
TA	1	MET	-	cloning artifact	UNP P03045
TA	2	GLY	-	cloning artifact	UNP P03045
TA	3	ASN	-	cloning artifact	UNP P03045
TA	4	ALA	-	cloning artifact	UNP P03045
TA	5	LYS	-	cloning artifact	UNP P03045
TA	6	THR	-	cloning artifact	UNP P03045
TA	24	ALA	-	linker	UNP P03045
TA	25	GLY	-	linker	UNP P03045
TA	26	ALA	-	linker	UNP P03045
TA	27	GLY	-	linker	UNP P03045
TA	28	ALA	-	linker	UNP P03045
TA	29	GLY	-	linker	UNP P03045
TA	30	ALA	-	linker	UNP P03045
TA	31	MET	-	linker	UNP P03045
TA	39	ASN	ILE	engineered mutation	UNP O66529
TA	42	VAL	GLU	engineered mutation	UNP O66529
TA	58	VAL	ILE	engineered mutation	UNP O66529
TA	61	ASP	GLY	engineered mutation	UNP O66529
TA	62	ILE	VAL	engineered mutation	UNP O66529
TA	97	TYR	PHE	engineered mutation	UNP O66529
TA	102	GLY	-	linker	UNP O66529
TA	103	THR	-	linker	UNP O66529
TA	104	GLY	-	linker	UNP O66529
TA	105	HIS	-	linker	UNP O66529
TA	106	HIS	-	linker	UNP O66529
TA	107	HIS	-	linker	UNP O66529
TA	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
TA	109	HIS	-	linker	UNP O66529
TA	110	HIS	-	linker	UNP O66529
TA	111	GLY	-	linker	UNP O66529
TA	112	SER	-	linker	UNP O66529
TA	113	SER	-	linker	UNP O66529
TA	114	ILE	MET	engineered mutation	UNP O66529
TA	115	GLU	GLN	engineered mutation	UNP O66529
TA	138	THR	ALA	engineered mutation	UNP O66529
TA	177	ASP	GLY	engineered mutation	UNP O66529
TA	191	PHE	ILE	engineered mutation	UNP O66529
TA	193	ASP	VAL	engineered mutation	UNP O66529
TB	1	MET	-	cloning artifact	UNP P03045
TB	2	GLY	-	cloning artifact	UNP P03045
TB	3	ASN	-	cloning artifact	UNP P03045
TB	4	ALA	-	cloning artifact	UNP P03045
TB	5	LYS	-	cloning artifact	UNP P03045
TB	6	THR	-	cloning artifact	UNP P03045
TB	24	ALA	-	linker	UNP P03045
TB	25	GLY	-	linker	UNP P03045
TB	26	ALA	-	linker	UNP P03045
TB	27	GLY	-	linker	UNP P03045
TB	28	ALA	-	linker	UNP P03045
TB	29	GLY	-	linker	UNP P03045
TB	30	ALA	-	linker	UNP P03045
TB	31	MET	-	linker	UNP P03045
TB	39	ASN	ILE	engineered mutation	UNP O66529
TB	42	VAL	GLU	engineered mutation	UNP O66529
TB	58	VAL	ILE	engineered mutation	UNP O66529
TB	61	ASP	GLY	engineered mutation	UNP O66529
TB	62	ILE	VAL	engineered mutation	UNP O66529
TB	97	TYR	PHE	engineered mutation	UNP O66529
TB	102	GLY	-	linker	UNP O66529
TB	103	THR	-	linker	UNP O66529
TB	104	GLY	-	linker	UNP O66529
TB	105	HIS	-	linker	UNP O66529
TB	106	HIS	-	linker	UNP O66529
TB	107	HIS	-	linker	UNP O66529
TB	108	HIS	-	linker	UNP O66529
TB	109	HIS	-	linker	UNP O66529
TB	110	HIS	-	linker	UNP O66529
TB	111	GLY	-	linker	UNP O66529
TB	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
TB	113	SER	-	linker	UNP O66529
TB	114	ILE	MET	engineered mutation	UNP O66529
TB	115	GLU	GLN	engineered mutation	UNP O66529
TB	138	THR	ALA	engineered mutation	UNP O66529
TB	177	ASP	GLY	engineered mutation	UNP O66529
TB	191	PHE	ILE	engineered mutation	UNP O66529
TB	193	ASP	VAL	engineered mutation	UNP O66529
TC	1	MET	-	cloning artifact	UNP P03045
TC	2	GLY	-	cloning artifact	UNP P03045
TC	3	ASN	-	cloning artifact	UNP P03045
TC	4	ALA	-	cloning artifact	UNP P03045
TC	5	LYS	-	cloning artifact	UNP P03045
TC	6	THR	-	cloning artifact	UNP P03045
TC	24	ALA	-	linker	UNP P03045
TC	25	GLY	-	linker	UNP P03045
TC	26	ALA	-	linker	UNP P03045
TC	27	GLY	-	linker	UNP P03045
TC	28	ALA	-	linker	UNP P03045
TC	29	GLY	-	linker	UNP P03045
TC	30	ALA	-	linker	UNP P03045
TC	31	MET	-	linker	UNP P03045
TC	39	ASN	ILE	engineered mutation	UNP O66529
TC	42	VAL	GLU	engineered mutation	UNP O66529
TC	58	VAL	ILE	engineered mutation	UNP O66529
TC	61	ASP	GLY	engineered mutation	UNP O66529
TC	62	ILE	VAL	engineered mutation	UNP O66529
TC	97	TYR	PHE	engineered mutation	UNP O66529
TC	102	GLY	-	linker	UNP O66529
TC	103	THR	-	linker	UNP O66529
TC	104	GLY	-	linker	UNP O66529
TC	105	HIS	-	linker	UNP O66529
TC	106	HIS	-	linker	UNP O66529
TC	107	HIS	-	linker	UNP O66529
TC	108	HIS	-	linker	UNP O66529
TC	109	HIS	-	linker	UNP O66529
TC	110	HIS	-	linker	UNP O66529
TC	111	GLY	-	linker	UNP O66529
TC	112	SER	-	linker	UNP O66529
TC	113	SER	-	linker	UNP O66529
TC	114	ILE	MET	engineered mutation	UNP O66529
TC	115	GLU	GLN	engineered mutation	UNP O66529
TC	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
TC	177	ASP	GLY	engineered mutation	UNP O66529
TC	191	PHE	ILE	engineered mutation	UNP O66529
TC	193	ASP	VAL	engineered mutation	UNP O66529
TD	1	MET	-	cloning artifact	UNP P03045
TD	2	GLY	-	cloning artifact	UNP P03045
TD	3	ASN	-	cloning artifact	UNP P03045
TD	4	ALA	-	cloning artifact	UNP P03045
TD	5	LYS	-	cloning artifact	UNP P03045
TD	6	THR	-	cloning artifact	UNP P03045
TD	24	ALA	-	linker	UNP P03045
TD	25	GLY	-	linker	UNP P03045
TD	26	ALA	-	linker	UNP P03045
TD	27	GLY	-	linker	UNP P03045
TD	28	ALA	-	linker	UNP P03045
TD	29	GLY	-	linker	UNP P03045
TD	30	ALA	-	linker	UNP P03045
TD	31	MET	-	linker	UNP P03045
TD	39	ASN	ILE	engineered mutation	UNP O66529
TD	42	VAL	GLU	engineered mutation	UNP O66529
TD	58	VAL	ILE	engineered mutation	UNP O66529
TD	61	ASP	GLY	engineered mutation	UNP O66529
TD	62	ILE	VAL	engineered mutation	UNP O66529
TD	97	TYR	PHE	engineered mutation	UNP O66529
TD	102	GLY	-	linker	UNP O66529
TD	103	THR	-	linker	UNP O66529
TD	104	GLY	-	linker	UNP O66529
TD	105	HIS	-	linker	UNP O66529
TD	106	HIS	-	linker	UNP O66529
TD	107	HIS	-	linker	UNP O66529
TD	108	HIS	-	linker	UNP O66529
TD	109	HIS	-	linker	UNP O66529
TD	110	HIS	-	linker	UNP O66529
TD	111	GLY	-	linker	UNP O66529
TD	112	SER	-	linker	UNP O66529
TD	113	SER	-	linker	UNP O66529
TD	114	ILE	MET	engineered mutation	UNP O66529
TD	115	GLU	GLN	engineered mutation	UNP O66529
TD	138	THR	ALA	engineered mutation	UNP O66529
TD	177	ASP	GLY	engineered mutation	UNP O66529
TD	191	PHE	ILE	engineered mutation	UNP O66529
TD	193	ASP	VAL	engineered mutation	UNP O66529
UA	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
UA	2	GLY	-	cloning artifact	UNP P03045
UA	3	ASN	-	cloning artifact	UNP P03045
UA	4	ALA	-	cloning artifact	UNP P03045
UA	5	LYS	-	cloning artifact	UNP P03045
UA	6	THR	-	cloning artifact	UNP P03045
UA	24	ALA	-	linker	UNP P03045
UA	25	GLY	-	linker	UNP P03045
UA	26	ALA	-	linker	UNP P03045
UA	27	GLY	-	linker	UNP P03045
UA	28	ALA	-	linker	UNP P03045
UA	29	GLY	-	linker	UNP P03045
UA	30	ALA	-	linker	UNP P03045
UA	31	MET	-	linker	UNP P03045
UA	39	ASN	ILE	engineered mutation	UNP O66529
UA	42	VAL	GLU	engineered mutation	UNP O66529
UA	58	VAL	ILE	engineered mutation	UNP O66529
UA	61	ASP	GLY	engineered mutation	UNP O66529
UA	62	ILE	VAL	engineered mutation	UNP O66529
UA	97	TYR	PHE	engineered mutation	UNP O66529
UA	102	GLY	-	linker	UNP O66529
UA	103	THR	-	linker	UNP O66529
UA	104	GLY	-	linker	UNP O66529
UA	105	HIS	-	linker	UNP O66529
UA	106	HIS	-	linker	UNP O66529
UA	107	HIS	-	linker	UNP O66529
UA	108	HIS	-	linker	UNP O66529
UA	109	HIS	-	linker	UNP O66529
UA	110	HIS	-	linker	UNP O66529
UA	111	GLY	-	linker	UNP O66529
UA	112	SER	-	linker	UNP O66529
UA	113	SER	-	linker	UNP O66529
UA	114	ILE	MET	engineered mutation	UNP O66529
UA	115	GLU	GLN	engineered mutation	UNP O66529
UA	138	THR	ALA	engineered mutation	UNP O66529
UA	177	ASP	GLY	engineered mutation	UNP O66529
UA	191	PHE	ILE	engineered mutation	UNP O66529
UA	193	ASP	VAL	engineered mutation	UNP O66529
UB	1	MET	-	cloning artifact	UNP P03045
UB	2	GLY	-	cloning artifact	UNP P03045
UB	3	ASN	-	cloning artifact	UNP P03045
UB	4	ALA	-	cloning artifact	UNP P03045
UB	5	LYS	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
UB	6	THR	-	cloning artifact	UNP P03045
UB	24	ALA	-	linker	UNP P03045
UB	25	GLY	-	linker	UNP P03045
UB	26	ALA	-	linker	UNP P03045
UB	27	GLY	-	linker	UNP P03045
UB	28	ALA	-	linker	UNP P03045
UB	29	GLY	-	linker	UNP P03045
UB	30	ALA	-	linker	UNP P03045
UB	31	MET	-	linker	UNP P03045
UB	39	ASN	ILE	engineered mutation	UNP O66529
UB	42	VAL	GLU	engineered mutation	UNP O66529
UB	58	VAL	ILE	engineered mutation	UNP O66529
UB	61	ASP	GLY	engineered mutation	UNP O66529
UB	62	ILE	VAL	engineered mutation	UNP O66529
UB	97	TYR	PHE	engineered mutation	UNP O66529
UB	102	GLY	-	linker	UNP O66529
UB	103	THR	-	linker	UNP O66529
UB	104	GLY	-	linker	UNP O66529
UB	105	HIS	-	linker	UNP O66529
UB	106	HIS	-	linker	UNP O66529
UB	107	HIS	-	linker	UNP O66529
UB	108	HIS	-	linker	UNP O66529
UB	109	HIS	-	linker	UNP O66529
UB	110	HIS	-	linker	UNP O66529
UB	111	GLY	-	linker	UNP O66529
UB	112	SER	-	linker	UNP O66529
UB	113	SER	-	linker	UNP O66529
UB	114	ILE	MET	engineered mutation	UNP O66529
UB	115	GLU	GLN	engineered mutation	UNP O66529
UB	138	THR	ALA	engineered mutation	UNP O66529
UB	177	ASP	GLY	engineered mutation	UNP O66529
UB	191	PHE	ILE	engineered mutation	UNP O66529
UB	193	ASP	VAL	engineered mutation	UNP O66529
UC	1	MET	-	cloning artifact	UNP P03045
UC	2	GLY	-	cloning artifact	UNP P03045
UC	3	ASN	-	cloning artifact	UNP P03045
UC	4	ALA	-	cloning artifact	UNP P03045
UC	5	LYS	-	cloning artifact	UNP P03045
UC	6	THR	-	cloning artifact	UNP P03045
UC	24	ALA	-	linker	UNP P03045
UC	25	GLY	-	linker	UNP P03045
UC	26	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
UC	27	GLY	-	linker	UNP P03045
UC	28	ALA	-	linker	UNP P03045
UC	29	GLY	-	linker	UNP P03045
UC	30	ALA	-	linker	UNP P03045
UC	31	MET	-	linker	UNP P03045
UC	39	ASN	ILE	engineered mutation	UNP O66529
UC	42	VAL	GLU	engineered mutation	UNP O66529
UC	58	VAL	ILE	engineered mutation	UNP O66529
UC	61	ASP	GLY	engineered mutation	UNP O66529
UC	62	ILE	VAL	engineered mutation	UNP O66529
UC	97	TYR	PHE	engineered mutation	UNP O66529
UC	102	GLY	-	linker	UNP O66529
UC	103	THR	-	linker	UNP O66529
UC	104	GLY	-	linker	UNP O66529
UC	105	HIS	-	linker	UNP O66529
UC	106	HIS	-	linker	UNP O66529
UC	107	HIS	-	linker	UNP O66529
UC	108	HIS	-	linker	UNP O66529
UC	109	HIS	-	linker	UNP O66529
UC	110	HIS	-	linker	UNP O66529
UC	111	GLY	-	linker	UNP O66529
UC	112	SER	-	linker	UNP O66529
UC	113	SER	-	linker	UNP O66529
UC	114	ILE	MET	engineered mutation	UNP O66529
UC	115	GLU	GLN	engineered mutation	UNP O66529
UC	138	THR	ALA	engineered mutation	UNP O66529
UC	177	ASP	GLY	engineered mutation	UNP O66529
UC	191	PHE	ILE	engineered mutation	UNP O66529
UC	193	ASP	VAL	engineered mutation	UNP O66529
UD	1	MET	-	cloning artifact	UNP P03045
UD	2	GLY	-	cloning artifact	UNP P03045
UD	3	ASN	-	cloning artifact	UNP P03045
UD	4	ALA	-	cloning artifact	UNP P03045
UD	5	LYS	-	cloning artifact	UNP P03045
UD	6	THR	-	cloning artifact	UNP P03045
UD	24	ALA	-	linker	UNP P03045
UD	25	GLY	-	linker	UNP P03045
UD	26	ALA	-	linker	UNP P03045
UD	27	GLY	-	linker	UNP P03045
UD	28	ALA	-	linker	UNP P03045
UD	29	GLY	-	linker	UNP P03045
UD	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
UD	31	MET	-	linker	UNP P03045
UD	39	ASN	ILE	engineered mutation	UNP O66529
UD	42	VAL	GLU	engineered mutation	UNP O66529
UD	58	VAL	ILE	engineered mutation	UNP O66529
UD	61	ASP	GLY	engineered mutation	UNP O66529
UD	62	ILE	VAL	engineered mutation	UNP O66529
UD	97	TYR	PHE	engineered mutation	UNP O66529
UD	102	GLY	-	linker	UNP O66529
UD	103	THR	-	linker	UNP O66529
UD	104	GLY	-	linker	UNP O66529
UD	105	HIS	-	linker	UNP O66529
UD	106	HIS	-	linker	UNP O66529
UD	107	HIS	-	linker	UNP O66529
UD	108	HIS	-	linker	UNP O66529
UD	109	HIS	-	linker	UNP O66529
UD	110	HIS	-	linker	UNP O66529
UD	111	GLY	-	linker	UNP O66529
UD	112	SER	-	linker	UNP O66529
UD	113	SER	-	linker	UNP O66529
UD	114	ILE	MET	engineered mutation	UNP O66529
UD	115	GLU	GLN	engineered mutation	UNP O66529
UD	138	THR	ALA	engineered mutation	UNP O66529
UD	177	ASP	GLY	engineered mutation	UNP O66529
UD	191	PHE	ILE	engineered mutation	UNP O66529
UD	193	ASP	VAL	engineered mutation	UNP O66529
VA	1	MET	-	cloning artifact	UNP P03045
VA	2	GLY	-	cloning artifact	UNP P03045
VA	3	ASN	-	cloning artifact	UNP P03045
VA	4	ALA	-	cloning artifact	UNP P03045
VA	5	LYS	-	cloning artifact	UNP P03045
VA	6	THR	-	cloning artifact	UNP P03045
VA	24	ALA	-	linker	UNP P03045
VA	25	GLY	-	linker	UNP P03045
VA	26	ALA	-	linker	UNP P03045
VA	27	GLY	-	linker	UNP P03045
VA	28	ALA	-	linker	UNP P03045
VA	29	GLY	-	linker	UNP P03045
VA	30	ALA	-	linker	UNP P03045
VA	31	MET	-	linker	UNP P03045
VA	39	ASN	ILE	engineered mutation	UNP O66529
VA	42	VAL	GLU	engineered mutation	UNP O66529
VA	58	VAL	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
VA	61	ASP	GLY	engineered mutation	UNP O66529
VA	62	ILE	VAL	engineered mutation	UNP O66529
VA	97	TYR	PHE	engineered mutation	UNP O66529
VA	102	GLY	-	linker	UNP O66529
VA	103	THR	-	linker	UNP O66529
VA	104	GLY	-	linker	UNP O66529
VA	105	HIS	-	linker	UNP O66529
VA	106	HIS	-	linker	UNP O66529
VA	107	HIS	-	linker	UNP O66529
VA	108	HIS	-	linker	UNP O66529
VA	109	HIS	-	linker	UNP O66529
VA	110	HIS	-	linker	UNP O66529
VA	111	GLY	-	linker	UNP O66529
VA	112	SER	-	linker	UNP O66529
VA	113	SER	-	linker	UNP O66529
VA	114	ILE	MET	engineered mutation	UNP O66529
VA	115	GLU	GLN	engineered mutation	UNP O66529
VA	138	THR	ALA	engineered mutation	UNP O66529
VA	177	ASP	GLY	engineered mutation	UNP O66529
VA	191	PHE	ILE	engineered mutation	UNP O66529
VA	193	ASP	VAL	engineered mutation	UNP O66529
VB	1	MET	-	cloning artifact	UNP P03045
VB	2	GLY	-	cloning artifact	UNP P03045
VB	3	ASN	-	cloning artifact	UNP P03045
VB	4	ALA	-	cloning artifact	UNP P03045
VB	5	LYS	-	cloning artifact	UNP P03045
VB	6	THR	-	cloning artifact	UNP P03045
VB	24	ALA	-	linker	UNP P03045
VB	25	GLY	-	linker	UNP P03045
VB	26	ALA	-	linker	UNP P03045
VB	27	GLY	-	linker	UNP P03045
VB	28	ALA	-	linker	UNP P03045
VB	29	GLY	-	linker	UNP P03045
VB	30	ALA	-	linker	UNP P03045
VB	31	MET	-	linker	UNP P03045
VB	39	ASN	ILE	engineered mutation	UNP O66529
VB	42	VAL	GLU	engineered mutation	UNP O66529
VB	58	VAL	ILE	engineered mutation	UNP O66529
VB	61	ASP	GLY	engineered mutation	UNP O66529
VB	62	ILE	VAL	engineered mutation	UNP O66529
VB	97	TYR	PHE	engineered mutation	UNP O66529
VB	102	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
VB	103	THR	-	linker	UNP O66529
VB	104	GLY	-	linker	UNP O66529
VB	105	HIS	-	linker	UNP O66529
VB	106	HIS	-	linker	UNP O66529
VB	107	HIS	-	linker	UNP O66529
VB	108	HIS	-	linker	UNP O66529
VB	109	HIS	-	linker	UNP O66529
VB	110	HIS	-	linker	UNP O66529
VB	111	GLY	-	linker	UNP O66529
VB	112	SER	-	linker	UNP O66529
VB	113	SER	-	linker	UNP O66529
VB	114	ILE	MET	engineered mutation	UNP O66529
VB	115	GLU	GLN	engineered mutation	UNP O66529
VB	138	THR	ALA	engineered mutation	UNP O66529
VB	177	ASP	GLY	engineered mutation	UNP O66529
VB	191	PHE	ILE	engineered mutation	UNP O66529
VB	193	ASP	VAL	engineered mutation	UNP O66529
VC	1	MET	-	cloning artifact	UNP P03045
VC	2	GLY	-	cloning artifact	UNP P03045
VC	3	ASN	-	cloning artifact	UNP P03045
VC	4	ALA	-	cloning artifact	UNP P03045
VC	5	LYS	-	cloning artifact	UNP P03045
VC	6	THR	-	cloning artifact	UNP P03045
VC	24	ALA	-	linker	UNP P03045
VC	25	GLY	-	linker	UNP P03045
VC	26	ALA	-	linker	UNP P03045
VC	27	GLY	-	linker	UNP P03045
VC	28	ALA	-	linker	UNP P03045
VC	29	GLY	-	linker	UNP P03045
VC	30	ALA	-	linker	UNP P03045
VC	31	MET	-	linker	UNP P03045
VC	39	ASN	ILE	engineered mutation	UNP O66529
VC	42	VAL	GLU	engineered mutation	UNP O66529
VC	58	VAL	ILE	engineered mutation	UNP O66529
VC	61	ASP	GLY	engineered mutation	UNP O66529
VC	62	ILE	VAL	engineered mutation	UNP O66529
VC	97	TYR	PHE	engineered mutation	UNP O66529
VC	102	GLY	-	linker	UNP O66529
VC	103	THR	-	linker	UNP O66529
VC	104	GLY	-	linker	UNP O66529
VC	105	HIS	-	linker	UNP O66529
VC	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
VC	107	HIS	-	linker	UNP O66529
VC	108	HIS	-	linker	UNP O66529
VC	109	HIS	-	linker	UNP O66529
VC	110	HIS	-	linker	UNP O66529
VC	111	GLY	-	linker	UNP O66529
VC	112	SER	-	linker	UNP O66529
VC	113	SER	-	linker	UNP O66529
VC	114	ILE	MET	engineered mutation	UNP O66529
VC	115	GLU	GLN	engineered mutation	UNP O66529
VC	138	THR	ALA	engineered mutation	UNP O66529
VC	177	ASP	GLY	engineered mutation	UNP O66529
VC	191	PHE	ILE	engineered mutation	UNP O66529
VC	193	ASP	VAL	engineered mutation	UNP O66529
VD	1	MET	-	cloning artifact	UNP P03045
VD	2	GLY	-	cloning artifact	UNP P03045
VD	3	ASN	-	cloning artifact	UNP P03045
VD	4	ALA	-	cloning artifact	UNP P03045
VD	5	LYS	-	cloning artifact	UNP P03045
VD	6	THR	-	cloning artifact	UNP P03045
VD	24	ALA	-	linker	UNP P03045
VD	25	GLY	-	linker	UNP P03045
VD	26	ALA	-	linker	UNP P03045
VD	27	GLY	-	linker	UNP P03045
VD	28	ALA	-	linker	UNP P03045
VD	29	GLY	-	linker	UNP P03045
VD	30	ALA	-	linker	UNP P03045
VD	31	MET	-	linker	UNP P03045
VD	39	ASN	ILE	engineered mutation	UNP O66529
VD	42	VAL	GLU	engineered mutation	UNP O66529
VD	58	VAL	ILE	engineered mutation	UNP O66529
VD	61	ASP	GLY	engineered mutation	UNP O66529
VD	62	ILE	VAL	engineered mutation	UNP O66529
VD	97	TYR	PHE	engineered mutation	UNP O66529
VD	102	GLY	-	linker	UNP O66529
VD	103	THR	-	linker	UNP O66529
VD	104	GLY	-	linker	UNP O66529
VD	105	HIS	-	linker	UNP O66529
VD	106	HIS	-	linker	UNP O66529
VD	107	HIS	-	linker	UNP O66529
VD	108	HIS	-	linker	UNP O66529
VD	109	HIS	-	linker	UNP O66529
VD	110	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
VD	111	GLY	-	linker	UNP O66529
VD	112	SER	-	linker	UNP O66529
VD	113	SER	-	linker	UNP O66529
VD	114	ILE	MET	engineered mutation	UNP O66529
VD	115	GLU	GLN	engineered mutation	UNP O66529
VD	138	THR	ALA	engineered mutation	UNP O66529
VD	177	ASP	GLY	engineered mutation	UNP O66529
VD	191	PHE	ILE	engineered mutation	UNP O66529
VD	193	ASP	VAL	engineered mutation	UNP O66529
WA	1	MET	-	cloning artifact	UNP P03045
WA	2	GLY	-	cloning artifact	UNP P03045
WA	3	ASN	-	cloning artifact	UNP P03045
WA	4	ALA	-	cloning artifact	UNP P03045
WA	5	LYS	-	cloning artifact	UNP P03045
WA	6	THR	-	cloning artifact	UNP P03045
WA	24	ALA	-	linker	UNP P03045
WA	25	GLY	-	linker	UNP P03045
WA	26	ALA	-	linker	UNP P03045
WA	27	GLY	-	linker	UNP P03045
WA	28	ALA	-	linker	UNP P03045
WA	29	GLY	-	linker	UNP P03045
WA	30	ALA	-	linker	UNP P03045
WA	31	MET	-	linker	UNP P03045
WA	39	ASN	ILE	engineered mutation	UNP O66529
WA	42	VAL	GLU	engineered mutation	UNP O66529
WA	58	VAL	ILE	engineered mutation	UNP O66529
WA	61	ASP	GLY	engineered mutation	UNP O66529
WA	62	ILE	VAL	engineered mutation	UNP O66529
WA	97	TYR	PHE	engineered mutation	UNP O66529
WA	102	GLY	-	linker	UNP O66529
WA	103	THR	-	linker	UNP O66529
WA	104	GLY	-	linker	UNP O66529
WA	105	HIS	-	linker	UNP O66529
WA	106	HIS	-	linker	UNP O66529
WA	107	HIS	-	linker	UNP O66529
WA	108	HIS	-	linker	UNP O66529
WA	109	HIS	-	linker	UNP O66529
WA	110	HIS	-	linker	UNP O66529
WA	111	GLY	-	linker	UNP O66529
WA	112	SER	-	linker	UNP O66529
WA	113	SER	-	linker	UNP O66529
WA	114	ILE	MET	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
WA	115	GLU	GLN	engineered mutation	UNP O66529
WA	138	THR	ALA	engineered mutation	UNP O66529
WA	177	ASP	GLY	engineered mutation	UNP O66529
WA	191	PHE	ILE	engineered mutation	UNP O66529
WA	193	ASP	VAL	engineered mutation	UNP O66529
WB	1	MET	-	cloning artifact	UNP P03045
WB	2	GLY	-	cloning artifact	UNP P03045
WB	3	ASN	-	cloning artifact	UNP P03045
WB	4	ALA	-	cloning artifact	UNP P03045
WB	5	LYS	-	cloning artifact	UNP P03045
WB	6	THR	-	cloning artifact	UNP P03045
WB	24	ALA	-	linker	UNP P03045
WB	25	GLY	-	linker	UNP P03045
WB	26	ALA	-	linker	UNP P03045
WB	27	GLY	-	linker	UNP P03045
WB	28	ALA	-	linker	UNP P03045
WB	29	GLY	-	linker	UNP P03045
WB	30	ALA	-	linker	UNP P03045
WB	31	MET	-	linker	UNP P03045
WB	39	ASN	ILE	engineered mutation	UNP O66529
WB	42	VAL	GLU	engineered mutation	UNP O66529
WB	58	VAL	ILE	engineered mutation	UNP O66529
WB	61	ASP	GLY	engineered mutation	UNP O66529
WB	62	ILE	VAL	engineered mutation	UNP O66529
WB	97	TYR	PHE	engineered mutation	UNP O66529
WB	102	GLY	-	linker	UNP O66529
WB	103	THR	-	linker	UNP O66529
WB	104	GLY	-	linker	UNP O66529
WB	105	HIS	-	linker	UNP O66529
WB	106	HIS	-	linker	UNP O66529
WB	107	HIS	-	linker	UNP O66529
WB	108	HIS	-	linker	UNP O66529
WB	109	HIS	-	linker	UNP O66529
WB	110	HIS	-	linker	UNP O66529
WB	111	GLY	-	linker	UNP O66529
WB	112	SER	-	linker	UNP O66529
WB	113	SER	-	linker	UNP O66529
WB	114	ILE	MET	engineered mutation	UNP O66529
WB	115	GLU	GLN	engineered mutation	UNP O66529
WB	138	THR	ALA	engineered mutation	UNP O66529
WB	177	ASP	GLY	engineered mutation	UNP O66529
WB	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
WB	193	ASP	VAL	engineered mutation	UNP O66529
WC	1	MET	-	cloning artifact	UNP P03045
WC	2	GLY	-	cloning artifact	UNP P03045
WC	3	ASN	-	cloning artifact	UNP P03045
WC	4	ALA	-	cloning artifact	UNP P03045
WC	5	LYS	-	cloning artifact	UNP P03045
WC	6	THR	-	cloning artifact	UNP P03045
WC	24	ALA	-	linker	UNP P03045
WC	25	GLY	-	linker	UNP P03045
WC	26	ALA	-	linker	UNP P03045
WC	27	GLY	-	linker	UNP P03045
WC	28	ALA	-	linker	UNP P03045
WC	29	GLY	-	linker	UNP P03045
WC	30	ALA	-	linker	UNP P03045
WC	31	MET	-	linker	UNP P03045
WC	39	ASN	ILE	engineered mutation	UNP O66529
WC	42	VAL	GLU	engineered mutation	UNP O66529
WC	58	VAL	ILE	engineered mutation	UNP O66529
WC	61	ASP	GLY	engineered mutation	UNP O66529
WC	62	ILE	VAL	engineered mutation	UNP O66529
WC	97	TYR	PHE	engineered mutation	UNP O66529
WC	102	GLY	-	linker	UNP O66529
WC	103	THR	-	linker	UNP O66529
WC	104	GLY	-	linker	UNP O66529
WC	105	HIS	-	linker	UNP O66529
WC	106	HIS	-	linker	UNP O66529
WC	107	HIS	-	linker	UNP O66529
WC	108	HIS	-	linker	UNP O66529
WC	109	HIS	-	linker	UNP O66529
WC	110	HIS	-	linker	UNP O66529
WC	111	GLY	-	linker	UNP O66529
WC	112	SER	-	linker	UNP O66529
WC	113	SER	-	linker	UNP O66529
WC	114	ILE	MET	engineered mutation	UNP O66529
WC	115	GLU	GLN	engineered mutation	UNP O66529
WC	138	THR	ALA	engineered mutation	UNP O66529
WC	177	ASP	GLY	engineered mutation	UNP O66529
WC	191	PHE	ILE	engineered mutation	UNP O66529
WC	193	ASP	VAL	engineered mutation	UNP O66529
WD	1	MET	-	cloning artifact	UNP P03045
WD	2	GLY	-	cloning artifact	UNP P03045
WD	3	ASN	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
WD	4	ALA	-	cloning artifact	UNP P03045
WD	5	LYS	-	cloning artifact	UNP P03045
WD	6	THR	-	cloning artifact	UNP P03045
WD	24	ALA	-	linker	UNP P03045
WD	25	GLY	-	linker	UNP P03045
WD	26	ALA	-	linker	UNP P03045
WD	27	GLY	-	linker	UNP P03045
WD	28	ALA	-	linker	UNP P03045
WD	29	GLY	-	linker	UNP P03045
WD	30	ALA	-	linker	UNP P03045
WD	31	MET	-	linker	UNP P03045
WD	39	ASN	ILE	engineered mutation	UNP O66529
WD	42	VAL	GLU	engineered mutation	UNP O66529
WD	58	VAL	ILE	engineered mutation	UNP O66529
WD	61	ASP	GLY	engineered mutation	UNP O66529
WD	62	ILE	VAL	engineered mutation	UNP O66529
WD	97	TYR	PHE	engineered mutation	UNP O66529
WD	102	GLY	-	linker	UNP O66529
WD	103	THR	-	linker	UNP O66529
WD	104	GLY	-	linker	UNP O66529
WD	105	HIS	-	linker	UNP O66529
WD	106	HIS	-	linker	UNP O66529
WD	107	HIS	-	linker	UNP O66529
WD	108	HIS	-	linker	UNP O66529
WD	109	HIS	-	linker	UNP O66529
WD	110	HIS	-	linker	UNP O66529
WD	111	GLY	-	linker	UNP O66529
WD	112	SER	-	linker	UNP O66529
WD	113	SER	-	linker	UNP O66529
WD	114	ILE	MET	engineered mutation	UNP O66529
WD	115	GLU	GLN	engineered mutation	UNP O66529
WD	138	THR	ALA	engineered mutation	UNP O66529
WD	177	ASP	GLY	engineered mutation	UNP O66529
WD	191	PHE	ILE	engineered mutation	UNP O66529
WD	193	ASP	VAL	engineered mutation	UNP O66529
XA	1	MET	-	cloning artifact	UNP P03045
XA	2	GLY	-	cloning artifact	UNP P03045
XA	3	ASN	-	cloning artifact	UNP P03045
XA	4	ALA	-	cloning artifact	UNP P03045
XA	5	LYS	-	cloning artifact	UNP P03045
XA	6	THR	-	cloning artifact	UNP P03045
XA	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
XA	25	GLY	-	linker	UNP P03045
XA	26	ALA	-	linker	UNP P03045
XA	27	GLY	-	linker	UNP P03045
XA	28	ALA	-	linker	UNP P03045
XA	29	GLY	-	linker	UNP P03045
XA	30	ALA	-	linker	UNP P03045
XA	31	MET	-	linker	UNP P03045
XA	39	ASN	ILE	engineered mutation	UNP O66529
XA	42	VAL	GLU	engineered mutation	UNP O66529
XA	58	VAL	ILE	engineered mutation	UNP O66529
XA	61	ASP	GLY	engineered mutation	UNP O66529
XA	62	ILE	VAL	engineered mutation	UNP O66529
XA	97	TYR	PHE	engineered mutation	UNP O66529
XA	102	GLY	-	linker	UNP O66529
XA	103	THR	-	linker	UNP O66529
XA	104	GLY	-	linker	UNP O66529
XA	105	HIS	-	linker	UNP O66529
XA	106	HIS	-	linker	UNP O66529
XA	107	HIS	-	linker	UNP O66529
XA	108	HIS	-	linker	UNP O66529
XA	109	HIS	-	linker	UNP O66529
XA	110	HIS	-	linker	UNP O66529
XA	111	GLY	-	linker	UNP O66529
XA	112	SER	-	linker	UNP O66529
XA	113	SER	-	linker	UNP O66529
XA	114	ILE	MET	engineered mutation	UNP O66529
XA	115	GLU	GLN	engineered mutation	UNP O66529
XA	138	THR	ALA	engineered mutation	UNP O66529
XA	177	ASP	GLY	engineered mutation	UNP O66529
XA	191	PHE	ILE	engineered mutation	UNP O66529
XA	193	ASP	VAL	engineered mutation	UNP O66529
XB	1	MET	-	cloning artifact	UNP P03045
XB	2	GLY	-	cloning artifact	UNP P03045
XB	3	ASN	-	cloning artifact	UNP P03045
XB	4	ALA	-	cloning artifact	UNP P03045
XB	5	LYS	-	cloning artifact	UNP P03045
XB	6	THR	-	cloning artifact	UNP P03045
XB	24	ALA	-	linker	UNP P03045
XB	25	GLY	-	linker	UNP P03045
XB	26	ALA	-	linker	UNP P03045
XB	27	GLY	-	linker	UNP P03045
XB	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
XB	29	GLY	-	linker	UNP P03045
XB	30	ALA	-	linker	UNP P03045
XB	31	MET	-	linker	UNP P03045
XB	39	ASN	ILE	engineered mutation	UNP O66529
XB	42	VAL	GLU	engineered mutation	UNP O66529
XB	58	VAL	ILE	engineered mutation	UNP O66529
XB	61	ASP	GLY	engineered mutation	UNP O66529
XB	62	ILE	VAL	engineered mutation	UNP O66529
XB	97	TYR	PHE	engineered mutation	UNP O66529
XB	102	GLY	-	linker	UNP O66529
XB	103	THR	-	linker	UNP O66529
XB	104	GLY	-	linker	UNP O66529
XB	105	HIS	-	linker	UNP O66529
XB	106	HIS	-	linker	UNP O66529
XB	107	HIS	-	linker	UNP O66529
XB	108	HIS	-	linker	UNP O66529
XB	109	HIS	-	linker	UNP O66529
XB	110	HIS	-	linker	UNP O66529
XB	111	GLY	-	linker	UNP O66529
XB	112	SER	-	linker	UNP O66529
XB	113	SER	-	linker	UNP O66529
XB	114	ILE	MET	engineered mutation	UNP O66529
XB	115	GLU	GLN	engineered mutation	UNP O66529
XB	138	THR	ALA	engineered mutation	UNP O66529
XB	177	ASP	GLY	engineered mutation	UNP O66529
XB	191	PHE	ILE	engineered mutation	UNP O66529
XB	193	ASP	VAL	engineered mutation	UNP O66529
XC	1	MET	-	cloning artifact	UNP P03045
XC	2	GLY	-	cloning artifact	UNP P03045
XC	3	ASN	-	cloning artifact	UNP P03045
XC	4	ALA	-	cloning artifact	UNP P03045
XC	5	LYS	-	cloning artifact	UNP P03045
XC	6	THR	-	cloning artifact	UNP P03045
XC	24	ALA	-	linker	UNP P03045
XC	25	GLY	-	linker	UNP P03045
XC	26	ALA	-	linker	UNP P03045
XC	27	GLY	-	linker	UNP P03045
XC	28	ALA	-	linker	UNP P03045
XC	29	GLY	-	linker	UNP P03045
XC	30	ALA	-	linker	UNP P03045
XC	31	MET	-	linker	UNP P03045
XC	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
XC	42	VAL	GLU	engineered mutation	UNP O66529
XC	58	VAL	ILE	engineered mutation	UNP O66529
XC	61	ASP	GLY	engineered mutation	UNP O66529
XC	62	ILE	VAL	engineered mutation	UNP O66529
XC	97	TYR	PHE	engineered mutation	UNP O66529
XC	102	GLY	-	linker	UNP O66529
XC	103	THR	-	linker	UNP O66529
XC	104	GLY	-	linker	UNP O66529
XC	105	HIS	-	linker	UNP O66529
XC	106	HIS	-	linker	UNP O66529
XC	107	HIS	-	linker	UNP O66529
XC	108	HIS	-	linker	UNP O66529
XC	109	HIS	-	linker	UNP O66529
XC	110	HIS	-	linker	UNP O66529
XC	111	GLY	-	linker	UNP O66529
XC	112	SER	-	linker	UNP O66529
XC	113	SER	-	linker	UNP O66529
XC	114	ILE	MET	engineered mutation	UNP O66529
XC	115	GLU	GLN	engineered mutation	UNP O66529
XC	138	THR	ALA	engineered mutation	UNP O66529
XC	177	ASP	GLY	engineered mutation	UNP O66529
XC	191	PHE	ILE	engineered mutation	UNP O66529
XC	193	ASP	VAL	engineered mutation	UNP O66529
XD	1	MET	-	cloning artifact	UNP P03045
XD	2	GLY	-	cloning artifact	UNP P03045
XD	3	ASN	-	cloning artifact	UNP P03045
XD	4	ALA	-	cloning artifact	UNP P03045
XD	5	LYS	-	cloning artifact	UNP P03045
XD	6	THR	-	cloning artifact	UNP P03045
XD	24	ALA	-	linker	UNP P03045
XD	25	GLY	-	linker	UNP P03045
XD	26	ALA	-	linker	UNP P03045
XD	27	GLY	-	linker	UNP P03045
XD	28	ALA	-	linker	UNP P03045
XD	29	GLY	-	linker	UNP P03045
XD	30	ALA	-	linker	UNP P03045
XD	31	MET	-	linker	UNP P03045
XD	39	ASN	ILE	engineered mutation	UNP O66529
XD	42	VAL	GLU	engineered mutation	UNP O66529
XD	58	VAL	ILE	engineered mutation	UNP O66529
XD	61	ASP	GLY	engineered mutation	UNP O66529
XD	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
XD	97	TYR	PHE	engineered mutation	UNP O66529
XD	102	GLY	-	linker	UNP O66529
XD	103	THR	-	linker	UNP O66529
XD	104	GLY	-	linker	UNP O66529
XD	105	HIS	-	linker	UNP O66529
XD	106	HIS	-	linker	UNP O66529
XD	107	HIS	-	linker	UNP O66529
XD	108	HIS	-	linker	UNP O66529
XD	109	HIS	-	linker	UNP O66529
XD	110	HIS	-	linker	UNP O66529
XD	111	GLY	-	linker	UNP O66529
XD	112	SER	-	linker	UNP O66529
XD	113	SER	-	linker	UNP O66529
XD	114	ILE	MET	engineered mutation	UNP O66529
XD	115	GLU	GLN	engineered mutation	UNP O66529
XD	138	THR	ALA	engineered mutation	UNP O66529
XD	177	ASP	GLY	engineered mutation	UNP O66529
XD	191	PHE	ILE	engineered mutation	UNP O66529
XD	193	ASP	VAL	engineered mutation	UNP O66529
YA	1	MET	-	cloning artifact	UNP P03045
YA	2	GLY	-	cloning artifact	UNP P03045
YA	3	ASN	-	cloning artifact	UNP P03045
YA	4	ALA	-	cloning artifact	UNP P03045
YA	5	LYS	-	cloning artifact	UNP P03045
YA	6	THR	-	cloning artifact	UNP P03045
YA	24	ALA	-	linker	UNP P03045
YA	25	GLY	-	linker	UNP P03045
YA	26	ALA	-	linker	UNP P03045
YA	27	GLY	-	linker	UNP P03045
YA	28	ALA	-	linker	UNP P03045
YA	29	GLY	-	linker	UNP P03045
YA	30	ALA	-	linker	UNP P03045
YA	31	MET	-	linker	UNP P03045
YA	39	ASN	ILE	engineered mutation	UNP O66529
YA	42	VAL	GLU	engineered mutation	UNP O66529
YA	58	VAL	ILE	engineered mutation	UNP O66529
YA	61	ASP	GLY	engineered mutation	UNP O66529
YA	62	ILE	VAL	engineered mutation	UNP O66529
YA	97	TYR	PHE	engineered mutation	UNP O66529
YA	102	GLY	-	linker	UNP O66529
YA	103	THR	-	linker	UNP O66529
YA	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
YA	105	HIS	-	linker	UNP O66529
YA	106	HIS	-	linker	UNP O66529
YA	107	HIS	-	linker	UNP O66529
YA	108	HIS	-	linker	UNP O66529
YA	109	HIS	-	linker	UNP O66529
YA	110	HIS	-	linker	UNP O66529
YA	111	GLY	-	linker	UNP O66529
YA	112	SER	-	linker	UNP O66529
YA	113	SER	-	linker	UNP O66529
YA	114	ILE	MET	engineered mutation	UNP O66529
YA	115	GLU	GLN	engineered mutation	UNP O66529
YA	138	THR	ALA	engineered mutation	UNP O66529
YA	177	ASP	GLY	engineered mutation	UNP O66529
YA	191	PHE	ILE	engineered mutation	UNP O66529
YA	193	ASP	VAL	engineered mutation	UNP O66529
YB	1	MET	-	cloning artifact	UNP P03045
YB	2	GLY	-	cloning artifact	UNP P03045
YB	3	ASN	-	cloning artifact	UNP P03045
YB	4	ALA	-	cloning artifact	UNP P03045
YB	5	LYS	-	cloning artifact	UNP P03045
YB	6	THR	-	cloning artifact	UNP P03045
YB	24	ALA	-	linker	UNP P03045
YB	25	GLY	-	linker	UNP P03045
YB	26	ALA	-	linker	UNP P03045
YB	27	GLY	-	linker	UNP P03045
YB	28	ALA	-	linker	UNP P03045
YB	29	GLY	-	linker	UNP P03045
YB	30	ALA	-	linker	UNP P03045
YB	31	MET	-	linker	UNP P03045
YB	39	ASN	ILE	engineered mutation	UNP O66529
YB	42	VAL	GLU	engineered mutation	UNP O66529
YB	58	VAL	ILE	engineered mutation	UNP O66529
YB	61	ASP	GLY	engineered mutation	UNP O66529
YB	62	ILE	VAL	engineered mutation	UNP O66529
YB	97	TYR	PHE	engineered mutation	UNP O66529
YB	102	GLY	-	linker	UNP O66529
YB	103	THR	-	linker	UNP O66529
YB	104	GLY	-	linker	UNP O66529
YB	105	HIS	-	linker	UNP O66529
YB	106	HIS	-	linker	UNP O66529
YB	107	HIS	-	linker	UNP O66529
YB	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
YB	109	HIS	-	linker	UNP O66529
YB	110	HIS	-	linker	UNP O66529
YB	111	GLY	-	linker	UNP O66529
YB	112	SER	-	linker	UNP O66529
YB	113	SER	-	linker	UNP O66529
YB	114	ILE	MET	engineered mutation	UNP O66529
YB	115	GLU	GLN	engineered mutation	UNP O66529
YB	138	THR	ALA	engineered mutation	UNP O66529
YB	177	ASP	GLY	engineered mutation	UNP O66529
YB	191	PHE	ILE	engineered mutation	UNP O66529
YB	193	ASP	VAL	engineered mutation	UNP O66529
YC	1	MET	-	cloning artifact	UNP P03045
YC	2	GLY	-	cloning artifact	UNP P03045
YC	3	ASN	-	cloning artifact	UNP P03045
YC	4	ALA	-	cloning artifact	UNP P03045
YC	5	LYS	-	cloning artifact	UNP P03045
YC	6	THR	-	cloning artifact	UNP P03045
YC	24	ALA	-	linker	UNP P03045
YC	25	GLY	-	linker	UNP P03045
YC	26	ALA	-	linker	UNP P03045
YC	27	GLY	-	linker	UNP P03045
YC	28	ALA	-	linker	UNP P03045
YC	29	GLY	-	linker	UNP P03045
YC	30	ALA	-	linker	UNP P03045
YC	31	MET	-	linker	UNP P03045
YC	39	ASN	ILE	engineered mutation	UNP O66529
YC	42	VAL	GLU	engineered mutation	UNP O66529
YC	58	VAL	ILE	engineered mutation	UNP O66529
YC	61	ASP	GLY	engineered mutation	UNP O66529
YC	62	ILE	VAL	engineered mutation	UNP O66529
YC	97	TYR	PHE	engineered mutation	UNP O66529
YC	102	GLY	-	linker	UNP O66529
YC	103	THR	-	linker	UNP O66529
YC	104	GLY	-	linker	UNP O66529
YC	105	HIS	-	linker	UNP O66529
YC	106	HIS	-	linker	UNP O66529
YC	107	HIS	-	linker	UNP O66529
YC	108	HIS	-	linker	UNP O66529
YC	109	HIS	-	linker	UNP O66529
YC	110	HIS	-	linker	UNP O66529
YC	111	GLY	-	linker	UNP O66529
YC	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
YC	113	SER	-	linker	UNP O66529
YC	114	ILE	MET	engineered mutation	UNP O66529
YC	115	GLU	GLN	engineered mutation	UNP O66529
YC	138	THR	ALA	engineered mutation	UNP O66529
YC	177	ASP	GLY	engineered mutation	UNP O66529
YC	191	PHE	ILE	engineered mutation	UNP O66529
YC	193	ASP	VAL	engineered mutation	UNP O66529
YD	1	MET	-	cloning artifact	UNP P03045
YD	2	GLY	-	cloning artifact	UNP P03045
YD	3	ASN	-	cloning artifact	UNP P03045
YD	4	ALA	-	cloning artifact	UNP P03045
YD	5	LYS	-	cloning artifact	UNP P03045
YD	6	THR	-	cloning artifact	UNP P03045
YD	24	ALA	-	linker	UNP P03045
YD	25	GLY	-	linker	UNP P03045
YD	26	ALA	-	linker	UNP P03045
YD	27	GLY	-	linker	UNP P03045
YD	28	ALA	-	linker	UNP P03045
YD	29	GLY	-	linker	UNP P03045
YD	30	ALA	-	linker	UNP P03045
YD	31	MET	-	linker	UNP P03045
YD	39	ASN	ILE	engineered mutation	UNP O66529
YD	42	VAL	GLU	engineered mutation	UNP O66529
YD	58	VAL	ILE	engineered mutation	UNP O66529
YD	61	ASP	GLY	engineered mutation	UNP O66529
YD	62	ILE	VAL	engineered mutation	UNP O66529
YD	97	TYR	PHE	engineered mutation	UNP O66529
YD	102	GLY	-	linker	UNP O66529
YD	103	THR	-	linker	UNP O66529
YD	104	GLY	-	linker	UNP O66529
YD	105	HIS	-	linker	UNP O66529
YD	106	HIS	-	linker	UNP O66529
YD	107	HIS	-	linker	UNP O66529
YD	108	HIS	-	linker	UNP O66529
YD	109	HIS	-	linker	UNP O66529
YD	110	HIS	-	linker	UNP O66529
YD	111	GLY	-	linker	UNP O66529
YD	112	SER	-	linker	UNP O66529
YD	113	SER	-	linker	UNP O66529
YD	114	ILE	MET	engineered mutation	UNP O66529
YD	115	GLU	GLN	engineered mutation	UNP O66529
YD	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
YD	177	ASP	GLY	engineered mutation	UNP O66529
YD	191	PHE	ILE	engineered mutation	UNP O66529
YD	193	ASP	VAL	engineered mutation	UNP O66529
ZA	1	MET	-	cloning artifact	UNP P03045
ZA	2	GLY	-	cloning artifact	UNP P03045
ZA	3	ASN	-	cloning artifact	UNP P03045
ZA	4	ALA	-	cloning artifact	UNP P03045
ZA	5	LYS	-	cloning artifact	UNP P03045
ZA	6	THR	-	cloning artifact	UNP P03045
ZA	24	ALA	-	linker	UNP P03045
ZA	25	GLY	-	linker	UNP P03045
ZA	26	ALA	-	linker	UNP P03045
ZA	27	GLY	-	linker	UNP P03045
ZA	28	ALA	-	linker	UNP P03045
ZA	29	GLY	-	linker	UNP P03045
ZA	30	ALA	-	linker	UNP P03045
ZA	31	MET	-	linker	UNP P03045
ZA	39	ASN	ILE	engineered mutation	UNP O66529
ZA	42	VAL	GLU	engineered mutation	UNP O66529
ZA	58	VAL	ILE	engineered mutation	UNP O66529
ZA	61	ASP	GLY	engineered mutation	UNP O66529
ZA	62	ILE	VAL	engineered mutation	UNP O66529
ZA	97	TYR	PHE	engineered mutation	UNP O66529
ZA	102	GLY	-	linker	UNP O66529
ZA	103	THR	-	linker	UNP O66529
ZA	104	GLY	-	linker	UNP O66529
ZA	105	HIS	-	linker	UNP O66529
ZA	106	HIS	-	linker	UNP O66529
ZA	107	HIS	-	linker	UNP O66529
ZA	108	HIS	-	linker	UNP O66529
ZA	109	HIS	-	linker	UNP O66529
ZA	110	HIS	-	linker	UNP O66529
ZA	111	GLY	-	linker	UNP O66529
ZA	112	SER	-	linker	UNP O66529
ZA	113	SER	-	linker	UNP O66529
ZA	114	ILE	MET	engineered mutation	UNP O66529
ZA	115	GLU	GLN	engineered mutation	UNP O66529
ZA	138	THR	ALA	engineered mutation	UNP O66529
ZA	177	ASP	GLY	engineered mutation	UNP O66529
ZA	191	PHE	ILE	engineered mutation	UNP O66529
ZA	193	ASP	VAL	engineered mutation	UNP O66529
ZB	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
ZB	2	GLY	-	cloning artifact	UNP P03045
ZB	3	ASN	-	cloning artifact	UNP P03045
ZB	4	ALA	-	cloning artifact	UNP P03045
ZB	5	LYS	-	cloning artifact	UNP P03045
ZB	6	THR	-	cloning artifact	UNP P03045
ZB	24	ALA	-	linker	UNP P03045
ZB	25	GLY	-	linker	UNP P03045
ZB	26	ALA	-	linker	UNP P03045
ZB	27	GLY	-	linker	UNP P03045
ZB	28	ALA	-	linker	UNP P03045
ZB	29	GLY	-	linker	UNP P03045
ZB	30	ALA	-	linker	UNP P03045
ZB	31	MET	-	linker	UNP P03045
ZB	39	ASN	ILE	engineered mutation	UNP O66529
ZB	42	VAL	GLU	engineered mutation	UNP O66529
ZB	58	VAL	ILE	engineered mutation	UNP O66529
ZB	61	ASP	GLY	engineered mutation	UNP O66529
ZB	62	ILE	VAL	engineered mutation	UNP O66529
ZB	97	TYR	PHE	engineered mutation	UNP O66529
ZB	102	GLY	-	linker	UNP O66529
ZB	103	THR	-	linker	UNP O66529
ZB	104	GLY	-	linker	UNP O66529
ZB	105	HIS	-	linker	UNP O66529
ZB	106	HIS	-	linker	UNP O66529
ZB	107	HIS	-	linker	UNP O66529
ZB	108	HIS	-	linker	UNP O66529
ZB	109	HIS	-	linker	UNP O66529
ZB	110	HIS	-	linker	UNP O66529
ZB	111	GLY	-	linker	UNP O66529
ZB	112	SER	-	linker	UNP O66529
ZB	113	SER	-	linker	UNP O66529
ZB	114	ILE	MET	engineered mutation	UNP O66529
ZB	115	GLU	GLN	engineered mutation	UNP O66529
ZB	138	THR	ALA	engineered mutation	UNP O66529
ZB	177	ASP	GLY	engineered mutation	UNP O66529
ZB	191	PHE	ILE	engineered mutation	UNP O66529
ZB	193	ASP	VAL	engineered mutation	UNP O66529
ZC	1	MET	-	cloning artifact	UNP P03045
ZC	2	GLY	-	cloning artifact	UNP P03045
ZC	3	ASN	-	cloning artifact	UNP P03045
ZC	4	ALA	-	cloning artifact	UNP P03045
ZC	5	LYS	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
ZC	6	THR	-	cloning artifact	UNP P03045
ZC	24	ALA	-	linker	UNP P03045
ZC	25	GLY	-	linker	UNP P03045
ZC	26	ALA	-	linker	UNP P03045
ZC	27	GLY	-	linker	UNP P03045
ZC	28	ALA	-	linker	UNP P03045
ZC	29	GLY	-	linker	UNP P03045
ZC	30	ALA	-	linker	UNP P03045
ZC	31	MET	-	linker	UNP P03045
ZC	39	ASN	ILE	engineered mutation	UNP O66529
ZC	42	VAL	GLU	engineered mutation	UNP O66529
ZC	58	VAL	ILE	engineered mutation	UNP O66529
ZC	61	ASP	GLY	engineered mutation	UNP O66529
ZC	62	ILE	VAL	engineered mutation	UNP O66529
ZC	97	TYR	PHE	engineered mutation	UNP O66529
ZC	102	GLY	-	linker	UNP O66529
ZC	103	THR	-	linker	UNP O66529
ZC	104	GLY	-	linker	UNP O66529
ZC	105	HIS	-	linker	UNP O66529
ZC	106	HIS	-	linker	UNP O66529
ZC	107	HIS	-	linker	UNP O66529
ZC	108	HIS	-	linker	UNP O66529
ZC	109	HIS	-	linker	UNP O66529
ZC	110	HIS	-	linker	UNP O66529
ZC	111	GLY	-	linker	UNP O66529
ZC	112	SER	-	linker	UNP O66529
ZC	113	SER	-	linker	UNP O66529
ZC	114	ILE	MET	engineered mutation	UNP O66529
ZC	115	GLU	GLN	engineered mutation	UNP O66529
ZC	138	THR	ALA	engineered mutation	UNP O66529
ZC	177	ASP	GLY	engineered mutation	UNP O66529
ZC	191	PHE	ILE	engineered mutation	UNP O66529
ZC	193	ASP	VAL	engineered mutation	UNP O66529
ZD	1	MET	-	cloning artifact	UNP P03045
ZD	2	GLY	-	cloning artifact	UNP P03045
ZD	3	ASN	-	cloning artifact	UNP P03045
ZD	4	ALA	-	cloning artifact	UNP P03045
ZD	5	LYS	-	cloning artifact	UNP P03045
ZD	6	THR	-	cloning artifact	UNP P03045
ZD	24	ALA	-	linker	UNP P03045
ZD	25	GLY	-	linker	UNP P03045
ZD	26	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
ZD	27	GLY	-	linker	UNP P03045
ZD	28	ALA	-	linker	UNP P03045
ZD	29	GLY	-	linker	UNP P03045
ZD	30	ALA	-	linker	UNP P03045
ZD	31	MET	-	linker	UNP P03045
ZD	39	ASN	ILE	engineered mutation	UNP O66529
ZD	42	VAL	GLU	engineered mutation	UNP O66529
ZD	58	VAL	ILE	engineered mutation	UNP O66529
ZD	61	ASP	GLY	engineered mutation	UNP O66529
ZD	62	ILE	VAL	engineered mutation	UNP O66529
ZD	97	TYR	PHE	engineered mutation	UNP O66529
ZD	102	GLY	-	linker	UNP O66529
ZD	103	THR	-	linker	UNP O66529
ZD	104	GLY	-	linker	UNP O66529
ZD	105	HIS	-	linker	UNP O66529
ZD	106	HIS	-	linker	UNP O66529
ZD	107	HIS	-	linker	UNP O66529
ZD	108	HIS	-	linker	UNP O66529
ZD	109	HIS	-	linker	UNP O66529
ZD	110	HIS	-	linker	UNP O66529
ZD	111	GLY	-	linker	UNP O66529
ZD	112	SER	-	linker	UNP O66529
ZD	113	SER	-	linker	UNP O66529
ZD	114	ILE	MET	engineered mutation	UNP O66529
ZD	115	GLU	GLN	engineered mutation	UNP O66529
ZD	138	THR	ALA	engineered mutation	UNP O66529
ZD	177	ASP	GLY	engineered mutation	UNP O66529
ZD	191	PHE	ILE	engineered mutation	UNP O66529
ZD	193	ASP	VAL	engineered mutation	UNP O66529
aA	1	MET	-	cloning artifact	UNP P03045
aA	2	GLY	-	cloning artifact	UNP P03045
aA	3	ASN	-	cloning artifact	UNP P03045
aA	4	ALA	-	cloning artifact	UNP P03045
aA	5	LYS	-	cloning artifact	UNP P03045
aA	6	THR	-	cloning artifact	UNP P03045
aA	24	ALA	-	linker	UNP P03045
aA	25	GLY	-	linker	UNP P03045
aA	26	ALA	-	linker	UNP P03045
aA	27	GLY	-	linker	UNP P03045
aA	28	ALA	-	linker	UNP P03045
aA	29	GLY	-	linker	UNP P03045
aA	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
aA	31	MET	-	linker	UNP P03045
aA	39	ASN	ILE	engineered mutation	UNP O66529
aA	42	VAL	GLU	engineered mutation	UNP O66529
aA	58	VAL	ILE	engineered mutation	UNP O66529
aA	61	ASP	GLY	engineered mutation	UNP O66529
aA	62	ILE	VAL	engineered mutation	UNP O66529
aA	97	TYR	PHE	engineered mutation	UNP O66529
aA	102	GLY	-	linker	UNP O66529
aA	103	THR	-	linker	UNP O66529
aA	104	GLY	-	linker	UNP O66529
aA	105	HIS	-	linker	UNP O66529
aA	106	HIS	-	linker	UNP O66529
aA	107	HIS	-	linker	UNP O66529
aA	108	HIS	-	linker	UNP O66529
aA	109	HIS	-	linker	UNP O66529
aA	110	HIS	-	linker	UNP O66529
aA	111	GLY	-	linker	UNP O66529
aA	112	SER	-	linker	UNP O66529
aA	113	SER	-	linker	UNP O66529
aA	114	ILE	MET	engineered mutation	UNP O66529
aA	115	GLU	GLN	engineered mutation	UNP O66529
aA	138	THR	ALA	engineered mutation	UNP O66529
aA	177	ASP	GLY	engineered mutation	UNP O66529
aA	191	PHE	ILE	engineered mutation	UNP O66529
aA	193	ASP	VAL	engineered mutation	UNP O66529
aB	1	MET	-	cloning artifact	UNP P03045
aB	2	GLY	-	cloning artifact	UNP P03045
aB	3	ASN	-	cloning artifact	UNP P03045
aB	4	ALA	-	cloning artifact	UNP P03045
aB	5	LYS	-	cloning artifact	UNP P03045
aB	6	THR	-	cloning artifact	UNP P03045
aB	24	ALA	-	linker	UNP P03045
aB	25	GLY	-	linker	UNP P03045
aB	26	ALA	-	linker	UNP P03045
aB	27	GLY	-	linker	UNP P03045
aB	28	ALA	-	linker	UNP P03045
aB	29	GLY	-	linker	UNP P03045
aB	30	ALA	-	linker	UNP P03045
aB	31	MET	-	linker	UNP P03045
aB	39	ASN	ILE	engineered mutation	UNP O66529
aB	42	VAL	GLU	engineered mutation	UNP O66529
aB	58	VAL	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
aB	61	ASP	GLY	engineered mutation	UNP O66529
aB	62	ILE	VAL	engineered mutation	UNP O66529
aB	97	TYR	PHE	engineered mutation	UNP O66529
aB	102	GLY	-	linker	UNP O66529
aB	103	THR	-	linker	UNP O66529
aB	104	GLY	-	linker	UNP O66529
aB	105	HIS	-	linker	UNP O66529
aB	106	HIS	-	linker	UNP O66529
aB	107	HIS	-	linker	UNP O66529
aB	108	HIS	-	linker	UNP O66529
aB	109	HIS	-	linker	UNP O66529
aB	110	HIS	-	linker	UNP O66529
aB	111	GLY	-	linker	UNP O66529
aB	112	SER	-	linker	UNP O66529
aB	113	SER	-	linker	UNP O66529
aB	114	ILE	MET	engineered mutation	UNP O66529
aB	115	GLU	GLN	engineered mutation	UNP O66529
aB	138	THR	ALA	engineered mutation	UNP O66529
aB	177	ASP	GLY	engineered mutation	UNP O66529
aB	191	PHE	ILE	engineered mutation	UNP O66529
aB	193	ASP	VAL	engineered mutation	UNP O66529
aC	1	MET	-	cloning artifact	UNP P03045
aC	2	GLY	-	cloning artifact	UNP P03045
aC	3	ASN	-	cloning artifact	UNP P03045
aC	4	ALA	-	cloning artifact	UNP P03045
aC	5	LYS	-	cloning artifact	UNP P03045
aC	6	THR	-	cloning artifact	UNP P03045
aC	24	ALA	-	linker	UNP P03045
aC	25	GLY	-	linker	UNP P03045
aC	26	ALA	-	linker	UNP P03045
aC	27	GLY	-	linker	UNP P03045
aC	28	ALA	-	linker	UNP P03045
aC	29	GLY	-	linker	UNP P03045
aC	30	ALA	-	linker	UNP P03045
aC	31	MET	-	linker	UNP P03045
aC	39	ASN	ILE	engineered mutation	UNP O66529
aC	42	VAL	GLU	engineered mutation	UNP O66529
aC	58	VAL	ILE	engineered mutation	UNP O66529
aC	61	ASP	GLY	engineered mutation	UNP O66529
aC	62	ILE	VAL	engineered mutation	UNP O66529
aC	97	TYR	PHE	engineered mutation	UNP O66529
aC	102	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
aC	103	THR	-	linker	UNP O66529
aC	104	GLY	-	linker	UNP O66529
aC	105	HIS	-	linker	UNP O66529
aC	106	HIS	-	linker	UNP O66529
aC	107	HIS	-	linker	UNP O66529
aC	108	HIS	-	linker	UNP O66529
aC	109	HIS	-	linker	UNP O66529
aC	110	HIS	-	linker	UNP O66529
aC	111	GLY	-	linker	UNP O66529
aC	112	SER	-	linker	UNP O66529
aC	113	SER	-	linker	UNP O66529
aC	114	ILE	MET	engineered mutation	UNP O66529
aC	115	GLU	GLN	engineered mutation	UNP O66529
aC	138	THR	ALA	engineered mutation	UNP O66529
aC	177	ASP	GLY	engineered mutation	UNP O66529
aC	191	PHE	ILE	engineered mutation	UNP O66529
aC	193	ASP	VAL	engineered mutation	UNP O66529
aD	1	MET	-	cloning artifact	UNP P03045
aD	2	GLY	-	cloning artifact	UNP P03045
aD	3	ASN	-	cloning artifact	UNP P03045
aD	4	ALA	-	cloning artifact	UNP P03045
aD	5	LYS	-	cloning artifact	UNP P03045
aD	6	THR	-	cloning artifact	UNP P03045
aD	24	ALA	-	linker	UNP P03045
aD	25	GLY	-	linker	UNP P03045
aD	26	ALA	-	linker	UNP P03045
aD	27	GLY	-	linker	UNP P03045
aD	28	ALA	-	linker	UNP P03045
aD	29	GLY	-	linker	UNP P03045
aD	30	ALA	-	linker	UNP P03045
aD	31	MET	-	linker	UNP P03045
aD	39	ASN	ILE	engineered mutation	UNP O66529
aD	42	VAL	GLU	engineered mutation	UNP O66529
aD	58	VAL	ILE	engineered mutation	UNP O66529
aD	61	ASP	GLY	engineered mutation	UNP O66529
aD	62	ILE	VAL	engineered mutation	UNP O66529
aD	97	TYR	PHE	engineered mutation	UNP O66529
aD	102	GLY	-	linker	UNP O66529
aD	103	THR	-	linker	UNP O66529
aD	104	GLY	-	linker	UNP O66529
aD	105	HIS	-	linker	UNP O66529
aD	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
aD	107	HIS	-	linker	UNP O66529
aD	108	HIS	-	linker	UNP O66529
aD	109	HIS	-	linker	UNP O66529
aD	110	HIS	-	linker	UNP O66529
aD	111	GLY	-	linker	UNP O66529
aD	112	SER	-	linker	UNP O66529
aD	113	SER	-	linker	UNP O66529
aD	114	ILE	MET	engineered mutation	UNP O66529
aD	115	GLU	GLN	engineered mutation	UNP O66529
aD	138	THR	ALA	engineered mutation	UNP O66529
aD	177	ASP	GLY	engineered mutation	UNP O66529
aD	191	PHE	ILE	engineered mutation	UNP O66529
aD	193	ASP	VAL	engineered mutation	UNP O66529
bA	1	MET	-	cloning artifact	UNP P03045
bA	2	GLY	-	cloning artifact	UNP P03045
bA	3	ASN	-	cloning artifact	UNP P03045
bA	4	ALA	-	cloning artifact	UNP P03045
bA	5	LYS	-	cloning artifact	UNP P03045
bA	6	THR	-	cloning artifact	UNP P03045
bA	24	ALA	-	linker	UNP P03045
bA	25	GLY	-	linker	UNP P03045
bA	26	ALA	-	linker	UNP P03045
bA	27	GLY	-	linker	UNP P03045
bA	28	ALA	-	linker	UNP P03045
bA	29	GLY	-	linker	UNP P03045
bA	30	ALA	-	linker	UNP P03045
bA	31	MET	-	linker	UNP P03045
bA	39	ASN	ILE	engineered mutation	UNP O66529
bA	42	VAL	GLU	engineered mutation	UNP O66529
bA	58	VAL	ILE	engineered mutation	UNP O66529
bA	61	ASP	GLY	engineered mutation	UNP O66529
bA	62	ILE	VAL	engineered mutation	UNP O66529
bA	97	TYR	PHE	engineered mutation	UNP O66529
bA	102	GLY	-	linker	UNP O66529
bA	103	THR	-	linker	UNP O66529
bA	104	GLY	-	linker	UNP O66529
bA	105	HIS	-	linker	UNP O66529
bA	106	HIS	-	linker	UNP O66529
bA	107	HIS	-	linker	UNP O66529
bA	108	HIS	-	linker	UNP O66529
bA	109	HIS	-	linker	UNP O66529
bA	110	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
bA	111	GLY	-	linker	UNP O66529
bA	112	SER	-	linker	UNP O66529
bA	113	SER	-	linker	UNP O66529
bA	114	ILE	MET	engineered mutation	UNP O66529
bA	115	GLU	GLN	engineered mutation	UNP O66529
bA	138	THR	ALA	engineered mutation	UNP O66529
bA	177	ASP	GLY	engineered mutation	UNP O66529
bA	191	PHE	ILE	engineered mutation	UNP O66529
bA	193	ASP	VAL	engineered mutation	UNP O66529
bB	1	MET	-	cloning artifact	UNP P03045
bB	2	GLY	-	cloning artifact	UNP P03045
bB	3	ASN	-	cloning artifact	UNP P03045
bB	4	ALA	-	cloning artifact	UNP P03045
bB	5	LYS	-	cloning artifact	UNP P03045
bB	6	THR	-	cloning artifact	UNP P03045
bB	24	ALA	-	linker	UNP P03045
bB	25	GLY	-	linker	UNP P03045
bB	26	ALA	-	linker	UNP P03045
bB	27	GLY	-	linker	UNP P03045
bB	28	ALA	-	linker	UNP P03045
bB	29	GLY	-	linker	UNP P03045
bB	30	ALA	-	linker	UNP P03045
bB	31	MET	-	linker	UNP P03045
bB	39	ASN	ILE	engineered mutation	UNP O66529
bB	42	VAL	GLU	engineered mutation	UNP O66529
bB	58	VAL	ILE	engineered mutation	UNP O66529
bB	61	ASP	GLY	engineered mutation	UNP O66529
bB	62	ILE	VAL	engineered mutation	UNP O66529
bB	97	TYR	PHE	engineered mutation	UNP O66529
bB	102	GLY	-	linker	UNP O66529
bB	103	THR	-	linker	UNP O66529
bB	104	GLY	-	linker	UNP O66529
bB	105	HIS	-	linker	UNP O66529
bB	106	HIS	-	linker	UNP O66529
bB	107	HIS	-	linker	UNP O66529
bB	108	HIS	-	linker	UNP O66529
bB	109	HIS	-	linker	UNP O66529
bB	110	HIS	-	linker	UNP O66529
bB	111	GLY	-	linker	UNP O66529
bB	112	SER	-	linker	UNP O66529
bB	113	SER	-	linker	UNP O66529
bB	114	ILE	MET	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
bB	115	GLU	GLN	engineered mutation	UNP O66529
bB	138	THR	ALA	engineered mutation	UNP O66529
bB	177	ASP	GLY	engineered mutation	UNP O66529
bB	191	PHE	ILE	engineered mutation	UNP O66529
bB	193	ASP	VAL	engineered mutation	UNP O66529
bC	1	MET	-	cloning artifact	UNP P03045
bC	2	GLY	-	cloning artifact	UNP P03045
bC	3	ASN	-	cloning artifact	UNP P03045
bC	4	ALA	-	cloning artifact	UNP P03045
bC	5	LYS	-	cloning artifact	UNP P03045
bC	6	THR	-	cloning artifact	UNP P03045
bC	24	ALA	-	linker	UNP P03045
bC	25	GLY	-	linker	UNP P03045
bC	26	ALA	-	linker	UNP P03045
bC	27	GLY	-	linker	UNP P03045
bC	28	ALA	-	linker	UNP P03045
bC	29	GLY	-	linker	UNP P03045
bC	30	ALA	-	linker	UNP P03045
bC	31	MET	-	linker	UNP P03045
bC	39	ASN	ILE	engineered mutation	UNP O66529
bC	42	VAL	GLU	engineered mutation	UNP O66529
bC	58	VAL	ILE	engineered mutation	UNP O66529
bC	61	ASP	GLY	engineered mutation	UNP O66529
bC	62	ILE	VAL	engineered mutation	UNP O66529
bC	97	TYR	PHE	engineered mutation	UNP O66529
bC	102	GLY	-	linker	UNP O66529
bC	103	THR	-	linker	UNP O66529
bC	104	GLY	-	linker	UNP O66529
bC	105	HIS	-	linker	UNP O66529
bC	106	HIS	-	linker	UNP O66529
bC	107	HIS	-	linker	UNP O66529
bC	108	HIS	-	linker	UNP O66529
bC	109	HIS	-	linker	UNP O66529
bC	110	HIS	-	linker	UNP O66529
bC	111	GLY	-	linker	UNP O66529
bC	112	SER	-	linker	UNP O66529
bC	113	SER	-	linker	UNP O66529
bC	114	ILE	MET	engineered mutation	UNP O66529
bC	115	GLU	GLN	engineered mutation	UNP O66529
bC	138	THR	ALA	engineered mutation	UNP O66529
bC	177	ASP	GLY	engineered mutation	UNP O66529
bC	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
bC	193	ASP	VAL	engineered mutation	UNP O66529
bD	1	MET	-	cloning artifact	UNP P03045
bD	2	GLY	-	cloning artifact	UNP P03045
bD	3	ASN	-	cloning artifact	UNP P03045
bD	4	ALA	-	cloning artifact	UNP P03045
bD	5	LYS	-	cloning artifact	UNP P03045
bD	6	THR	-	cloning artifact	UNP P03045
bD	24	ALA	-	linker	UNP P03045
bD	25	GLY	-	linker	UNP P03045
bD	26	ALA	-	linker	UNP P03045
bD	27	GLY	-	linker	UNP P03045
bD	28	ALA	-	linker	UNP P03045
bD	29	GLY	-	linker	UNP P03045
bD	30	ALA	-	linker	UNP P03045
bD	31	MET	-	linker	UNP P03045
bD	39	ASN	ILE	engineered mutation	UNP O66529
bD	42	VAL	GLU	engineered mutation	UNP O66529
bD	58	VAL	ILE	engineered mutation	UNP O66529
bD	61	ASP	GLY	engineered mutation	UNP O66529
bD	62	ILE	VAL	engineered mutation	UNP O66529
bD	97	TYR	PHE	engineered mutation	UNP O66529
bD	102	GLY	-	linker	UNP O66529
bD	103	THR	-	linker	UNP O66529
bD	104	GLY	-	linker	UNP O66529
bD	105	HIS	-	linker	UNP O66529
bD	106	HIS	-	linker	UNP O66529
bD	107	HIS	-	linker	UNP O66529
bD	108	HIS	-	linker	UNP O66529
bD	109	HIS	-	linker	UNP O66529
bD	110	HIS	-	linker	UNP O66529
bD	111	GLY	-	linker	UNP O66529
bD	112	SER	-	linker	UNP O66529
bD	113	SER	-	linker	UNP O66529
bD	114	ILE	MET	engineered mutation	UNP O66529
bD	115	GLU	GLN	engineered mutation	UNP O66529
bD	138	THR	ALA	engineered mutation	UNP O66529
bD	177	ASP	GLY	engineered mutation	UNP O66529
bD	191	PHE	ILE	engineered mutation	UNP O66529
bD	193	ASP	VAL	engineered mutation	UNP O66529
cA	1	MET	-	cloning artifact	UNP P03045
cA	2	GLY	-	cloning artifact	UNP P03045
cA	3	ASN	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
cA	4	ALA	-	cloning artifact	UNP P03045
cA	5	LYS	-	cloning artifact	UNP P03045
cA	6	THR	-	cloning artifact	UNP P03045
cA	24	ALA	-	linker	UNP P03045
cA	25	GLY	-	linker	UNP P03045
cA	26	ALA	-	linker	UNP P03045
cA	27	GLY	-	linker	UNP P03045
cA	28	ALA	-	linker	UNP P03045
cA	29	GLY	-	linker	UNP P03045
cA	30	ALA	-	linker	UNP P03045
cA	31	MET	-	linker	UNP P03045
cA	39	ASN	ILE	engineered mutation	UNP O66529
cA	42	VAL	GLU	engineered mutation	UNP O66529
cA	58	VAL	ILE	engineered mutation	UNP O66529
cA	61	ASP	GLY	engineered mutation	UNP O66529
cA	62	ILE	VAL	engineered mutation	UNP O66529
cA	97	TYR	PHE	engineered mutation	UNP O66529
cA	102	GLY	-	linker	UNP O66529
cA	103	THR	-	linker	UNP O66529
cA	104	GLY	-	linker	UNP O66529
cA	105	HIS	-	linker	UNP O66529
cA	106	HIS	-	linker	UNP O66529
cA	107	HIS	-	linker	UNP O66529
cA	108	HIS	-	linker	UNP O66529
cA	109	HIS	-	linker	UNP O66529
cA	110	HIS	-	linker	UNP O66529
cA	111	GLY	-	linker	UNP O66529
cA	112	SER	-	linker	UNP O66529
cA	113	SER	-	linker	UNP O66529
cA	114	ILE	MET	engineered mutation	UNP O66529
cA	115	GLU	GLN	engineered mutation	UNP O66529
cA	138	THR	ALA	engineered mutation	UNP O66529
cA	177	ASP	GLY	engineered mutation	UNP O66529
cA	191	PHE	ILE	engineered mutation	UNP O66529
cA	193	ASP	VAL	engineered mutation	UNP O66529
cB	1	MET	-	cloning artifact	UNP P03045
cB	2	GLY	-	cloning artifact	UNP P03045
cB	3	ASN	-	cloning artifact	UNP P03045
cB	4	ALA	-	cloning artifact	UNP P03045
cB	5	LYS	-	cloning artifact	UNP P03045
cB	6	THR	-	cloning artifact	UNP P03045
cB	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
cB	25	GLY	-	linker	UNP P03045
cB	26	ALA	-	linker	UNP P03045
cB	27	GLY	-	linker	UNP P03045
cB	28	ALA	-	linker	UNP P03045
cB	29	GLY	-	linker	UNP P03045
cB	30	ALA	-	linker	UNP P03045
cB	31	MET	-	linker	UNP P03045
cB	39	ASN	ILE	engineered mutation	UNP O66529
cB	42	VAL	GLU	engineered mutation	UNP O66529
cB	58	VAL	ILE	engineered mutation	UNP O66529
cB	61	ASP	GLY	engineered mutation	UNP O66529
cB	62	ILE	VAL	engineered mutation	UNP O66529
cB	97	TYR	PHE	engineered mutation	UNP O66529
cB	102	GLY	-	linker	UNP O66529
cB	103	THR	-	linker	UNP O66529
cB	104	GLY	-	linker	UNP O66529
cB	105	HIS	-	linker	UNP O66529
cB	106	HIS	-	linker	UNP O66529
cB	107	HIS	-	linker	UNP O66529
cB	108	HIS	-	linker	UNP O66529
cB	109	HIS	-	linker	UNP O66529
cB	110	HIS	-	linker	UNP O66529
cB	111	GLY	-	linker	UNP O66529
cB	112	SER	-	linker	UNP O66529
cB	113	SER	-	linker	UNP O66529
cB	114	ILE	MET	engineered mutation	UNP O66529
cB	115	GLU	GLN	engineered mutation	UNP O66529
cB	138	THR	ALA	engineered mutation	UNP O66529
cB	177	ASP	GLY	engineered mutation	UNP O66529
cB	191	PHE	ILE	engineered mutation	UNP O66529
cB	193	ASP	VAL	engineered mutation	UNP O66529
cC	1	MET	-	cloning artifact	UNP P03045
cC	2	GLY	-	cloning artifact	UNP P03045
cC	3	ASN	-	cloning artifact	UNP P03045
cC	4	ALA	-	cloning artifact	UNP P03045
cC	5	LYS	-	cloning artifact	UNP P03045
cC	6	THR	-	cloning artifact	UNP P03045
cC	24	ALA	-	linker	UNP P03045
cC	25	GLY	-	linker	UNP P03045
cC	26	ALA	-	linker	UNP P03045
cC	27	GLY	-	linker	UNP P03045
cC	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
cC	29	GLY	-	linker	UNP P03045
cC	30	ALA	-	linker	UNP P03045
cC	31	MET	-	linker	UNP P03045
cC	39	ASN	ILE	engineered mutation	UNP O66529
cC	42	VAL	GLU	engineered mutation	UNP O66529
cC	58	VAL	ILE	engineered mutation	UNP O66529
cC	61	ASP	GLY	engineered mutation	UNP O66529
cC	62	ILE	VAL	engineered mutation	UNP O66529
cC	97	TYR	PHE	engineered mutation	UNP O66529
cC	102	GLY	-	linker	UNP O66529
cC	103	THR	-	linker	UNP O66529
cC	104	GLY	-	linker	UNP O66529
cC	105	HIS	-	linker	UNP O66529
cC	106	HIS	-	linker	UNP O66529
cC	107	HIS	-	linker	UNP O66529
cC	108	HIS	-	linker	UNP O66529
cC	109	HIS	-	linker	UNP O66529
cC	110	HIS	-	linker	UNP O66529
cC	111	GLY	-	linker	UNP O66529
cC	112	SER	-	linker	UNP O66529
cC	113	SER	-	linker	UNP O66529
cC	114	ILE	MET	engineered mutation	UNP O66529
cC	115	GLU	GLN	engineered mutation	UNP O66529
cC	138	THR	ALA	engineered mutation	UNP O66529
cC	177	ASP	GLY	engineered mutation	UNP O66529
cC	191	PHE	ILE	engineered mutation	UNP O66529
cC	193	ASP	VAL	engineered mutation	UNP O66529
cD	1	MET	-	cloning artifact	UNP P03045
cD	2	GLY	-	cloning artifact	UNP P03045
cD	3	ASN	-	cloning artifact	UNP P03045
cD	4	ALA	-	cloning artifact	UNP P03045
cD	5	LYS	-	cloning artifact	UNP P03045
cD	6	THR	-	cloning artifact	UNP P03045
cD	24	ALA	-	linker	UNP P03045
cD	25	GLY	-	linker	UNP P03045
cD	26	ALA	-	linker	UNP P03045
cD	27	GLY	-	linker	UNP P03045
cD	28	ALA	-	linker	UNP P03045
cD	29	GLY	-	linker	UNP P03045
cD	30	ALA	-	linker	UNP P03045
cD	31	MET	-	linker	UNP P03045
cD	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
cD	42	VAL	GLU	engineered mutation	UNP O66529
cD	58	VAL	ILE	engineered mutation	UNP O66529
cD	61	ASP	GLY	engineered mutation	UNP O66529
cD	62	ILE	VAL	engineered mutation	UNP O66529
cD	97	TYR	PHE	engineered mutation	UNP O66529
cD	102	GLY	-	linker	UNP O66529
cD	103	THR	-	linker	UNP O66529
cD	104	GLY	-	linker	UNP O66529
cD	105	HIS	-	linker	UNP O66529
cD	106	HIS	-	linker	UNP O66529
cD	107	HIS	-	linker	UNP O66529
cD	108	HIS	-	linker	UNP O66529
cD	109	HIS	-	linker	UNP O66529
cD	110	HIS	-	linker	UNP O66529
cD	111	GLY	-	linker	UNP O66529
cD	112	SER	-	linker	UNP O66529
cD	113	SER	-	linker	UNP O66529
cD	114	ILE	MET	engineered mutation	UNP O66529
cD	115	GLU	GLN	engineered mutation	UNP O66529
cD	138	THR	ALA	engineered mutation	UNP O66529
cD	177	ASP	GLY	engineered mutation	UNP O66529
cD	191	PHE	ILE	engineered mutation	UNP O66529
cD	193	ASP	VAL	engineered mutation	UNP O66529
dA	1	MET	-	cloning artifact	UNP P03045
dA	2	GLY	-	cloning artifact	UNP P03045
dA	3	ASN	-	cloning artifact	UNP P03045
dA	4	ALA	-	cloning artifact	UNP P03045
dA	5	LYS	-	cloning artifact	UNP P03045
dA	6	THR	-	cloning artifact	UNP P03045
dA	24	ALA	-	linker	UNP P03045
dA	25	GLY	-	linker	UNP P03045
dA	26	ALA	-	linker	UNP P03045
dA	27	GLY	-	linker	UNP P03045
dA	28	ALA	-	linker	UNP P03045
dA	29	GLY	-	linker	UNP P03045
dA	30	ALA	-	linker	UNP P03045
dA	31	MET	-	linker	UNP P03045
dA	39	ASN	ILE	engineered mutation	UNP O66529
dA	42	VAL	GLU	engineered mutation	UNP O66529
dA	58	VAL	ILE	engineered mutation	UNP O66529
dA	61	ASP	GLY	engineered mutation	UNP O66529
dA	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
dA	97	TYR	PHE	engineered mutation	UNP O66529
dA	102	GLY	-	linker	UNP O66529
dA	103	THR	-	linker	UNP O66529
dA	104	GLY	-	linker	UNP O66529
dA	105	HIS	-	linker	UNP O66529
dA	106	HIS	-	linker	UNP O66529
dA	107	HIS	-	linker	UNP O66529
dA	108	HIS	-	linker	UNP O66529
dA	109	HIS	-	linker	UNP O66529
dA	110	HIS	-	linker	UNP O66529
dA	111	GLY	-	linker	UNP O66529
dA	112	SER	-	linker	UNP O66529
dA	113	SER	-	linker	UNP O66529
dA	114	ILE	MET	engineered mutation	UNP O66529
dA	115	GLU	GLN	engineered mutation	UNP O66529
dA	138	THR	ALA	engineered mutation	UNP O66529
dA	177	ASP	GLY	engineered mutation	UNP O66529
dA	191	PHE	ILE	engineered mutation	UNP O66529
dA	193	ASP	VAL	engineered mutation	UNP O66529
dB	1	MET	-	cloning artifact	UNP P03045
dB	2	GLY	-	cloning artifact	UNP P03045
dB	3	ASN	-	cloning artifact	UNP P03045
dB	4	ALA	-	cloning artifact	UNP P03045
dB	5	LYS	-	cloning artifact	UNP P03045
dB	6	THR	-	cloning artifact	UNP P03045
dB	24	ALA	-	linker	UNP P03045
dB	25	GLY	-	linker	UNP P03045
dB	26	ALA	-	linker	UNP P03045
dB	27	GLY	-	linker	UNP P03045
dB	28	ALA	-	linker	UNP P03045
dB	29	GLY	-	linker	UNP P03045
dB	30	ALA	-	linker	UNP P03045
dB	31	MET	-	linker	UNP P03045
dB	39	ASN	ILE	engineered mutation	UNP O66529
dB	42	VAL	GLU	engineered mutation	UNP O66529
dB	58	VAL	ILE	engineered mutation	UNP O66529
dB	61	ASP	GLY	engineered mutation	UNP O66529
dB	62	ILE	VAL	engineered mutation	UNP O66529
dB	97	TYR	PHE	engineered mutation	UNP O66529
dB	102	GLY	-	linker	UNP O66529
dB	103	THR	-	linker	UNP O66529
dB	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
dB	105	HIS	-	linker	UNP O66529
dB	106	HIS	-	linker	UNP O66529
dB	107	HIS	-	linker	UNP O66529
dB	108	HIS	-	linker	UNP O66529
dB	109	HIS	-	linker	UNP O66529
dB	110	HIS	-	linker	UNP O66529
dB	111	GLY	-	linker	UNP O66529
dB	112	SER	-	linker	UNP O66529
dB	113	SER	-	linker	UNP O66529
dB	114	ILE	MET	engineered mutation	UNP O66529
dB	115	GLU	GLN	engineered mutation	UNP O66529
dB	138	THR	ALA	engineered mutation	UNP O66529
dB	177	ASP	GLY	engineered mutation	UNP O66529
dB	191	PHE	ILE	engineered mutation	UNP O66529
dB	193	ASP	VAL	engineered mutation	UNP O66529
dC	1	MET	-	cloning artifact	UNP P03045
dC	2	GLY	-	cloning artifact	UNP P03045
dC	3	ASN	-	cloning artifact	UNP P03045
dC	4	ALA	-	cloning artifact	UNP P03045
dC	5	LYS	-	cloning artifact	UNP P03045
dC	6	THR	-	cloning artifact	UNP P03045
dC	24	ALA	-	linker	UNP P03045
dC	25	GLY	-	linker	UNP P03045
dC	26	ALA	-	linker	UNP P03045
dC	27	GLY	-	linker	UNP P03045
dC	28	ALA	-	linker	UNP P03045
dC	29	GLY	-	linker	UNP P03045
dC	30	ALA	-	linker	UNP P03045
dC	31	MET	-	linker	UNP P03045
dC	39	ASN	ILE	engineered mutation	UNP O66529
dC	42	VAL	GLU	engineered mutation	UNP O66529
dC	58	VAL	ILE	engineered mutation	UNP O66529
dC	61	ASP	GLY	engineered mutation	UNP O66529
dC	62	ILE	VAL	engineered mutation	UNP O66529
dC	97	TYR	PHE	engineered mutation	UNP O66529
dC	102	GLY	-	linker	UNP O66529
dC	103	THR	-	linker	UNP O66529
dC	104	GLY	-	linker	UNP O66529
dC	105	HIS	-	linker	UNP O66529
dC	106	HIS	-	linker	UNP O66529
dC	107	HIS	-	linker	UNP O66529
dC	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
dC	109	HIS	-	linker	UNP O66529
dC	110	HIS	-	linker	UNP O66529
dC	111	GLY	-	linker	UNP O66529
dC	112	SER	-	linker	UNP O66529
dC	113	SER	-	linker	UNP O66529
dC	114	ILE	MET	engineered mutation	UNP O66529
dC	115	GLU	GLN	engineered mutation	UNP O66529
dC	138	THR	ALA	engineered mutation	UNP O66529
dC	177	ASP	GLY	engineered mutation	UNP O66529
dC	191	PHE	ILE	engineered mutation	UNP O66529
dC	193	ASP	VAL	engineered mutation	UNP O66529
dD	1	MET	-	cloning artifact	UNP P03045
dD	2	GLY	-	cloning artifact	UNP P03045
dD	3	ASN	-	cloning artifact	UNP P03045
dD	4	ALA	-	cloning artifact	UNP P03045
dD	5	LYS	-	cloning artifact	UNP P03045
dD	6	THR	-	cloning artifact	UNP P03045
dD	24	ALA	-	linker	UNP P03045
dD	25	GLY	-	linker	UNP P03045
dD	26	ALA	-	linker	UNP P03045
dD	27	GLY	-	linker	UNP P03045
dD	28	ALA	-	linker	UNP P03045
dD	29	GLY	-	linker	UNP P03045
dD	30	ALA	-	linker	UNP P03045
dD	31	MET	-	linker	UNP P03045
dD	39	ASN	ILE	engineered mutation	UNP O66529
dD	42	VAL	GLU	engineered mutation	UNP O66529
dD	58	VAL	ILE	engineered mutation	UNP O66529
dD	61	ASP	GLY	engineered mutation	UNP O66529
dD	62	ILE	VAL	engineered mutation	UNP O66529
dD	97	TYR	PHE	engineered mutation	UNP O66529
dD	102	GLY	-	linker	UNP O66529
dD	103	THR	-	linker	UNP O66529
dD	104	GLY	-	linker	UNP O66529
dD	105	HIS	-	linker	UNP O66529
dD	106	HIS	-	linker	UNP O66529
dD	107	HIS	-	linker	UNP O66529
dD	108	HIS	-	linker	UNP O66529
dD	109	HIS	-	linker	UNP O66529
dD	110	HIS	-	linker	UNP O66529
dD	111	GLY	-	linker	UNP O66529
dD	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
dD	113	SER	-	linker	UNP O66529
dD	114	ILE	MET	engineered mutation	UNP O66529
dD	115	GLU	GLN	engineered mutation	UNP O66529
dD	138	THR	ALA	engineered mutation	UNP O66529
dD	177	ASP	GLY	engineered mutation	UNP O66529
dD	191	PHE	ILE	engineered mutation	UNP O66529
dD	193	ASP	VAL	engineered mutation	UNP O66529
eA	1	MET	-	cloning artifact	UNP P03045
eA	2	GLY	-	cloning artifact	UNP P03045
eA	3	ASN	-	cloning artifact	UNP P03045
eA	4	ALA	-	cloning artifact	UNP P03045
eA	5	LYS	-	cloning artifact	UNP P03045
eA	6	THR	-	cloning artifact	UNP P03045
eA	24	ALA	-	linker	UNP P03045
eA	25	GLY	-	linker	UNP P03045
eA	26	ALA	-	linker	UNP P03045
eA	27	GLY	-	linker	UNP P03045
eA	28	ALA	-	linker	UNP P03045
eA	29	GLY	-	linker	UNP P03045
eA	30	ALA	-	linker	UNP P03045
eA	31	MET	-	linker	UNP P03045
eA	39	ASN	ILE	engineered mutation	UNP O66529
eA	42	VAL	GLU	engineered mutation	UNP O66529
eA	58	VAL	ILE	engineered mutation	UNP O66529
eA	61	ASP	GLY	engineered mutation	UNP O66529
eA	62	ILE	VAL	engineered mutation	UNP O66529
eA	97	TYR	PHE	engineered mutation	UNP O66529
eA	102	GLY	-	linker	UNP O66529
eA	103	THR	-	linker	UNP O66529
eA	104	GLY	-	linker	UNP O66529
eA	105	HIS	-	linker	UNP O66529
eA	106	HIS	-	linker	UNP O66529
eA	107	HIS	-	linker	UNP O66529
eA	108	HIS	-	linker	UNP O66529
eA	109	HIS	-	linker	UNP O66529
eA	110	HIS	-	linker	UNP O66529
eA	111	GLY	-	linker	UNP O66529
eA	112	SER	-	linker	UNP O66529
eA	113	SER	-	linker	UNP O66529
eA	114	ILE	MET	engineered mutation	UNP O66529
eA	115	GLU	GLN	engineered mutation	UNP O66529
eA	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
eA	177	ASP	GLY	engineered mutation	UNP O66529
eA	191	PHE	ILE	engineered mutation	UNP O66529
eA	193	ASP	VAL	engineered mutation	UNP O66529
eB	1	MET	-	cloning artifact	UNP P03045
eB	2	GLY	-	cloning artifact	UNP P03045
eB	3	ASN	-	cloning artifact	UNP P03045
eB	4	ALA	-	cloning artifact	UNP P03045
eB	5	LYS	-	cloning artifact	UNP P03045
eB	6	THR	-	cloning artifact	UNP P03045
eB	24	ALA	-	linker	UNP P03045
eB	25	GLY	-	linker	UNP P03045
eB	26	ALA	-	linker	UNP P03045
eB	27	GLY	-	linker	UNP P03045
eB	28	ALA	-	linker	UNP P03045
eB	29	GLY	-	linker	UNP P03045
eB	30	ALA	-	linker	UNP P03045
eB	31	MET	-	linker	UNP P03045
eB	39	ASN	ILE	engineered mutation	UNP O66529
eB	42	VAL	GLU	engineered mutation	UNP O66529
eB	58	VAL	ILE	engineered mutation	UNP O66529
eB	61	ASP	GLY	engineered mutation	UNP O66529
eB	62	ILE	VAL	engineered mutation	UNP O66529
eB	97	TYR	PHE	engineered mutation	UNP O66529
eB	102	GLY	-	linker	UNP O66529
eB	103	THR	-	linker	UNP O66529
eB	104	GLY	-	linker	UNP O66529
eB	105	HIS	-	linker	UNP O66529
eB	106	HIS	-	linker	UNP O66529
eB	107	HIS	-	linker	UNP O66529
eB	108	HIS	-	linker	UNP O66529
eB	109	HIS	-	linker	UNP O66529
eB	110	HIS	-	linker	UNP O66529
eB	111	GLY	-	linker	UNP O66529
eB	112	SER	-	linker	UNP O66529
eB	113	SER	-	linker	UNP O66529
eB	114	ILE	MET	engineered mutation	UNP O66529
eB	115	GLU	GLN	engineered mutation	UNP O66529
eB	138	THR	ALA	engineered mutation	UNP O66529
eB	177	ASP	GLY	engineered mutation	UNP O66529
eB	191	PHE	ILE	engineered mutation	UNP O66529
eB	193	ASP	VAL	engineered mutation	UNP O66529
eC	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
eC	2	GLY	-	cloning artifact	UNP P03045
eC	3	ASN	-	cloning artifact	UNP P03045
eC	4	ALA	-	cloning artifact	UNP P03045
eC	5	LYS	-	cloning artifact	UNP P03045
eC	6	THR	-	cloning artifact	UNP P03045
eC	24	ALA	-	linker	UNP P03045
eC	25	GLY	-	linker	UNP P03045
eC	26	ALA	-	linker	UNP P03045
eC	27	GLY	-	linker	UNP P03045
eC	28	ALA	-	linker	UNP P03045
eC	29	GLY	-	linker	UNP P03045
eC	30	ALA	-	linker	UNP P03045
eC	31	MET	-	linker	UNP P03045
eC	39	ASN	ILE	engineered mutation	UNP O66529
eC	42	VAL	GLU	engineered mutation	UNP O66529
eC	58	VAL	ILE	engineered mutation	UNP O66529
eC	61	ASP	GLY	engineered mutation	UNP O66529
eC	62	ILE	VAL	engineered mutation	UNP O66529
eC	97	TYR	PHE	engineered mutation	UNP O66529
eC	102	GLY	-	linker	UNP O66529
eC	103	THR	-	linker	UNP O66529
eC	104	GLY	-	linker	UNP O66529
eC	105	HIS	-	linker	UNP O66529
eC	106	HIS	-	linker	UNP O66529
eC	107	HIS	-	linker	UNP O66529
eC	108	HIS	-	linker	UNP O66529
eC	109	HIS	-	linker	UNP O66529
eC	110	HIS	-	linker	UNP O66529
eC	111	GLY	-	linker	UNP O66529
eC	112	SER	-	linker	UNP O66529
eC	113	SER	-	linker	UNP O66529
eC	114	ILE	MET	engineered mutation	UNP O66529
eC	115	GLU	GLN	engineered mutation	UNP O66529
eC	138	THR	ALA	engineered mutation	UNP O66529
eC	177	ASP	GLY	engineered mutation	UNP O66529
eC	191	PHE	ILE	engineered mutation	UNP O66529
eC	193	ASP	VAL	engineered mutation	UNP O66529
eD	1	MET	-	cloning artifact	UNP P03045
eD	2	GLY	-	cloning artifact	UNP P03045
eD	3	ASN	-	cloning artifact	UNP P03045
eD	4	ALA	-	cloning artifact	UNP P03045
eD	5	LYS	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
eD	6	THR	-	cloning artifact	UNP P03045
eD	24	ALA	-	linker	UNP P03045
eD	25	GLY	-	linker	UNP P03045
eD	26	ALA	-	linker	UNP P03045
eD	27	GLY	-	linker	UNP P03045
eD	28	ALA	-	linker	UNP P03045
eD	29	GLY	-	linker	UNP P03045
eD	30	ALA	-	linker	UNP P03045
eD	31	MET	-	linker	UNP P03045
eD	39	ASN	ILE	engineered mutation	UNP O66529
eD	42	VAL	GLU	engineered mutation	UNP O66529
eD	58	VAL	ILE	engineered mutation	UNP O66529
eD	61	ASP	GLY	engineered mutation	UNP O66529
eD	62	ILE	VAL	engineered mutation	UNP O66529
eD	97	TYR	PHE	engineered mutation	UNP O66529
eD	102	GLY	-	linker	UNP O66529
eD	103	THR	-	linker	UNP O66529
eD	104	GLY	-	linker	UNP O66529
eD	105	HIS	-	linker	UNP O66529
eD	106	HIS	-	linker	UNP O66529
eD	107	HIS	-	linker	UNP O66529
eD	108	HIS	-	linker	UNP O66529
eD	109	HIS	-	linker	UNP O66529
eD	110	HIS	-	linker	UNP O66529
eD	111	GLY	-	linker	UNP O66529
eD	112	SER	-	linker	UNP O66529
eD	113	SER	-	linker	UNP O66529
eD	114	ILE	MET	engineered mutation	UNP O66529
eD	115	GLU	GLN	engineered mutation	UNP O66529
eD	138	THR	ALA	engineered mutation	UNP O66529
eD	177	ASP	GLY	engineered mutation	UNP O66529
eD	191	PHE	ILE	engineered mutation	UNP O66529
eD	193	ASP	VAL	engineered mutation	UNP O66529
fA	1	MET	-	cloning artifact	UNP P03045
fA	2	GLY	-	cloning artifact	UNP P03045
fA	3	ASN	-	cloning artifact	UNP P03045
fA	4	ALA	-	cloning artifact	UNP P03045
fA	5	LYS	-	cloning artifact	UNP P03045
fA	6	THR	-	cloning artifact	UNP P03045
fA	24	ALA	-	linker	UNP P03045
fA	25	GLY	-	linker	UNP P03045
fA	26	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
fA	27	GLY	-	linker	UNP P03045
fA	28	ALA	-	linker	UNP P03045
fA	29	GLY	-	linker	UNP P03045
fA	30	ALA	-	linker	UNP P03045
fA	31	MET	-	linker	UNP P03045
fA	39	ASN	ILE	engineered mutation	UNP O66529
fA	42	VAL	GLU	engineered mutation	UNP O66529
fA	58	VAL	ILE	engineered mutation	UNP O66529
fA	61	ASP	GLY	engineered mutation	UNP O66529
fA	62	ILE	VAL	engineered mutation	UNP O66529
fA	97	TYR	PHE	engineered mutation	UNP O66529
fA	102	GLY	-	linker	UNP O66529
fA	103	THR	-	linker	UNP O66529
fA	104	GLY	-	linker	UNP O66529
fA	105	HIS	-	linker	UNP O66529
fA	106	HIS	-	linker	UNP O66529
fA	107	HIS	-	linker	UNP O66529
fA	108	HIS	-	linker	UNP O66529
fA	109	HIS	-	linker	UNP O66529
fA	110	HIS	-	linker	UNP O66529
fA	111	GLY	-	linker	UNP O66529
fA	112	SER	-	linker	UNP O66529
fA	113	SER	-	linker	UNP O66529
fA	114	ILE	MET	engineered mutation	UNP O66529
fA	115	GLU	GLN	engineered mutation	UNP O66529
fA	138	THR	ALA	engineered mutation	UNP O66529
fA	177	ASP	GLY	engineered mutation	UNP O66529
fA	191	PHE	ILE	engineered mutation	UNP O66529
fA	193	ASP	VAL	engineered mutation	UNP O66529
fB	1	MET	-	cloning artifact	UNP P03045
fB	2	GLY	-	cloning artifact	UNP P03045
fB	3	ASN	-	cloning artifact	UNP P03045
fB	4	ALA	-	cloning artifact	UNP P03045
fB	5	LYS	-	cloning artifact	UNP P03045
fB	6	THR	-	cloning artifact	UNP P03045
fB	24	ALA	-	linker	UNP P03045
fB	25	GLY	-	linker	UNP P03045
fB	26	ALA	-	linker	UNP P03045
fB	27	GLY	-	linker	UNP P03045
fB	28	ALA	-	linker	UNP P03045
fB	29	GLY	-	linker	UNP P03045
fB	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
fB	31	MET	-	linker	UNP P03045
fB	39	ASN	ILE	engineered mutation	UNP O66529
fB	42	VAL	GLU	engineered mutation	UNP O66529
fB	58	VAL	ILE	engineered mutation	UNP O66529
fB	61	ASP	GLY	engineered mutation	UNP O66529
fB	62	ILE	VAL	engineered mutation	UNP O66529
fB	97	TYR	PHE	engineered mutation	UNP O66529
fB	102	GLY	-	linker	UNP O66529
fB	103	THR	-	linker	UNP O66529
fB	104	GLY	-	linker	UNP O66529
fB	105	HIS	-	linker	UNP O66529
fB	106	HIS	-	linker	UNP O66529
fB	107	HIS	-	linker	UNP O66529
fB	108	HIS	-	linker	UNP O66529
fB	109	HIS	-	linker	UNP O66529
fB	110	HIS	-	linker	UNP O66529
fB	111	GLY	-	linker	UNP O66529
fB	112	SER	-	linker	UNP O66529
fB	113	SER	-	linker	UNP O66529
fB	114	ILE	MET	engineered mutation	UNP O66529
fB	115	GLU	GLN	engineered mutation	UNP O66529
fB	138	THR	ALA	engineered mutation	UNP O66529
fB	177	ASP	GLY	engineered mutation	UNP O66529
fB	191	PHE	ILE	engineered mutation	UNP O66529
fB	193	ASP	VAL	engineered mutation	UNP O66529
fC	1	MET	-	cloning artifact	UNP P03045
fC	2	GLY	-	cloning artifact	UNP P03045
fC	3	ASN	-	cloning artifact	UNP P03045
fC	4	ALA	-	cloning artifact	UNP P03045
fC	5	LYS	-	cloning artifact	UNP P03045
fC	6	THR	-	cloning artifact	UNP P03045
fC	24	ALA	-	linker	UNP P03045
fC	25	GLY	-	linker	UNP P03045
fC	26	ALA	-	linker	UNP P03045
fC	27	GLY	-	linker	UNP P03045
fC	28	ALA	-	linker	UNP P03045
fC	29	GLY	-	linker	UNP P03045
fC	30	ALA	-	linker	UNP P03045
fC	31	MET	-	linker	UNP P03045
fC	39	ASN	ILE	engineered mutation	UNP O66529
fC	42	VAL	GLU	engineered mutation	UNP O66529
fC	58	VAL	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
fC	61	ASP	GLY	engineered mutation	UNP O66529
fC	62	ILE	VAL	engineered mutation	UNP O66529
fC	97	TYR	PHE	engineered mutation	UNP O66529
fC	102	GLY	-	linker	UNP O66529
fC	103	THR	-	linker	UNP O66529
fC	104	GLY	-	linker	UNP O66529
fC	105	HIS	-	linker	UNP O66529
fC	106	HIS	-	linker	UNP O66529
fC	107	HIS	-	linker	UNP O66529
fC	108	HIS	-	linker	UNP O66529
fC	109	HIS	-	linker	UNP O66529
fC	110	HIS	-	linker	UNP O66529
fC	111	GLY	-	linker	UNP O66529
fC	112	SER	-	linker	UNP O66529
fC	113	SER	-	linker	UNP O66529
fC	114	ILE	MET	engineered mutation	UNP O66529
fC	115	GLU	GLN	engineered mutation	UNP O66529
fC	138	THR	ALA	engineered mutation	UNP O66529
fC	177	ASP	GLY	engineered mutation	UNP O66529
fC	191	PHE	ILE	engineered mutation	UNP O66529
fC	193	ASP	VAL	engineered mutation	UNP O66529
fD	1	MET	-	cloning artifact	UNP P03045
fD	2	GLY	-	cloning artifact	UNP P03045
fD	3	ASN	-	cloning artifact	UNP P03045
fD	4	ALA	-	cloning artifact	UNP P03045
fD	5	LYS	-	cloning artifact	UNP P03045
fD	6	THR	-	cloning artifact	UNP P03045
fD	24	ALA	-	linker	UNP P03045
fD	25	GLY	-	linker	UNP P03045
fD	26	ALA	-	linker	UNP P03045
fD	27	GLY	-	linker	UNP P03045
fD	28	ALA	-	linker	UNP P03045
fD	29	GLY	-	linker	UNP P03045
fD	30	ALA	-	linker	UNP P03045
fD	31	MET	-	linker	UNP P03045
fD	39	ASN	ILE	engineered mutation	UNP O66529
fD	42	VAL	GLU	engineered mutation	UNP O66529
fD	58	VAL	ILE	engineered mutation	UNP O66529
fD	61	ASP	GLY	engineered mutation	UNP O66529
fD	62	ILE	VAL	engineered mutation	UNP O66529
fD	97	TYR	PHE	engineered mutation	UNP O66529
fD	102	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
fD	103	THR	-	linker	UNP O66529
fD	104	GLY	-	linker	UNP O66529
fD	105	HIS	-	linker	UNP O66529
fD	106	HIS	-	linker	UNP O66529
fD	107	HIS	-	linker	UNP O66529
fD	108	HIS	-	linker	UNP O66529
fD	109	HIS	-	linker	UNP O66529
fD	110	HIS	-	linker	UNP O66529
fD	111	GLY	-	linker	UNP O66529
fD	112	SER	-	linker	UNP O66529
fD	113	SER	-	linker	UNP O66529
fD	114	ILE	MET	engineered mutation	UNP O66529
fD	115	GLU	GLN	engineered mutation	UNP O66529
fD	138	THR	ALA	engineered mutation	UNP O66529
fD	177	ASP	GLY	engineered mutation	UNP O66529
fD	191	PHE	ILE	engineered mutation	UNP O66529
fD	193	ASP	VAL	engineered mutation	UNP O66529
gA	1	MET	-	cloning artifact	UNP P03045
gA	2	GLY	-	cloning artifact	UNP P03045
gA	3	ASN	-	cloning artifact	UNP P03045
gA	4	ALA	-	cloning artifact	UNP P03045
gA	5	LYS	-	cloning artifact	UNP P03045
gA	6	THR	-	cloning artifact	UNP P03045
gA	24	ALA	-	linker	UNP P03045
gA	25	GLY	-	linker	UNP P03045
gA	26	ALA	-	linker	UNP P03045
gA	27	GLY	-	linker	UNP P03045
gA	28	ALA	-	linker	UNP P03045
gA	29	GLY	-	linker	UNP P03045
gA	30	ALA	-	linker	UNP P03045
gA	31	MET	-	linker	UNP P03045
gA	39	ASN	ILE	engineered mutation	UNP O66529
gA	42	VAL	GLU	engineered mutation	UNP O66529
gA	58	VAL	ILE	engineered mutation	UNP O66529
gA	61	ASP	GLY	engineered mutation	UNP O66529
gA	62	ILE	VAL	engineered mutation	UNP O66529
gA	97	TYR	PHE	engineered mutation	UNP O66529
gA	102	GLY	-	linker	UNP O66529
gA	103	THR	-	linker	UNP O66529
gA	104	GLY	-	linker	UNP O66529
gA	105	HIS	-	linker	UNP O66529
gA	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
gA	107	HIS	-	linker	UNP O66529
gA	108	HIS	-	linker	UNP O66529
gA	109	HIS	-	linker	UNP O66529
gA	110	HIS	-	linker	UNP O66529
gA	111	GLY	-	linker	UNP O66529
gA	112	SER	-	linker	UNP O66529
gA	113	SER	-	linker	UNP O66529
gA	114	ILE	MET	engineered mutation	UNP O66529
gA	115	GLU	GLN	engineered mutation	UNP O66529
gA	138	THR	ALA	engineered mutation	UNP O66529
gA	177	ASP	GLY	engineered mutation	UNP O66529
gA	191	PHE	ILE	engineered mutation	UNP O66529
gA	193	ASP	VAL	engineered mutation	UNP O66529
gB	1	MET	-	cloning artifact	UNP P03045
gB	2	GLY	-	cloning artifact	UNP P03045
gB	3	ASN	-	cloning artifact	UNP P03045
gB	4	ALA	-	cloning artifact	UNP P03045
gB	5	LYS	-	cloning artifact	UNP P03045
gB	6	THR	-	cloning artifact	UNP P03045
gB	24	ALA	-	linker	UNP P03045
gB	25	GLY	-	linker	UNP P03045
gB	26	ALA	-	linker	UNP P03045
gB	27	GLY	-	linker	UNP P03045
gB	28	ALA	-	linker	UNP P03045
gB	29	GLY	-	linker	UNP P03045
gB	30	ALA	-	linker	UNP P03045
gB	31	MET	-	linker	UNP P03045
gB	39	ASN	ILE	engineered mutation	UNP O66529
gB	42	VAL	GLU	engineered mutation	UNP O66529
gB	58	VAL	ILE	engineered mutation	UNP O66529
gB	61	ASP	GLY	engineered mutation	UNP O66529
gB	62	ILE	VAL	engineered mutation	UNP O66529
gB	97	TYR	PHE	engineered mutation	UNP O66529
gB	102	GLY	-	linker	UNP O66529
gB	103	THR	-	linker	UNP O66529
gB	104	GLY	-	linker	UNP O66529
gB	105	HIS	-	linker	UNP O66529
gB	106	HIS	-	linker	UNP O66529
gB	107	HIS	-	linker	UNP O66529
gB	108	HIS	-	linker	UNP O66529
gB	109	HIS	-	linker	UNP O66529
gB	110	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
gB	111	GLY	-	linker	UNP O66529
gB	112	SER	-	linker	UNP O66529
gB	113	SER	-	linker	UNP O66529
gB	114	ILE	MET	engineered mutation	UNP O66529
gB	115	GLU	GLN	engineered mutation	UNP O66529
gB	138	THR	ALA	engineered mutation	UNP O66529
gB	177	ASP	GLY	engineered mutation	UNP O66529
gB	191	PHE	ILE	engineered mutation	UNP O66529
gB	193	ASP	VAL	engineered mutation	UNP O66529
gC	1	MET	-	cloning artifact	UNP P03045
gC	2	GLY	-	cloning artifact	UNP P03045
gC	3	ASN	-	cloning artifact	UNP P03045
gC	4	ALA	-	cloning artifact	UNP P03045
gC	5	LYS	-	cloning artifact	UNP P03045
gC	6	THR	-	cloning artifact	UNP P03045
gC	24	ALA	-	linker	UNP P03045
gC	25	GLY	-	linker	UNP P03045
gC	26	ALA	-	linker	UNP P03045
gC	27	GLY	-	linker	UNP P03045
gC	28	ALA	-	linker	UNP P03045
gC	29	GLY	-	linker	UNP P03045
gC	30	ALA	-	linker	UNP P03045
gC	31	MET	-	linker	UNP P03045
gC	39	ASN	ILE	engineered mutation	UNP O66529
gC	42	VAL	GLU	engineered mutation	UNP O66529
gC	58	VAL	ILE	engineered mutation	UNP O66529
gC	61	ASP	GLY	engineered mutation	UNP O66529
gC	62	ILE	VAL	engineered mutation	UNP O66529
gC	97	TYR	PHE	engineered mutation	UNP O66529
gC	102	GLY	-	linker	UNP O66529
gC	103	THR	-	linker	UNP O66529
gC	104	GLY	-	linker	UNP O66529
gC	105	HIS	-	linker	UNP O66529
gC	106	HIS	-	linker	UNP O66529
gC	107	HIS	-	linker	UNP O66529
gC	108	HIS	-	linker	UNP O66529
gC	109	HIS	-	linker	UNP O66529
gC	110	HIS	-	linker	UNP O66529
gC	111	GLY	-	linker	UNP O66529
gC	112	SER	-	linker	UNP O66529
gC	113	SER	-	linker	UNP O66529
gC	114	ILE	MET	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
gC	115	GLU	GLN	engineered mutation	UNP O66529
gC	138	THR	ALA	engineered mutation	UNP O66529
gC	177	ASP	GLY	engineered mutation	UNP O66529
gC	191	PHE	ILE	engineered mutation	UNP O66529
gC	193	ASP	VAL	engineered mutation	UNP O66529
gD	1	MET	-	cloning artifact	UNP P03045
gD	2	GLY	-	cloning artifact	UNP P03045
gD	3	ASN	-	cloning artifact	UNP P03045
gD	4	ALA	-	cloning artifact	UNP P03045
gD	5	LYS	-	cloning artifact	UNP P03045
gD	6	THR	-	cloning artifact	UNP P03045
gD	24	ALA	-	linker	UNP P03045
gD	25	GLY	-	linker	UNP P03045
gD	26	ALA	-	linker	UNP P03045
gD	27	GLY	-	linker	UNP P03045
gD	28	ALA	-	linker	UNP P03045
gD	29	GLY	-	linker	UNP P03045
gD	30	ALA	-	linker	UNP P03045
gD	31	MET	-	linker	UNP P03045
gD	39	ASN	ILE	engineered mutation	UNP O66529
gD	42	VAL	GLU	engineered mutation	UNP O66529
gD	58	VAL	ILE	engineered mutation	UNP O66529
gD	61	ASP	GLY	engineered mutation	UNP O66529
gD	62	ILE	VAL	engineered mutation	UNP O66529
gD	97	TYR	PHE	engineered mutation	UNP O66529
gD	102	GLY	-	linker	UNP O66529
gD	103	THR	-	linker	UNP O66529
gD	104	GLY	-	linker	UNP O66529
gD	105	HIS	-	linker	UNP O66529
gD	106	HIS	-	linker	UNP O66529
gD	107	HIS	-	linker	UNP O66529
gD	108	HIS	-	linker	UNP O66529
gD	109	HIS	-	linker	UNP O66529
gD	110	HIS	-	linker	UNP O66529
gD	111	GLY	-	linker	UNP O66529
gD	112	SER	-	linker	UNP O66529
gD	113	SER	-	linker	UNP O66529
gD	114	ILE	MET	engineered mutation	UNP O66529
gD	115	GLU	GLN	engineered mutation	UNP O66529
gD	138	THR	ALA	engineered mutation	UNP O66529
gD	177	ASP	GLY	engineered mutation	UNP O66529
gD	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
gD	193	ASP	VAL	engineered mutation	UNP O66529
hA	1	MET	-	cloning artifact	UNP P03045
hA	2	GLY	-	cloning artifact	UNP P03045
hA	3	ASN	-	cloning artifact	UNP P03045
hA	4	ALA	-	cloning artifact	UNP P03045
hA	5	LYS	-	cloning artifact	UNP P03045
hA	6	THR	-	cloning artifact	UNP P03045
hA	24	ALA	-	linker	UNP P03045
hA	25	GLY	-	linker	UNP P03045
hA	26	ALA	-	linker	UNP P03045
hA	27	GLY	-	linker	UNP P03045
hA	28	ALA	-	linker	UNP P03045
hA	29	GLY	-	linker	UNP P03045
hA	30	ALA	-	linker	UNP P03045
hA	31	MET	-	linker	UNP P03045
hA	39	ASN	ILE	engineered mutation	UNP O66529
hA	42	VAL	GLU	engineered mutation	UNP O66529
hA	58	VAL	ILE	engineered mutation	UNP O66529
hA	61	ASP	GLY	engineered mutation	UNP O66529
hA	62	ILE	VAL	engineered mutation	UNP O66529
hA	97	TYR	PHE	engineered mutation	UNP O66529
hA	102	GLY	-	linker	UNP O66529
hA	103	THR	-	linker	UNP O66529
hA	104	GLY	-	linker	UNP O66529
hA	105	HIS	-	linker	UNP O66529
hA	106	HIS	-	linker	UNP O66529
hA	107	HIS	-	linker	UNP O66529
hA	108	HIS	-	linker	UNP O66529
hA	109	HIS	-	linker	UNP O66529
hA	110	HIS	-	linker	UNP O66529
hA	111	GLY	-	linker	UNP O66529
hA	112	SER	-	linker	UNP O66529
hA	113	SER	-	linker	UNP O66529
hA	114	ILE	MET	engineered mutation	UNP O66529
hA	115	GLU	GLN	engineered mutation	UNP O66529
hA	138	THR	ALA	engineered mutation	UNP O66529
hA	177	ASP	GLY	engineered mutation	UNP O66529
hA	191	PHE	ILE	engineered mutation	UNP O66529
hA	193	ASP	VAL	engineered mutation	UNP O66529
hB	1	MET	-	cloning artifact	UNP P03045
hB	2	GLY	-	cloning artifact	UNP P03045
hB	3	ASN	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
hB	4	ALA	-	cloning artifact	UNP P03045
hB	5	LYS	-	cloning artifact	UNP P03045
hB	6	THR	-	cloning artifact	UNP P03045
hB	24	ALA	-	linker	UNP P03045
hB	25	GLY	-	linker	UNP P03045
hB	26	ALA	-	linker	UNP P03045
hB	27	GLY	-	linker	UNP P03045
hB	28	ALA	-	linker	UNP P03045
hB	29	GLY	-	linker	UNP P03045
hB	30	ALA	-	linker	UNP P03045
hB	31	MET	-	linker	UNP P03045
hB	39	ASN	ILE	engineered mutation	UNP O66529
hB	42	VAL	GLU	engineered mutation	UNP O66529
hB	58	VAL	ILE	engineered mutation	UNP O66529
hB	61	ASP	GLY	engineered mutation	UNP O66529
hB	62	ILE	VAL	engineered mutation	UNP O66529
hB	97	TYR	PHE	engineered mutation	UNP O66529
hB	102	GLY	-	linker	UNP O66529
hB	103	THR	-	linker	UNP O66529
hB	104	GLY	-	linker	UNP O66529
hB	105	HIS	-	linker	UNP O66529
hB	106	HIS	-	linker	UNP O66529
hB	107	HIS	-	linker	UNP O66529
hB	108	HIS	-	linker	UNP O66529
hB	109	HIS	-	linker	UNP O66529
hB	110	HIS	-	linker	UNP O66529
hB	111	GLY	-	linker	UNP O66529
hB	112	SER	-	linker	UNP O66529
hB	113	SER	-	linker	UNP O66529
hB	114	ILE	MET	engineered mutation	UNP O66529
hB	115	GLU	GLN	engineered mutation	UNP O66529
hB	138	THR	ALA	engineered mutation	UNP O66529
hB	177	ASP	GLY	engineered mutation	UNP O66529
hB	191	PHE	ILE	engineered mutation	UNP O66529
hB	193	ASP	VAL	engineered mutation	UNP O66529
hC	1	MET	-	cloning artifact	UNP P03045
hC	2	GLY	-	cloning artifact	UNP P03045
hC	3	ASN	-	cloning artifact	UNP P03045
hC	4	ALA	-	cloning artifact	UNP P03045
hC	5	LYS	-	cloning artifact	UNP P03045
hC	6	THR	-	cloning artifact	UNP P03045
hC	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
hC	25	GLY	-	linker	UNP P03045
hC	26	ALA	-	linker	UNP P03045
hC	27	GLY	-	linker	UNP P03045
hC	28	ALA	-	linker	UNP P03045
hC	29	GLY	-	linker	UNP P03045
hC	30	ALA	-	linker	UNP P03045
hC	31	MET	-	linker	UNP P03045
hC	39	ASN	ILE	engineered mutation	UNP O66529
hC	42	VAL	GLU	engineered mutation	UNP O66529
hC	58	VAL	ILE	engineered mutation	UNP O66529
hC	61	ASP	GLY	engineered mutation	UNP O66529
hC	62	ILE	VAL	engineered mutation	UNP O66529
hC	97	TYR	PHE	engineered mutation	UNP O66529
hC	102	GLY	-	linker	UNP O66529
hC	103	THR	-	linker	UNP O66529
hC	104	GLY	-	linker	UNP O66529
hC	105	HIS	-	linker	UNP O66529
hC	106	HIS	-	linker	UNP O66529
hC	107	HIS	-	linker	UNP O66529
hC	108	HIS	-	linker	UNP O66529
hC	109	HIS	-	linker	UNP O66529
hC	110	HIS	-	linker	UNP O66529
hC	111	GLY	-	linker	UNP O66529
hC	112	SER	-	linker	UNP O66529
hC	113	SER	-	linker	UNP O66529
hC	114	ILE	MET	engineered mutation	UNP O66529
hC	115	GLU	GLN	engineered mutation	UNP O66529
hC	138	THR	ALA	engineered mutation	UNP O66529
hC	177	ASP	GLY	engineered mutation	UNP O66529
hC	191	PHE	ILE	engineered mutation	UNP O66529
hC	193	ASP	VAL	engineered mutation	UNP O66529
hD	1	MET	-	cloning artifact	UNP P03045
hD	2	GLY	-	cloning artifact	UNP P03045
hD	3	ASN	-	cloning artifact	UNP P03045
hD	4	ALA	-	cloning artifact	UNP P03045
hD	5	LYS	-	cloning artifact	UNP P03045
hD	6	THR	-	cloning artifact	UNP P03045
hD	24	ALA	-	linker	UNP P03045
hD	25	GLY	-	linker	UNP P03045
hD	26	ALA	-	linker	UNP P03045
hD	27	GLY	-	linker	UNP P03045
hD	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
hD	29	GLY	-	linker	UNP P03045
hD	30	ALA	-	linker	UNP P03045
hD	31	MET	-	linker	UNP P03045
hD	39	ASN	ILE	engineered mutation	UNP O66529
hD	42	VAL	GLU	engineered mutation	UNP O66529
hD	58	VAL	ILE	engineered mutation	UNP O66529
hD	61	ASP	GLY	engineered mutation	UNP O66529
hD	62	ILE	VAL	engineered mutation	UNP O66529
hD	97	TYR	PHE	engineered mutation	UNP O66529
hD	102	GLY	-	linker	UNP O66529
hD	103	THR	-	linker	UNP O66529
hD	104	GLY	-	linker	UNP O66529
hD	105	HIS	-	linker	UNP O66529
hD	106	HIS	-	linker	UNP O66529
hD	107	HIS	-	linker	UNP O66529
hD	108	HIS	-	linker	UNP O66529
hD	109	HIS	-	linker	UNP O66529
hD	110	HIS	-	linker	UNP O66529
hD	111	GLY	-	linker	UNP O66529
hD	112	SER	-	linker	UNP O66529
hD	113	SER	-	linker	UNP O66529
hD	114	ILE	MET	engineered mutation	UNP O66529
hD	115	GLU	GLN	engineered mutation	UNP O66529
hD	138	THR	ALA	engineered mutation	UNP O66529
hD	177	ASP	GLY	engineered mutation	UNP O66529
hD	191	PHE	ILE	engineered mutation	UNP O66529
hD	193	ASP	VAL	engineered mutation	UNP O66529
iA	1	MET	-	cloning artifact	UNP P03045
iA	2	GLY	-	cloning artifact	UNP P03045
iA	3	ASN	-	cloning artifact	UNP P03045
iA	4	ALA	-	cloning artifact	UNP P03045
iA	5	LYS	-	cloning artifact	UNP P03045
iA	6	THR	-	cloning artifact	UNP P03045
iA	24	ALA	-	linker	UNP P03045
iA	25	GLY	-	linker	UNP P03045
iA	26	ALA	-	linker	UNP P03045
iA	27	GLY	-	linker	UNP P03045
iA	28	ALA	-	linker	UNP P03045
iA	29	GLY	-	linker	UNP P03045
iA	30	ALA	-	linker	UNP P03045
iA	31	MET	-	linker	UNP P03045
iA	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
iA	42	VAL	GLU	engineered mutation	UNP O66529
iA	58	VAL	ILE	engineered mutation	UNP O66529
iA	61	ASP	GLY	engineered mutation	UNP O66529
iA	62	ILE	VAL	engineered mutation	UNP O66529
iA	97	TYR	PHE	engineered mutation	UNP O66529
iA	102	GLY	-	linker	UNP O66529
iA	103	THR	-	linker	UNP O66529
iA	104	GLY	-	linker	UNP O66529
iA	105	HIS	-	linker	UNP O66529
iA	106	HIS	-	linker	UNP O66529
iA	107	HIS	-	linker	UNP O66529
iA	108	HIS	-	linker	UNP O66529
iA	109	HIS	-	linker	UNP O66529
iA	110	HIS	-	linker	UNP O66529
iA	111	GLY	-	linker	UNP O66529
iA	112	SER	-	linker	UNP O66529
iA	113	SER	-	linker	UNP O66529
iA	114	ILE	MET	engineered mutation	UNP O66529
iA	115	GLU	GLN	engineered mutation	UNP O66529
iA	138	THR	ALA	engineered mutation	UNP O66529
iA	177	ASP	GLY	engineered mutation	UNP O66529
iA	191	PHE	ILE	engineered mutation	UNP O66529
iA	193	ASP	VAL	engineered mutation	UNP O66529
iB	1	MET	-	cloning artifact	UNP P03045
iB	2	GLY	-	cloning artifact	UNP P03045
iB	3	ASN	-	cloning artifact	UNP P03045
iB	4	ALA	-	cloning artifact	UNP P03045
iB	5	LYS	-	cloning artifact	UNP P03045
iB	6	THR	-	cloning artifact	UNP P03045
iB	24	ALA	-	linker	UNP P03045
iB	25	GLY	-	linker	UNP P03045
iB	26	ALA	-	linker	UNP P03045
iB	27	GLY	-	linker	UNP P03045
iB	28	ALA	-	linker	UNP P03045
iB	29	GLY	-	linker	UNP P03045
iB	30	ALA	-	linker	UNP P03045
iB	31	MET	-	linker	UNP P03045
iB	39	ASN	ILE	engineered mutation	UNP O66529
iB	42	VAL	GLU	engineered mutation	UNP O66529
iB	58	VAL	ILE	engineered mutation	UNP O66529
iB	61	ASP	GLY	engineered mutation	UNP O66529
iB	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
iB	97	TYR	PHE	engineered mutation	UNP O66529
iB	102	GLY	-	linker	UNP O66529
iB	103	THR	-	linker	UNP O66529
iB	104	GLY	-	linker	UNP O66529
iB	105	HIS	-	linker	UNP O66529
iB	106	HIS	-	linker	UNP O66529
iB	107	HIS	-	linker	UNP O66529
iB	108	HIS	-	linker	UNP O66529
iB	109	HIS	-	linker	UNP O66529
iB	110	HIS	-	linker	UNP O66529
iB	111	GLY	-	linker	UNP O66529
iB	112	SER	-	linker	UNP O66529
iB	113	SER	-	linker	UNP O66529
iB	114	ILE	MET	engineered mutation	UNP O66529
iB	115	GLU	GLN	engineered mutation	UNP O66529
iB	138	THR	ALA	engineered mutation	UNP O66529
iB	177	ASP	GLY	engineered mutation	UNP O66529
iB	191	PHE	ILE	engineered mutation	UNP O66529
iB	193	ASP	VAL	engineered mutation	UNP O66529
iC	1	MET	-	cloning artifact	UNP P03045
iC	2	GLY	-	cloning artifact	UNP P03045
iC	3	ASN	-	cloning artifact	UNP P03045
iC	4	ALA	-	cloning artifact	UNP P03045
iC	5	LYS	-	cloning artifact	UNP P03045
iC	6	THR	-	cloning artifact	UNP P03045
iC	24	ALA	-	linker	UNP P03045
iC	25	GLY	-	linker	UNP P03045
iC	26	ALA	-	linker	UNP P03045
iC	27	GLY	-	linker	UNP P03045
iC	28	ALA	-	linker	UNP P03045
iC	29	GLY	-	linker	UNP P03045
iC	30	ALA	-	linker	UNP P03045
iC	31	MET	-	linker	UNP P03045
iC	39	ASN	ILE	engineered mutation	UNP O66529
iC	42	VAL	GLU	engineered mutation	UNP O66529
iC	58	VAL	ILE	engineered mutation	UNP O66529
iC	61	ASP	GLY	engineered mutation	UNP O66529
iC	62	ILE	VAL	engineered mutation	UNP O66529
iC	97	TYR	PHE	engineered mutation	UNP O66529
iC	102	GLY	-	linker	UNP O66529
iC	103	THR	-	linker	UNP O66529
iC	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
iC	105	HIS	-	linker	UNP O66529
iC	106	HIS	-	linker	UNP O66529
iC	107	HIS	-	linker	UNP O66529
iC	108	HIS	-	linker	UNP O66529
iC	109	HIS	-	linker	UNP O66529
iC	110	HIS	-	linker	UNP O66529
iC	111	GLY	-	linker	UNP O66529
iC	112	SER	-	linker	UNP O66529
iC	113	SER	-	linker	UNP O66529
iC	114	ILE	MET	engineered mutation	UNP O66529
iC	115	GLU	GLN	engineered mutation	UNP O66529
iC	138	THR	ALA	engineered mutation	UNP O66529
iC	177	ASP	GLY	engineered mutation	UNP O66529
iC	191	PHE	ILE	engineered mutation	UNP O66529
iC	193	ASP	VAL	engineered mutation	UNP O66529
iD	1	MET	-	cloning artifact	UNP P03045
iD	2	GLY	-	cloning artifact	UNP P03045
iD	3	ASN	-	cloning artifact	UNP P03045
iD	4	ALA	-	cloning artifact	UNP P03045
iD	5	LYS	-	cloning artifact	UNP P03045
iD	6	THR	-	cloning artifact	UNP P03045
iD	24	ALA	-	linker	UNP P03045
iD	25	GLY	-	linker	UNP P03045
iD	26	ALA	-	linker	UNP P03045
iD	27	GLY	-	linker	UNP P03045
iD	28	ALA	-	linker	UNP P03045
iD	29	GLY	-	linker	UNP P03045
iD	30	ALA	-	linker	UNP P03045
iD	31	MET	-	linker	UNP P03045
iD	39	ASN	ILE	engineered mutation	UNP O66529
iD	42	VAL	GLU	engineered mutation	UNP O66529
iD	58	VAL	ILE	engineered mutation	UNP O66529
iD	61	ASP	GLY	engineered mutation	UNP O66529
iD	62	ILE	VAL	engineered mutation	UNP O66529
iD	97	TYR	PHE	engineered mutation	UNP O66529
iD	102	GLY	-	linker	UNP O66529
iD	103	THR	-	linker	UNP O66529
iD	104	GLY	-	linker	UNP O66529
iD	105	HIS	-	linker	UNP O66529
iD	106	HIS	-	linker	UNP O66529
iD	107	HIS	-	linker	UNP O66529
iD	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
iD	109	HIS	-	linker	UNP O66529
iD	110	HIS	-	linker	UNP O66529
iD	111	GLY	-	linker	UNP O66529
iD	112	SER	-	linker	UNP O66529
iD	113	SER	-	linker	UNP O66529
iD	114	ILE	MET	engineered mutation	UNP O66529
iD	115	GLU	GLN	engineered mutation	UNP O66529
iD	138	THR	ALA	engineered mutation	UNP O66529
iD	177	ASP	GLY	engineered mutation	UNP O66529
iD	191	PHE	ILE	engineered mutation	UNP O66529
iD	193	ASP	VAL	engineered mutation	UNP O66529
jA	1	MET	-	cloning artifact	UNP P03045
jA	2	GLY	-	cloning artifact	UNP P03045
jA	3	ASN	-	cloning artifact	UNP P03045
jA	4	ALA	-	cloning artifact	UNP P03045
jA	5	LYS	-	cloning artifact	UNP P03045
jA	6	THR	-	cloning artifact	UNP P03045
jA	24	ALA	-	linker	UNP P03045
jA	25	GLY	-	linker	UNP P03045
jA	26	ALA	-	linker	UNP P03045
jA	27	GLY	-	linker	UNP P03045
jA	28	ALA	-	linker	UNP P03045
jA	29	GLY	-	linker	UNP P03045
jA	30	ALA	-	linker	UNP P03045
jA	31	MET	-	linker	UNP P03045
jA	39	ASN	ILE	engineered mutation	UNP O66529
jA	42	VAL	GLU	engineered mutation	UNP O66529
jA	58	VAL	ILE	engineered mutation	UNP O66529
jA	61	ASP	GLY	engineered mutation	UNP O66529
jA	62	ILE	VAL	engineered mutation	UNP O66529
jA	97	TYR	PHE	engineered mutation	UNP O66529
jA	102	GLY	-	linker	UNP O66529
jA	103	THR	-	linker	UNP O66529
jA	104	GLY	-	linker	UNP O66529
jA	105	HIS	-	linker	UNP O66529
jA	106	HIS	-	linker	UNP O66529
jA	107	HIS	-	linker	UNP O66529
jA	108	HIS	-	linker	UNP O66529
jA	109	HIS	-	linker	UNP O66529
jA	110	HIS	-	linker	UNP O66529
jA	111	GLY	-	linker	UNP O66529
jA	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
jA	113	SER	-	linker	UNP O66529
jA	114	ILE	MET	engineered mutation	UNP O66529
jA	115	GLU	GLN	engineered mutation	UNP O66529
jA	138	THR	ALA	engineered mutation	UNP O66529
jA	177	ASP	GLY	engineered mutation	UNP O66529
jA	191	PHE	ILE	engineered mutation	UNP O66529
jA	193	ASP	VAL	engineered mutation	UNP O66529
jB	1	MET	-	cloning artifact	UNP P03045
jB	2	GLY	-	cloning artifact	UNP P03045
jB	3	ASN	-	cloning artifact	UNP P03045
jB	4	ALA	-	cloning artifact	UNP P03045
jB	5	LYS	-	cloning artifact	UNP P03045
jB	6	THR	-	cloning artifact	UNP P03045
jB	24	ALA	-	linker	UNP P03045
jB	25	GLY	-	linker	UNP P03045
jB	26	ALA	-	linker	UNP P03045
jB	27	GLY	-	linker	UNP P03045
jB	28	ALA	-	linker	UNP P03045
jB	29	GLY	-	linker	UNP P03045
jB	30	ALA	-	linker	UNP P03045
jB	31	MET	-	linker	UNP P03045
jB	39	ASN	ILE	engineered mutation	UNP O66529
jB	42	VAL	GLU	engineered mutation	UNP O66529
jB	58	VAL	ILE	engineered mutation	UNP O66529
jB	61	ASP	GLY	engineered mutation	UNP O66529
jB	62	ILE	VAL	engineered mutation	UNP O66529
jB	97	TYR	PHE	engineered mutation	UNP O66529
jB	102	GLY	-	linker	UNP O66529
jB	103	THR	-	linker	UNP O66529
jB	104	GLY	-	linker	UNP O66529
jB	105	HIS	-	linker	UNP O66529
jB	106	HIS	-	linker	UNP O66529
jB	107	HIS	-	linker	UNP O66529
jB	108	HIS	-	linker	UNP O66529
jB	109	HIS	-	linker	UNP O66529
jB	110	HIS	-	linker	UNP O66529
jB	111	GLY	-	linker	UNP O66529
jB	112	SER	-	linker	UNP O66529
jB	113	SER	-	linker	UNP O66529
jB	114	ILE	MET	engineered mutation	UNP O66529
jB	115	GLU	GLN	engineered mutation	UNP O66529
jB	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
jB	177	ASP	GLY	engineered mutation	UNP O66529
jB	191	PHE	ILE	engineered mutation	UNP O66529
jB	193	ASP	VAL	engineered mutation	UNP O66529
jC	1	MET	-	cloning artifact	UNP P03045
jC	2	GLY	-	cloning artifact	UNP P03045
jC	3	ASN	-	cloning artifact	UNP P03045
jC	4	ALA	-	cloning artifact	UNP P03045
jC	5	LYS	-	cloning artifact	UNP P03045
jC	6	THR	-	cloning artifact	UNP P03045
jC	24	ALA	-	linker	UNP P03045
jC	25	GLY	-	linker	UNP P03045
jC	26	ALA	-	linker	UNP P03045
jC	27	GLY	-	linker	UNP P03045
jC	28	ALA	-	linker	UNP P03045
jC	29	GLY	-	linker	UNP P03045
jC	30	ALA	-	linker	UNP P03045
jC	31	MET	-	linker	UNP P03045
jC	39	ASN	ILE	engineered mutation	UNP O66529
jC	42	VAL	GLU	engineered mutation	UNP O66529
jC	58	VAL	ILE	engineered mutation	UNP O66529
jC	61	ASP	GLY	engineered mutation	UNP O66529
jC	62	ILE	VAL	engineered mutation	UNP O66529
jC	97	TYR	PHE	engineered mutation	UNP O66529
jC	102	GLY	-	linker	UNP O66529
jC	103	THR	-	linker	UNP O66529
jC	104	GLY	-	linker	UNP O66529
jC	105	HIS	-	linker	UNP O66529
jC	106	HIS	-	linker	UNP O66529
jC	107	HIS	-	linker	UNP O66529
jC	108	HIS	-	linker	UNP O66529
jC	109	HIS	-	linker	UNP O66529
jC	110	HIS	-	linker	UNP O66529
jC	111	GLY	-	linker	UNP O66529
jC	112	SER	-	linker	UNP O66529
jC	113	SER	-	linker	UNP O66529
jC	114	ILE	MET	engineered mutation	UNP O66529
jC	115	GLU	GLN	engineered mutation	UNP O66529
jC	138	THR	ALA	engineered mutation	UNP O66529
jC	177	ASP	GLY	engineered mutation	UNP O66529
jC	191	PHE	ILE	engineered mutation	UNP O66529
jC	193	ASP	VAL	engineered mutation	UNP O66529
jD	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
jD	2	GLY	-	cloning artifact	UNP P03045
jD	3	ASN	-	cloning artifact	UNP P03045
jD	4	ALA	-	cloning artifact	UNP P03045
jD	5	LYS	-	cloning artifact	UNP P03045
jD	6	THR	-	cloning artifact	UNP P03045
jD	24	ALA	-	linker	UNP P03045
jD	25	GLY	-	linker	UNP P03045
jD	26	ALA	-	linker	UNP P03045
jD	27	GLY	-	linker	UNP P03045
jD	28	ALA	-	linker	UNP P03045
jD	29	GLY	-	linker	UNP P03045
jD	30	ALA	-	linker	UNP P03045
jD	31	MET	-	linker	UNP P03045
jD	39	ASN	ILE	engineered mutation	UNP O66529
jD	42	VAL	GLU	engineered mutation	UNP O66529
jD	58	VAL	ILE	engineered mutation	UNP O66529
jD	61	ASP	GLY	engineered mutation	UNP O66529
jD	62	ILE	VAL	engineered mutation	UNP O66529
jD	97	TYR	PHE	engineered mutation	UNP O66529
jD	102	GLY	-	linker	UNP O66529
jD	103	THR	-	linker	UNP O66529
jD	104	GLY	-	linker	UNP O66529
jD	105	HIS	-	linker	UNP O66529
jD	106	HIS	-	linker	UNP O66529
jD	107	HIS	-	linker	UNP O66529
jD	108	HIS	-	linker	UNP O66529
jD	109	HIS	-	linker	UNP O66529
jD	110	HIS	-	linker	UNP O66529
jD	111	GLY	-	linker	UNP O66529
jD	112	SER	-	linker	UNP O66529
jD	113	SER	-	linker	UNP O66529
jD	114	ILE	MET	engineered mutation	UNP O66529
jD	115	GLU	GLN	engineered mutation	UNP O66529
jD	138	THR	ALA	engineered mutation	UNP O66529
jD	177	ASP	GLY	engineered mutation	UNP O66529
jD	191	PHE	ILE	engineered mutation	UNP O66529
jD	193	ASP	VAL	engineered mutation	UNP O66529
kA	1	MET	-	cloning artifact	UNP P03045
kA	2	GLY	-	cloning artifact	UNP P03045
kA	3	ASN	-	cloning artifact	UNP P03045
kA	4	ALA	-	cloning artifact	UNP P03045
kA	5	LYS	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
kA	6	THR	-	cloning artifact	UNP P03045
kA	24	ALA	-	linker	UNP P03045
kA	25	GLY	-	linker	UNP P03045
kA	26	ALA	-	linker	UNP P03045
kA	27	GLY	-	linker	UNP P03045
kA	28	ALA	-	linker	UNP P03045
kA	29	GLY	-	linker	UNP P03045
kA	30	ALA	-	linker	UNP P03045
kA	31	MET	-	linker	UNP P03045
kA	39	ASN	ILE	engineered mutation	UNP O66529
kA	42	VAL	GLU	engineered mutation	UNP O66529
kA	58	VAL	ILE	engineered mutation	UNP O66529
kA	61	ASP	GLY	engineered mutation	UNP O66529
kA	62	ILE	VAL	engineered mutation	UNP O66529
kA	97	TYR	PHE	engineered mutation	UNP O66529
kA	102	GLY	-	linker	UNP O66529
kA	103	THR	-	linker	UNP O66529
kA	104	GLY	-	linker	UNP O66529
kA	105	HIS	-	linker	UNP O66529
kA	106	HIS	-	linker	UNP O66529
kA	107	HIS	-	linker	UNP O66529
kA	108	HIS	-	linker	UNP O66529
kA	109	HIS	-	linker	UNP O66529
kA	110	HIS	-	linker	UNP O66529
kA	111	GLY	-	linker	UNP O66529
kA	112	SER	-	linker	UNP O66529
kA	113	SER	-	linker	UNP O66529
kA	114	ILE	MET	engineered mutation	UNP O66529
kA	115	GLU	GLN	engineered mutation	UNP O66529
kA	138	THR	ALA	engineered mutation	UNP O66529
kA	177	ASP	GLY	engineered mutation	UNP O66529
kA	191	PHE	ILE	engineered mutation	UNP O66529
kA	193	ASP	VAL	engineered mutation	UNP O66529
kB	1	MET	-	cloning artifact	UNP P03045
kB	2	GLY	-	cloning artifact	UNP P03045
kB	3	ASN	-	cloning artifact	UNP P03045
kB	4	ALA	-	cloning artifact	UNP P03045
kB	5	LYS	-	cloning artifact	UNP P03045
kB	6	THR	-	cloning artifact	UNP P03045
kB	24	ALA	-	linker	UNP P03045
kB	25	GLY	-	linker	UNP P03045
kB	26	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
kB	27	GLY	-	linker	UNP P03045
kB	28	ALA	-	linker	UNP P03045
kB	29	GLY	-	linker	UNP P03045
kB	30	ALA	-	linker	UNP P03045
kB	31	MET	-	linker	UNP P03045
kB	39	ASN	ILE	engineered mutation	UNP O66529
kB	42	VAL	GLU	engineered mutation	UNP O66529
kB	58	VAL	ILE	engineered mutation	UNP O66529
kB	61	ASP	GLY	engineered mutation	UNP O66529
kB	62	ILE	VAL	engineered mutation	UNP O66529
kB	97	TYR	PHE	engineered mutation	UNP O66529
kB	102	GLY	-	linker	UNP O66529
kB	103	THR	-	linker	UNP O66529
kB	104	GLY	-	linker	UNP O66529
kB	105	HIS	-	linker	UNP O66529
kB	106	HIS	-	linker	UNP O66529
kB	107	HIS	-	linker	UNP O66529
kB	108	HIS	-	linker	UNP O66529
kB	109	HIS	-	linker	UNP O66529
kB	110	HIS	-	linker	UNP O66529
kB	111	GLY	-	linker	UNP O66529
kB	112	SER	-	linker	UNP O66529
kB	113	SER	-	linker	UNP O66529
kB	114	ILE	MET	engineered mutation	UNP O66529
kB	115	GLU	GLN	engineered mutation	UNP O66529
kB	138	THR	ALA	engineered mutation	UNP O66529
kB	177	ASP	GLY	engineered mutation	UNP O66529
kB	191	PHE	ILE	engineered mutation	UNP O66529
kB	193	ASP	VAL	engineered mutation	UNP O66529
kC	1	MET	-	cloning artifact	UNP P03045
kC	2	GLY	-	cloning artifact	UNP P03045
kC	3	ASN	-	cloning artifact	UNP P03045
kC	4	ALA	-	cloning artifact	UNP P03045
kC	5	LYS	-	cloning artifact	UNP P03045
kC	6	THR	-	cloning artifact	UNP P03045
kC	24	ALA	-	linker	UNP P03045
kC	25	GLY	-	linker	UNP P03045
kC	26	ALA	-	linker	UNP P03045
kC	27	GLY	-	linker	UNP P03045
kC	28	ALA	-	linker	UNP P03045
kC	29	GLY	-	linker	UNP P03045
kC	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
kC	31	MET	-	linker	UNP P03045
kC	39	ASN	ILE	engineered mutation	UNP O66529
kC	42	VAL	GLU	engineered mutation	UNP O66529
kC	58	VAL	ILE	engineered mutation	UNP O66529
kC	61	ASP	GLY	engineered mutation	UNP O66529
kC	62	ILE	VAL	engineered mutation	UNP O66529
kC	97	TYR	PHE	engineered mutation	UNP O66529
kC	102	GLY	-	linker	UNP O66529
kC	103	THR	-	linker	UNP O66529
kC	104	GLY	-	linker	UNP O66529
kC	105	HIS	-	linker	UNP O66529
kC	106	HIS	-	linker	UNP O66529
kC	107	HIS	-	linker	UNP O66529
kC	108	HIS	-	linker	UNP O66529
kC	109	HIS	-	linker	UNP O66529
kC	110	HIS	-	linker	UNP O66529
kC	111	GLY	-	linker	UNP O66529
kC	112	SER	-	linker	UNP O66529
kC	113	SER	-	linker	UNP O66529
kC	114	ILE	MET	engineered mutation	UNP O66529
kC	115	GLU	GLN	engineered mutation	UNP O66529
kC	138	THR	ALA	engineered mutation	UNP O66529
kC	177	ASP	GLY	engineered mutation	UNP O66529
kC	191	PHE	ILE	engineered mutation	UNP O66529
kC	193	ASP	VAL	engineered mutation	UNP O66529
kD	1	MET	-	cloning artifact	UNP P03045
kD	2	GLY	-	cloning artifact	UNP P03045
kD	3	ASN	-	cloning artifact	UNP P03045
kD	4	ALA	-	cloning artifact	UNP P03045
kD	5	LYS	-	cloning artifact	UNP P03045
kD	6	THR	-	cloning artifact	UNP P03045
kD	24	ALA	-	linker	UNP P03045
kD	25	GLY	-	linker	UNP P03045
kD	26	ALA	-	linker	UNP P03045
kD	27	GLY	-	linker	UNP P03045
kD	28	ALA	-	linker	UNP P03045
kD	29	GLY	-	linker	UNP P03045
kD	30	ALA	-	linker	UNP P03045
kD	31	MET	-	linker	UNP P03045
kD	39	ASN	ILE	engineered mutation	UNP O66529
kD	42	VAL	GLU	engineered mutation	UNP O66529
kD	58	VAL	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
kD	61	ASP	GLY	engineered mutation	UNP O66529
kD	62	ILE	VAL	engineered mutation	UNP O66529
kD	97	TYR	PHE	engineered mutation	UNP O66529
kD	102	GLY	-	linker	UNP O66529
kD	103	THR	-	linker	UNP O66529
kD	104	GLY	-	linker	UNP O66529
kD	105	HIS	-	linker	UNP O66529
kD	106	HIS	-	linker	UNP O66529
kD	107	HIS	-	linker	UNP O66529
kD	108	HIS	-	linker	UNP O66529
kD	109	HIS	-	linker	UNP O66529
kD	110	HIS	-	linker	UNP O66529
kD	111	GLY	-	linker	UNP O66529
kD	112	SER	-	linker	UNP O66529
kD	113	SER	-	linker	UNP O66529
kD	114	ILE	MET	engineered mutation	UNP O66529
kD	115	GLU	GLN	engineered mutation	UNP O66529
kD	138	THR	ALA	engineered mutation	UNP O66529
kD	177	ASP	GLY	engineered mutation	UNP O66529
kD	191	PHE	ILE	engineered mutation	UNP O66529
kD	193	ASP	VAL	engineered mutation	UNP O66529
lA	1	MET	-	cloning artifact	UNP P03045
lA	2	GLY	-	cloning artifact	UNP P03045
lA	3	ASN	-	cloning artifact	UNP P03045
lA	4	ALA	-	cloning artifact	UNP P03045
lA	5	LYS	-	cloning artifact	UNP P03045
lA	6	THR	-	cloning artifact	UNP P03045
lA	24	ALA	-	linker	UNP P03045
lA	25	GLY	-	linker	UNP P03045
lA	26	ALA	-	linker	UNP P03045
lA	27	GLY	-	linker	UNP P03045
lA	28	ALA	-	linker	UNP P03045
lA	29	GLY	-	linker	UNP P03045
lA	30	ALA	-	linker	UNP P03045
lA	31	MET	-	linker	UNP P03045
lA	39	ASN	ILE	engineered mutation	UNP O66529
lA	42	VAL	GLU	engineered mutation	UNP O66529
lA	58	VAL	ILE	engineered mutation	UNP O66529
lA	61	ASP	GLY	engineered mutation	UNP O66529
lA	62	ILE	VAL	engineered mutation	UNP O66529
lA	97	TYR	PHE	engineered mutation	UNP O66529
lA	102	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
lA	103	THR	-	linker	UNP O66529
lA	104	GLY	-	linker	UNP O66529
lA	105	HIS	-	linker	UNP O66529
lA	106	HIS	-	linker	UNP O66529
lA	107	HIS	-	linker	UNP O66529
lA	108	HIS	-	linker	UNP O66529
lA	109	HIS	-	linker	UNP O66529
lA	110	HIS	-	linker	UNP O66529
lA	111	GLY	-	linker	UNP O66529
lA	112	SER	-	linker	UNP O66529
lA	113	SER	-	linker	UNP O66529
lA	114	ILE	MET	engineered mutation	UNP O66529
lA	115	GLU	GLN	engineered mutation	UNP O66529
lA	138	THR	ALA	engineered mutation	UNP O66529
lA	177	ASP	GLY	engineered mutation	UNP O66529
lA	191	PHE	ILE	engineered mutation	UNP O66529
lA	193	ASP	VAL	engineered mutation	UNP O66529
lB	1	MET	-	cloning artifact	UNP P03045
lB	2	GLY	-	cloning artifact	UNP P03045
lB	3	ASN	-	cloning artifact	UNP P03045
lB	4	ALA	-	cloning artifact	UNP P03045
lB	5	LYS	-	cloning artifact	UNP P03045
lB	6	THR	-	cloning artifact	UNP P03045
lB	24	ALA	-	linker	UNP P03045
lB	25	GLY	-	linker	UNP P03045
lB	26	ALA	-	linker	UNP P03045
lB	27	GLY	-	linker	UNP P03045
lB	28	ALA	-	linker	UNP P03045
lB	29	GLY	-	linker	UNP P03045
lB	30	ALA	-	linker	UNP P03045
lB	31	MET	-	linker	UNP P03045
lB	39	ASN	ILE	engineered mutation	UNP O66529
lB	42	VAL	GLU	engineered mutation	UNP O66529
lB	58	VAL	ILE	engineered mutation	UNP O66529
lB	61	ASP	GLY	engineered mutation	UNP O66529
lB	62	ILE	VAL	engineered mutation	UNP O66529
lB	97	TYR	PHE	engineered mutation	UNP O66529
lB	102	GLY	-	linker	UNP O66529
lB	103	THR	-	linker	UNP O66529
lB	104	GLY	-	linker	UNP O66529
lB	105	HIS	-	linker	UNP O66529
lB	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
lB	107	HIS	-	linker	UNP O66529
lB	108	HIS	-	linker	UNP O66529
lB	109	HIS	-	linker	UNP O66529
lB	110	HIS	-	linker	UNP O66529
lB	111	GLY	-	linker	UNP O66529
lB	112	SER	-	linker	UNP O66529
lB	113	SER	-	linker	UNP O66529
lB	114	ILE	MET	engineered mutation	UNP O66529
lB	115	GLU	GLN	engineered mutation	UNP O66529
lB	138	THR	ALA	engineered mutation	UNP O66529
lB	177	ASP	GLY	engineered mutation	UNP O66529
lB	191	PHE	ILE	engineered mutation	UNP O66529
lB	193	ASP	VAL	engineered mutation	UNP O66529
lC	1	MET	-	cloning artifact	UNP P03045
lC	2	GLY	-	cloning artifact	UNP P03045
lC	3	ASN	-	cloning artifact	UNP P03045
lC	4	ALA	-	cloning artifact	UNP P03045
lC	5	LYS	-	cloning artifact	UNP P03045
lC	6	THR	-	cloning artifact	UNP P03045
lC	24	ALA	-	linker	UNP P03045
lC	25	GLY	-	linker	UNP P03045
lC	26	ALA	-	linker	UNP P03045
lC	27	GLY	-	linker	UNP P03045
lC	28	ALA	-	linker	UNP P03045
lC	29	GLY	-	linker	UNP P03045
lC	30	ALA	-	linker	UNP P03045
lC	31	MET	-	linker	UNP P03045
lC	39	ASN	ILE	engineered mutation	UNP O66529
lC	42	VAL	GLU	engineered mutation	UNP O66529
lC	58	VAL	ILE	engineered mutation	UNP O66529
lC	61	ASP	GLY	engineered mutation	UNP O66529
lC	62	ILE	VAL	engineered mutation	UNP O66529
lC	97	TYR	PHE	engineered mutation	UNP O66529
lC	102	GLY	-	linker	UNP O66529
lC	103	THR	-	linker	UNP O66529
lC	104	GLY	-	linker	UNP O66529
lC	105	HIS	-	linker	UNP O66529
lC	106	HIS	-	linker	UNP O66529
lC	107	HIS	-	linker	UNP O66529
lC	108	HIS	-	linker	UNP O66529
lC	109	HIS	-	linker	UNP O66529
lC	110	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
lC	111	GLY	-	linker	UNP O66529
lC	112	SER	-	linker	UNP O66529
lC	113	SER	-	linker	UNP O66529
lC	114	ILE	MET	engineered mutation	UNP O66529
lC	115	GLU	GLN	engineered mutation	UNP O66529
lC	138	THR	ALA	engineered mutation	UNP O66529
lC	177	ASP	GLY	engineered mutation	UNP O66529
lC	191	PHE	ILE	engineered mutation	UNP O66529
lC	193	ASP	VAL	engineered mutation	UNP O66529
lD	1	MET	-	cloning artifact	UNP P03045
lD	2	GLY	-	cloning artifact	UNP P03045
lD	3	ASN	-	cloning artifact	UNP P03045
lD	4	ALA	-	cloning artifact	UNP P03045
lD	5	LYS	-	cloning artifact	UNP P03045
lD	6	THR	-	cloning artifact	UNP P03045
lD	24	ALA	-	linker	UNP P03045
lD	25	GLY	-	linker	UNP P03045
lD	26	ALA	-	linker	UNP P03045
lD	27	GLY	-	linker	UNP P03045
lD	28	ALA	-	linker	UNP P03045
lD	29	GLY	-	linker	UNP P03045
lD	30	ALA	-	linker	UNP P03045
lD	31	MET	-	linker	UNP P03045
lD	39	ASN	ILE	engineered mutation	UNP O66529
lD	42	VAL	GLU	engineered mutation	UNP O66529
lD	58	VAL	ILE	engineered mutation	UNP O66529
lD	61	ASP	GLY	engineered mutation	UNP O66529
lD	62	ILE	VAL	engineered mutation	UNP O66529
lD	97	TYR	PHE	engineered mutation	UNP O66529
lD	102	GLY	-	linker	UNP O66529
lD	103	THR	-	linker	UNP O66529
lD	104	GLY	-	linker	UNP O66529
lD	105	HIS	-	linker	UNP O66529
lD	106	HIS	-	linker	UNP O66529
lD	107	HIS	-	linker	UNP O66529
lD	108	HIS	-	linker	UNP O66529
lD	109	HIS	-	linker	UNP O66529
lD	110	HIS	-	linker	UNP O66529
lD	111	GLY	-	linker	UNP O66529
lD	112	SER	-	linker	UNP O66529
lD	113	SER	-	linker	UNP O66529
lD	114	ILE	MET	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
lD	115	GLU	GLN	engineered mutation	UNP O66529
lD	138	THR	ALA	engineered mutation	UNP O66529
lD	177	ASP	GLY	engineered mutation	UNP O66529
lD	191	PHE	ILE	engineered mutation	UNP O66529
lD	193	ASP	VAL	engineered mutation	UNP O66529
mA	1	MET	-	cloning artifact	UNP P03045
mA	2	GLY	-	cloning artifact	UNP P03045
mA	3	ASN	-	cloning artifact	UNP P03045
mA	4	ALA	-	cloning artifact	UNP P03045
mA	5	LYS	-	cloning artifact	UNP P03045
mA	6	THR	-	cloning artifact	UNP P03045
mA	24	ALA	-	linker	UNP P03045
mA	25	GLY	-	linker	UNP P03045
mA	26	ALA	-	linker	UNP P03045
mA	27	GLY	-	linker	UNP P03045
mA	28	ALA	-	linker	UNP P03045
mA	29	GLY	-	linker	UNP P03045
mA	30	ALA	-	linker	UNP P03045
mA	31	MET	-	linker	UNP P03045
mA	39	ASN	ILE	engineered mutation	UNP O66529
mA	42	VAL	GLU	engineered mutation	UNP O66529
mA	58	VAL	ILE	engineered mutation	UNP O66529
mA	61	ASP	GLY	engineered mutation	UNP O66529
mA	62	ILE	VAL	engineered mutation	UNP O66529
mA	97	TYR	PHE	engineered mutation	UNP O66529
mA	102	GLY	-	linker	UNP O66529
mA	103	THR	-	linker	UNP O66529
mA	104	GLY	-	linker	UNP O66529
mA	105	HIS	-	linker	UNP O66529
mA	106	HIS	-	linker	UNP O66529
mA	107	HIS	-	linker	UNP O66529
mA	108	HIS	-	linker	UNP O66529
mA	109	HIS	-	linker	UNP O66529
mA	110	HIS	-	linker	UNP O66529
mA	111	GLY	-	linker	UNP O66529
mA	112	SER	-	linker	UNP O66529
mA	113	SER	-	linker	UNP O66529
mA	114	ILE	MET	engineered mutation	UNP O66529
mA	115	GLU	GLN	engineered mutation	UNP O66529
mA	138	THR	ALA	engineered mutation	UNP O66529
mA	177	ASP	GLY	engineered mutation	UNP O66529
mA	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
mA	193	ASP	VAL	engineered mutation	UNP O66529
mB	1	MET	-	cloning artifact	UNP P03045
mB	2	GLY	-	cloning artifact	UNP P03045
mB	3	ASN	-	cloning artifact	UNP P03045
mB	4	ALA	-	cloning artifact	UNP P03045
mB	5	LYS	-	cloning artifact	UNP P03045
mB	6	THR	-	cloning artifact	UNP P03045
mB	24	ALA	-	linker	UNP P03045
mB	25	GLY	-	linker	UNP P03045
mB	26	ALA	-	linker	UNP P03045
mB	27	GLY	-	linker	UNP P03045
mB	28	ALA	-	linker	UNP P03045
mB	29	GLY	-	linker	UNP P03045
mB	30	ALA	-	linker	UNP P03045
mB	31	MET	-	linker	UNP P03045
mB	39	ASN	ILE	engineered mutation	UNP O66529
mB	42	VAL	GLU	engineered mutation	UNP O66529
mB	58	VAL	ILE	engineered mutation	UNP O66529
mB	61	ASP	GLY	engineered mutation	UNP O66529
mB	62	ILE	VAL	engineered mutation	UNP O66529
mB	97	TYR	PHE	engineered mutation	UNP O66529
mB	102	GLY	-	linker	UNP O66529
mB	103	THR	-	linker	UNP O66529
mB	104	GLY	-	linker	UNP O66529
mB	105	HIS	-	linker	UNP O66529
mB	106	HIS	-	linker	UNP O66529
mB	107	HIS	-	linker	UNP O66529
mB	108	HIS	-	linker	UNP O66529
mB	109	HIS	-	linker	UNP O66529
mB	110	HIS	-	linker	UNP O66529
mB	111	GLY	-	linker	UNP O66529
mB	112	SER	-	linker	UNP O66529
mB	113	SER	-	linker	UNP O66529
mB	114	ILE	MET	engineered mutation	UNP O66529
mB	115	GLU	GLN	engineered mutation	UNP O66529
mB	138	THR	ALA	engineered mutation	UNP O66529
mB	177	ASP	GLY	engineered mutation	UNP O66529
mB	191	PHE	ILE	engineered mutation	UNP O66529
mB	193	ASP	VAL	engineered mutation	UNP O66529
mC	1	MET	-	cloning artifact	UNP P03045
mC	2	GLY	-	cloning artifact	UNP P03045
mC	3	ASN	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
mC	4	ALA	-	cloning artifact	UNP P03045
mC	5	LYS	-	cloning artifact	UNP P03045
mC	6	THR	-	cloning artifact	UNP P03045
mC	24	ALA	-	linker	UNP P03045
mC	25	GLY	-	linker	UNP P03045
mC	26	ALA	-	linker	UNP P03045
mC	27	GLY	-	linker	UNP P03045
mC	28	ALA	-	linker	UNP P03045
mC	29	GLY	-	linker	UNP P03045
mC	30	ALA	-	linker	UNP P03045
mC	31	MET	-	linker	UNP P03045
mC	39	ASN	ILE	engineered mutation	UNP O66529
mC	42	VAL	GLU	engineered mutation	UNP O66529
mC	58	VAL	ILE	engineered mutation	UNP O66529
mC	61	ASP	GLY	engineered mutation	UNP O66529
mC	62	ILE	VAL	engineered mutation	UNP O66529
mC	97	TYR	PHE	engineered mutation	UNP O66529
mC	102	GLY	-	linker	UNP O66529
mC	103	THR	-	linker	UNP O66529
mC	104	GLY	-	linker	UNP O66529
mC	105	HIS	-	linker	UNP O66529
mC	106	HIS	-	linker	UNP O66529
mC	107	HIS	-	linker	UNP O66529
mC	108	HIS	-	linker	UNP O66529
mC	109	HIS	-	linker	UNP O66529
mC	110	HIS	-	linker	UNP O66529
mC	111	GLY	-	linker	UNP O66529
mC	112	SER	-	linker	UNP O66529
mC	113	SER	-	linker	UNP O66529
mC	114	ILE	MET	engineered mutation	UNP O66529
mC	115	GLU	GLN	engineered mutation	UNP O66529
mC	138	THR	ALA	engineered mutation	UNP O66529
mC	177	ASP	GLY	engineered mutation	UNP O66529
mC	191	PHE	ILE	engineered mutation	UNP O66529
mC	193	ASP	VAL	engineered mutation	UNP O66529
mD	1	MET	-	cloning artifact	UNP P03045
mD	2	GLY	-	cloning artifact	UNP P03045
mD	3	ASN	-	cloning artifact	UNP P03045
mD	4	ALA	-	cloning artifact	UNP P03045
mD	5	LYS	-	cloning artifact	UNP P03045
mD	6	THR	-	cloning artifact	UNP P03045
mD	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
mD	25	GLY	-	linker	UNP P03045
mD	26	ALA	-	linker	UNP P03045
mD	27	GLY	-	linker	UNP P03045
mD	28	ALA	-	linker	UNP P03045
mD	29	GLY	-	linker	UNP P03045
mD	30	ALA	-	linker	UNP P03045
mD	31	MET	-	linker	UNP P03045
mD	39	ASN	ILE	engineered mutation	UNP O66529
mD	42	VAL	GLU	engineered mutation	UNP O66529
mD	58	VAL	ILE	engineered mutation	UNP O66529
mD	61	ASP	GLY	engineered mutation	UNP O66529
mD	62	ILE	VAL	engineered mutation	UNP O66529
mD	97	TYR	PHE	engineered mutation	UNP O66529
mD	102	GLY	-	linker	UNP O66529
mD	103	THR	-	linker	UNP O66529
mD	104	GLY	-	linker	UNP O66529
mD	105	HIS	-	linker	UNP O66529
mD	106	HIS	-	linker	UNP O66529
mD	107	HIS	-	linker	UNP O66529
mD	108	HIS	-	linker	UNP O66529
mD	109	HIS	-	linker	UNP O66529
mD	110	HIS	-	linker	UNP O66529
mD	111	GLY	-	linker	UNP O66529
mD	112	SER	-	linker	UNP O66529
mD	113	SER	-	linker	UNP O66529
mD	114	ILE	MET	engineered mutation	UNP O66529
mD	115	GLU	GLN	engineered mutation	UNP O66529
mD	138	THR	ALA	engineered mutation	UNP O66529
mD	177	ASP	GLY	engineered mutation	UNP O66529
mD	191	PHE	ILE	engineered mutation	UNP O66529
mD	193	ASP	VAL	engineered mutation	UNP O66529
nA	1	MET	-	cloning artifact	UNP P03045
nA	2	GLY	-	cloning artifact	UNP P03045
nA	3	ASN	-	cloning artifact	UNP P03045
nA	4	ALA	-	cloning artifact	UNP P03045
nA	5	LYS	-	cloning artifact	UNP P03045
nA	6	THR	-	cloning artifact	UNP P03045
nA	24	ALA	-	linker	UNP P03045
nA	25	GLY	-	linker	UNP P03045
nA	26	ALA	-	linker	UNP P03045
nA	27	GLY	-	linker	UNP P03045
nA	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
nA	29	GLY	-	linker	UNP P03045
nA	30	ALA	-	linker	UNP P03045
nA	31	MET	-	linker	UNP P03045
nA	39	ASN	ILE	engineered mutation	UNP O66529
nA	42	VAL	GLU	engineered mutation	UNP O66529
nA	58	VAL	ILE	engineered mutation	UNP O66529
nA	61	ASP	GLY	engineered mutation	UNP O66529
nA	62	ILE	VAL	engineered mutation	UNP O66529
nA	97	TYR	PHE	engineered mutation	UNP O66529
nA	102	GLY	-	linker	UNP O66529
nA	103	THR	-	linker	UNP O66529
nA	104	GLY	-	linker	UNP O66529
nA	105	HIS	-	linker	UNP O66529
nA	106	HIS	-	linker	UNP O66529
nA	107	HIS	-	linker	UNP O66529
nA	108	HIS	-	linker	UNP O66529
nA	109	HIS	-	linker	UNP O66529
nA	110	HIS	-	linker	UNP O66529
nA	111	GLY	-	linker	UNP O66529
nA	112	SER	-	linker	UNP O66529
nA	113	SER	-	linker	UNP O66529
nA	114	ILE	MET	engineered mutation	UNP O66529
nA	115	GLU	GLN	engineered mutation	UNP O66529
nA	138	THR	ALA	engineered mutation	UNP O66529
nA	177	ASP	GLY	engineered mutation	UNP O66529
nA	191	PHE	ILE	engineered mutation	UNP O66529
nA	193	ASP	VAL	engineered mutation	UNP O66529
nB	1	MET	-	cloning artifact	UNP P03045
nB	2	GLY	-	cloning artifact	UNP P03045
nB	3	ASN	-	cloning artifact	UNP P03045
nB	4	ALA	-	cloning artifact	UNP P03045
nB	5	LYS	-	cloning artifact	UNP P03045
nB	6	THR	-	cloning artifact	UNP P03045
nB	24	ALA	-	linker	UNP P03045
nB	25	GLY	-	linker	UNP P03045
nB	26	ALA	-	linker	UNP P03045
nB	27	GLY	-	linker	UNP P03045
nB	28	ALA	-	linker	UNP P03045
nB	29	GLY	-	linker	UNP P03045
nB	30	ALA	-	linker	UNP P03045
nB	31	MET	-	linker	UNP P03045
nB	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
nB	42	VAL	GLU	engineered mutation	UNP O66529
nB	58	VAL	ILE	engineered mutation	UNP O66529
nB	61	ASP	GLY	engineered mutation	UNP O66529
nB	62	ILE	VAL	engineered mutation	UNP O66529
nB	97	TYR	PHE	engineered mutation	UNP O66529
nB	102	GLY	-	linker	UNP O66529
nB	103	THR	-	linker	UNP O66529
nB	104	GLY	-	linker	UNP O66529
nB	105	HIS	-	linker	UNP O66529
nB	106	HIS	-	linker	UNP O66529
nB	107	HIS	-	linker	UNP O66529
nB	108	HIS	-	linker	UNP O66529
nB	109	HIS	-	linker	UNP O66529
nB	110	HIS	-	linker	UNP O66529
nB	111	GLY	-	linker	UNP O66529
nB	112	SER	-	linker	UNP O66529
nB	113	SER	-	linker	UNP O66529
nB	114	ILE	MET	engineered mutation	UNP O66529
nB	115	GLU	GLN	engineered mutation	UNP O66529
nB	138	THR	ALA	engineered mutation	UNP O66529
nB	177	ASP	GLY	engineered mutation	UNP O66529
nB	191	PHE	ILE	engineered mutation	UNP O66529
nB	193	ASP	VAL	engineered mutation	UNP O66529
nC	1	MET	-	cloning artifact	UNP P03045
nC	2	GLY	-	cloning artifact	UNP P03045
nC	3	ASN	-	cloning artifact	UNP P03045
nC	4	ALA	-	cloning artifact	UNP P03045
nC	5	LYS	-	cloning artifact	UNP P03045
nC	6	THR	-	cloning artifact	UNP P03045
nC	24	ALA	-	linker	UNP P03045
nC	25	GLY	-	linker	UNP P03045
nC	26	ALA	-	linker	UNP P03045
nC	27	GLY	-	linker	UNP P03045
nC	28	ALA	-	linker	UNP P03045
nC	29	GLY	-	linker	UNP P03045
nC	30	ALA	-	linker	UNP P03045
nC	31	MET	-	linker	UNP P03045
nC	39	ASN	ILE	engineered mutation	UNP O66529
nC	42	VAL	GLU	engineered mutation	UNP O66529
nC	58	VAL	ILE	engineered mutation	UNP O66529
nC	61	ASP	GLY	engineered mutation	UNP O66529
nC	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
nC	97	TYR	PHE	engineered mutation	UNP O66529
nC	102	GLY	-	linker	UNP O66529
nC	103	THR	-	linker	UNP O66529
nC	104	GLY	-	linker	UNP O66529
nC	105	HIS	-	linker	UNP O66529
nC	106	HIS	-	linker	UNP O66529
nC	107	HIS	-	linker	UNP O66529
nC	108	HIS	-	linker	UNP O66529
nC	109	HIS	-	linker	UNP O66529
nC	110	HIS	-	linker	UNP O66529
nC	111	GLY	-	linker	UNP O66529
nC	112	SER	-	linker	UNP O66529
nC	113	SER	-	linker	UNP O66529
nC	114	ILE	MET	engineered mutation	UNP O66529
nC	115	GLU	GLN	engineered mutation	UNP O66529
nC	138	THR	ALA	engineered mutation	UNP O66529
nC	177	ASP	GLY	engineered mutation	UNP O66529
nC	191	PHE	ILE	engineered mutation	UNP O66529
nC	193	ASP	VAL	engineered mutation	UNP O66529
nD	1	MET	-	cloning artifact	UNP P03045
nD	2	GLY	-	cloning artifact	UNP P03045
nD	3	ASN	-	cloning artifact	UNP P03045
nD	4	ALA	-	cloning artifact	UNP P03045
nD	5	LYS	-	cloning artifact	UNP P03045
nD	6	THR	-	cloning artifact	UNP P03045
nD	24	ALA	-	linker	UNP P03045
nD	25	GLY	-	linker	UNP P03045
nD	26	ALA	-	linker	UNP P03045
nD	27	GLY	-	linker	UNP P03045
nD	28	ALA	-	linker	UNP P03045
nD	29	GLY	-	linker	UNP P03045
nD	30	ALA	-	linker	UNP P03045
nD	31	MET	-	linker	UNP P03045
nD	39	ASN	ILE	engineered mutation	UNP O66529
nD	42	VAL	GLU	engineered mutation	UNP O66529
nD	58	VAL	ILE	engineered mutation	UNP O66529
nD	61	ASP	GLY	engineered mutation	UNP O66529
nD	62	ILE	VAL	engineered mutation	UNP O66529
nD	97	TYR	PHE	engineered mutation	UNP O66529
nD	102	GLY	-	linker	UNP O66529
nD	103	THR	-	linker	UNP O66529
nD	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
nD	105	HIS	-	linker	UNP O66529
nD	106	HIS	-	linker	UNP O66529
nD	107	HIS	-	linker	UNP O66529
nD	108	HIS	-	linker	UNP O66529
nD	109	HIS	-	linker	UNP O66529
nD	110	HIS	-	linker	UNP O66529
nD	111	GLY	-	linker	UNP O66529
nD	112	SER	-	linker	UNP O66529
nD	113	SER	-	linker	UNP O66529
nD	114	ILE	MET	engineered mutation	UNP O66529
nD	115	GLU	GLN	engineered mutation	UNP O66529
nD	138	THR	ALA	engineered mutation	UNP O66529
nD	177	ASP	GLY	engineered mutation	UNP O66529
nD	191	PHE	ILE	engineered mutation	UNP O66529
nD	193	ASP	VAL	engineered mutation	UNP O66529
oA	1	MET	-	cloning artifact	UNP P03045
oA	2	GLY	-	cloning artifact	UNP P03045
oA	3	ASN	-	cloning artifact	UNP P03045
oA	4	ALA	-	cloning artifact	UNP P03045
oA	5	LYS	-	cloning artifact	UNP P03045
oA	6	THR	-	cloning artifact	UNP P03045
oA	24	ALA	-	linker	UNP P03045
oA	25	GLY	-	linker	UNP P03045
oA	26	ALA	-	linker	UNP P03045
oA	27	GLY	-	linker	UNP P03045
oA	28	ALA	-	linker	UNP P03045
oA	29	GLY	-	linker	UNP P03045
oA	30	ALA	-	linker	UNP P03045
oA	31	MET	-	linker	UNP P03045
oA	39	ASN	ILE	engineered mutation	UNP O66529
oA	42	VAL	GLU	engineered mutation	UNP O66529
oA	58	VAL	ILE	engineered mutation	UNP O66529
oA	61	ASP	GLY	engineered mutation	UNP O66529
oA	62	ILE	VAL	engineered mutation	UNP O66529
oA	97	TYR	PHE	engineered mutation	UNP O66529
oA	102	GLY	-	linker	UNP O66529
oA	103	THR	-	linker	UNP O66529
oA	104	GLY	-	linker	UNP O66529
oA	105	HIS	-	linker	UNP O66529
oA	106	HIS	-	linker	UNP O66529
oA	107	HIS	-	linker	UNP O66529
oA	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
oA	109	HIS	-	linker	UNP O66529
oA	110	HIS	-	linker	UNP O66529
oA	111	GLY	-	linker	UNP O66529
oA	112	SER	-	linker	UNP O66529
oA	113	SER	-	linker	UNP O66529
oA	114	ILE	MET	engineered mutation	UNP O66529
oA	115	GLU	GLN	engineered mutation	UNP O66529
oA	138	THR	ALA	engineered mutation	UNP O66529
oA	177	ASP	GLY	engineered mutation	UNP O66529
oA	191	PHE	ILE	engineered mutation	UNP O66529
oA	193	ASP	VAL	engineered mutation	UNP O66529
oB	1	MET	-	cloning artifact	UNP P03045
oB	2	GLY	-	cloning artifact	UNP P03045
oB	3	ASN	-	cloning artifact	UNP P03045
oB	4	ALA	-	cloning artifact	UNP P03045
oB	5	LYS	-	cloning artifact	UNP P03045
oB	6	THR	-	cloning artifact	UNP P03045
oB	24	ALA	-	linker	UNP P03045
oB	25	GLY	-	linker	UNP P03045
oB	26	ALA	-	linker	UNP P03045
oB	27	GLY	-	linker	UNP P03045
oB	28	ALA	-	linker	UNP P03045
oB	29	GLY	-	linker	UNP P03045
oB	30	ALA	-	linker	UNP P03045
oB	31	MET	-	linker	UNP P03045
oB	39	ASN	ILE	engineered mutation	UNP O66529
oB	42	VAL	GLU	engineered mutation	UNP O66529
oB	58	VAL	ILE	engineered mutation	UNP O66529
oB	61	ASP	GLY	engineered mutation	UNP O66529
oB	62	ILE	VAL	engineered mutation	UNP O66529
oB	97	TYR	PHE	engineered mutation	UNP O66529
oB	102	GLY	-	linker	UNP O66529
oB	103	THR	-	linker	UNP O66529
oB	104	GLY	-	linker	UNP O66529
oB	105	HIS	-	linker	UNP O66529
oB	106	HIS	-	linker	UNP O66529
oB	107	HIS	-	linker	UNP O66529
oB	108	HIS	-	linker	UNP O66529
oB	109	HIS	-	linker	UNP O66529
oB	110	HIS	-	linker	UNP O66529
oB	111	GLY	-	linker	UNP O66529
oB	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
oB	113	SER	-	linker	UNP O66529
oB	114	ILE	MET	engineered mutation	UNP O66529
oB	115	GLU	GLN	engineered mutation	UNP O66529
oB	138	THR	ALA	engineered mutation	UNP O66529
oB	177	ASP	GLY	engineered mutation	UNP O66529
oB	191	PHE	ILE	engineered mutation	UNP O66529
oB	193	ASP	VAL	engineered mutation	UNP O66529
oC	1	MET	-	cloning artifact	UNP P03045
oC	2	GLY	-	cloning artifact	UNP P03045
oC	3	ASN	-	cloning artifact	UNP P03045
oC	4	ALA	-	cloning artifact	UNP P03045
oC	5	LYS	-	cloning artifact	UNP P03045
oC	6	THR	-	cloning artifact	UNP P03045
oC	24	ALA	-	linker	UNP P03045
oC	25	GLY	-	linker	UNP P03045
oC	26	ALA	-	linker	UNP P03045
oC	27	GLY	-	linker	UNP P03045
oC	28	ALA	-	linker	UNP P03045
oC	29	GLY	-	linker	UNP P03045
oC	30	ALA	-	linker	UNP P03045
oC	31	MET	-	linker	UNP P03045
oC	39	ASN	ILE	engineered mutation	UNP O66529
oC	42	VAL	GLU	engineered mutation	UNP O66529
oC	58	VAL	ILE	engineered mutation	UNP O66529
oC	61	ASP	GLY	engineered mutation	UNP O66529
oC	62	ILE	VAL	engineered mutation	UNP O66529
oC	97	TYR	PHE	engineered mutation	UNP O66529
oC	102	GLY	-	linker	UNP O66529
oC	103	THR	-	linker	UNP O66529
oC	104	GLY	-	linker	UNP O66529
oC	105	HIS	-	linker	UNP O66529
oC	106	HIS	-	linker	UNP O66529
oC	107	HIS	-	linker	UNP O66529
oC	108	HIS	-	linker	UNP O66529
oC	109	HIS	-	linker	UNP O66529
oC	110	HIS	-	linker	UNP O66529
oC	111	GLY	-	linker	UNP O66529
oC	112	SER	-	linker	UNP O66529
oC	113	SER	-	linker	UNP O66529
oC	114	ILE	MET	engineered mutation	UNP O66529
oC	115	GLU	GLN	engineered mutation	UNP O66529
oC	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
oC	177	ASP	GLY	engineered mutation	UNP O66529
oC	191	PHE	ILE	engineered mutation	UNP O66529
oC	193	ASP	VAL	engineered mutation	UNP O66529
oD	1	MET	-	cloning artifact	UNP P03045
oD	2	GLY	-	cloning artifact	UNP P03045
oD	3	ASN	-	cloning artifact	UNP P03045
oD	4	ALA	-	cloning artifact	UNP P03045
oD	5	LYS	-	cloning artifact	UNP P03045
oD	6	THR	-	cloning artifact	UNP P03045
oD	24	ALA	-	linker	UNP P03045
oD	25	GLY	-	linker	UNP P03045
oD	26	ALA	-	linker	UNP P03045
oD	27	GLY	-	linker	UNP P03045
oD	28	ALA	-	linker	UNP P03045
oD	29	GLY	-	linker	UNP P03045
oD	30	ALA	-	linker	UNP P03045
oD	31	MET	-	linker	UNP P03045
oD	39	ASN	ILE	engineered mutation	UNP O66529
oD	42	VAL	GLU	engineered mutation	UNP O66529
oD	58	VAL	ILE	engineered mutation	UNP O66529
oD	61	ASP	GLY	engineered mutation	UNP O66529
oD	62	ILE	VAL	engineered mutation	UNP O66529
oD	97	TYR	PHE	engineered mutation	UNP O66529
oD	102	GLY	-	linker	UNP O66529
oD	103	THR	-	linker	UNP O66529
oD	104	GLY	-	linker	UNP O66529
oD	105	HIS	-	linker	UNP O66529
oD	106	HIS	-	linker	UNP O66529
oD	107	HIS	-	linker	UNP O66529
oD	108	HIS	-	linker	UNP O66529
oD	109	HIS	-	linker	UNP O66529
oD	110	HIS	-	linker	UNP O66529
oD	111	GLY	-	linker	UNP O66529
oD	112	SER	-	linker	UNP O66529
oD	113	SER	-	linker	UNP O66529
oD	114	ILE	MET	engineered mutation	UNP O66529
oD	115	GLU	GLN	engineered mutation	UNP O66529
oD	138	THR	ALA	engineered mutation	UNP O66529
oD	177	ASP	GLY	engineered mutation	UNP O66529
oD	191	PHE	ILE	engineered mutation	UNP O66529
oD	193	ASP	VAL	engineered mutation	UNP O66529
pA	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
pA	2	GLY	-	cloning artifact	UNP P03045
pA	3	ASN	-	cloning artifact	UNP P03045
pA	4	ALA	-	cloning artifact	UNP P03045
pA	5	LYS	-	cloning artifact	UNP P03045
pA	6	THR	-	cloning artifact	UNP P03045
pA	24	ALA	-	linker	UNP P03045
pA	25	GLY	-	linker	UNP P03045
pA	26	ALA	-	linker	UNP P03045
pA	27	GLY	-	linker	UNP P03045
pA	28	ALA	-	linker	UNP P03045
pA	29	GLY	-	linker	UNP P03045
pA	30	ALA	-	linker	UNP P03045
pA	31	MET	-	linker	UNP P03045
pA	39	ASN	ILE	engineered mutation	UNP O66529
pA	42	VAL	GLU	engineered mutation	UNP O66529
pA	58	VAL	ILE	engineered mutation	UNP O66529
pA	61	ASP	GLY	engineered mutation	UNP O66529
pA	62	ILE	VAL	engineered mutation	UNP O66529
pA	97	TYR	PHE	engineered mutation	UNP O66529
pA	102	GLY	-	linker	UNP O66529
pA	103	THR	-	linker	UNP O66529
pA	104	GLY	-	linker	UNP O66529
pA	105	HIS	-	linker	UNP O66529
pA	106	HIS	-	linker	UNP O66529
pA	107	HIS	-	linker	UNP O66529
pA	108	HIS	-	linker	UNP O66529
pA	109	HIS	-	linker	UNP O66529
pA	110	HIS	-	linker	UNP O66529
pA	111	GLY	-	linker	UNP O66529
pA	112	SER	-	linker	UNP O66529
pA	113	SER	-	linker	UNP O66529
pA	114	ILE	MET	engineered mutation	UNP O66529
pA	115	GLU	GLN	engineered mutation	UNP O66529
pA	138	THR	ALA	engineered mutation	UNP O66529
pA	177	ASP	GLY	engineered mutation	UNP O66529
pA	191	PHE	ILE	engineered mutation	UNP O66529
pA	193	ASP	VAL	engineered mutation	UNP O66529
pB	1	MET	-	cloning artifact	UNP P03045
pB	2	GLY	-	cloning artifact	UNP P03045
pB	3	ASN	-	cloning artifact	UNP P03045
pB	4	ALA	-	cloning artifact	UNP P03045
pB	5	LYS	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
pB	6	THR	-	cloning artifact	UNP P03045
pB	24	ALA	-	linker	UNP P03045
pB	25	GLY	-	linker	UNP P03045
pB	26	ALA	-	linker	UNP P03045
pB	27	GLY	-	linker	UNP P03045
pB	28	ALA	-	linker	UNP P03045
pB	29	GLY	-	linker	UNP P03045
pB	30	ALA	-	linker	UNP P03045
pB	31	MET	-	linker	UNP P03045
pB	39	ASN	ILE	engineered mutation	UNP O66529
pB	42	VAL	GLU	engineered mutation	UNP O66529
pB	58	VAL	ILE	engineered mutation	UNP O66529
pB	61	ASP	GLY	engineered mutation	UNP O66529
pB	62	ILE	VAL	engineered mutation	UNP O66529
pB	97	TYR	PHE	engineered mutation	UNP O66529
pB	102	GLY	-	linker	UNP O66529
pB	103	THR	-	linker	UNP O66529
pB	104	GLY	-	linker	UNP O66529
pB	105	HIS	-	linker	UNP O66529
pB	106	HIS	-	linker	UNP O66529
pB	107	HIS	-	linker	UNP O66529
pB	108	HIS	-	linker	UNP O66529
pB	109	HIS	-	linker	UNP O66529
pB	110	HIS	-	linker	UNP O66529
pB	111	GLY	-	linker	UNP O66529
pB	112	SER	-	linker	UNP O66529
pB	113	SER	-	linker	UNP O66529
pB	114	ILE	MET	engineered mutation	UNP O66529
pB	115	GLU	GLN	engineered mutation	UNP O66529
pB	138	THR	ALA	engineered mutation	UNP O66529
pB	177	ASP	GLY	engineered mutation	UNP O66529
pB	191	PHE	ILE	engineered mutation	UNP O66529
pB	193	ASP	VAL	engineered mutation	UNP O66529
pC	1	MET	-	cloning artifact	UNP P03045
pC	2	GLY	-	cloning artifact	UNP P03045
pC	3	ASN	-	cloning artifact	UNP P03045
pC	4	ALA	-	cloning artifact	UNP P03045
pC	5	LYS	-	cloning artifact	UNP P03045
pC	6	THR	-	cloning artifact	UNP P03045
pC	24	ALA	-	linker	UNP P03045
pC	25	GLY	-	linker	UNP P03045
pC	26	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
pC	27	GLY	-	linker	UNP P03045
pC	28	ALA	-	linker	UNP P03045
pC	29	GLY	-	linker	UNP P03045
pC	30	ALA	-	linker	UNP P03045
pC	31	MET	-	linker	UNP P03045
pC	39	ASN	ILE	engineered mutation	UNP O66529
pC	42	VAL	GLU	engineered mutation	UNP O66529
pC	58	VAL	ILE	engineered mutation	UNP O66529
pC	61	ASP	GLY	engineered mutation	UNP O66529
pC	62	ILE	VAL	engineered mutation	UNP O66529
pC	97	TYR	PHE	engineered mutation	UNP O66529
pC	102	GLY	-	linker	UNP O66529
pC	103	THR	-	linker	UNP O66529
pC	104	GLY	-	linker	UNP O66529
pC	105	HIS	-	linker	UNP O66529
pC	106	HIS	-	linker	UNP O66529
pC	107	HIS	-	linker	UNP O66529
pC	108	HIS	-	linker	UNP O66529
pC	109	HIS	-	linker	UNP O66529
pC	110	HIS	-	linker	UNP O66529
pC	111	GLY	-	linker	UNP O66529
pC	112	SER	-	linker	UNP O66529
pC	113	SER	-	linker	UNP O66529
pC	114	ILE	MET	engineered mutation	UNP O66529
pC	115	GLU	GLN	engineered mutation	UNP O66529
pC	138	THR	ALA	engineered mutation	UNP O66529
pC	177	ASP	GLY	engineered mutation	UNP O66529
pC	191	PHE	ILE	engineered mutation	UNP O66529
pC	193	ASP	VAL	engineered mutation	UNP O66529
pD	1	MET	-	cloning artifact	UNP P03045
pD	2	GLY	-	cloning artifact	UNP P03045
pD	3	ASN	-	cloning artifact	UNP P03045
pD	4	ALA	-	cloning artifact	UNP P03045
pD	5	LYS	-	cloning artifact	UNP P03045
pD	6	THR	-	cloning artifact	UNP P03045
pD	24	ALA	-	linker	UNP P03045
pD	25	GLY	-	linker	UNP P03045
pD	26	ALA	-	linker	UNP P03045
pD	27	GLY	-	linker	UNP P03045
pD	28	ALA	-	linker	UNP P03045
pD	29	GLY	-	linker	UNP P03045
pD	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
pD	31	MET	-	linker	UNP P03045
pD	39	ASN	ILE	engineered mutation	UNP O66529
pD	42	VAL	GLU	engineered mutation	UNP O66529
pD	58	VAL	ILE	engineered mutation	UNP O66529
pD	61	ASP	GLY	engineered mutation	UNP O66529
pD	62	ILE	VAL	engineered mutation	UNP O66529
pD	97	TYR	PHE	engineered mutation	UNP O66529
pD	102	GLY	-	linker	UNP O66529
pD	103	THR	-	linker	UNP O66529
pD	104	GLY	-	linker	UNP O66529
pD	105	HIS	-	linker	UNP O66529
pD	106	HIS	-	linker	UNP O66529
pD	107	HIS	-	linker	UNP O66529
pD	108	HIS	-	linker	UNP O66529
pD	109	HIS	-	linker	UNP O66529
pD	110	HIS	-	linker	UNP O66529
pD	111	GLY	-	linker	UNP O66529
pD	112	SER	-	linker	UNP O66529
pD	113	SER	-	linker	UNP O66529
pD	114	ILE	MET	engineered mutation	UNP O66529
pD	115	GLU	GLN	engineered mutation	UNP O66529
pD	138	THR	ALA	engineered mutation	UNP O66529
pD	177	ASP	GLY	engineered mutation	UNP O66529
pD	191	PHE	ILE	engineered mutation	UNP O66529
pD	193	ASP	VAL	engineered mutation	UNP O66529
qA	1	MET	-	cloning artifact	UNP P03045
qA	2	GLY	-	cloning artifact	UNP P03045
qA	3	ASN	-	cloning artifact	UNP P03045
qA	4	ALA	-	cloning artifact	UNP P03045
qA	5	LYS	-	cloning artifact	UNP P03045
qA	6	THR	-	cloning artifact	UNP P03045
qA	24	ALA	-	linker	UNP P03045
qA	25	GLY	-	linker	UNP P03045
qA	26	ALA	-	linker	UNP P03045
qA	27	GLY	-	linker	UNP P03045
qA	28	ALA	-	linker	UNP P03045
qA	29	GLY	-	linker	UNP P03045
qA	30	ALA	-	linker	UNP P03045
qA	31	MET	-	linker	UNP P03045
qA	39	ASN	ILE	engineered mutation	UNP O66529
qA	42	VAL	GLU	engineered mutation	UNP O66529
qA	58	VAL	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
qA	61	ASP	GLY	engineered mutation	UNP O66529
qA	62	ILE	VAL	engineered mutation	UNP O66529
qA	97	TYR	PHE	engineered mutation	UNP O66529
qA	102	GLY	-	linker	UNP O66529
qA	103	THR	-	linker	UNP O66529
qA	104	GLY	-	linker	UNP O66529
qA	105	HIS	-	linker	UNP O66529
qA	106	HIS	-	linker	UNP O66529
qA	107	HIS	-	linker	UNP O66529
qA	108	HIS	-	linker	UNP O66529
qA	109	HIS	-	linker	UNP O66529
qA	110	HIS	-	linker	UNP O66529
qA	111	GLY	-	linker	UNP O66529
qA	112	SER	-	linker	UNP O66529
qA	113	SER	-	linker	UNP O66529
qA	114	ILE	MET	engineered mutation	UNP O66529
qA	115	GLU	GLN	engineered mutation	UNP O66529
qA	138	THR	ALA	engineered mutation	UNP O66529
qA	177	ASP	GLY	engineered mutation	UNP O66529
qA	191	PHE	ILE	engineered mutation	UNP O66529
qA	193	ASP	VAL	engineered mutation	UNP O66529
qB	1	MET	-	cloning artifact	UNP P03045
qB	2	GLY	-	cloning artifact	UNP P03045
qB	3	ASN	-	cloning artifact	UNP P03045
qB	4	ALA	-	cloning artifact	UNP P03045
qB	5	LYS	-	cloning artifact	UNP P03045
qB	6	THR	-	cloning artifact	UNP P03045
qB	24	ALA	-	linker	UNP P03045
qB	25	GLY	-	linker	UNP P03045
qB	26	ALA	-	linker	UNP P03045
qB	27	GLY	-	linker	UNP P03045
qB	28	ALA	-	linker	UNP P03045
qB	29	GLY	-	linker	UNP P03045
qB	30	ALA	-	linker	UNP P03045
qB	31	MET	-	linker	UNP P03045
qB	39	ASN	ILE	engineered mutation	UNP O66529
qB	42	VAL	GLU	engineered mutation	UNP O66529
qB	58	VAL	ILE	engineered mutation	UNP O66529
qB	61	ASP	GLY	engineered mutation	UNP O66529
qB	62	ILE	VAL	engineered mutation	UNP O66529
qB	97	TYR	PHE	engineered mutation	UNP O66529
qB	102	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
qB	103	THR	-	linker	UNP O66529
qB	104	GLY	-	linker	UNP O66529
qB	105	HIS	-	linker	UNP O66529
qB	106	HIS	-	linker	UNP O66529
qB	107	HIS	-	linker	UNP O66529
qB	108	HIS	-	linker	UNP O66529
qB	109	HIS	-	linker	UNP O66529
qB	110	HIS	-	linker	UNP O66529
qB	111	GLY	-	linker	UNP O66529
qB	112	SER	-	linker	UNP O66529
qB	113	SER	-	linker	UNP O66529
qB	114	ILE	MET	engineered mutation	UNP O66529
qB	115	GLU	GLN	engineered mutation	UNP O66529
qB	138	THR	ALA	engineered mutation	UNP O66529
qB	177	ASP	GLY	engineered mutation	UNP O66529
qB	191	PHE	ILE	engineered mutation	UNP O66529
qB	193	ASP	VAL	engineered mutation	UNP O66529
qC	1	MET	-	cloning artifact	UNP P03045
qC	2	GLY	-	cloning artifact	UNP P03045
qC	3	ASN	-	cloning artifact	UNP P03045
qC	4	ALA	-	cloning artifact	UNP P03045
qC	5	LYS	-	cloning artifact	UNP P03045
qC	6	THR	-	cloning artifact	UNP P03045
qC	24	ALA	-	linker	UNP P03045
qC	25	GLY	-	linker	UNP P03045
qC	26	ALA	-	linker	UNP P03045
qC	27	GLY	-	linker	UNP P03045
qC	28	ALA	-	linker	UNP P03045
qC	29	GLY	-	linker	UNP P03045
qC	30	ALA	-	linker	UNP P03045
qC	31	MET	-	linker	UNP P03045
qC	39	ASN	ILE	engineered mutation	UNP O66529
qC	42	VAL	GLU	engineered mutation	UNP O66529
qC	58	VAL	ILE	engineered mutation	UNP O66529
qC	61	ASP	GLY	engineered mutation	UNP O66529
qC	62	ILE	VAL	engineered mutation	UNP O66529
qC	97	TYR	PHE	engineered mutation	UNP O66529
qC	102	GLY	-	linker	UNP O66529
qC	103	THR	-	linker	UNP O66529
qC	104	GLY	-	linker	UNP O66529
qC	105	HIS	-	linker	UNP O66529
qC	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
qC	107	HIS	-	linker	UNP O66529
qC	108	HIS	-	linker	UNP O66529
qC	109	HIS	-	linker	UNP O66529
qC	110	HIS	-	linker	UNP O66529
qC	111	GLY	-	linker	UNP O66529
qC	112	SER	-	linker	UNP O66529
qC	113	SER	-	linker	UNP O66529
qC	114	ILE	MET	engineered mutation	UNP O66529
qC	115	GLU	GLN	engineered mutation	UNP O66529
qC	138	THR	ALA	engineered mutation	UNP O66529
qC	177	ASP	GLY	engineered mutation	UNP O66529
qC	191	PHE	ILE	engineered mutation	UNP O66529
qC	193	ASP	VAL	engineered mutation	UNP O66529
qD	1	MET	-	cloning artifact	UNP P03045
qD	2	GLY	-	cloning artifact	UNP P03045
qD	3	ASN	-	cloning artifact	UNP P03045
qD	4	ALA	-	cloning artifact	UNP P03045
qD	5	LYS	-	cloning artifact	UNP P03045
qD	6	THR	-	cloning artifact	UNP P03045
qD	24	ALA	-	linker	UNP P03045
qD	25	GLY	-	linker	UNP P03045
qD	26	ALA	-	linker	UNP P03045
qD	27	GLY	-	linker	UNP P03045
qD	28	ALA	-	linker	UNP P03045
qD	29	GLY	-	linker	UNP P03045
qD	30	ALA	-	linker	UNP P03045
qD	31	MET	-	linker	UNP P03045
qD	39	ASN	ILE	engineered mutation	UNP O66529
qD	42	VAL	GLU	engineered mutation	UNP O66529
qD	58	VAL	ILE	engineered mutation	UNP O66529
qD	61	ASP	GLY	engineered mutation	UNP O66529
qD	62	ILE	VAL	engineered mutation	UNP O66529
qD	97	TYR	PHE	engineered mutation	UNP O66529
qD	102	GLY	-	linker	UNP O66529
qD	103	THR	-	linker	UNP O66529
qD	104	GLY	-	linker	UNP O66529
qD	105	HIS	-	linker	UNP O66529
qD	106	HIS	-	linker	UNP O66529
qD	107	HIS	-	linker	UNP O66529
qD	108	HIS	-	linker	UNP O66529
qD	109	HIS	-	linker	UNP O66529
qD	110	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
qD	111	GLY	-	linker	UNP O66529
qD	112	SER	-	linker	UNP O66529
qD	113	SER	-	linker	UNP O66529
qD	114	ILE	MET	engineered mutation	UNP O66529
qD	115	GLU	GLN	engineered mutation	UNP O66529
qD	138	THR	ALA	engineered mutation	UNP O66529
qD	177	ASP	GLY	engineered mutation	UNP O66529
qD	191	PHE	ILE	engineered mutation	UNP O66529
qD	193	ASP	VAL	engineered mutation	UNP O66529
rA	1	MET	-	cloning artifact	UNP P03045
rA	2	GLY	-	cloning artifact	UNP P03045
rA	3	ASN	-	cloning artifact	UNP P03045
rA	4	ALA	-	cloning artifact	UNP P03045
rA	5	LYS	-	cloning artifact	UNP P03045
rA	6	THR	-	cloning artifact	UNP P03045
rA	24	ALA	-	linker	UNP P03045
rA	25	GLY	-	linker	UNP P03045
rA	26	ALA	-	linker	UNP P03045
rA	27	GLY	-	linker	UNP P03045
rA	28	ALA	-	linker	UNP P03045
rA	29	GLY	-	linker	UNP P03045
rA	30	ALA	-	linker	UNP P03045
rA	31	MET	-	linker	UNP P03045
rA	39	ASN	ILE	engineered mutation	UNP O66529
rA	42	VAL	GLU	engineered mutation	UNP O66529
rA	58	VAL	ILE	engineered mutation	UNP O66529
rA	61	ASP	GLY	engineered mutation	UNP O66529
rA	62	ILE	VAL	engineered mutation	UNP O66529
rA	97	TYR	PHE	engineered mutation	UNP O66529
rA	102	GLY	-	linker	UNP O66529
rA	103	THR	-	linker	UNP O66529
rA	104	GLY	-	linker	UNP O66529
rA	105	HIS	-	linker	UNP O66529
rA	106	HIS	-	linker	UNP O66529
rA	107	HIS	-	linker	UNP O66529
rA	108	HIS	-	linker	UNP O66529
rA	109	HIS	-	linker	UNP O66529
rA	110	HIS	-	linker	UNP O66529
rA	111	GLY	-	linker	UNP O66529
rA	112	SER	-	linker	UNP O66529
rA	113	SER	-	linker	UNP O66529
rA	114	ILE	MET	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
rA	115	GLU	GLN	engineered mutation	UNP O66529
rA	138	THR	ALA	engineered mutation	UNP O66529
rA	177	ASP	GLY	engineered mutation	UNP O66529
rA	191	PHE	ILE	engineered mutation	UNP O66529
rA	193	ASP	VAL	engineered mutation	UNP O66529
rB	1	MET	-	cloning artifact	UNP P03045
rB	2	GLY	-	cloning artifact	UNP P03045
rB	3	ASN	-	cloning artifact	UNP P03045
rB	4	ALA	-	cloning artifact	UNP P03045
rB	5	LYS	-	cloning artifact	UNP P03045
rB	6	THR	-	cloning artifact	UNP P03045
rB	24	ALA	-	linker	UNP P03045
rB	25	GLY	-	linker	UNP P03045
rB	26	ALA	-	linker	UNP P03045
rB	27	GLY	-	linker	UNP P03045
rB	28	ALA	-	linker	UNP P03045
rB	29	GLY	-	linker	UNP P03045
rB	30	ALA	-	linker	UNP P03045
rB	31	MET	-	linker	UNP P03045
rB	39	ASN	ILE	engineered mutation	UNP O66529
rB	42	VAL	GLU	engineered mutation	UNP O66529
rB	58	VAL	ILE	engineered mutation	UNP O66529
rB	61	ASP	GLY	engineered mutation	UNP O66529
rB	62	ILE	VAL	engineered mutation	UNP O66529
rB	97	TYR	PHE	engineered mutation	UNP O66529
rB	102	GLY	-	linker	UNP O66529
rB	103	THR	-	linker	UNP O66529
rB	104	GLY	-	linker	UNP O66529
rB	105	HIS	-	linker	UNP O66529
rB	106	HIS	-	linker	UNP O66529
rB	107	HIS	-	linker	UNP O66529
rB	108	HIS	-	linker	UNP O66529
rB	109	HIS	-	linker	UNP O66529
rB	110	HIS	-	linker	UNP O66529
rB	111	GLY	-	linker	UNP O66529
rB	112	SER	-	linker	UNP O66529
rB	113	SER	-	linker	UNP O66529
rB	114	ILE	MET	engineered mutation	UNP O66529
rB	115	GLU	GLN	engineered mutation	UNP O66529
rB	138	THR	ALA	engineered mutation	UNP O66529
rB	177	ASP	GLY	engineered mutation	UNP O66529
rB	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
rB	193	ASP	VAL	engineered mutation	UNP O66529
rC	1	MET	-	cloning artifact	UNP P03045
rC	2	GLY	-	cloning artifact	UNP P03045
rC	3	ASN	-	cloning artifact	UNP P03045
rC	4	ALA	-	cloning artifact	UNP P03045
rC	5	LYS	-	cloning artifact	UNP P03045
rC	6	THR	-	cloning artifact	UNP P03045
rC	24	ALA	-	linker	UNP P03045
rC	25	GLY	-	linker	UNP P03045
rC	26	ALA	-	linker	UNP P03045
rC	27	GLY	-	linker	UNP P03045
rC	28	ALA	-	linker	UNP P03045
rC	29	GLY	-	linker	UNP P03045
rC	30	ALA	-	linker	UNP P03045
rC	31	MET	-	linker	UNP P03045
rC	39	ASN	ILE	engineered mutation	UNP O66529
rC	42	VAL	GLU	engineered mutation	UNP O66529
rC	58	VAL	ILE	engineered mutation	UNP O66529
rC	61	ASP	GLY	engineered mutation	UNP O66529
rC	62	ILE	VAL	engineered mutation	UNP O66529
rC	97	TYR	PHE	engineered mutation	UNP O66529
rC	102	GLY	-	linker	UNP O66529
rC	103	THR	-	linker	UNP O66529
rC	104	GLY	-	linker	UNP O66529
rC	105	HIS	-	linker	UNP O66529
rC	106	HIS	-	linker	UNP O66529
rC	107	HIS	-	linker	UNP O66529
rC	108	HIS	-	linker	UNP O66529
rC	109	HIS	-	linker	UNP O66529
rC	110	HIS	-	linker	UNP O66529
rC	111	GLY	-	linker	UNP O66529
rC	112	SER	-	linker	UNP O66529
rC	113	SER	-	linker	UNP O66529
rC	114	ILE	MET	engineered mutation	UNP O66529
rC	115	GLU	GLN	engineered mutation	UNP O66529
rC	138	THR	ALA	engineered mutation	UNP O66529
rC	177	ASP	GLY	engineered mutation	UNP O66529
rC	191	PHE	ILE	engineered mutation	UNP O66529
rC	193	ASP	VAL	engineered mutation	UNP O66529
rD	1	MET	-	cloning artifact	UNP P03045
rD	2	GLY	-	cloning artifact	UNP P03045
rD	3	ASN	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
rD	4	ALA	-	cloning artifact	UNP P03045
rD	5	LYS	-	cloning artifact	UNP P03045
rD	6	THR	-	cloning artifact	UNP P03045
rD	24	ALA	-	linker	UNP P03045
rD	25	GLY	-	linker	UNP P03045
rD	26	ALA	-	linker	UNP P03045
rD	27	GLY	-	linker	UNP P03045
rD	28	ALA	-	linker	UNP P03045
rD	29	GLY	-	linker	UNP P03045
rD	30	ALA	-	linker	UNP P03045
rD	31	MET	-	linker	UNP P03045
rD	39	ASN	ILE	engineered mutation	UNP O66529
rD	42	VAL	GLU	engineered mutation	UNP O66529
rD	58	VAL	ILE	engineered mutation	UNP O66529
rD	61	ASP	GLY	engineered mutation	UNP O66529
rD	62	ILE	VAL	engineered mutation	UNP O66529
rD	97	TYR	PHE	engineered mutation	UNP O66529
rD	102	GLY	-	linker	UNP O66529
rD	103	THR	-	linker	UNP O66529
rD	104	GLY	-	linker	UNP O66529
rD	105	HIS	-	linker	UNP O66529
rD	106	HIS	-	linker	UNP O66529
rD	107	HIS	-	linker	UNP O66529
rD	108	HIS	-	linker	UNP O66529
rD	109	HIS	-	linker	UNP O66529
rD	110	HIS	-	linker	UNP O66529
rD	111	GLY	-	linker	UNP O66529
rD	112	SER	-	linker	UNP O66529
rD	113	SER	-	linker	UNP O66529
rD	114	ILE	MET	engineered mutation	UNP O66529
rD	115	GLU	GLN	engineered mutation	UNP O66529
rD	138	THR	ALA	engineered mutation	UNP O66529
rD	177	ASP	GLY	engineered mutation	UNP O66529
rD	191	PHE	ILE	engineered mutation	UNP O66529
rD	193	ASP	VAL	engineered mutation	UNP O66529
sA	1	MET	-	cloning artifact	UNP P03045
sA	2	GLY	-	cloning artifact	UNP P03045
sA	3	ASN	-	cloning artifact	UNP P03045
sA	4	ALA	-	cloning artifact	UNP P03045
sA	5	LYS	-	cloning artifact	UNP P03045
sA	6	THR	-	cloning artifact	UNP P03045
sA	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
sA	25	GLY	-	linker	UNP P03045
sA	26	ALA	-	linker	UNP P03045
sA	27	GLY	-	linker	UNP P03045
sA	28	ALA	-	linker	UNP P03045
sA	29	GLY	-	linker	UNP P03045
sA	30	ALA	-	linker	UNP P03045
sA	31	MET	-	linker	UNP P03045
sA	39	ASN	ILE	engineered mutation	UNP O66529
sA	42	VAL	GLU	engineered mutation	UNP O66529
sA	58	VAL	ILE	engineered mutation	UNP O66529
sA	61	ASP	GLY	engineered mutation	UNP O66529
sA	62	ILE	VAL	engineered mutation	UNP O66529
sA	97	TYR	PHE	engineered mutation	UNP O66529
sA	102	GLY	-	linker	UNP O66529
sA	103	THR	-	linker	UNP O66529
sA	104	GLY	-	linker	UNP O66529
sA	105	HIS	-	linker	UNP O66529
sA	106	HIS	-	linker	UNP O66529
sA	107	HIS	-	linker	UNP O66529
sA	108	HIS	-	linker	UNP O66529
sA	109	HIS	-	linker	UNP O66529
sA	110	HIS	-	linker	UNP O66529
sA	111	GLY	-	linker	UNP O66529
sA	112	SER	-	linker	UNP O66529
sA	113	SER	-	linker	UNP O66529
sA	114	ILE	MET	engineered mutation	UNP O66529
sA	115	GLU	GLN	engineered mutation	UNP O66529
sA	138	THR	ALA	engineered mutation	UNP O66529
sA	177	ASP	GLY	engineered mutation	UNP O66529
sA	191	PHE	ILE	engineered mutation	UNP O66529
sA	193	ASP	VAL	engineered mutation	UNP O66529
sB	1	MET	-	cloning artifact	UNP P03045
sB	2	GLY	-	cloning artifact	UNP P03045
sB	3	ASN	-	cloning artifact	UNP P03045
sB	4	ALA	-	cloning artifact	UNP P03045
sB	5	LYS	-	cloning artifact	UNP P03045
sB	6	THR	-	cloning artifact	UNP P03045
sB	24	ALA	-	linker	UNP P03045
sB	25	GLY	-	linker	UNP P03045
sB	26	ALA	-	linker	UNP P03045
sB	27	GLY	-	linker	UNP P03045
sB	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
sB	29	GLY	-	linker	UNP P03045
sB	30	ALA	-	linker	UNP P03045
sB	31	MET	-	linker	UNP P03045
sB	39	ASN	ILE	engineered mutation	UNP O66529
sB	42	VAL	GLU	engineered mutation	UNP O66529
sB	58	VAL	ILE	engineered mutation	UNP O66529
sB	61	ASP	GLY	engineered mutation	UNP O66529
sB	62	ILE	VAL	engineered mutation	UNP O66529
sB	97	TYR	PHE	engineered mutation	UNP O66529
sB	102	GLY	-	linker	UNP O66529
sB	103	THR	-	linker	UNP O66529
sB	104	GLY	-	linker	UNP O66529
sB	105	HIS	-	linker	UNP O66529
sB	106	HIS	-	linker	UNP O66529
sB	107	HIS	-	linker	UNP O66529
sB	108	HIS	-	linker	UNP O66529
sB	109	HIS	-	linker	UNP O66529
sB	110	HIS	-	linker	UNP O66529
sB	111	GLY	-	linker	UNP O66529
sB	112	SER	-	linker	UNP O66529
sB	113	SER	-	linker	UNP O66529
sB	114	ILE	MET	engineered mutation	UNP O66529
sB	115	GLU	GLN	engineered mutation	UNP O66529
sB	138	THR	ALA	engineered mutation	UNP O66529
sB	177	ASP	GLY	engineered mutation	UNP O66529
sB	191	PHE	ILE	engineered mutation	UNP O66529
sB	193	ASP	VAL	engineered mutation	UNP O66529
sC	1	MET	-	cloning artifact	UNP P03045
sC	2	GLY	-	cloning artifact	UNP P03045
sC	3	ASN	-	cloning artifact	UNP P03045
sC	4	ALA	-	cloning artifact	UNP P03045
sC	5	LYS	-	cloning artifact	UNP P03045
sC	6	THR	-	cloning artifact	UNP P03045
sC	24	ALA	-	linker	UNP P03045
sC	25	GLY	-	linker	UNP P03045
sC	26	ALA	-	linker	UNP P03045
sC	27	GLY	-	linker	UNP P03045
sC	28	ALA	-	linker	UNP P03045
sC	29	GLY	-	linker	UNP P03045
sC	30	ALA	-	linker	UNP P03045
sC	31	MET	-	linker	UNP P03045
sC	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
sC	42	VAL	GLU	engineered mutation	UNP O66529
sC	58	VAL	ILE	engineered mutation	UNP O66529
sC	61	ASP	GLY	engineered mutation	UNP O66529
sC	62	ILE	VAL	engineered mutation	UNP O66529
sC	97	TYR	PHE	engineered mutation	UNP O66529
sC	102	GLY	-	linker	UNP O66529
sC	103	THR	-	linker	UNP O66529
sC	104	GLY	-	linker	UNP O66529
sC	105	HIS	-	linker	UNP O66529
sC	106	HIS	-	linker	UNP O66529
sC	107	HIS	-	linker	UNP O66529
sC	108	HIS	-	linker	UNP O66529
sC	109	HIS	-	linker	UNP O66529
sC	110	HIS	-	linker	UNP O66529
sC	111	GLY	-	linker	UNP O66529
sC	112	SER	-	linker	UNP O66529
sC	113	SER	-	linker	UNP O66529
sC	114	ILE	MET	engineered mutation	UNP O66529
sC	115	GLU	GLN	engineered mutation	UNP O66529
sC	138	THR	ALA	engineered mutation	UNP O66529
sC	177	ASP	GLY	engineered mutation	UNP O66529
sC	191	PHE	ILE	engineered mutation	UNP O66529
sC	193	ASP	VAL	engineered mutation	UNP O66529
sD	1	MET	-	cloning artifact	UNP P03045
sD	2	GLY	-	cloning artifact	UNP P03045
sD	3	ASN	-	cloning artifact	UNP P03045
sD	4	ALA	-	cloning artifact	UNP P03045
sD	5	LYS	-	cloning artifact	UNP P03045
sD	6	THR	-	cloning artifact	UNP P03045
sD	24	ALA	-	linker	UNP P03045
sD	25	GLY	-	linker	UNP P03045
sD	26	ALA	-	linker	UNP P03045
sD	27	GLY	-	linker	UNP P03045
sD	28	ALA	-	linker	UNP P03045
sD	29	GLY	-	linker	UNP P03045
sD	30	ALA	-	linker	UNP P03045
sD	31	MET	-	linker	UNP P03045
sD	39	ASN	ILE	engineered mutation	UNP O66529
sD	42	VAL	GLU	engineered mutation	UNP O66529
sD	58	VAL	ILE	engineered mutation	UNP O66529
sD	61	ASP	GLY	engineered mutation	UNP O66529
sD	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
sD	97	TYR	PHE	engineered mutation	UNP O66529
sD	102	GLY	-	linker	UNP O66529
sD	103	THR	-	linker	UNP O66529
sD	104	GLY	-	linker	UNP O66529
sD	105	HIS	-	linker	UNP O66529
sD	106	HIS	-	linker	UNP O66529
sD	107	HIS	-	linker	UNP O66529
sD	108	HIS	-	linker	UNP O66529
sD	109	HIS	-	linker	UNP O66529
sD	110	HIS	-	linker	UNP O66529
sD	111	GLY	-	linker	UNP O66529
sD	112	SER	-	linker	UNP O66529
sD	113	SER	-	linker	UNP O66529
sD	114	ILE	MET	engineered mutation	UNP O66529
sD	115	GLU	GLN	engineered mutation	UNP O66529
sD	138	THR	ALA	engineered mutation	UNP O66529
sD	177	ASP	GLY	engineered mutation	UNP O66529
sD	191	PHE	ILE	engineered mutation	UNP O66529
sD	193	ASP	VAL	engineered mutation	UNP O66529
tA	1	MET	-	cloning artifact	UNP P03045
tA	2	GLY	-	cloning artifact	UNP P03045
tA	3	ASN	-	cloning artifact	UNP P03045
tA	4	ALA	-	cloning artifact	UNP P03045
tA	5	LYS	-	cloning artifact	UNP P03045
tA	6	THR	-	cloning artifact	UNP P03045
tA	24	ALA	-	linker	UNP P03045
tA	25	GLY	-	linker	UNP P03045
tA	26	ALA	-	linker	UNP P03045
tA	27	GLY	-	linker	UNP P03045
tA	28	ALA	-	linker	UNP P03045
tA	29	GLY	-	linker	UNP P03045
tA	30	ALA	-	linker	UNP P03045
tA	31	MET	-	linker	UNP P03045
tA	39	ASN	ILE	engineered mutation	UNP O66529
tA	42	VAL	GLU	engineered mutation	UNP O66529
tA	58	VAL	ILE	engineered mutation	UNP O66529
tA	61	ASP	GLY	engineered mutation	UNP O66529
tA	62	ILE	VAL	engineered mutation	UNP O66529
tA	97	TYR	PHE	engineered mutation	UNP O66529
tA	102	GLY	-	linker	UNP O66529
tA	103	THR	-	linker	UNP O66529
tA	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
tA	105	HIS	-	linker	UNP O66529
tA	106	HIS	-	linker	UNP O66529
tA	107	HIS	-	linker	UNP O66529
tA	108	HIS	-	linker	UNP O66529
tA	109	HIS	-	linker	UNP O66529
tA	110	HIS	-	linker	UNP O66529
tA	111	GLY	-	linker	UNP O66529
tA	112	SER	-	linker	UNP O66529
tA	113	SER	-	linker	UNP O66529
tA	114	ILE	MET	engineered mutation	UNP O66529
tA	115	GLU	GLN	engineered mutation	UNP O66529
tA	138	THR	ALA	engineered mutation	UNP O66529
tA	177	ASP	GLY	engineered mutation	UNP O66529
tA	191	PHE	ILE	engineered mutation	UNP O66529
tA	193	ASP	VAL	engineered mutation	UNP O66529
tB	1	MET	-	cloning artifact	UNP P03045
tB	2	GLY	-	cloning artifact	UNP P03045
tB	3	ASN	-	cloning artifact	UNP P03045
tB	4	ALA	-	cloning artifact	UNP P03045
tB	5	LYS	-	cloning artifact	UNP P03045
tB	6	THR	-	cloning artifact	UNP P03045
tB	24	ALA	-	linker	UNP P03045
tB	25	GLY	-	linker	UNP P03045
tB	26	ALA	-	linker	UNP P03045
tB	27	GLY	-	linker	UNP P03045
tB	28	ALA	-	linker	UNP P03045
tB	29	GLY	-	linker	UNP P03045
tB	30	ALA	-	linker	UNP P03045
tB	31	MET	-	linker	UNP P03045
tB	39	ASN	ILE	engineered mutation	UNP O66529
tB	42	VAL	GLU	engineered mutation	UNP O66529
tB	58	VAL	ILE	engineered mutation	UNP O66529
tB	61	ASP	GLY	engineered mutation	UNP O66529
tB	62	ILE	VAL	engineered mutation	UNP O66529
tB	97	TYR	PHE	engineered mutation	UNP O66529
tB	102	GLY	-	linker	UNP O66529
tB	103	THR	-	linker	UNP O66529
tB	104	GLY	-	linker	UNP O66529
tB	105	HIS	-	linker	UNP O66529
tB	106	HIS	-	linker	UNP O66529
tB	107	HIS	-	linker	UNP O66529
tB	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
tB	109	HIS	-	linker	UNP O66529
tB	110	HIS	-	linker	UNP O66529
tB	111	GLY	-	linker	UNP O66529
tB	112	SER	-	linker	UNP O66529
tB	113	SER	-	linker	UNP O66529
tB	114	ILE	MET	engineered mutation	UNP O66529
tB	115	GLU	GLN	engineered mutation	UNP O66529
tB	138	THR	ALA	engineered mutation	UNP O66529
tB	177	ASP	GLY	engineered mutation	UNP O66529
tB	191	PHE	ILE	engineered mutation	UNP O66529
tB	193	ASP	VAL	engineered mutation	UNP O66529
tC	1	MET	-	cloning artifact	UNP P03045
tC	2	GLY	-	cloning artifact	UNP P03045
tC	3	ASN	-	cloning artifact	UNP P03045
tC	4	ALA	-	cloning artifact	UNP P03045
tC	5	LYS	-	cloning artifact	UNP P03045
tC	6	THR	-	cloning artifact	UNP P03045
tC	24	ALA	-	linker	UNP P03045
tC	25	GLY	-	linker	UNP P03045
tC	26	ALA	-	linker	UNP P03045
tC	27	GLY	-	linker	UNP P03045
tC	28	ALA	-	linker	UNP P03045
tC	29	GLY	-	linker	UNP P03045
tC	30	ALA	-	linker	UNP P03045
tC	31	MET	-	linker	UNP P03045
tC	39	ASN	ILE	engineered mutation	UNP O66529
tC	42	VAL	GLU	engineered mutation	UNP O66529
tC	58	VAL	ILE	engineered mutation	UNP O66529
tC	61	ASP	GLY	engineered mutation	UNP O66529
tC	62	ILE	VAL	engineered mutation	UNP O66529
tC	97	TYR	PHE	engineered mutation	UNP O66529
tC	102	GLY	-	linker	UNP O66529
tC	103	THR	-	linker	UNP O66529
tC	104	GLY	-	linker	UNP O66529
tC	105	HIS	-	linker	UNP O66529
tC	106	HIS	-	linker	UNP O66529
tC	107	HIS	-	linker	UNP O66529
tC	108	HIS	-	linker	UNP O66529
tC	109	HIS	-	linker	UNP O66529
tC	110	HIS	-	linker	UNP O66529
tC	111	GLY	-	linker	UNP O66529
tC	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
tC	113	SER	-	linker	UNP O66529
tC	114	ILE	MET	engineered mutation	UNP O66529
tC	115	GLU	GLN	engineered mutation	UNP O66529
tC	138	THR	ALA	engineered mutation	UNP O66529
tC	177	ASP	GLY	engineered mutation	UNP O66529
tC	191	PHE	ILE	engineered mutation	UNP O66529
tC	193	ASP	VAL	engineered mutation	UNP O66529
tD	1	MET	-	cloning artifact	UNP P03045
tD	2	GLY	-	cloning artifact	UNP P03045
tD	3	ASN	-	cloning artifact	UNP P03045
tD	4	ALA	-	cloning artifact	UNP P03045
tD	5	LYS	-	cloning artifact	UNP P03045
tD	6	THR	-	cloning artifact	UNP P03045
tD	24	ALA	-	linker	UNP P03045
tD	25	GLY	-	linker	UNP P03045
tD	26	ALA	-	linker	UNP P03045
tD	27	GLY	-	linker	UNP P03045
tD	28	ALA	-	linker	UNP P03045
tD	29	GLY	-	linker	UNP P03045
tD	30	ALA	-	linker	UNP P03045
tD	31	MET	-	linker	UNP P03045
tD	39	ASN	ILE	engineered mutation	UNP O66529
tD	42	VAL	GLU	engineered mutation	UNP O66529
tD	58	VAL	ILE	engineered mutation	UNP O66529
tD	61	ASP	GLY	engineered mutation	UNP O66529
tD	62	ILE	VAL	engineered mutation	UNP O66529
tD	97	TYR	PHE	engineered mutation	UNP O66529
tD	102	GLY	-	linker	UNP O66529
tD	103	THR	-	linker	UNP O66529
tD	104	GLY	-	linker	UNP O66529
tD	105	HIS	-	linker	UNP O66529
tD	106	HIS	-	linker	UNP O66529
tD	107	HIS	-	linker	UNP O66529
tD	108	HIS	-	linker	UNP O66529
tD	109	HIS	-	linker	UNP O66529
tD	110	HIS	-	linker	UNP O66529
tD	111	GLY	-	linker	UNP O66529
tD	112	SER	-	linker	UNP O66529
tD	113	SER	-	linker	UNP O66529
tD	114	ILE	MET	engineered mutation	UNP O66529
tD	115	GLU	GLN	engineered mutation	UNP O66529
tD	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
tD	177	ASP	GLY	engineered mutation	UNP O66529
tD	191	PHE	ILE	engineered mutation	UNP O66529
tD	193	ASP	VAL	engineered mutation	UNP O66529
uA	1	MET	-	cloning artifact	UNP P03045
uA	2	GLY	-	cloning artifact	UNP P03045
uA	3	ASN	-	cloning artifact	UNP P03045
uA	4	ALA	-	cloning artifact	UNP P03045
uA	5	LYS	-	cloning artifact	UNP P03045
uA	6	THR	-	cloning artifact	UNP P03045
uA	24	ALA	-	linker	UNP P03045
uA	25	GLY	-	linker	UNP P03045
uA	26	ALA	-	linker	UNP P03045
uA	27	GLY	-	linker	UNP P03045
uA	28	ALA	-	linker	UNP P03045
uA	29	GLY	-	linker	UNP P03045
uA	30	ALA	-	linker	UNP P03045
uA	31	MET	-	linker	UNP P03045
uA	39	ASN	ILE	engineered mutation	UNP O66529
uA	42	VAL	GLU	engineered mutation	UNP O66529
uA	58	VAL	ILE	engineered mutation	UNP O66529
uA	61	ASP	GLY	engineered mutation	UNP O66529
uA	62	ILE	VAL	engineered mutation	UNP O66529
uA	97	TYR	PHE	engineered mutation	UNP O66529
uA	102	GLY	-	linker	UNP O66529
uA	103	THR	-	linker	UNP O66529
uA	104	GLY	-	linker	UNP O66529
uA	105	HIS	-	linker	UNP O66529
uA	106	HIS	-	linker	UNP O66529
uA	107	HIS	-	linker	UNP O66529
uA	108	HIS	-	linker	UNP O66529
uA	109	HIS	-	linker	UNP O66529
uA	110	HIS	-	linker	UNP O66529
uA	111	GLY	-	linker	UNP O66529
uA	112	SER	-	linker	UNP O66529
uA	113	SER	-	linker	UNP O66529
uA	114	ILE	MET	engineered mutation	UNP O66529
uA	115	GLU	GLN	engineered mutation	UNP O66529
uA	138	THR	ALA	engineered mutation	UNP O66529
uA	177	ASP	GLY	engineered mutation	UNP O66529
uA	191	PHE	ILE	engineered mutation	UNP O66529
uA	193	ASP	VAL	engineered mutation	UNP O66529
uB	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
uB	2	GLY	-	cloning artifact	UNP P03045
uB	3	ASN	-	cloning artifact	UNP P03045
uB	4	ALA	-	cloning artifact	UNP P03045
uB	5	LYS	-	cloning artifact	UNP P03045
uB	6	THR	-	cloning artifact	UNP P03045
uB	24	ALA	-	linker	UNP P03045
uB	25	GLY	-	linker	UNP P03045
uB	26	ALA	-	linker	UNP P03045
uB	27	GLY	-	linker	UNP P03045
uB	28	ALA	-	linker	UNP P03045
uB	29	GLY	-	linker	UNP P03045
uB	30	ALA	-	linker	UNP P03045
uB	31	MET	-	linker	UNP P03045
uB	39	ASN	ILE	engineered mutation	UNP O66529
uB	42	VAL	GLU	engineered mutation	UNP O66529
uB	58	VAL	ILE	engineered mutation	UNP O66529
uB	61	ASP	GLY	engineered mutation	UNP O66529
uB	62	ILE	VAL	engineered mutation	UNP O66529
uB	97	TYR	PHE	engineered mutation	UNP O66529
uB	102	GLY	-	linker	UNP O66529
uB	103	THR	-	linker	UNP O66529
uB	104	GLY	-	linker	UNP O66529
uB	105	HIS	-	linker	UNP O66529
uB	106	HIS	-	linker	UNP O66529
uB	107	HIS	-	linker	UNP O66529
uB	108	HIS	-	linker	UNP O66529
uB	109	HIS	-	linker	UNP O66529
uB	110	HIS	-	linker	UNP O66529
uB	111	GLY	-	linker	UNP O66529
uB	112	SER	-	linker	UNP O66529
uB	113	SER	-	linker	UNP O66529
uB	114	ILE	MET	engineered mutation	UNP O66529
uB	115	GLU	GLN	engineered mutation	UNP O66529
uB	138	THR	ALA	engineered mutation	UNP O66529
uB	177	ASP	GLY	engineered mutation	UNP O66529
uB	191	PHE	ILE	engineered mutation	UNP O66529
uB	193	ASP	VAL	engineered mutation	UNP O66529
uC	1	MET	-	cloning artifact	UNP P03045
uC	2	GLY	-	cloning artifact	UNP P03045
uC	3	ASN	-	cloning artifact	UNP P03045
uC	4	ALA	-	cloning artifact	UNP P03045
uC	5	LYS	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
uC	6	THR	-	cloning artifact	UNP P03045
uC	24	ALA	-	linker	UNP P03045
uC	25	GLY	-	linker	UNP P03045
uC	26	ALA	-	linker	UNP P03045
uC	27	GLY	-	linker	UNP P03045
uC	28	ALA	-	linker	UNP P03045
uC	29	GLY	-	linker	UNP P03045
uC	30	ALA	-	linker	UNP P03045
uC	31	MET	-	linker	UNP P03045
uC	39	ASN	ILE	engineered mutation	UNP O66529
uC	42	VAL	GLU	engineered mutation	UNP O66529
uC	58	VAL	ILE	engineered mutation	UNP O66529
uC	61	ASP	GLY	engineered mutation	UNP O66529
uC	62	ILE	VAL	engineered mutation	UNP O66529
uC	97	TYR	PHE	engineered mutation	UNP O66529
uC	102	GLY	-	linker	UNP O66529
uC	103	THR	-	linker	UNP O66529
uC	104	GLY	-	linker	UNP O66529
uC	105	HIS	-	linker	UNP O66529
uC	106	HIS	-	linker	UNP O66529
uC	107	HIS	-	linker	UNP O66529
uC	108	HIS	-	linker	UNP O66529
uC	109	HIS	-	linker	UNP O66529
uC	110	HIS	-	linker	UNP O66529
uC	111	GLY	-	linker	UNP O66529
uC	112	SER	-	linker	UNP O66529
uC	113	SER	-	linker	UNP O66529
uC	114	ILE	MET	engineered mutation	UNP O66529
uC	115	GLU	GLN	engineered mutation	UNP O66529
uC	138	THR	ALA	engineered mutation	UNP O66529
uC	177	ASP	GLY	engineered mutation	UNP O66529
uC	191	PHE	ILE	engineered mutation	UNP O66529
uC	193	ASP	VAL	engineered mutation	UNP O66529
uD	1	MET	-	cloning artifact	UNP P03045
uD	2	GLY	-	cloning artifact	UNP P03045
uD	3	ASN	-	cloning artifact	UNP P03045
uD	4	ALA	-	cloning artifact	UNP P03045
uD	5	LYS	-	cloning artifact	UNP P03045
uD	6	THR	-	cloning artifact	UNP P03045
uD	24	ALA	-	linker	UNP P03045
uD	25	GLY	-	linker	UNP P03045
uD	26	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
uD	27	GLY	-	linker	UNP P03045
uD	28	ALA	-	linker	UNP P03045
uD	29	GLY	-	linker	UNP P03045
uD	30	ALA	-	linker	UNP P03045
uD	31	MET	-	linker	UNP P03045
uD	39	ASN	ILE	engineered mutation	UNP O66529
uD	42	VAL	GLU	engineered mutation	UNP O66529
uD	58	VAL	ILE	engineered mutation	UNP O66529
uD	61	ASP	GLY	engineered mutation	UNP O66529
uD	62	ILE	VAL	engineered mutation	UNP O66529
uD	97	TYR	PHE	engineered mutation	UNP O66529
uD	102	GLY	-	linker	UNP O66529
uD	103	THR	-	linker	UNP O66529
uD	104	GLY	-	linker	UNP O66529
uD	105	HIS	-	linker	UNP O66529
uD	106	HIS	-	linker	UNP O66529
uD	107	HIS	-	linker	UNP O66529
uD	108	HIS	-	linker	UNP O66529
uD	109	HIS	-	linker	UNP O66529
uD	110	HIS	-	linker	UNP O66529
uD	111	GLY	-	linker	UNP O66529
uD	112	SER	-	linker	UNP O66529
uD	113	SER	-	linker	UNP O66529
uD	114	ILE	MET	engineered mutation	UNP O66529
uD	115	GLU	GLN	engineered mutation	UNP O66529
uD	138	THR	ALA	engineered mutation	UNP O66529
uD	177	ASP	GLY	engineered mutation	UNP O66529
uD	191	PHE	ILE	engineered mutation	UNP O66529
uD	193	ASP	VAL	engineered mutation	UNP O66529
vA	1	MET	-	cloning artifact	UNP P03045
vA	2	GLY	-	cloning artifact	UNP P03045
vA	3	ASN	-	cloning artifact	UNP P03045
vA	4	ALA	-	cloning artifact	UNP P03045
vA	5	LYS	-	cloning artifact	UNP P03045
vA	6	THR	-	cloning artifact	UNP P03045
vA	24	ALA	-	linker	UNP P03045
vA	25	GLY	-	linker	UNP P03045
vA	26	ALA	-	linker	UNP P03045
vA	27	GLY	-	linker	UNP P03045
vA	28	ALA	-	linker	UNP P03045
vA	29	GLY	-	linker	UNP P03045
vA	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
vA	31	MET	-	linker	UNP P03045
vA	39	ASN	ILE	engineered mutation	UNP O66529
vA	42	VAL	GLU	engineered mutation	UNP O66529
vA	58	VAL	ILE	engineered mutation	UNP O66529
vA	61	ASP	GLY	engineered mutation	UNP O66529
vA	62	ILE	VAL	engineered mutation	UNP O66529
vA	97	TYR	PHE	engineered mutation	UNP O66529
vA	102	GLY	-	linker	UNP O66529
vA	103	THR	-	linker	UNP O66529
vA	104	GLY	-	linker	UNP O66529
vA	105	HIS	-	linker	UNP O66529
vA	106	HIS	-	linker	UNP O66529
vA	107	HIS	-	linker	UNP O66529
vA	108	HIS	-	linker	UNP O66529
vA	109	HIS	-	linker	UNP O66529
vA	110	HIS	-	linker	UNP O66529
vA	111	GLY	-	linker	UNP O66529
vA	112	SER	-	linker	UNP O66529
vA	113	SER	-	linker	UNP O66529
vA	114	ILE	MET	engineered mutation	UNP O66529
vA	115	GLU	GLN	engineered mutation	UNP O66529
vA	138	THR	ALA	engineered mutation	UNP O66529
vA	177	ASP	GLY	engineered mutation	UNP O66529
vA	191	PHE	ILE	engineered mutation	UNP O66529
vA	193	ASP	VAL	engineered mutation	UNP O66529
vB	1	MET	-	cloning artifact	UNP P03045
vB	2	GLY	-	cloning artifact	UNP P03045
vB	3	ASN	-	cloning artifact	UNP P03045
vB	4	ALA	-	cloning artifact	UNP P03045
vB	5	LYS	-	cloning artifact	UNP P03045
vB	6	THR	-	cloning artifact	UNP P03045
vB	24	ALA	-	linker	UNP P03045
vB	25	GLY	-	linker	UNP P03045
vB	26	ALA	-	linker	UNP P03045
vB	27	GLY	-	linker	UNP P03045
vB	28	ALA	-	linker	UNP P03045
vB	29	GLY	-	linker	UNP P03045
vB	30	ALA	-	linker	UNP P03045
vB	31	MET	-	linker	UNP P03045
vB	39	ASN	ILE	engineered mutation	UNP O66529
vB	42	VAL	GLU	engineered mutation	UNP O66529
vB	58	VAL	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
vB	61	ASP	GLY	engineered mutation	UNP O66529
vB	62	ILE	VAL	engineered mutation	UNP O66529
vB	97	TYR	PHE	engineered mutation	UNP O66529
vB	102	GLY	-	linker	UNP O66529
vB	103	THR	-	linker	UNP O66529
vB	104	GLY	-	linker	UNP O66529
vB	105	HIS	-	linker	UNP O66529
vB	106	HIS	-	linker	UNP O66529
vB	107	HIS	-	linker	UNP O66529
vB	108	HIS	-	linker	UNP O66529
vB	109	HIS	-	linker	UNP O66529
vB	110	HIS	-	linker	UNP O66529
vB	111	GLY	-	linker	UNP O66529
vB	112	SER	-	linker	UNP O66529
vB	113	SER	-	linker	UNP O66529
vB	114	ILE	MET	engineered mutation	UNP O66529
vB	115	GLU	GLN	engineered mutation	UNP O66529
vB	138	THR	ALA	engineered mutation	UNP O66529
vB	177	ASP	GLY	engineered mutation	UNP O66529
vB	191	PHE	ILE	engineered mutation	UNP O66529
vB	193	ASP	VAL	engineered mutation	UNP O66529
vC	1	MET	-	cloning artifact	UNP P03045
vC	2	GLY	-	cloning artifact	UNP P03045
vC	3	ASN	-	cloning artifact	UNP P03045
vC	4	ALA	-	cloning artifact	UNP P03045
vC	5	LYS	-	cloning artifact	UNP P03045
vC	6	THR	-	cloning artifact	UNP P03045
vC	24	ALA	-	linker	UNP P03045
vC	25	GLY	-	linker	UNP P03045
vC	26	ALA	-	linker	UNP P03045
vC	27	GLY	-	linker	UNP P03045
vC	28	ALA	-	linker	UNP P03045
vC	29	GLY	-	linker	UNP P03045
vC	30	ALA	-	linker	UNP P03045
vC	31	MET	-	linker	UNP P03045
vC	39	ASN	ILE	engineered mutation	UNP O66529
vC	42	VAL	GLU	engineered mutation	UNP O66529
vC	58	VAL	ILE	engineered mutation	UNP O66529
vC	61	ASP	GLY	engineered mutation	UNP O66529
vC	62	ILE	VAL	engineered mutation	UNP O66529
vC	97	TYR	PHE	engineered mutation	UNP O66529
vC	102	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
vC	103	THR	-	linker	UNP O66529
vC	104	GLY	-	linker	UNP O66529
vC	105	HIS	-	linker	UNP O66529
vC	106	HIS	-	linker	UNP O66529
vC	107	HIS	-	linker	UNP O66529
vC	108	HIS	-	linker	UNP O66529
vC	109	HIS	-	linker	UNP O66529
vC	110	HIS	-	linker	UNP O66529
vC	111	GLY	-	linker	UNP O66529
vC	112	SER	-	linker	UNP O66529
vC	113	SER	-	linker	UNP O66529
vC	114	ILE	MET	engineered mutation	UNP O66529
vC	115	GLU	GLN	engineered mutation	UNP O66529
vC	138	THR	ALA	engineered mutation	UNP O66529
vC	177	ASP	GLY	engineered mutation	UNP O66529
vC	191	PHE	ILE	engineered mutation	UNP O66529
vC	193	ASP	VAL	engineered mutation	UNP O66529
vD	1	MET	-	cloning artifact	UNP P03045
vD	2	GLY	-	cloning artifact	UNP P03045
vD	3	ASN	-	cloning artifact	UNP P03045
vD	4	ALA	-	cloning artifact	UNP P03045
vD	5	LYS	-	cloning artifact	UNP P03045
vD	6	THR	-	cloning artifact	UNP P03045
vD	24	ALA	-	linker	UNP P03045
vD	25	GLY	-	linker	UNP P03045
vD	26	ALA	-	linker	UNP P03045
vD	27	GLY	-	linker	UNP P03045
vD	28	ALA	-	linker	UNP P03045
vD	29	GLY	-	linker	UNP P03045
vD	30	ALA	-	linker	UNP P03045
vD	31	MET	-	linker	UNP P03045
vD	39	ASN	ILE	engineered mutation	UNP O66529
vD	42	VAL	GLU	engineered mutation	UNP O66529
vD	58	VAL	ILE	engineered mutation	UNP O66529
vD	61	ASP	GLY	engineered mutation	UNP O66529
vD	62	ILE	VAL	engineered mutation	UNP O66529
vD	97	TYR	PHE	engineered mutation	UNP O66529
vD	102	GLY	-	linker	UNP O66529
vD	103	THR	-	linker	UNP O66529
vD	104	GLY	-	linker	UNP O66529
vD	105	HIS	-	linker	UNP O66529
vD	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
vD	107	HIS	-	linker	UNP O66529
vD	108	HIS	-	linker	UNP O66529
vD	109	HIS	-	linker	UNP O66529
vD	110	HIS	-	linker	UNP O66529
vD	111	GLY	-	linker	UNP O66529
vD	112	SER	-	linker	UNP O66529
vD	113	SER	-	linker	UNP O66529
vD	114	ILE	MET	engineered mutation	UNP O66529
vD	115	GLU	GLN	engineered mutation	UNP O66529
vD	138	THR	ALA	engineered mutation	UNP O66529
vD	177	ASP	GLY	engineered mutation	UNP O66529
vD	191	PHE	ILE	engineered mutation	UNP O66529
vD	193	ASP	VAL	engineered mutation	UNP O66529
wA	1	MET	-	cloning artifact	UNP P03045
wA	2	GLY	-	cloning artifact	UNP P03045
wA	3	ASN	-	cloning artifact	UNP P03045
wA	4	ALA	-	cloning artifact	UNP P03045
wA	5	LYS	-	cloning artifact	UNP P03045
wA	6	THR	-	cloning artifact	UNP P03045
wA	24	ALA	-	linker	UNP P03045
wA	25	GLY	-	linker	UNP P03045
wA	26	ALA	-	linker	UNP P03045
wA	27	GLY	-	linker	UNP P03045
wA	28	ALA	-	linker	UNP P03045
wA	29	GLY	-	linker	UNP P03045
wA	30	ALA	-	linker	UNP P03045
wA	31	MET	-	linker	UNP P03045
wA	39	ASN	ILE	engineered mutation	UNP O66529
wA	42	VAL	GLU	engineered mutation	UNP O66529
wA	58	VAL	ILE	engineered mutation	UNP O66529
wA	61	ASP	GLY	engineered mutation	UNP O66529
wA	62	ILE	VAL	engineered mutation	UNP O66529
wA	97	TYR	PHE	engineered mutation	UNP O66529
wA	102	GLY	-	linker	UNP O66529
wA	103	THR	-	linker	UNP O66529
wA	104	GLY	-	linker	UNP O66529
wA	105	HIS	-	linker	UNP O66529
wA	106	HIS	-	linker	UNP O66529
wA	107	HIS	-	linker	UNP O66529
wA	108	HIS	-	linker	UNP O66529
wA	109	HIS	-	linker	UNP O66529
wA	110	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
wA	111	GLY	-	linker	UNP O66529
wA	112	SER	-	linker	UNP O66529
wA	113	SER	-	linker	UNP O66529
wA	114	ILE	MET	engineered mutation	UNP O66529
wA	115	GLU	GLN	engineered mutation	UNP O66529
wA	138	THR	ALA	engineered mutation	UNP O66529
wA	177	ASP	GLY	engineered mutation	UNP O66529
wA	191	PHE	ILE	engineered mutation	UNP O66529
wA	193	ASP	VAL	engineered mutation	UNP O66529
wB	1	MET	-	cloning artifact	UNP P03045
wB	2	GLY	-	cloning artifact	UNP P03045
wB	3	ASN	-	cloning artifact	UNP P03045
wB	4	ALA	-	cloning artifact	UNP P03045
wB	5	LYS	-	cloning artifact	UNP P03045
wB	6	THR	-	cloning artifact	UNP P03045
wB	24	ALA	-	linker	UNP P03045
wB	25	GLY	-	linker	UNP P03045
wB	26	ALA	-	linker	UNP P03045
wB	27	GLY	-	linker	UNP P03045
wB	28	ALA	-	linker	UNP P03045
wB	29	GLY	-	linker	UNP P03045
wB	30	ALA	-	linker	UNP P03045
wB	31	MET	-	linker	UNP P03045
wB	39	ASN	ILE	engineered mutation	UNP O66529
wB	42	VAL	GLU	engineered mutation	UNP O66529
wB	58	VAL	ILE	engineered mutation	UNP O66529
wB	61	ASP	GLY	engineered mutation	UNP O66529
wB	62	ILE	VAL	engineered mutation	UNP O66529
wB	97	TYR	PHE	engineered mutation	UNP O66529
wB	102	GLY	-	linker	UNP O66529
wB	103	THR	-	linker	UNP O66529
wB	104	GLY	-	linker	UNP O66529
wB	105	HIS	-	linker	UNP O66529
wB	106	HIS	-	linker	UNP O66529
wB	107	HIS	-	linker	UNP O66529
wB	108	HIS	-	linker	UNP O66529
wB	109	HIS	-	linker	UNP O66529
wB	110	HIS	-	linker	UNP O66529
wB	111	GLY	-	linker	UNP O66529
wB	112	SER	-	linker	UNP O66529
wB	113	SER	-	linker	UNP O66529
wB	114	ILE	MET	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
wB	115	GLU	GLN	engineered mutation	UNP O66529
wB	138	THR	ALA	engineered mutation	UNP O66529
wB	177	ASP	GLY	engineered mutation	UNP O66529
wB	191	PHE	ILE	engineered mutation	UNP O66529
wB	193	ASP	VAL	engineered mutation	UNP O66529
wC	1	MET	-	cloning artifact	UNP P03045
wC	2	GLY	-	cloning artifact	UNP P03045
wC	3	ASN	-	cloning artifact	UNP P03045
wC	4	ALA	-	cloning artifact	UNP P03045
wC	5	LYS	-	cloning artifact	UNP P03045
wC	6	THR	-	cloning artifact	UNP P03045
wC	24	ALA	-	linker	UNP P03045
wC	25	GLY	-	linker	UNP P03045
wC	26	ALA	-	linker	UNP P03045
wC	27	GLY	-	linker	UNP P03045
wC	28	ALA	-	linker	UNP P03045
wC	29	GLY	-	linker	UNP P03045
wC	30	ALA	-	linker	UNP P03045
wC	31	MET	-	linker	UNP P03045
wC	39	ASN	ILE	engineered mutation	UNP O66529
wC	42	VAL	GLU	engineered mutation	UNP O66529
wC	58	VAL	ILE	engineered mutation	UNP O66529
wC	61	ASP	GLY	engineered mutation	UNP O66529
wC	62	ILE	VAL	engineered mutation	UNP O66529
wC	97	TYR	PHE	engineered mutation	UNP O66529
wC	102	GLY	-	linker	UNP O66529
wC	103	THR	-	linker	UNP O66529
wC	104	GLY	-	linker	UNP O66529
wC	105	HIS	-	linker	UNP O66529
wC	106	HIS	-	linker	UNP O66529
wC	107	HIS	-	linker	UNP O66529
wC	108	HIS	-	linker	UNP O66529
wC	109	HIS	-	linker	UNP O66529
wC	110	HIS	-	linker	UNP O66529
wC	111	GLY	-	linker	UNP O66529
wC	112	SER	-	linker	UNP O66529
wC	113	SER	-	linker	UNP O66529
wC	114	ILE	MET	engineered mutation	UNP O66529
wC	115	GLU	GLN	engineered mutation	UNP O66529
wC	138	THR	ALA	engineered mutation	UNP O66529
wC	177	ASP	GLY	engineered mutation	UNP O66529
wC	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
wC	193	ASP	VAL	engineered mutation	UNP O66529
wD	1	MET	-	cloning artifact	UNP P03045
wD	2	GLY	-	cloning artifact	UNP P03045
wD	3	ASN	-	cloning artifact	UNP P03045
wD	4	ALA	-	cloning artifact	UNP P03045
wD	5	LYS	-	cloning artifact	UNP P03045
wD	6	THR	-	cloning artifact	UNP P03045
wD	24	ALA	-	linker	UNP P03045
wD	25	GLY	-	linker	UNP P03045
wD	26	ALA	-	linker	UNP P03045
wD	27	GLY	-	linker	UNP P03045
wD	28	ALA	-	linker	UNP P03045
wD	29	GLY	-	linker	UNP P03045
wD	30	ALA	-	linker	UNP P03045
wD	31	MET	-	linker	UNP P03045
wD	39	ASN	ILE	engineered mutation	UNP O66529
wD	42	VAL	GLU	engineered mutation	UNP O66529
wD	58	VAL	ILE	engineered mutation	UNP O66529
wD	61	ASP	GLY	engineered mutation	UNP O66529
wD	62	ILE	VAL	engineered mutation	UNP O66529
wD	97	TYR	PHE	engineered mutation	UNP O66529
wD	102	GLY	-	linker	UNP O66529
wD	103	THR	-	linker	UNP O66529
wD	104	GLY	-	linker	UNP O66529
wD	105	HIS	-	linker	UNP O66529
wD	106	HIS	-	linker	UNP O66529
wD	107	HIS	-	linker	UNP O66529
wD	108	HIS	-	linker	UNP O66529
wD	109	HIS	-	linker	UNP O66529
wD	110	HIS	-	linker	UNP O66529
wD	111	GLY	-	linker	UNP O66529
wD	112	SER	-	linker	UNP O66529
wD	113	SER	-	linker	UNP O66529
wD	114	ILE	MET	engineered mutation	UNP O66529
wD	115	GLU	GLN	engineered mutation	UNP O66529
wD	138	THR	ALA	engineered mutation	UNP O66529
wD	177	ASP	GLY	engineered mutation	UNP O66529
wD	191	PHE	ILE	engineered mutation	UNP O66529
wD	193	ASP	VAL	engineered mutation	UNP O66529
xA	1	MET	-	cloning artifact	UNP P03045
xA	2	GLY	-	cloning artifact	UNP P03045
xA	3	ASN	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
xA	4	ALA	-	cloning artifact	UNP P03045
xA	5	LYS	-	cloning artifact	UNP P03045
xA	6	THR	-	cloning artifact	UNP P03045
xA	24	ALA	-	linker	UNP P03045
xA	25	GLY	-	linker	UNP P03045
xA	26	ALA	-	linker	UNP P03045
xA	27	GLY	-	linker	UNP P03045
xA	28	ALA	-	linker	UNP P03045
xA	29	GLY	-	linker	UNP P03045
xA	30	ALA	-	linker	UNP P03045
xA	31	MET	-	linker	UNP P03045
xA	39	ASN	ILE	engineered mutation	UNP O66529
xA	42	VAL	GLU	engineered mutation	UNP O66529
xA	58	VAL	ILE	engineered mutation	UNP O66529
xA	61	ASP	GLY	engineered mutation	UNP O66529
xA	62	ILE	VAL	engineered mutation	UNP O66529
xA	97	TYR	PHE	engineered mutation	UNP O66529
xA	102	GLY	-	linker	UNP O66529
xA	103	THR	-	linker	UNP O66529
xA	104	GLY	-	linker	UNP O66529
xA	105	HIS	-	linker	UNP O66529
xA	106	HIS	-	linker	UNP O66529
xA	107	HIS	-	linker	UNP O66529
xA	108	HIS	-	linker	UNP O66529
xA	109	HIS	-	linker	UNP O66529
xA	110	HIS	-	linker	UNP O66529
xA	111	GLY	-	linker	UNP O66529
xA	112	SER	-	linker	UNP O66529
xA	113	SER	-	linker	UNP O66529
xA	114	ILE	MET	engineered mutation	UNP O66529
xA	115	GLU	GLN	engineered mutation	UNP O66529
xA	138	THR	ALA	engineered mutation	UNP O66529
xA	177	ASP	GLY	engineered mutation	UNP O66529
xA	191	PHE	ILE	engineered mutation	UNP O66529
xA	193	ASP	VAL	engineered mutation	UNP O66529
xB	1	MET	-	cloning artifact	UNP P03045
xB	2	GLY	-	cloning artifact	UNP P03045
xB	3	ASN	-	cloning artifact	UNP P03045
xB	4	ALA	-	cloning artifact	UNP P03045
xB	5	LYS	-	cloning artifact	UNP P03045
xB	6	THR	-	cloning artifact	UNP P03045
xB	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
xB	25	GLY	-	linker	UNP P03045
xB	26	ALA	-	linker	UNP P03045
xB	27	GLY	-	linker	UNP P03045
xB	28	ALA	-	linker	UNP P03045
xB	29	GLY	-	linker	UNP P03045
xB	30	ALA	-	linker	UNP P03045
xB	31	MET	-	linker	UNP P03045
xB	39	ASN	ILE	engineered mutation	UNP O66529
xB	42	VAL	GLU	engineered mutation	UNP O66529
xB	58	VAL	ILE	engineered mutation	UNP O66529
xB	61	ASP	GLY	engineered mutation	UNP O66529
xB	62	ILE	VAL	engineered mutation	UNP O66529
xB	97	TYR	PHE	engineered mutation	UNP O66529
xB	102	GLY	-	linker	UNP O66529
xB	103	THR	-	linker	UNP O66529
xB	104	GLY	-	linker	UNP O66529
xB	105	HIS	-	linker	UNP O66529
xB	106	HIS	-	linker	UNP O66529
xB	107	HIS	-	linker	UNP O66529
xB	108	HIS	-	linker	UNP O66529
xB	109	HIS	-	linker	UNP O66529
xB	110	HIS	-	linker	UNP O66529
xB	111	GLY	-	linker	UNP O66529
xB	112	SER	-	linker	UNP O66529
xB	113	SER	-	linker	UNP O66529
xB	114	ILE	MET	engineered mutation	UNP O66529
xB	115	GLU	GLN	engineered mutation	UNP O66529
xB	138	THR	ALA	engineered mutation	UNP O66529
xB	177	ASP	GLY	engineered mutation	UNP O66529
xB	191	PHE	ILE	engineered mutation	UNP O66529
xB	193	ASP	VAL	engineered mutation	UNP O66529
xC	1	MET	-	cloning artifact	UNP P03045
xC	2	GLY	-	cloning artifact	UNP P03045
xC	3	ASN	-	cloning artifact	UNP P03045
xC	4	ALA	-	cloning artifact	UNP P03045
xC	5	LYS	-	cloning artifact	UNP P03045
xC	6	THR	-	cloning artifact	UNP P03045
xC	24	ALA	-	linker	UNP P03045
xC	25	GLY	-	linker	UNP P03045
xC	26	ALA	-	linker	UNP P03045
xC	27	GLY	-	linker	UNP P03045
xC	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
xC	29	GLY	-	linker	UNP P03045
xC	30	ALA	-	linker	UNP P03045
xC	31	MET	-	linker	UNP P03045
xC	39	ASN	ILE	engineered mutation	UNP O66529
xC	42	VAL	GLU	engineered mutation	UNP O66529
xC	58	VAL	ILE	engineered mutation	UNP O66529
xC	61	ASP	GLY	engineered mutation	UNP O66529
xC	62	ILE	VAL	engineered mutation	UNP O66529
xC	97	TYR	PHE	engineered mutation	UNP O66529
xC	102	GLY	-	linker	UNP O66529
xC	103	THR	-	linker	UNP O66529
xC	104	GLY	-	linker	UNP O66529
xC	105	HIS	-	linker	UNP O66529
xC	106	HIS	-	linker	UNP O66529
xC	107	HIS	-	linker	UNP O66529
xC	108	HIS	-	linker	UNP O66529
xC	109	HIS	-	linker	UNP O66529
xC	110	HIS	-	linker	UNP O66529
xC	111	GLY	-	linker	UNP O66529
xC	112	SER	-	linker	UNP O66529
xC	113	SER	-	linker	UNP O66529
xC	114	ILE	MET	engineered mutation	UNP O66529
xC	115	GLU	GLN	engineered mutation	UNP O66529
xC	138	THR	ALA	engineered mutation	UNP O66529
xC	177	ASP	GLY	engineered mutation	UNP O66529
xC	191	PHE	ILE	engineered mutation	UNP O66529
xC	193	ASP	VAL	engineered mutation	UNP O66529
xD	1	MET	-	cloning artifact	UNP P03045
xD	2	GLY	-	cloning artifact	UNP P03045
xD	3	ASN	-	cloning artifact	UNP P03045
xD	4	ALA	-	cloning artifact	UNP P03045
xD	5	LYS	-	cloning artifact	UNP P03045
xD	6	THR	-	cloning artifact	UNP P03045
xD	24	ALA	-	linker	UNP P03045
xD	25	GLY	-	linker	UNP P03045
xD	26	ALA	-	linker	UNP P03045
xD	27	GLY	-	linker	UNP P03045
xD	28	ALA	-	linker	UNP P03045
xD	29	GLY	-	linker	UNP P03045
xD	30	ALA	-	linker	UNP P03045
xD	31	MET	-	linker	UNP P03045
xD	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
xD	42	VAL	GLU	engineered mutation	UNP O66529
xD	58	VAL	ILE	engineered mutation	UNP O66529
xD	61	ASP	GLY	engineered mutation	UNP O66529
xD	62	ILE	VAL	engineered mutation	UNP O66529
xD	97	TYR	PHE	engineered mutation	UNP O66529
xD	102	GLY	-	linker	UNP O66529
xD	103	THR	-	linker	UNP O66529
xD	104	GLY	-	linker	UNP O66529
xD	105	HIS	-	linker	UNP O66529
xD	106	HIS	-	linker	UNP O66529
xD	107	HIS	-	linker	UNP O66529
xD	108	HIS	-	linker	UNP O66529
xD	109	HIS	-	linker	UNP O66529
xD	110	HIS	-	linker	UNP O66529
xD	111	GLY	-	linker	UNP O66529
xD	112	SER	-	linker	UNP O66529
xD	113	SER	-	linker	UNP O66529
xD	114	ILE	MET	engineered mutation	UNP O66529
xD	115	GLU	GLN	engineered mutation	UNP O66529
xD	138	THR	ALA	engineered mutation	UNP O66529
xD	177	ASP	GLY	engineered mutation	UNP O66529
xD	191	PHE	ILE	engineered mutation	UNP O66529
xD	193	ASP	VAL	engineered mutation	UNP O66529
yA	1	MET	-	cloning artifact	UNP P03045
yA	2	GLY	-	cloning artifact	UNP P03045
yA	3	ASN	-	cloning artifact	UNP P03045
yA	4	ALA	-	cloning artifact	UNP P03045
yA	5	LYS	-	cloning artifact	UNP P03045
yA	6	THR	-	cloning artifact	UNP P03045
yA	24	ALA	-	linker	UNP P03045
yA	25	GLY	-	linker	UNP P03045
yA	26	ALA	-	linker	UNP P03045
yA	27	GLY	-	linker	UNP P03045
yA	28	ALA	-	linker	UNP P03045
yA	29	GLY	-	linker	UNP P03045
yA	30	ALA	-	linker	UNP P03045
yA	31	MET	-	linker	UNP P03045
yA	39	ASN	ILE	engineered mutation	UNP O66529
yA	42	VAL	GLU	engineered mutation	UNP O66529
yA	58	VAL	ILE	engineered mutation	UNP O66529
yA	61	ASP	GLY	engineered mutation	UNP O66529
yA	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
yA	97	TYR	PHE	engineered mutation	UNP O66529
yA	102	GLY	-	linker	UNP O66529
yA	103	THR	-	linker	UNP O66529
yA	104	GLY	-	linker	UNP O66529
yA	105	HIS	-	linker	UNP O66529
yA	106	HIS	-	linker	UNP O66529
yA	107	HIS	-	linker	UNP O66529
yA	108	HIS	-	linker	UNP O66529
yA	109	HIS	-	linker	UNP O66529
yA	110	HIS	-	linker	UNP O66529
yA	111	GLY	-	linker	UNP O66529
yA	112	SER	-	linker	UNP O66529
yA	113	SER	-	linker	UNP O66529
yA	114	ILE	MET	engineered mutation	UNP O66529
yA	115	GLU	GLN	engineered mutation	UNP O66529
yA	138	THR	ALA	engineered mutation	UNP O66529
yA	177	ASP	GLY	engineered mutation	UNP O66529
yA	191	PHE	ILE	engineered mutation	UNP O66529
yA	193	ASP	VAL	engineered mutation	UNP O66529
yB	1	MET	-	cloning artifact	UNP P03045
yB	2	GLY	-	cloning artifact	UNP P03045
yB	3	ASN	-	cloning artifact	UNP P03045
yB	4	ALA	-	cloning artifact	UNP P03045
yB	5	LYS	-	cloning artifact	UNP P03045
yB	6	THR	-	cloning artifact	UNP P03045
yB	24	ALA	-	linker	UNP P03045
yB	25	GLY	-	linker	UNP P03045
yB	26	ALA	-	linker	UNP P03045
yB	27	GLY	-	linker	UNP P03045
yB	28	ALA	-	linker	UNP P03045
yB	29	GLY	-	linker	UNP P03045
yB	30	ALA	-	linker	UNP P03045
yB	31	MET	-	linker	UNP P03045
yB	39	ASN	ILE	engineered mutation	UNP O66529
yB	42	VAL	GLU	engineered mutation	UNP O66529
yB	58	VAL	ILE	engineered mutation	UNP O66529
yB	61	ASP	GLY	engineered mutation	UNP O66529
yB	62	ILE	VAL	engineered mutation	UNP O66529
yB	97	TYR	PHE	engineered mutation	UNP O66529
yB	102	GLY	-	linker	UNP O66529
yB	103	THR	-	linker	UNP O66529
yB	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
yB	105	HIS	-	linker	UNP O66529
yB	106	HIS	-	linker	UNP O66529
yB	107	HIS	-	linker	UNP O66529
yB	108	HIS	-	linker	UNP O66529
yB	109	HIS	-	linker	UNP O66529
yB	110	HIS	-	linker	UNP O66529
yB	111	GLY	-	linker	UNP O66529
yB	112	SER	-	linker	UNP O66529
yB	113	SER	-	linker	UNP O66529
yB	114	ILE	MET	engineered mutation	UNP O66529
yB	115	GLU	GLN	engineered mutation	UNP O66529
yB	138	THR	ALA	engineered mutation	UNP O66529
yB	177	ASP	GLY	engineered mutation	UNP O66529
yB	191	PHE	ILE	engineered mutation	UNP O66529
yB	193	ASP	VAL	engineered mutation	UNP O66529
yC	1	MET	-	cloning artifact	UNP P03045
yC	2	GLY	-	cloning artifact	UNP P03045
yC	3	ASN	-	cloning artifact	UNP P03045
yC	4	ALA	-	cloning artifact	UNP P03045
yC	5	LYS	-	cloning artifact	UNP P03045
yC	6	THR	-	cloning artifact	UNP P03045
yC	24	ALA	-	linker	UNP P03045
yC	25	GLY	-	linker	UNP P03045
yC	26	ALA	-	linker	UNP P03045
yC	27	GLY	-	linker	UNP P03045
yC	28	ALA	-	linker	UNP P03045
yC	29	GLY	-	linker	UNP P03045
yC	30	ALA	-	linker	UNP P03045
yC	31	MET	-	linker	UNP P03045
yC	39	ASN	ILE	engineered mutation	UNP O66529
yC	42	VAL	GLU	engineered mutation	UNP O66529
yC	58	VAL	ILE	engineered mutation	UNP O66529
yC	61	ASP	GLY	engineered mutation	UNP O66529
yC	62	ILE	VAL	engineered mutation	UNP O66529
yC	97	TYR	PHE	engineered mutation	UNP O66529
yC	102	GLY	-	linker	UNP O66529
yC	103	THR	-	linker	UNP O66529
yC	104	GLY	-	linker	UNP O66529
yC	105	HIS	-	linker	UNP O66529
yC	106	HIS	-	linker	UNP O66529
yC	107	HIS	-	linker	UNP O66529
yC	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
yC	109	HIS	-	linker	UNP O66529
yC	110	HIS	-	linker	UNP O66529
yC	111	GLY	-	linker	UNP O66529
yC	112	SER	-	linker	UNP O66529
yC	113	SER	-	linker	UNP O66529
yC	114	ILE	MET	engineered mutation	UNP O66529
yC	115	GLU	GLN	engineered mutation	UNP O66529
yC	138	THR	ALA	engineered mutation	UNP O66529
yC	177	ASP	GLY	engineered mutation	UNP O66529
yC	191	PHE	ILE	engineered mutation	UNP O66529
yC	193	ASP	VAL	engineered mutation	UNP O66529
yD	1	MET	-	cloning artifact	UNP P03045
yD	2	GLY	-	cloning artifact	UNP P03045
yD	3	ASN	-	cloning artifact	UNP P03045
yD	4	ALA	-	cloning artifact	UNP P03045
yD	5	LYS	-	cloning artifact	UNP P03045
yD	6	THR	-	cloning artifact	UNP P03045
yD	24	ALA	-	linker	UNP P03045
yD	25	GLY	-	linker	UNP P03045
yD	26	ALA	-	linker	UNP P03045
yD	27	GLY	-	linker	UNP P03045
yD	28	ALA	-	linker	UNP P03045
yD	29	GLY	-	linker	UNP P03045
yD	30	ALA	-	linker	UNP P03045
yD	31	MET	-	linker	UNP P03045
yD	39	ASN	ILE	engineered mutation	UNP O66529
yD	42	VAL	GLU	engineered mutation	UNP O66529
yD	58	VAL	ILE	engineered mutation	UNP O66529
yD	61	ASP	GLY	engineered mutation	UNP O66529
yD	62	ILE	VAL	engineered mutation	UNP O66529
yD	97	TYR	PHE	engineered mutation	UNP O66529
yD	102	GLY	-	linker	UNP O66529
yD	103	THR	-	linker	UNP O66529
yD	104	GLY	-	linker	UNP O66529
yD	105	HIS	-	linker	UNP O66529
yD	106	HIS	-	linker	UNP O66529
yD	107	HIS	-	linker	UNP O66529
yD	108	HIS	-	linker	UNP O66529
yD	109	HIS	-	linker	UNP O66529
yD	110	HIS	-	linker	UNP O66529
yD	111	GLY	-	linker	UNP O66529
yD	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
yD	113	SER	-	linker	UNP O66529
yD	114	ILE	MET	engineered mutation	UNP O66529
yD	115	GLU	GLN	engineered mutation	UNP O66529
yD	138	THR	ALA	engineered mutation	UNP O66529
yD	177	ASP	GLY	engineered mutation	UNP O66529
yD	191	PHE	ILE	engineered mutation	UNP O66529
yD	193	ASP	VAL	engineered mutation	UNP O66529
zA	1	MET	-	cloning artifact	UNP P03045
zA	2	GLY	-	cloning artifact	UNP P03045
zA	3	ASN	-	cloning artifact	UNP P03045
zA	4	ALA	-	cloning artifact	UNP P03045
zA	5	LYS	-	cloning artifact	UNP P03045
zA	6	THR	-	cloning artifact	UNP P03045
zA	24	ALA	-	linker	UNP P03045
zA	25	GLY	-	linker	UNP P03045
zA	26	ALA	-	linker	UNP P03045
zA	27	GLY	-	linker	UNP P03045
zA	28	ALA	-	linker	UNP P03045
zA	29	GLY	-	linker	UNP P03045
zA	30	ALA	-	linker	UNP P03045
zA	31	MET	-	linker	UNP P03045
zA	39	ASN	ILE	engineered mutation	UNP O66529
zA	42	VAL	GLU	engineered mutation	UNP O66529
zA	58	VAL	ILE	engineered mutation	UNP O66529
zA	61	ASP	GLY	engineered mutation	UNP O66529
zA	62	ILE	VAL	engineered mutation	UNP O66529
zA	97	TYR	PHE	engineered mutation	UNP O66529
zA	102	GLY	-	linker	UNP O66529
zA	103	THR	-	linker	UNP O66529
zA	104	GLY	-	linker	UNP O66529
zA	105	HIS	-	linker	UNP O66529
zA	106	HIS	-	linker	UNP O66529
zA	107	HIS	-	linker	UNP O66529
zA	108	HIS	-	linker	UNP O66529
zA	109	HIS	-	linker	UNP O66529
zA	110	HIS	-	linker	UNP O66529
zA	111	GLY	-	linker	UNP O66529
zA	112	SER	-	linker	UNP O66529
zA	113	SER	-	linker	UNP O66529
zA	114	ILE	MET	engineered mutation	UNP O66529
zA	115	GLU	GLN	engineered mutation	UNP O66529
zA	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
zA	177	ASP	GLY	engineered mutation	UNP O66529
zA	191	PHE	ILE	engineered mutation	UNP O66529
zA	193	ASP	VAL	engineered mutation	UNP O66529
zB	1	MET	-	cloning artifact	UNP P03045
zB	2	GLY	-	cloning artifact	UNP P03045
zB	3	ASN	-	cloning artifact	UNP P03045
zB	4	ALA	-	cloning artifact	UNP P03045
zB	5	LYS	-	cloning artifact	UNP P03045
zB	6	THR	-	cloning artifact	UNP P03045
zB	24	ALA	-	linker	UNP P03045
zB	25	GLY	-	linker	UNP P03045
zB	26	ALA	-	linker	UNP P03045
zB	27	GLY	-	linker	UNP P03045
zB	28	ALA	-	linker	UNP P03045
zB	29	GLY	-	linker	UNP P03045
zB	30	ALA	-	linker	UNP P03045
zB	31	MET	-	linker	UNP P03045
zB	39	ASN	ILE	engineered mutation	UNP O66529
zB	42	VAL	GLU	engineered mutation	UNP O66529
zB	58	VAL	ILE	engineered mutation	UNP O66529
zB	61	ASP	GLY	engineered mutation	UNP O66529
zB	62	ILE	VAL	engineered mutation	UNP O66529
zB	97	TYR	PHE	engineered mutation	UNP O66529
zB	102	GLY	-	linker	UNP O66529
zB	103	THR	-	linker	UNP O66529
zB	104	GLY	-	linker	UNP O66529
zB	105	HIS	-	linker	UNP O66529
zB	106	HIS	-	linker	UNP O66529
zB	107	HIS	-	linker	UNP O66529
zB	108	HIS	-	linker	UNP O66529
zB	109	HIS	-	linker	UNP O66529
zB	110	HIS	-	linker	UNP O66529
zB	111	GLY	-	linker	UNP O66529
zB	112	SER	-	linker	UNP O66529
zB	113	SER	-	linker	UNP O66529
zB	114	ILE	MET	engineered mutation	UNP O66529
zB	115	GLU	GLN	engineered mutation	UNP O66529
zB	138	THR	ALA	engineered mutation	UNP O66529
zB	177	ASP	GLY	engineered mutation	UNP O66529
zB	191	PHE	ILE	engineered mutation	UNP O66529
zB	193	ASP	VAL	engineered mutation	UNP O66529
zC	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
zC	2	GLY	-	cloning artifact	UNP P03045
zC	3	ASN	-	cloning artifact	UNP P03045
zC	4	ALA	-	cloning artifact	UNP P03045
zC	5	LYS	-	cloning artifact	UNP P03045
zC	6	THR	-	cloning artifact	UNP P03045
zC	24	ALA	-	linker	UNP P03045
zC	25	GLY	-	linker	UNP P03045
zC	26	ALA	-	linker	UNP P03045
zC	27	GLY	-	linker	UNP P03045
zC	28	ALA	-	linker	UNP P03045
zC	29	GLY	-	linker	UNP P03045
zC	30	ALA	-	linker	UNP P03045
zC	31	MET	-	linker	UNP P03045
zC	39	ASN	ILE	engineered mutation	UNP O66529
zC	42	VAL	GLU	engineered mutation	UNP O66529
zC	58	VAL	ILE	engineered mutation	UNP O66529
zC	61	ASP	GLY	engineered mutation	UNP O66529
zC	62	ILE	VAL	engineered mutation	UNP O66529
zC	97	TYR	PHE	engineered mutation	UNP O66529
zC	102	GLY	-	linker	UNP O66529
zC	103	THR	-	linker	UNP O66529
zC	104	GLY	-	linker	UNP O66529
zC	105	HIS	-	linker	UNP O66529
zC	106	HIS	-	linker	UNP O66529
zC	107	HIS	-	linker	UNP O66529
zC	108	HIS	-	linker	UNP O66529
zC	109	HIS	-	linker	UNP O66529
zC	110	HIS	-	linker	UNP O66529
zC	111	GLY	-	linker	UNP O66529
zC	112	SER	-	linker	UNP O66529
zC	113	SER	-	linker	UNP O66529
zC	114	ILE	MET	engineered mutation	UNP O66529
zC	115	GLU	GLN	engineered mutation	UNP O66529
zC	138	THR	ALA	engineered mutation	UNP O66529
zC	177	ASP	GLY	engineered mutation	UNP O66529
zC	191	PHE	ILE	engineered mutation	UNP O66529
zC	193	ASP	VAL	engineered mutation	UNP O66529
zD	1	MET	-	cloning artifact	UNP P03045
zD	2	GLY	-	cloning artifact	UNP P03045
zD	3	ASN	-	cloning artifact	UNP P03045
zD	4	ALA	-	cloning artifact	UNP P03045
zD	5	LYS	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
zD	6	THR	-	cloning artifact	UNP P03045
zD	24	ALA	-	linker	UNP P03045
zD	25	GLY	-	linker	UNP P03045
zD	26	ALA	-	linker	UNP P03045
zD	27	GLY	-	linker	UNP P03045
zD	28	ALA	-	linker	UNP P03045
zD	29	GLY	-	linker	UNP P03045
zD	30	ALA	-	linker	UNP P03045
zD	31	MET	-	linker	UNP P03045
zD	39	ASN	ILE	engineered mutation	UNP O66529
zD	42	VAL	GLU	engineered mutation	UNP O66529
zD	58	VAL	ILE	engineered mutation	UNP O66529
zD	61	ASP	GLY	engineered mutation	UNP O66529
zD	62	ILE	VAL	engineered mutation	UNP O66529
zD	97	TYR	PHE	engineered mutation	UNP O66529
zD	102	GLY	-	linker	UNP O66529
zD	103	THR	-	linker	UNP O66529
zD	104	GLY	-	linker	UNP O66529
zD	105	HIS	-	linker	UNP O66529
zD	106	HIS	-	linker	UNP O66529
zD	107	HIS	-	linker	UNP O66529
zD	108	HIS	-	linker	UNP O66529
zD	109	HIS	-	linker	UNP O66529
zD	110	HIS	-	linker	UNP O66529
zD	111	GLY	-	linker	UNP O66529
zD	112	SER	-	linker	UNP O66529
zD	113	SER	-	linker	UNP O66529
zD	114	ILE	MET	engineered mutation	UNP O66529
zD	115	GLU	GLN	engineered mutation	UNP O66529
zD	138	THR	ALA	engineered mutation	UNP O66529
zD	177	ASP	GLY	engineered mutation	UNP O66529
zD	191	PHE	ILE	engineered mutation	UNP O66529
zD	193	ASP	VAL	engineered mutation	UNP O66529
0A	1	MET	-	cloning artifact	UNP P03045
0A	2	GLY	-	cloning artifact	UNP P03045
0A	3	ASN	-	cloning artifact	UNP P03045
0A	4	ALA	-	cloning artifact	UNP P03045
0A	5	LYS	-	cloning artifact	UNP P03045
0A	6	THR	-	cloning artifact	UNP P03045
0A	24	ALA	-	linker	UNP P03045
0A	25	GLY	-	linker	UNP P03045
0A	26	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
0A	27	GLY	-	linker	UNP P03045
0A	28	ALA	-	linker	UNP P03045
0A	29	GLY	-	linker	UNP P03045
0A	30	ALA	-	linker	UNP P03045
0A	31	MET	-	linker	UNP P03045
0A	39	ASN	ILE	engineered mutation	UNP O66529
0A	42	VAL	GLU	engineered mutation	UNP O66529
0A	58	VAL	ILE	engineered mutation	UNP O66529
0A	61	ASP	GLY	engineered mutation	UNP O66529
0A	62	ILE	VAL	engineered mutation	UNP O66529
0A	97	TYR	PHE	engineered mutation	UNP O66529
0A	102	GLY	-	linker	UNP O66529
0A	103	THR	-	linker	UNP O66529
0A	104	GLY	-	linker	UNP O66529
0A	105	HIS	-	linker	UNP O66529
0A	106	HIS	-	linker	UNP O66529
0A	107	HIS	-	linker	UNP O66529
0A	108	HIS	-	linker	UNP O66529
0A	109	HIS	-	linker	UNP O66529
0A	110	HIS	-	linker	UNP O66529
0A	111	GLY	-	linker	UNP O66529
0A	112	SER	-	linker	UNP O66529
0A	113	SER	-	linker	UNP O66529
0A	114	ILE	MET	engineered mutation	UNP O66529
0A	115	GLU	GLN	engineered mutation	UNP O66529
0A	138	THR	ALA	engineered mutation	UNP O66529
0A	177	ASP	GLY	engineered mutation	UNP O66529
0A	191	PHE	ILE	engineered mutation	UNP O66529
0A	193	ASP	VAL	engineered mutation	UNP O66529
0B	1	MET	-	cloning artifact	UNP P03045
0B	2	GLY	-	cloning artifact	UNP P03045
0B	3	ASN	-	cloning artifact	UNP P03045
0B	4	ALA	-	cloning artifact	UNP P03045
0B	5	LYS	-	cloning artifact	UNP P03045
0B	6	THR	-	cloning artifact	UNP P03045
0B	24	ALA	-	linker	UNP P03045
0B	25	GLY	-	linker	UNP P03045
0B	26	ALA	-	linker	UNP P03045
0B	27	GLY	-	linker	UNP P03045
0B	28	ALA	-	linker	UNP P03045
0B	29	GLY	-	linker	UNP P03045
0B	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
0B	31	MET	-	linker	UNP P03045
0B	39	ASN	ILE	engineered mutation	UNP O66529
0B	42	VAL	GLU	engineered mutation	UNP O66529
0B	58	VAL	ILE	engineered mutation	UNP O66529
0B	61	ASP	GLY	engineered mutation	UNP O66529
0B	62	ILE	VAL	engineered mutation	UNP O66529
0B	97	TYR	PHE	engineered mutation	UNP O66529
0B	102	GLY	-	linker	UNP O66529
0B	103	THR	-	linker	UNP O66529
0B	104	GLY	-	linker	UNP O66529
0B	105	HIS	-	linker	UNP O66529
0B	106	HIS	-	linker	UNP O66529
0B	107	HIS	-	linker	UNP O66529
0B	108	HIS	-	linker	UNP O66529
0B	109	HIS	-	linker	UNP O66529
0B	110	HIS	-	linker	UNP O66529
0B	111	GLY	-	linker	UNP O66529
0B	112	SER	-	linker	UNP O66529
0B	113	SER	-	linker	UNP O66529
0B	114	ILE	MET	engineered mutation	UNP O66529
0B	115	GLU	GLN	engineered mutation	UNP O66529
0B	138	THR	ALA	engineered mutation	UNP O66529
0B	177	ASP	GLY	engineered mutation	UNP O66529
0B	191	PHE	ILE	engineered mutation	UNP O66529
0B	193	ASP	VAL	engineered mutation	UNP O66529
0C	1	MET	-	cloning artifact	UNP P03045
0C	2	GLY	-	cloning artifact	UNP P03045
0C	3	ASN	-	cloning artifact	UNP P03045
0C	4	ALA	-	cloning artifact	UNP P03045
0C	5	LYS	-	cloning artifact	UNP P03045
0C	6	THR	-	cloning artifact	UNP P03045
0C	24	ALA	-	linker	UNP P03045
0C	25	GLY	-	linker	UNP P03045
0C	26	ALA	-	linker	UNP P03045
0C	27	GLY	-	linker	UNP P03045
0C	28	ALA	-	linker	UNP P03045
0C	29	GLY	-	linker	UNP P03045
0C	30	ALA	-	linker	UNP P03045
0C	31	MET	-	linker	UNP P03045
0C	39	ASN	ILE	engineered mutation	UNP O66529
0C	42	VAL	GLU	engineered mutation	UNP O66529
0C	58	VAL	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
0C	61	ASP	GLY	engineered mutation	UNP O66529
0C	62	ILE	VAL	engineered mutation	UNP O66529
0C	97	TYR	PHE	engineered mutation	UNP O66529
0C	102	GLY	-	linker	UNP O66529
0C	103	THR	-	linker	UNP O66529
0C	104	GLY	-	linker	UNP O66529
0C	105	HIS	-	linker	UNP O66529
0C	106	HIS	-	linker	UNP O66529
0C	107	HIS	-	linker	UNP O66529
0C	108	HIS	-	linker	UNP O66529
0C	109	HIS	-	linker	UNP O66529
0C	110	HIS	-	linker	UNP O66529
0C	111	GLY	-	linker	UNP O66529
0C	112	SER	-	linker	UNP O66529
0C	113	SER	-	linker	UNP O66529
0C	114	ILE	MET	engineered mutation	UNP O66529
0C	115	GLU	GLN	engineered mutation	UNP O66529
0C	138	THR	ALA	engineered mutation	UNP O66529
0C	177	ASP	GLY	engineered mutation	UNP O66529
0C	191	PHE	ILE	engineered mutation	UNP O66529
0C	193	ASP	VAL	engineered mutation	UNP O66529
0D	1	MET	-	cloning artifact	UNP P03045
0D	2	GLY	-	cloning artifact	UNP P03045
0D	3	ASN	-	cloning artifact	UNP P03045
0D	4	ALA	-	cloning artifact	UNP P03045
0D	5	LYS	-	cloning artifact	UNP P03045
0D	6	THR	-	cloning artifact	UNP P03045
0D	24	ALA	-	linker	UNP P03045
0D	25	GLY	-	linker	UNP P03045
0D	26	ALA	-	linker	UNP P03045
0D	27	GLY	-	linker	UNP P03045
0D	28	ALA	-	linker	UNP P03045
0D	29	GLY	-	linker	UNP P03045
0D	30	ALA	-	linker	UNP P03045
0D	31	MET	-	linker	UNP P03045
0D	39	ASN	ILE	engineered mutation	UNP O66529
0D	42	VAL	GLU	engineered mutation	UNP O66529
0D	58	VAL	ILE	engineered mutation	UNP O66529
0D	61	ASP	GLY	engineered mutation	UNP O66529
0D	62	ILE	VAL	engineered mutation	UNP O66529
0D	97	TYR	PHE	engineered mutation	UNP O66529
0D	102	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
0D	103	THR	-	linker	UNP O66529
0D	104	GLY	-	linker	UNP O66529
0D	105	HIS	-	linker	UNP O66529
0D	106	HIS	-	linker	UNP O66529
0D	107	HIS	-	linker	UNP O66529
0D	108	HIS	-	linker	UNP O66529
0D	109	HIS	-	linker	UNP O66529
0D	110	HIS	-	linker	UNP O66529
0D	111	GLY	-	linker	UNP O66529
0D	112	SER	-	linker	UNP O66529
0D	113	SER	-	linker	UNP O66529
0D	114	ILE	MET	engineered mutation	UNP O66529
0D	115	GLU	GLN	engineered mutation	UNP O66529
0D	138	THR	ALA	engineered mutation	UNP O66529
0D	177	ASP	GLY	engineered mutation	UNP O66529
0D	191	PHE	ILE	engineered mutation	UNP O66529
0D	193	ASP	VAL	engineered mutation	UNP O66529
1A	1	MET	-	cloning artifact	UNP P03045
1A	2	GLY	-	cloning artifact	UNP P03045
1A	3	ASN	-	cloning artifact	UNP P03045
1A	4	ALA	-	cloning artifact	UNP P03045
1A	5	LYS	-	cloning artifact	UNP P03045
1A	6	THR	-	cloning artifact	UNP P03045
1A	24	ALA	-	linker	UNP P03045
1A	25	GLY	-	linker	UNP P03045
1A	26	ALA	-	linker	UNP P03045
1A	27	GLY	-	linker	UNP P03045
1A	28	ALA	-	linker	UNP P03045
1A	29	GLY	-	linker	UNP P03045
1A	30	ALA	-	linker	UNP P03045
1A	31	MET	-	linker	UNP P03045
1A	39	ASN	ILE	engineered mutation	UNP O66529
1A	42	VAL	GLU	engineered mutation	UNP O66529
1A	58	VAL	ILE	engineered mutation	UNP O66529
1A	61	ASP	GLY	engineered mutation	UNP O66529
1A	62	ILE	VAL	engineered mutation	UNP O66529
1A	97	TYR	PHE	engineered mutation	UNP O66529
1A	102	GLY	-	linker	UNP O66529
1A	103	THR	-	linker	UNP O66529
1A	104	GLY	-	linker	UNP O66529
1A	105	HIS	-	linker	UNP O66529
1A	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
1A	107	HIS	-	linker	UNP O66529
1A	108	HIS	-	linker	UNP O66529
1A	109	HIS	-	linker	UNP O66529
1A	110	HIS	-	linker	UNP O66529
1A	111	GLY	-	linker	UNP O66529
1A	112	SER	-	linker	UNP O66529
1A	113	SER	-	linker	UNP O66529
1A	114	ILE	MET	engineered mutation	UNP O66529
1A	115	GLU	GLN	engineered mutation	UNP O66529
1A	138	THR	ALA	engineered mutation	UNP O66529
1A	177	ASP	GLY	engineered mutation	UNP O66529
1A	191	PHE	ILE	engineered mutation	UNP O66529
1A	193	ASP	VAL	engineered mutation	UNP O66529
1B	1	MET	-	cloning artifact	UNP P03045
1B	2	GLY	-	cloning artifact	UNP P03045
1B	3	ASN	-	cloning artifact	UNP P03045
1B	4	ALA	-	cloning artifact	UNP P03045
1B	5	LYS	-	cloning artifact	UNP P03045
1B	6	THR	-	cloning artifact	UNP P03045
1B	24	ALA	-	linker	UNP P03045
1B	25	GLY	-	linker	UNP P03045
1B	26	ALA	-	linker	UNP P03045
1B	27	GLY	-	linker	UNP P03045
1B	28	ALA	-	linker	UNP P03045
1B	29	GLY	-	linker	UNP P03045
1B	30	ALA	-	linker	UNP P03045
1B	31	MET	-	linker	UNP P03045
1B	39	ASN	ILE	engineered mutation	UNP O66529
1B	42	VAL	GLU	engineered mutation	UNP O66529
1B	58	VAL	ILE	engineered mutation	UNP O66529
1B	61	ASP	GLY	engineered mutation	UNP O66529
1B	62	ILE	VAL	engineered mutation	UNP O66529
1B	97	TYR	PHE	engineered mutation	UNP O66529
1B	102	GLY	-	linker	UNP O66529
1B	103	THR	-	linker	UNP O66529
1B	104	GLY	-	linker	UNP O66529
1B	105	HIS	-	linker	UNP O66529
1B	106	HIS	-	linker	UNP O66529
1B	107	HIS	-	linker	UNP O66529
1B	108	HIS	-	linker	UNP O66529
1B	109	HIS	-	linker	UNP O66529
1B	110	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
1B	111	GLY	-	linker	UNP O66529
1B	112	SER	-	linker	UNP O66529
1B	113	SER	-	linker	UNP O66529
1B	114	ILE	MET	engineered mutation	UNP O66529
1B	115	GLU	GLN	engineered mutation	UNP O66529
1B	138	THR	ALA	engineered mutation	UNP O66529
1B	177	ASP	GLY	engineered mutation	UNP O66529
1B	191	PHE	ILE	engineered mutation	UNP O66529
1B	193	ASP	VAL	engineered mutation	UNP O66529
1C	1	MET	-	cloning artifact	UNP P03045
1C	2	GLY	-	cloning artifact	UNP P03045
1C	3	ASN	-	cloning artifact	UNP P03045
1C	4	ALA	-	cloning artifact	UNP P03045
1C	5	LYS	-	cloning artifact	UNP P03045
1C	6	THR	-	cloning artifact	UNP P03045
1C	24	ALA	-	linker	UNP P03045
1C	25	GLY	-	linker	UNP P03045
1C	26	ALA	-	linker	UNP P03045
1C	27	GLY	-	linker	UNP P03045
1C	28	ALA	-	linker	UNP P03045
1C	29	GLY	-	linker	UNP P03045
1C	30	ALA	-	linker	UNP P03045
1C	31	MET	-	linker	UNP P03045
1C	39	ASN	ILE	engineered mutation	UNP O66529
1C	42	VAL	GLU	engineered mutation	UNP O66529
1C	58	VAL	ILE	engineered mutation	UNP O66529
1C	61	ASP	GLY	engineered mutation	UNP O66529
1C	62	ILE	VAL	engineered mutation	UNP O66529
1C	97	TYR	PHE	engineered mutation	UNP O66529
1C	102	GLY	-	linker	UNP O66529
1C	103	THR	-	linker	UNP O66529
1C	104	GLY	-	linker	UNP O66529
1C	105	HIS	-	linker	UNP O66529
1C	106	HIS	-	linker	UNP O66529
1C	107	HIS	-	linker	UNP O66529
1C	108	HIS	-	linker	UNP O66529
1C	109	HIS	-	linker	UNP O66529
1C	110	HIS	-	linker	UNP O66529
1C	111	GLY	-	linker	UNP O66529
1C	112	SER	-	linker	UNP O66529
1C	113	SER	-	linker	UNP O66529
1C	114	ILE	MET	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
1C	115	GLU	GLN	engineered mutation	UNP O66529
1C	138	THR	ALA	engineered mutation	UNP O66529
1C	177	ASP	GLY	engineered mutation	UNP O66529
1C	191	PHE	ILE	engineered mutation	UNP O66529
1C	193	ASP	VAL	engineered mutation	UNP O66529
1D	1	MET	-	cloning artifact	UNP P03045
1D	2	GLY	-	cloning artifact	UNP P03045
1D	3	ASN	-	cloning artifact	UNP P03045
1D	4	ALA	-	cloning artifact	UNP P03045
1D	5	LYS	-	cloning artifact	UNP P03045
1D	6	THR	-	cloning artifact	UNP P03045
1D	24	ALA	-	linker	UNP P03045
1D	25	GLY	-	linker	UNP P03045
1D	26	ALA	-	linker	UNP P03045
1D	27	GLY	-	linker	UNP P03045
1D	28	ALA	-	linker	UNP P03045
1D	29	GLY	-	linker	UNP P03045
1D	30	ALA	-	linker	UNP P03045
1D	31	MET	-	linker	UNP P03045
1D	39	ASN	ILE	engineered mutation	UNP O66529
1D	42	VAL	GLU	engineered mutation	UNP O66529
1D	58	VAL	ILE	engineered mutation	UNP O66529
1D	61	ASP	GLY	engineered mutation	UNP O66529
1D	62	ILE	VAL	engineered mutation	UNP O66529
1D	97	TYR	PHE	engineered mutation	UNP O66529
1D	102	GLY	-	linker	UNP O66529
1D	103	THR	-	linker	UNP O66529
1D	104	GLY	-	linker	UNP O66529
1D	105	HIS	-	linker	UNP O66529
1D	106	HIS	-	linker	UNP O66529
1D	107	HIS	-	linker	UNP O66529
1D	108	HIS	-	linker	UNP O66529
1D	109	HIS	-	linker	UNP O66529
1D	110	HIS	-	linker	UNP O66529
1D	111	GLY	-	linker	UNP O66529
1D	112	SER	-	linker	UNP O66529
1D	113	SER	-	linker	UNP O66529
1D	114	ILE	MET	engineered mutation	UNP O66529
1D	115	GLU	GLN	engineered mutation	UNP O66529
1D	138	THR	ALA	engineered mutation	UNP O66529
1D	177	ASP	GLY	engineered mutation	UNP O66529
1D	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
1D	193	ASP	VAL	engineered mutation	UNP O66529
2A	1	MET	-	cloning artifact	UNP P03045
2A	2	GLY	-	cloning artifact	UNP P03045
2A	3	ASN	-	cloning artifact	UNP P03045
2A	4	ALA	-	cloning artifact	UNP P03045
2A	5	LYS	-	cloning artifact	UNP P03045
2A	6	THR	-	cloning artifact	UNP P03045
2A	24	ALA	-	linker	UNP P03045
2A	25	GLY	-	linker	UNP P03045
2A	26	ALA	-	linker	UNP P03045
2A	27	GLY	-	linker	UNP P03045
2A	28	ALA	-	linker	UNP P03045
2A	29	GLY	-	linker	UNP P03045
2A	30	ALA	-	linker	UNP P03045
2A	31	MET	-	linker	UNP P03045
2A	39	ASN	ILE	engineered mutation	UNP O66529
2A	42	VAL	GLU	engineered mutation	UNP O66529
2A	58	VAL	ILE	engineered mutation	UNP O66529
2A	61	ASP	GLY	engineered mutation	UNP O66529
2A	62	ILE	VAL	engineered mutation	UNP O66529
2A	97	TYR	PHE	engineered mutation	UNP O66529
2A	102	GLY	-	linker	UNP O66529
2A	103	THR	-	linker	UNP O66529
2A	104	GLY	-	linker	UNP O66529
2A	105	HIS	-	linker	UNP O66529
2A	106	HIS	-	linker	UNP O66529
2A	107	HIS	-	linker	UNP O66529
2A	108	HIS	-	linker	UNP O66529
2A	109	HIS	-	linker	UNP O66529
2A	110	HIS	-	linker	UNP O66529
2A	111	GLY	-	linker	UNP O66529
2A	112	SER	-	linker	UNP O66529
2A	113	SER	-	linker	UNP O66529
2A	114	ILE	MET	engineered mutation	UNP O66529
2A	115	GLU	GLN	engineered mutation	UNP O66529
2A	138	THR	ALA	engineered mutation	UNP O66529
2A	177	ASP	GLY	engineered mutation	UNP O66529
2A	191	PHE	ILE	engineered mutation	UNP O66529
2A	193	ASP	VAL	engineered mutation	UNP O66529
2B	1	MET	-	cloning artifact	UNP P03045
2B	2	GLY	-	cloning artifact	UNP P03045
2B	3	ASN	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
2B	4	ALA	-	cloning artifact	UNP P03045
2B	5	LYS	-	cloning artifact	UNP P03045
2B	6	THR	-	cloning artifact	UNP P03045
2B	24	ALA	-	linker	UNP P03045
2B	25	GLY	-	linker	UNP P03045
2B	26	ALA	-	linker	UNP P03045
2B	27	GLY	-	linker	UNP P03045
2B	28	ALA	-	linker	UNP P03045
2B	29	GLY	-	linker	UNP P03045
2B	30	ALA	-	linker	UNP P03045
2B	31	MET	-	linker	UNP P03045
2B	39	ASN	ILE	engineered mutation	UNP O66529
2B	42	VAL	GLU	engineered mutation	UNP O66529
2B	58	VAL	ILE	engineered mutation	UNP O66529
2B	61	ASP	GLY	engineered mutation	UNP O66529
2B	62	ILE	VAL	engineered mutation	UNP O66529
2B	97	TYR	PHE	engineered mutation	UNP O66529
2B	102	GLY	-	linker	UNP O66529
2B	103	THR	-	linker	UNP O66529
2B	104	GLY	-	linker	UNP O66529
2B	105	HIS	-	linker	UNP O66529
2B	106	HIS	-	linker	UNP O66529
2B	107	HIS	-	linker	UNP O66529
2B	108	HIS	-	linker	UNP O66529
2B	109	HIS	-	linker	UNP O66529
2B	110	HIS	-	linker	UNP O66529
2B	111	GLY	-	linker	UNP O66529
2B	112	SER	-	linker	UNP O66529
2B	113	SER	-	linker	UNP O66529
2B	114	ILE	MET	engineered mutation	UNP O66529
2B	115	GLU	GLN	engineered mutation	UNP O66529
2B	138	THR	ALA	engineered mutation	UNP O66529
2B	177	ASP	GLY	engineered mutation	UNP O66529
2B	191	PHE	ILE	engineered mutation	UNP O66529
2B	193	ASP	VAL	engineered mutation	UNP O66529
2C	1	MET	-	cloning artifact	UNP P03045
2C	2	GLY	-	cloning artifact	UNP P03045
2C	3	ASN	-	cloning artifact	UNP P03045
2C	4	ALA	-	cloning artifact	UNP P03045
2C	5	LYS	-	cloning artifact	UNP P03045
2C	6	THR	-	cloning artifact	UNP P03045
2C	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
2C	25	GLY	-	linker	UNP P03045
2C	26	ALA	-	linker	UNP P03045
2C	27	GLY	-	linker	UNP P03045
2C	28	ALA	-	linker	UNP P03045
2C	29	GLY	-	linker	UNP P03045
2C	30	ALA	-	linker	UNP P03045
2C	31	MET	-	linker	UNP P03045
2C	39	ASN	ILE	engineered mutation	UNP O66529
2C	42	VAL	GLU	engineered mutation	UNP O66529
2C	58	VAL	ILE	engineered mutation	UNP O66529
2C	61	ASP	GLY	engineered mutation	UNP O66529
2C	62	ILE	VAL	engineered mutation	UNP O66529
2C	97	TYR	PHE	engineered mutation	UNP O66529
2C	102	GLY	-	linker	UNP O66529
2C	103	THR	-	linker	UNP O66529
2C	104	GLY	-	linker	UNP O66529
2C	105	HIS	-	linker	UNP O66529
2C	106	HIS	-	linker	UNP O66529
2C	107	HIS	-	linker	UNP O66529
2C	108	HIS	-	linker	UNP O66529
2C	109	HIS	-	linker	UNP O66529
2C	110	HIS	-	linker	UNP O66529
2C	111	GLY	-	linker	UNP O66529
2C	112	SER	-	linker	UNP O66529
2C	113	SER	-	linker	UNP O66529
2C	114	ILE	MET	engineered mutation	UNP O66529
2C	115	GLU	GLN	engineered mutation	UNP O66529
2C	138	THR	ALA	engineered mutation	UNP O66529
2C	177	ASP	GLY	engineered mutation	UNP O66529
2C	191	PHE	ILE	engineered mutation	UNP O66529
2C	193	ASP	VAL	engineered mutation	UNP O66529
2D	1	MET	-	cloning artifact	UNP P03045
2D	2	GLY	-	cloning artifact	UNP P03045
2D	3	ASN	-	cloning artifact	UNP P03045
2D	4	ALA	-	cloning artifact	UNP P03045
2D	5	LYS	-	cloning artifact	UNP P03045
2D	6	THR	-	cloning artifact	UNP P03045
2D	24	ALA	-	linker	UNP P03045
2D	25	GLY	-	linker	UNP P03045
2D	26	ALA	-	linker	UNP P03045
2D	27	GLY	-	linker	UNP P03045
2D	28	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
2D	29	GLY	-	linker	UNP P03045
2D	30	ALA	-	linker	UNP P03045
2D	31	MET	-	linker	UNP P03045
2D	39	ASN	ILE	engineered mutation	UNP O66529
2D	42	VAL	GLU	engineered mutation	UNP O66529
2D	58	VAL	ILE	engineered mutation	UNP O66529
2D	61	ASP	GLY	engineered mutation	UNP O66529
2D	62	ILE	VAL	engineered mutation	UNP O66529
2D	97	TYR	PHE	engineered mutation	UNP O66529
2D	102	GLY	-	linker	UNP O66529
2D	103	THR	-	linker	UNP O66529
2D	104	GLY	-	linker	UNP O66529
2D	105	HIS	-	linker	UNP O66529
2D	106	HIS	-	linker	UNP O66529
2D	107	HIS	-	linker	UNP O66529
2D	108	HIS	-	linker	UNP O66529
2D	109	HIS	-	linker	UNP O66529
2D	110	HIS	-	linker	UNP O66529
2D	111	GLY	-	linker	UNP O66529
2D	112	SER	-	linker	UNP O66529
2D	113	SER	-	linker	UNP O66529
2D	114	ILE	MET	engineered mutation	UNP O66529
2D	115	GLU	GLN	engineered mutation	UNP O66529
2D	138	THR	ALA	engineered mutation	UNP O66529
2D	177	ASP	GLY	engineered mutation	UNP O66529
2D	191	PHE	ILE	engineered mutation	UNP O66529
2D	193	ASP	VAL	engineered mutation	UNP O66529
3A	1	MET	-	cloning artifact	UNP P03045
3A	2	GLY	-	cloning artifact	UNP P03045
3A	3	ASN	-	cloning artifact	UNP P03045
3A	4	ALA	-	cloning artifact	UNP P03045
3A	5	LYS	-	cloning artifact	UNP P03045
3A	6	THR	-	cloning artifact	UNP P03045
3A	24	ALA	-	linker	UNP P03045
3A	25	GLY	-	linker	UNP P03045
3A	26	ALA	-	linker	UNP P03045
3A	27	GLY	-	linker	UNP P03045
3A	28	ALA	-	linker	UNP P03045
3A	29	GLY	-	linker	UNP P03045
3A	30	ALA	-	linker	UNP P03045
3A	31	MET	-	linker	UNP P03045
3A	39	ASN	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
3A	42	VAL	GLU	engineered mutation	UNP O66529
3A	58	VAL	ILE	engineered mutation	UNP O66529
3A	61	ASP	GLY	engineered mutation	UNP O66529
3A	62	ILE	VAL	engineered mutation	UNP O66529
3A	97	TYR	PHE	engineered mutation	UNP O66529
3A	102	GLY	-	linker	UNP O66529
3A	103	THR	-	linker	UNP O66529
3A	104	GLY	-	linker	UNP O66529
3A	105	HIS	-	linker	UNP O66529
3A	106	HIS	-	linker	UNP O66529
3A	107	HIS	-	linker	UNP O66529
3A	108	HIS	-	linker	UNP O66529
3A	109	HIS	-	linker	UNP O66529
3A	110	HIS	-	linker	UNP O66529
3A	111	GLY	-	linker	UNP O66529
3A	112	SER	-	linker	UNP O66529
3A	113	SER	-	linker	UNP O66529
3A	114	ILE	MET	engineered mutation	UNP O66529
3A	115	GLU	GLN	engineered mutation	UNP O66529
3A	138	THR	ALA	engineered mutation	UNP O66529
3A	177	ASP	GLY	engineered mutation	UNP O66529
3A	191	PHE	ILE	engineered mutation	UNP O66529
3A	193	ASP	VAL	engineered mutation	UNP O66529
3B	1	MET	-	cloning artifact	UNP P03045
3B	2	GLY	-	cloning artifact	UNP P03045
3B	3	ASN	-	cloning artifact	UNP P03045
3B	4	ALA	-	cloning artifact	UNP P03045
3B	5	LYS	-	cloning artifact	UNP P03045
3B	6	THR	-	cloning artifact	UNP P03045
3B	24	ALA	-	linker	UNP P03045
3B	25	GLY	-	linker	UNP P03045
3B	26	ALA	-	linker	UNP P03045
3B	27	GLY	-	linker	UNP P03045
3B	28	ALA	-	linker	UNP P03045
3B	29	GLY	-	linker	UNP P03045
3B	30	ALA	-	linker	UNP P03045
3B	31	MET	-	linker	UNP P03045
3B	39	ASN	ILE	engineered mutation	UNP O66529
3B	42	VAL	GLU	engineered mutation	UNP O66529
3B	58	VAL	ILE	engineered mutation	UNP O66529
3B	61	ASP	GLY	engineered mutation	UNP O66529
3B	62	ILE	VAL	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
3B	97	TYR	PHE	engineered mutation	UNP O66529
3B	102	GLY	-	linker	UNP O66529
3B	103	THR	-	linker	UNP O66529
3B	104	GLY	-	linker	UNP O66529
3B	105	HIS	-	linker	UNP O66529
3B	106	HIS	-	linker	UNP O66529
3B	107	HIS	-	linker	UNP O66529
3B	108	HIS	-	linker	UNP O66529
3B	109	HIS	-	linker	UNP O66529
3B	110	HIS	-	linker	UNP O66529
3B	111	GLY	-	linker	UNP O66529
3B	112	SER	-	linker	UNP O66529
3B	113	SER	-	linker	UNP O66529
3B	114	ILE	MET	engineered mutation	UNP O66529
3B	115	GLU	GLN	engineered mutation	UNP O66529
3B	138	THR	ALA	engineered mutation	UNP O66529
3B	177	ASP	GLY	engineered mutation	UNP O66529
3B	191	PHE	ILE	engineered mutation	UNP O66529
3B	193	ASP	VAL	engineered mutation	UNP O66529
3C	1	MET	-	cloning artifact	UNP P03045
3C	2	GLY	-	cloning artifact	UNP P03045
3C	3	ASN	-	cloning artifact	UNP P03045
3C	4	ALA	-	cloning artifact	UNP P03045
3C	5	LYS	-	cloning artifact	UNP P03045
3C	6	THR	-	cloning artifact	UNP P03045
3C	24	ALA	-	linker	UNP P03045
3C	25	GLY	-	linker	UNP P03045
3C	26	ALA	-	linker	UNP P03045
3C	27	GLY	-	linker	UNP P03045
3C	28	ALA	-	linker	UNP P03045
3C	29	GLY	-	linker	UNP P03045
3C	30	ALA	-	linker	UNP P03045
3C	31	MET	-	linker	UNP P03045
3C	39	ASN	ILE	engineered mutation	UNP O66529
3C	42	VAL	GLU	engineered mutation	UNP O66529
3C	58	VAL	ILE	engineered mutation	UNP O66529
3C	61	ASP	GLY	engineered mutation	UNP O66529
3C	62	ILE	VAL	engineered mutation	UNP O66529
3C	97	TYR	PHE	engineered mutation	UNP O66529
3C	102	GLY	-	linker	UNP O66529
3C	103	THR	-	linker	UNP O66529
3C	104	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
3C	105	HIS	-	linker	UNP O66529
3C	106	HIS	-	linker	UNP O66529
3C	107	HIS	-	linker	UNP O66529
3C	108	HIS	-	linker	UNP O66529
3C	109	HIS	-	linker	UNP O66529
3C	110	HIS	-	linker	UNP O66529
3C	111	GLY	-	linker	UNP O66529
3C	112	SER	-	linker	UNP O66529
3C	113	SER	-	linker	UNP O66529
3C	114	ILE	MET	engineered mutation	UNP O66529
3C	115	GLU	GLN	engineered mutation	UNP O66529
3C	138	THR	ALA	engineered mutation	UNP O66529
3C	177	ASP	GLY	engineered mutation	UNP O66529
3C	191	PHE	ILE	engineered mutation	UNP O66529
3C	193	ASP	VAL	engineered mutation	UNP O66529
3D	1	MET	-	cloning artifact	UNP P03045
3D	2	GLY	-	cloning artifact	UNP P03045
3D	3	ASN	-	cloning artifact	UNP P03045
3D	4	ALA	-	cloning artifact	UNP P03045
3D	5	LYS	-	cloning artifact	UNP P03045
3D	6	THR	-	cloning artifact	UNP P03045
3D	24	ALA	-	linker	UNP P03045
3D	25	GLY	-	linker	UNP P03045
3D	26	ALA	-	linker	UNP P03045
3D	27	GLY	-	linker	UNP P03045
3D	28	ALA	-	linker	UNP P03045
3D	29	GLY	-	linker	UNP P03045
3D	30	ALA	-	linker	UNP P03045
3D	31	MET	-	linker	UNP P03045
3D	39	ASN	ILE	engineered mutation	UNP O66529
3D	42	VAL	GLU	engineered mutation	UNP O66529
3D	58	VAL	ILE	engineered mutation	UNP O66529
3D	61	ASP	GLY	engineered mutation	UNP O66529
3D	62	ILE	VAL	engineered mutation	UNP O66529
3D	97	TYR	PHE	engineered mutation	UNP O66529
3D	102	GLY	-	linker	UNP O66529
3D	103	THR	-	linker	UNP O66529
3D	104	GLY	-	linker	UNP O66529
3D	105	HIS	-	linker	UNP O66529
3D	106	HIS	-	linker	UNP O66529
3D	107	HIS	-	linker	UNP O66529
3D	108	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
3D	109	HIS	-	linker	UNP O66529
3D	110	HIS	-	linker	UNP O66529
3D	111	GLY	-	linker	UNP O66529
3D	112	SER	-	linker	UNP O66529
3D	113	SER	-	linker	UNP O66529
3D	114	ILE	MET	engineered mutation	UNP O66529
3D	115	GLU	GLN	engineered mutation	UNP O66529
3D	138	THR	ALA	engineered mutation	UNP O66529
3D	177	ASP	GLY	engineered mutation	UNP O66529
3D	191	PHE	ILE	engineered mutation	UNP O66529
3D	193	ASP	VAL	engineered mutation	UNP O66529
4A	1	MET	-	cloning artifact	UNP P03045
4A	2	GLY	-	cloning artifact	UNP P03045
4A	3	ASN	-	cloning artifact	UNP P03045
4A	4	ALA	-	cloning artifact	UNP P03045
4A	5	LYS	-	cloning artifact	UNP P03045
4A	6	THR	-	cloning artifact	UNP P03045
4A	24	ALA	-	linker	UNP P03045
4A	25	GLY	-	linker	UNP P03045
4A	26	ALA	-	linker	UNP P03045
4A	27	GLY	-	linker	UNP P03045
4A	28	ALA	-	linker	UNP P03045
4A	29	GLY	-	linker	UNP P03045
4A	30	ALA	-	linker	UNP P03045
4A	31	MET	-	linker	UNP P03045
4A	39	ASN	ILE	engineered mutation	UNP O66529
4A	42	VAL	GLU	engineered mutation	UNP O66529
4A	58	VAL	ILE	engineered mutation	UNP O66529
4A	61	ASP	GLY	engineered mutation	UNP O66529
4A	62	ILE	VAL	engineered mutation	UNP O66529
4A	97	TYR	PHE	engineered mutation	UNP O66529
4A	102	GLY	-	linker	UNP O66529
4A	103	THR	-	linker	UNP O66529
4A	104	GLY	-	linker	UNP O66529
4A	105	HIS	-	linker	UNP O66529
4A	106	HIS	-	linker	UNP O66529
4A	107	HIS	-	linker	UNP O66529
4A	108	HIS	-	linker	UNP O66529
4A	109	HIS	-	linker	UNP O66529
4A	110	HIS	-	linker	UNP O66529
4A	111	GLY	-	linker	UNP O66529
4A	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
4A	113	SER	-	linker	UNP O66529
4A	114	ILE	MET	engineered mutation	UNP O66529
4A	115	GLU	GLN	engineered mutation	UNP O66529
4A	138	THR	ALA	engineered mutation	UNP O66529
4A	177	ASP	GLY	engineered mutation	UNP O66529
4A	191	PHE	ILE	engineered mutation	UNP O66529
4A	193	ASP	VAL	engineered mutation	UNP O66529
4B	1	MET	-	cloning artifact	UNP P03045
4B	2	GLY	-	cloning artifact	UNP P03045
4B	3	ASN	-	cloning artifact	UNP P03045
4B	4	ALA	-	cloning artifact	UNP P03045
4B	5	LYS	-	cloning artifact	UNP P03045
4B	6	THR	-	cloning artifact	UNP P03045
4B	24	ALA	-	linker	UNP P03045
4B	25	GLY	-	linker	UNP P03045
4B	26	ALA	-	linker	UNP P03045
4B	27	GLY	-	linker	UNP P03045
4B	28	ALA	-	linker	UNP P03045
4B	29	GLY	-	linker	UNP P03045
4B	30	ALA	-	linker	UNP P03045
4B	31	MET	-	linker	UNP P03045
4B	39	ASN	ILE	engineered mutation	UNP O66529
4B	42	VAL	GLU	engineered mutation	UNP O66529
4B	58	VAL	ILE	engineered mutation	UNP O66529
4B	61	ASP	GLY	engineered mutation	UNP O66529
4B	62	ILE	VAL	engineered mutation	UNP O66529
4B	97	TYR	PHE	engineered mutation	UNP O66529
4B	102	GLY	-	linker	UNP O66529
4B	103	THR	-	linker	UNP O66529
4B	104	GLY	-	linker	UNP O66529
4B	105	HIS	-	linker	UNP O66529
4B	106	HIS	-	linker	UNP O66529
4B	107	HIS	-	linker	UNP O66529
4B	108	HIS	-	linker	UNP O66529
4B	109	HIS	-	linker	UNP O66529
4B	110	HIS	-	linker	UNP O66529
4B	111	GLY	-	linker	UNP O66529
4B	112	SER	-	linker	UNP O66529
4B	113	SER	-	linker	UNP O66529
4B	114	ILE	MET	engineered mutation	UNP O66529
4B	115	GLU	GLN	engineered mutation	UNP O66529
4B	138	THR	ALA	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
4B	177	ASP	GLY	engineered mutation	UNP O66529
4B	191	PHE	ILE	engineered mutation	UNP O66529
4B	193	ASP	VAL	engineered mutation	UNP O66529
4C	1	MET	-	cloning artifact	UNP P03045
4C	2	GLY	-	cloning artifact	UNP P03045
4C	3	ASN	-	cloning artifact	UNP P03045
4C	4	ALA	-	cloning artifact	UNP P03045
4C	5	LYS	-	cloning artifact	UNP P03045
4C	6	THR	-	cloning artifact	UNP P03045
4C	24	ALA	-	linker	UNP P03045
4C	25	GLY	-	linker	UNP P03045
4C	26	ALA	-	linker	UNP P03045
4C	27	GLY	-	linker	UNP P03045
4C	28	ALA	-	linker	UNP P03045
4C	29	GLY	-	linker	UNP P03045
4C	30	ALA	-	linker	UNP P03045
4C	31	MET	-	linker	UNP P03045
4C	39	ASN	ILE	engineered mutation	UNP O66529
4C	42	VAL	GLU	engineered mutation	UNP O66529
4C	58	VAL	ILE	engineered mutation	UNP O66529
4C	61	ASP	GLY	engineered mutation	UNP O66529
4C	62	ILE	VAL	engineered mutation	UNP O66529
4C	97	TYR	PHE	engineered mutation	UNP O66529
4C	102	GLY	-	linker	UNP O66529
4C	103	THR	-	linker	UNP O66529
4C	104	GLY	-	linker	UNP O66529
4C	105	HIS	-	linker	UNP O66529
4C	106	HIS	-	linker	UNP O66529
4C	107	HIS	-	linker	UNP O66529
4C	108	HIS	-	linker	UNP O66529
4C	109	HIS	-	linker	UNP O66529
4C	110	HIS	-	linker	UNP O66529
4C	111	GLY	-	linker	UNP O66529
4C	112	SER	-	linker	UNP O66529
4C	113	SER	-	linker	UNP O66529
4C	114	ILE	MET	engineered mutation	UNP O66529
4C	115	GLU	GLN	engineered mutation	UNP O66529
4C	138	THR	ALA	engineered mutation	UNP O66529
4C	177	ASP	GLY	engineered mutation	UNP O66529
4C	191	PHE	ILE	engineered mutation	UNP O66529
4C	193	ASP	VAL	engineered mutation	UNP O66529
4D	1	MET	-	cloning artifact	UNP P03045

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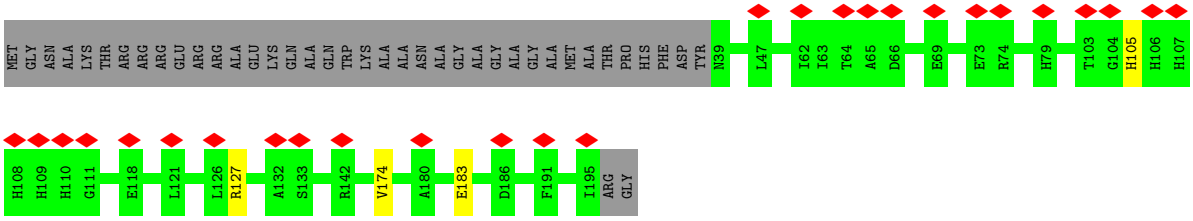
Chain	Residue	Modelled	Actual	Comment	Reference
4D	2	GLY	-	cloning artifact	UNP P03045
4D	3	ASN	-	cloning artifact	UNP P03045
4D	4	ALA	-	cloning artifact	UNP P03045
4D	5	LYS	-	cloning artifact	UNP P03045
4D	6	THR	-	cloning artifact	UNP P03045
4D	24	ALA	-	linker	UNP P03045
4D	25	GLY	-	linker	UNP P03045
4D	26	ALA	-	linker	UNP P03045
4D	27	GLY	-	linker	UNP P03045
4D	28	ALA	-	linker	UNP P03045
4D	29	GLY	-	linker	UNP P03045
4D	30	ALA	-	linker	UNP P03045
4D	31	MET	-	linker	UNP P03045
4D	39	ASN	ILE	engineered mutation	UNP O66529
4D	42	VAL	GLU	engineered mutation	UNP O66529
4D	58	VAL	ILE	engineered mutation	UNP O66529
4D	61	ASP	GLY	engineered mutation	UNP O66529
4D	62	ILE	VAL	engineered mutation	UNP O66529
4D	97	TYR	PHE	engineered mutation	UNP O66529
4D	102	GLY	-	linker	UNP O66529
4D	103	THR	-	linker	UNP O66529
4D	104	GLY	-	linker	UNP O66529
4D	105	HIS	-	linker	UNP O66529
4D	106	HIS	-	linker	UNP O66529
4D	107	HIS	-	linker	UNP O66529
4D	108	HIS	-	linker	UNP O66529
4D	109	HIS	-	linker	UNP O66529
4D	110	HIS	-	linker	UNP O66529
4D	111	GLY	-	linker	UNP O66529
4D	112	SER	-	linker	UNP O66529
4D	113	SER	-	linker	UNP O66529
4D	114	ILE	MET	engineered mutation	UNP O66529
4D	115	GLU	GLN	engineered mutation	UNP O66529
4D	138	THR	ALA	engineered mutation	UNP O66529
4D	177	ASP	GLY	engineered mutation	UNP O66529
4D	191	PHE	ILE	engineered mutation	UNP O66529
4D	193	ASP	VAL	engineered mutation	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.

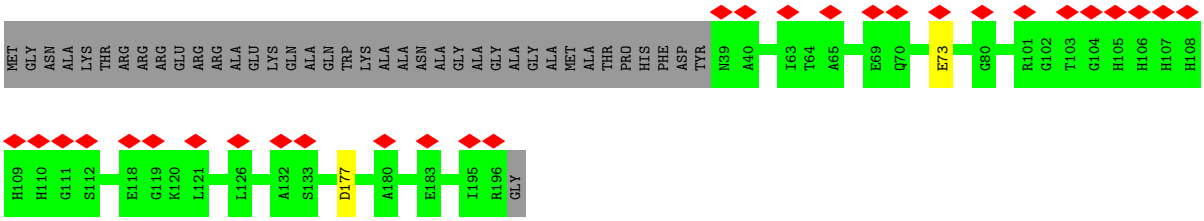
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AA:



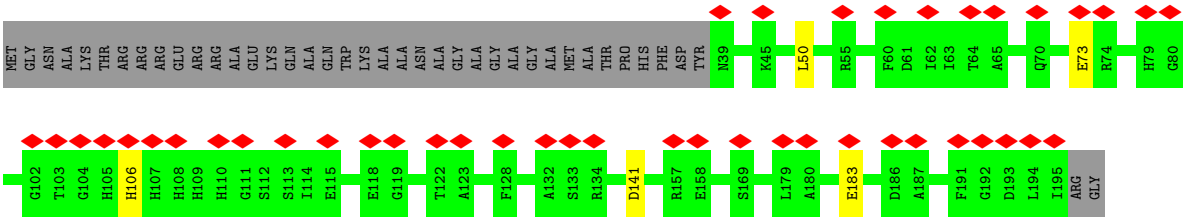
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AB:



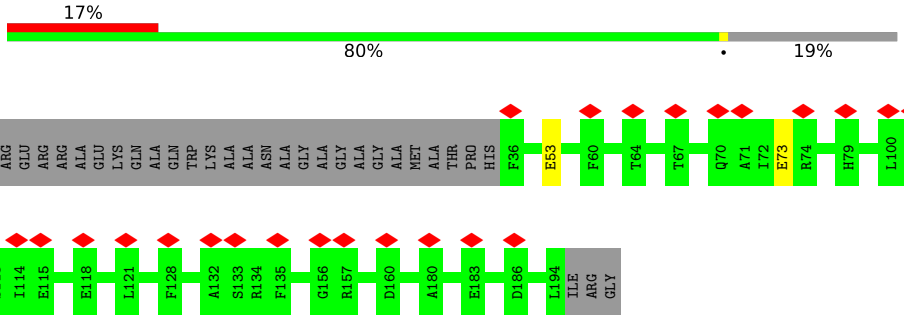
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AC:



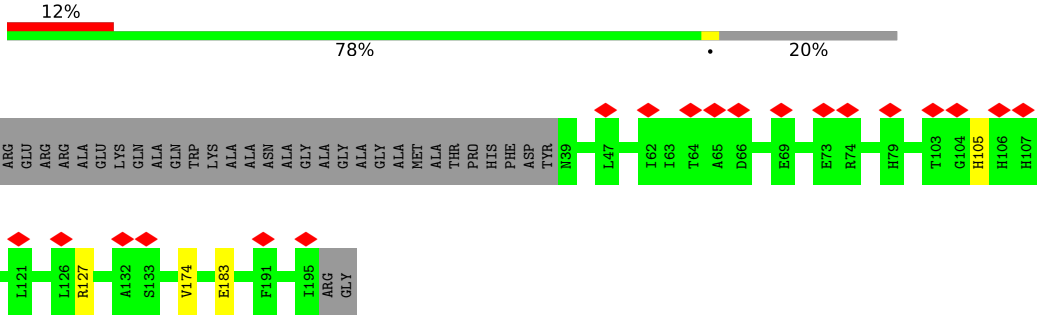
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AD:



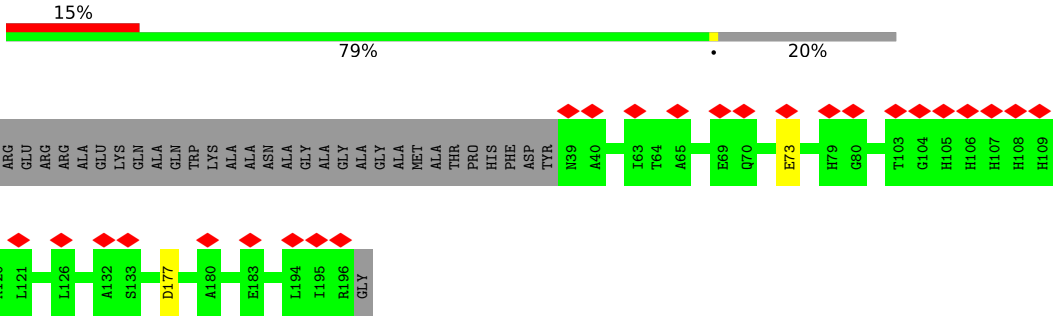
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BA:



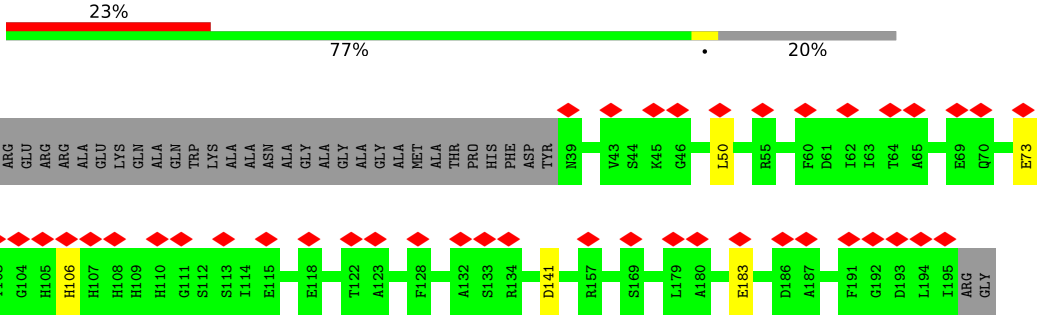
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BB:



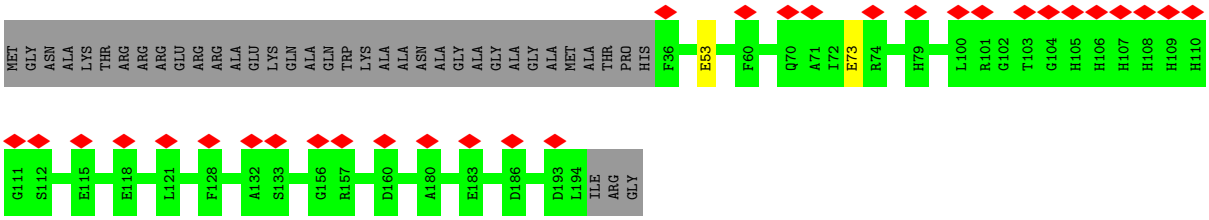
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BC:



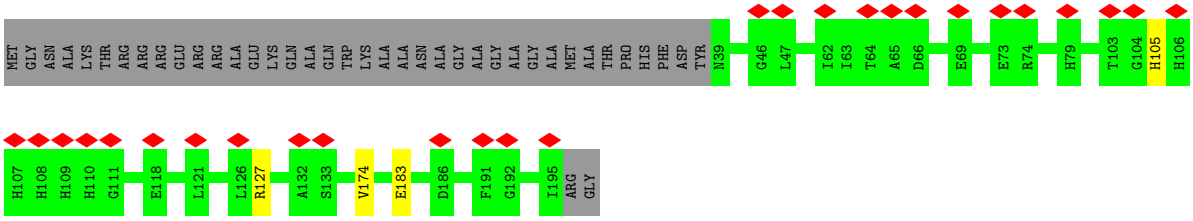
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BD:



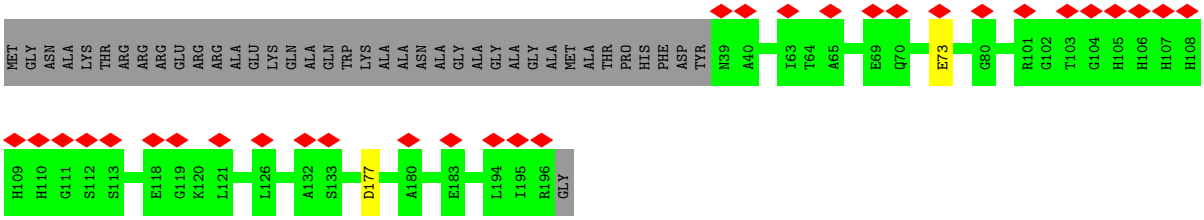
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CA:



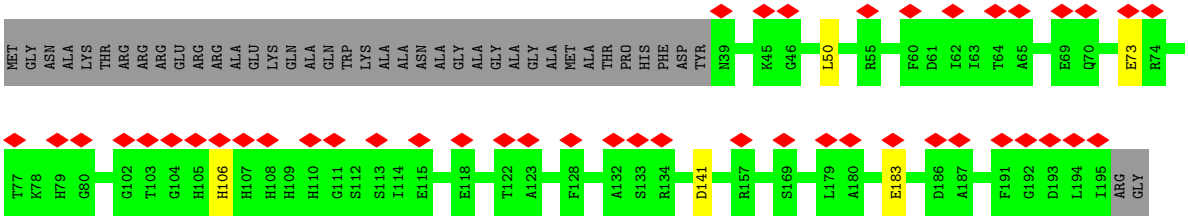
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CB:



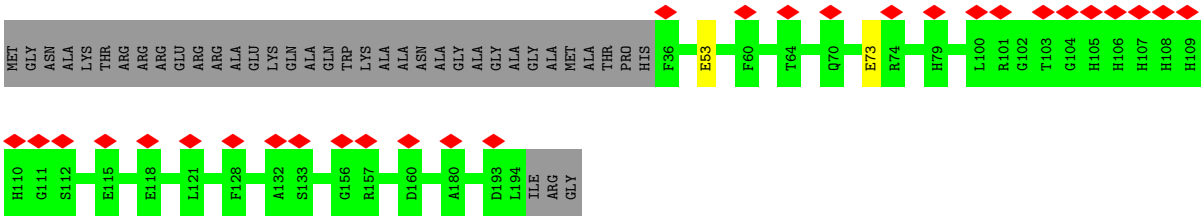
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CC:



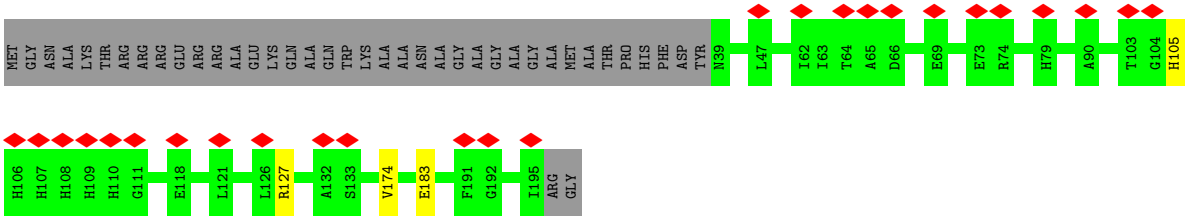
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CD:



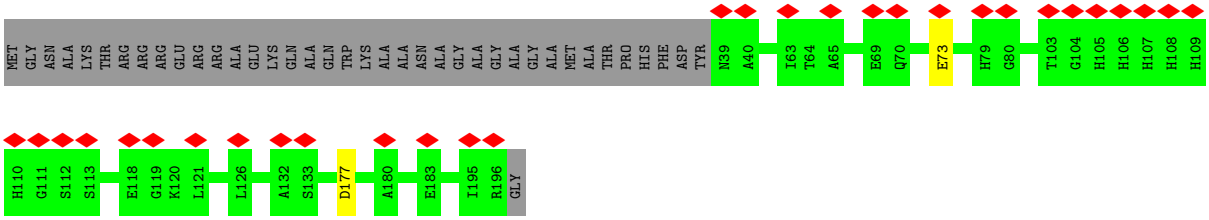
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DA:



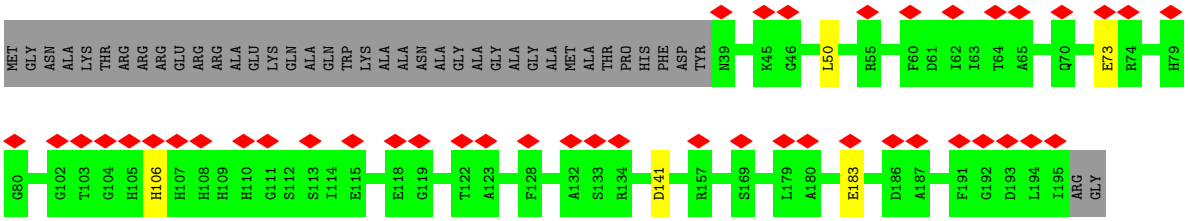
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DB:



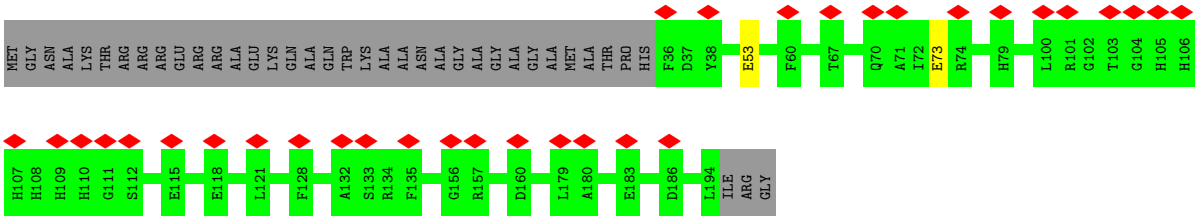
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DC:



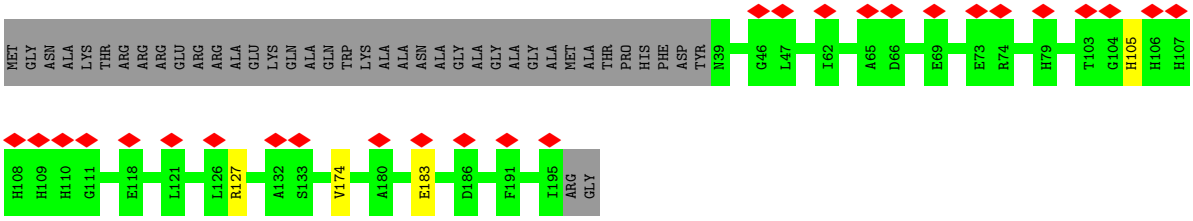
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DD:



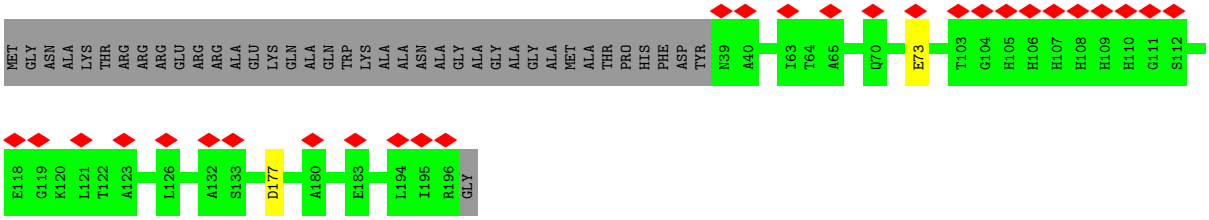
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EA:



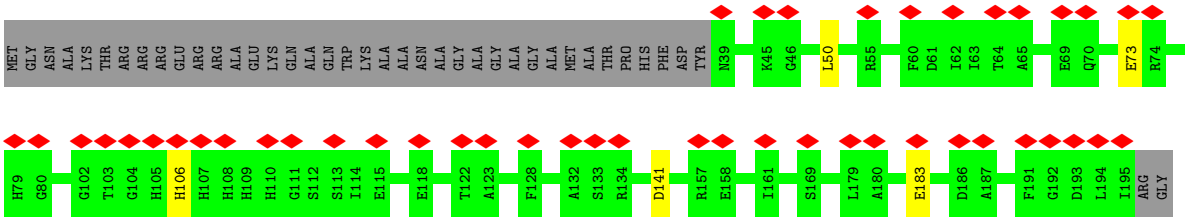
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EB:



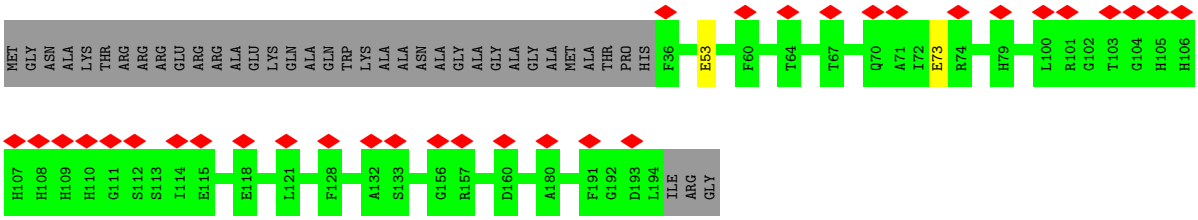
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EC:



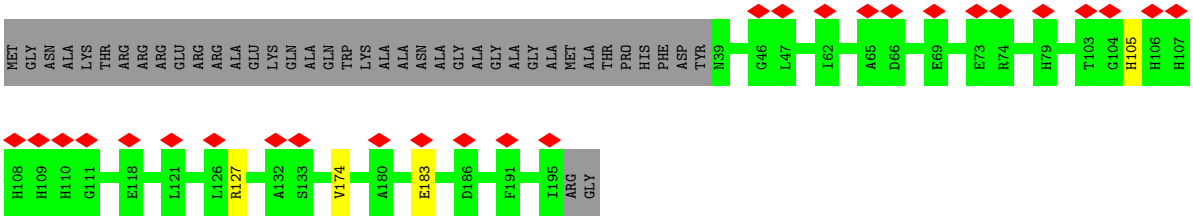
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain ED:



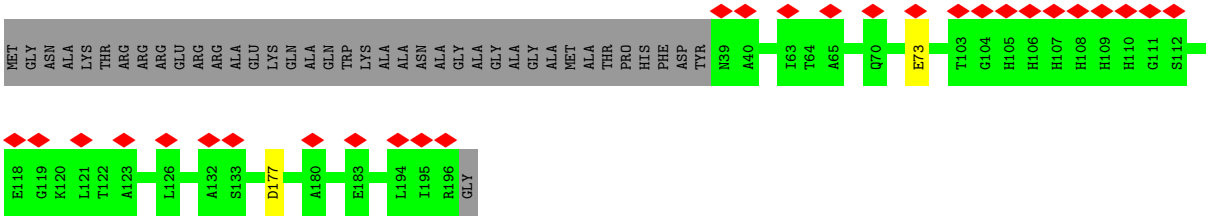
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FA:



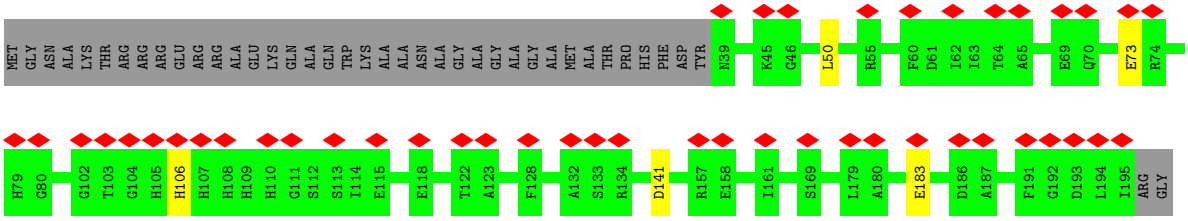
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FB:



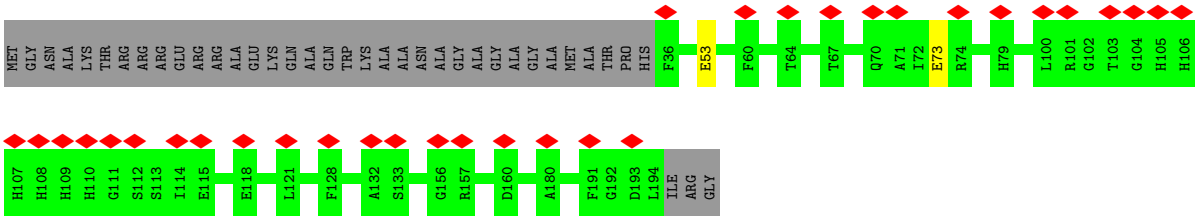
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FC:



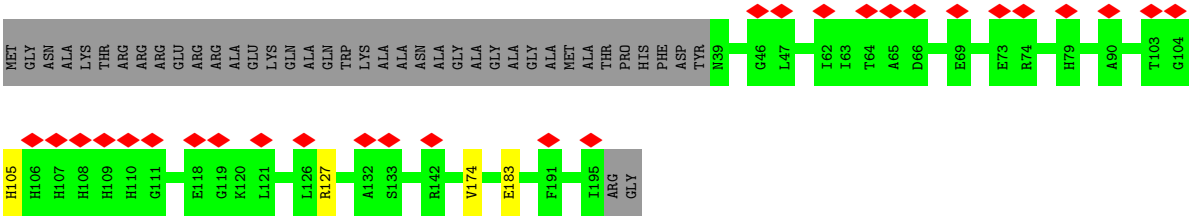
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FD:



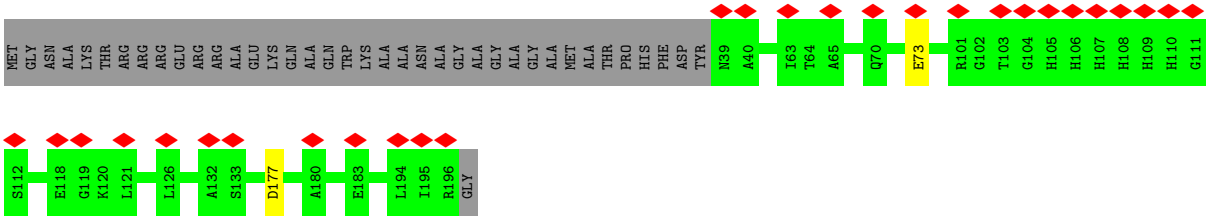
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain GA:



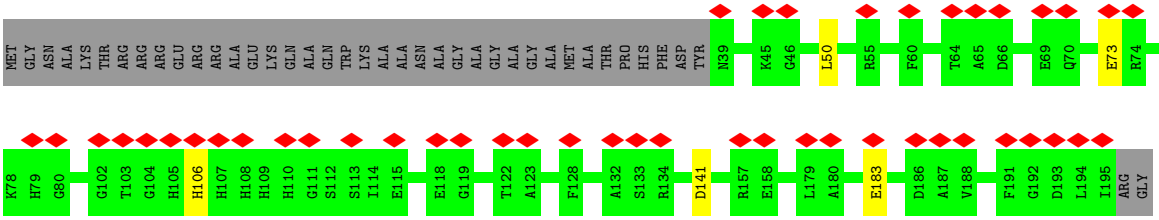
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain GB:



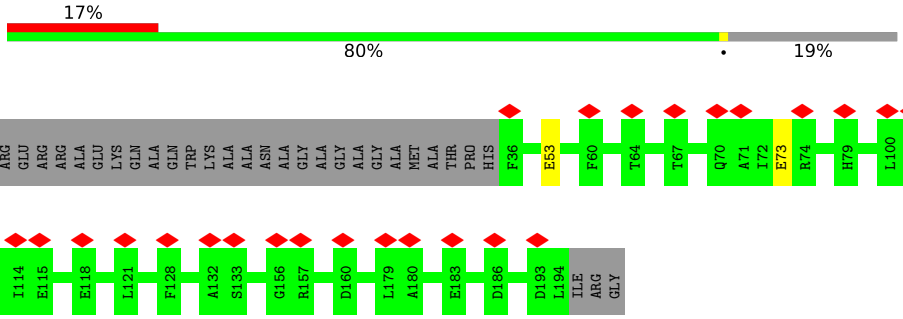
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain GC:



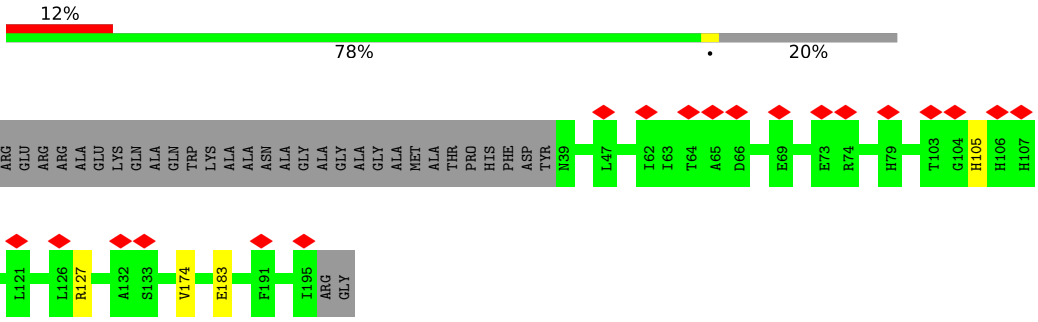
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain GD:



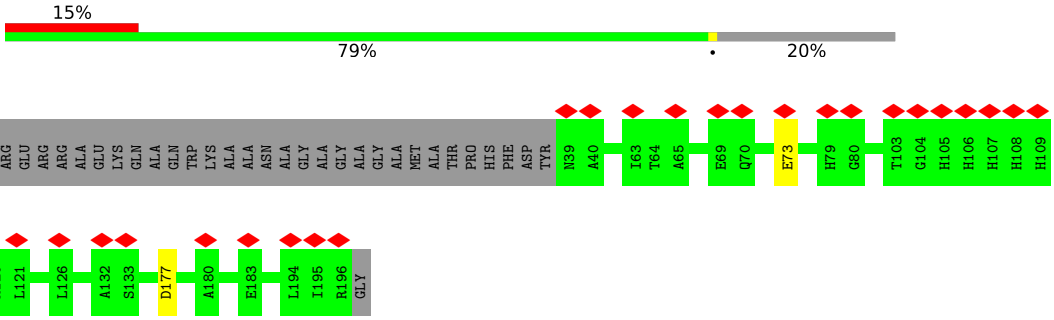
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HA:



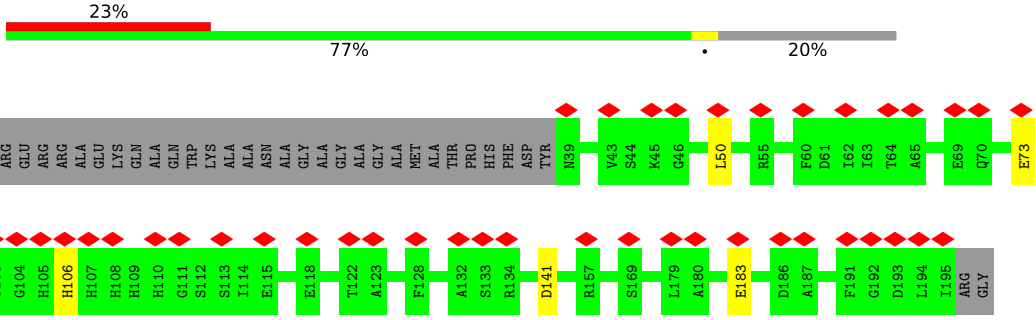
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HB:



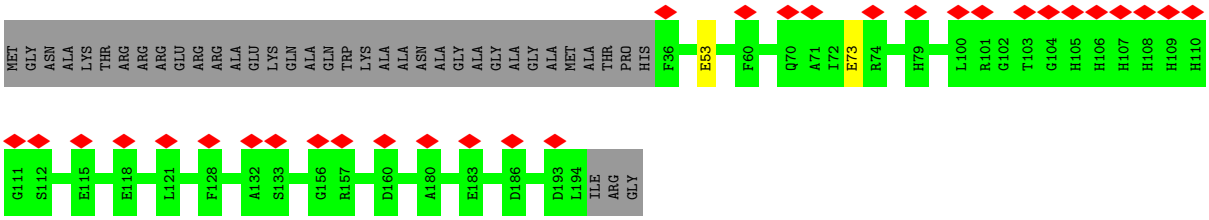
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HC:



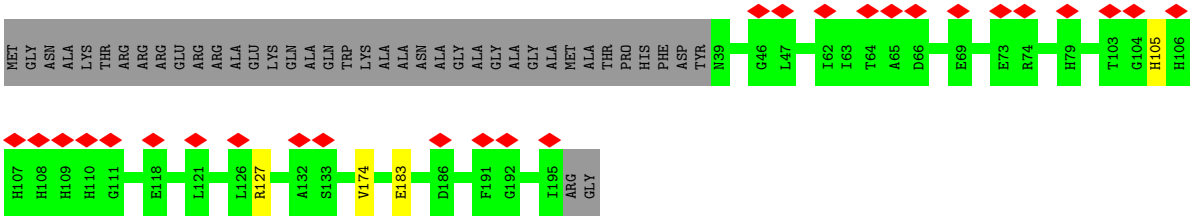
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HD:



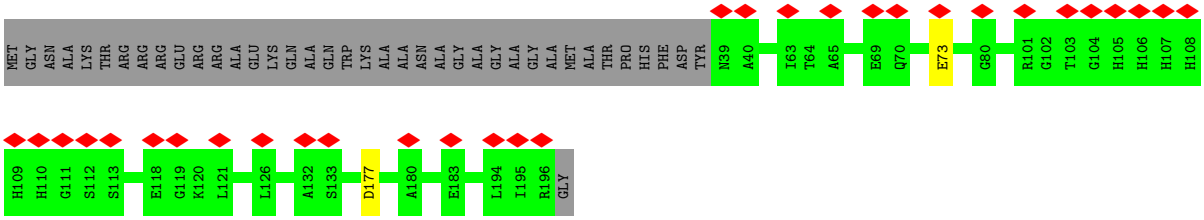
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IA:



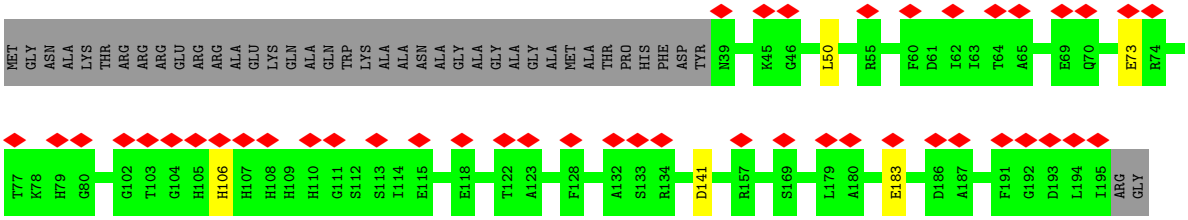
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IB:



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

Chain IC:



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

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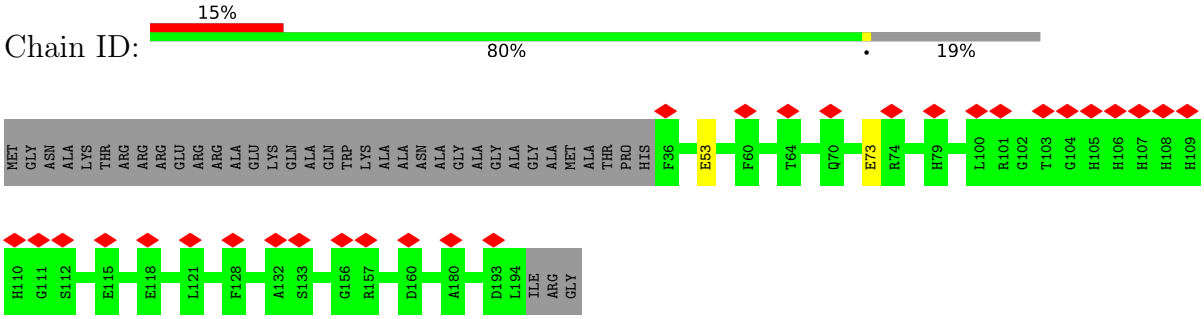
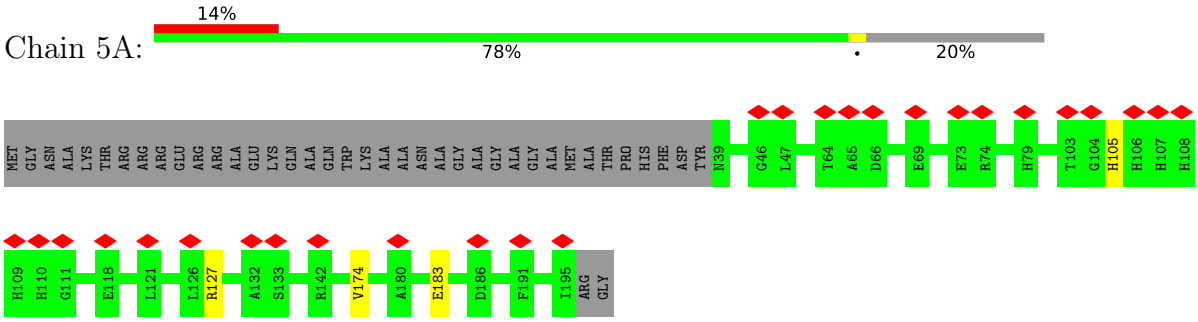


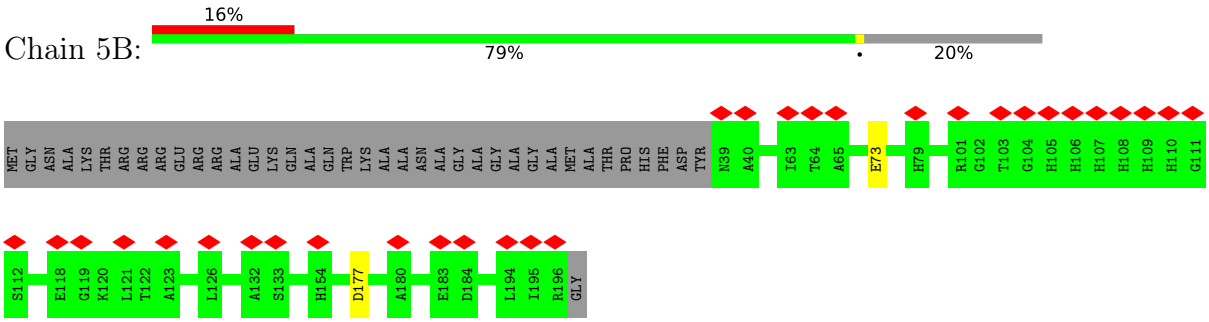
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 5A:



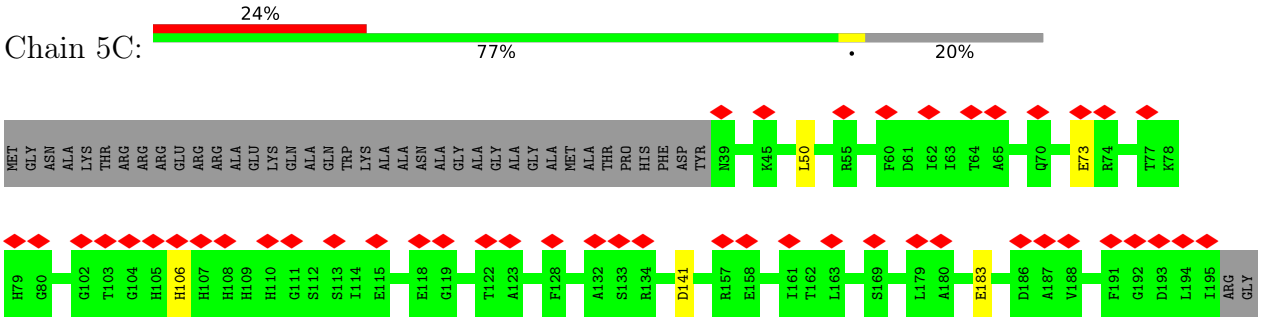
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 5B:



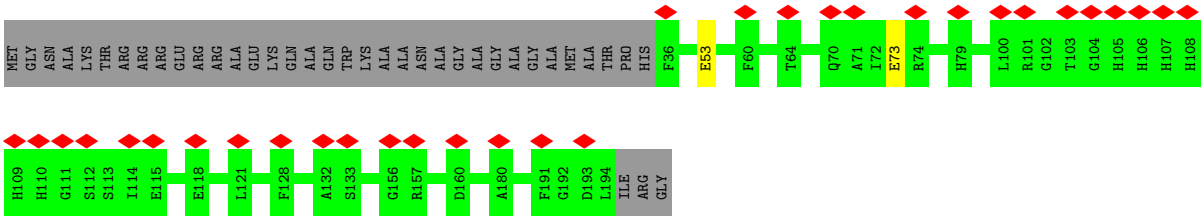
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 5C:



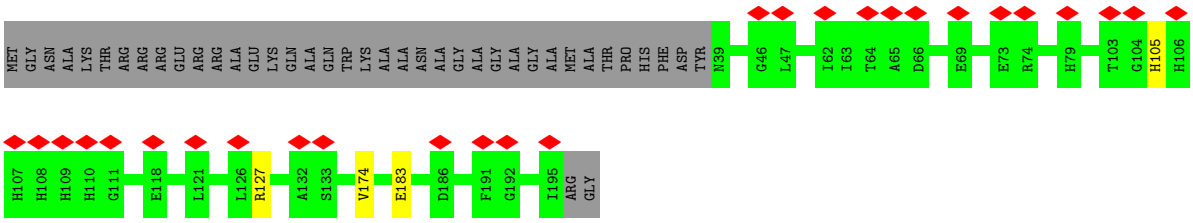
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 5D:



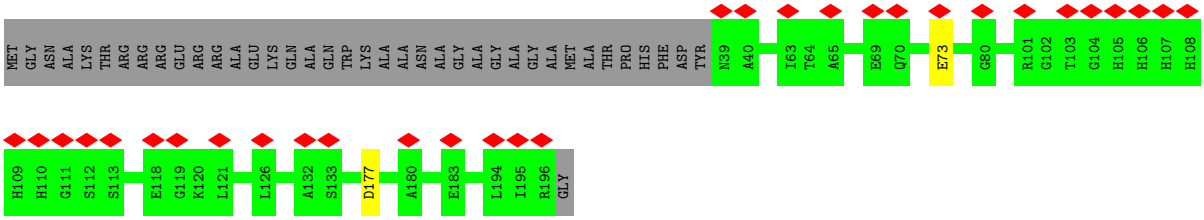
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JA:



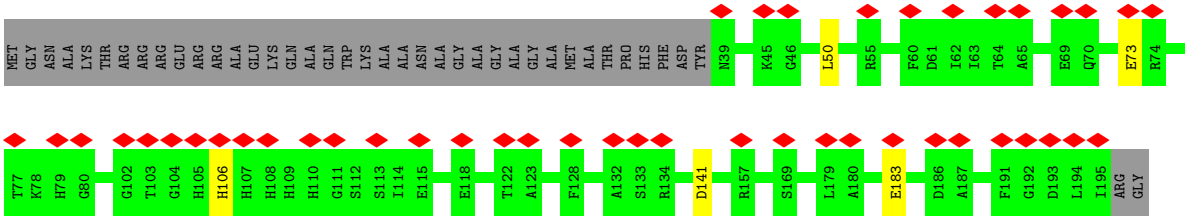
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JB:



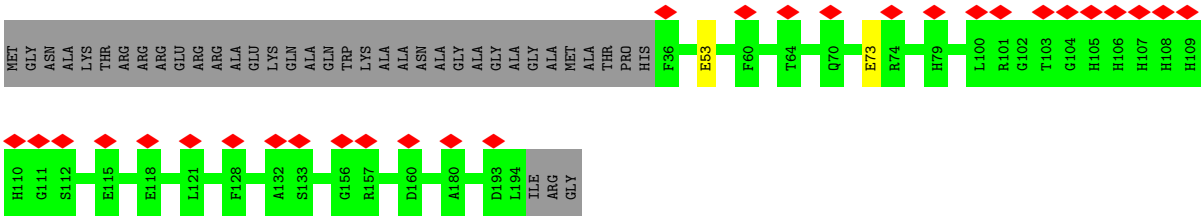
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JC:



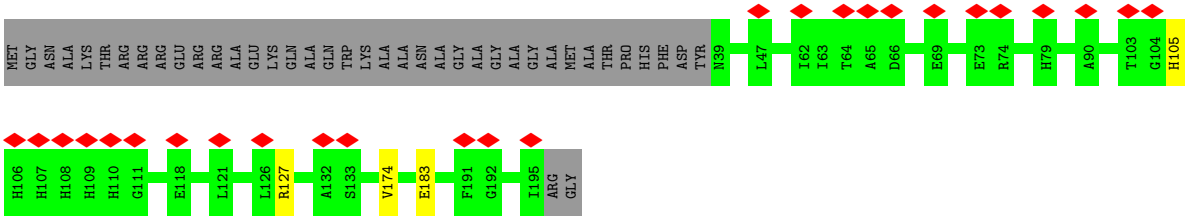
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JD:



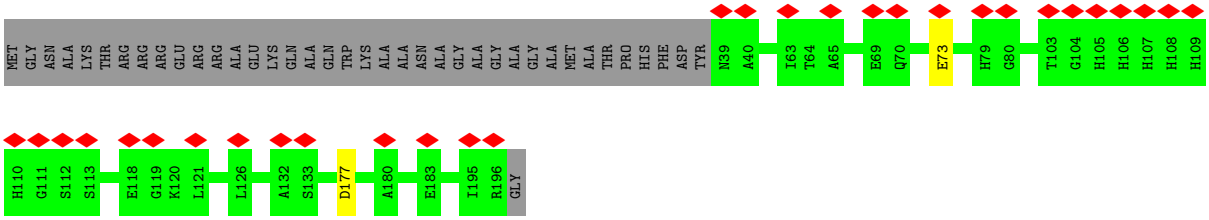
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KA:



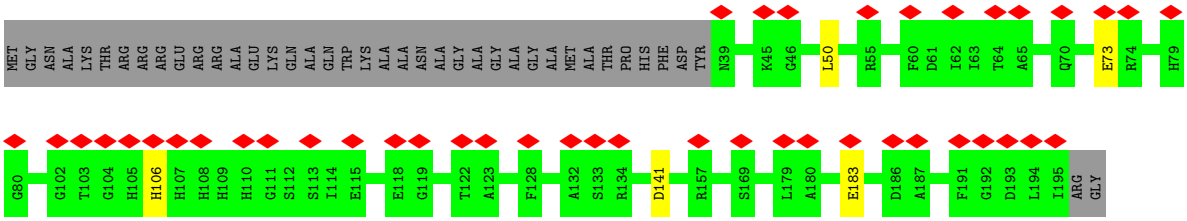
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KB:



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

Chain KC:



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

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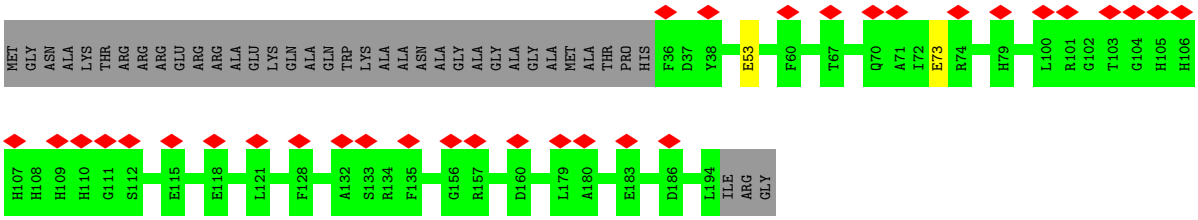
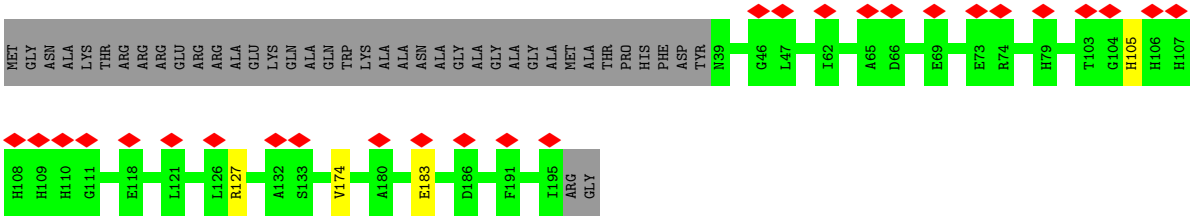


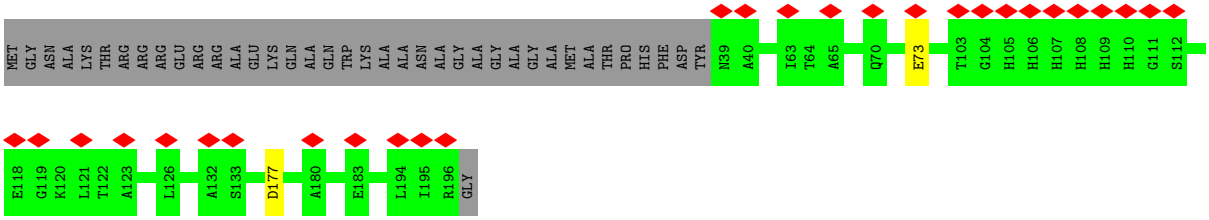
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LA:



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

Chain LB:



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

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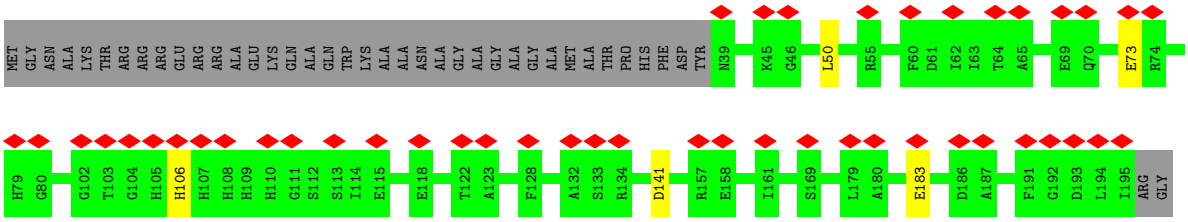
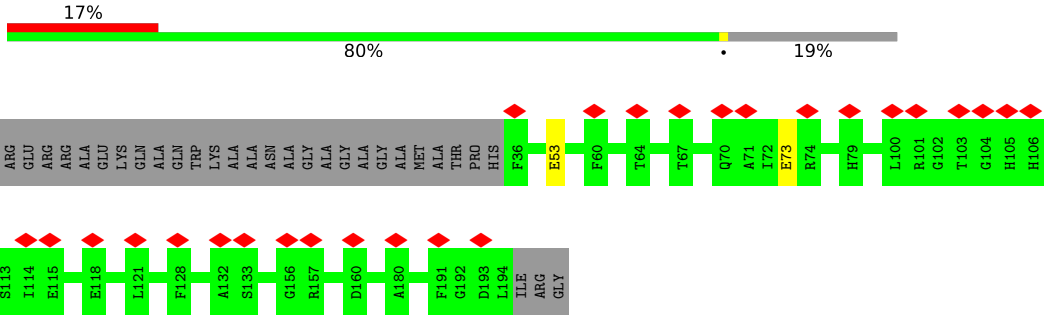


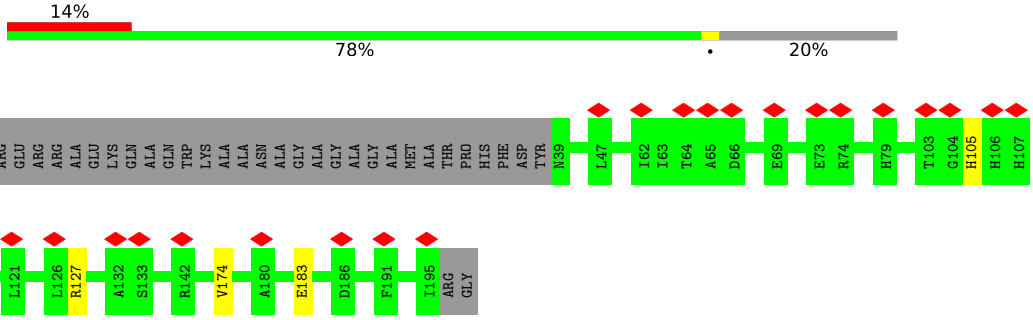
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LD:



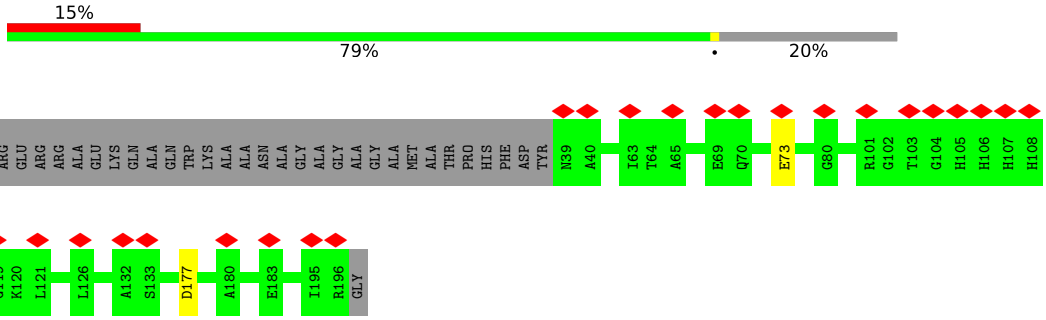
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain MA:



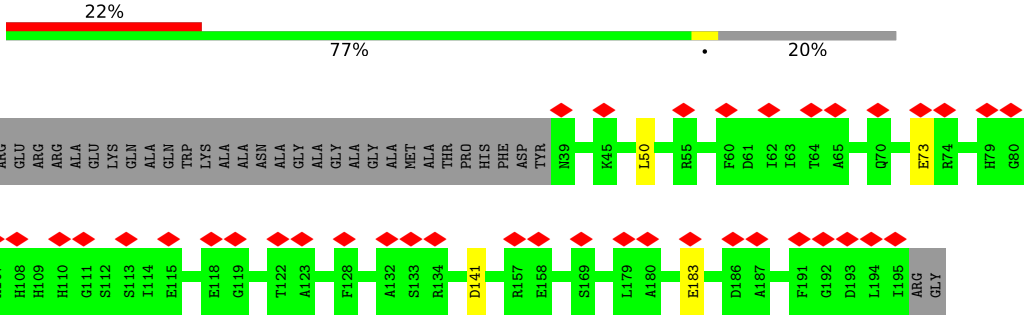
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain MB:



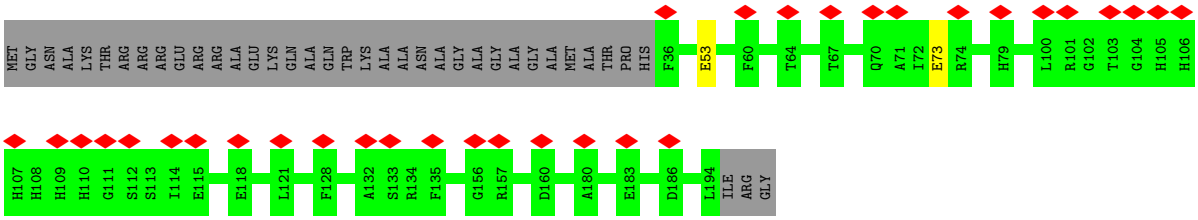
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain MC:



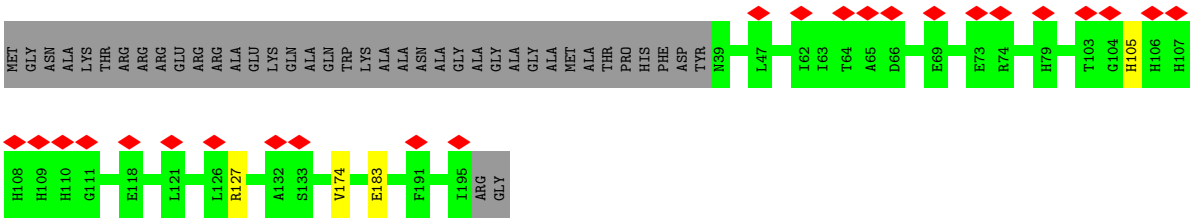
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain MD:



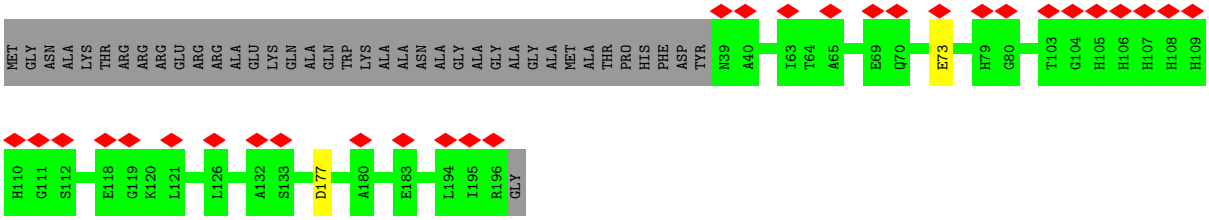
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain NA:



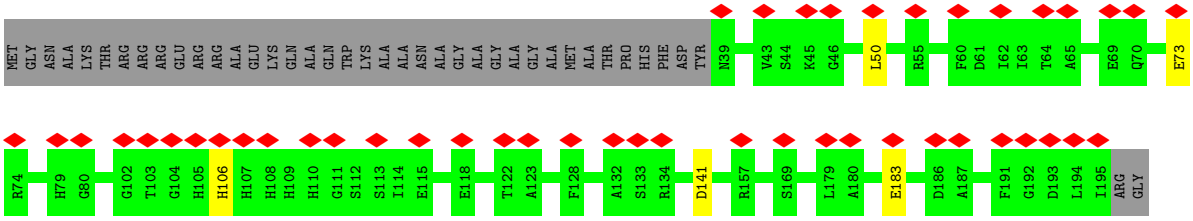
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain NB:



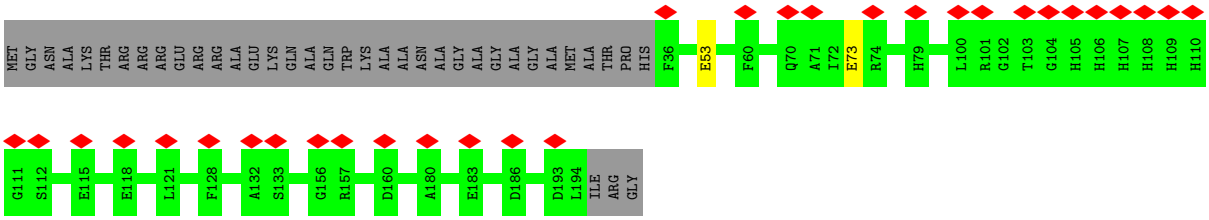
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain NC:



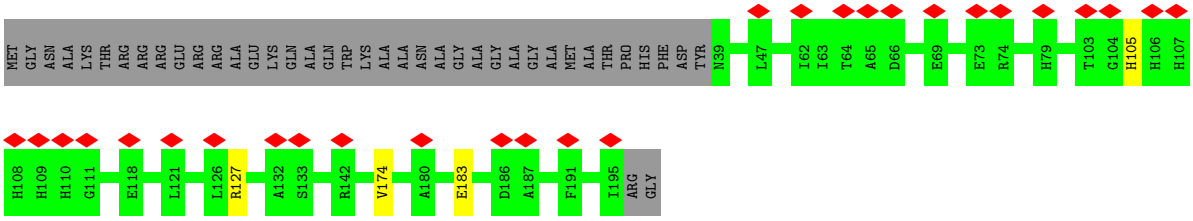
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain ND:



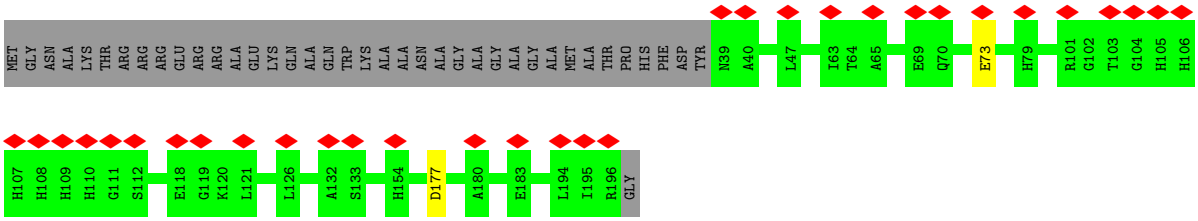
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain OA:



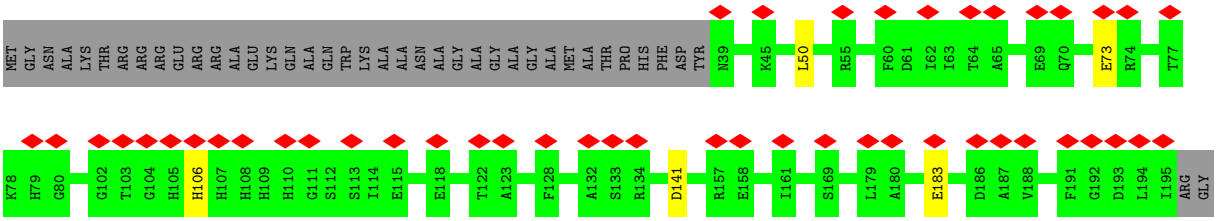
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain OB:



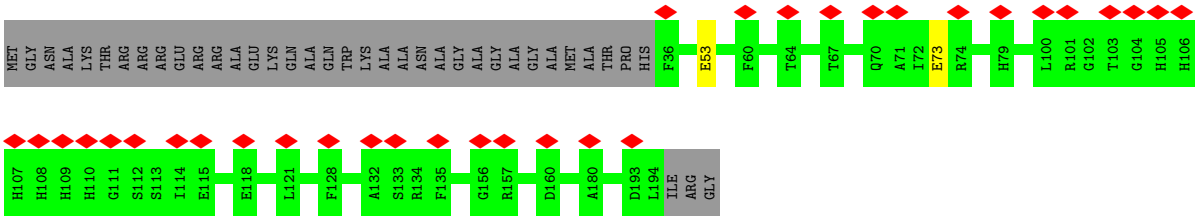
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain OC:



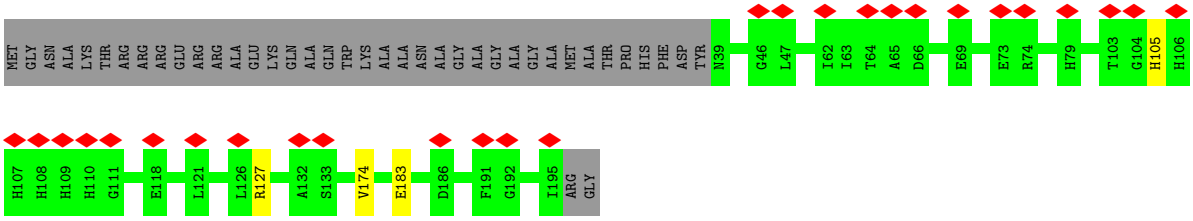
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain OD:



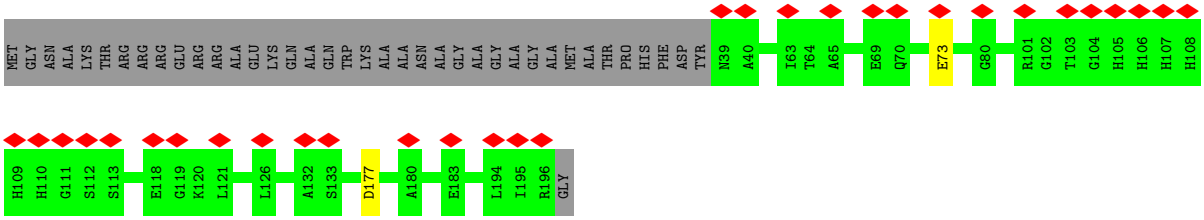
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain PA:



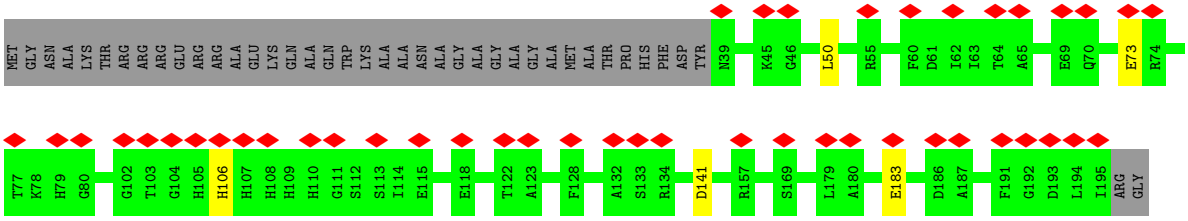
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain PB:



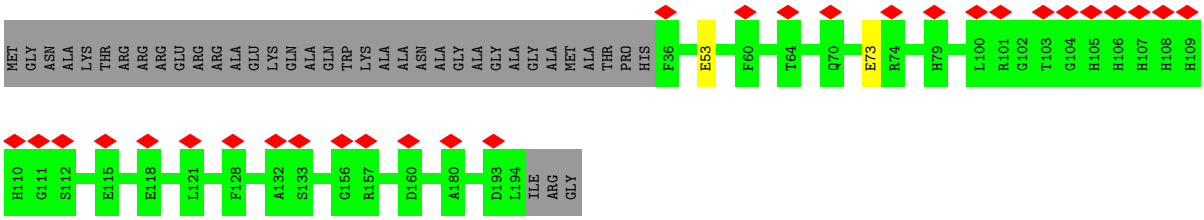
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain PC:



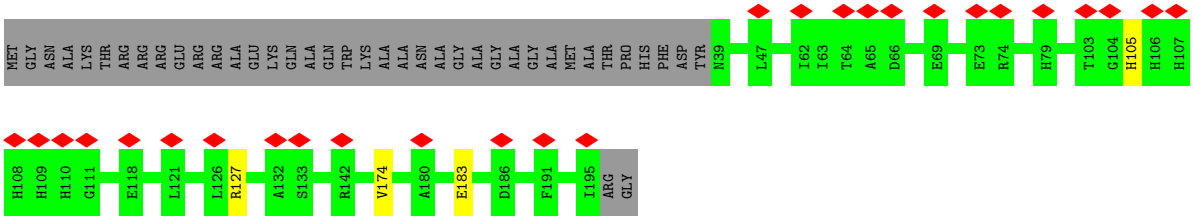
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain PD:



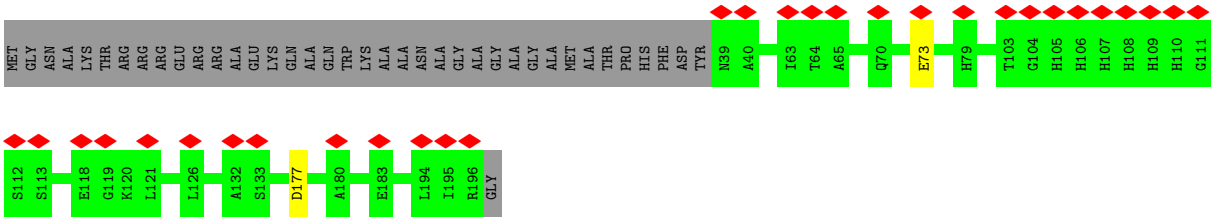
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 6A:



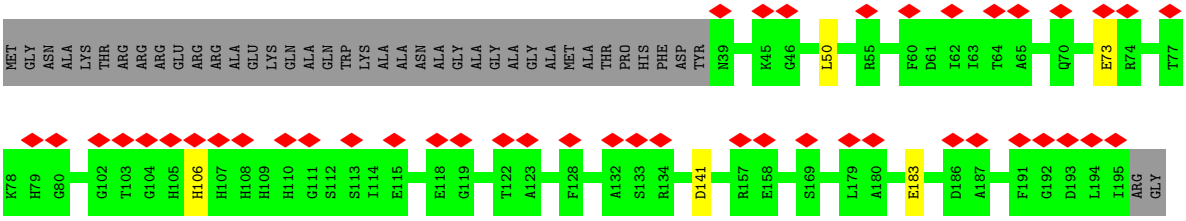
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 6B:



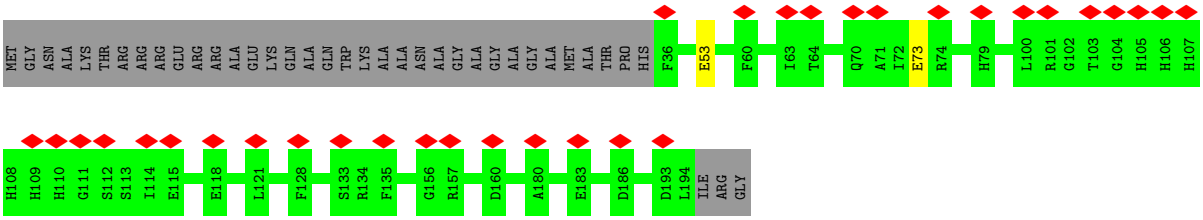
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 6C:



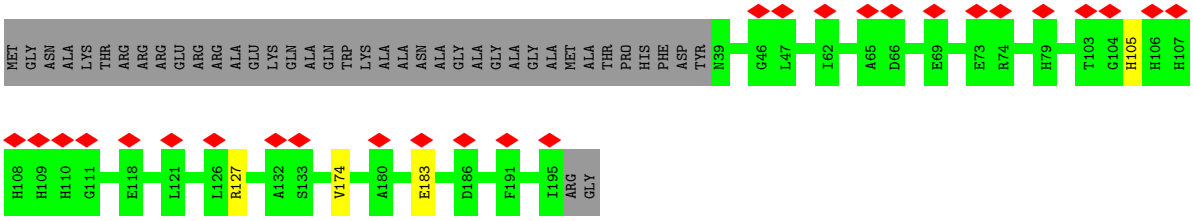
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 6D:



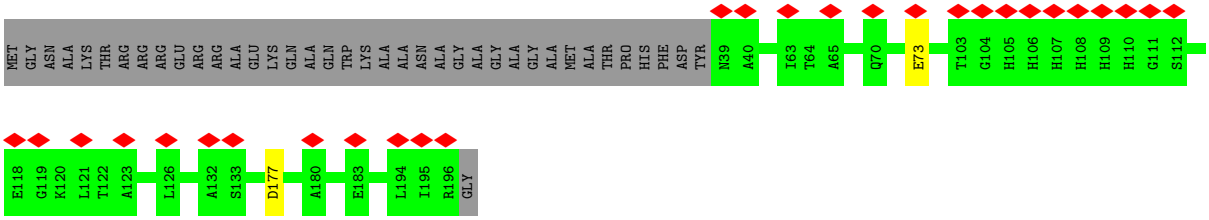
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 7A:



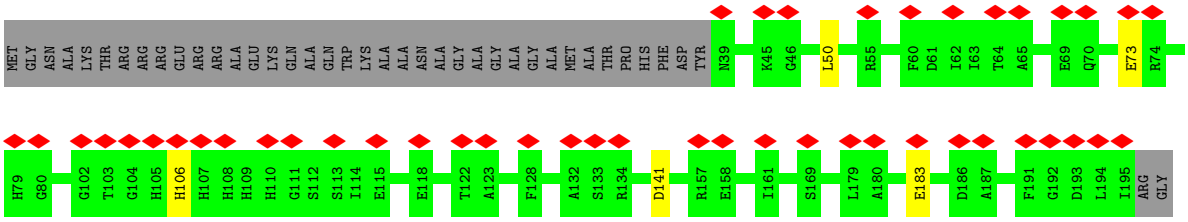
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 7B:



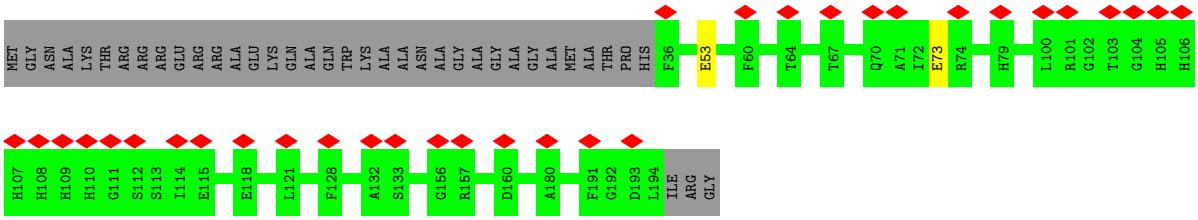
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 7C:



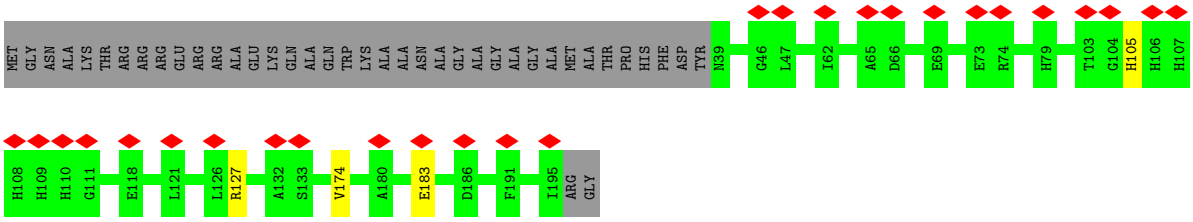
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 7D:



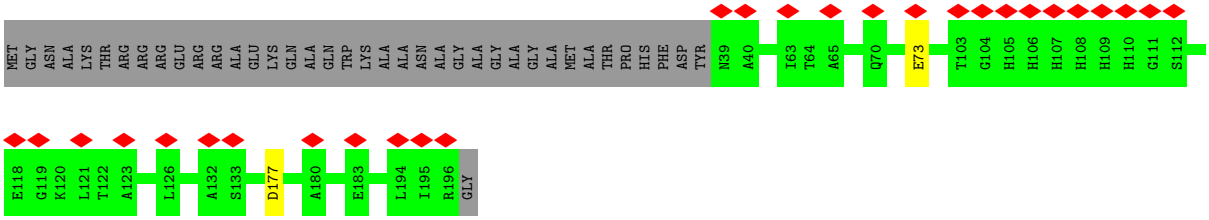
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain QA:



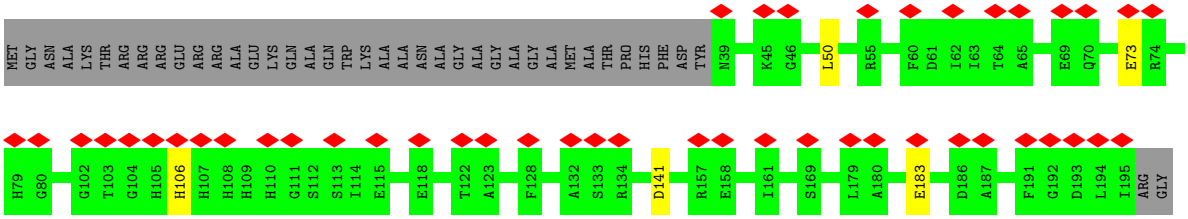
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain QB:



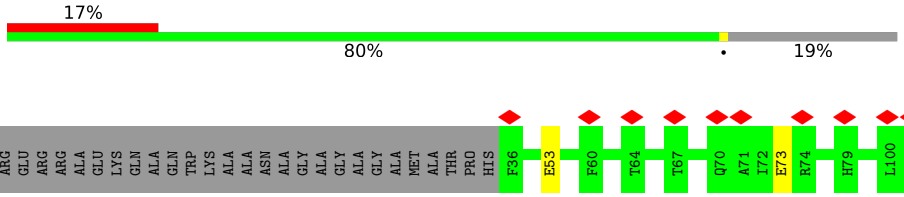
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

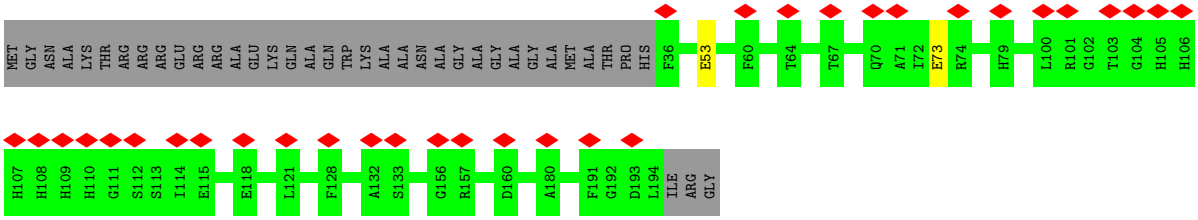
Chain QC:



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

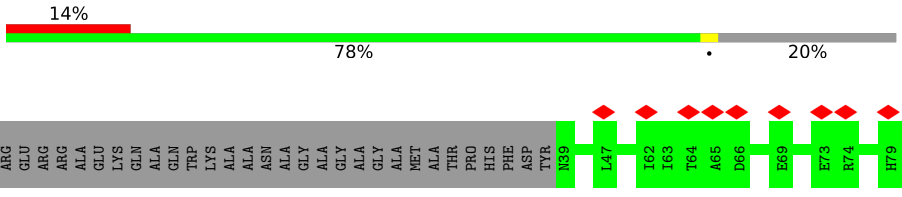
Chain QD:

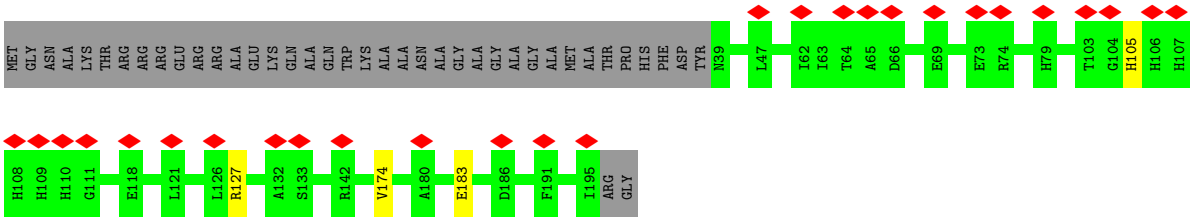




• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

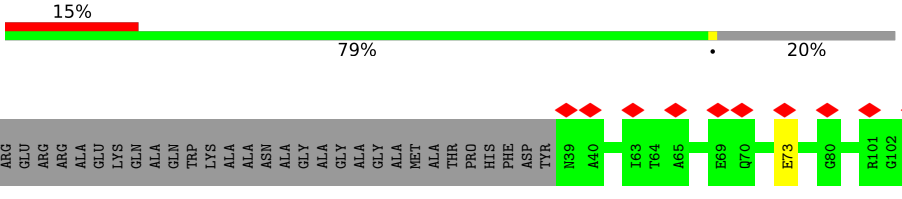
Chain RA:

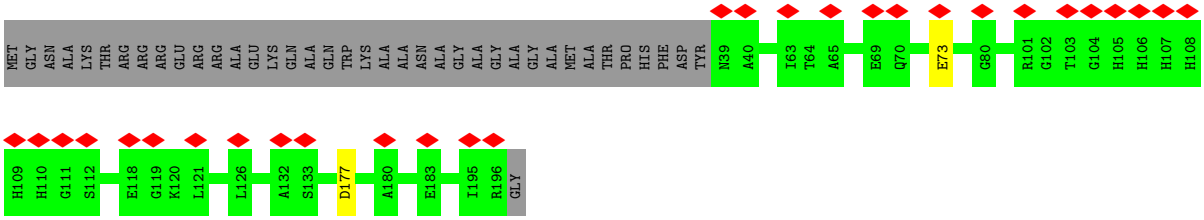




• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain RB:





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

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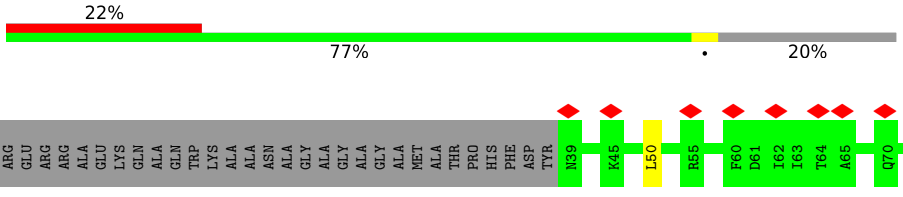
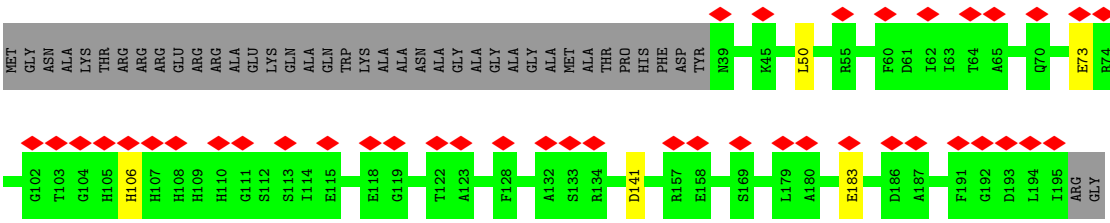
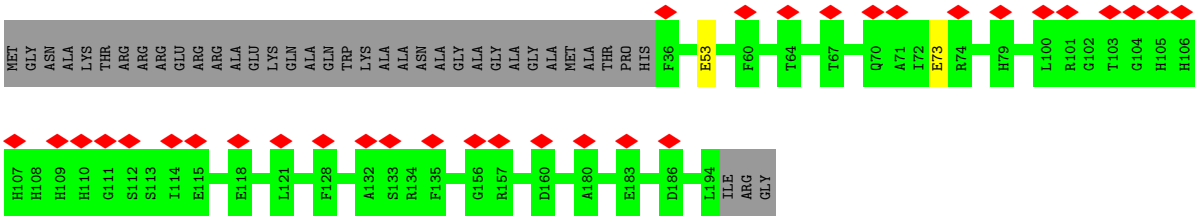




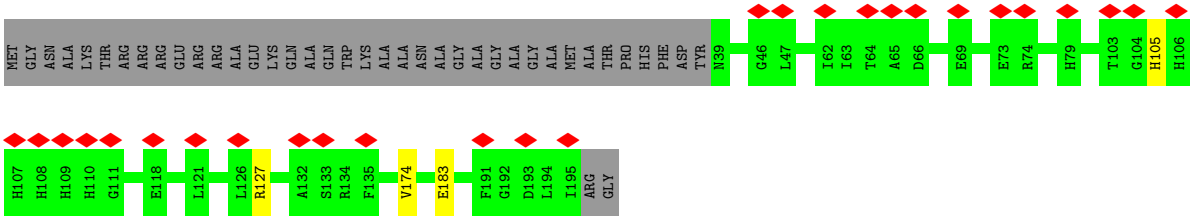
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain RD:



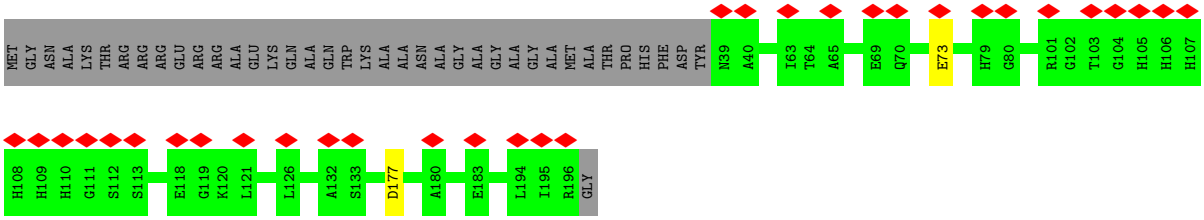
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain SA:



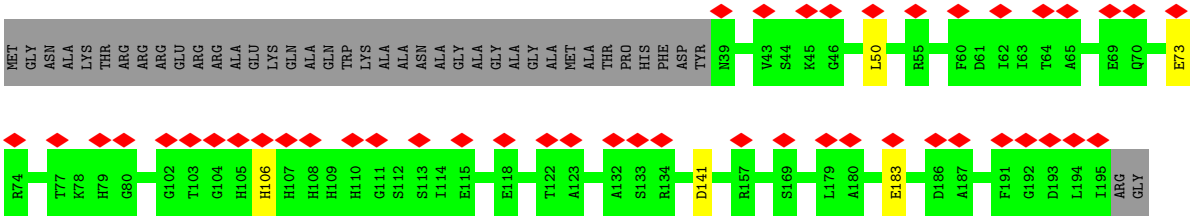
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain SB:



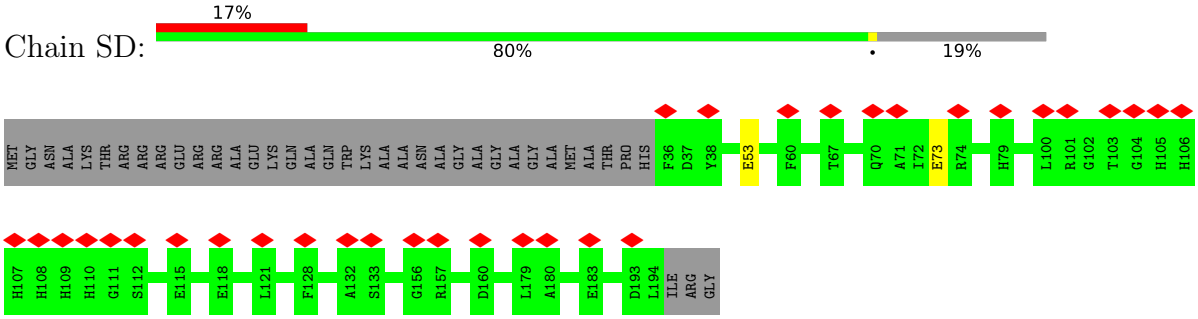
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain SC:



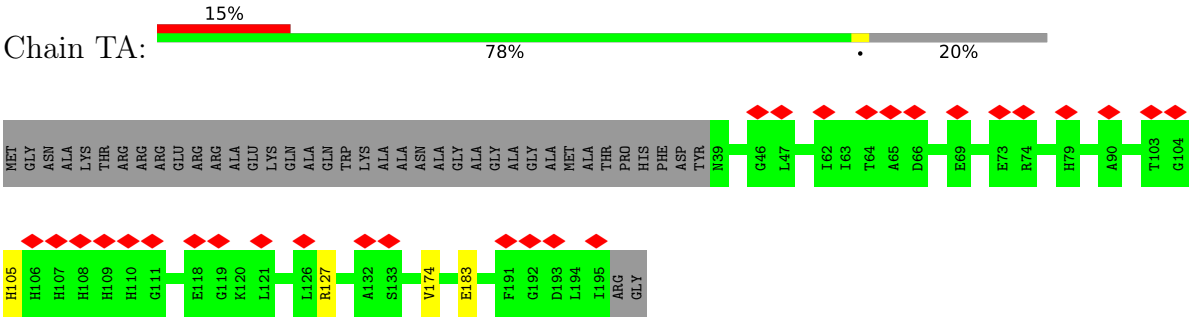
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain SD:



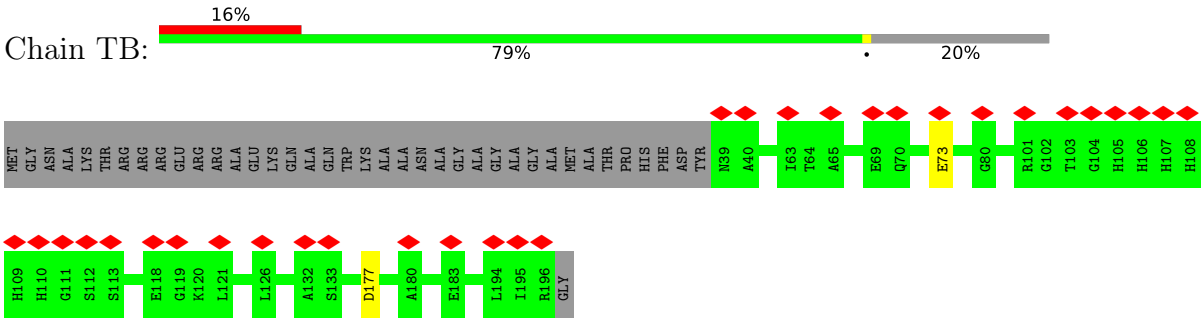
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain TA:



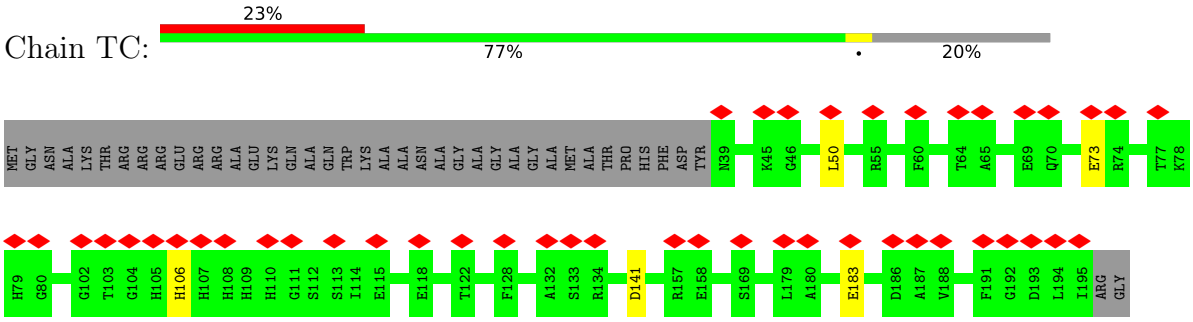
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain TB:



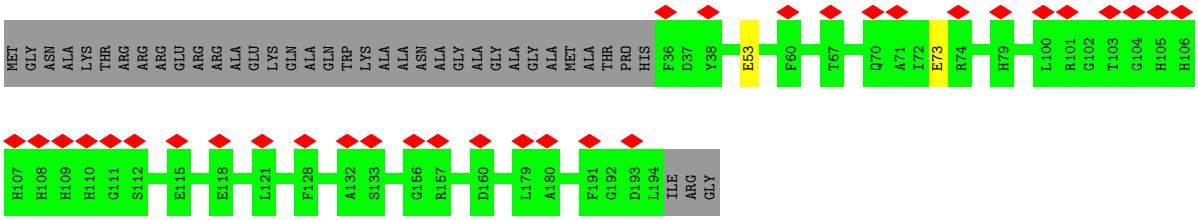
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain TC:



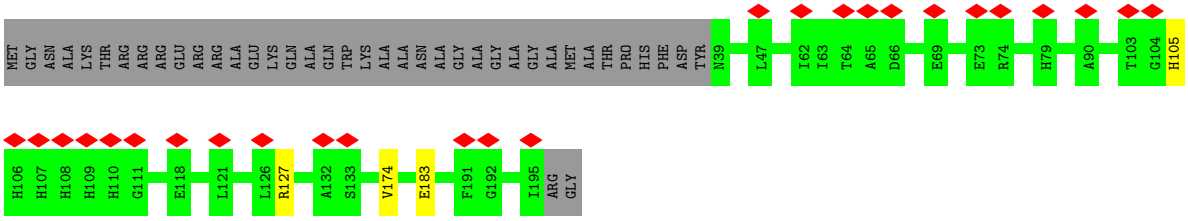
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain TD:



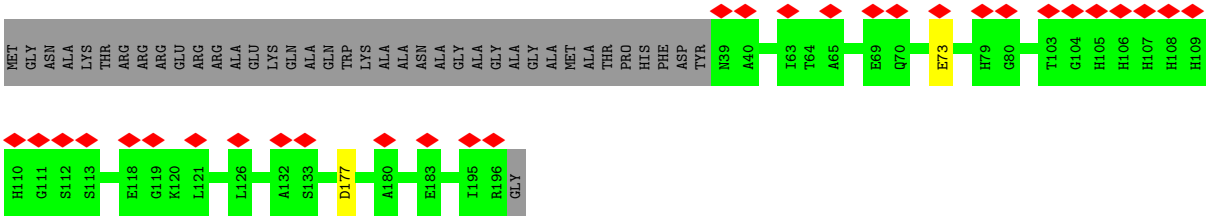
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain UA:



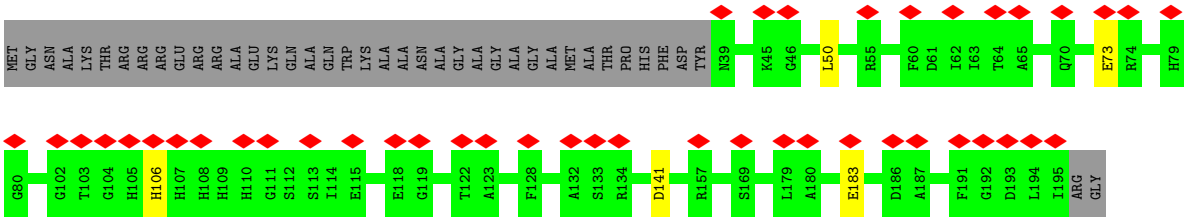
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain UB:



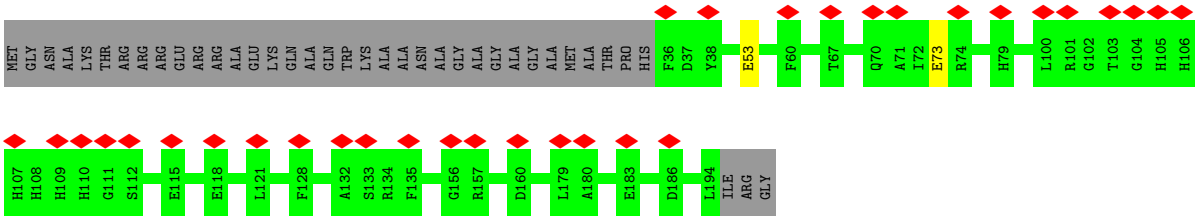
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain UC:



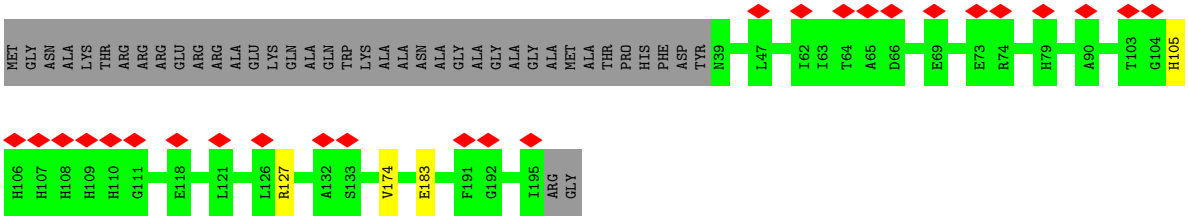
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain UD:



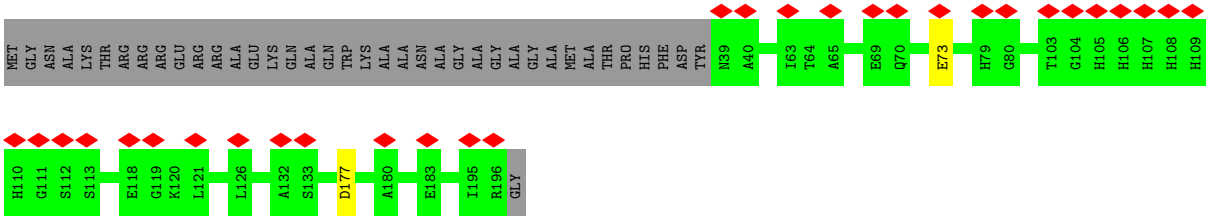
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain VA:



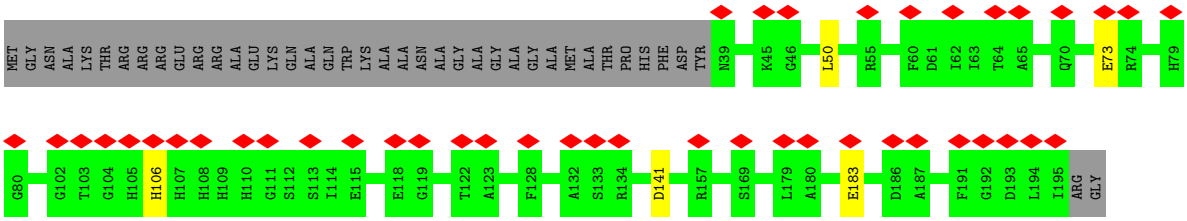
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain VB:



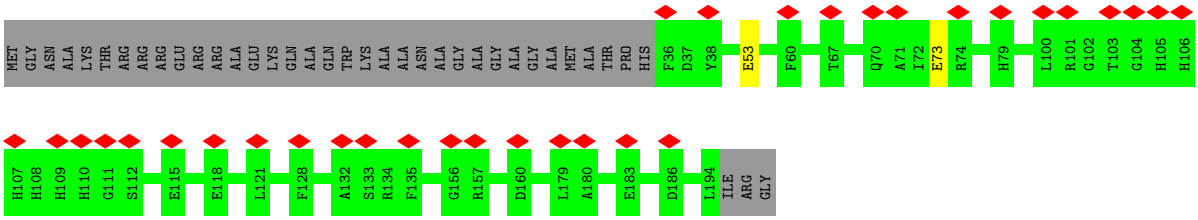
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain VC:



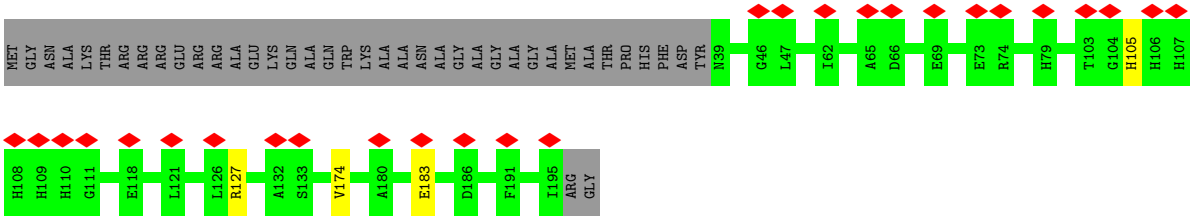
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain VD:



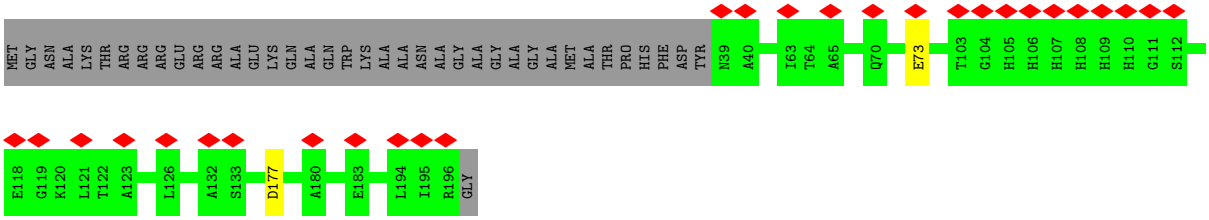
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain WA:



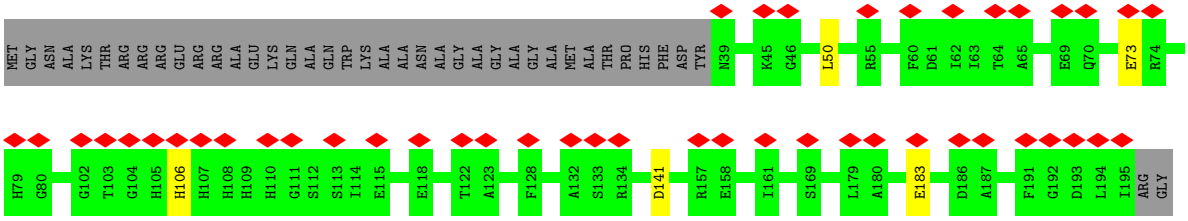
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain WB:



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

Chain WC:



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

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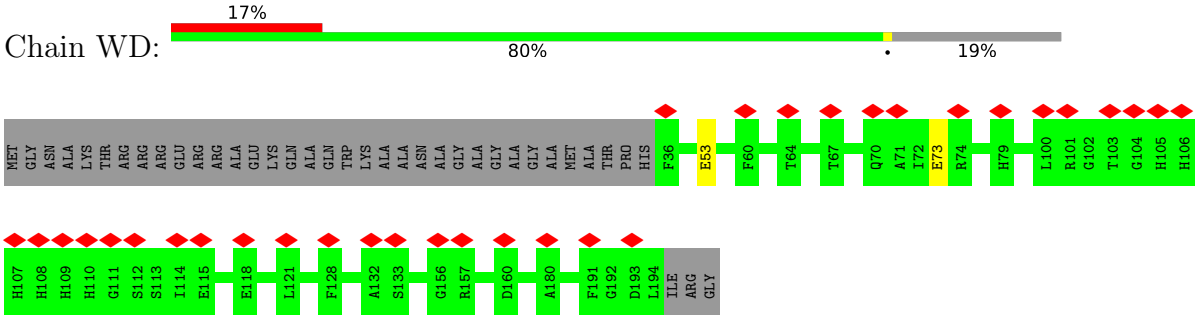
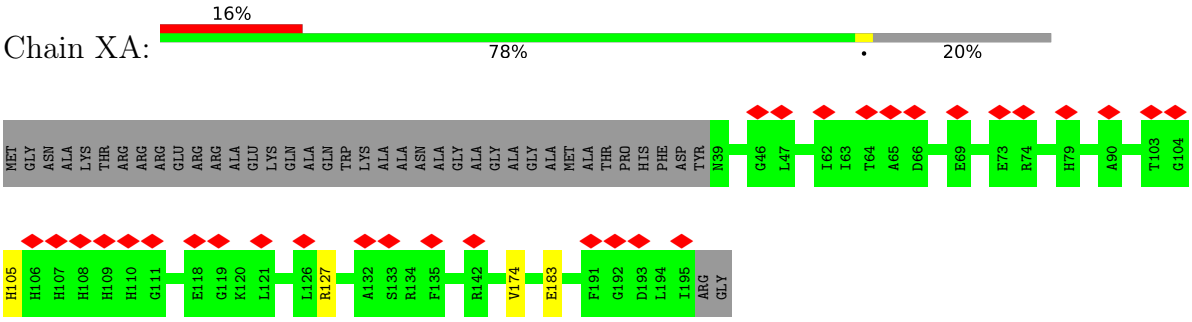


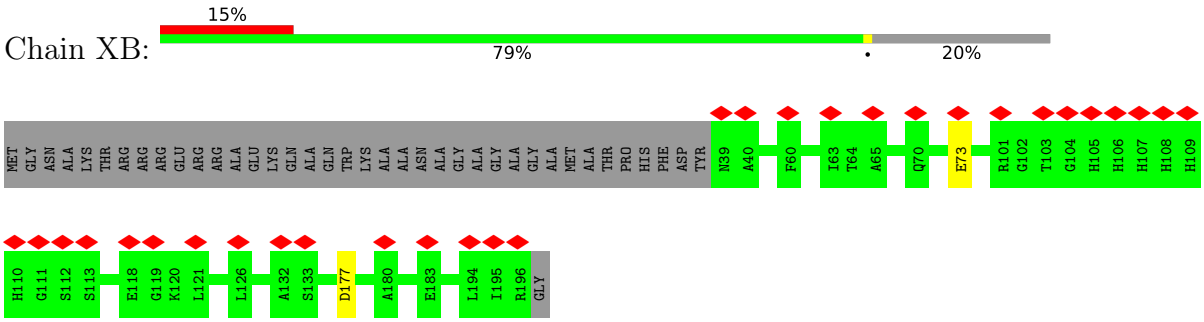
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain XA:



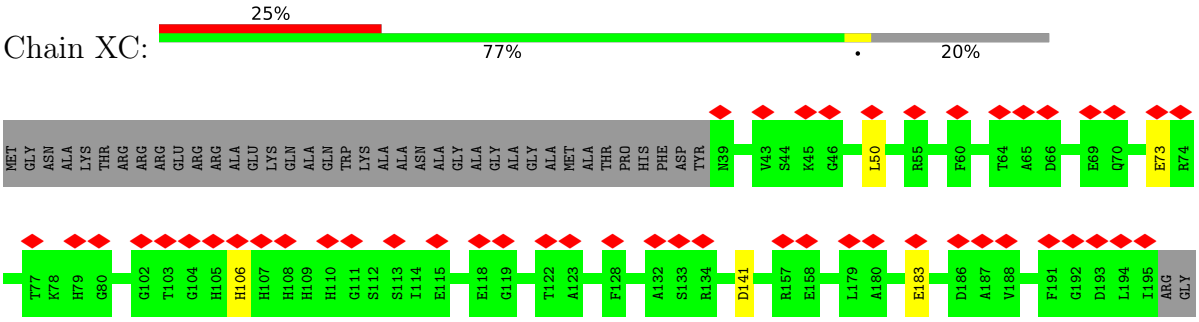
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain XB:



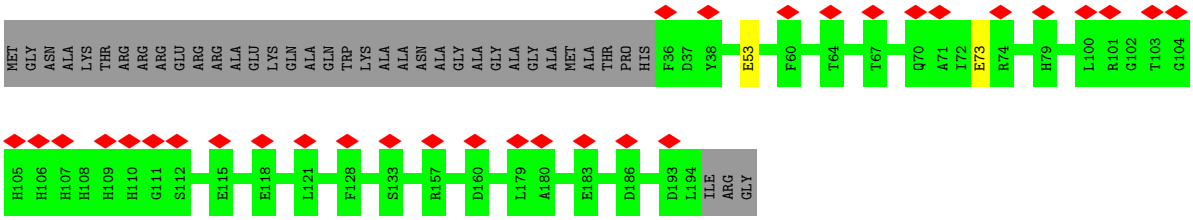
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain XC:



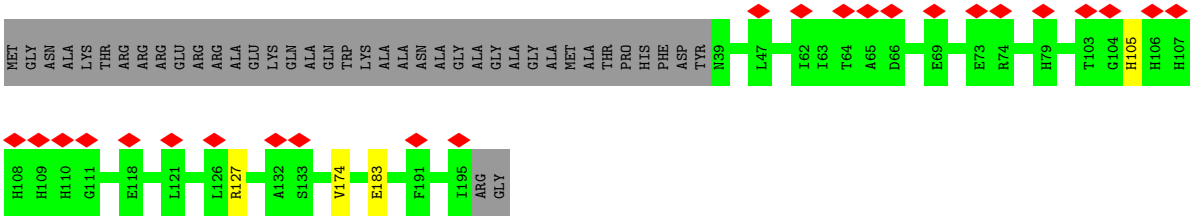
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain XD:



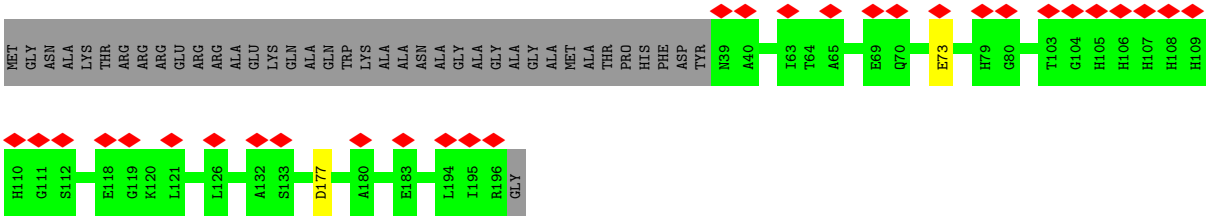
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain YA:



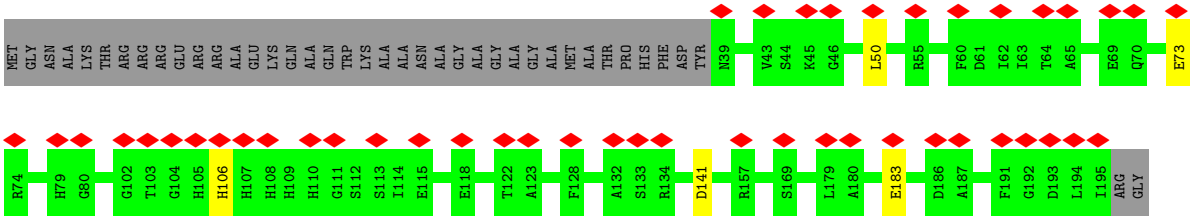
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain YB:



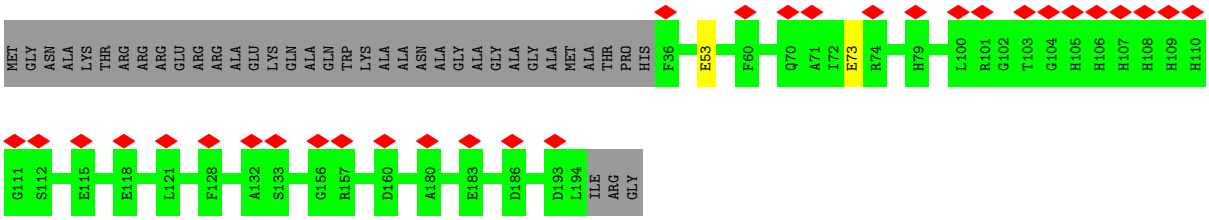
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain YC:



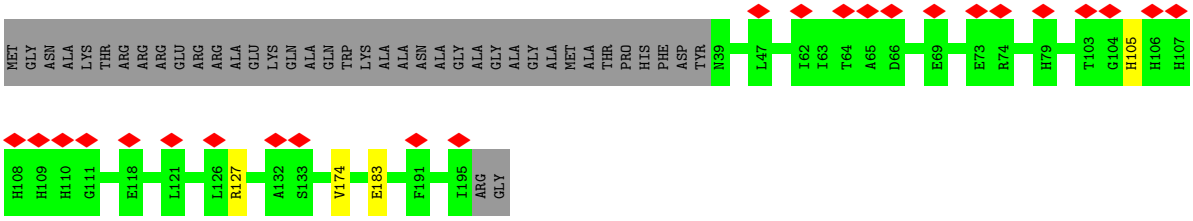
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain YD:



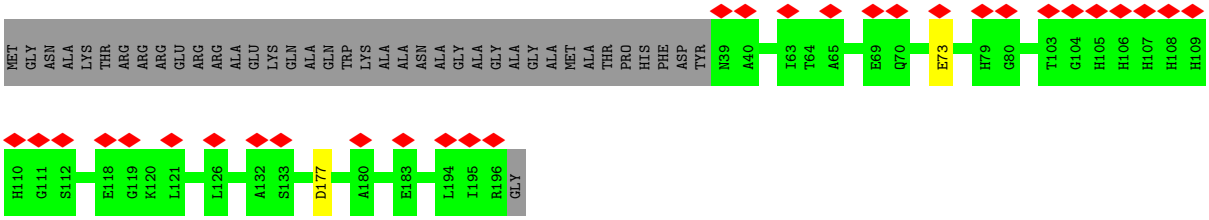
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain ZA:



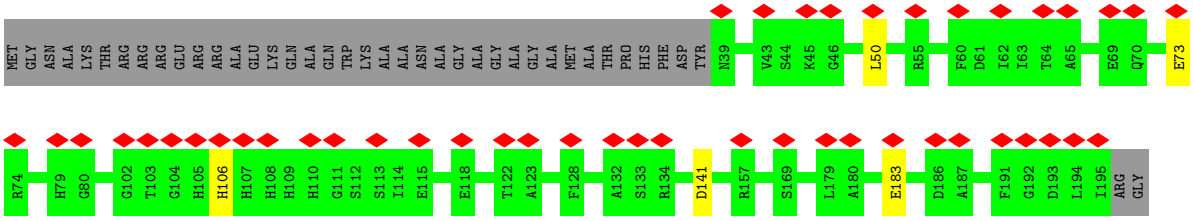
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain ZB:



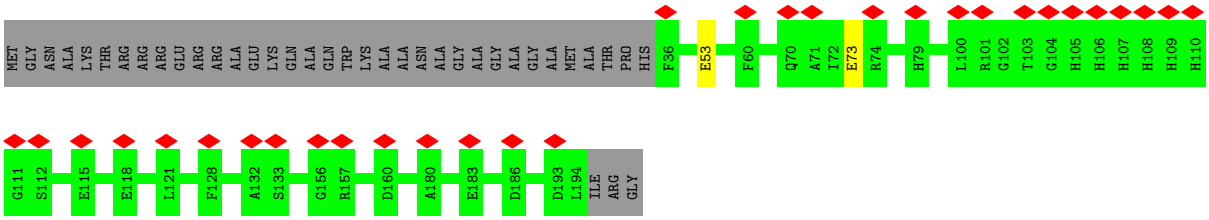
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain ZC:



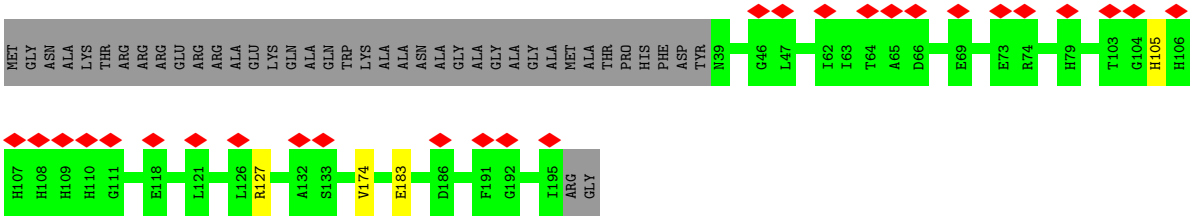
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain ZD:



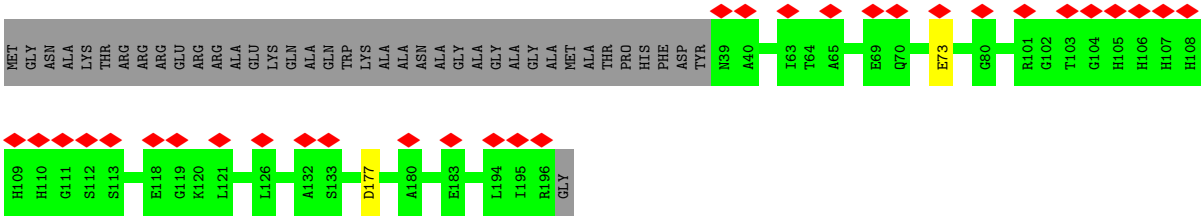
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain aA:



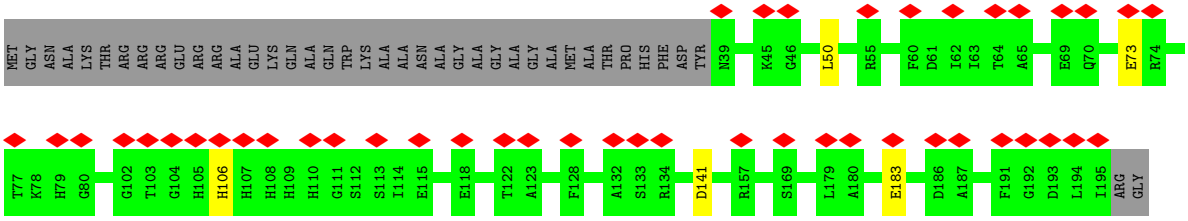
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain aB:



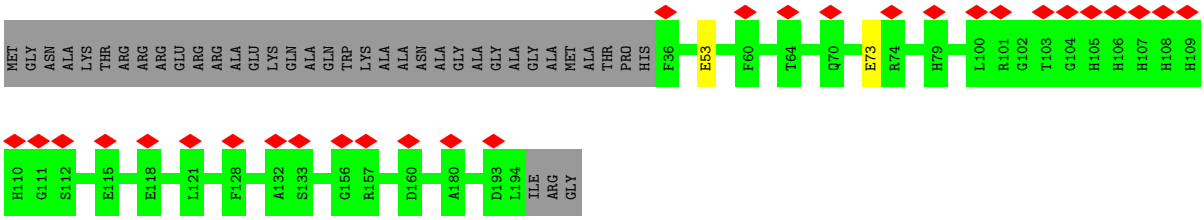
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain aC:



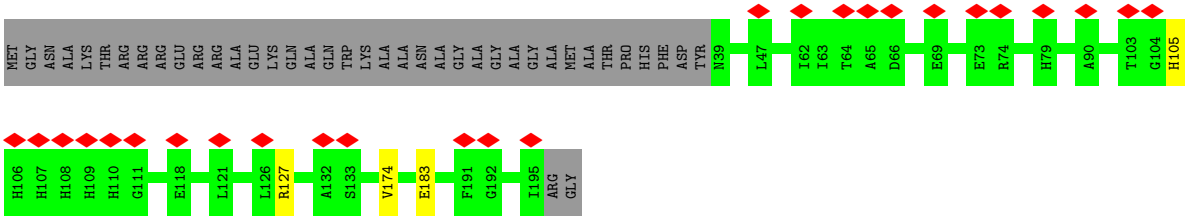
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain aD:



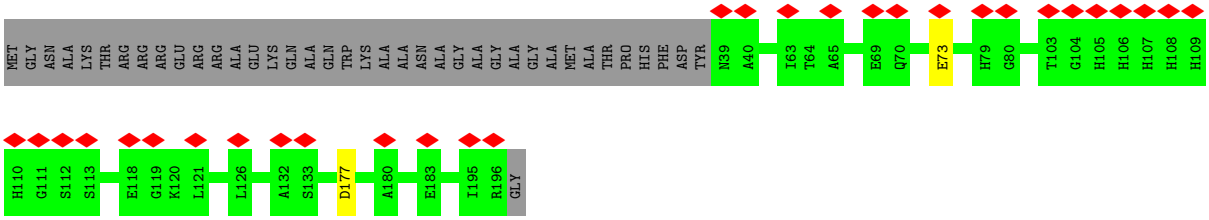
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain bA:



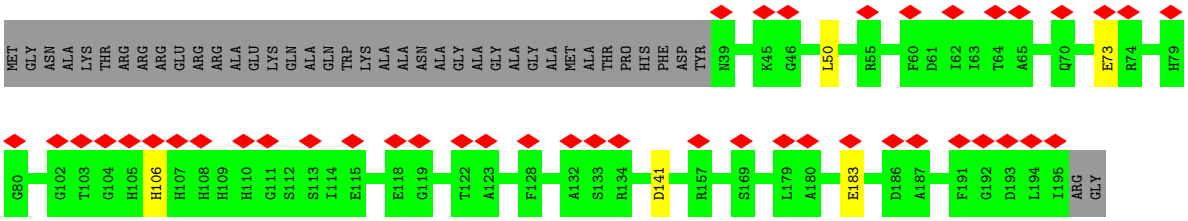
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain bB:



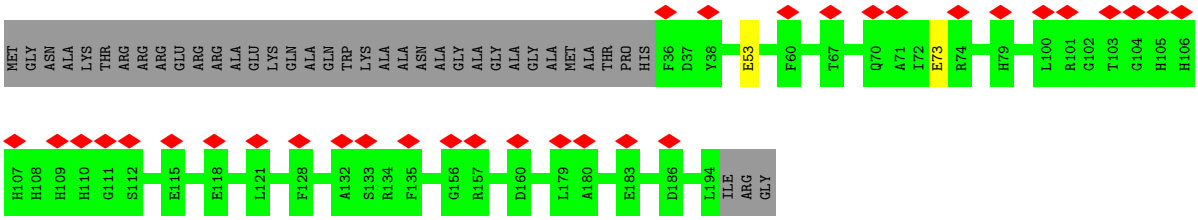
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain bC:



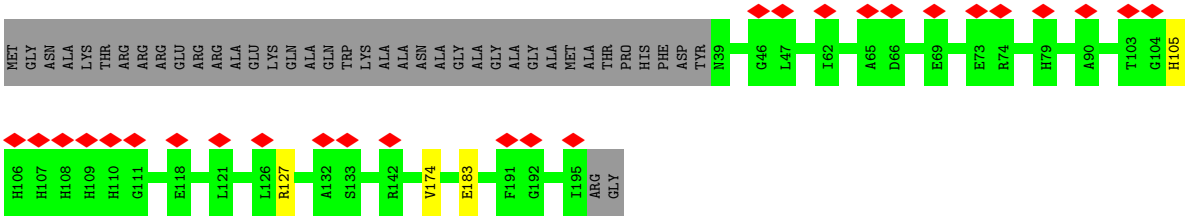
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain bD:



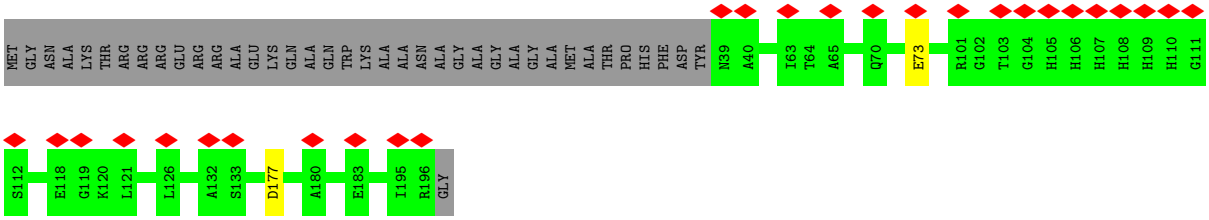
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain cA:



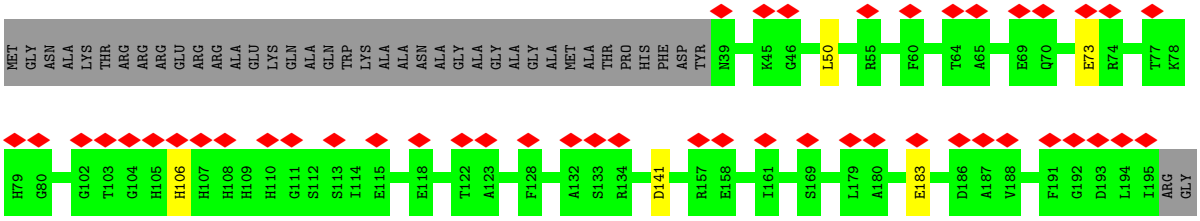
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain cB:



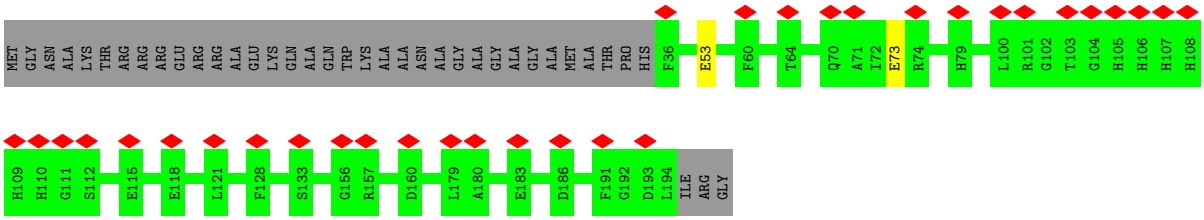
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain cC:



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

Chain cD:



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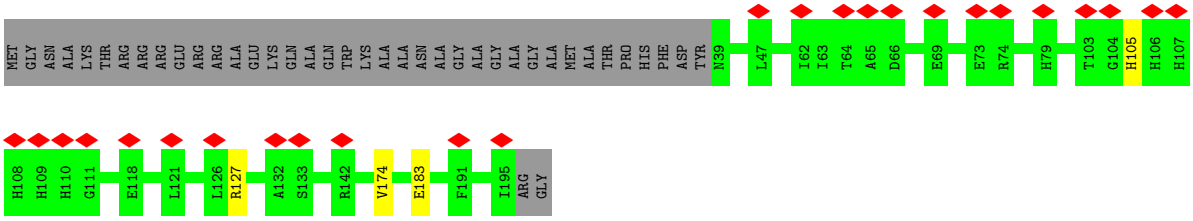
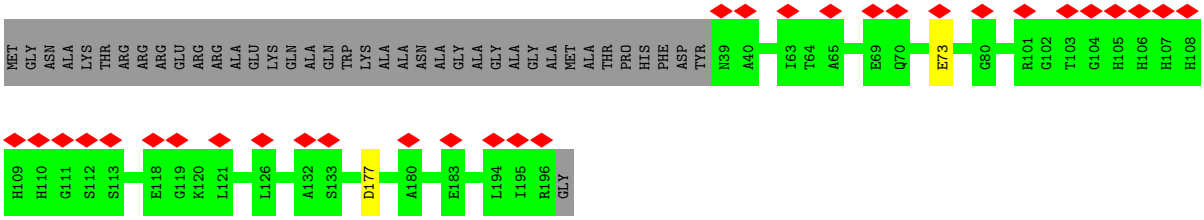
Chain dA:



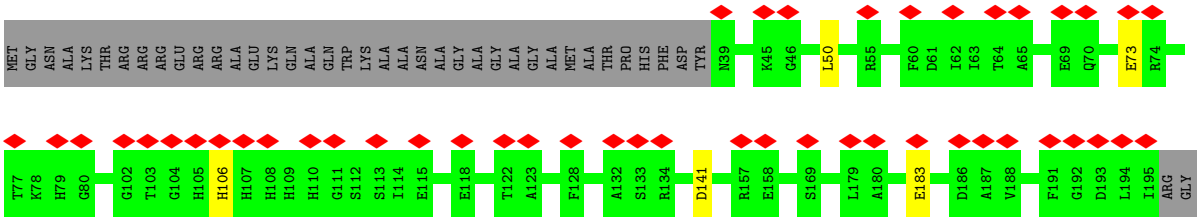
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain dB:



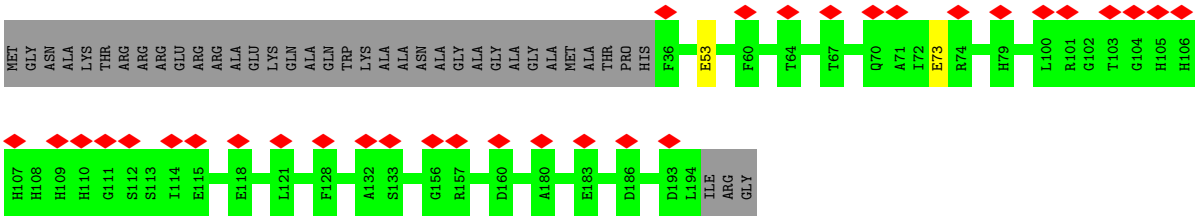
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain dC:



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

Chain dD:



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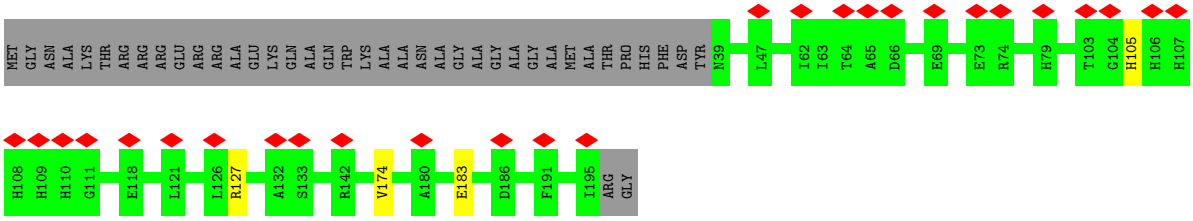
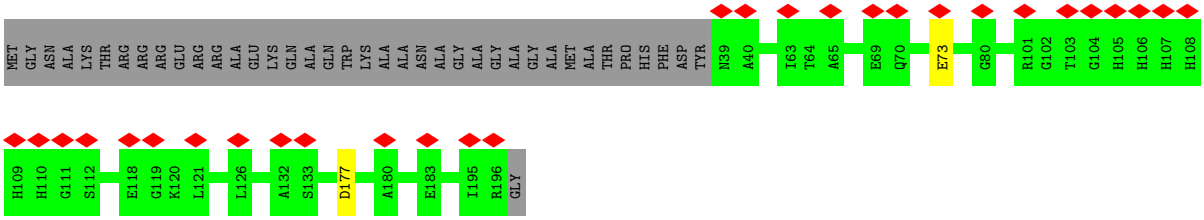
Chain eA:



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

Chain eB:



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

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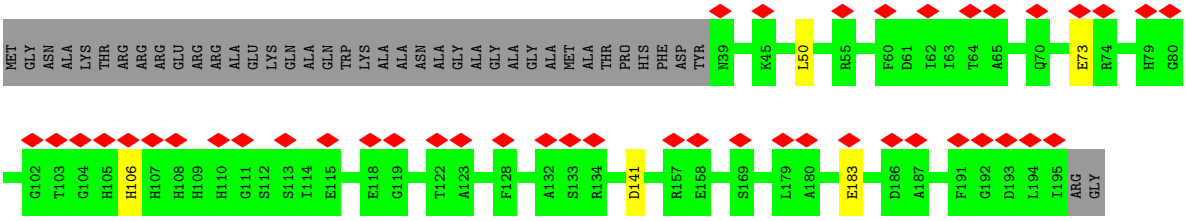
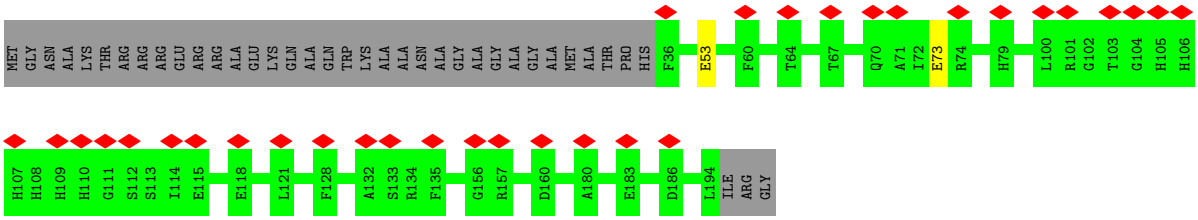


• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain eD:



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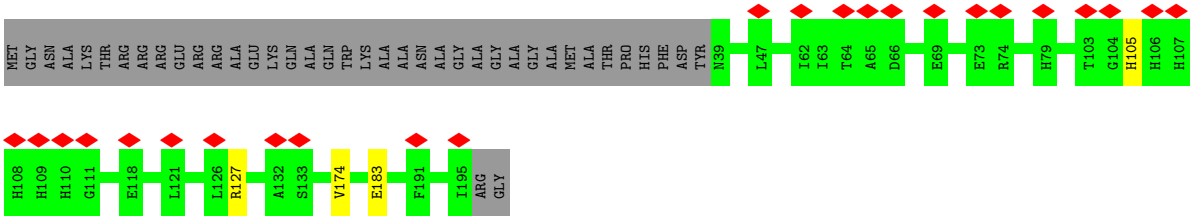
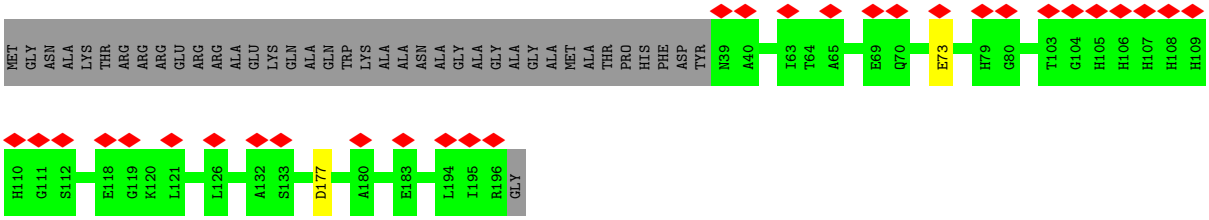
Chain fA:



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

Chain fB:



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

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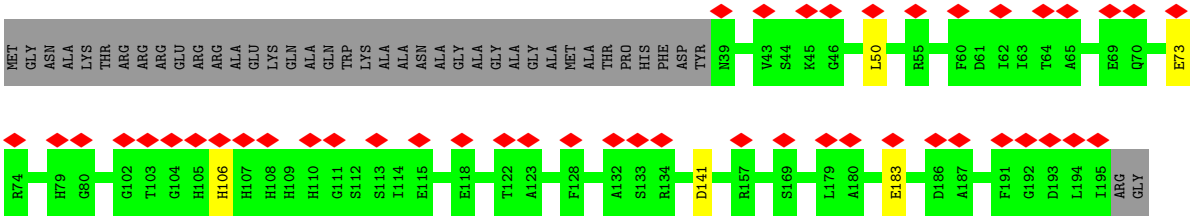

• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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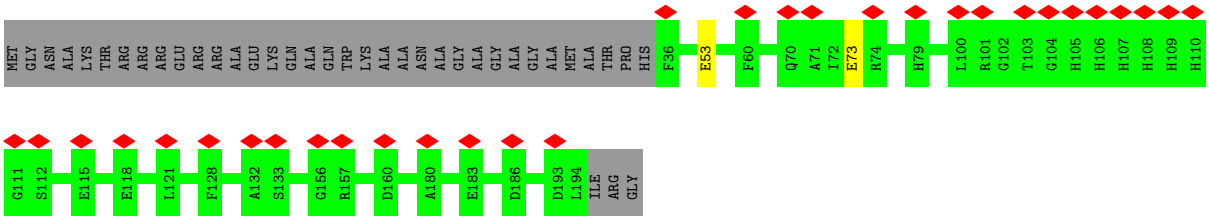
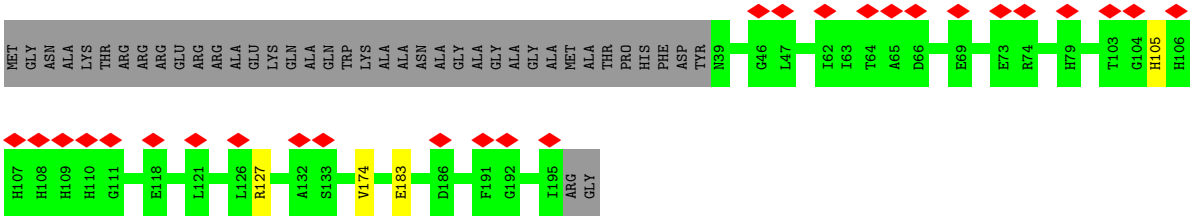


• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain gA:



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

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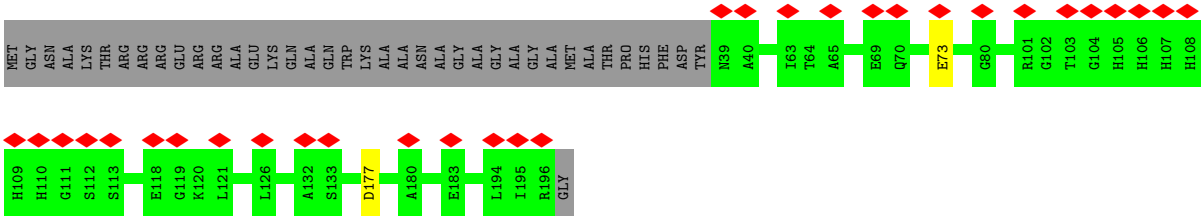
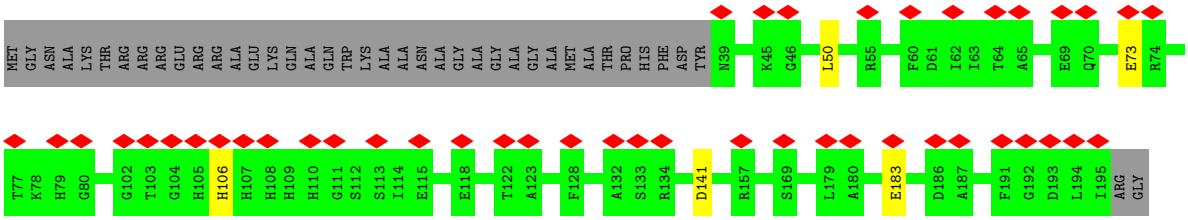


• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain gC:



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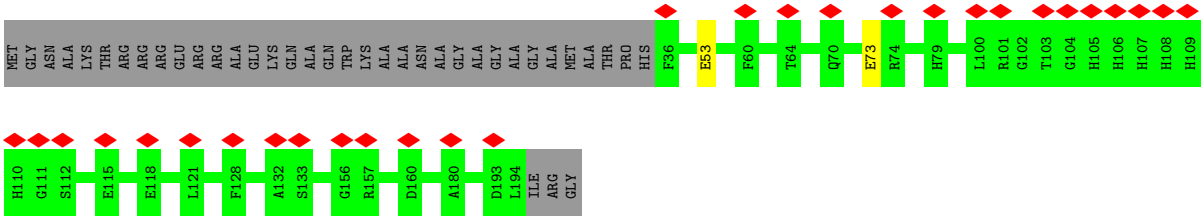

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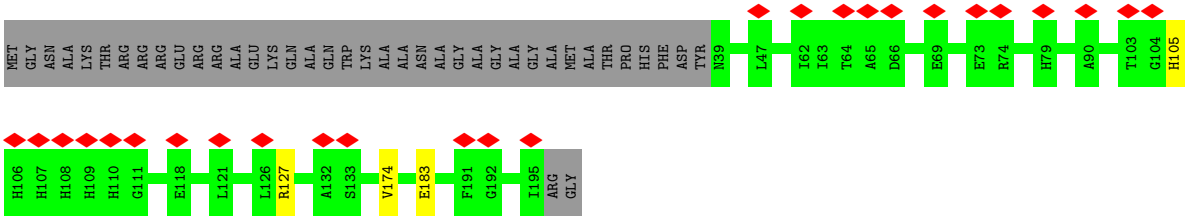
Chain hA:



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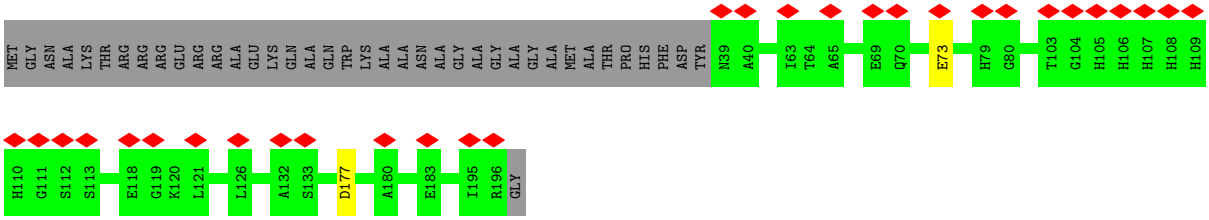

• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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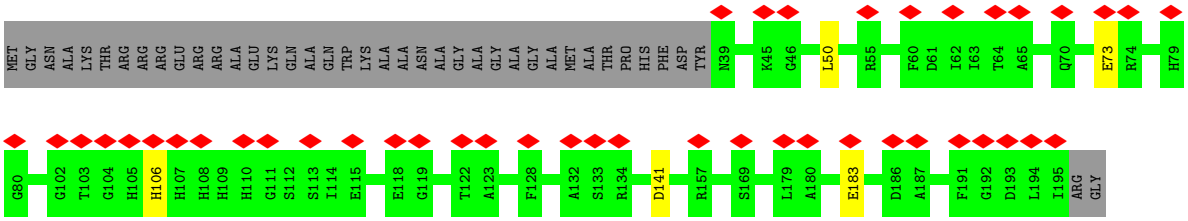
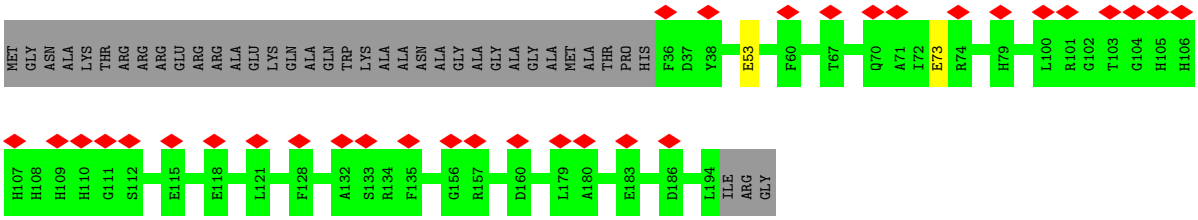


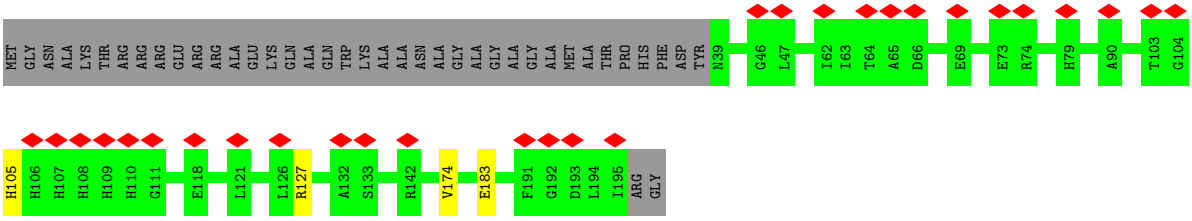
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain hD:



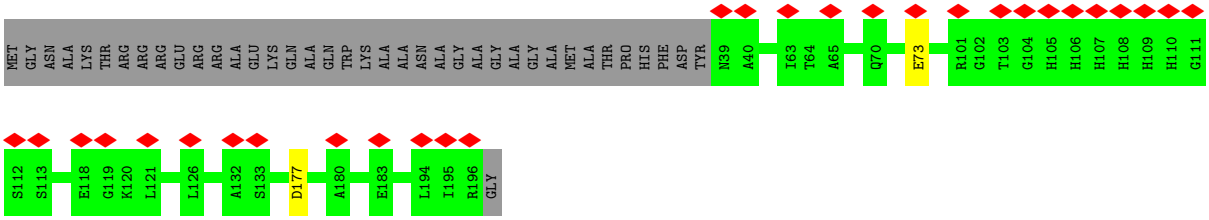
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain iA:



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

Chain iB:



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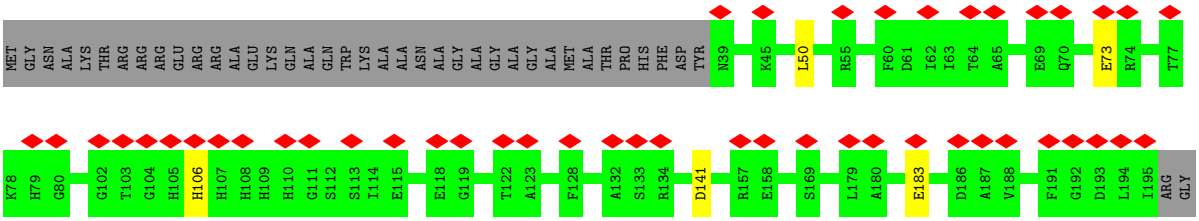

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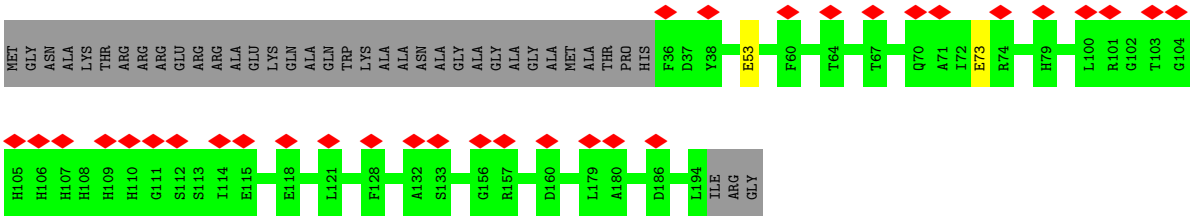

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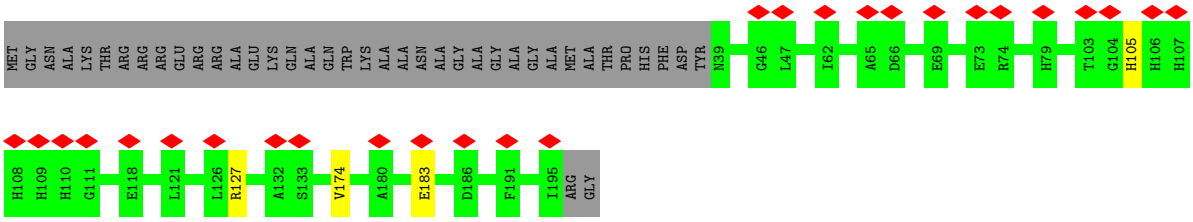
Chain jA:



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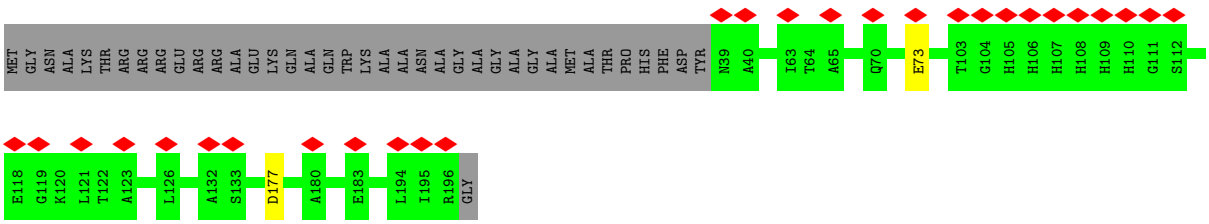

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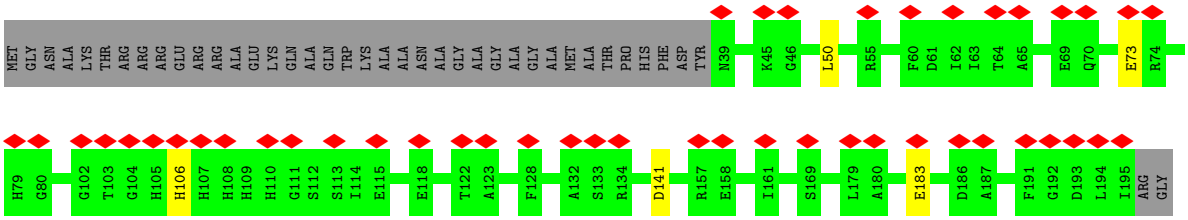

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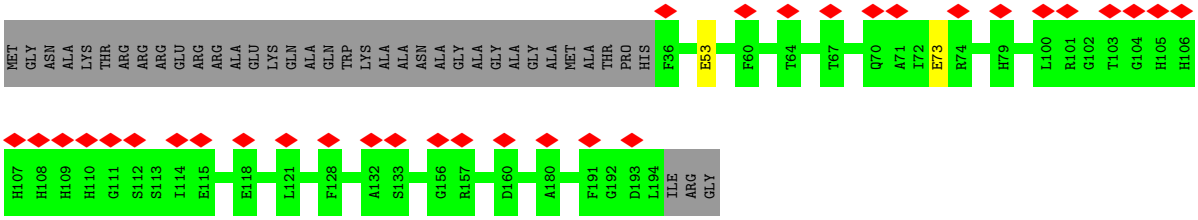

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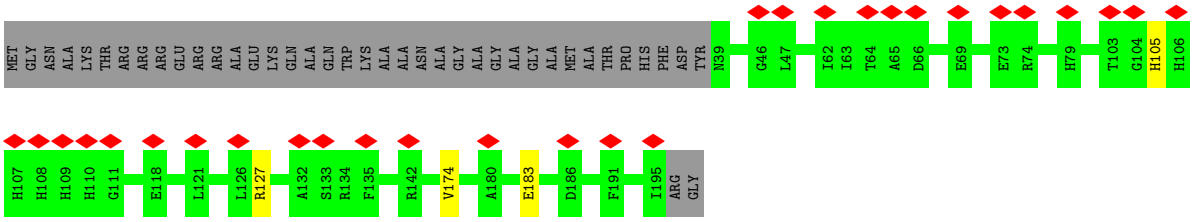
Chain kA:



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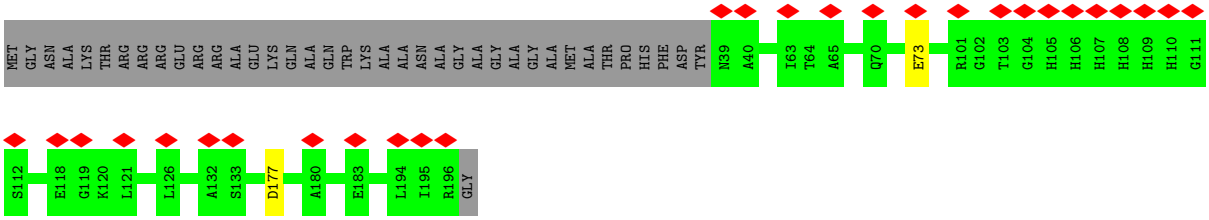

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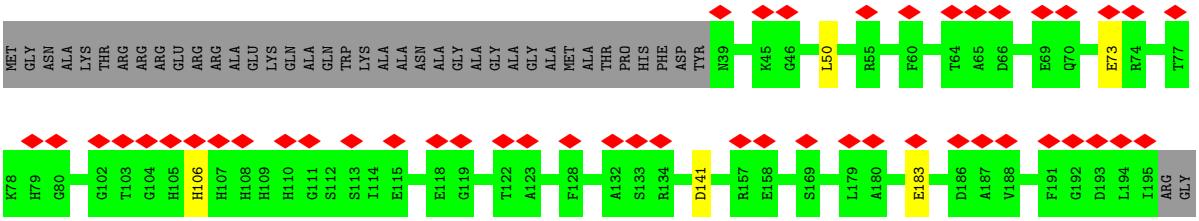

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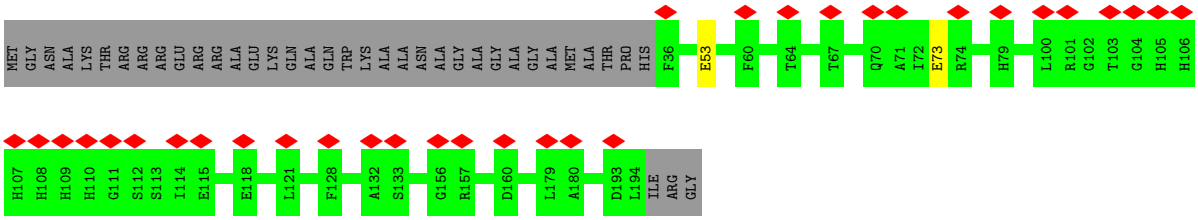
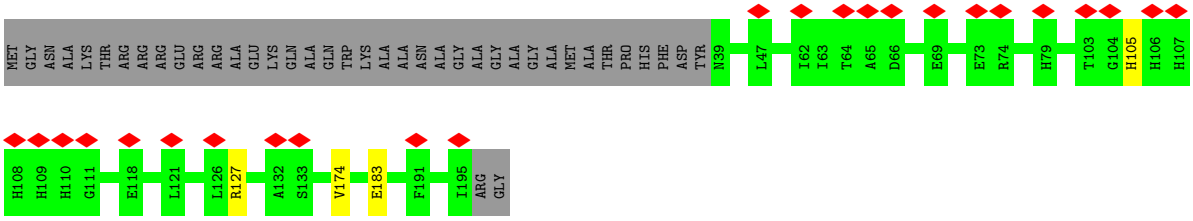


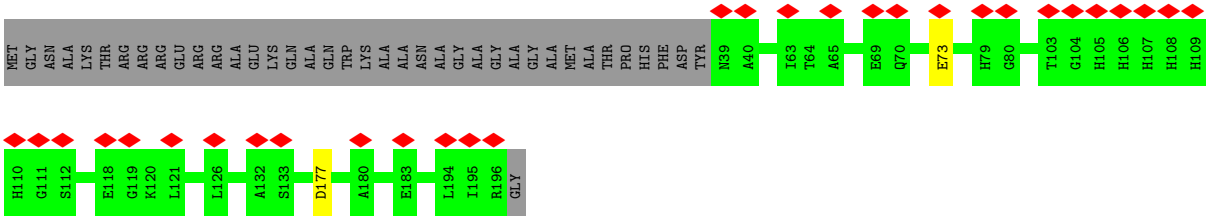
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain lA:



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

Chain lB:



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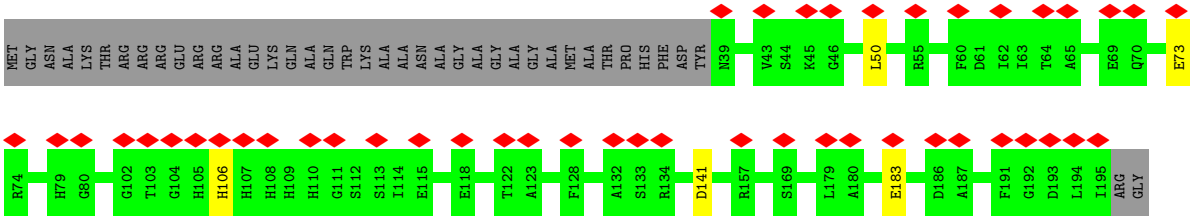

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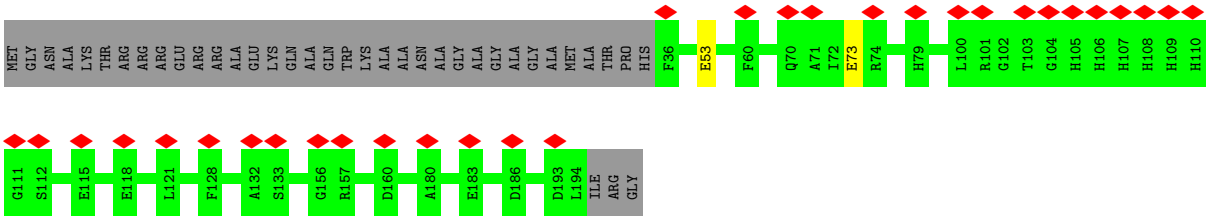
Chain lD:



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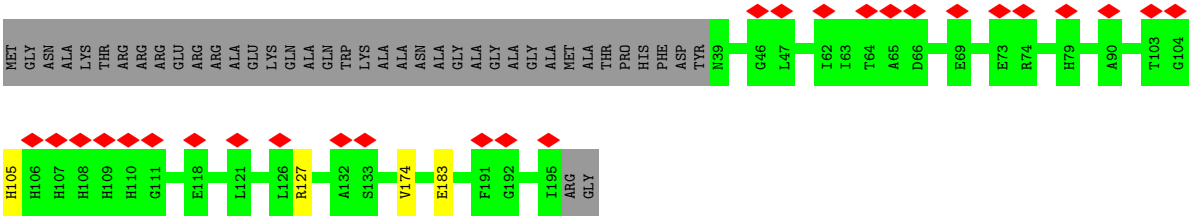
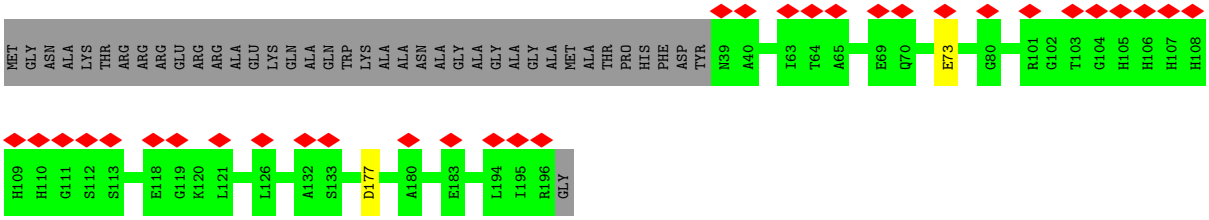
Chain mA:



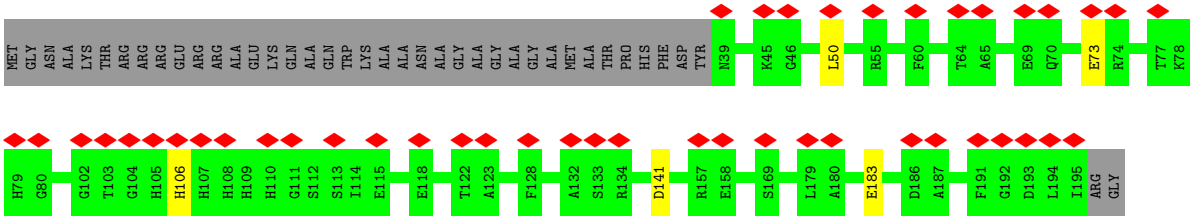
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain mB:



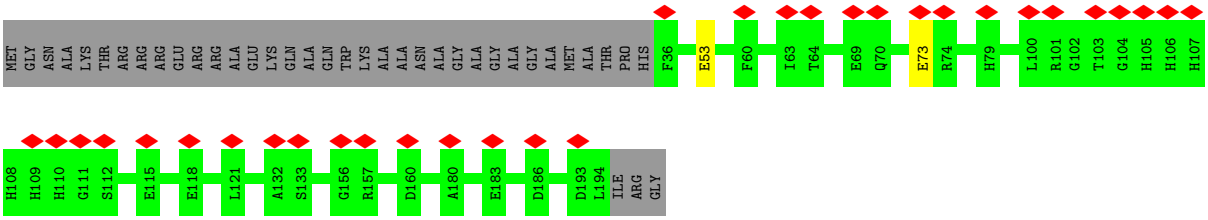
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain mC:



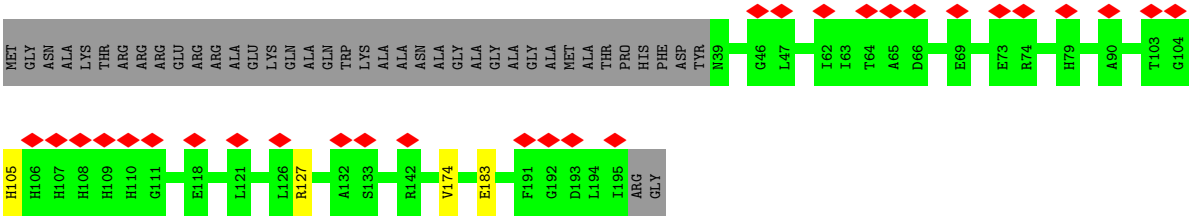
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain mD:



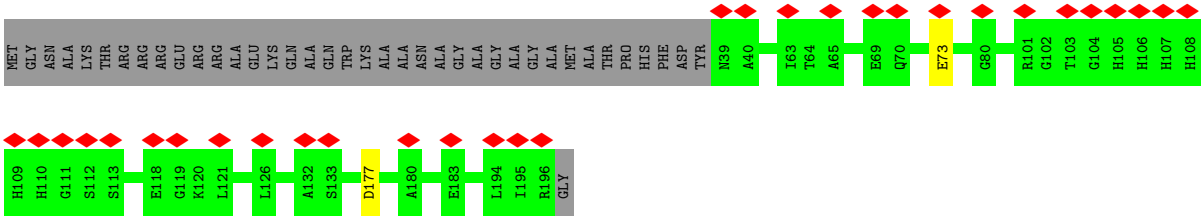
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain nA:



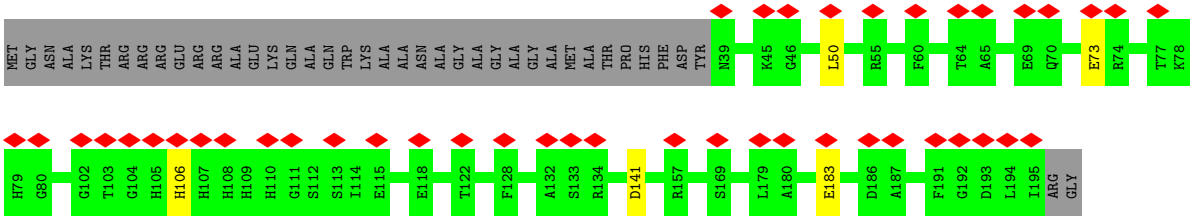
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain nB:



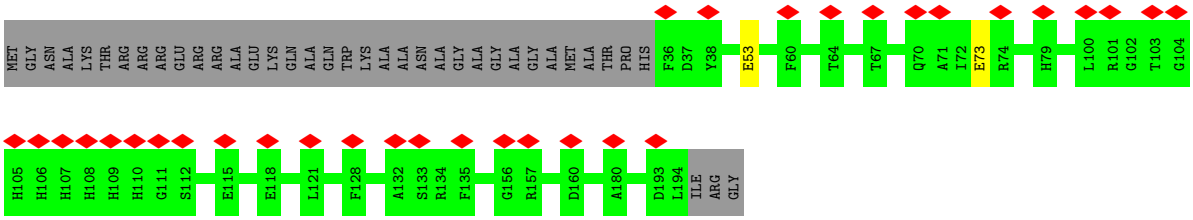
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain nC:



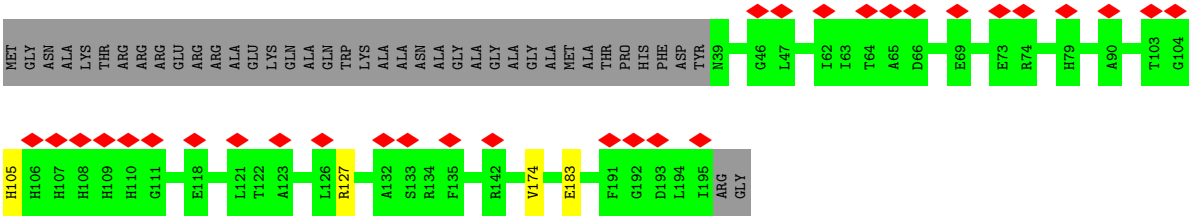
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain nD:



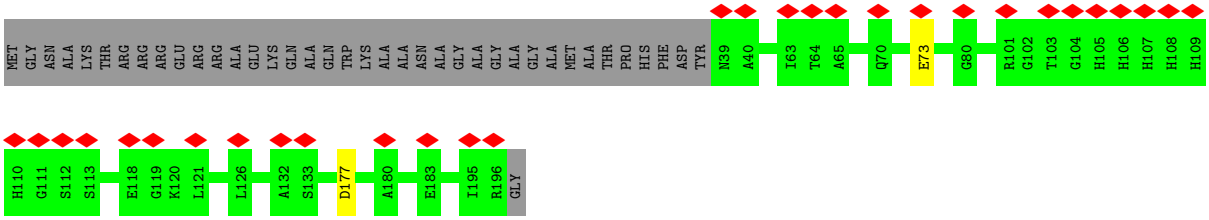
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain oA:



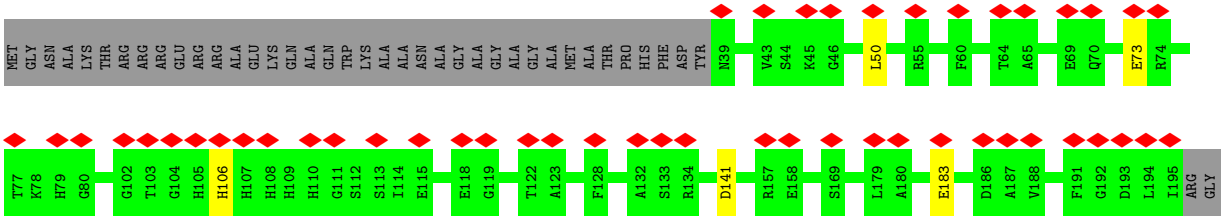
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain oB:



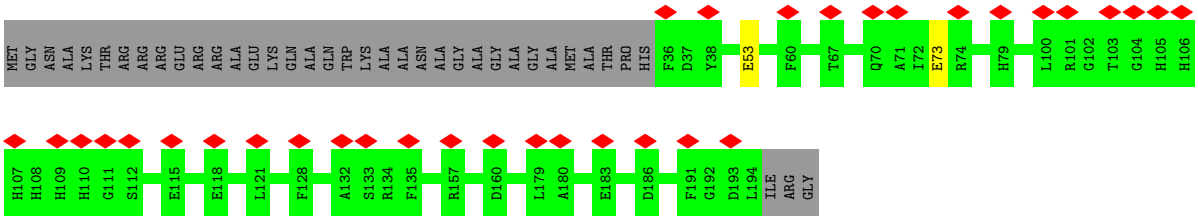
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain oC:



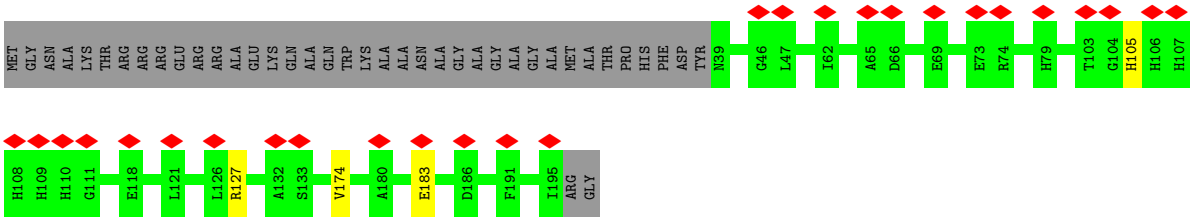
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain oD:



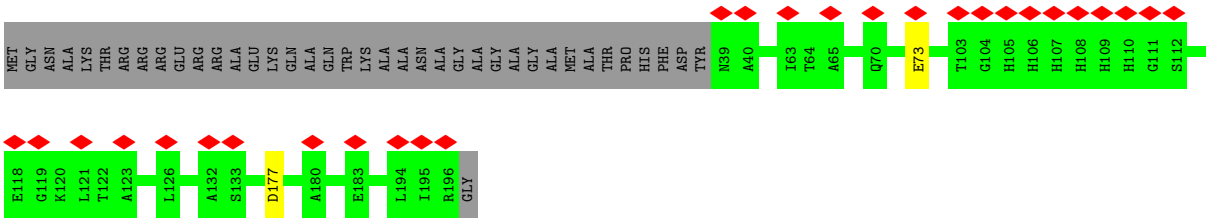
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain pA:



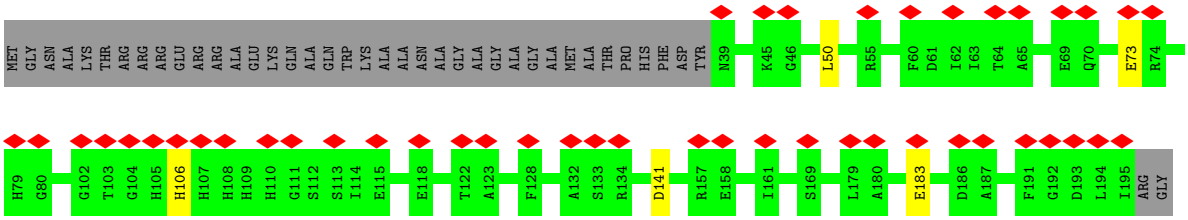
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain pB:



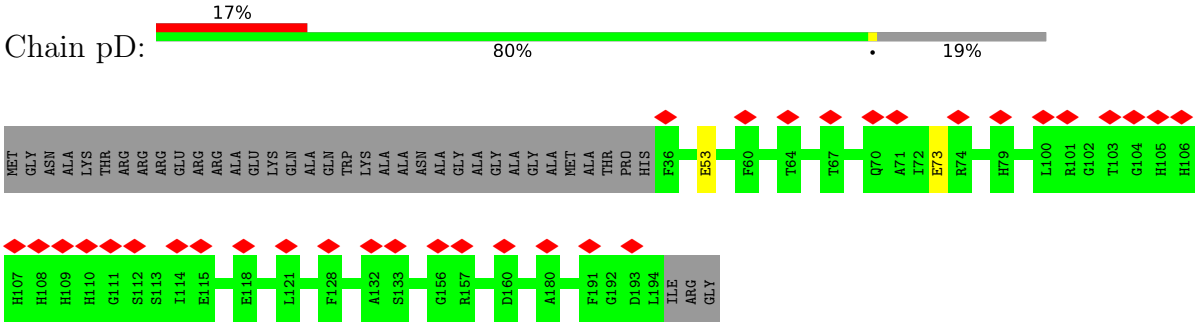
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain pC:



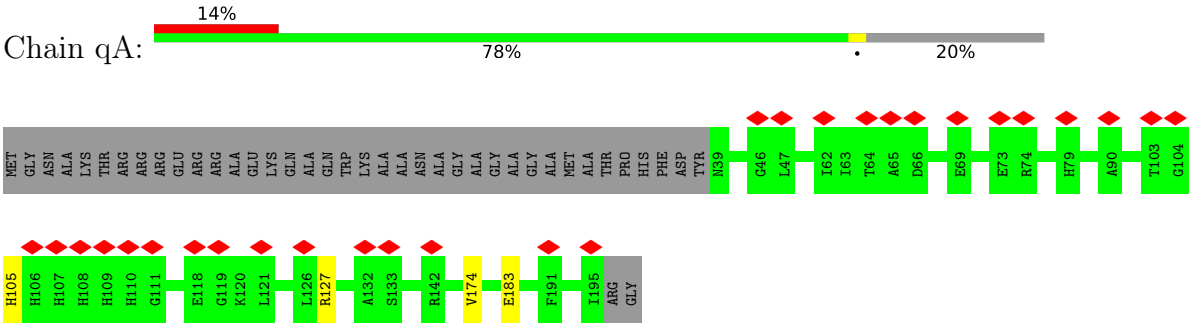
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain pD:



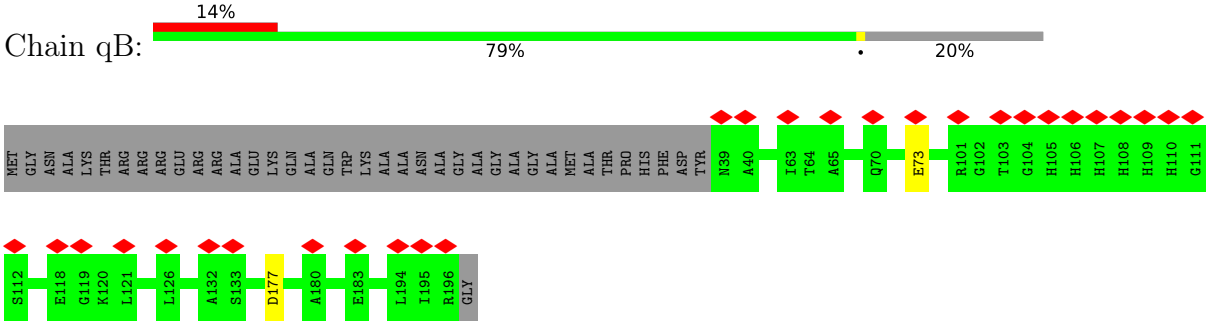
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain qA:



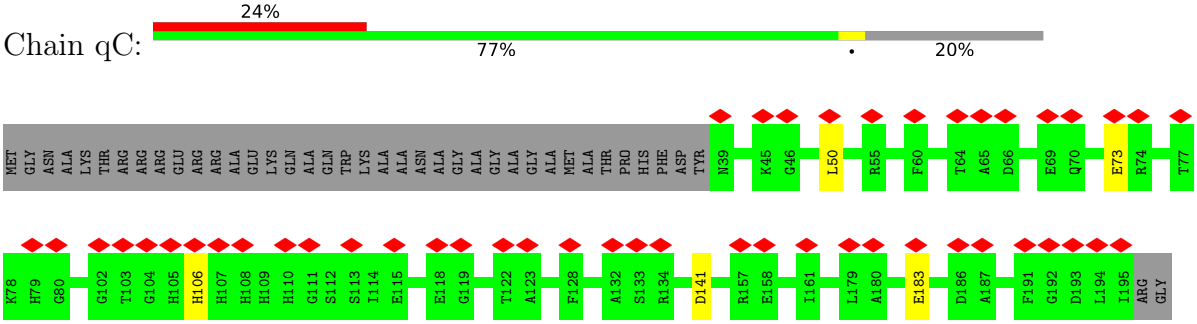
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain qB:



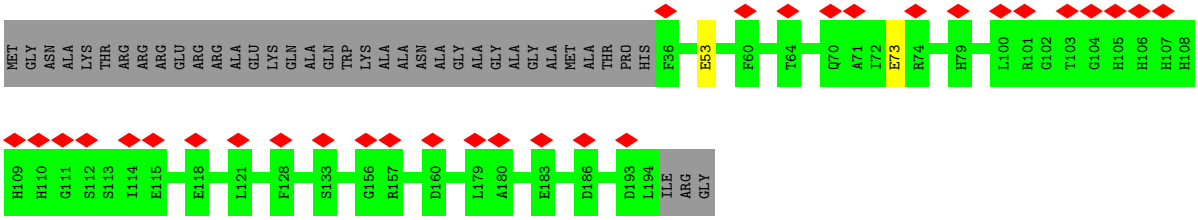
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain qC:



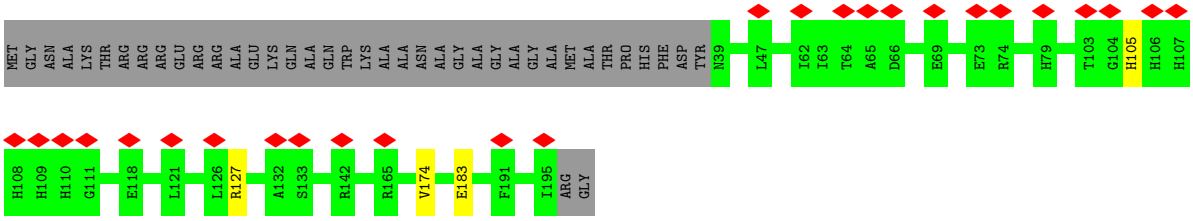
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain qD:



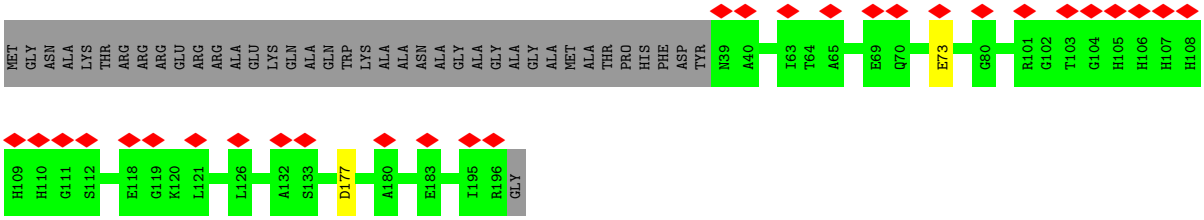
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain rA:



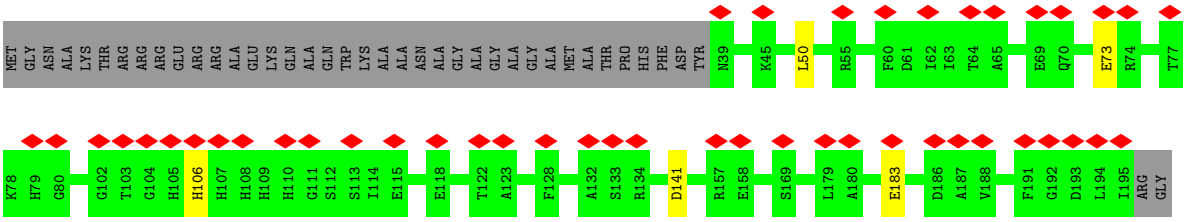
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain rB:



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

Chain rC:



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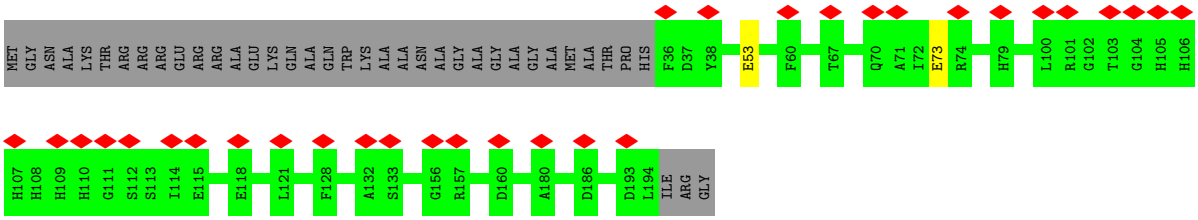
Chain rD:



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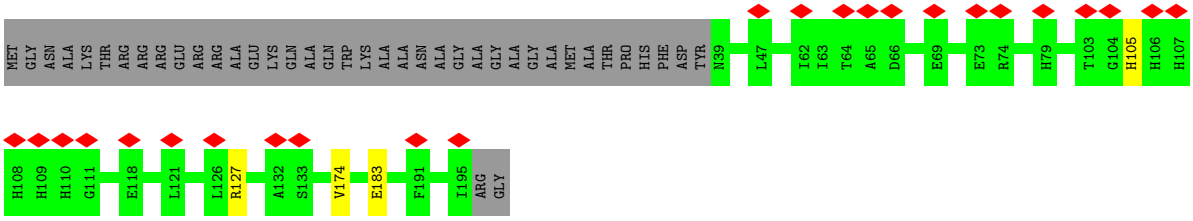
Chain sA:



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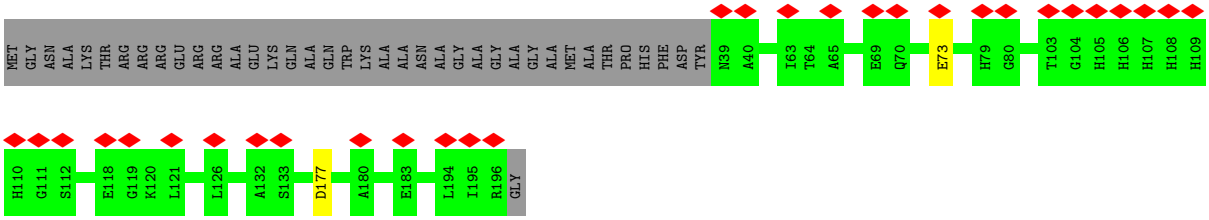
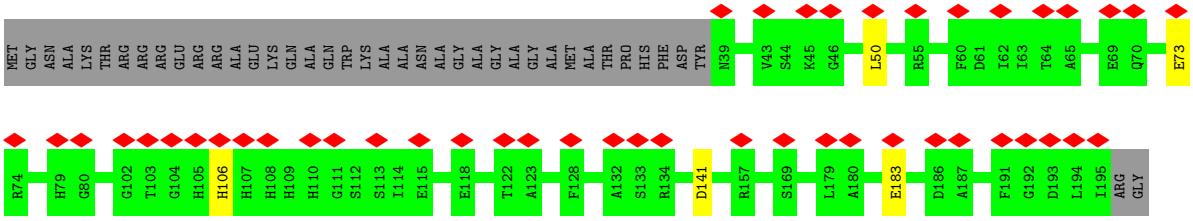
Chain sB:



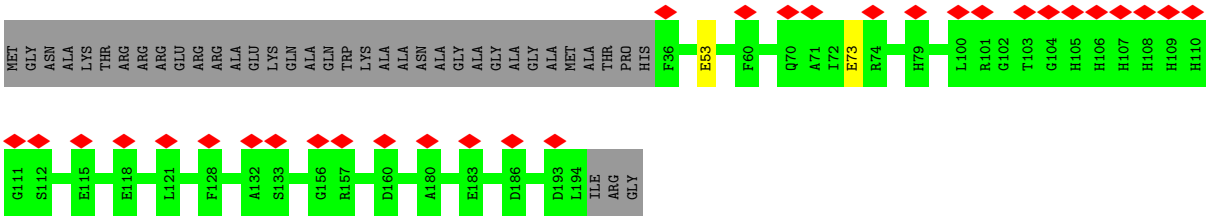
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain sC:



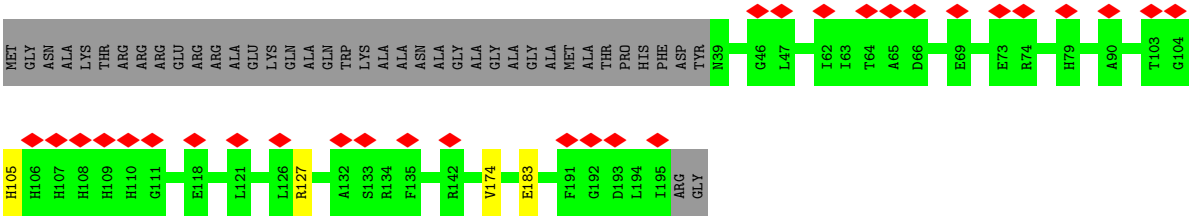
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain sD:



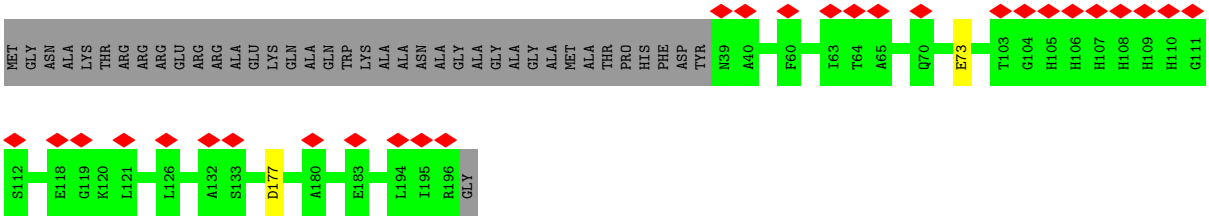
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain tA:



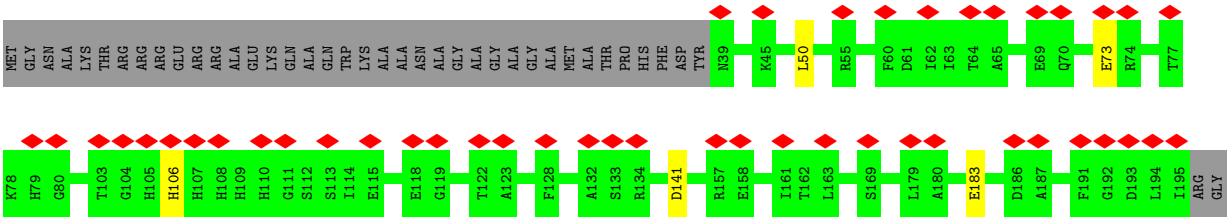
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain tB:



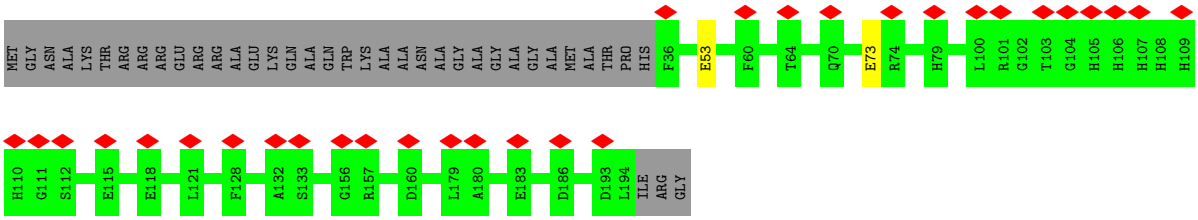
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain tC:



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

Chain tD:



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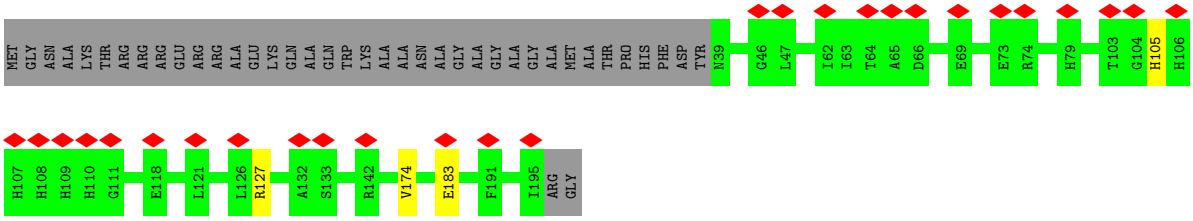
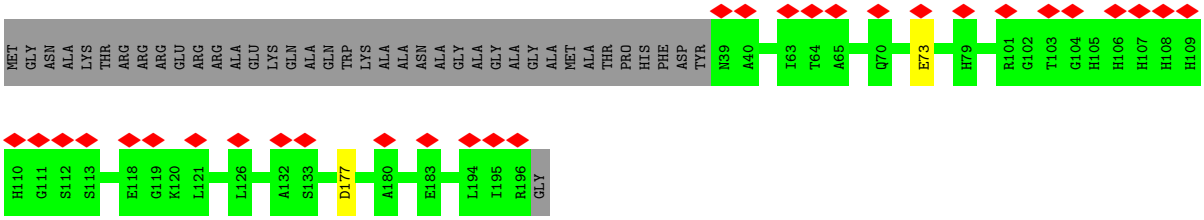
Chain uA:



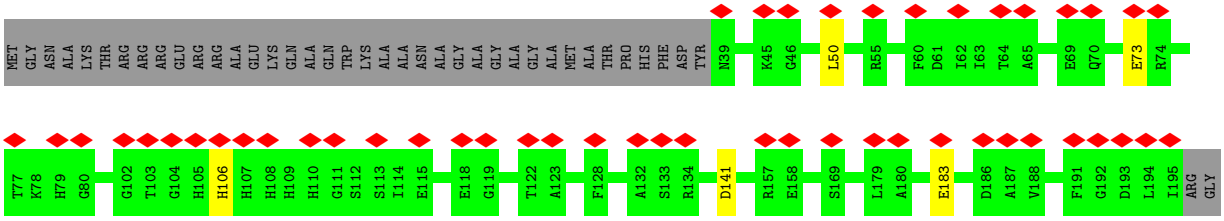
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain uB:



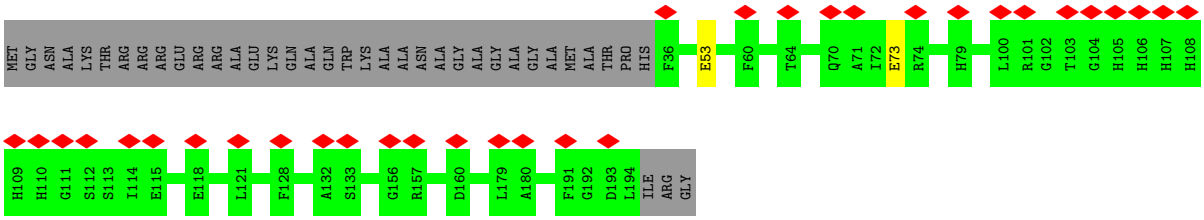
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain uC:



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

Chain uD:



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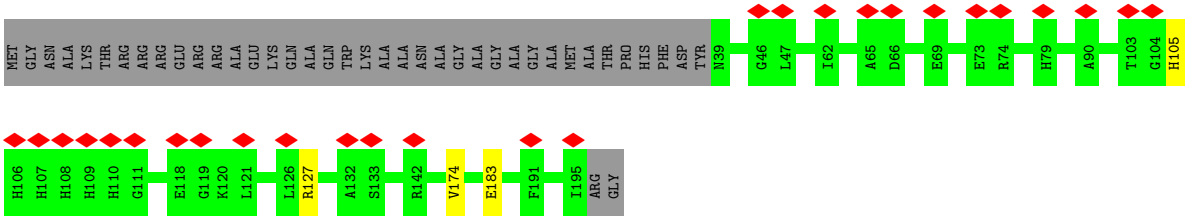
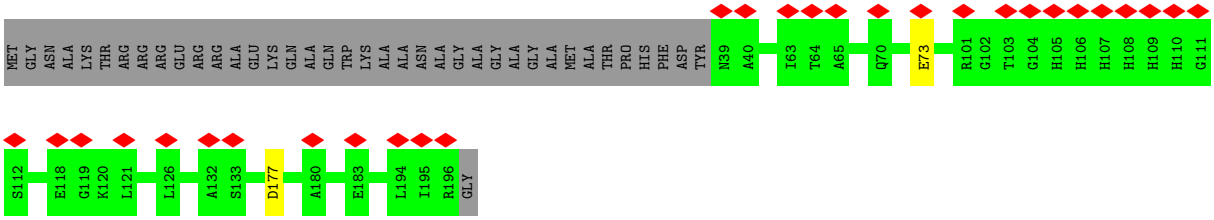
Chain vA:



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

Chain vB:



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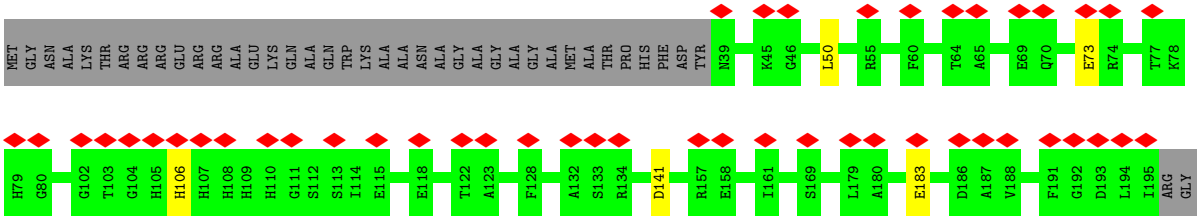
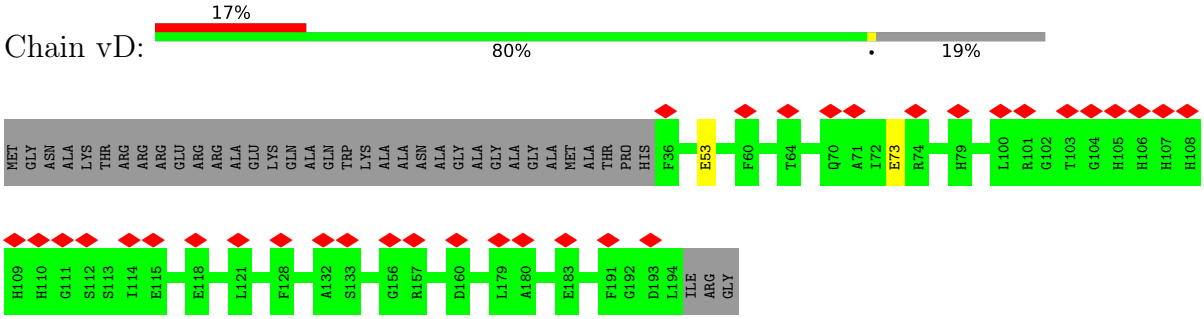


• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain vD:



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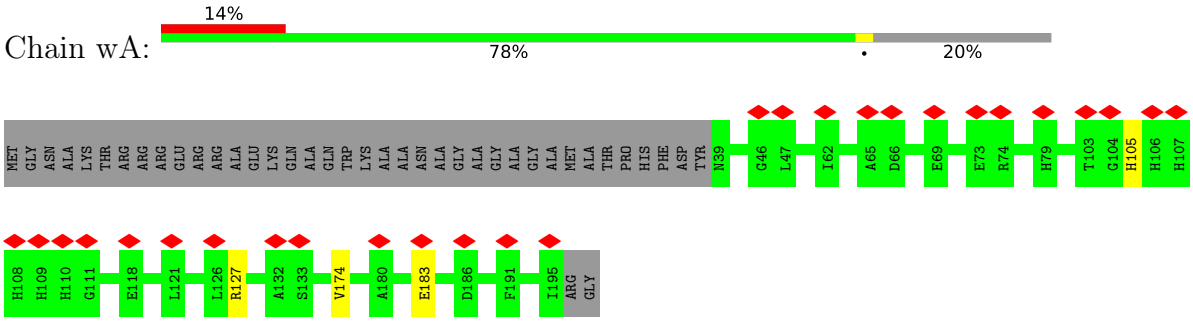
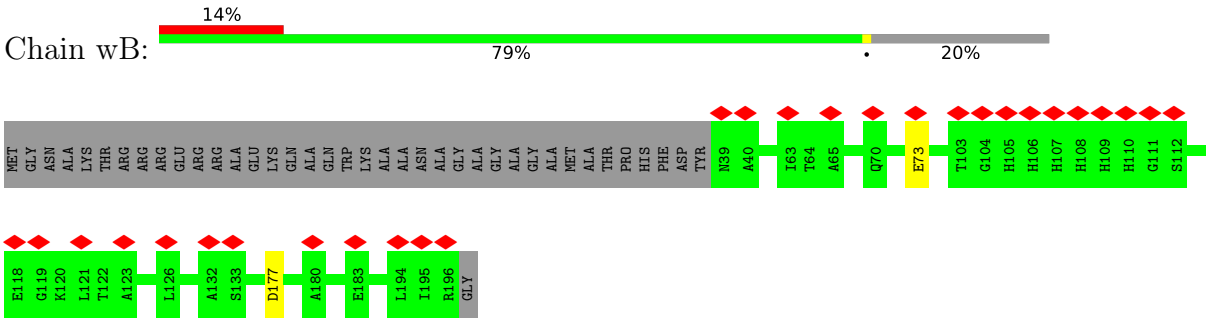
Chain wA:



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

Chain wB:



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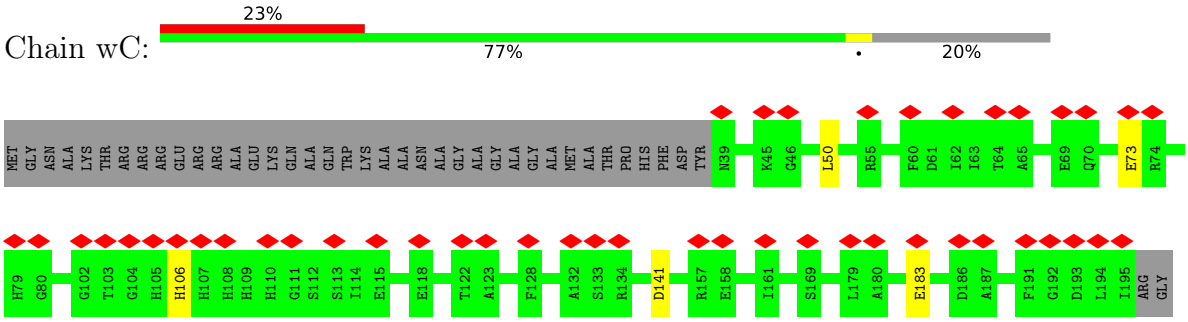
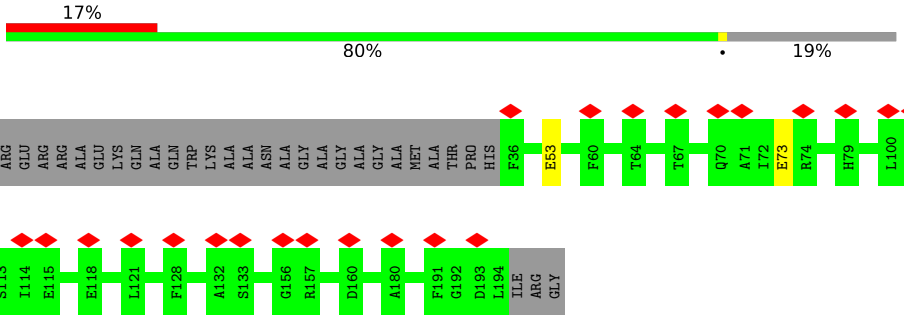


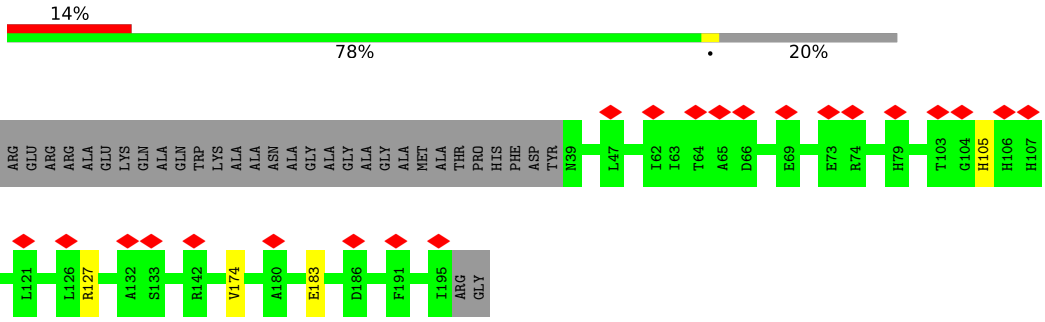
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain wD:



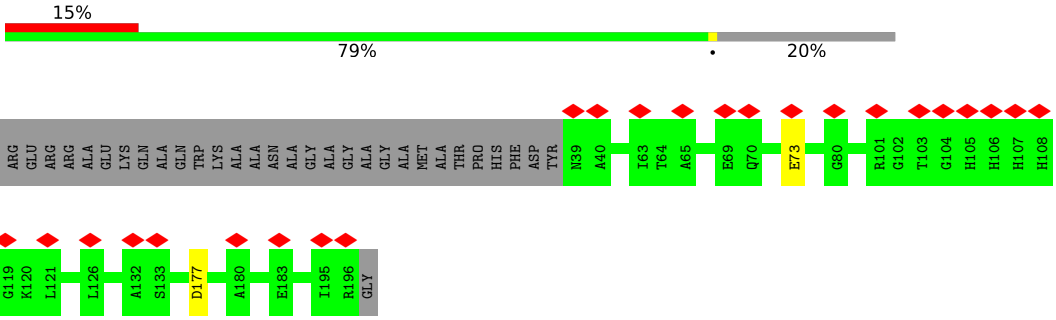
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain xA:



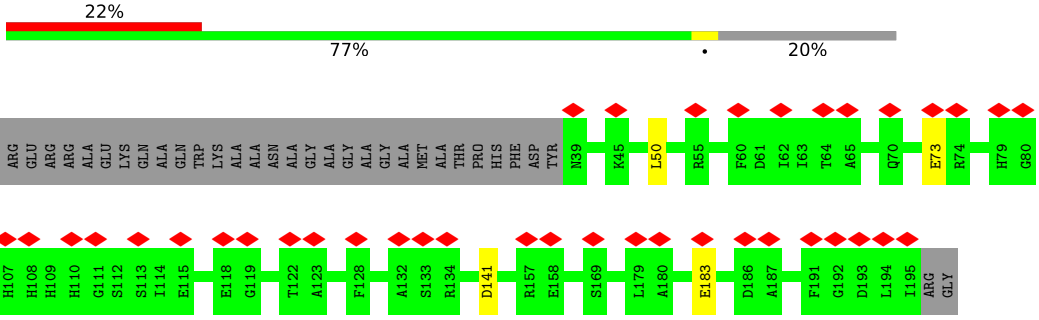
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain xB:



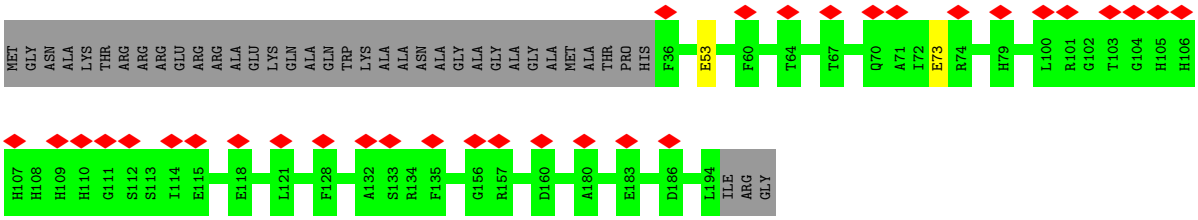
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain xC:



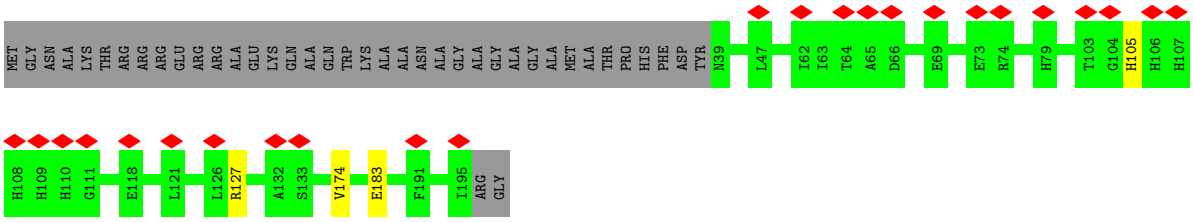
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain xD:



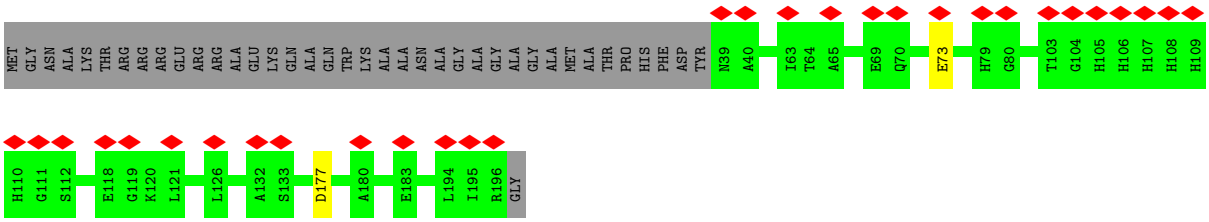
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain yA:



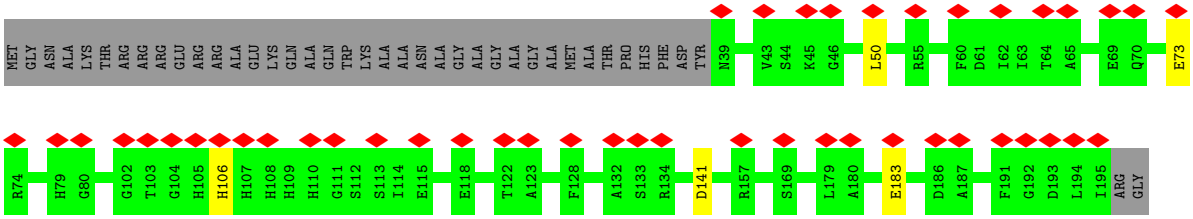
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain yB:



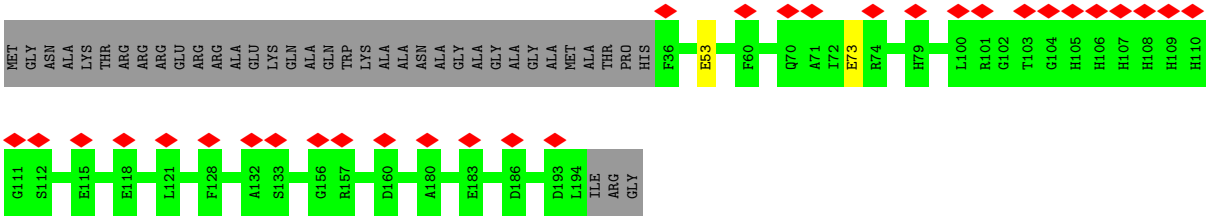
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain yC:



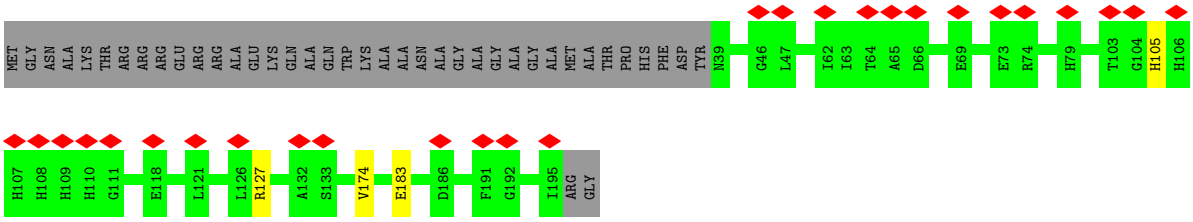
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain yD:



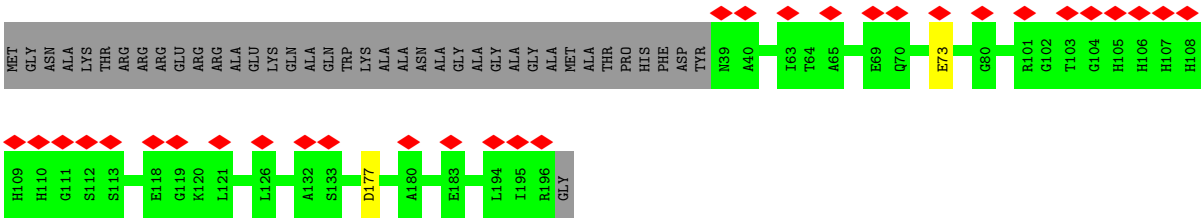
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain zA:



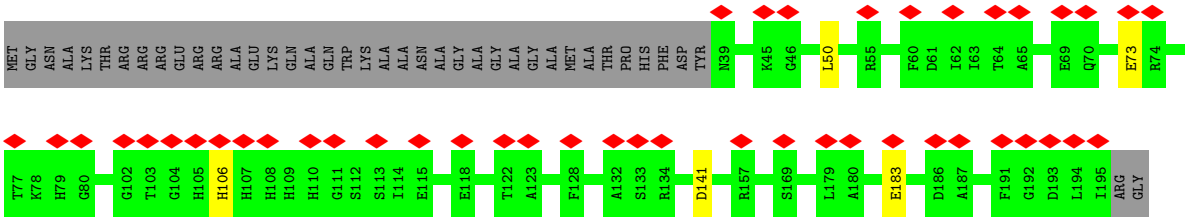
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain zB:



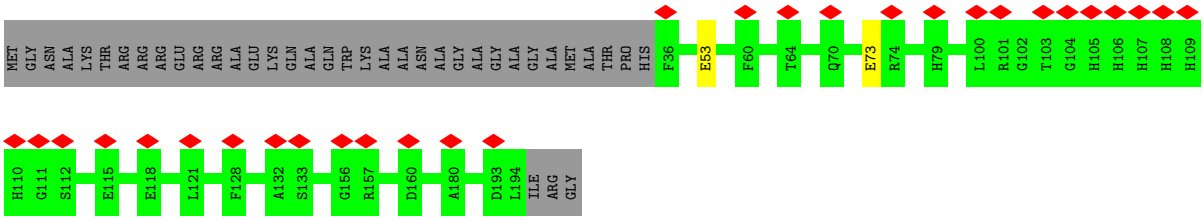
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain zC:



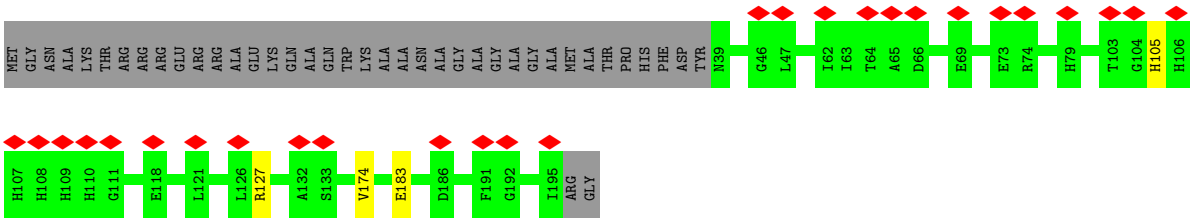
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain zD:



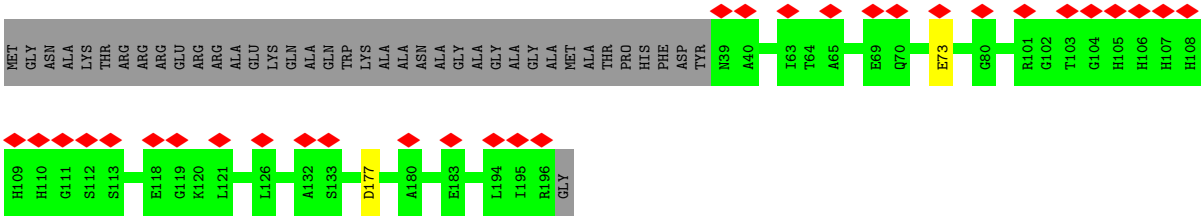
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 0A:



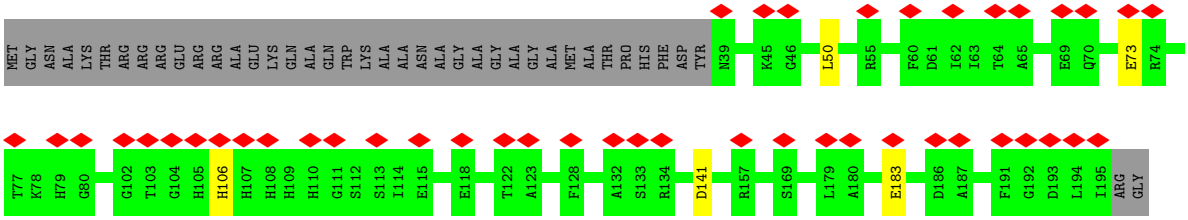
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 0B:



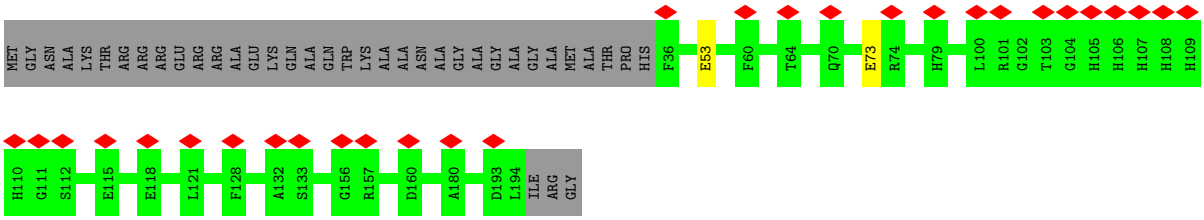
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 0C:



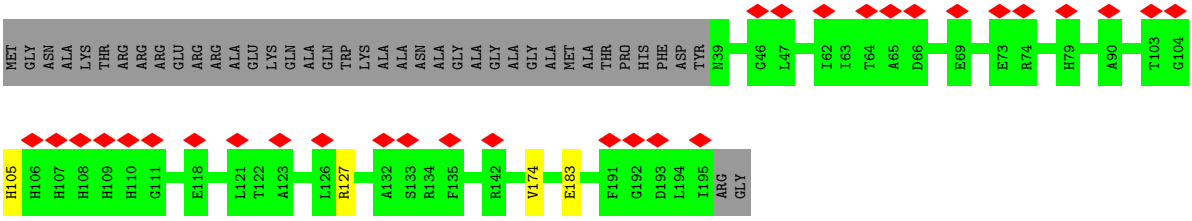
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 0D:



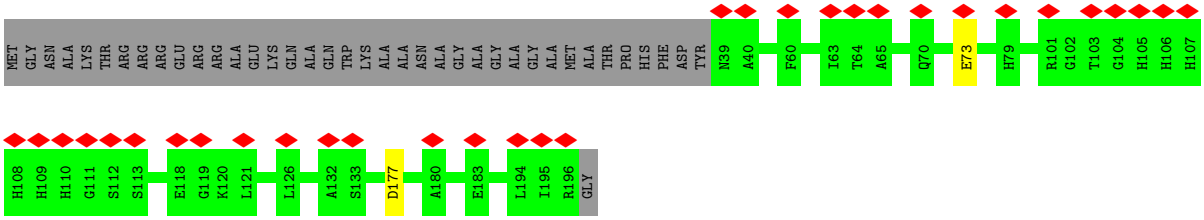
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 1A:



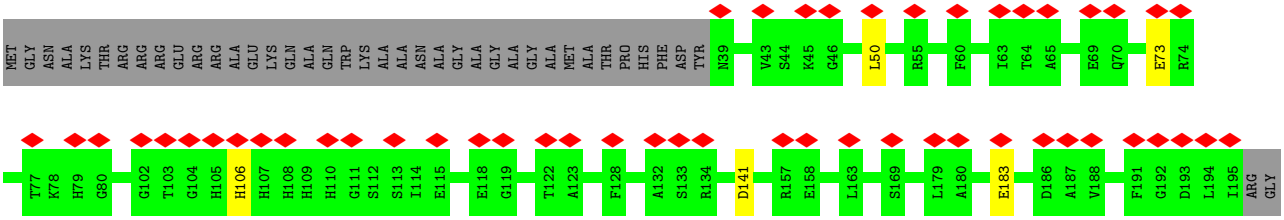
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 1B:



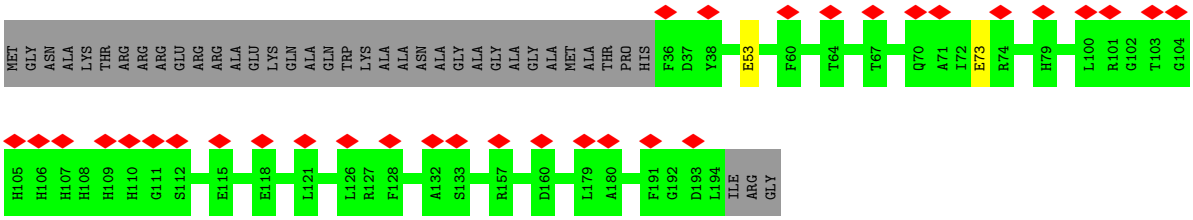
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 1C:



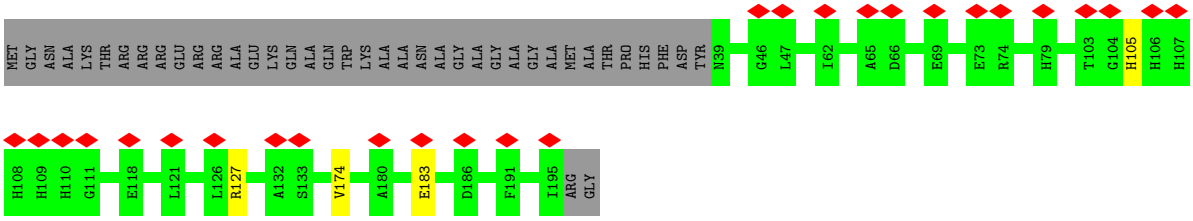
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 1D:



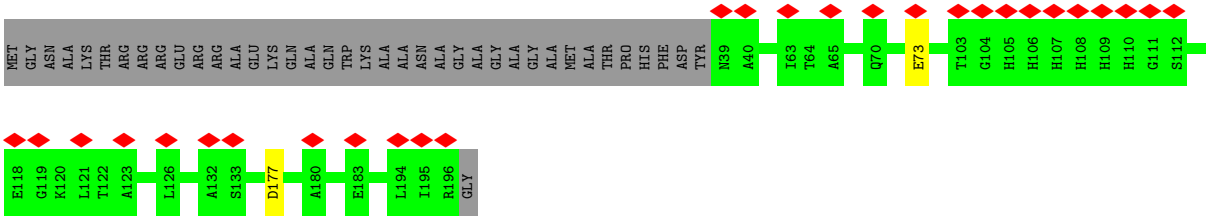
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 2A:



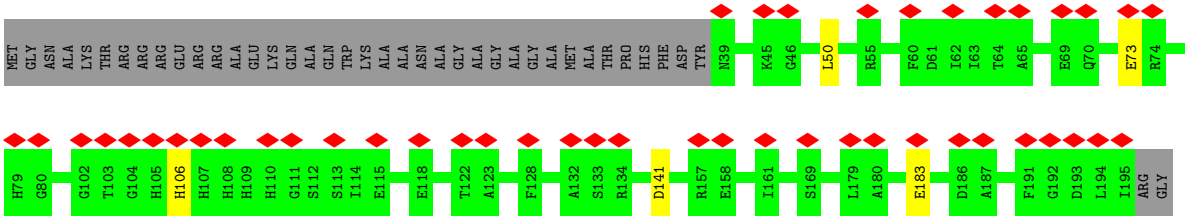
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 2B:



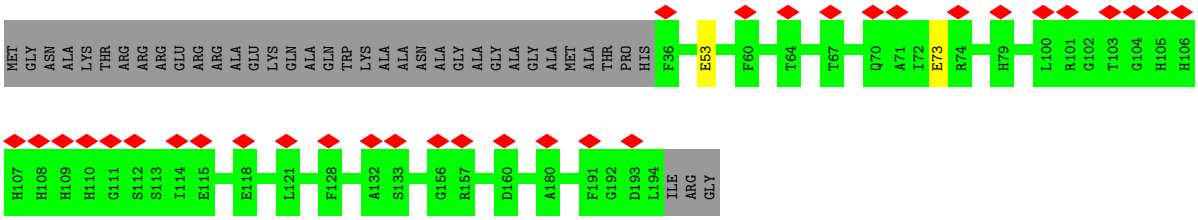
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 2C:



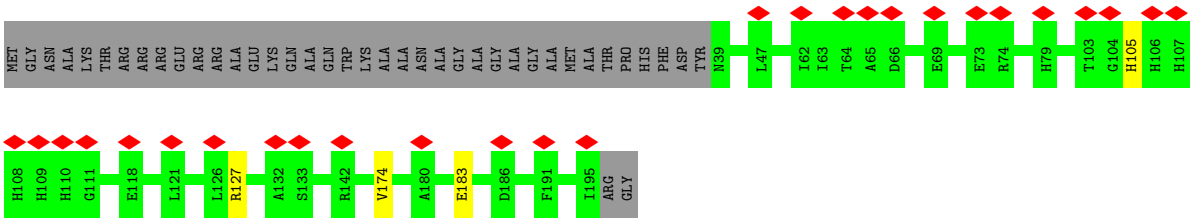
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 2D:



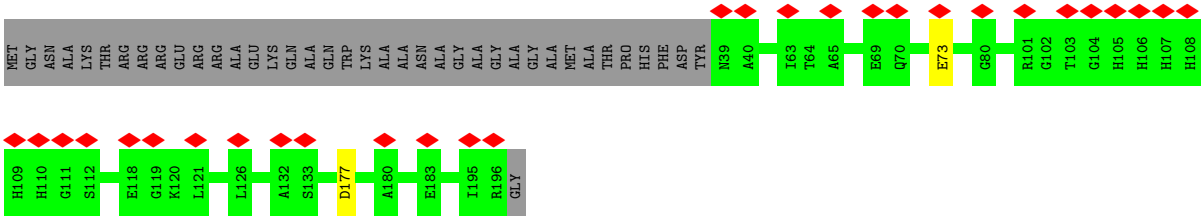
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 3A:



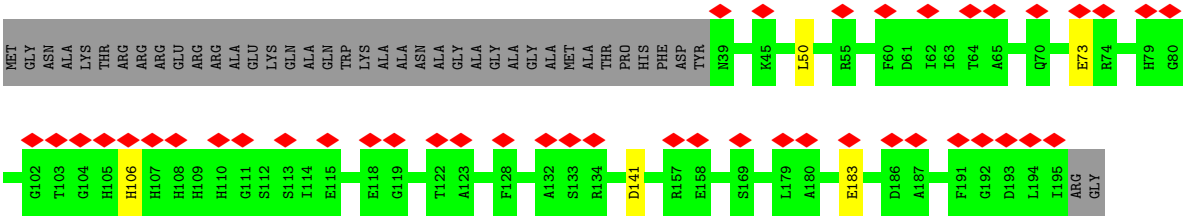
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 3B:



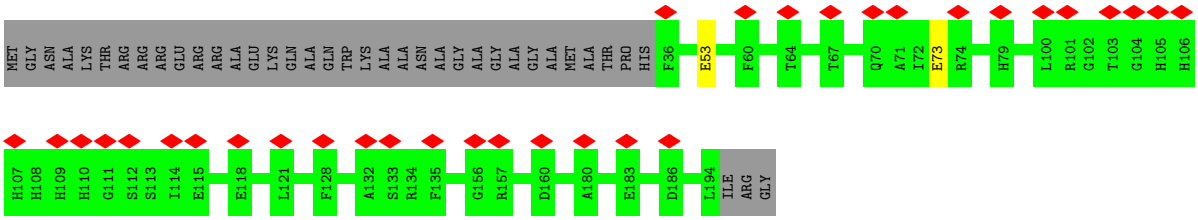
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 3C:



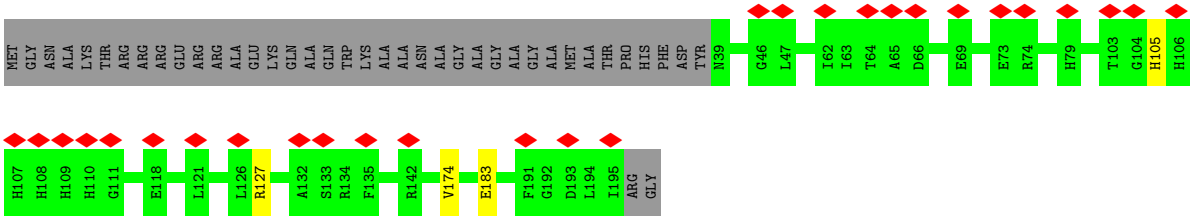
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 3D:



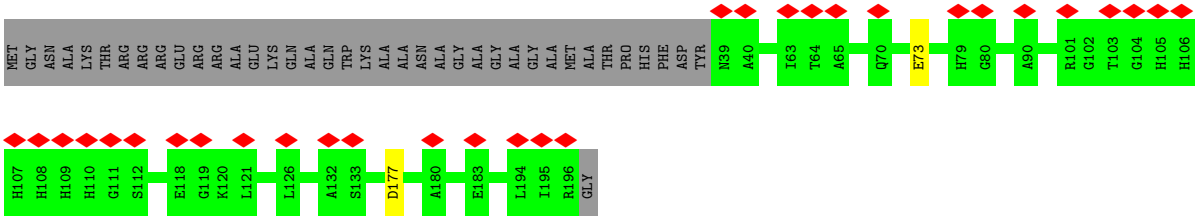
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 4A:



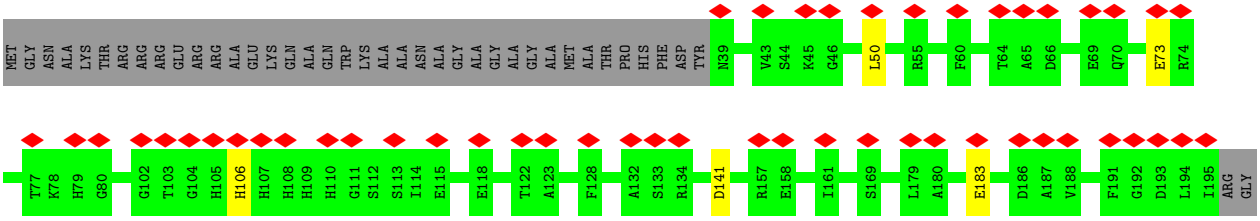
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 4B:



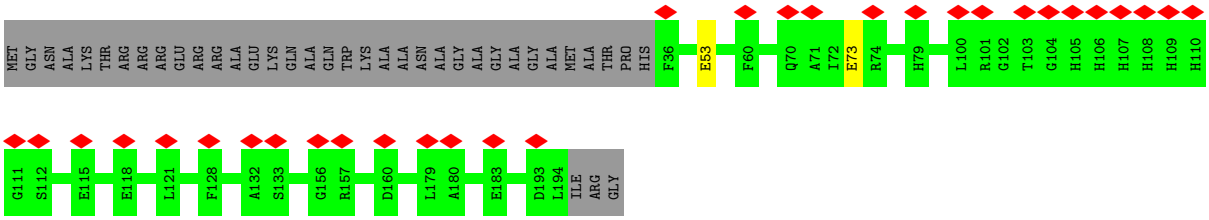
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain 4C:



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

Chain 4D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	3815	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	62000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.185	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0509	Depositor
Map size (Å)	648.0, 648.0, 648.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.8, 1.8, 1.8	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	0A	0.24	0/1226	0.41	0/1658
1	0B	0.25	0/1231	0.41	0/1665
1	0C	0.26	0/1226	0.44	0/1658
1	0D	0.25	0/1244	0.43	0/1683
1	1A	0.24	0/1226	0.41	0/1658
1	1B	0.25	0/1231	0.41	0/1665
1	1C	0.26	0/1226	0.44	0/1658
1	1D	0.25	0/1244	0.43	0/1683
1	2A	0.24	0/1226	0.41	0/1658
1	2B	0.25	0/1231	0.41	0/1665
1	2C	0.26	0/1226	0.44	0/1658
1	2D	0.25	0/1244	0.43	0/1683
1	3A	0.24	0/1226	0.41	0/1658
1	3B	0.25	0/1231	0.41	0/1665
1	3C	0.26	0/1226	0.44	0/1658
1	3D	0.25	0/1244	0.43	0/1683
1	4A	0.24	0/1226	0.41	0/1658
1	4B	0.25	0/1231	0.41	0/1665
1	4C	0.26	0/1226	0.44	0/1658
1	4D	0.25	0/1244	0.43	0/1683
1	5A	0.24	0/1226	0.41	0/1658
1	5B	0.25	0/1231	0.41	0/1665
1	5C	0.26	0/1226	0.44	0/1658
1	5D	0.25	0/1244	0.43	0/1683
1	6A	0.24	0/1226	0.41	0/1658
1	6B	0.25	0/1231	0.41	0/1665
1	6C	0.26	0/1226	0.44	0/1658
1	6D	0.25	0/1244	0.43	0/1683
1	7A	0.24	0/1226	0.41	0/1658
1	7B	0.25	0/1231	0.41	0/1665
1	7C	0.26	0/1226	0.44	0/1658
1	7D	0.25	0/1244	0.43	0/1683
1	AA	0.24	0/1226	0.41	0/1658
1	AB	0.25	0/1231	0.41	0/1665

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	AC	0.26	0/1226	0.44	0/1658
1	AD	0.25	0/1244	0.43	0/1683
1	BA	0.24	0/1226	0.41	0/1658
1	BB	0.25	0/1231	0.41	0/1665
1	BC	0.26	0/1226	0.44	0/1658
1	BD	0.25	0/1244	0.43	0/1683
1	CA	0.24	0/1226	0.41	0/1658
1	CB	0.25	0/1231	0.41	0/1665
1	CC	0.26	0/1226	0.44	0/1658
1	CD	0.25	0/1244	0.43	0/1683
1	DA	0.24	0/1226	0.41	0/1658
1	DB	0.25	0/1231	0.41	0/1665
1	DC	0.26	0/1226	0.44	0/1658
1	DD	0.25	0/1244	0.43	0/1683
1	EA	0.24	0/1226	0.41	0/1658
1	EB	0.25	0/1231	0.41	0/1665
1	EC	0.26	0/1226	0.44	0/1658
1	ED	0.25	0/1244	0.43	0/1683
1	FA	0.24	0/1226	0.41	0/1658
1	FB	0.25	0/1231	0.41	0/1665
1	FC	0.26	0/1226	0.44	0/1658
1	FD	0.25	0/1244	0.43	0/1683
1	GA	0.24	0/1226	0.41	0/1658
1	GB	0.25	0/1231	0.41	0/1665
1	GC	0.26	0/1226	0.44	0/1658
1	GD	0.25	0/1244	0.43	0/1683
1	HA	0.24	0/1226	0.41	0/1658
1	HB	0.25	0/1231	0.41	0/1665
1	HC	0.26	0/1226	0.44	0/1658
1	HD	0.25	0/1244	0.43	0/1683
1	IA	0.24	0/1226	0.41	0/1658
1	IB	0.25	0/1231	0.41	0/1665
1	IC	0.26	0/1226	0.44	0/1658
1	ID	0.25	0/1244	0.43	0/1683
1	JA	0.24	0/1226	0.41	0/1658
1	JB	0.25	0/1231	0.41	0/1665
1	JC	0.26	0/1226	0.44	0/1658
1	JD	0.25	0/1244	0.43	0/1683
1	KA	0.24	0/1226	0.41	0/1658
1	KB	0.25	0/1231	0.41	0/1665
1	KC	0.26	0/1226	0.44	0/1658
1	KD	0.25	0/1244	0.43	0/1683
1	LA	0.24	0/1226	0.41	0/1658

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	LB	0.25	0/1231	0.41	0/1665
1	LC	0.26	0/1226	0.44	0/1658
1	LD	0.25	0/1244	0.43	0/1683
1	MA	0.24	0/1226	0.41	0/1658
1	MB	0.25	0/1231	0.41	0/1665
1	MC	0.26	0/1226	0.44	0/1658
1	MD	0.25	0/1244	0.43	0/1683
1	NA	0.24	0/1226	0.41	0/1658
1	NB	0.25	0/1231	0.41	0/1665
1	NC	0.26	0/1226	0.44	0/1658
1	ND	0.25	0/1244	0.43	0/1683
1	OA	0.24	0/1226	0.41	0/1658
1	OB	0.25	0/1231	0.41	0/1665
1	OC	0.26	0/1226	0.44	0/1658
1	OD	0.25	0/1244	0.43	0/1683
1	PA	0.24	0/1226	0.41	0/1658
1	PB	0.25	0/1231	0.41	0/1665
1	PC	0.26	0/1226	0.44	0/1658
1	PD	0.25	0/1244	0.43	0/1683
1	QA	0.24	0/1226	0.41	0/1658
1	QB	0.25	0/1231	0.41	0/1665
1	QC	0.26	0/1226	0.44	0/1658
1	QD	0.25	0/1244	0.43	0/1683
1	RA	0.24	0/1226	0.41	0/1658
1	RB	0.25	0/1231	0.41	0/1665
1	RC	0.26	0/1226	0.44	0/1658
1	RD	0.25	0/1244	0.43	0/1683
1	SA	0.24	0/1226	0.41	0/1658
1	SB	0.25	0/1231	0.41	0/1665
1	SC	0.26	0/1226	0.44	0/1658
1	SD	0.25	0/1244	0.43	0/1683
1	TA	0.24	0/1226	0.41	0/1658
1	TB	0.25	0/1231	0.41	0/1665
1	TC	0.26	0/1226	0.44	0/1658
1	TD	0.25	0/1244	0.43	0/1683
1	UA	0.24	0/1226	0.41	0/1658
1	UB	0.25	0/1231	0.41	0/1665
1	UC	0.26	0/1226	0.44	0/1658
1	UD	0.25	0/1244	0.43	0/1683
1	VA	0.24	0/1226	0.41	0/1658
1	VB	0.25	0/1231	0.41	0/1665
1	VC	0.26	0/1226	0.44	0/1658
1	VD	0.25	0/1244	0.43	0/1683

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	WA	0.24	0/1226	0.41	0/1658
1	WB	0.25	0/1231	0.41	0/1665
1	WC	0.26	0/1226	0.44	0/1658
1	WD	0.25	0/1244	0.43	0/1683
1	XA	0.24	0/1226	0.41	0/1658
1	XB	0.25	0/1231	0.41	0/1665
1	XC	0.26	0/1226	0.44	0/1658
1	XD	0.25	0/1244	0.43	0/1683
1	YA	0.24	0/1226	0.41	0/1658
1	YB	0.25	0/1231	0.41	0/1665
1	YC	0.26	0/1226	0.44	0/1658
1	YD	0.25	0/1244	0.43	0/1683
1	ZA	0.24	0/1226	0.41	0/1658
1	ZB	0.25	0/1231	0.41	0/1665
1	ZC	0.26	0/1226	0.44	0/1658
1	ZD	0.25	0/1244	0.43	0/1683
1	aA	0.24	0/1226	0.41	0/1658
1	aB	0.25	0/1231	0.41	0/1665
1	aC	0.26	0/1226	0.44	0/1658
1	aD	0.25	0/1244	0.43	0/1683
1	bA	0.24	0/1226	0.41	0/1658
1	bB	0.25	0/1231	0.41	0/1665
1	bC	0.26	0/1226	0.44	0/1658
1	bD	0.25	0/1244	0.43	0/1683
1	cA	0.24	0/1226	0.41	0/1658
1	cB	0.25	0/1231	0.41	0/1665
1	cC	0.26	0/1226	0.44	0/1658
1	cD	0.25	0/1244	0.43	0/1683
1	dA	0.24	0/1226	0.41	0/1658
1	dB	0.25	0/1231	0.41	0/1665
1	dC	0.26	0/1226	0.44	0/1658
1	dD	0.25	0/1244	0.43	0/1683
1	eA	0.24	0/1226	0.41	0/1658
1	eB	0.25	0/1231	0.41	0/1665
1	eC	0.26	0/1226	0.44	0/1658
1	eD	0.25	0/1244	0.43	0/1683
1	fA	0.24	0/1226	0.41	0/1658
1	fB	0.25	0/1231	0.41	0/1665
1	fC	0.26	0/1226	0.44	0/1658
1	fD	0.25	0/1244	0.42	0/1683
1	gA	0.24	0/1226	0.41	0/1658
1	gB	0.25	0/1231	0.41	0/1665
1	gC	0.26	0/1226	0.44	0/1658

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	gD	0.25	0/1244	0.43	0/1683
1	hA	0.24	0/1226	0.41	0/1658
1	hB	0.25	0/1231	0.41	0/1665
1	hC	0.26	0/1226	0.44	0/1658
1	hD	0.25	0/1244	0.43	0/1683
1	iA	0.24	0/1226	0.41	0/1658
1	iB	0.25	0/1231	0.41	0/1665
1	iC	0.26	0/1226	0.44	0/1658
1	iD	0.25	0/1244	0.43	0/1683
1	jA	0.24	0/1226	0.41	0/1658
1	jB	0.25	0/1231	0.41	0/1665
1	jC	0.26	0/1226	0.44	0/1658
1	jD	0.25	0/1244	0.43	0/1683
1	kA	0.24	0/1226	0.41	0/1658
1	kB	0.25	0/1231	0.41	0/1665
1	kC	0.26	0/1226	0.44	0/1658
1	kD	0.25	0/1244	0.43	0/1683
1	lA	0.24	0/1226	0.41	0/1658
1	lB	0.25	0/1231	0.41	0/1665
1	lC	0.26	0/1226	0.44	0/1658
1	lD	0.25	0/1244	0.43	0/1683
1	mA	0.24	0/1226	0.41	0/1658
1	mB	0.25	0/1231	0.41	0/1665
1	mC	0.26	0/1226	0.44	0/1658
1	mD	0.25	0/1244	0.43	0/1683
1	nA	0.24	0/1226	0.41	0/1658
1	nB	0.25	0/1231	0.41	0/1665
1	nC	0.26	0/1226	0.44	0/1658
1	nD	0.25	0/1244	0.43	0/1683
1	oA	0.24	0/1226	0.41	0/1658
1	oB	0.25	0/1231	0.41	0/1665
1	oC	0.26	0/1226	0.44	0/1658
1	oD	0.25	0/1244	0.43	0/1683
1	pA	0.24	0/1226	0.41	0/1658
1	pB	0.25	0/1231	0.41	0/1665
1	pC	0.26	0/1226	0.44	0/1658
1	pD	0.25	0/1244	0.43	0/1683
1	qA	0.24	0/1226	0.41	0/1658
1	qB	0.25	0/1231	0.41	0/1665
1	qC	0.26	0/1226	0.44	0/1658
1	qD	0.25	0/1244	0.43	0/1683
1	rA	0.24	0/1226	0.41	0/1658
1	rB	0.25	0/1231	0.41	0/1665

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	rC	0.26	0/1226	0.44	0/1658
1	rD	0.25	0/1244	0.43	0/1683
1	sA	0.24	0/1226	0.41	0/1658
1	sB	0.25	0/1231	0.41	0/1665
1	sC	0.26	0/1226	0.44	0/1658
1	sD	0.25	0/1244	0.43	0/1683
1	tA	0.24	0/1226	0.41	0/1658
1	tB	0.25	0/1231	0.41	0/1665
1	tC	0.26	0/1226	0.44	0/1658
1	tD	0.25	0/1244	0.43	0/1683
1	uA	0.24	0/1226	0.41	0/1658
1	uB	0.25	0/1231	0.41	0/1665
1	uC	0.26	0/1226	0.44	0/1658
1	uD	0.25	0/1244	0.43	0/1683
1	vA	0.24	0/1226	0.41	0/1658
1	vB	0.25	0/1231	0.41	0/1665
1	vC	0.26	0/1226	0.44	0/1658
1	vD	0.25	0/1244	0.43	0/1683
1	wA	0.24	0/1226	0.41	0/1658
1	wB	0.25	0/1231	0.41	0/1665
1	wC	0.26	0/1226	0.44	0/1658
1	wD	0.25	0/1244	0.42	0/1683
1	xA	0.24	0/1226	0.41	0/1658
1	xB	0.25	0/1231	0.41	0/1665
1	xC	0.26	0/1226	0.44	0/1658
1	xD	0.25	0/1244	0.43	0/1683
1	yA	0.24	0/1226	0.41	0/1658
1	yB	0.25	0/1231	0.41	0/1665
1	yC	0.26	0/1226	0.44	0/1658
1	yD	0.25	0/1244	0.43	0/1683
1	zA	0.24	0/1226	0.41	0/1658
1	zB	0.25	0/1231	0.41	0/1665
1	zC	0.26	0/1226	0.44	0/1658
1	zD	0.25	0/1244	0.42	0/1683
All	All	0.25	0/295620	0.42	0/399840

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0A	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	0B	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	0C	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	0D	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	1A	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	1B	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	1C	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	1D	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	2A	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	2B	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	2C	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	2D	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	3A	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	3B	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	3C	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	3D	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	4A	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	4B	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	4C	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	4D	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	5A	155/197 (79%)	150 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5B	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	5C	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	5D	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	6A	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	6B	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	6C	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	6D	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	7A	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	7B	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	7C	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	7D	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	AA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	AB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	AC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	AD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	BA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	BB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	BC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	BD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	CA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	CB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	CC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	CD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	DA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	DB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	DC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	DD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	EA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	EB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	EC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	ED	157/197 (80%)	151 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	FB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	FC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	FD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	GA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	GB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	GC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	GD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	HA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	HB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	HC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	HD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	IA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	IB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	IC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	ID	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	JA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	JB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	JC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	JD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	KA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	KB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	KC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	KD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	LA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	LB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	LC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	LD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	MA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	MB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	MC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	MD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	NA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	NB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	NC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	ND	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	OA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	OB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	OC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	OD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	PA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	PB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	PC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	PD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	QA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	QB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	QC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	QD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	RA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	RB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	RC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	RD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	SA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	SB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	SC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	SD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	TA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	TB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	TC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	TD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	UA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	UB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	UD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	VA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	VB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	VC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	VD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	WA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	WB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	WC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	WD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	XA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	XB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	XC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	XD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	YA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	YB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	YC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	YD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	ZA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	ZB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	ZC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	ZD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	aA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	aB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	aC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	aD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	bA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	bB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	bC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	bD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	cA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	cB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	cC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	cD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	dA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	dB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	dC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	dD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	eA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	eB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	eC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	eD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	fA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	fB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	fC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	fD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	gA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	gB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	gC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	gD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	hA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	hB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	hC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	hD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	iA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	iB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	iC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	iD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	jA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	jB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	jC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	jD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	kA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	kB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	kC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	kD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	lA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	lB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	lC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	lD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	mA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	mB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	mC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	mD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	nA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	nB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	nC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	nD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	oA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	oB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	oC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	oD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	pA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	pB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	pC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	pD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	qA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	qB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	qC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	qD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	rA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	rB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	rC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	rD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	sA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	sB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	sC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	sD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	tA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	tB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	tC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	tD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	uA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	uB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	uC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	uD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	vA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	vB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	vC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	vD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	wA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	wB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	wC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	wD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	xA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	xB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	xC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	xD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	yA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	yB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100
1	yC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	yD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
1	zA	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
1	zB	156/197 (79%)	153 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	zC	155/197 (79%)	153 (99%)	2 (1%)	0	100	100
1	zD	157/197 (80%)	151 (96%)	6 (4%)	0	100	100
All	All	37380/47280 (79%)	36420 (97%)	960 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	0A	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	0B	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	0C	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	0D	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	1A	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	1B	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	1C	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	1D	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	2A	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	2B	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	2C	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	2D	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	3A	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	3B	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	3C	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	3D	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	4A	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	4B	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	4C	125/150 (83%)	120 (96%)	5 (4%)	31	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4D	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	5A	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	5B	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	5C	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	5D	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	6A	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	6B	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	6C	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	6D	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	7A	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	7B	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	7C	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	7D	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	AA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	AB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	AC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	AD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	BA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	BB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	BC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	BD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	CA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	CB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	CC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	CD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	DA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	DB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	DC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	DD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	EA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	EB	125/150 (83%)	123 (98%)	2 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	ED	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	FA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	FB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	FC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	FD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	GA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	GB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	GC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	GD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	HA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	HB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	HC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	HD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	IA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	IB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	IC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	ID	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	JA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	JB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	JC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	JD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	KA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	KB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	KC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	KD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	LA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	LB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	LC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	LD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	MA	125/150 (83%)	121 (97%)	4 (3%)	39	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	MB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	MC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	MD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	NA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	NB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	NC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	ND	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	OA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	OB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	OC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	OD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	PA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	PB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	PC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	PD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	QA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	QB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	QC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	QD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	RA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	RB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	RC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	RD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	SA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	SB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	SC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	SD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	TA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	TB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	TC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	TD	126/150 (84%)	124 (98%)	2 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	UB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	UC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	UD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	VA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	VB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	VC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	VD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	WA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	WB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	WC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	WD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	XA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	XB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	XC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	XD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	YA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	YB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	YC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	YD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	ZA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	ZB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	ZC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	ZD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	aA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	aB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	aC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	aD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	bA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	bB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	bC	125/150 (83%)	120 (96%)	5 (4%)	31	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	bD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	cA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	cB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	cC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	cD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	dA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	dB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	dC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	dD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	eA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	eB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	eC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	eD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	fA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	fB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	fC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	fD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	gA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	gB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	gC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	gD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	hA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	hB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	hC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	hD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	iA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	iB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	iC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	iD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	jA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	jB	125/150 (83%)	123 (98%)	2 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	jC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	jD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	kA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	kB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	kC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	kD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	lA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	lB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	lC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	lD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	mA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	mB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	mC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	mD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	nA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	nB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	nC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	nD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	oA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	oB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	oC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	oD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	pA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	pB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	pC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	pD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	qA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	qB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	qC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	qD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	rA	125/150 (83%)	121 (97%)	4 (3%)	39	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	rB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	rC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	rD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	sA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	sB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	sC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	sD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	tA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	tB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	tC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	tD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	uA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	uB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	uC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	uD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	vA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	vB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	vC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	vD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	wA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	wB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	wC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	wD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	xA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	xB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	xC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	xD	126/150 (84%)	124 (98%)	2 (2%)	62	79
1	yA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	yB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	yC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	yD	126/150 (84%)	124 (98%)	2 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	zA	125/150 (83%)	121 (97%)	4 (3%)	39	61
1	zB	125/150 (83%)	123 (98%)	2 (2%)	62	79
1	zC	125/150 (83%)	120 (96%)	5 (4%)	31	55
1	zD	126/150 (84%)	124 (98%)	2 (2%)	62	79
All	All	30060/36000 (84%)	29280 (97%)	780 (3%)	49	66

All (780) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	105	HIS
1	AA	127	ARG
1	AA	174	VAL
1	AA	183	GLU
1	AB	73	GLU
1	AB	177	ASP
1	AC	50	LEU
1	AC	73	GLU
1	AC	106	HIS
1	AC	141	ASP
1	AC	183	GLU
1	AD	53	GLU
1	AD	73	GLU
1	BA	105	HIS
1	BA	127	ARG
1	BA	174	VAL
1	BA	183	GLU
1	BB	73	GLU
1	BB	177	ASP
1	BC	50	LEU
1	BC	73	GLU
1	BC	106	HIS
1	BC	141	ASP
1	BC	183	GLU
1	BD	53	GLU
1	BD	73	GLU
1	CA	105	HIS
1	CA	127	ARG
1	CA	174	VAL
1	CA	183	GLU
1	CB	73	GLU
1	CB	177	ASP

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Mol	Chain	Res	Type
1	CC	50	LEU
1	CC	73	GLU
1	CC	106	HIS
1	CC	141	ASP
1	CC	183	GLU
1	CD	53	GLU
1	CD	73	GLU
1	DA	105	HIS
1	DA	127	ARG
1	DA	174	VAL
1	DA	183	GLU
1	DB	73	GLU
1	DB	177	ASP
1	DC	50	LEU
1	DC	73	GLU
1	DC	106	HIS
1	DC	141	ASP
1	DC	183	GLU
1	DD	53	GLU
1	DD	73	GLU
1	EA	105	HIS
1	EA	127	ARG
1	EA	174	VAL
1	EA	183	GLU
1	EB	73	GLU
1	EB	177	ASP
1	EC	50	LEU
1	EC	73	GLU
1	EC	106	HIS
1	EC	141	ASP
1	EC	183	GLU
1	ED	53	GLU
1	ED	73	GLU
1	FA	105	HIS
1	FA	127	ARG
1	FA	174	VAL
1	FA	183	GLU
1	FB	73	GLU
1	FB	177	ASP
1	FC	50	LEU
1	FC	73	GLU
1	FC	106	HIS

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Mol	Chain	Res	Type
1	FC	141	ASP
1	FC	183	GLU
1	FD	53	GLU
1	FD	73	GLU
1	GA	105	HIS
1	GA	127	ARG
1	GA	174	VAL
1	GA	183	GLU
1	GB	73	GLU
1	GB	177	ASP
1	GC	50	LEU
1	GC	73	GLU
1	GC	106	HIS
1	GC	141	ASP
1	GC	183	GLU
1	GD	53	GLU
1	GD	73	GLU
1	HA	105	HIS
1	HA	127	ARG
1	HA	174	VAL
1	HA	183	GLU
1	HB	73	GLU
1	HB	177	ASP
1	HC	50	LEU
1	HC	73	GLU
1	HC	106	HIS
1	HC	141	ASP
1	HC	183	GLU
1	HD	53	GLU
1	HD	73	GLU
1	IA	105	HIS
1	IA	127	ARG
1	IA	174	VAL
1	IA	183	GLU
1	IB	73	GLU
1	IB	177	ASP
1	IC	50	LEU
1	IC	73	GLU
1	IC	106	HIS
1	IC	141	ASP
1	IC	183	GLU
1	ID	53	GLU

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Mol	Chain	Res	Type
1	ID	73	GLU
1	5A	105	HIS
1	5A	127	ARG
1	5A	174	VAL
1	5A	183	GLU
1	5B	73	GLU
1	5B	177	ASP
1	5C	50	LEU
1	5C	73	GLU
1	5C	106	HIS
1	5C	141	ASP
1	5C	183	GLU
1	5D	53	GLU
1	5D	73	GLU
1	JA	105	HIS
1	JA	127	ARG
1	JA	174	VAL
1	JA	183	GLU
1	JB	73	GLU
1	JB	177	ASP
1	JC	50	LEU
1	JC	73	GLU
1	JC	106	HIS
1	JC	141	ASP
1	JC	183	GLU
1	JD	53	GLU
1	JD	73	GLU
1	KA	105	HIS
1	KA	127	ARG
1	KA	174	VAL
1	KA	183	GLU
1	KB	73	GLU
1	KB	177	ASP
1	KC	50	LEU
1	KC	73	GLU
1	KC	106	HIS
1	KC	141	ASP
1	KC	183	GLU
1	KD	53	GLU
1	KD	73	GLU
1	LA	105	HIS
1	LA	127	ARG

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Mol	Chain	Res	Type
1	LA	174	VAL
1	LA	183	GLU
1	LB	73	GLU
1	LB	177	ASP
1	LC	50	LEU
1	LC	73	GLU
1	LC	106	HIS
1	LC	141	ASP
1	LC	183	GLU
1	LD	53	GLU
1	LD	73	GLU
1	MA	105	HIS
1	MA	127	ARG
1	MA	174	VAL
1	MA	183	GLU
1	MB	73	GLU
1	MB	177	ASP
1	MC	50	LEU
1	MC	73	GLU
1	MC	106	HIS
1	MC	141	ASP
1	MC	183	GLU
1	MD	53	GLU
1	MD	73	GLU
1	NA	105	HIS
1	NA	127	ARG
1	NA	174	VAL
1	NA	183	GLU
1	NB	73	GLU
1	NB	177	ASP
1	NC	50	LEU
1	NC	73	GLU
1	NC	106	HIS
1	NC	141	ASP
1	NC	183	GLU
1	ND	53	GLU
1	ND	73	GLU
1	OA	105	HIS
1	OA	127	ARG
1	OA	174	VAL
1	OA	183	GLU
1	OB	73	GLU

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Mol	Chain	Res	Type
1	OB	177	ASP
1	OC	50	LEU
1	OC	73	GLU
1	OC	106	HIS
1	OC	141	ASP
1	OC	183	GLU
1	OD	53	GLU
1	OD	73	GLU
1	PA	105	HIS
1	PA	127	ARG
1	PA	174	VAL
1	PA	183	GLU
1	PB	73	GLU
1	PB	177	ASP
1	PC	50	LEU
1	PC	73	GLU
1	PC	106	HIS
1	PC	141	ASP
1	PC	183	GLU
1	PD	53	GLU
1	PD	73	GLU
1	6A	105	HIS
1	6A	127	ARG
1	6A	174	VAL
1	6A	183	GLU
1	6B	73	GLU
1	6B	177	ASP
1	6C	50	LEU
1	6C	73	GLU
1	6C	106	HIS
1	6C	141	ASP
1	6C	183	GLU
1	6D	53	GLU
1	6D	73	GLU
1	7A	105	HIS
1	7A	127	ARG
1	7A	174	VAL
1	7A	183	GLU
1	7B	73	GLU
1	7B	177	ASP
1	7C	50	LEU
1	7C	73	GLU

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Mol	Chain	Res	Type
1	7C	106	HIS
1	7C	141	ASP
1	7C	183	GLU
1	7D	53	GLU
1	7D	73	GLU
1	QA	105	HIS
1	QA	127	ARG
1	QA	174	VAL
1	QA	183	GLU
1	QB	73	GLU
1	QB	177	ASP
1	QC	50	LEU
1	QC	73	GLU
1	QC	106	HIS
1	QC	141	ASP
1	QC	183	GLU
1	QD	53	GLU
1	QD	73	GLU
1	RA	105	HIS
1	RA	127	ARG
1	RA	174	VAL
1	RA	183	GLU
1	RB	73	GLU
1	RB	177	ASP
1	RC	50	LEU
1	RC	73	GLU
1	RC	106	HIS
1	RC	141	ASP
1	RC	183	GLU
1	RD	53	GLU
1	RD	73	GLU
1	SA	105	HIS
1	SA	127	ARG
1	SA	174	VAL
1	SA	183	GLU
1	SB	73	GLU
1	SB	177	ASP
1	SC	50	LEU
1	SC	73	GLU
1	SC	106	HIS
1	SC	141	ASP
1	SC	183	GLU

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Mol	Chain	Res	Type
1	SD	53	GLU
1	SD	73	GLU
1	TA	105	HIS
1	TA	127	ARG
1	TA	174	VAL
1	TA	183	GLU
1	TB	73	GLU
1	TB	177	ASP
1	TC	50	LEU
1	TC	73	GLU
1	TC	106	HIS
1	TC	141	ASP
1	TC	183	GLU
1	TD	53	GLU
1	TD	73	GLU
1	UA	105	HIS
1	UA	127	ARG
1	UA	174	VAL
1	UA	183	GLU
1	UB	73	GLU
1	UB	177	ASP
1	UC	50	LEU
1	UC	73	GLU
1	UC	106	HIS
1	UC	141	ASP
1	UC	183	GLU
1	UD	53	GLU
1	UD	73	GLU
1	VA	105	HIS
1	VA	127	ARG
1	VA	174	VAL
1	VA	183	GLU
1	VB	73	GLU
1	VB	177	ASP
1	VC	50	LEU
1	VC	73	GLU
1	VC	106	HIS
1	VC	141	ASP
1	VC	183	GLU
1	VD	53	GLU
1	VD	73	GLU
1	WA	105	HIS

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Mol	Chain	Res	Type
1	WA	127	ARG
1	WA	174	VAL
1	WA	183	GLU
1	WB	73	GLU
1	WB	177	ASP
1	WC	50	LEU
1	WC	73	GLU
1	WC	106	HIS
1	WC	141	ASP
1	WC	183	GLU
1	WD	53	GLU
1	WD	73	GLU
1	XA	105	HIS
1	XA	127	ARG
1	XA	174	VAL
1	XA	183	GLU
1	XB	73	GLU
1	XB	177	ASP
1	XC	50	LEU
1	XC	73	GLU
1	XC	106	HIS
1	XC	141	ASP
1	XC	183	GLU
1	XD	53	GLU
1	XD	73	GLU
1	YA	105	HIS
1	YA	127	ARG
1	YA	174	VAL
1	YA	183	GLU
1	YB	73	GLU
1	YB	177	ASP
1	YC	50	LEU
1	YC	73	GLU
1	YC	106	HIS
1	YC	141	ASP
1	YC	183	GLU
1	YD	53	GLU
1	YD	73	GLU
1	ZA	105	HIS
1	ZA	127	ARG
1	ZA	174	VAL
1	ZA	183	GLU

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Mol	Chain	Res	Type
1	ZB	73	GLU
1	ZB	177	ASP
1	ZC	50	LEU
1	ZC	73	GLU
1	ZC	106	HIS
1	ZC	141	ASP
1	ZC	183	GLU
1	ZD	53	GLU
1	ZD	73	GLU
1	aA	105	HIS
1	aA	127	ARG
1	aA	174	VAL
1	aA	183	GLU
1	aB	73	GLU
1	aB	177	ASP
1	aC	50	LEU
1	aC	73	GLU
1	aC	106	HIS
1	aC	141	ASP
1	aC	183	GLU
1	aD	53	GLU
1	aD	73	GLU
1	bA	105	HIS
1	bA	127	ARG
1	bA	174	VAL
1	bA	183	GLU
1	bB	73	GLU
1	bB	177	ASP
1	bC	50	LEU
1	bC	73	GLU
1	bC	106	HIS
1	bC	141	ASP
1	bC	183	GLU
1	bD	53	GLU
1	bD	73	GLU
1	cA	105	HIS
1	cA	127	ARG
1	cA	174	VAL
1	cA	183	GLU
1	cB	73	GLU
1	cB	177	ASP
1	cC	50	LEU

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Mol	Chain	Res	Type
1	cC	73	GLU
1	cC	106	HIS
1	cC	141	ASP
1	cC	183	GLU
1	cD	53	GLU
1	cD	73	GLU
1	dA	105	HIS
1	dA	127	ARG
1	dA	174	VAL
1	dA	183	GLU
1	dB	73	GLU
1	dB	177	ASP
1	dC	50	LEU
1	dC	73	GLU
1	dC	106	HIS
1	dC	141	ASP
1	dC	183	GLU
1	dD	53	GLU
1	dD	73	GLU
1	eA	105	HIS
1	eA	127	ARG
1	eA	174	VAL
1	eA	183	GLU
1	eB	73	GLU
1	eB	177	ASP
1	eC	50	LEU
1	eC	73	GLU
1	eC	106	HIS
1	eC	141	ASP
1	eC	183	GLU
1	eD	53	GLU
1	eD	73	GLU
1	fA	105	HIS
1	fA	127	ARG
1	fA	174	VAL
1	fA	183	GLU
1	fB	73	GLU
1	fB	177	ASP
1	fC	50	LEU
1	fC	73	GLU
1	fC	106	HIS
1	fC	141	ASP

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Mol	Chain	Res	Type
1	fC	183	GLU
1	fD	53	GLU
1	fD	73	GLU
1	gA	105	HIS
1	gA	127	ARG
1	gA	174	VAL
1	gA	183	GLU
1	gB	73	GLU
1	gB	177	ASP
1	gC	50	LEU
1	gC	73	GLU
1	gC	106	HIS
1	gC	141	ASP
1	gC	183	GLU
1	gD	53	GLU
1	gD	73	GLU
1	hA	105	HIS
1	hA	127	ARG
1	hA	174	VAL
1	hA	183	GLU
1	hB	73	GLU
1	hB	177	ASP
1	hC	50	LEU
1	hC	73	GLU
1	hC	106	HIS
1	hC	141	ASP
1	hC	183	GLU
1	hD	53	GLU
1	hD	73	GLU
1	iA	105	HIS
1	iA	127	ARG
1	iA	174	VAL
1	iA	183	GLU
1	iB	73	GLU
1	iB	177	ASP
1	iC	50	LEU
1	iC	73	GLU
1	iC	106	HIS
1	iC	141	ASP
1	iC	183	GLU
1	iD	53	GLU
1	iD	73	GLU

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Mol	Chain	Res	Type
1	jA	105	HIS
1	jA	127	ARG
1	jA	174	VAL
1	jA	183	GLU
1	jB	73	GLU
1	jB	177	ASP
1	jC	50	LEU
1	jC	73	GLU
1	jC	106	HIS
1	jC	141	ASP
1	jC	183	GLU
1	jD	53	GLU
1	jD	73	GLU
1	kA	105	HIS
1	kA	127	ARG
1	kA	174	VAL
1	kA	183	GLU
1	kB	73	GLU
1	kB	177	ASP
1	kC	50	LEU
1	kC	73	GLU
1	kC	106	HIS
1	kC	141	ASP
1	kC	183	GLU
1	kD	53	GLU
1	kD	73	GLU
1	lA	105	HIS
1	lA	127	ARG
1	lA	174	VAL
1	lA	183	GLU
1	lB	73	GLU
1	lB	177	ASP
1	lC	50	LEU
1	lC	73	GLU
1	lC	106	HIS
1	lC	141	ASP
1	lC	183	GLU
1	lD	53	GLU
1	lD	73	GLU
1	mA	105	HIS
1	mA	127	ARG
1	mA	174	VAL

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Mol	Chain	Res	Type
1	mA	183	GLU
1	mB	73	GLU
1	mB	177	ASP
1	mC	50	LEU
1	mC	73	GLU
1	mC	106	HIS
1	mC	141	ASP
1	mC	183	GLU
1	mD	53	GLU
1	mD	73	GLU
1	nA	105	HIS
1	nA	127	ARG
1	nA	174	VAL
1	nA	183	GLU
1	nB	73	GLU
1	nB	177	ASP
1	nC	50	LEU
1	nC	73	GLU
1	nC	106	HIS
1	nC	141	ASP
1	nC	183	GLU
1	nD	53	GLU
1	nD	73	GLU
1	oA	105	HIS
1	oA	127	ARG
1	oA	174	VAL
1	oA	183	GLU
1	oB	73	GLU
1	oB	177	ASP
1	oC	50	LEU
1	oC	73	GLU
1	oC	106	HIS
1	oC	141	ASP
1	oC	183	GLU
1	oD	53	GLU
1	oD	73	GLU
1	pA	105	HIS
1	pA	127	ARG
1	pA	174	VAL
1	pA	183	GLU
1	pB	73	GLU
1	pB	177	ASP

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Mol	Chain	Res	Type
1	pC	50	LEU
1	pC	73	GLU
1	pC	106	HIS
1	pC	141	ASP
1	pC	183	GLU
1	pD	53	GLU
1	pD	73	GLU
1	qA	105	HIS
1	qA	127	ARG
1	qA	174	VAL
1	qA	183	GLU
1	qB	73	GLU
1	qB	177	ASP
1	qC	50	LEU
1	qC	73	GLU
1	qC	106	HIS
1	qC	141	ASP
1	qC	183	GLU
1	qD	53	GLU
1	qD	73	GLU
1	rA	105	HIS
1	rA	127	ARG
1	rA	174	VAL
1	rA	183	GLU
1	rB	73	GLU
1	rB	177	ASP
1	rC	50	LEU
1	rC	73	GLU
1	rC	106	HIS
1	rC	141	ASP
1	rC	183	GLU
1	rD	53	GLU
1	rD	73	GLU
1	sA	105	HIS
1	sA	127	ARG
1	sA	174	VAL
1	sA	183	GLU
1	sB	73	GLU
1	sB	177	ASP
1	sC	50	LEU
1	sC	73	GLU
1	sC	106	HIS

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Mol	Chain	Res	Type
1	sC	141	ASP
1	sC	183	GLU
1	sD	53	GLU
1	sD	73	GLU
1	tA	105	HIS
1	tA	127	ARG
1	tA	174	VAL
1	tA	183	GLU
1	tB	73	GLU
1	tB	177	ASP
1	tC	50	LEU
1	tC	73	GLU
1	tC	106	HIS
1	tC	141	ASP
1	tC	183	GLU
1	tD	53	GLU
1	tD	73	GLU
1	uA	105	HIS
1	uA	127	ARG
1	uA	174	VAL
1	uA	183	GLU
1	uB	73	GLU
1	uB	177	ASP
1	uC	50	LEU
1	uC	73	GLU
1	uC	106	HIS
1	uC	141	ASP
1	uC	183	GLU
1	uD	53	GLU
1	uD	73	GLU
1	vA	105	HIS
1	vA	127	ARG
1	vA	174	VAL
1	vA	183	GLU
1	vB	73	GLU
1	vB	177	ASP
1	vC	50	LEU
1	vC	73	GLU
1	vC	106	HIS
1	vC	141	ASP
1	vC	183	GLU
1	vD	53	GLU

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Mol	Chain	Res	Type
1	vD	73	GLU
1	wA	105	HIS
1	wA	127	ARG
1	wA	174	VAL
1	wA	183	GLU
1	wB	73	GLU
1	wB	177	ASP
1	wC	50	LEU
1	wC	73	GLU
1	wC	106	HIS
1	wC	141	ASP
1	wC	183	GLU
1	wD	53	GLU
1	wD	73	GLU
1	xA	105	HIS
1	xA	127	ARG
1	xA	174	VAL
1	xA	183	GLU
1	xB	73	GLU
1	xB	177	ASP
1	xC	50	LEU
1	xC	73	GLU
1	xC	106	HIS
1	xC	141	ASP
1	xC	183	GLU
1	xD	53	GLU
1	xD	73	GLU
1	yA	105	HIS
1	yA	127	ARG
1	yA	174	VAL
1	yA	183	GLU
1	yB	73	GLU
1	yB	177	ASP
1	yC	50	LEU
1	yC	73	GLU
1	yC	106	HIS
1	yC	141	ASP
1	yC	183	GLU
1	yD	53	GLU
1	yD	73	GLU
1	zA	105	HIS
1	zA	127	ARG

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Mol	Chain	Res	Type
1	zA	174	VAL
1	zA	183	GLU
1	zB	73	GLU
1	zB	177	ASP
1	zC	50	LEU
1	zC	73	GLU
1	zC	106	HIS
1	zC	141	ASP
1	zC	183	GLU
1	zD	53	GLU
1	zD	73	GLU
1	0A	105	HIS
1	0A	127	ARG
1	0A	174	VAL
1	0A	183	GLU
1	0B	73	GLU
1	0B	177	ASP
1	0C	50	LEU
1	0C	73	GLU
1	0C	106	HIS
1	0C	141	ASP
1	0C	183	GLU
1	0D	53	GLU
1	0D	73	GLU
1	1A	105	HIS
1	1A	127	ARG
1	1A	174	VAL
1	1A	183	GLU
1	1B	73	GLU
1	1B	177	ASP
1	1C	50	LEU
1	1C	73	GLU
1	1C	106	HIS
1	1C	141	ASP
1	1C	183	GLU
1	1D	53	GLU
1	1D	73	GLU
1	2A	105	HIS
1	2A	127	ARG
1	2A	174	VAL
1	2A	183	GLU
1	2B	73	GLU

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Mol	Chain	Res	Type
1	2B	177	ASP
1	2C	50	LEU
1	2C	73	GLU
1	2C	106	HIS
1	2C	141	ASP
1	2C	183	GLU
1	2D	53	GLU
1	2D	73	GLU
1	3A	105	HIS
1	3A	127	ARG
1	3A	174	VAL
1	3A	183	GLU
1	3B	73	GLU
1	3B	177	ASP
1	3C	50	LEU
1	3C	73	GLU
1	3C	106	HIS
1	3C	141	ASP
1	3C	183	GLU
1	3D	53	GLU
1	3D	73	GLU
1	4A	105	HIS
1	4A	127	ARG
1	4A	174	VAL
1	4A	183	GLU
1	4B	73	GLU
1	4B	177	ASP
1	4C	50	LEU
1	4C	73	GLU
1	4C	106	HIS
1	4C	141	ASP
1	4C	183	GLU
1	4D	53	GLU
1	4D	73	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	HD	79	HIS
1	RD	79	HIS
1	XD	79	HIS
1	YD	79	HIS

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Mol	Chain	Res	Type
1	ZD	79	HIS
1	eD	79	HIS
1	lD	79	HIS
1	oD	79	HIS
1	sD	79	HIS
1	zD	79	HIS

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.

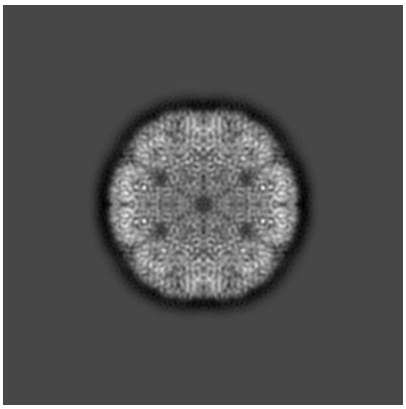
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11634. These allow visual inspection of the internal detail of the map and identification of artifacts.

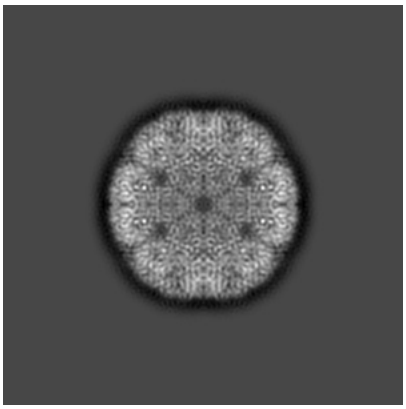
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

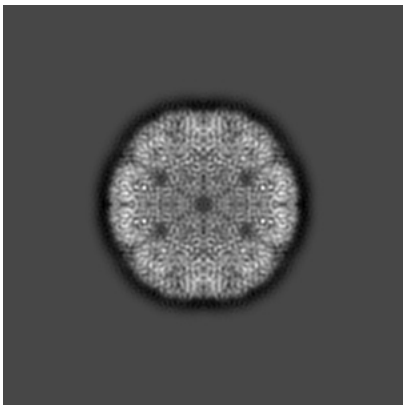
6.1.1 Primary map



X

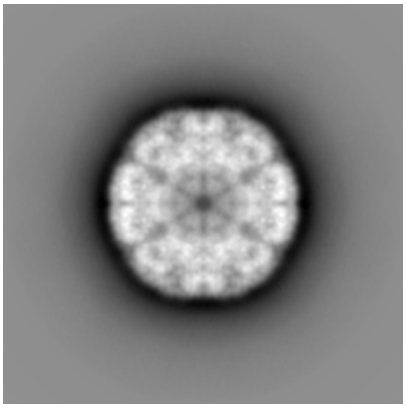


Y

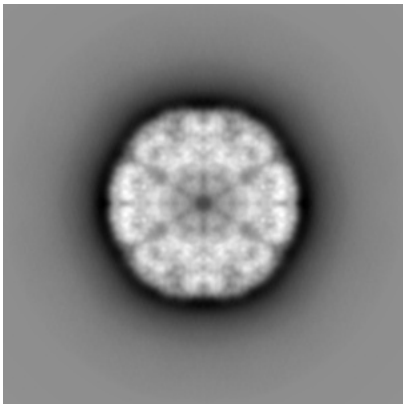


Z

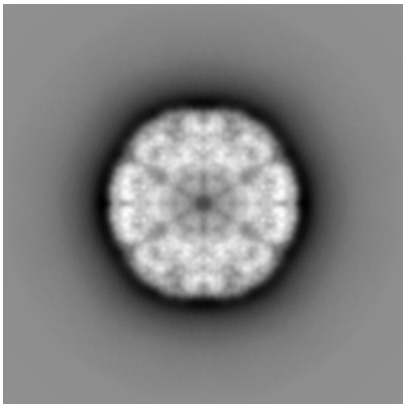
6.1.2 Raw map



X



Y

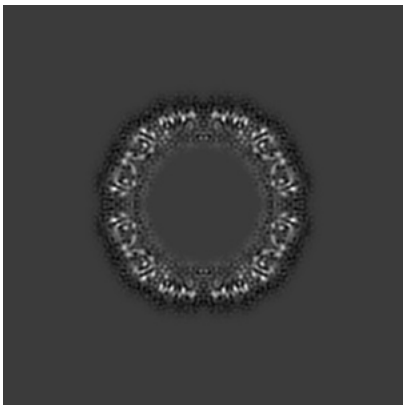


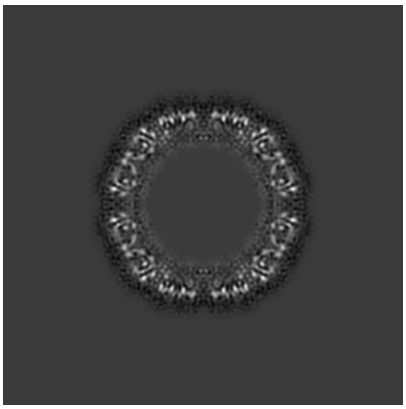
Z

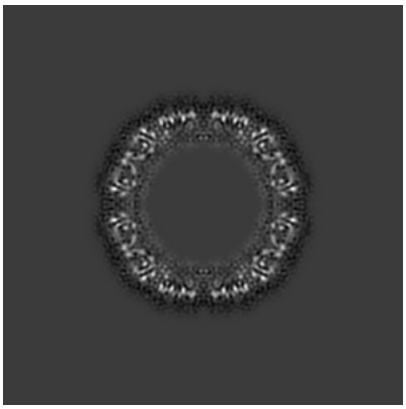
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

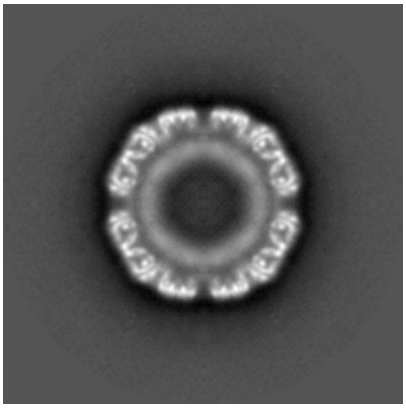
6.2.1 Primary map

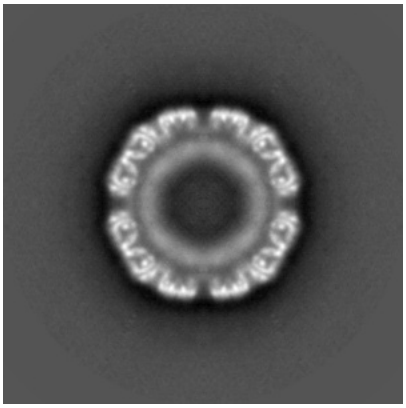

X Index: 180

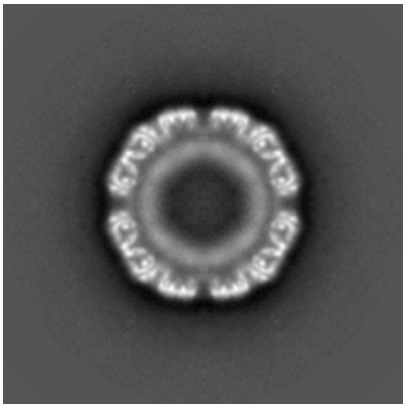

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

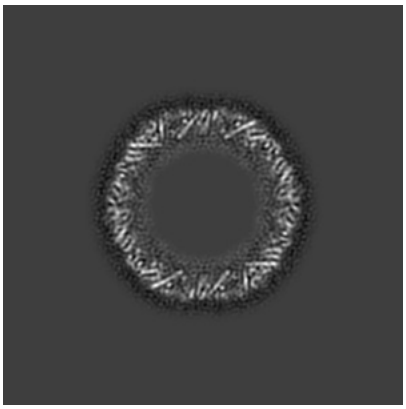

Y Index: 180


Z Index: 180

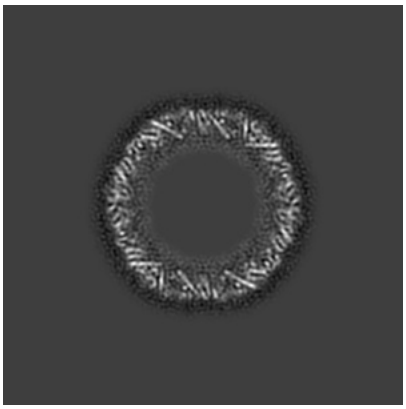
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

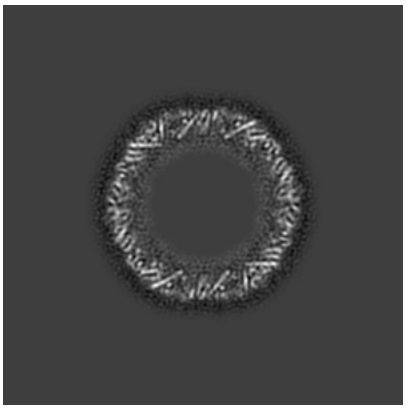
6.3.1 Primary map



X Index: 195

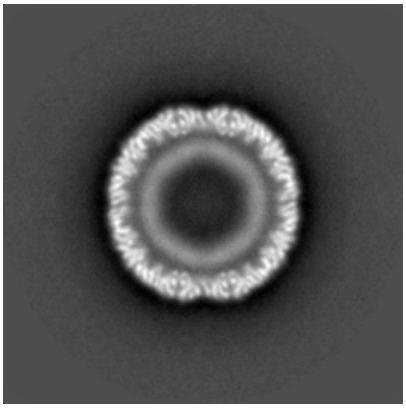


Y Index: 165

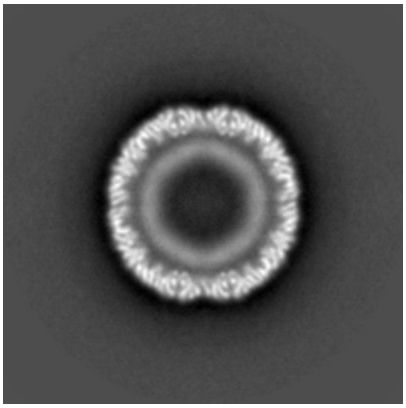


Z Index: 195

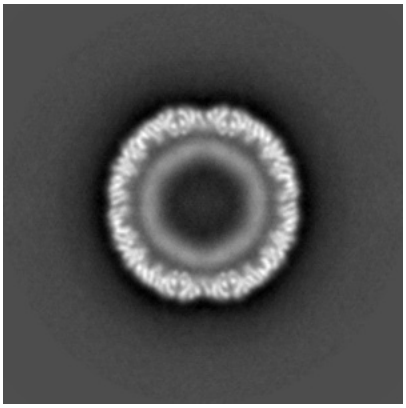
6.3.2 Raw map



X Index: 171



Y Index: 171

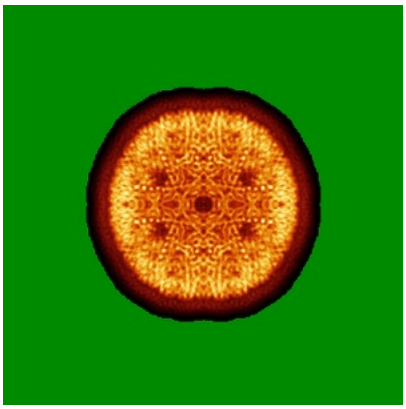


Z Index: 171

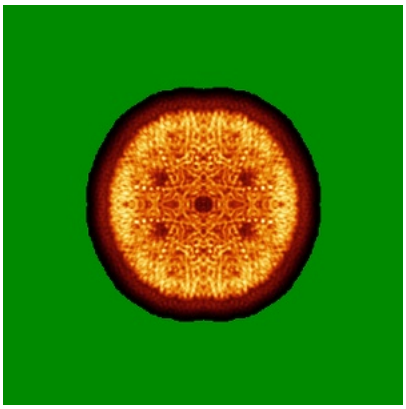
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

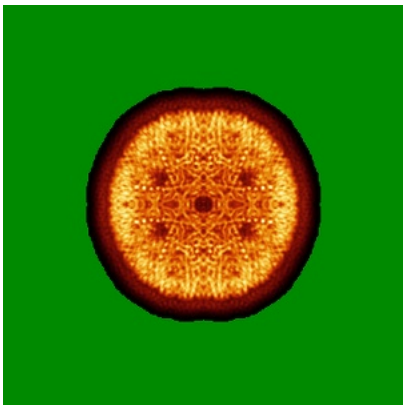
6.4.1 Primary map



X

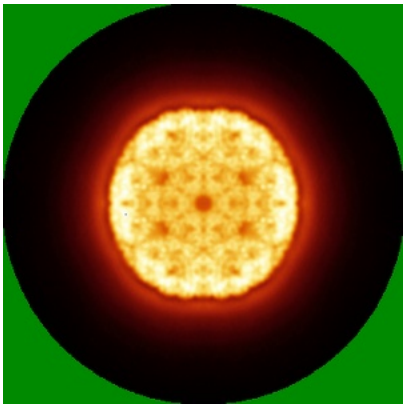


Y

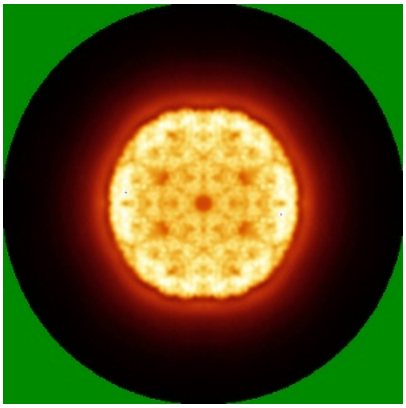


Z

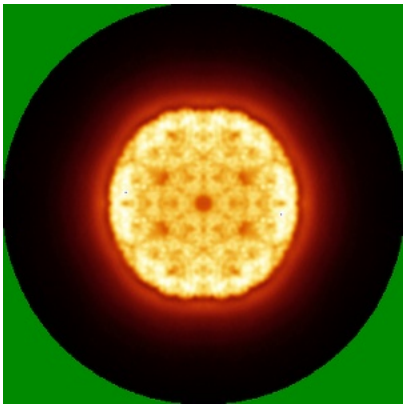
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

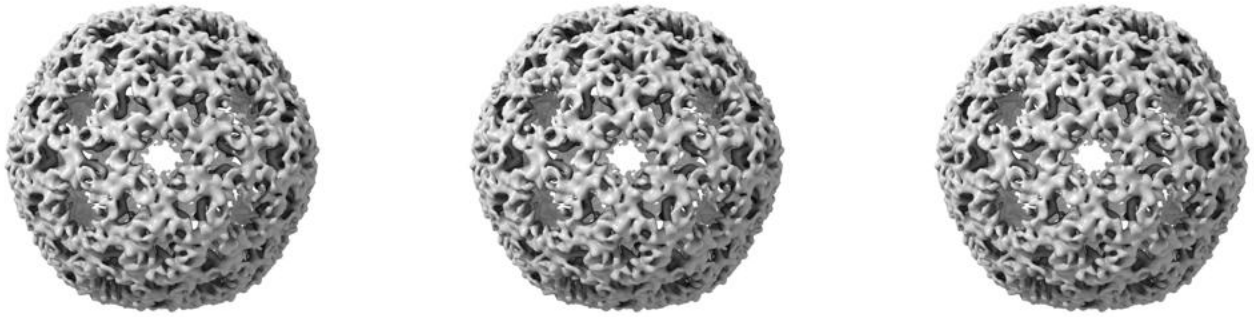
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0509. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

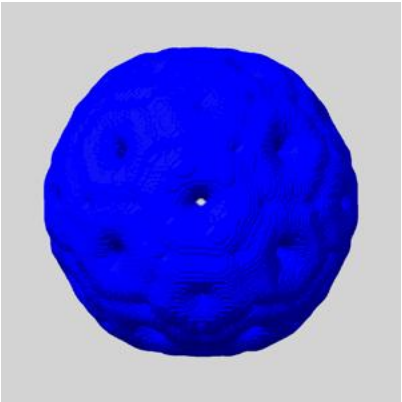
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

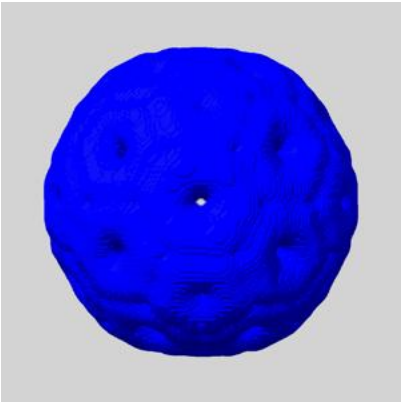
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

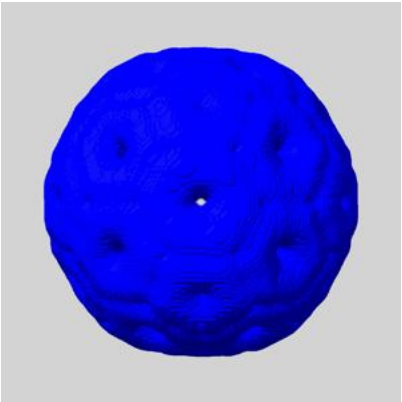
6.6.1 emd_11634_msk_1.map (i)



X



Y

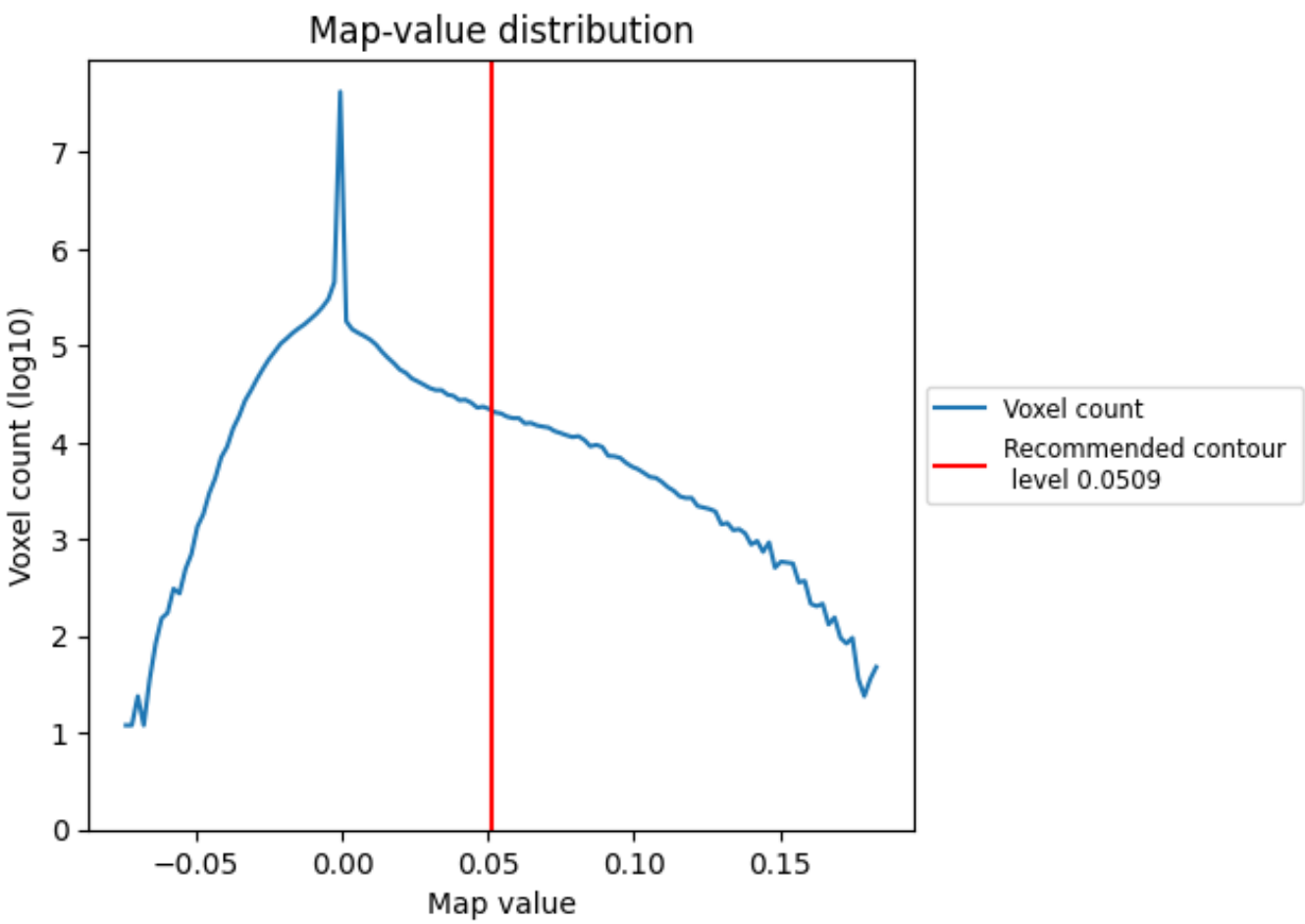


Z

7 Map analysis (i)

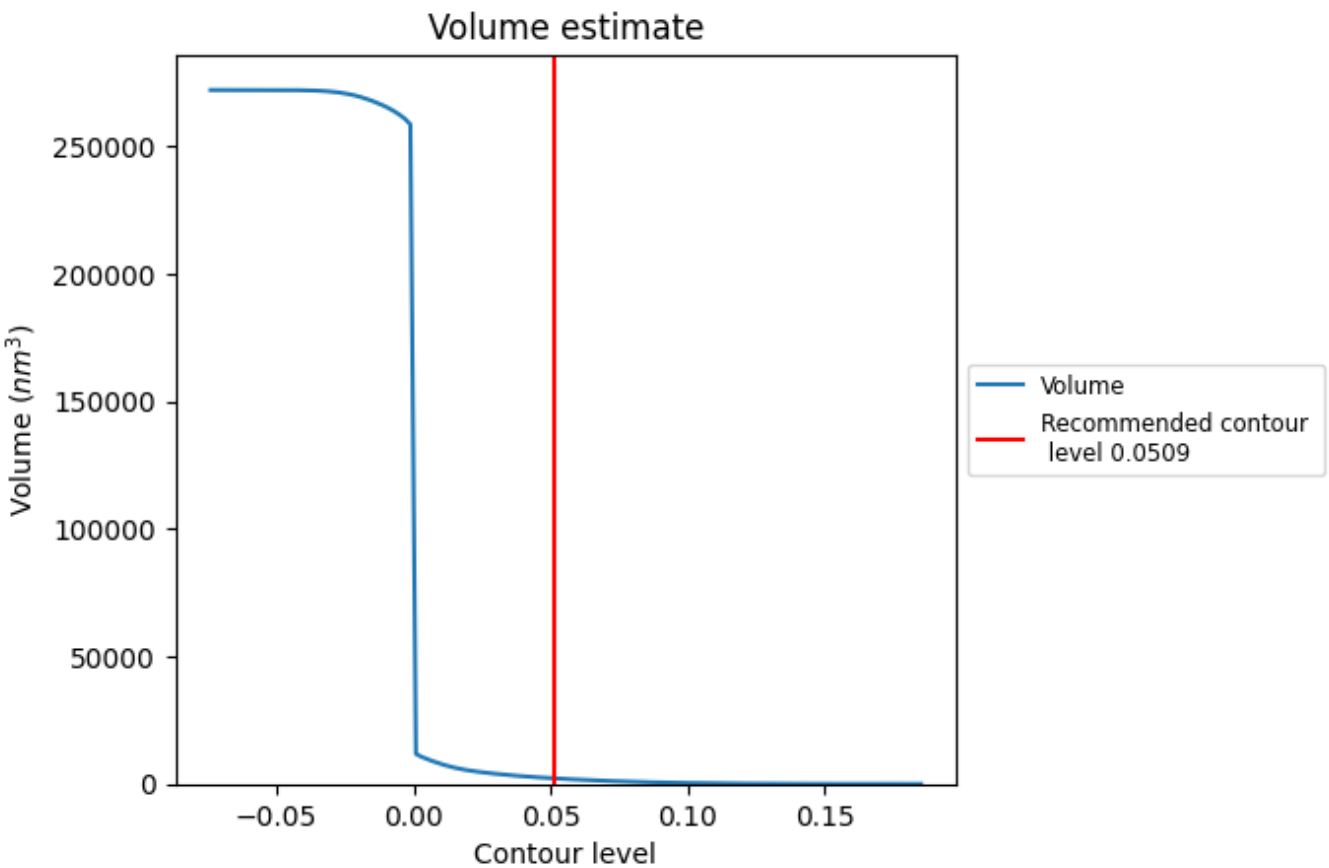
This section contains the results of statistical analysis of the map.

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.

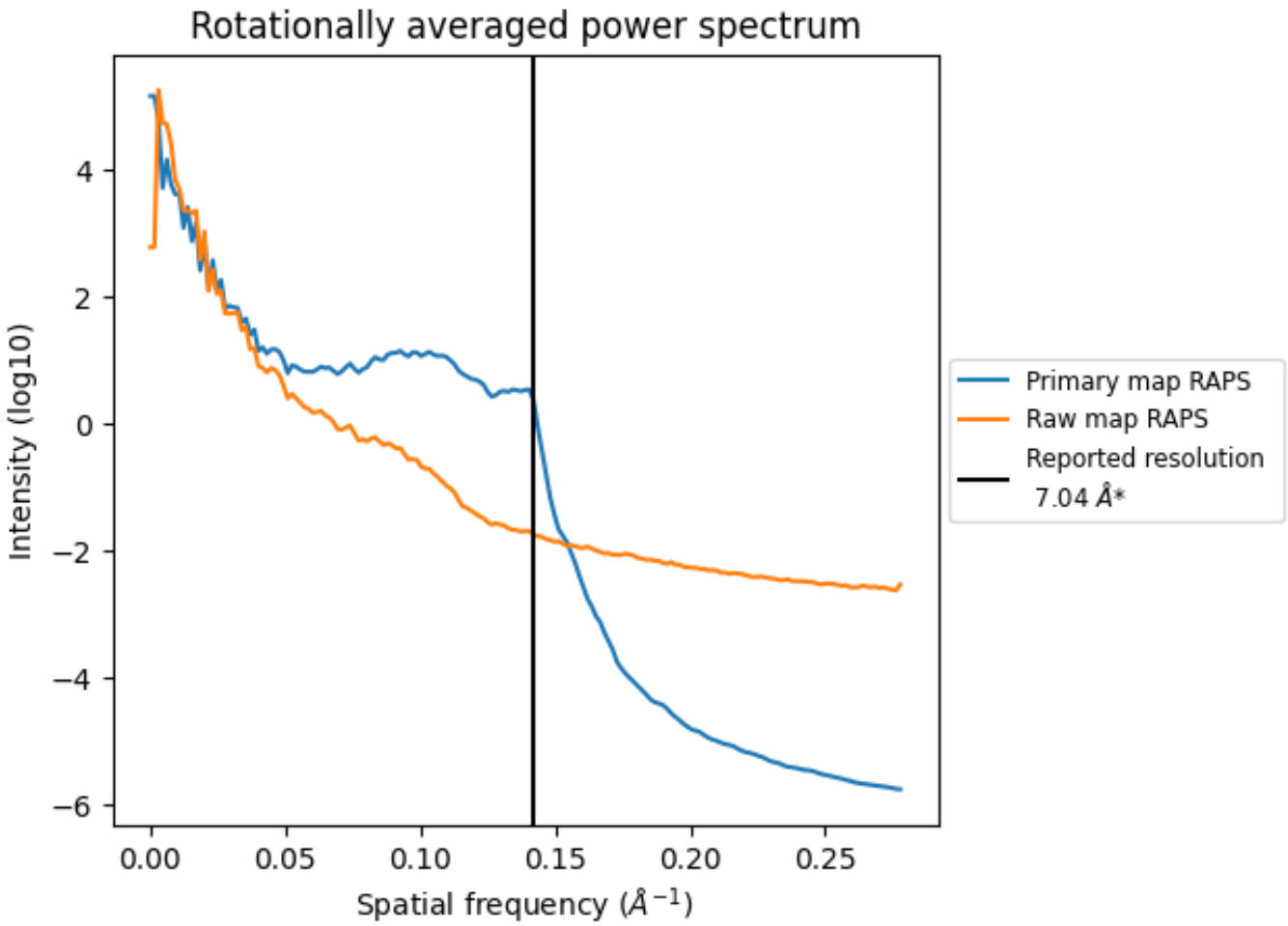
7.2 Volume estimate (i)



The volume at the recommended contour level is 2215 nm^3; this corresponds to an approximate mass of 2001 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)

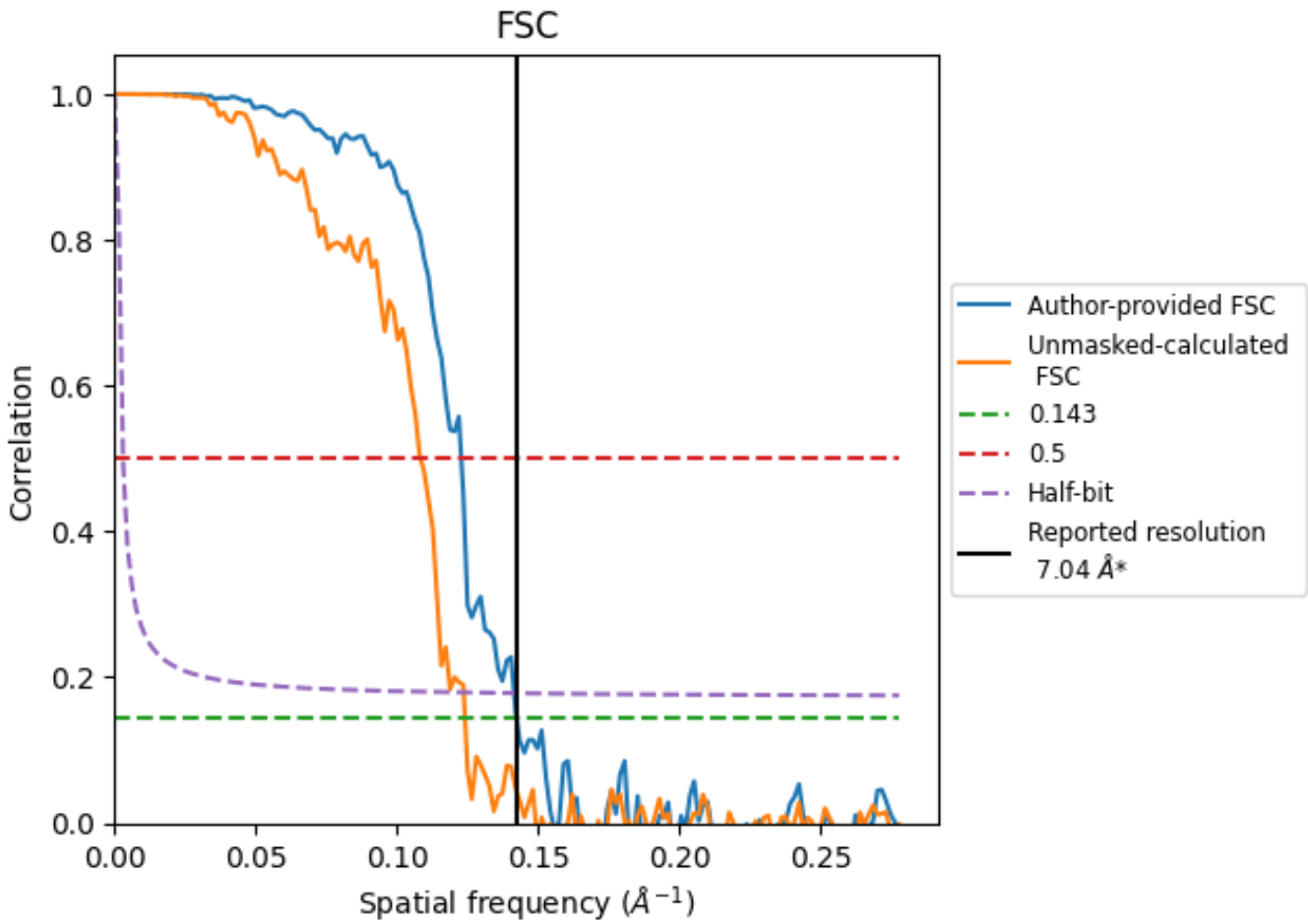


*Reported resolution corresponds to spatial frequency of 0.142 Å^{-1}

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 0.142 Å^{-1}

8.2 Resolution estimates (i)

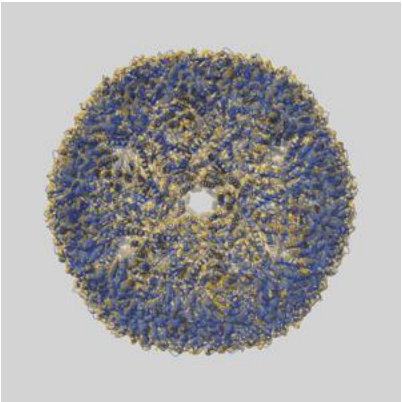
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.04	-	-
Author-provided FSC curve	7.03	8.15	7.07
Unmasked-calculated*	8.06	9.23	8.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.06 differs from the reported value 7.04 by more than 10 %

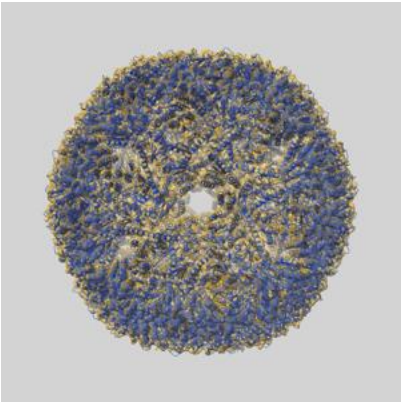
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11634 and PDB model 7A4I. Per-residue inclusion information can be found in section 3 on page 242.

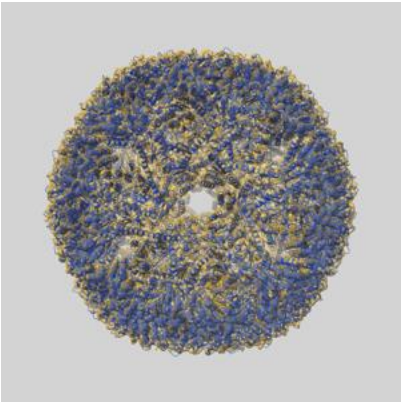
9.1 Map-model overlay (i)



X



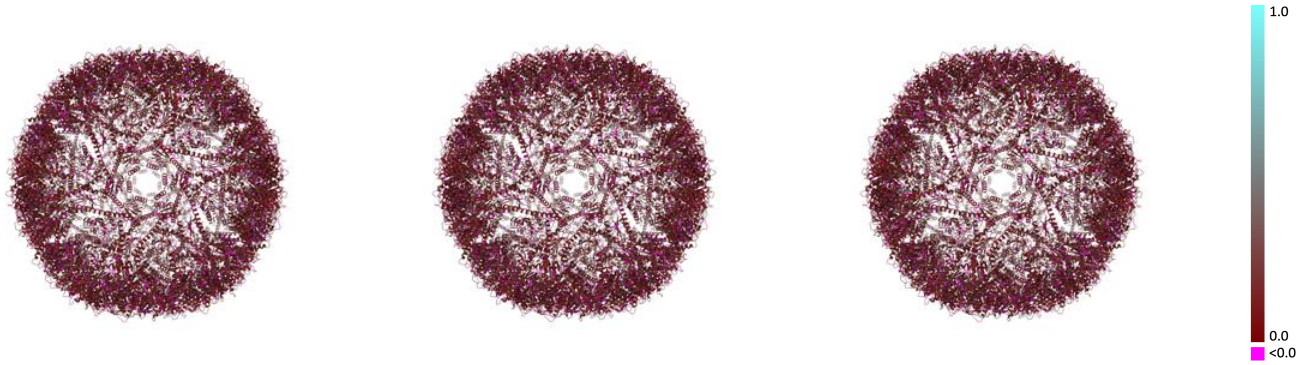
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0509 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.

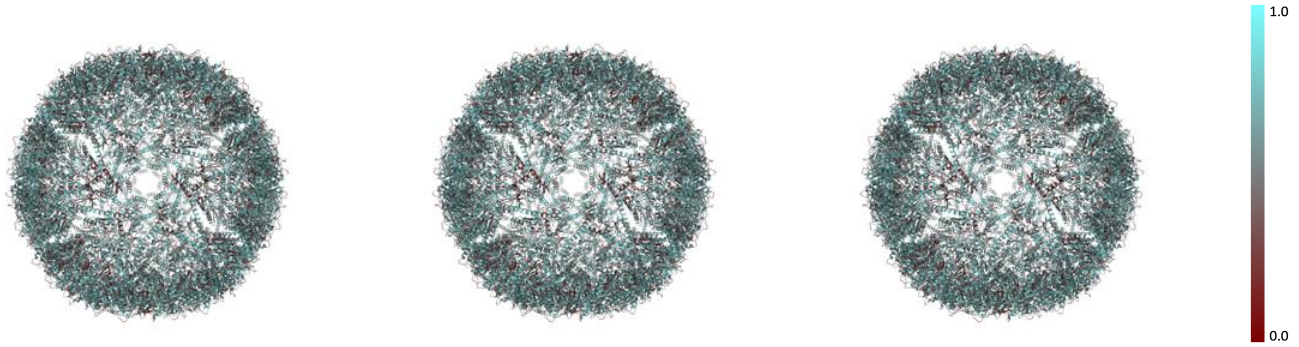
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

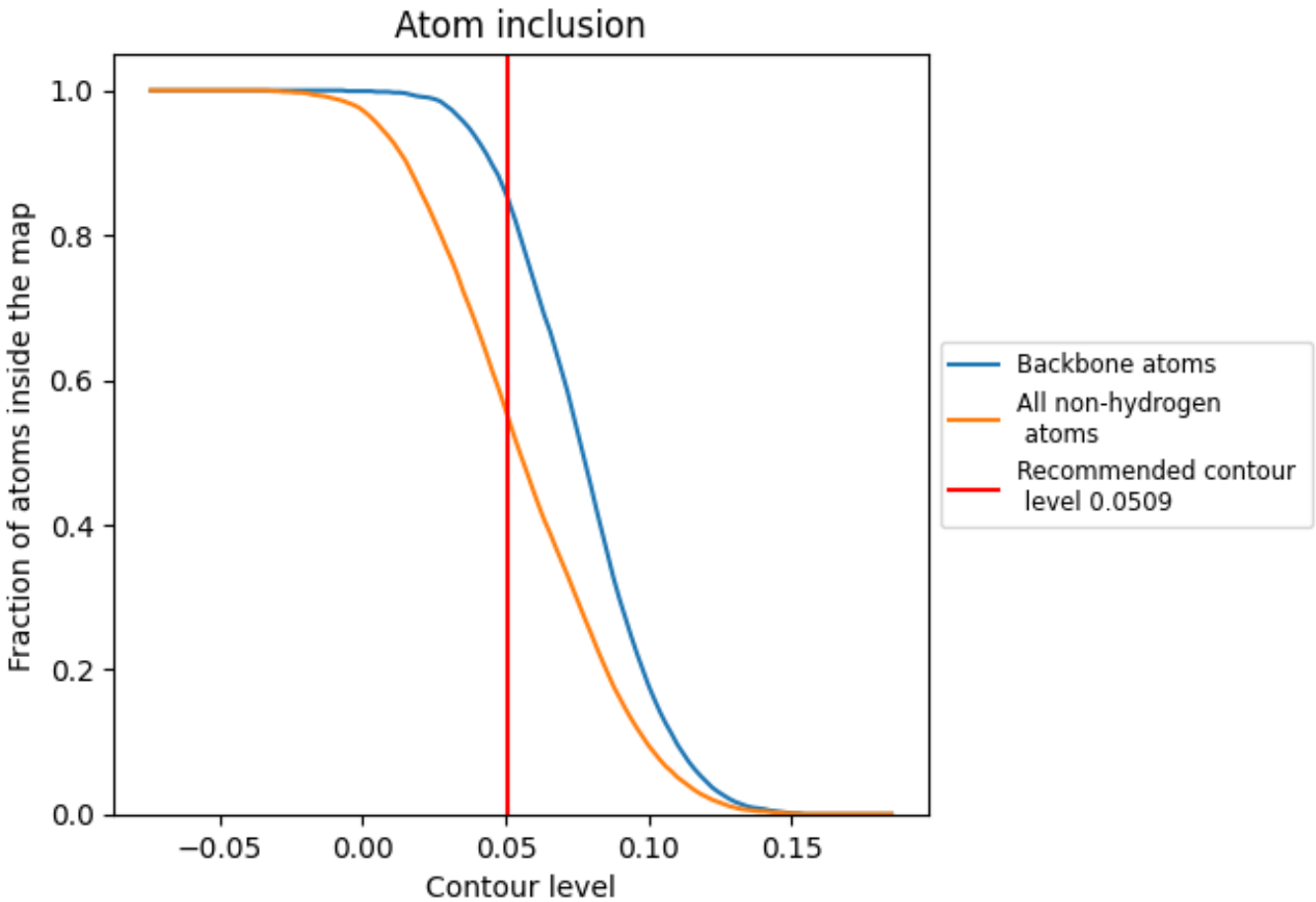
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0509).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 55% 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 (0.0509) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5480	0.1630
0A	0.5500	0.1580
0B	0.5570	0.1710
0C	0.5170	0.1570
0D	0.5610	0.1680
1A	0.5490	0.1540
1B	0.5510	0.1730
1C	0.5130	0.1550
1D	0.5620	0.1630
2A	0.5540	0.1560
2B	0.5630	0.1740
2C	0.5220	0.1590
2D	0.5620	0.1690
3A	0.5550	0.1570
3B	0.5620	0.1780
3C	0.5220	0.1620
3D	0.5590	0.1650
4A	0.5460	0.1560
4B	0.5520	0.1700
4C	0.5090	0.1530
4D	0.5680	0.1640
5A	0.5500	0.1550
5B	0.5560	0.1730
5C	0.5170	0.1530
5D	0.5660	0.1690
6A	0.5530	0.1550
6B	0.5530	0.1740
6C	0.5210	0.1590
6D	0.5660	0.1640
7A	0.5540	0.1580
7B	0.5630	0.1750
7C	0.5220	0.1600
7D	0.5620	0.1690
AA	0.5550	0.1550
AB	0.5620	0.1750

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Chain	Atom inclusion	Q-score
AC	0.5220	0.1590
AD	0.5590	0.1670
BA	0.5530	0.1520
BB	0.5540	0.1710
BC	0.5180	0.1610
BD	0.5660	0.1580
CA	0.5500	0.1550
CB	0.5570	0.1690
CC	0.5170	0.1580
CD	0.5610	0.1660
DA	0.5580	0.1530
DB	0.5610	0.1740
DC	0.5200	0.1610
DD	0.5620	0.1620
EA	0.5540	0.1570
EB	0.5640	0.1760
EC	0.5220	0.1590
ED	0.5620	0.1700
FA	0.5540	0.1570
FB	0.5630	0.1740
FC	0.5220	0.1590
FD	0.5620	0.1690
GA	0.5520	0.1570
GB	0.5590	0.1760
GC	0.5160	0.1580
GD	0.5620	0.1650
HA	0.5530	0.1550
HB	0.5540	0.1720
HC	0.5180	0.1610
HD	0.5660	0.1610
IA	0.5500	0.1570
IB	0.5570	0.1700
IC	0.5170	0.1580
ID	0.5610	0.1680
JA	0.5500	0.1560
JB	0.5570	0.1730
JC	0.5170	0.1620
JD	0.5610	0.1680
KA	0.5590	0.1560
KB	0.5610	0.1750
KC	0.5200	0.1620
KD	0.5620	0.1640

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Chain	Atom inclusion	Q-score
LA	0.5540	0.1560
LB	0.5630	0.1760
LC	0.5220	0.1580
LD	0.5620	0.1680
MA	0.5550	0.1550
MB	0.5620	0.1760
MC	0.5220	0.1610
MD	0.5590	0.1670
NA	0.5530	0.1530
NB	0.5540	0.1710
NC	0.5180	0.1610
ND	0.5660	0.1600
OA	0.5550	0.1530
OB	0.5540	0.1700
OC	0.5180	0.1570
OD	0.5630	0.1610
PA	0.5500	0.1560
PB	0.5570	0.1700
PC	0.5170	0.1580
PD	0.5610	0.1700
QA	0.5540	0.1550
QB	0.5640	0.1730
QC	0.5220	0.1580
QD	0.5620	0.1660
RA	0.5550	0.1550
RB	0.5620	0.1740
RC	0.5220	0.1610
RD	0.5590	0.1660
SA	0.5490	0.1550
SB	0.5540	0.1720
SC	0.5180	0.1590
SD	0.5620	0.1610
TA	0.5500	0.1560
TB	0.5550	0.1710
TC	0.5110	0.1570
TD	0.5590	0.1670
UA	0.5580	0.1520
UB	0.5610	0.1740
UC	0.5190	0.1620
UD	0.5620	0.1630
VA	0.5580	0.1570
VB	0.5610	0.1750

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Chain	Atom inclusion	Q-score
VC	0.5200	0.1610
VD	0.5620	0.1630
WA	0.5540	0.1540
WB	0.5640	0.1750
WC	0.5220	0.1600
WD	0.5620	0.1690
XA	0.5490	0.1560
XB	0.5540	0.1750
XC	0.5110	0.1590
XD	0.5600	0.1640
YA	0.5530	0.1520
YB	0.5550	0.1720
YC	0.5180	0.1620
YD	0.5660	0.1640
ZA	0.5530	0.1540
ZB	0.5550	0.1710
ZC	0.5180	0.1560
ZD	0.5660	0.1620
aA	0.5500	0.1570
aB	0.5570	0.1730
aC	0.5170	0.1590
aD	0.5610	0.1660
bA	0.5580	0.1540
bB	0.5610	0.1760
bC	0.5200	0.1630
bD	0.5620	0.1630
cA	0.5490	0.1580
cB	0.5640	0.1770
cC	0.5210	0.1630
cD	0.5640	0.1670
dA	0.5550	0.1560
dB	0.5590	0.1770
dC	0.5160	0.1580
dD	0.5580	0.1650
eA	0.5540	0.1560
eB	0.5620	0.1770
eC	0.5220	0.1610
eD	0.5590	0.1660
fA	0.5530	0.1530
fB	0.5540	0.1720
fC	0.5180	0.1600
fD	0.5660	0.1610

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Chain	Atom inclusion	Q-score
gA	0.5500	0.1570
gB	0.5570	0.1700
gC	0.5170	0.1600
gD	0.5610	0.1690
hA	0.5590	0.1530
hB	0.5610	0.1770
hC	0.5190	0.1640
hD	0.5620	0.1630
iA	0.5540	0.1530
iB	0.5570	0.1760
iC	0.5110	0.1570
iD	0.5640	0.1650
jA	0.5540	0.1560
jB	0.5630	0.1750
jC	0.5220	0.1630
jD	0.5620	0.1670
kA	0.5490	0.1540
kB	0.5620	0.1760
kC	0.5120	0.1560
kD	0.5570	0.1660
lA	0.5530	0.1530
lB	0.5540	0.1720
lC	0.5180	0.1600
lD	0.5660	0.1610
mA	0.5490	0.1550
mB	0.5550	0.1700
mC	0.5130	0.1600
mD	0.5630	0.1660
nA	0.5490	0.1580
nB	0.5530	0.1710
nC	0.5160	0.1590
nD	0.5570	0.1660
oA	0.5480	0.1570
oB	0.5560	0.1750
oC	0.5210	0.1580
oD	0.5590	0.1640
pA	0.5550	0.1570
pB	0.5640	0.1720
pC	0.5220	0.1580
pD	0.5620	0.1680
qA	0.5490	0.1590
qB	0.5610	0.1750

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Chain	Atom inclusion	Q-score
qC	0.5160	0.1560
qD	0.5630	0.1650
rA	0.5530	0.1520
rB	0.5590	0.1770
rC	0.5160	0.1610
rD	0.5590	0.1670
sA	0.5530	0.1540
sB	0.5540	0.1690
sC	0.5180	0.1610
sD	0.5660	0.1610
tA	0.5490	0.1580
tB	0.5560	0.1690
tC	0.5160	0.1540
tD	0.5600	0.1670
uA	0.5500	0.1550
uB	0.5550	0.1760
uC	0.5160	0.1560
uD	0.5610	0.1690
vA	0.5490	0.1550
vB	0.5610	0.1740
vC	0.5180	0.1580
vD	0.5600	0.1660
wA	0.5540	0.1550
wB	0.5640	0.1730
wC	0.5220	0.1600
wD	0.5620	0.1670
xA	0.5540	0.1550
xB	0.5620	0.1750
xC	0.5220	0.1620
xD	0.5590	0.1640
yA	0.5530	0.1560
yB	0.5550	0.1710
yC	0.5180	0.1590
yD	0.5660	0.1610
zA	0.5500	0.1550
zB	0.5570	0.1700
zC	0.5170	0.1570
zD	0.5610	0.1700