Full wwPDB EM Validation Report

Mar 22, 2026 – 05:17 PM UTC

PDB ID	:	7A4H / pdb_00007a4h
EMDB ID	:	EMD-11633
Title	:	Aquifex aeolicus lumazine synthase-derived nucleocapsid variant NC-2 (180-mer)
Authors	:	Tetter, S.; Hilvert, D.
Deposited on	:	2020-08-19
Resolution	:	4.50 Å(reported)
Based on initial model	:	1HQK

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:

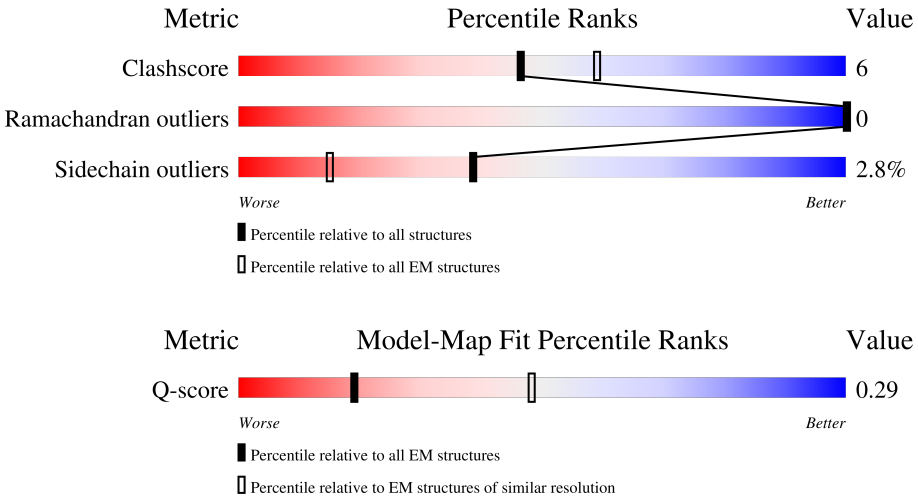
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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

Mol	Chain	Length	Quality of chain
1	AA	197	65% 11% 23%
1	AB	197	6% 64% 11% 25%
1	AC	197	5% 68% 9% 23%
1	AD	197	61% 14% 24%

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Mol	Chain	Length	Quality of chain
1	AE	197	64% 11% 24%
1	AF	197	59% 15% 25%
1	AG	197	62% 14% 24%
1	AH	197	62% 11% 25%
1	AI	197	66% 11% 23%
1	AJ	197	63% 12% 24%
1	AK	197	6% 63% 12% 24%
1	AL	197	62% 13% 23%
1	AM	197	59% 15% 25%
1	AN	197	8% 59% 16% 25%
1	AO	197	8% 65% 11% 24%
1	BA	197	65% 11% 23%
1	BB	197	6% 63% 12% 25%
1	BC	197	5% 68% 10% 23%
1	BD	197	63% 12% 24%
1	BE	197	64% 11% 24%
1	BF	197	59% 15% 25%
1	BG	197	61% 15% 24%
1	BH	197	62% 11% 25%
1	BI	197	66% 11% 23%
1	BJ	197	63% 12% 24%
1	BK	197	8% 63% 13% 24%
1	BL	197	62% 13% 23%
1	BM	197	61% 14% 25%
1	BN	197	8% 59% 16% 25%

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Mol	Chain	Length	Quality of chain
1	BO	197	8% 64% 12% 24%
1	CA	197	65% 11% 23%
1	CB	197	5% 63% 12% 25%
1	CC	197	68% 9% 23%
1	CD	197	61% 13% 24%
1	CE	197	64% 11% 24%
1	CF	197	59% 15% 25%
1	CG	197	61% 15% 24%
1	CH	197	62% 12% 25%
1	CI	197	68% 10% 23%
1	CJ	197	63% 12% 24%
1	CK	197	6% 63% 13% 24%
1	CL	197	61% 14% 23%
1	CM	197	5% 60% 14% 25%
1	CN	197	9% 59% 16% 25%
1	CO	197	7% 64% 12% 24%
1	DA	197	65% 11% 23%
1	DB	197	6% 64% 11% 25%
1	DC	197	6% 68% 10% 23%
1	DD	197	62% 13% 24%
1	DE	197	64% 11% 24%
1	DF	197	58% 16% 25%
1	DG	197	61% 14% 24%
1	DH	197	63% 10% 25%
1	DI	197	68% 10% 23%

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Mol	Chain	Length	Quality of chain
1	DJ	197	62% 13% 24%
1	DK	197	7% 64% 11% 24%
1	DL	197	63% 13% 23%
1	DM	197	61% 14% 25%
1	DN	197	9% 59% 16% 25%
1	DO	197	9% 64% 12% 24%
1	EA	197	65% 11% 23%
1	EB	197	6% 64% 11% 25%
1	EC	197	5% 68% 10% 23%
1	ED	197	61% 13% 24%
1	EE	197	63% 12% 24%
1	EF	197	6% 59% 15% 25%
1	EG	197	61% 15% 24%
1	EH	197	62% 11% 25%
1	EI	197	67% 10% 23%
1	EJ	197	62% 13% 24%
1	EK	197	8% 62% 14% 24%
1	EL	197	62% 13% 23%
1	EM	197	59% 15% 25%
1	EN	197	9% 59% 16% 25%
1	EO	197	7% 64% 12% 24%
1	FA	197	64% 12% 23%
1	FB	197	6% 64% 11% 25%
1	FC	197	5% 68% 9% 23%
1	FD	197	62% 13% 24%

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Mol	Chain	Length	Quality of chain
1	FE	197	65% 10% 24%
1	FF	197	5% 59% 15% 25%
1	FG	197	61% 14% 24%
1	FH	197	63% 11% 25%
1	FI	197	68% 10% 23%
1	FJ	197	63% 12% 24%
1	FK	197	7% 63% 12% 24%
1	FL	197	62% 14% 23%
1	FM	197	61% 13% 25%
1	FN	197	9% 59% 16% 25%
1	FO	197	8% 64% 12% 24%
1	GA	197	64% 12% 23%
1	GB	197	6% 63% 12% 25%
1	GC	197	5% 68% 10% 23%
1	GD	197	62% 12% 24%
1	GE	197	63% 12% 24%
1	GF	197	59% 15% 25%
1	GG	197	62% 14% 24%
1	GH	197	63% 11% 25%
1	GI	197	67% 10% 23%
1	GJ	197	63% 12% 24%
1	GK	197	6% 63% 13% 24%
1	GL	197	62% 14% 23%
1	GM	197	59% 15% 25%
1	GN	197	8% 59% 16% 25%

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Mol	Chain	Length	Quality of chain
1	GO	197	8% 65% 11% 24%
1	HA	197	65% 11% 23%
1	HB	197	7% 63% 12% 25%
1	HC	197	68% 10% 23%
1	HD	197	62% 12% 24%
1	HE	197	65% 10% 24%
1	HF	197	59% 15% 25%
1	HG	197	62% 14% 24%
1	HH	197	62% 11% 25%
1	HI	197	66% 11% 23%
1	HJ	197	62% 13% 24%
1	HK	197	7% 64% 11% 24%
1	HL	197	63% 13% 23%
1	HM	197	60% 14% 25%
1	HN	197	8% 59% 16% 25%
1	HO	197	9% 64% 12% 24%
1	IA	197	65% 11% 23%
1	IB	197	6% 63% 12% 25%
1	IC	197	68% 10% 23%
1	ID	197	61% 13% 24%
1	IE	197	64% 11% 24%
1	IF	197	59% 15% 25%
1	IG	197	61% 14% 24%
1	IH	197	64% 10% 25%
1	II	197	67% 10% 23%

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Mol	Chain	Length	Quality of chain
1	IJ	197	63% 12% 24%
1	IK	197	7% 63% 13% 24%
1	IL	197	62% 13% 23%
1	IM	197	60% 14% 25%
1	IN	197	9% 59% 16% 25%
1	IO	197	8% 64% 12% 24%
1	JA	197	63% 13% 23%
1	JB	197	64% 11% 25%
1	JC	197	5% 68% 9% 23%
1	JD	197	62% 13% 24%
1	JE	197	63% 12% 24%
1	JF	197	59% 15% 25%
1	JG	197	61% 14% 24%
1	JH	197	63% 10% 25%
1	JI	197	67% 10% 23%
1	JJ	197	63% 12% 24%
1	JK	197	6% 63% 12% 24%
1	JL	197	63% 12% 23%
1	JM	197	5% 60% 15% 25%
1	JN	197	9% 59% 16% 25%
1	JO	197	7% 64% 12% 24%
1	KA	197	64% 12% 23%
1	KB	197	6% 64% 11% 25%
1	KC	197	5% 68% 9% 23%
1	KD	197	61% 14% 24%

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Mol	Chain	Length	Quality of chain
1	KE	197	63% 12% 24%
1	KF	197	60% 14% 25%
1	KG	197	62% 13% 24%
1	KH	197	63% 11% 25%
1	KI	197	68% 10% 23%
1	KJ	197	64% 11% 24%
1	KK	197	6% 64% 12% 24%
1	KL	197	62% 14% 23%
1	KM	197	61% 14% 25%
1	KN	197	9% 59% 16% 25%
1	KO	197	9% 64% 12% 24%
1	LA	197	63% 13% 23%
1	LB	197	6% 63% 12% 25%
1	LC	197	68% 10% 23%
1	LD	197	62% 13% 24%
1	LE	197	63% 12% 24%
1	LF	197	59% 15% 25%
1	LG	197	62% 14% 24%
1	LH	197	63% 11% 25%
1	LI	197	66% 11% 23%
1	LJ	197	61% 14% 24%
1	LK	197	6% 64% 11% 24%
1	LL	197	61% 14% 23%
1	LM	197	59% 15% 25%
1	LN	197	8% 59% 16% 25%

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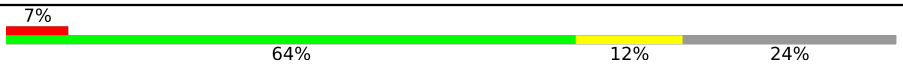
Mol	Chain	Length	Quality of chain
1	LO	197	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 204396 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
1	BA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		
1	BB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	BC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	BD	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	BE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	BF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	BG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	BH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	BI	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	BJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	BK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	BL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	BM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		
1	BN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	BO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	AA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	AC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	AD	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	AE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	AF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	AG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	AH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	AI	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	AJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	AK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	AL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	AM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		
1	AN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	AO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	CA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		
1	CB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	CC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	CD	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	CE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	CF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	CG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	CI	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	CJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	CK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	CL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	CM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		
1	CN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	CO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	DA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		
1	DB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	DC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	DD	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	DE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	DF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	DG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	DH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	DI	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	DJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	DK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	DL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	DM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	DO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	EA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		
1	EB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	EC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	ED	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	EE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	EF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	EG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	EH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	EI	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	EJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	EK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	EL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	EM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		
1	EN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	EO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	FA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		
1	FB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	FC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	FD	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	FE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	FF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	FG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	FH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	FI	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	FJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	FK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	FL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	FM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		
1	FN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	FO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	GA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		
1	GB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	GC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	GD	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	GE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	GF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	GG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	GH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	GI	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	GJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	GK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	GL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	GM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		
1	GN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	GO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	HA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		
1	HB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	HC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	HD	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	HE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	HF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	HG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	HH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	HI	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	HJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	HK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	HL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	HM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		
1	HN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	HO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	IA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	IC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	ID	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	IE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	IF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	IG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	IH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	II	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	IJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	IK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	IL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	IM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		
1	IN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	IO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	JA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		
1	JB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	JC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	JD	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	JE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	JF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	JG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	JH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	JI	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	JJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	JK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	JL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	JM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		
1	JN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	JO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	KA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		
1	KB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	KC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	KD	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	KE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	KF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	KG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	KH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	KI	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	KJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	KK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	KL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	KM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	KN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	KO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	LA	152	Total	C	N	O	S	0	0
			1150	725	202	220	3		
1	LB	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	LC	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	LD	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	LE	150	Total	C	N	O	S	0	0
			1140	720	200	217	3		
1	LF	148	Total	C	N	O	S	0	0
			1122	710	195	214	3		
1	LG	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		
1	LH	147	Total	C	N	O	S	0	0
			1118	708	194	213	3		
1	LI	152	Total	C	N	O	S	0	0
			1149	724	202	220	3		
1	LJ	149	Total	C	N	O	S	0	0
			1135	717	199	216	3		
1	LK	150	Total	C	N	O	S	0	0
			1141	720	200	218	3		
1	LL	151	Total	C	N	O	S	0	0
			1145	722	201	219	3		
1	LM	148	Total	C	N	O	S	0	0
			1123	711	195	214	3		
1	LN	148	Total	C	N	O	S	0	0
			1129	714	198	214	3		
1	LO	149	Total	C	N	O	S	0	0
			1134	716	199	216	3		

There are 5940 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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
BA	111	GLY	-	linker	UNP O66529
BA	112	SER	-	linker	UNP O66529
BA	113	SER	-	linker	UNP O66529
BA	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	115	GLU	GLN	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	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	115	GLU	GLN	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	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	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	115	GLU	GLN	engineered mutation	UNP O66529
BD	191	PHE	ILE	engineered mutation	UNP O66529

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
BO	6	THR	-	cloning artifact	UNP P03045
BO	24	ALA	-	linker	UNP P03045
BO	25	GLY	-	linker	UNP P03045
BO	26	ALA	-	linker	UNP P03045
BO	27	GLY	-	linker	UNP P03045
BO	28	ALA	-	linker	UNP P03045
BO	29	GLY	-	linker	UNP P03045
BO	30	ALA	-	linker	UNP P03045
BO	31	MET	-	linker	UNP P03045
BO	42	VAL	GLU	engineered mutation	UNP O66529
BO	58	VAL	ILE	engineered mutation	UNP O66529
BO	61	ASP	GLY	engineered mutation	UNP O66529
BO	62	ILE	VAL	engineered mutation	UNP O66529
BO	102	GLY	-	linker	UNP O66529
BO	103	THR	-	linker	UNP O66529
BO	104	GLY	-	linker	UNP O66529
BO	105	HIS	-	linker	UNP O66529
BO	106	HIS	-	linker	UNP O66529
BO	107	HIS	-	linker	UNP O66529
BO	108	HIS	-	linker	UNP O66529
BO	109	HIS	-	linker	UNP O66529
BO	110	HIS	-	linker	UNP O66529
BO	111	GLY	-	linker	UNP O66529
BO	112	SER	-	linker	UNP O66529
BO	113	SER	-	linker	UNP O66529
BO	115	GLU	GLN	engineered mutation	UNP O66529
BO	191	PHE	ILE	engineered mutation	UNP O66529
BO	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
AA	31	MET	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	115	GLU	GLN	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	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	115	GLU	GLN	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	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	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	115	GLU	GLN	engineered mutation	UNP O66529
AC	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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
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	115	GLU	GLN	engineered mutation	UNP O66529
AD	191	PHE	ILE	engineered mutation	UNP O66529
AD	193	ASP	VAL	engineered mutation	UNP O66529
AE	1	MET	-	cloning artifact	UNP P03045
AE	2	GLY	-	cloning artifact	UNP P03045
AE	3	ASN	-	cloning artifact	UNP P03045
AE	4	ALA	-	cloning artifact	UNP P03045
AE	5	LYS	-	cloning artifact	UNP P03045
AE	6	THR	-	cloning artifact	UNP P03045
AE	24	ALA	-	linker	UNP P03045
AE	25	GLY	-	linker	UNP P03045

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
AO	42	VAL	GLU	engineered mutation	UNP O66529
AO	58	VAL	ILE	engineered mutation	UNP O66529
AO	61	ASP	GLY	engineered mutation	UNP O66529
AO	62	ILE	VAL	engineered mutation	UNP O66529
AO	102	GLY	-	linker	UNP O66529
AO	103	THR	-	linker	UNP O66529
AO	104	GLY	-	linker	UNP O66529
AO	105	HIS	-	linker	UNP O66529
AO	106	HIS	-	linker	UNP O66529
AO	107	HIS	-	linker	UNP O66529
AO	108	HIS	-	linker	UNP O66529
AO	109	HIS	-	linker	UNP O66529
AO	110	HIS	-	linker	UNP O66529
AO	111	GLY	-	linker	UNP O66529
AO	112	SER	-	linker	UNP O66529
AO	113	SER	-	linker	UNP O66529
AO	115	GLU	GLN	engineered mutation	UNP O66529
AO	191	PHE	ILE	engineered mutation	UNP O66529
AO	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
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	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	115	GLU	GLN	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
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	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	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	115	GLU	GLN	engineered mutation	UNP O66529
CB	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
CC	29	GLY	-	linker	UNP P03045
CC	30	ALA	-	linker	UNP P03045
CC	31	MET	-	linker	UNP P03045
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	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	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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	115	GLU	GLN	engineered mutation	UNP O66529
CD	191	PHE	ILE	engineered mutation	UNP O66529
CD	193	ASP	VAL	engineered mutation	UNP O66529
CE	1	MET	-	cloning artifact	UNP P03045
CE	2	GLY	-	cloning artifact	UNP P03045
CE	3	ASN	-	cloning artifact	UNP P03045
CE	4	ALA	-	cloning artifact	UNP P03045
CE	5	LYS	-	cloning artifact	UNP P03045
CE	6	THR	-	cloning artifact	UNP P03045
CE	24	ALA	-	linker	UNP P03045
CE	25	GLY	-	linker	UNP P03045
CE	26	ALA	-	linker	UNP P03045
CE	27	GLY	-	linker	UNP P03045
CE	28	ALA	-	linker	UNP P03045
CE	29	GLY	-	linker	UNP P03045
CE	30	ALA	-	linker	UNP P03045
CE	31	MET	-	linker	UNP P03045
CE	42	VAL	GLU	engineered mutation	UNP O66529
CE	58	VAL	ILE	engineered mutation	UNP O66529
CE	61	ASP	GLY	engineered mutation	UNP O66529

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
CO	107	HIS	-	linker	UNP O66529
CO	108	HIS	-	linker	UNP O66529
CO	109	HIS	-	linker	UNP O66529
CO	110	HIS	-	linker	UNP O66529
CO	111	GLY	-	linker	UNP O66529
CO	112	SER	-	linker	UNP O66529
CO	113	SER	-	linker	UNP O66529
CO	115	GLU	GLN	engineered mutation	UNP O66529
CO	191	PHE	ILE	engineered mutation	UNP O66529
CO	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	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
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	115	GLU	GLN	engineered mutation	UNP O66529
DA	191	PHE	ILE	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	102	GLY	-	linker	UNP O66529
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	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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
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	115	GLU	GLN	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	42	VAL	GLU	engineered mutation	UNP O66529
DD	58	VAL	ILE	engineered mutation	UNP O66529
DD	61	ASP	GLY	engineered mutation	UNP O66529

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

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
DO	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	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	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	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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	115	GLU	GLN	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
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	42	VAL	GLU	engineered mutation	UNP O66529
EC	58	VAL	ILE	engineered mutation	UNP O66529
EC	61	ASP	GLY	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
EC	62	ILE	VAL	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	115	GLU	GLN	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
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	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	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

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

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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	115	GLU	GLN	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
FB	31	MET	-	linker	UNP P03045
FB	42	VAL	GLU	engineered mutation	UNP O66529
FB	58	VAL	ILE	engineered mutation	UNP O66529
FB	61	ASP	GLY	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
FB	62	ILE	VAL	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	115	GLU	GLN	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	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	115	GLU	GLN	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	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	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	115	GLU	GLN	engineered mutation	UNP O66529
FD	191	PHE	ILE	engineered mutation	UNP O66529
FD	193	ASP	VAL	engineered mutation	UNP O66529
FE	1	MET	-	cloning artifact	UNP P03045
FE	2	GLY	-	cloning artifact	UNP P03045

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
FO	26	ALA	-	linker	UNP P03045
FO	27	GLY	-	linker	UNP P03045
FO	28	ALA	-	linker	UNP P03045
FO	29	GLY	-	linker	UNP P03045
FO	30	ALA	-	linker	UNP P03045
FO	31	MET	-	linker	UNP P03045
FO	42	VAL	GLU	engineered mutation	UNP O66529
FO	58	VAL	ILE	engineered mutation	UNP O66529
FO	61	ASP	GLY	engineered mutation	UNP O66529
FO	62	ILE	VAL	engineered mutation	UNP O66529
FO	102	GLY	-	linker	UNP O66529
FO	103	THR	-	linker	UNP O66529
FO	104	GLY	-	linker	UNP O66529
FO	105	HIS	-	linker	UNP O66529
FO	106	HIS	-	linker	UNP O66529
FO	107	HIS	-	linker	UNP O66529
FO	108	HIS	-	linker	UNP O66529
FO	109	HIS	-	linker	UNP O66529
FO	110	HIS	-	linker	UNP O66529
FO	111	GLY	-	linker	UNP O66529
FO	112	SER	-	linker	UNP O66529
FO	113	SER	-	linker	UNP O66529
FO	115	GLU	GLN	engineered mutation	UNP O66529
FO	191	PHE	ILE	engineered mutation	UNP O66529
FO	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	42	VAL	GLU	engineered mutation	UNP O66529
GA	58	VAL	ILE	engineered mutation	UNP O66529
GA	61	ASP	GLY	engineered mutation	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
GA	62	ILE	VAL	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
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	115	GLU	GLN	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	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	115	GLU	GLN	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	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	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	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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	115	GLU	GLN	engineered mutation	UNP O66529
GD	191	PHE	ILE	engineered mutation	UNP O66529
GD	193	ASP	VAL	engineered mutation	UNP O66529
GE	1	MET	-	cloning artifact	UNP P03045
GE	2	GLY	-	cloning artifact	UNP P03045
GE	3	ASN	-	cloning artifact	UNP P03045
GE	4	ALA	-	cloning artifact	UNP P03045
GE	5	LYS	-	cloning artifact	UNP P03045
GE	6	THR	-	cloning artifact	UNP P03045
GE	24	ALA	-	linker	UNP P03045
GE	25	GLY	-	linker	UNP P03045
GE	26	ALA	-	linker	UNP P03045
GE	27	GLY	-	linker	UNP P03045
GE	28	ALA	-	linker	UNP P03045

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
GO	62	ILE	VAL	engineered mutation	UNP O66529
GO	102	GLY	-	linker	UNP O66529
GO	103	THR	-	linker	UNP O66529
GO	104	GLY	-	linker	UNP O66529
GO	105	HIS	-	linker	UNP O66529
GO	106	HIS	-	linker	UNP O66529
GO	107	HIS	-	linker	UNP O66529
GO	108	HIS	-	linker	UNP O66529
GO	109	HIS	-	linker	UNP O66529
GO	110	HIS	-	linker	UNP O66529
GO	111	GLY	-	linker	UNP O66529
GO	112	SER	-	linker	UNP O66529
GO	113	SER	-	linker	UNP O66529
GO	115	GLU	GLN	engineered mutation	UNP O66529
GO	191	PHE	ILE	engineered mutation	UNP O66529
GO	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	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	115	GLU	GLN	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
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	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	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	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	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	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	115	GLU	GLN	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	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	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	115	GLU	GLN	engineered mutation	UNP O66529
HD	191	PHE	ILE	engineered mutation	UNP O66529
HD	193	ASP	VAL	engineered mutation	UNP O66529
HE	1	MET	-	cloning artifact	UNP P03045
HE	2	GLY	-	cloning artifact	UNP P03045
HE	3	ASN	-	cloning artifact	UNP P03045
HE	4	ALA	-	cloning artifact	UNP P03045
HE	5	LYS	-	cloning artifact	UNP P03045
HE	6	THR	-	cloning artifact	UNP P03045
HE	24	ALA	-	linker	UNP P03045
HE	25	GLY	-	linker	UNP P03045
HE	26	ALA	-	linker	UNP P03045
HE	27	GLY	-	linker	UNP P03045
HE	28	ALA	-	linker	UNP P03045
HE	29	GLY	-	linker	UNP P03045
HE	30	ALA	-	linker	UNP P03045
HE	31	MET	-	linker	UNP P03045
HE	42	VAL	GLU	engineered mutation	UNP O66529
HE	58	VAL	ILE	engineered mutation	UNP O66529
HE	61	ASP	GLY	engineered mutation	UNP O66529
HE	62	ILE	VAL	engineered mutation	UNP O66529
HE	102	GLY	-	linker	UNP O66529
HE	103	THR	-	linker	UNP O66529

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
HO	110	HIS	-	linker	UNP O66529
HO	111	GLY	-	linker	UNP O66529
HO	112	SER	-	linker	UNP O66529
HO	113	SER	-	linker	UNP O66529
HO	115	GLU	GLN	engineered mutation	UNP O66529
HO	191	PHE	ILE	engineered mutation	UNP O66529
HO	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	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	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	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
IC	29	GLY	-	linker	UNP P03045
IC	30	ALA	-	linker	UNP P03045
IC	31	MET	-	linker	UNP P03045
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	102	GLY	-	linker	UNP O66529
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	115	GLU	GLN	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	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	102	GLY	-	linker	UNP O66529
ID	103	THR	-	linker	UNP O66529

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

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
JB	29	GLY	-	linker	UNP P03045
JB	30	ALA	-	linker	UNP P03045
JB	31	MET	-	linker	UNP P03045
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	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	115	GLU	GLN	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	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	102	GLY	-	linker	UNP O66529
JC	103	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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	115	GLU	GLN	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	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	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

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

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
KA	29	GLY	-	linker	UNP P03045
KA	30	ALA	-	linker	UNP P03045
KA	31	MET	-	linker	UNP P03045
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	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	115	GLU	GLN	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	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	102	GLY	-	linker	UNP O66529
KB	103	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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	115	GLU	GLN	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	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
KC	113	SER	-	linker	UNP O66529
KC	115	GLU	GLN	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	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	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	115	GLU	GLN	engineered mutation	UNP O66529
KD	191	PHE	ILE	engineered mutation	UNP O66529
KD	193	ASP	VAL	engineered mutation	UNP O66529
KE	1	MET	-	cloning artifact	UNP P03045
KE	2	GLY	-	cloning artifact	UNP P03045
KE	3	ASN	-	cloning artifact	UNP P03045
KE	4	ALA	-	cloning artifact	UNP P03045
KE	5	LYS	-	cloning artifact	UNP P03045

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
KO	29	GLY	-	linker	UNP P03045
KO	30	ALA	-	linker	UNP P03045
KO	31	MET	-	linker	UNP P03045
KO	42	VAL	GLU	engineered mutation	UNP O66529
KO	58	VAL	ILE	engineered mutation	UNP O66529
KO	61	ASP	GLY	engineered mutation	UNP O66529
KO	62	ILE	VAL	engineered mutation	UNP O66529
KO	102	GLY	-	linker	UNP O66529
KO	103	THR	-	linker	UNP O66529
KO	104	GLY	-	linker	UNP O66529
KO	105	HIS	-	linker	UNP O66529
KO	106	HIS	-	linker	UNP O66529
KO	107	HIS	-	linker	UNP O66529
KO	108	HIS	-	linker	UNP O66529
KO	109	HIS	-	linker	UNP O66529
KO	110	HIS	-	linker	UNP O66529
KO	111	GLY	-	linker	UNP O66529
KO	112	SER	-	linker	UNP O66529
KO	113	SER	-	linker	UNP O66529
KO	115	GLU	GLN	engineered mutation	UNP O66529
KO	191	PHE	ILE	engineered mutation	UNP O66529
KO	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	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	102	GLY	-	linker	UNP O66529
LA	103	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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	115	GLU	GLN	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	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
LB	113	SER	-	linker	UNP O66529
LB	115	GLU	GLN	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	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	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	115	GLU	GLN	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	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	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	115	GLU	GLN	engineered mutation	UNP O66529
LD	191	PHE	ILE	engineered mutation	UNP O66529
LD	193	ASP	VAL	engineered mutation	UNP O66529
LE	1	MET	-	cloning artifact	UNP P03045
LE	2	GLY	-	cloning artifact	UNP P03045
LE	3	ASN	-	cloning artifact	UNP P03045
LE	4	ALA	-	cloning artifact	UNP P03045
LE	5	LYS	-	cloning artifact	UNP P03045
LE	6	THR	-	cloning artifact	UNP P03045
LE	24	ALA	-	linker	UNP P03045
LE	25	GLY	-	linker	UNP P03045
LE	26	ALA	-	linker	UNP P03045
LE	27	GLY	-	linker	UNP P03045
LE	28	ALA	-	linker	UNP P03045
LE	29	GLY	-	linker	UNP P03045
LE	30	ALA	-	linker	UNP P03045
LE	31	MET	-	linker	UNP P03045

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

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

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

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

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

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

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

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

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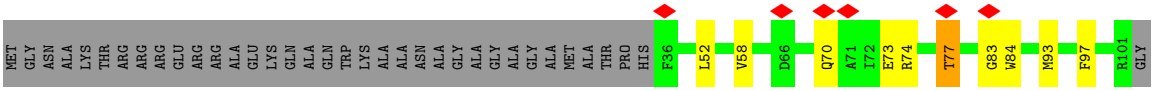
Chain	Residue	Modelled	Actual	Comment	Reference
LO	104	GLY	-	linker	UNP O66529
LO	105	HIS	-	linker	UNP O66529
LO	106	HIS	-	linker	UNP O66529
LO	107	HIS	-	linker	UNP O66529
LO	108	HIS	-	linker	UNP O66529
LO	109	HIS	-	linker	UNP O66529
LO	110	HIS	-	linker	UNP O66529
LO	111	GLY	-	linker	UNP O66529
LO	112	SER	-	linker	UNP O66529
LO	113	SER	-	linker	UNP O66529
LO	115	GLU	GLN	engineered mutation	UNP O66529
LO	191	PHE	ILE	engineered mutation	UNP O66529
LO	193	ASP	VAL	engineered mutation	UNP O66529

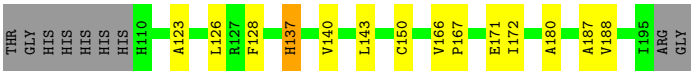
3 Residue-property plots (i)

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

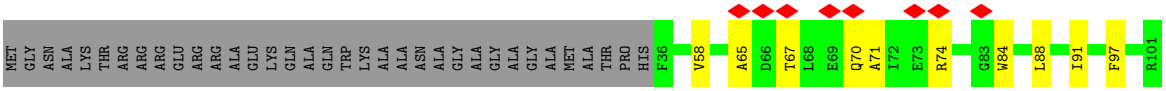
Chain BA:

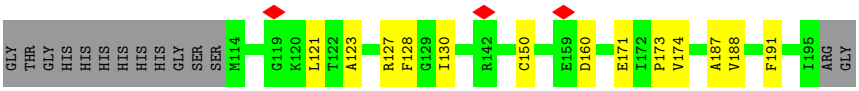




• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

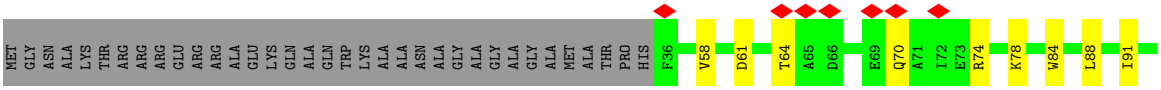
Chain BB:

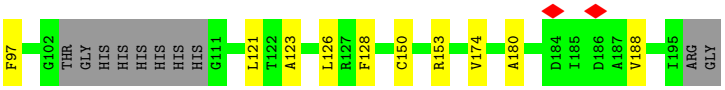




• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

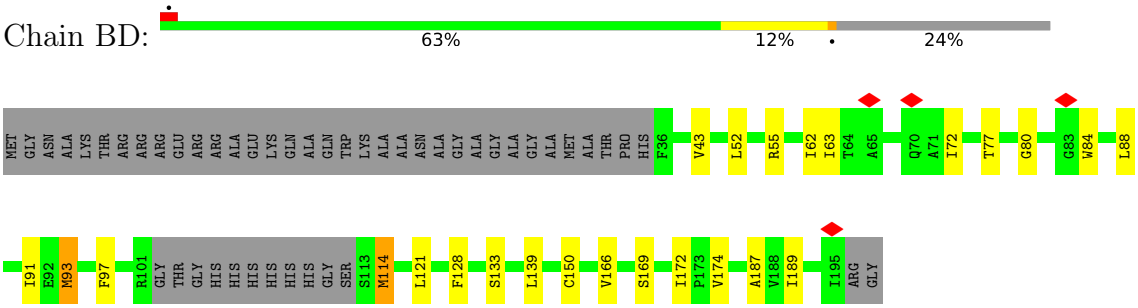
Chain BC:





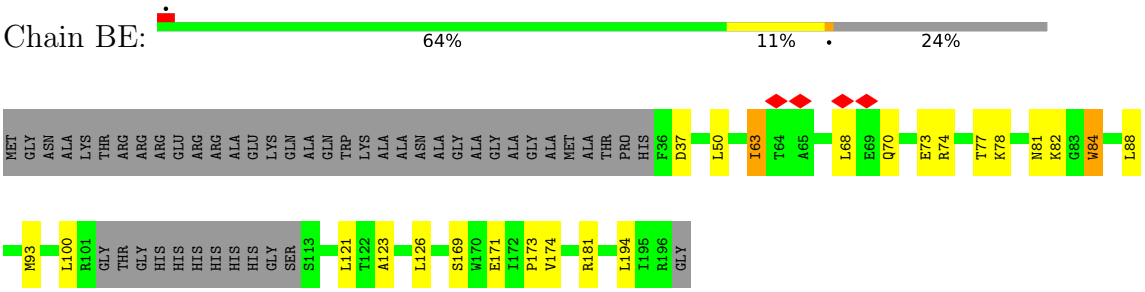
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BD:



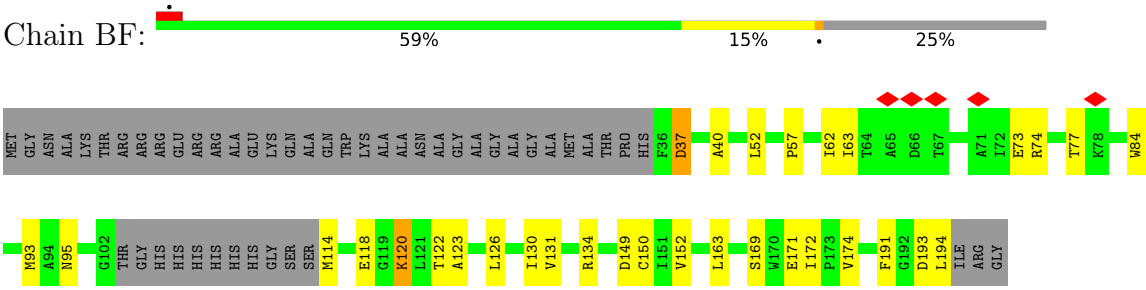
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BE:



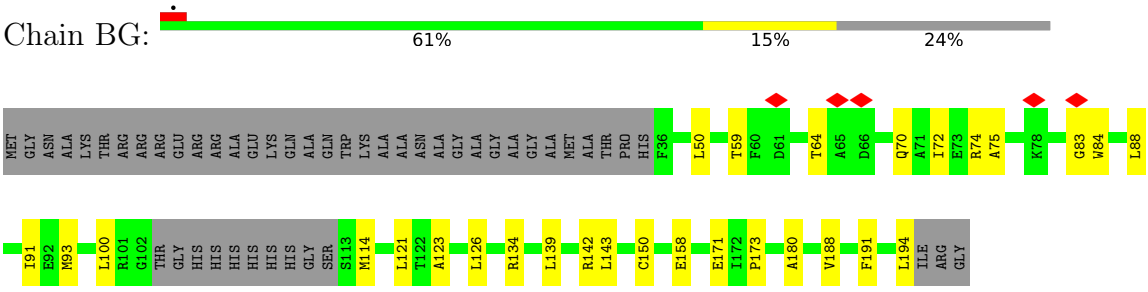
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BF:



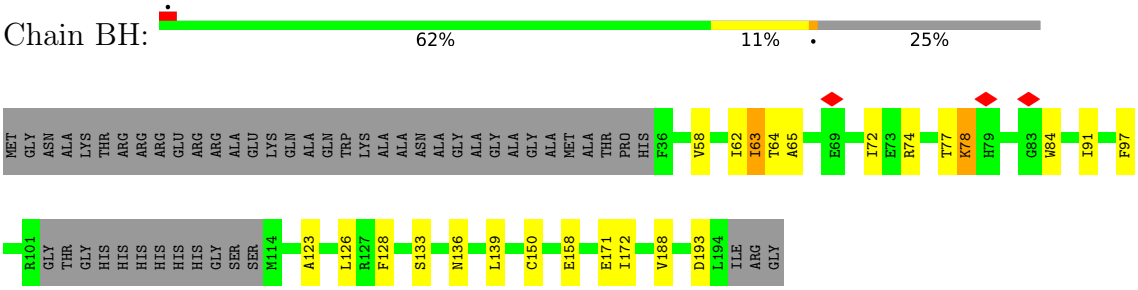
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BG:



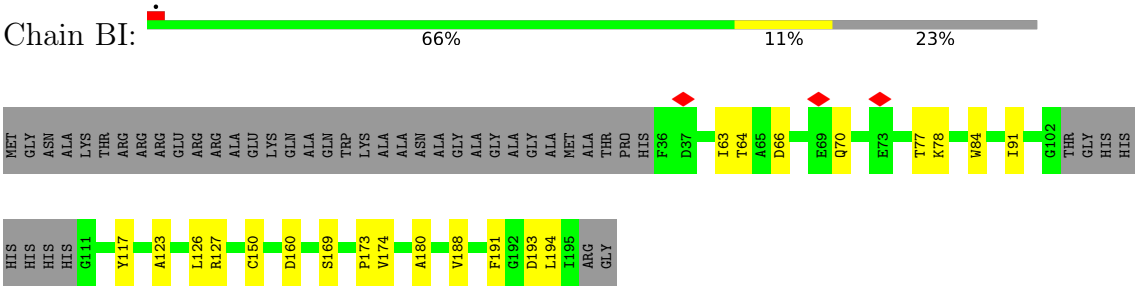
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BH:



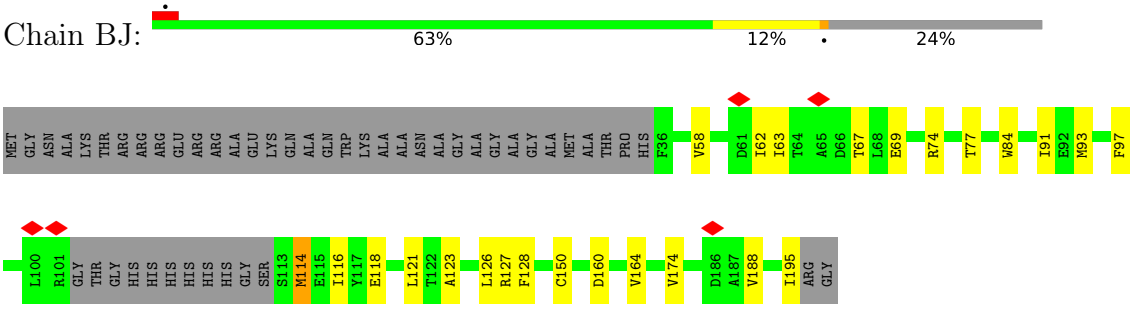
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BI:



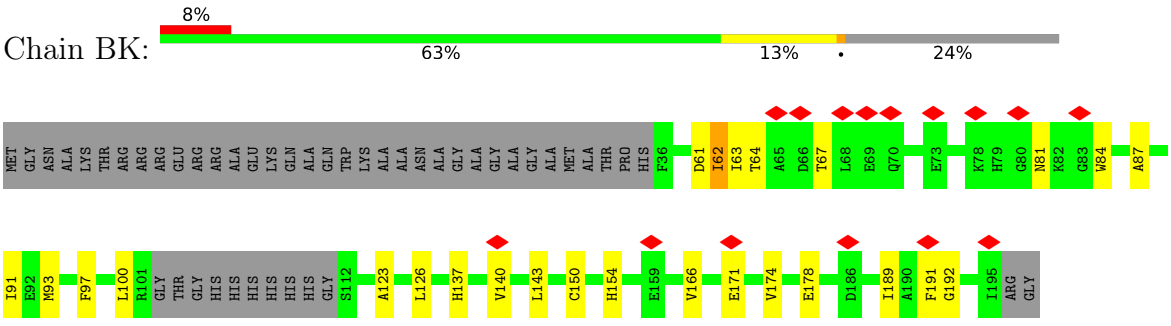
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BJ:



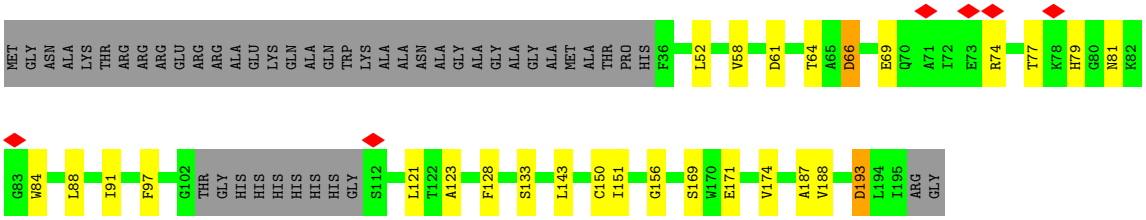
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BK:



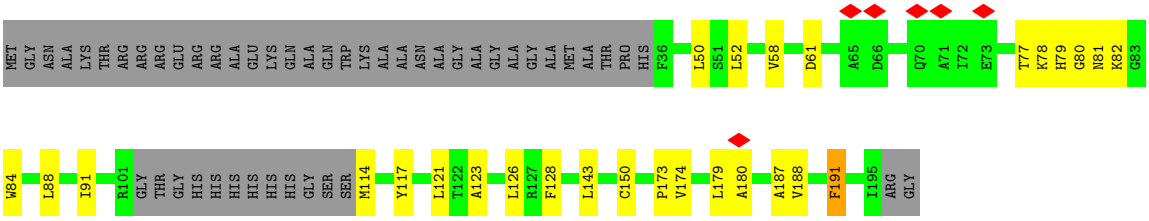
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BL:



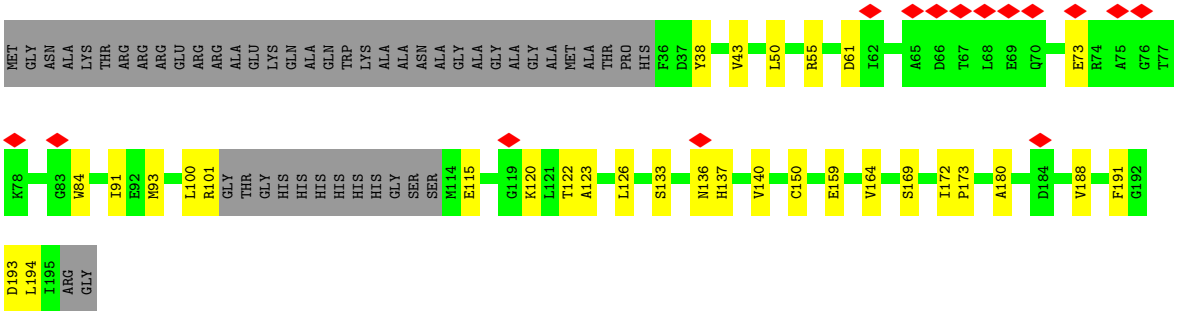
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BM:



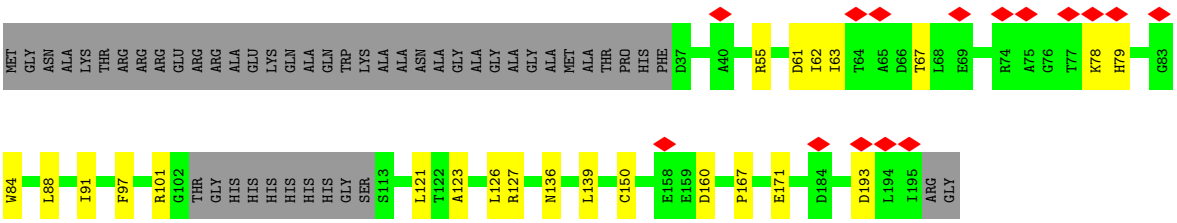
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BN:



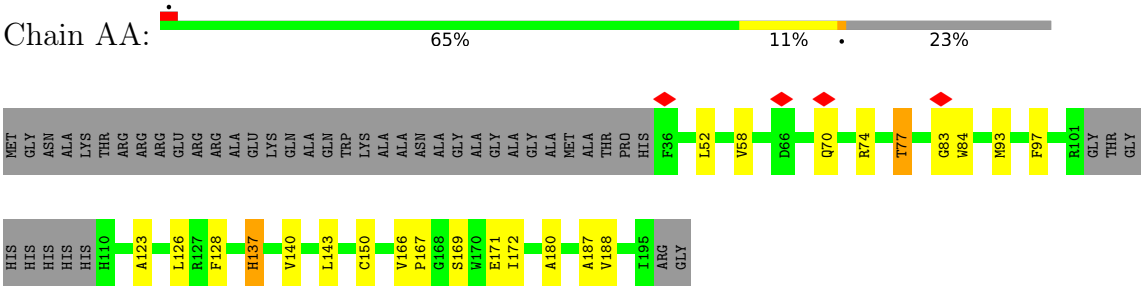
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BO:



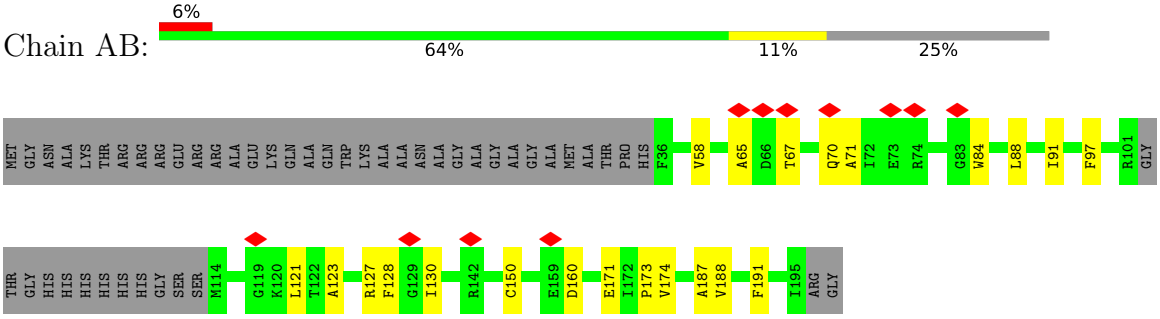
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AA:



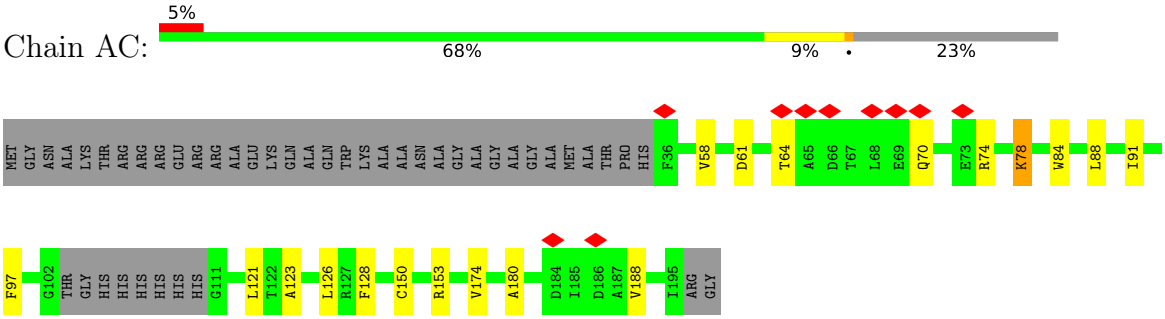
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AB:



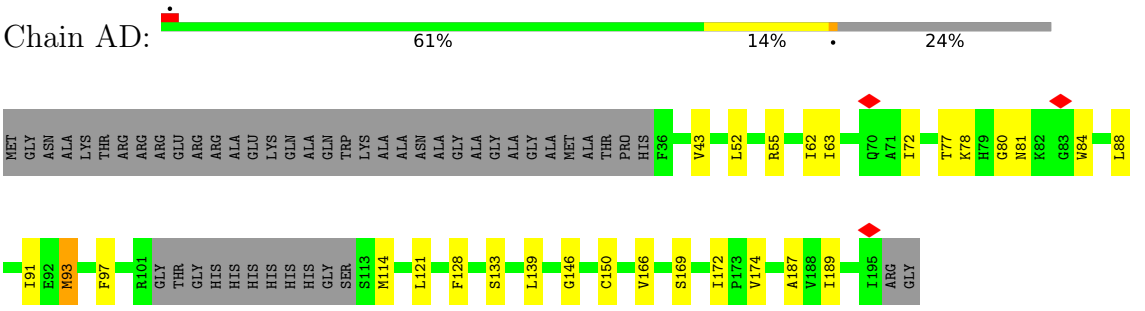
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AC:



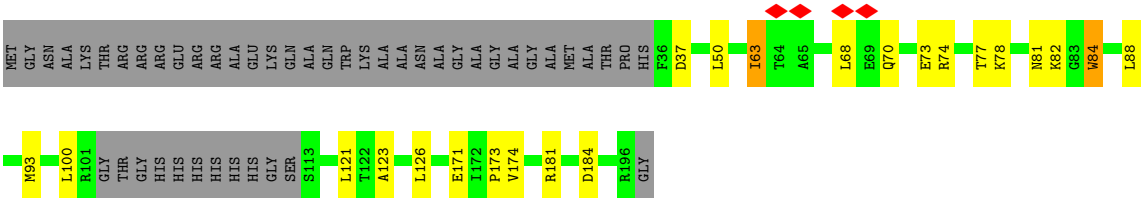
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AD:



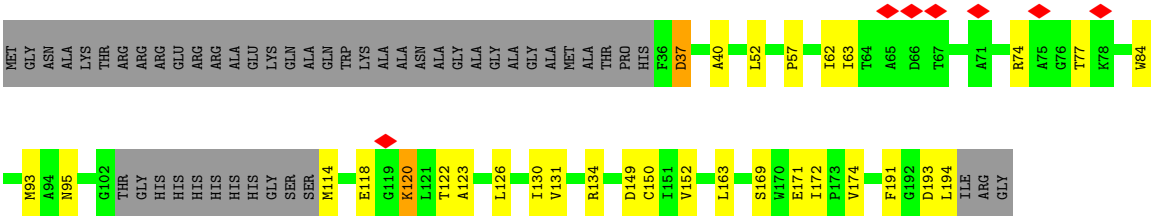
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AE:



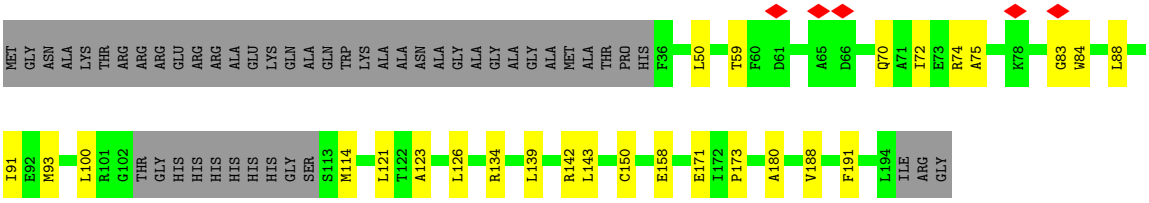
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AF:



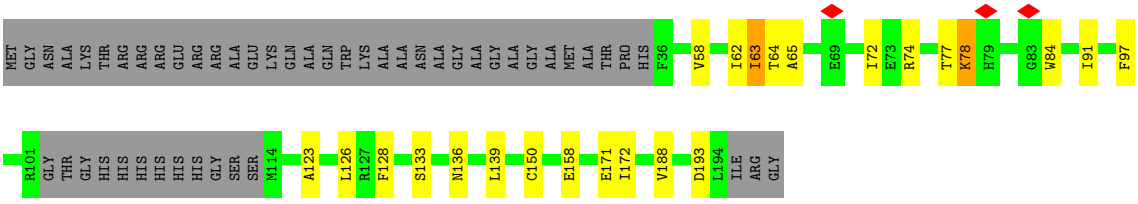
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AG:



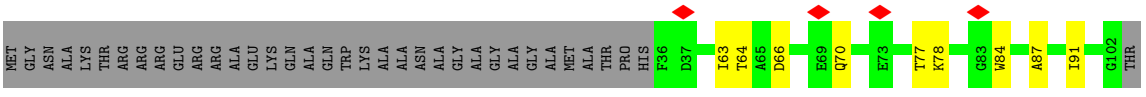
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AH:



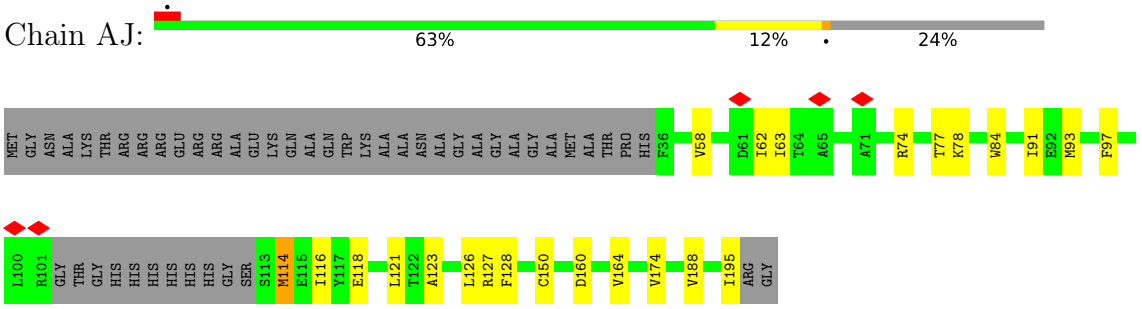
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AI:



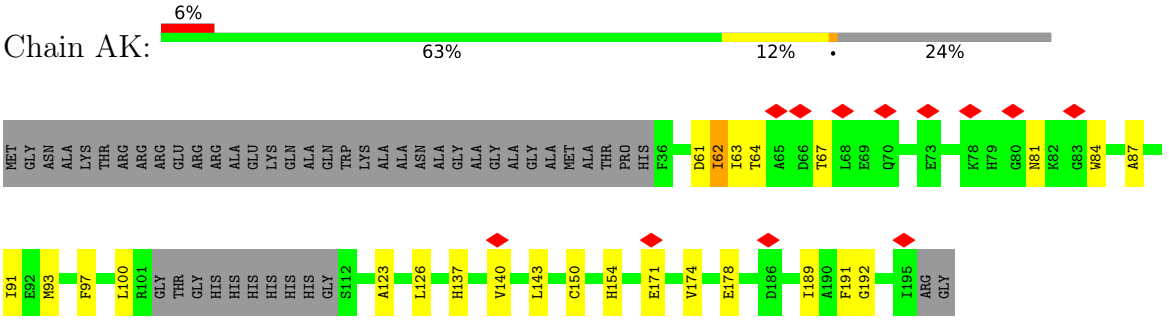
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AJ:



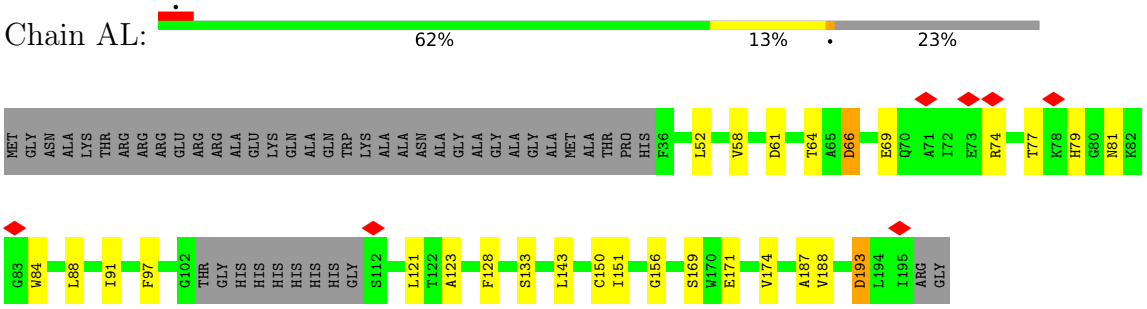
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AK:



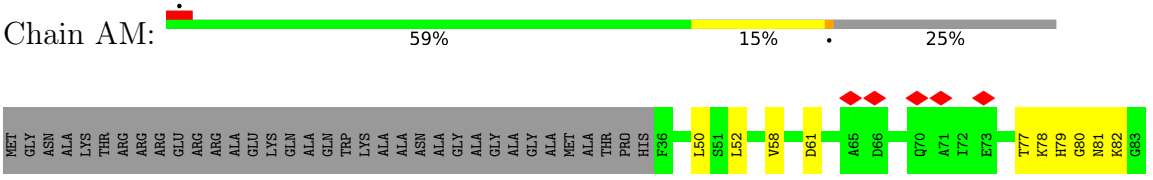
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

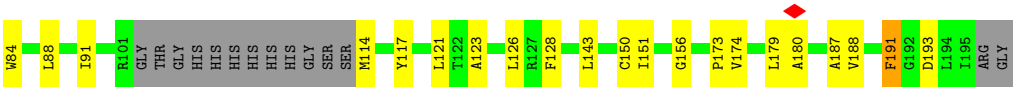
Chain AL:



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

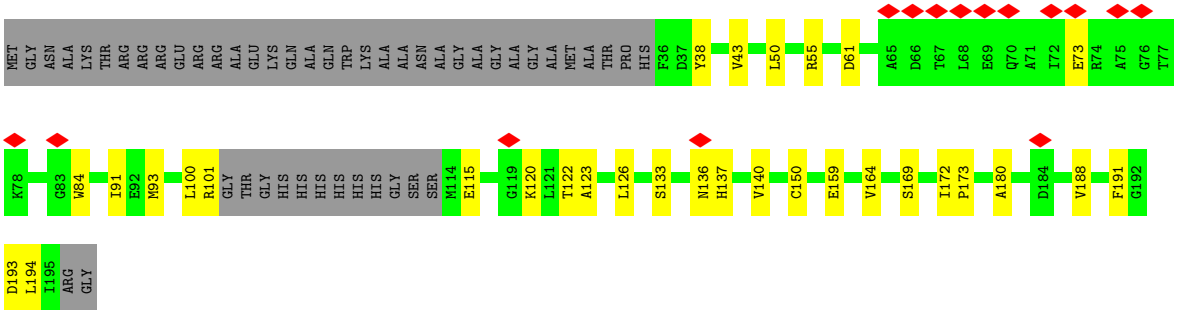
Chain AM:





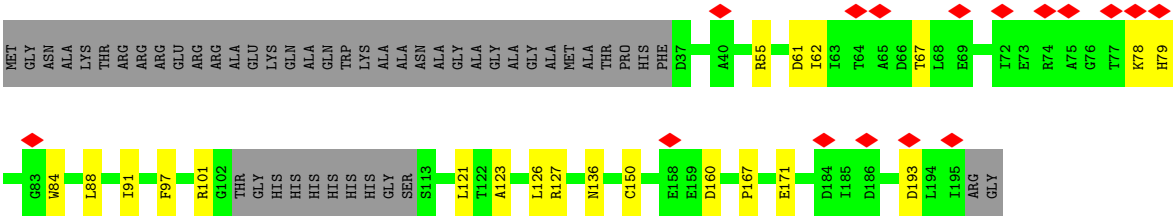
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AN:



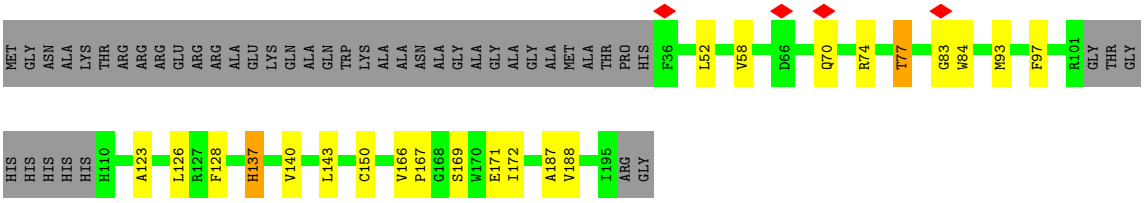
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AO:



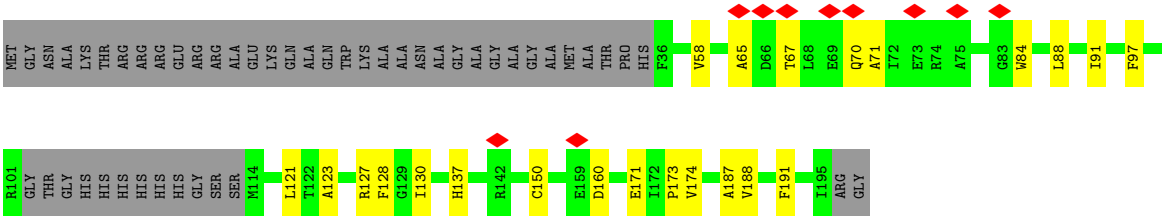
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CA:



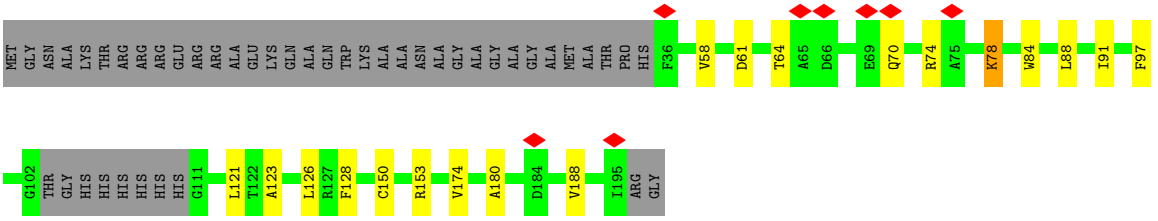
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CB:



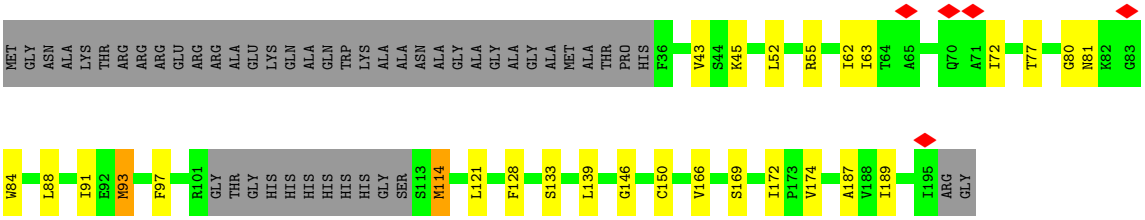
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CC:



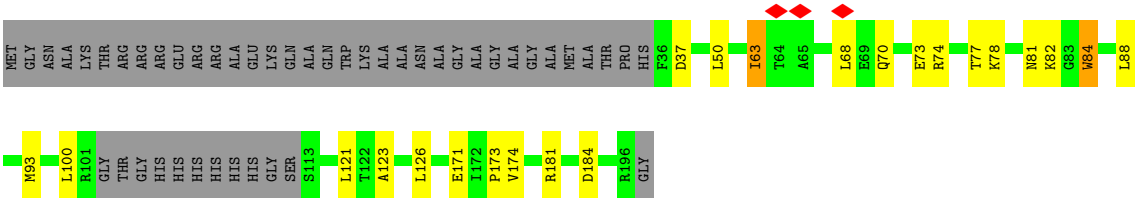
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CD:



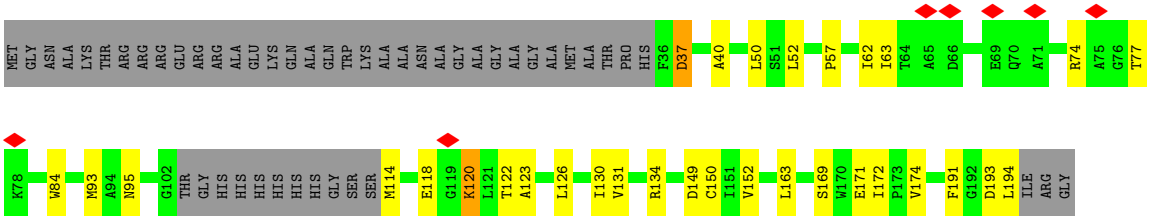
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CE:



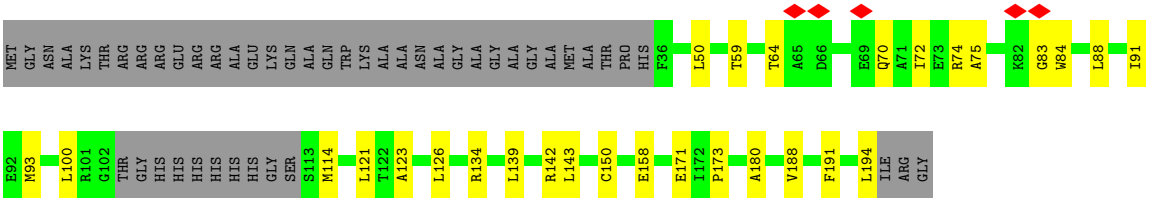
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CF:



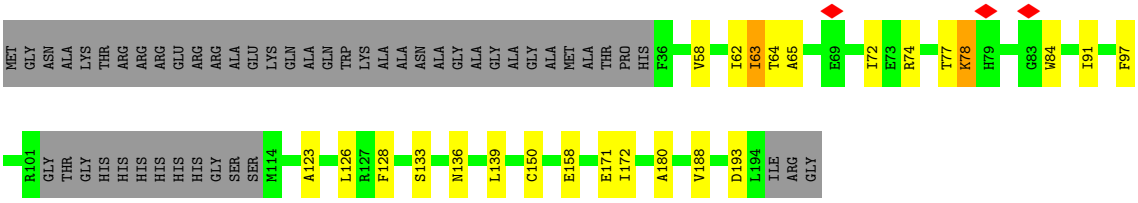
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CG:



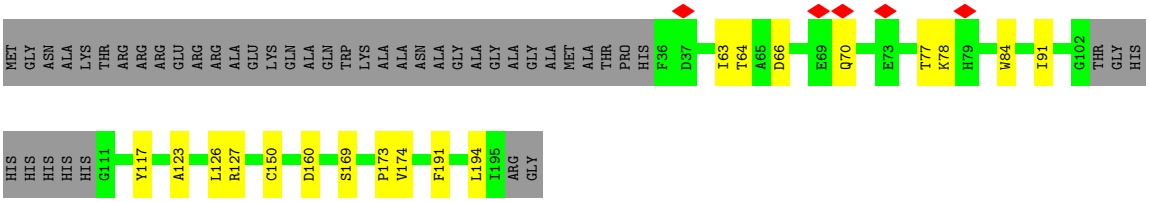
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CH:



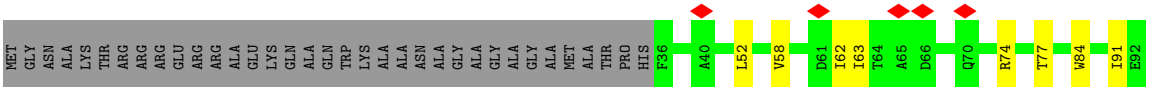
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

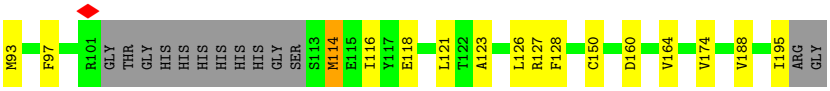
Chain CI:



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

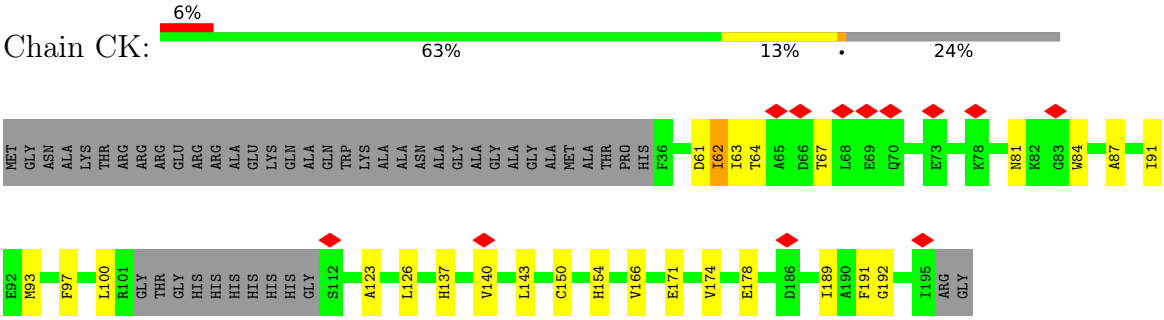
Chain CJ:





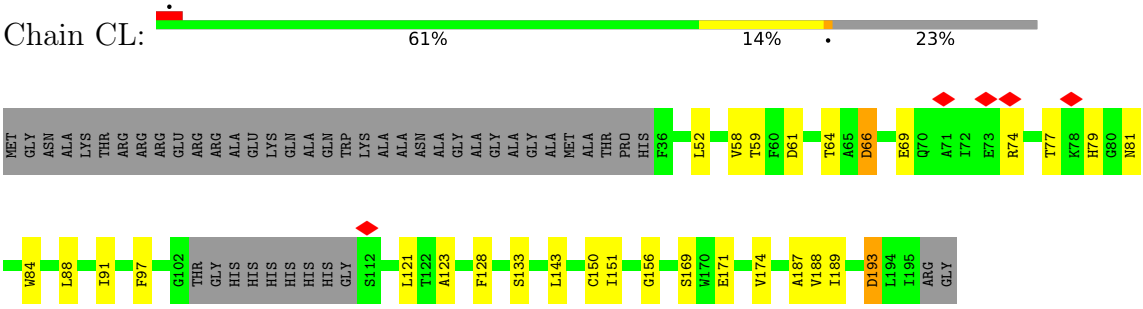
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CK:



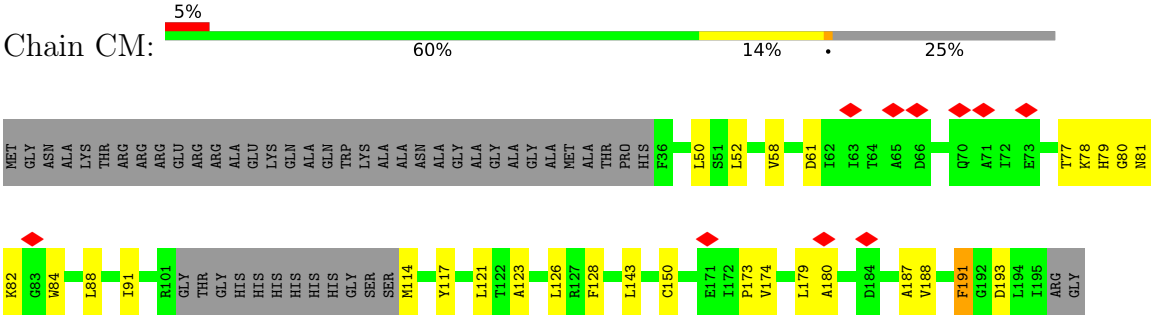
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CL:



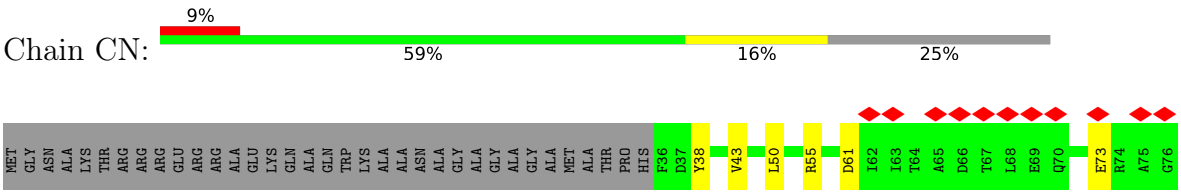
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

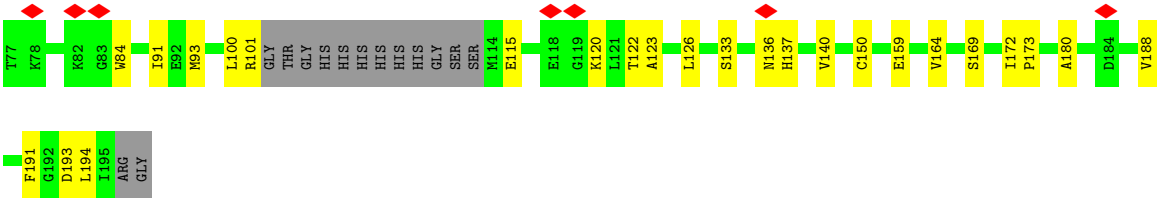
Chain CM:



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

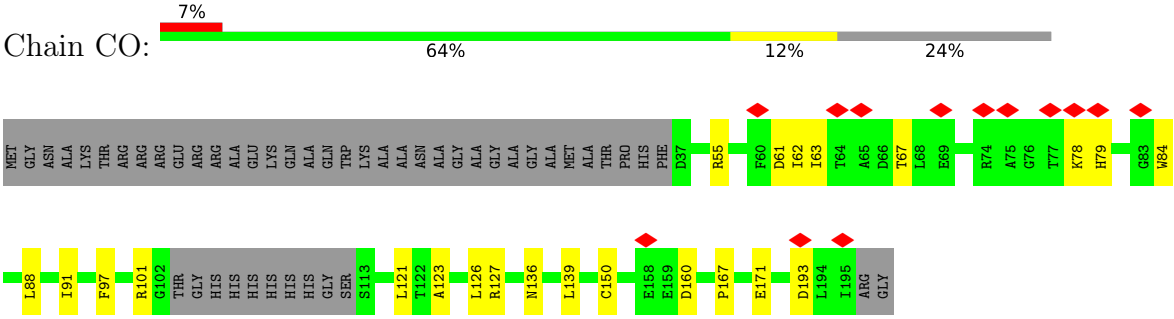
Chain CN:





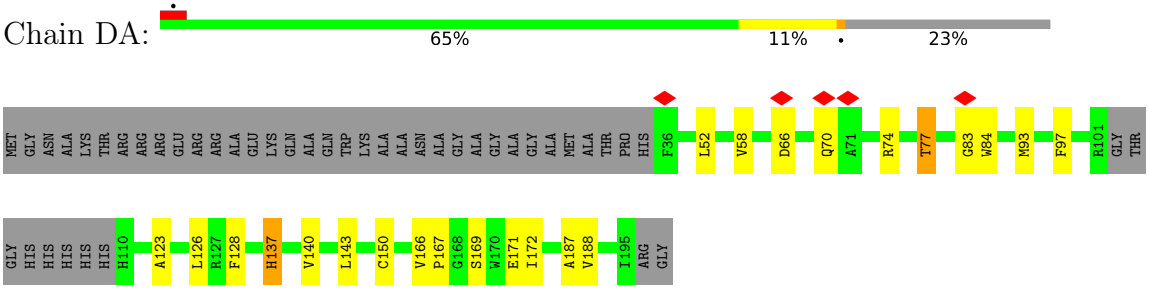
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CO:



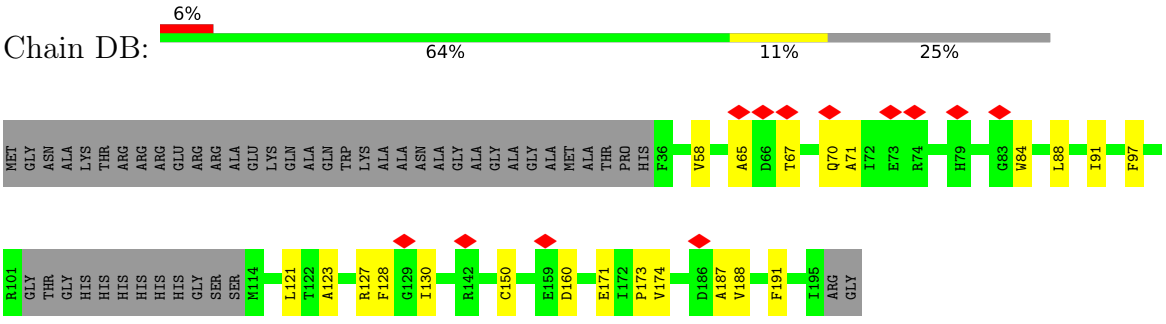
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DA:



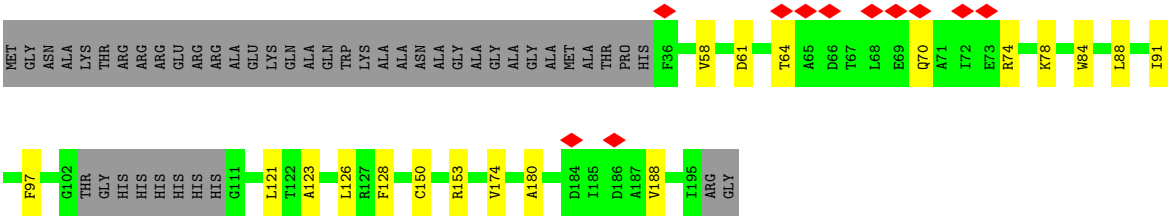
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DB:



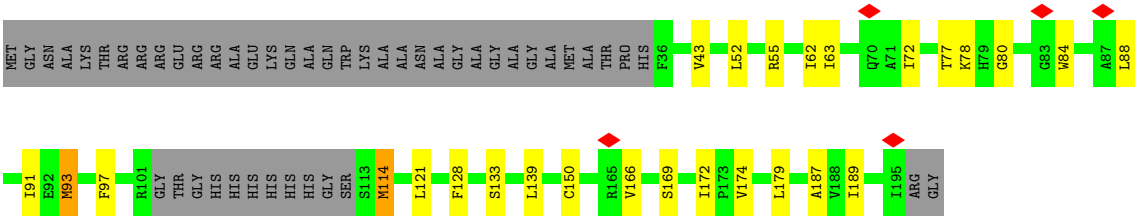
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DC:



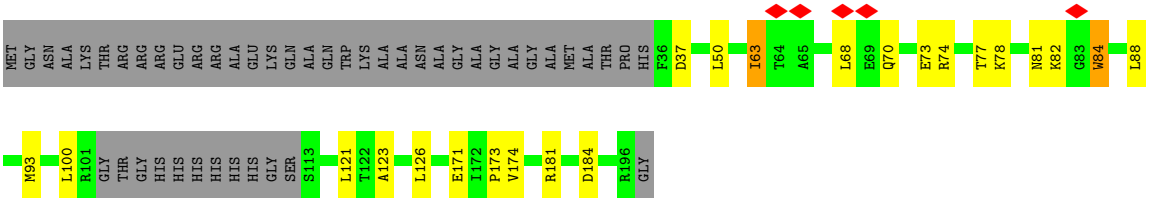
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DD:



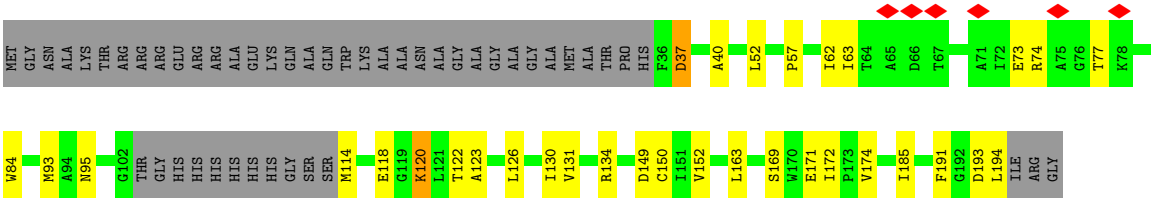
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DE:



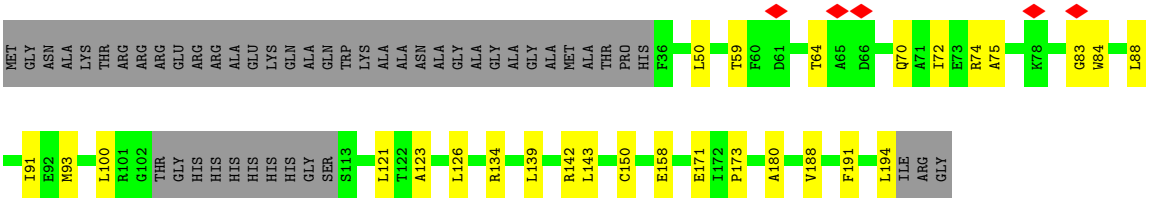
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DF:



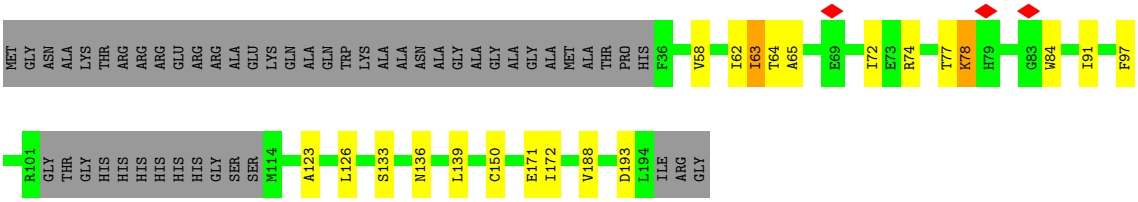
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DG:



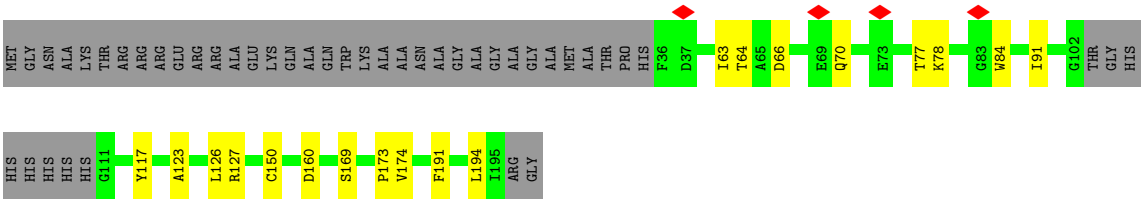
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DH:



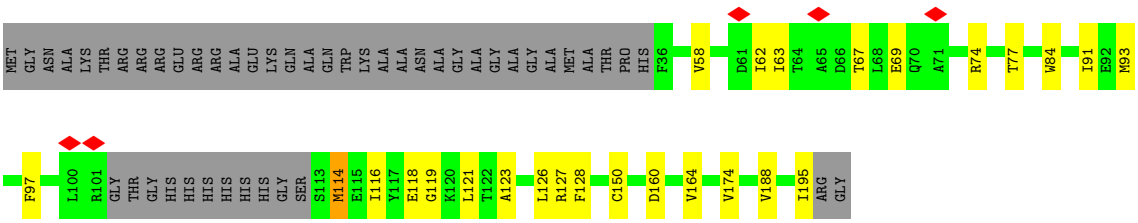
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DI:



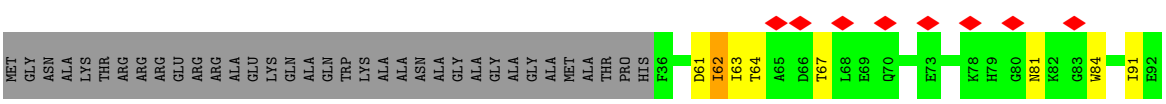
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

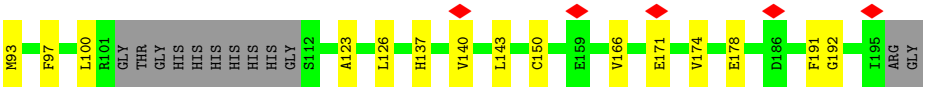
Chain DJ:



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

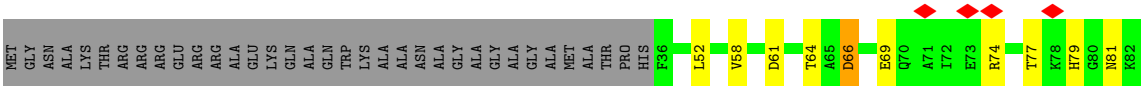
Chain DK:

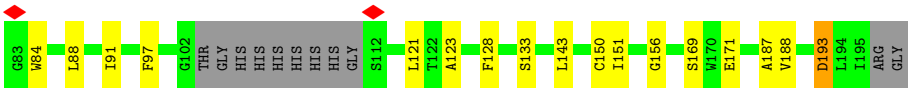




• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

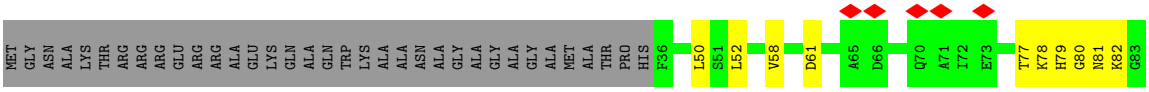
Chain DL:

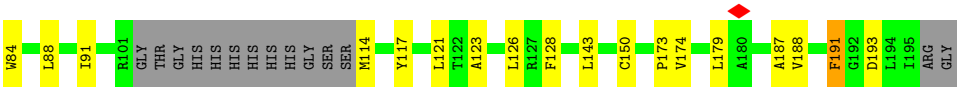




• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

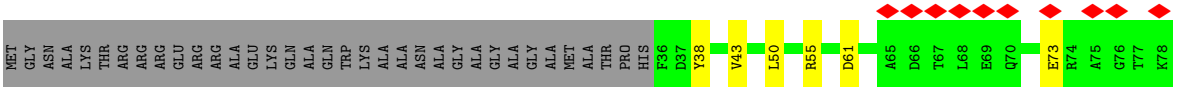
Chain DM:

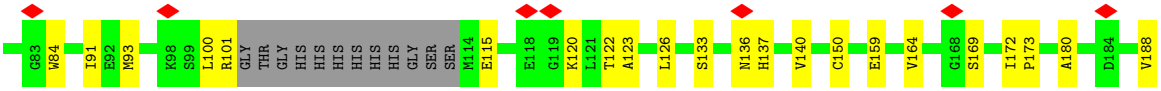


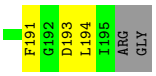


• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DN:

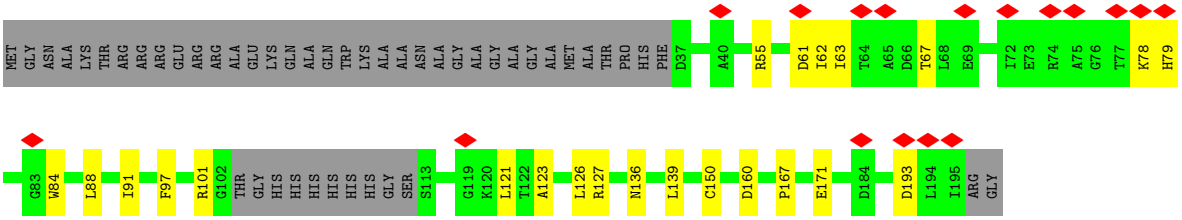






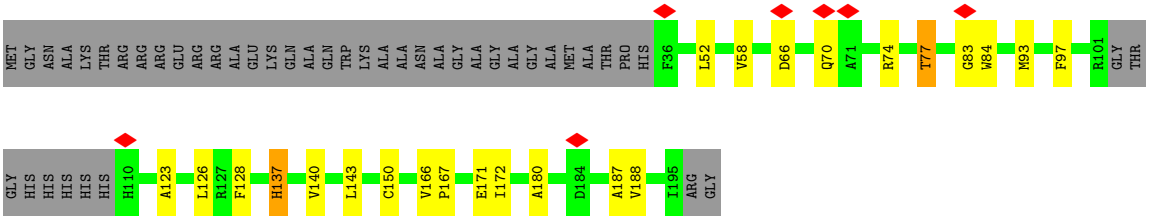
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DO:



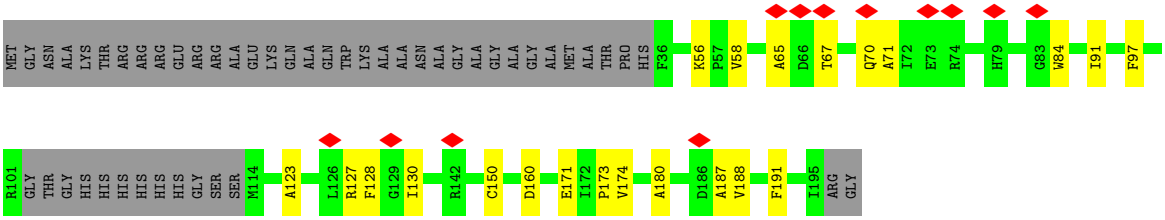
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EA:



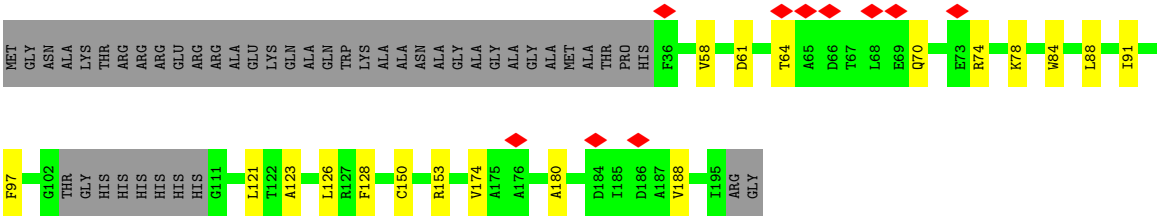
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EB:



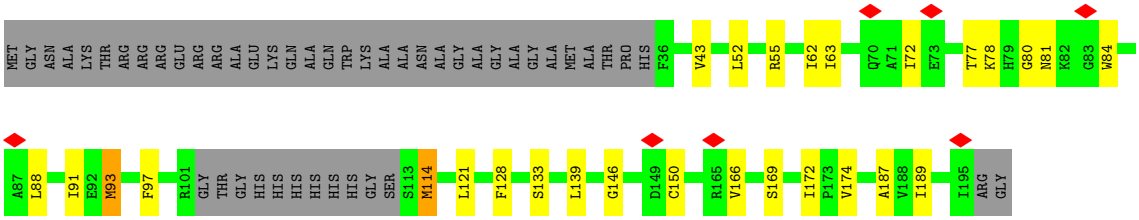
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EC:



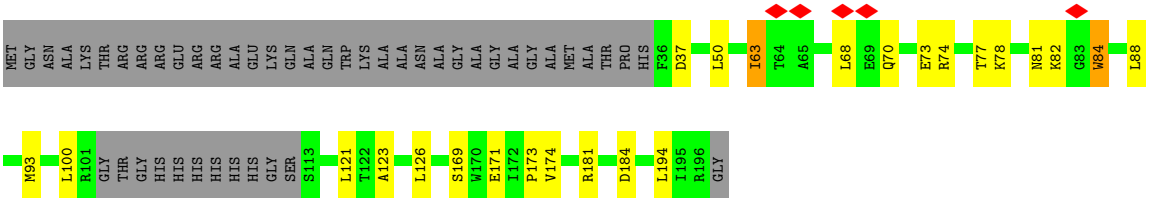
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain ED:



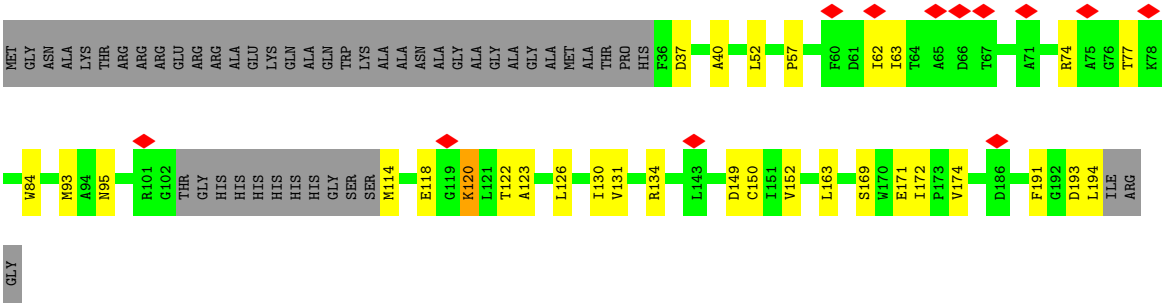
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EE:



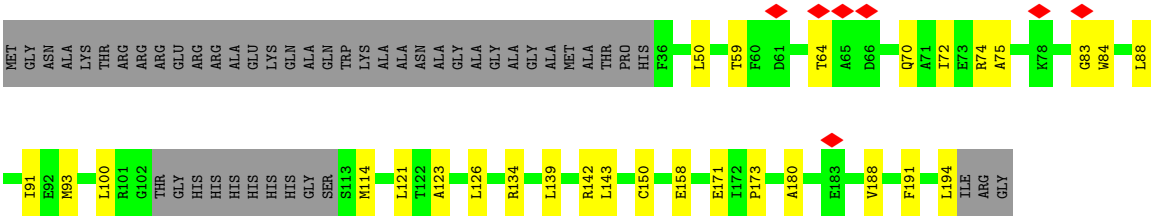
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EF:



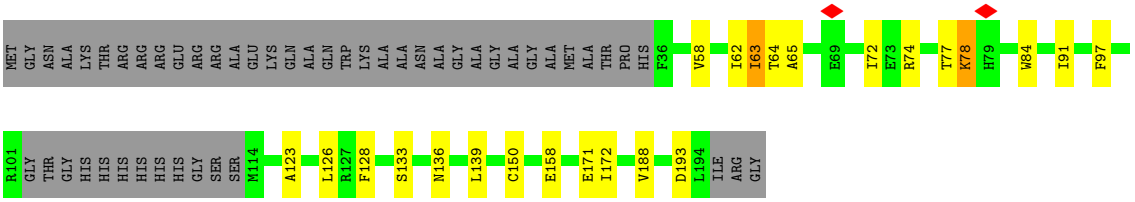
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EG:



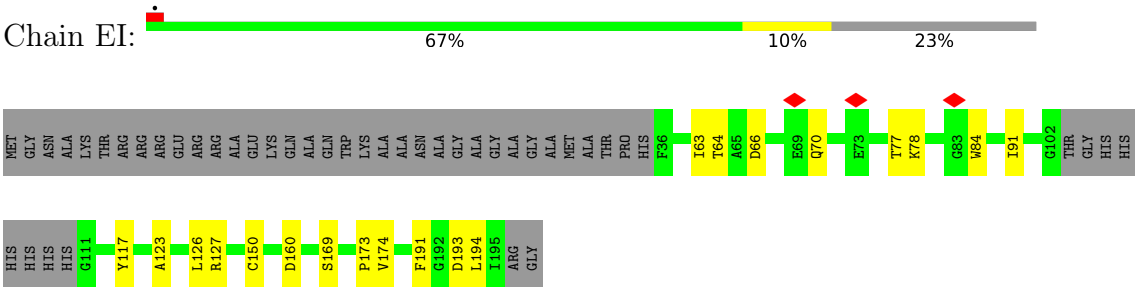
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EH:



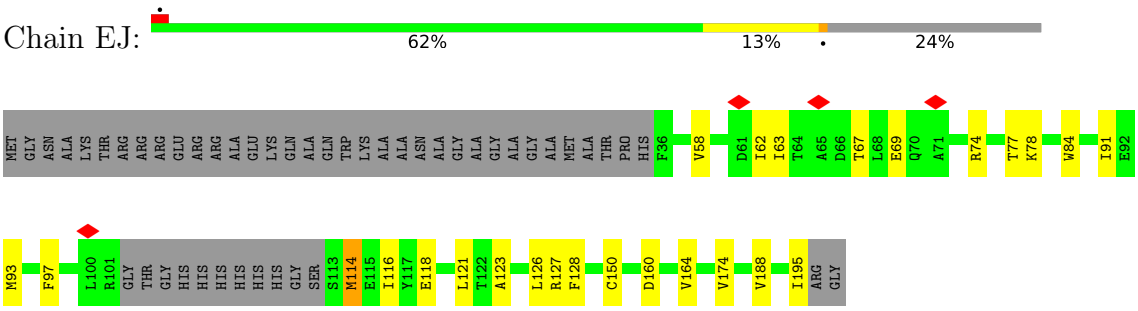
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EI:



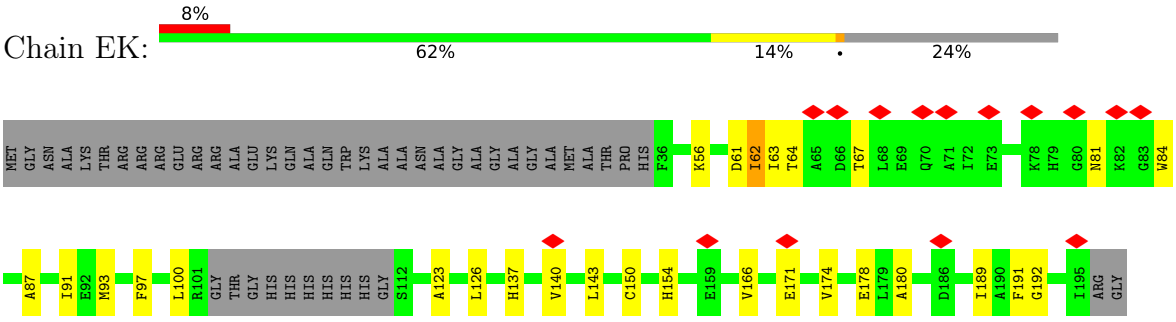
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EJ:



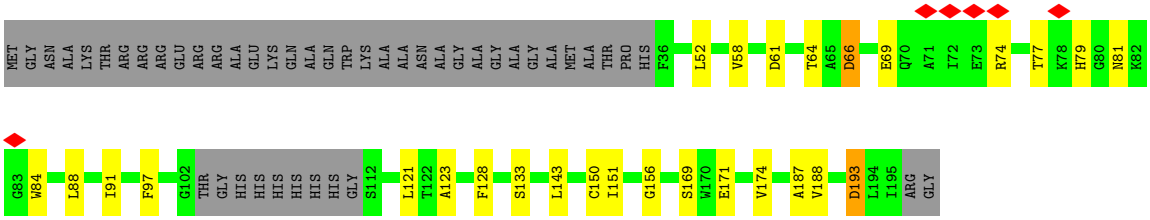
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EK:



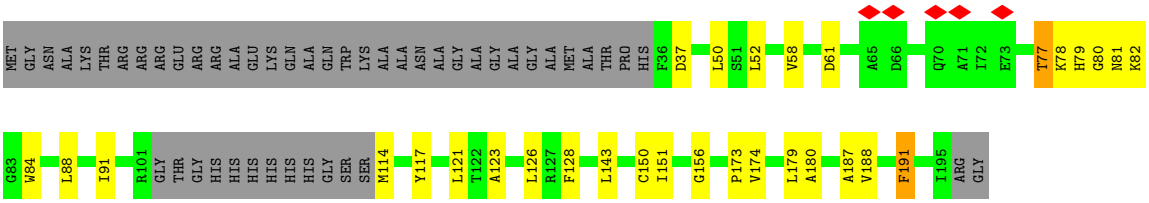
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EL:



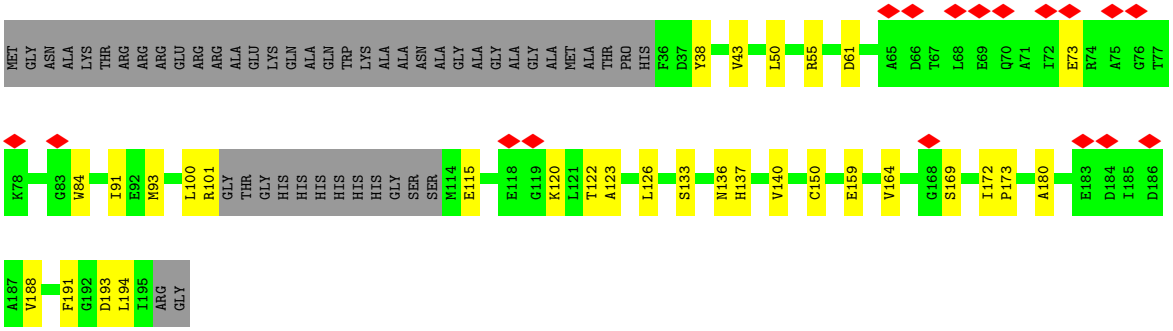
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EM:



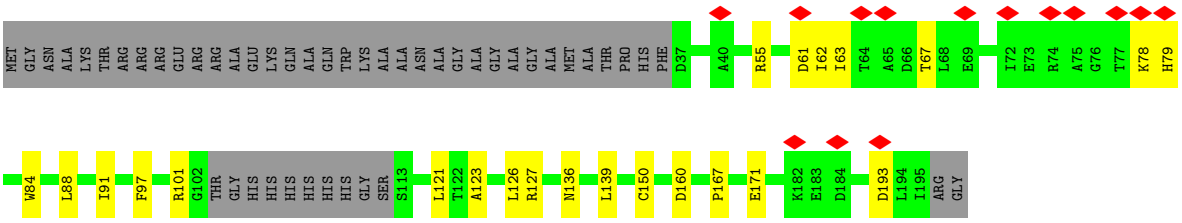
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EN:



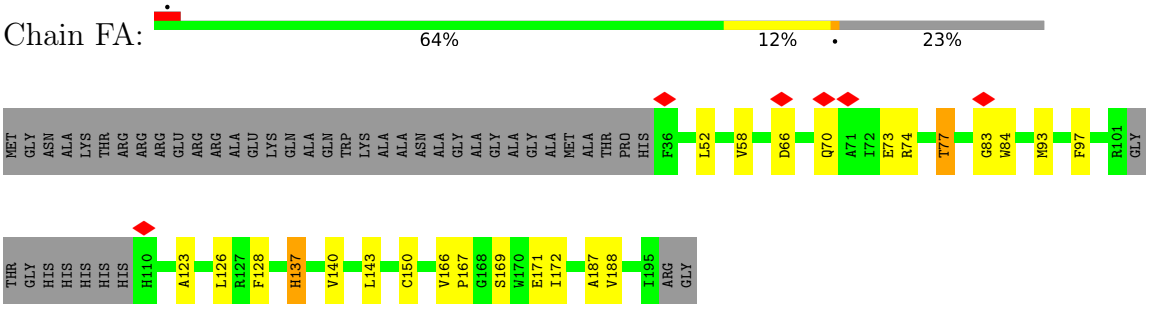
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EO:



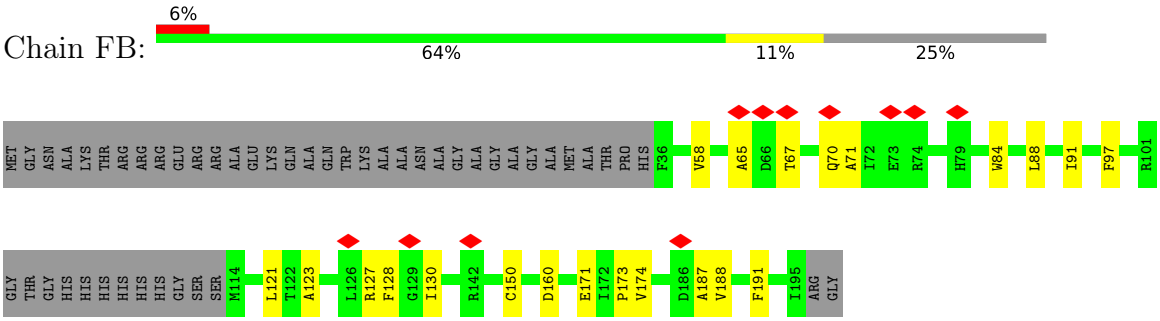
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FA:



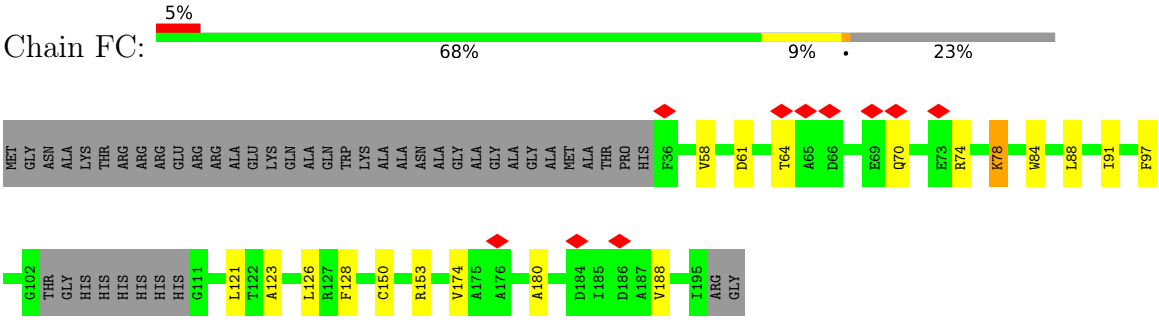
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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

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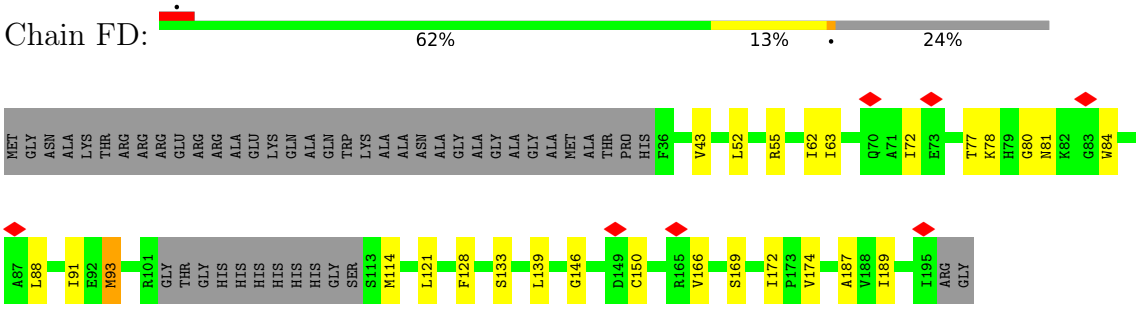

• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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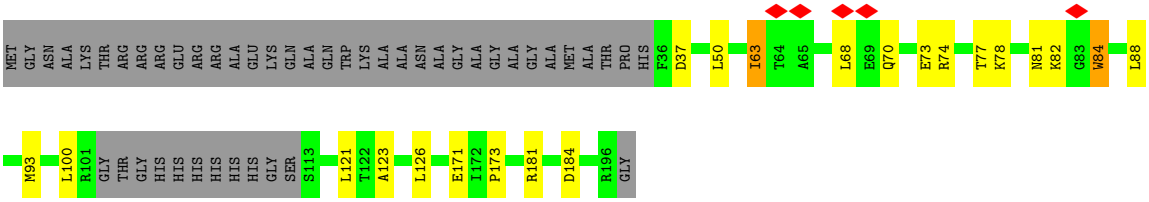

• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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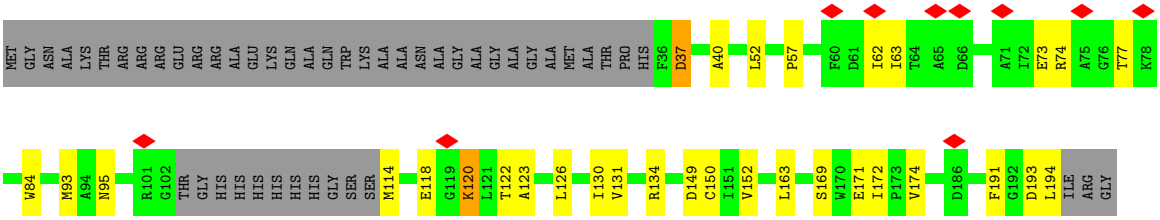
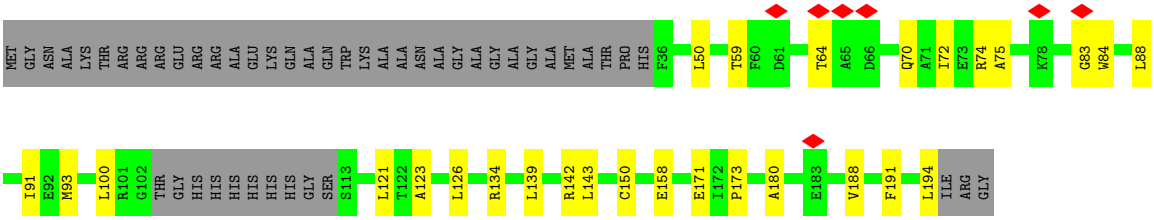


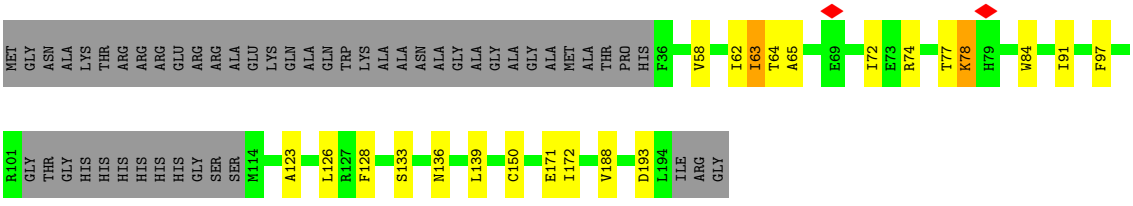
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FG:



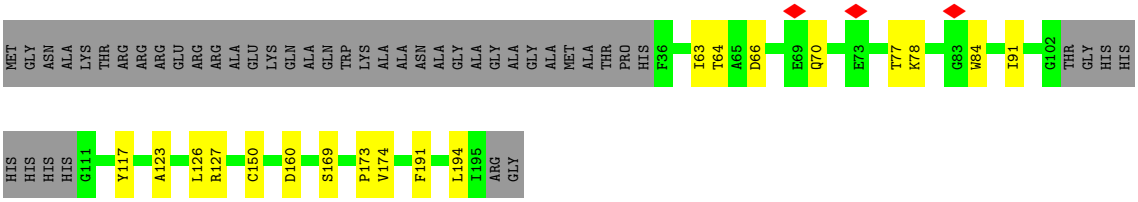
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FH:



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

Chain FI:



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

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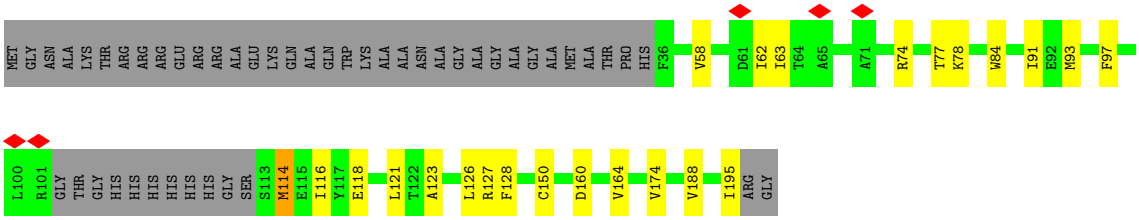

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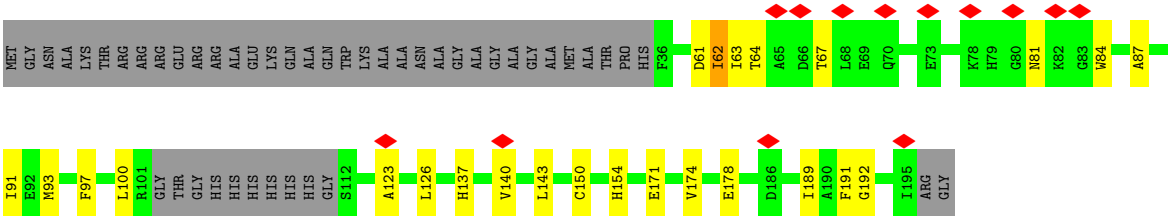
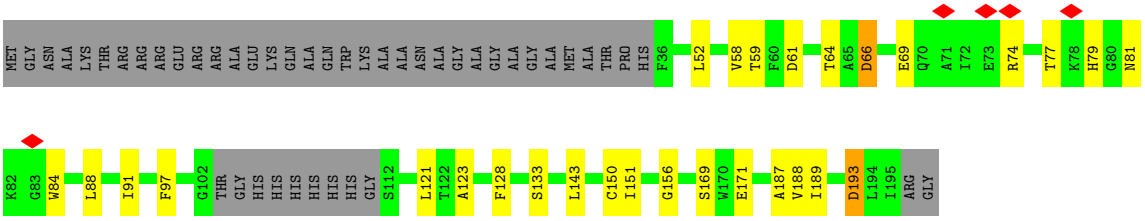
Chain FK:



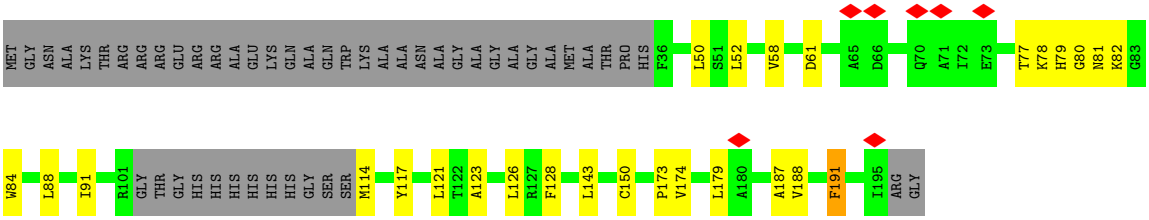
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FL:



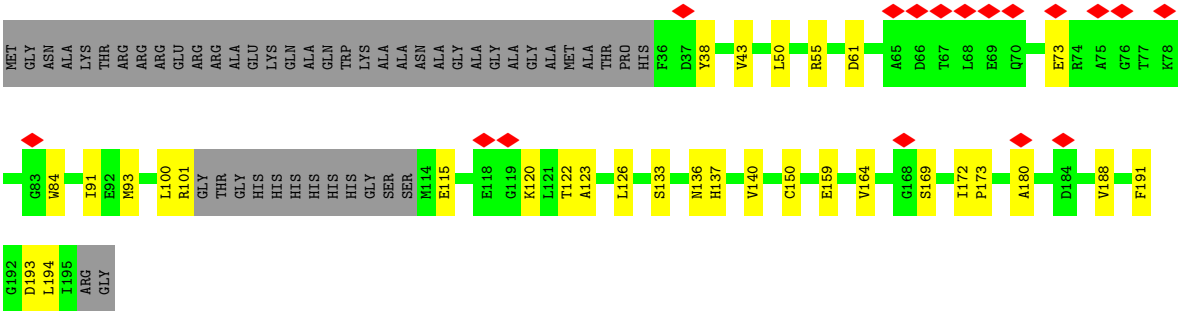
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FM:



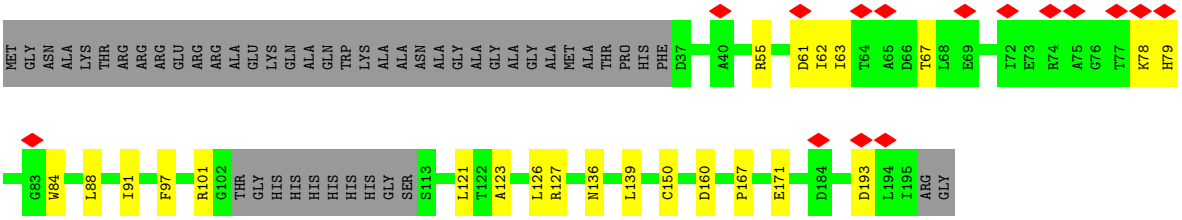
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FN:



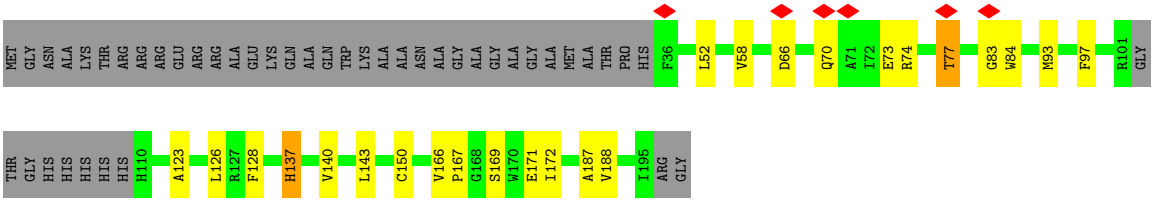
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FO:



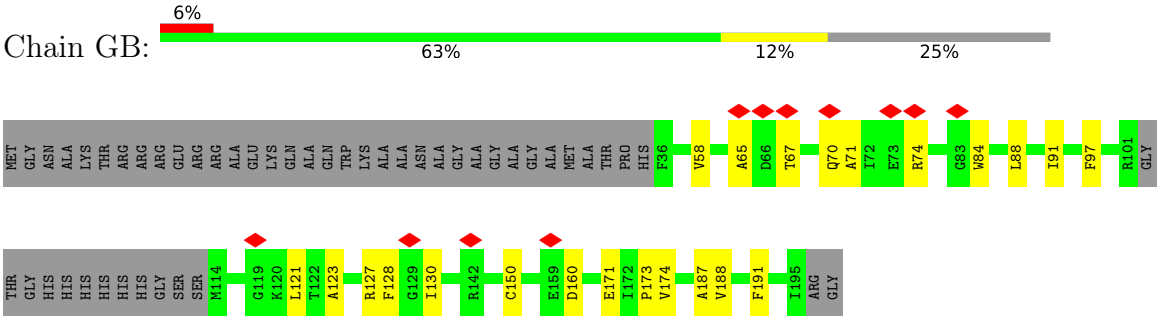
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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

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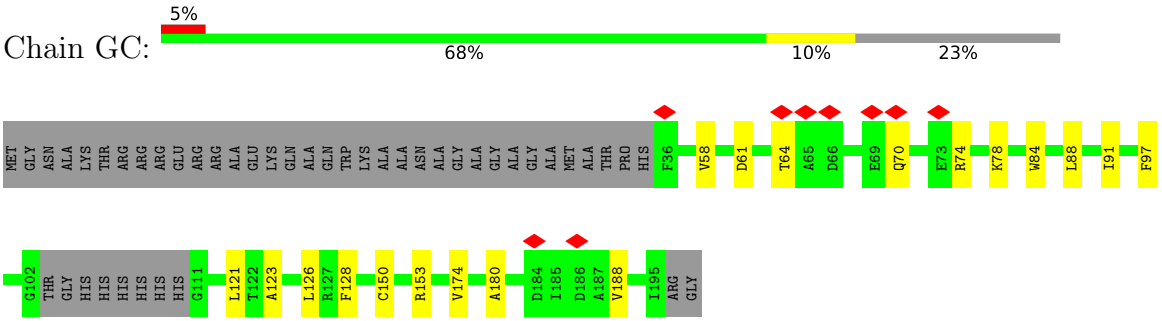

• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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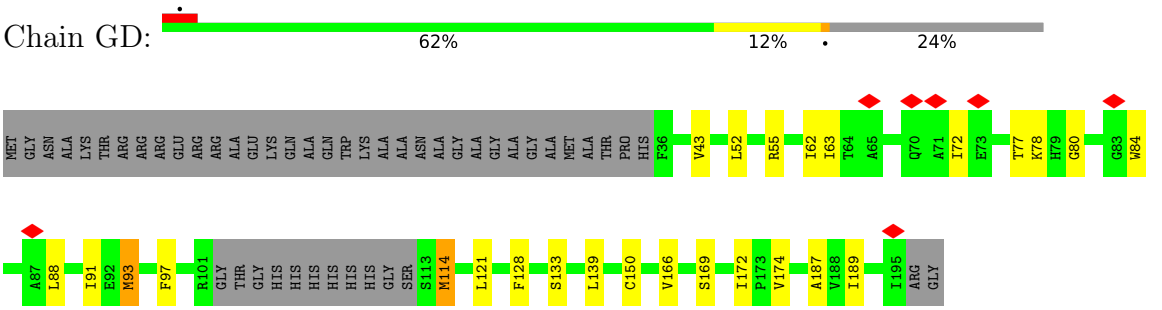

• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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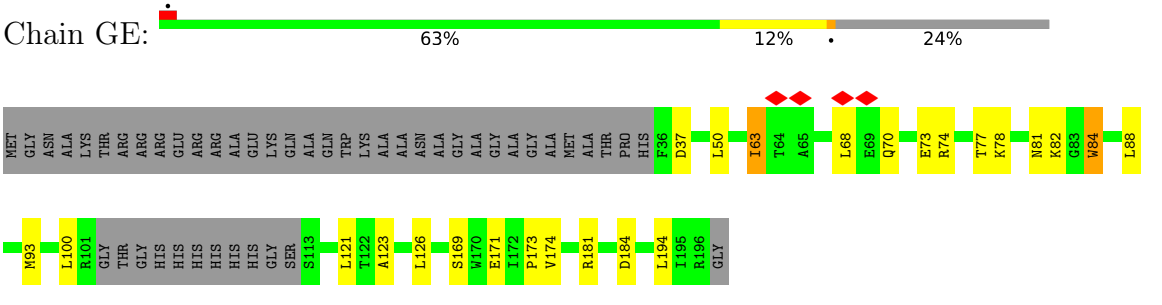

• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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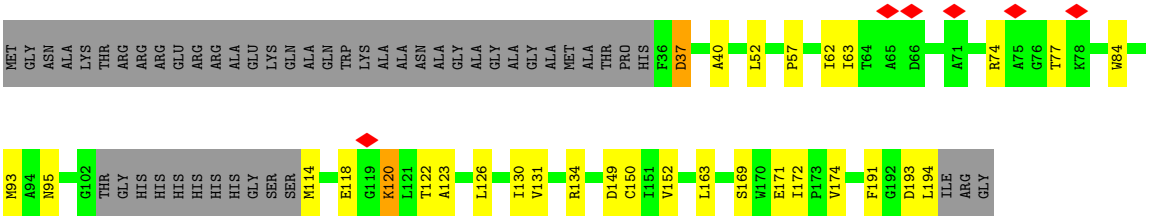

• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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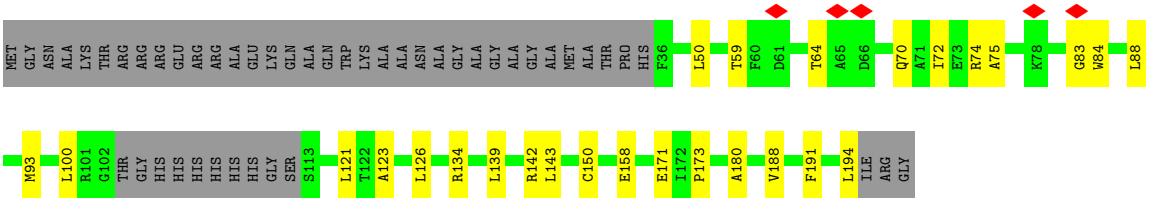

• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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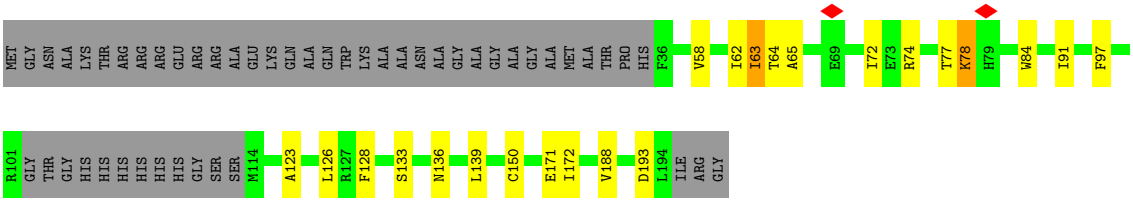
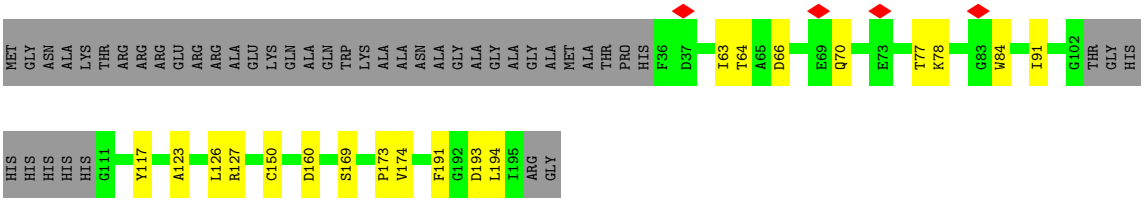


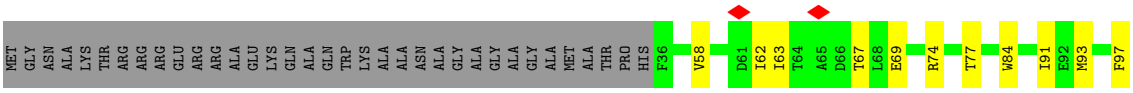
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

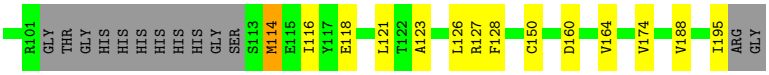
Chain GI:



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

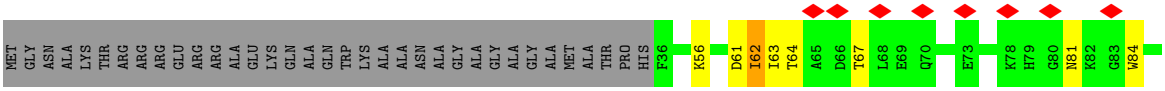
Chain GJ:

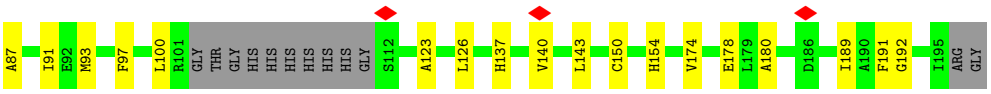




• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

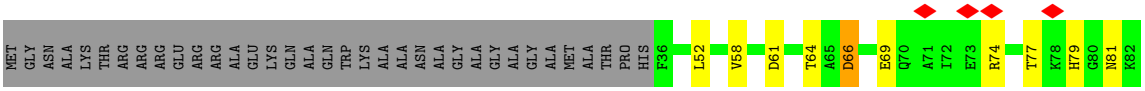
Chain GK:

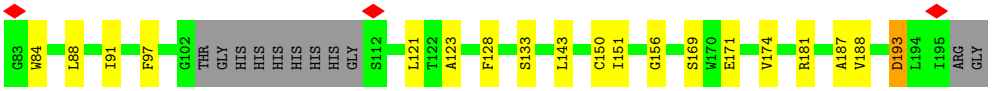




• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

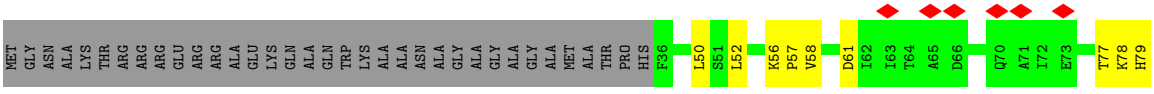
Chain GL:

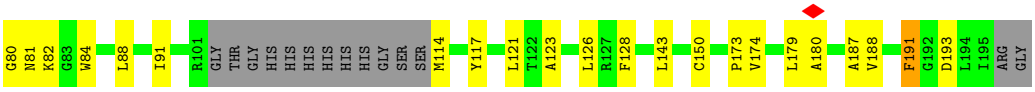




• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

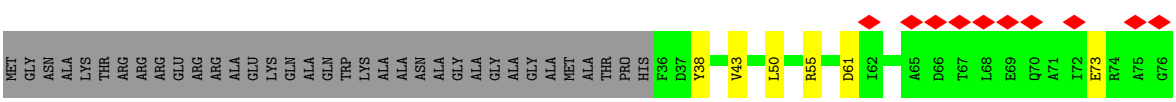
Chain GM:

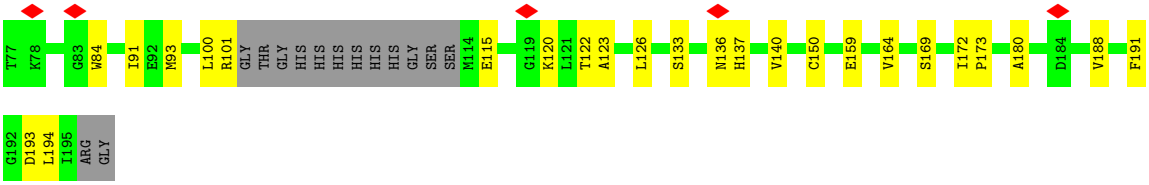




• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

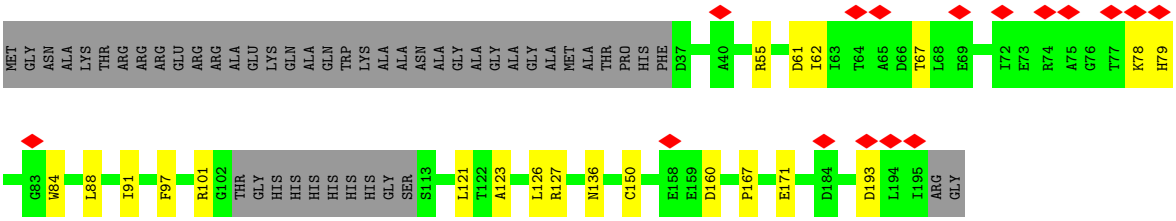
Chain GN:





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

Chain GO:



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

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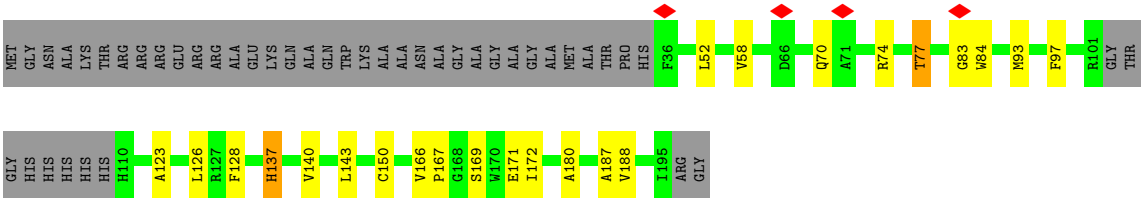
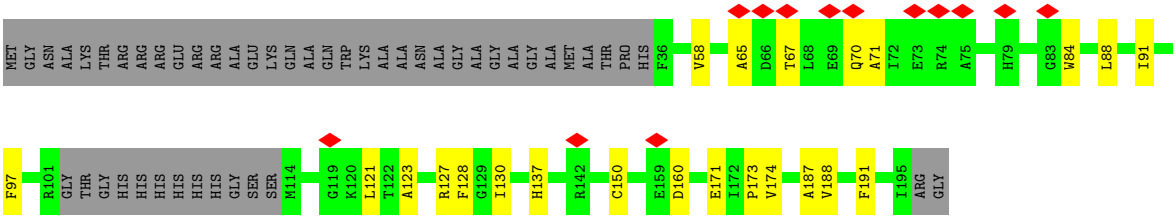


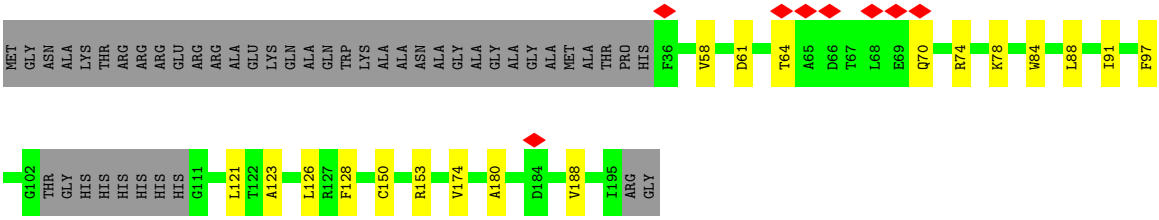
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-rityllumazine synthase,6,7-dimethyl-8-rityllumazine synthase

Chain HB:



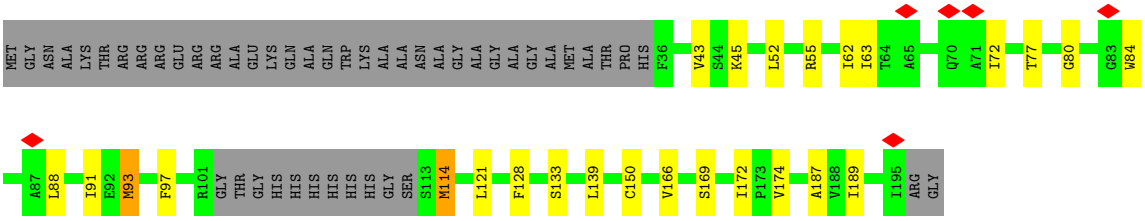
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-rityllumazine synthase,6,7-dimethyl-8-rityllumazine synthase

Chain HC:



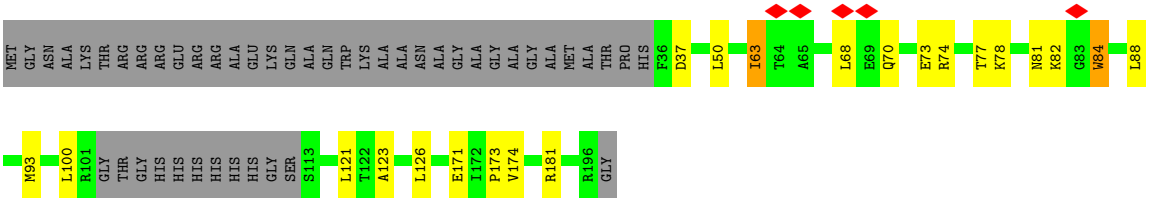
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HD:



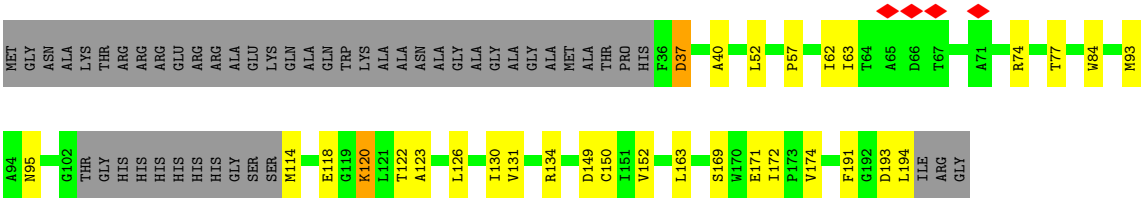
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HE:



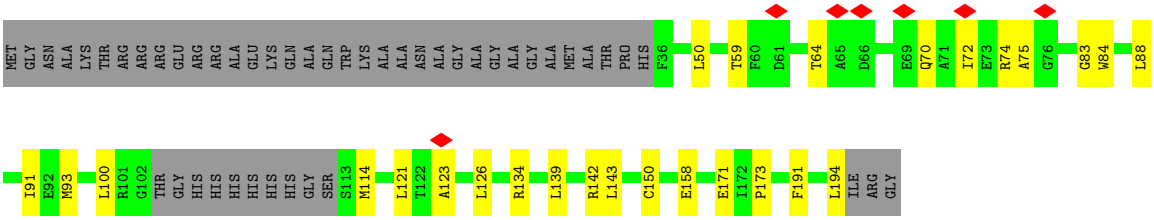
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HF:



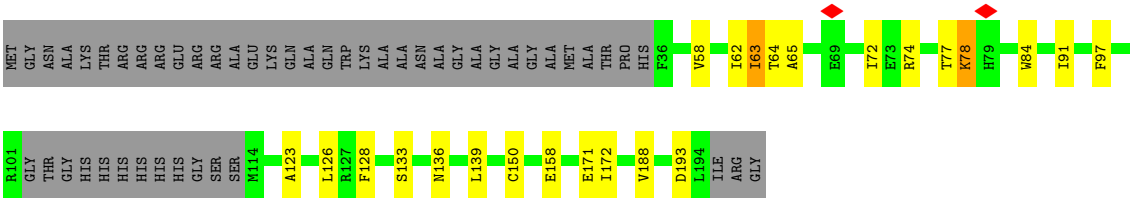
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HG:



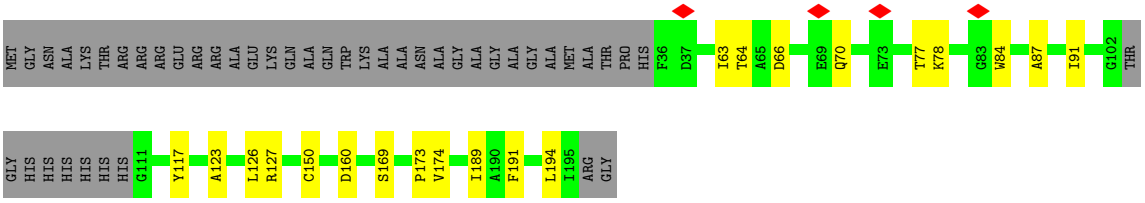
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HH:



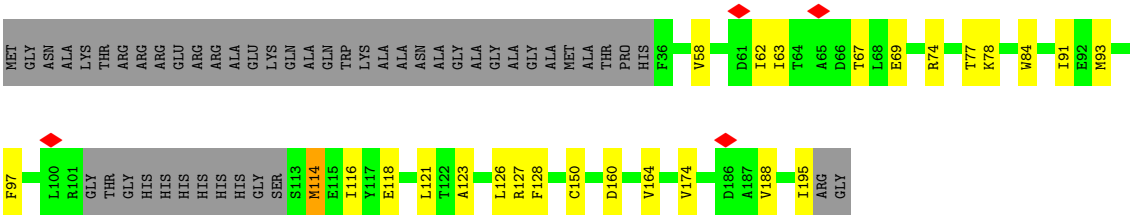
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HI:



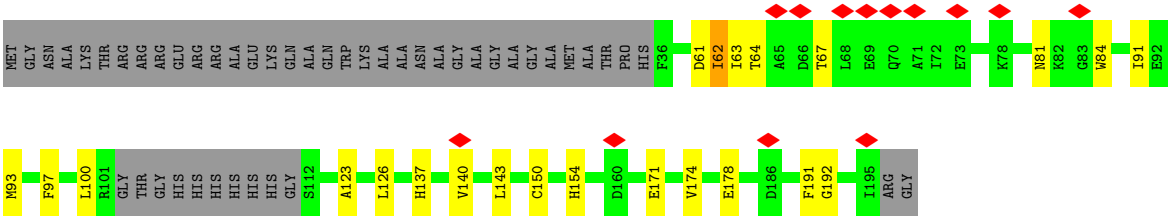
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HJ:



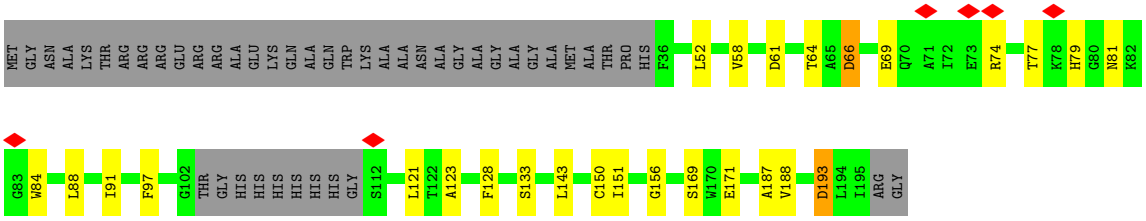
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HK:



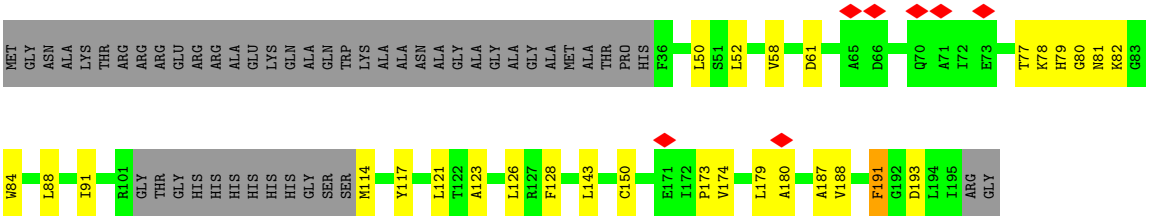
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HL:



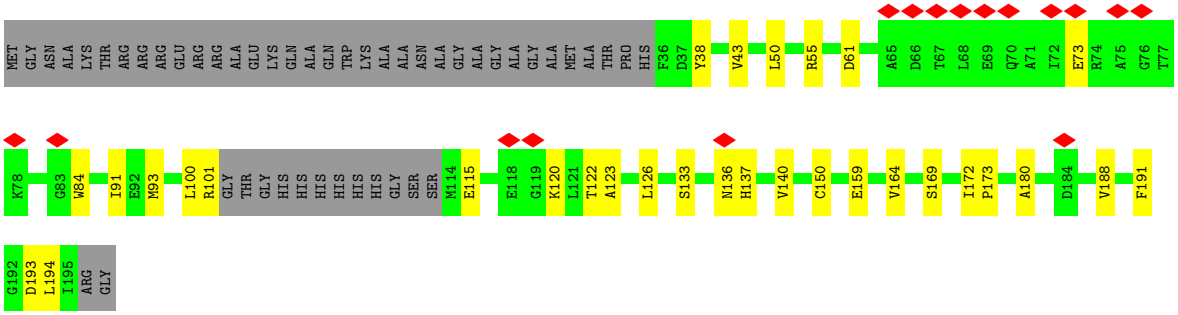
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HM:



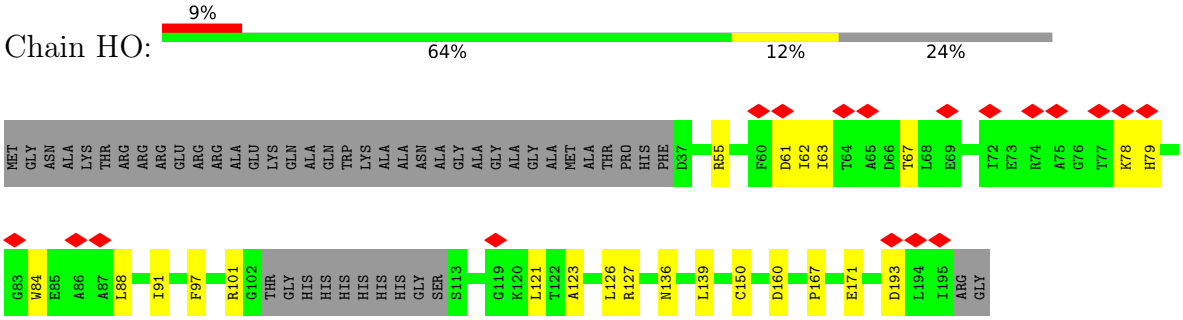
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HN:



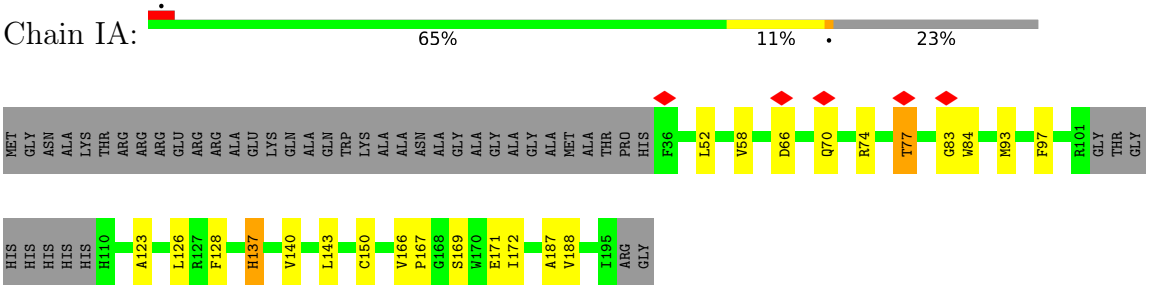
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HO:



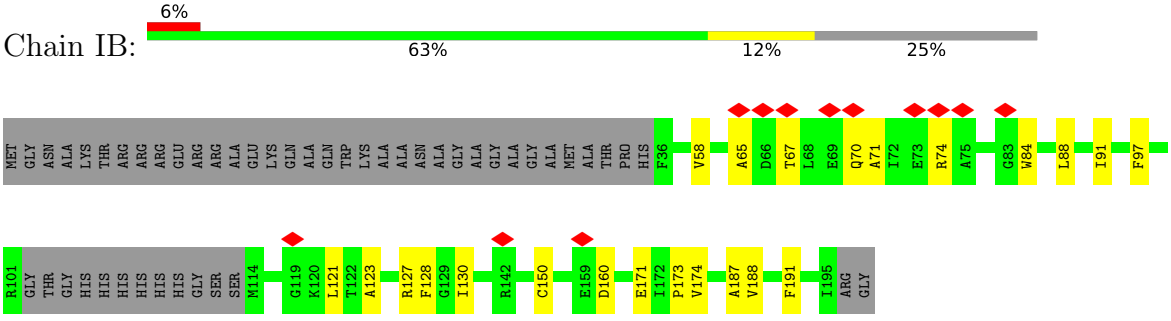
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IA:



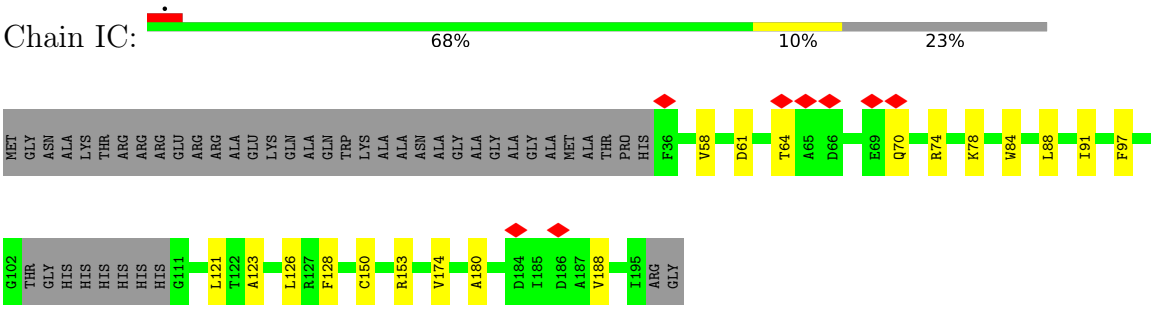
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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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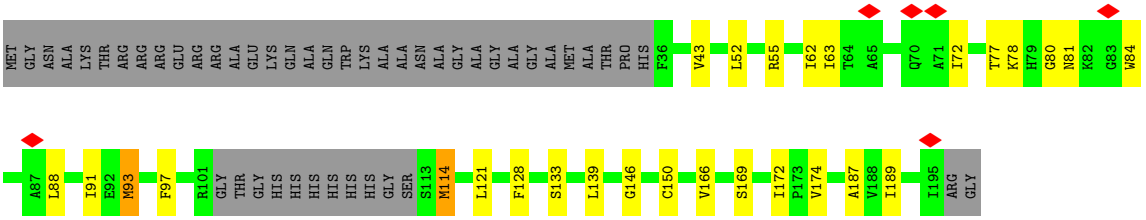
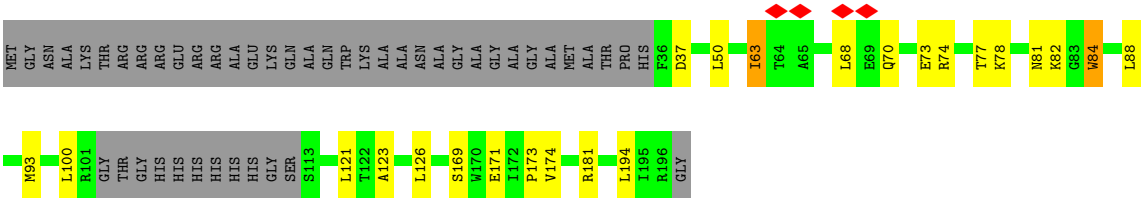


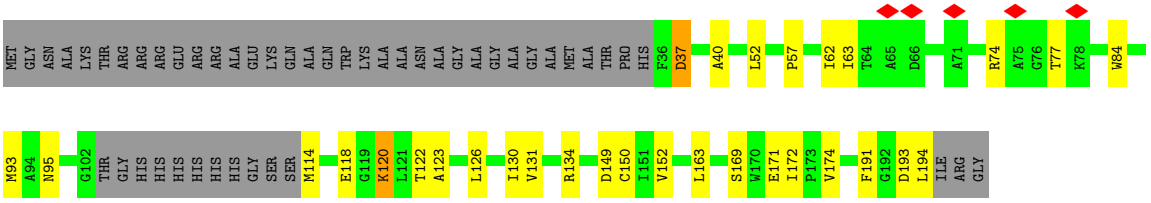
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IE:



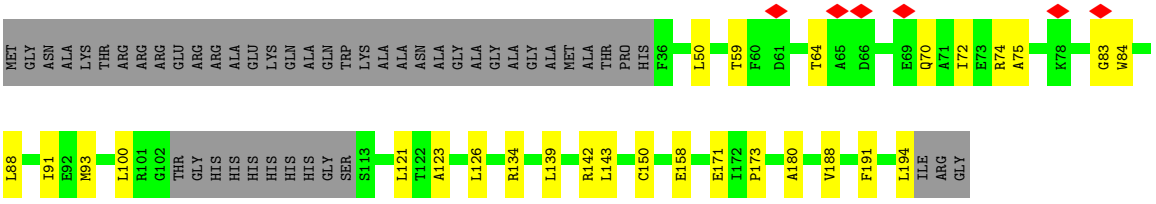
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IF:



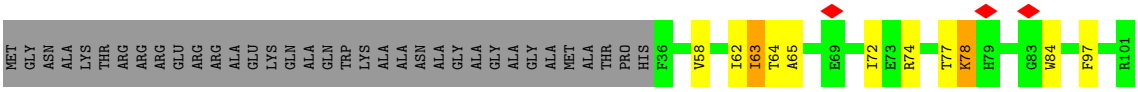
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IG:



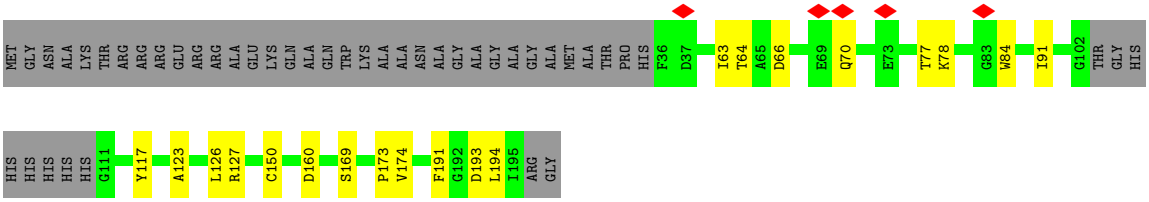
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IH:



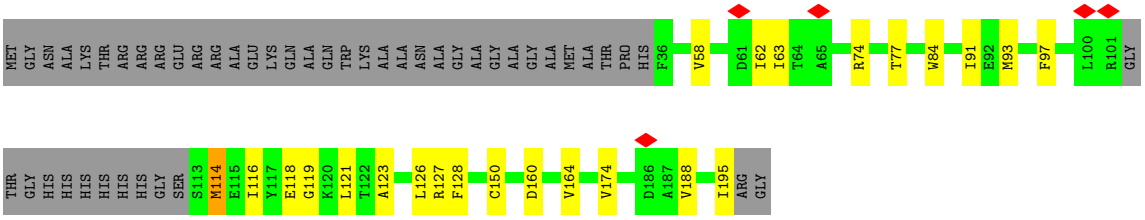
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain II:



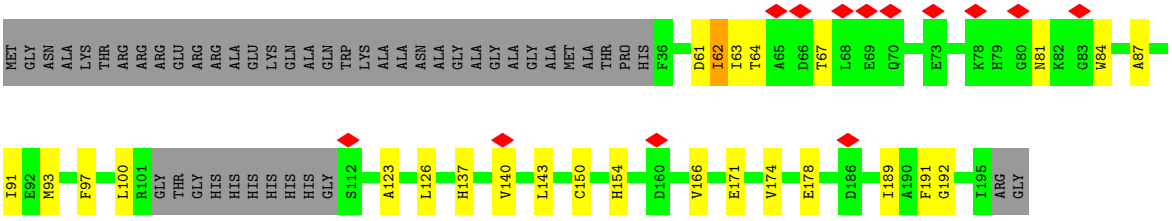
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IJ:



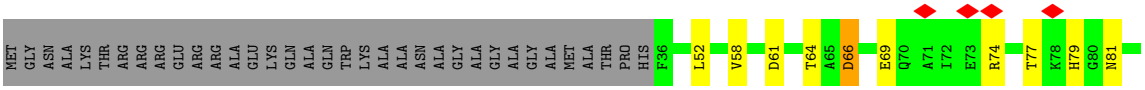
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IK:



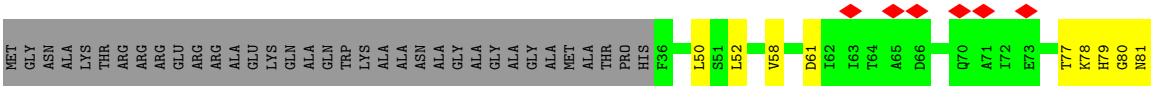
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

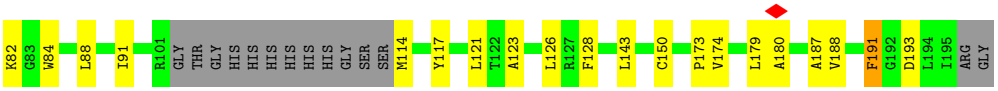
Chain IL:



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

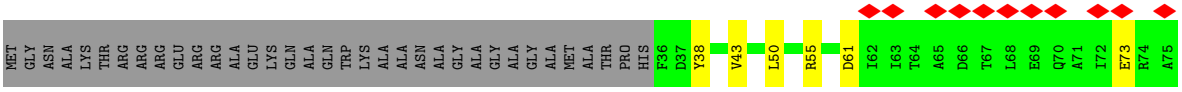
Chain IM:

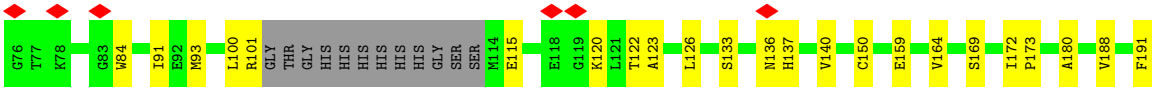


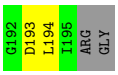


• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IN:

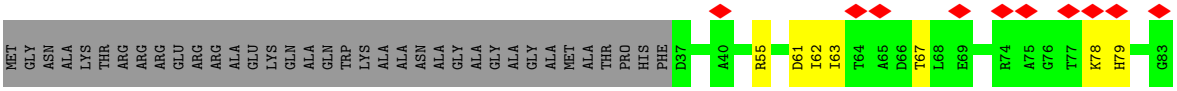






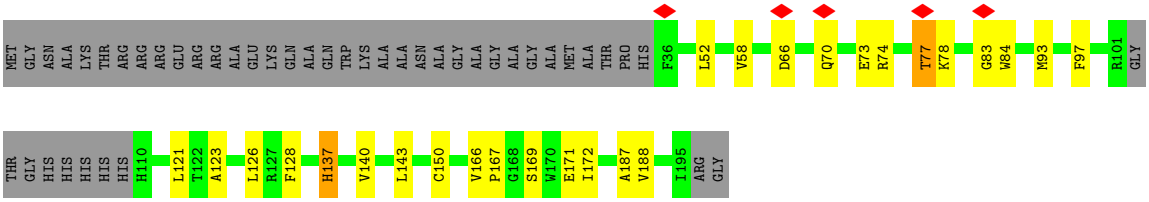
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IO:



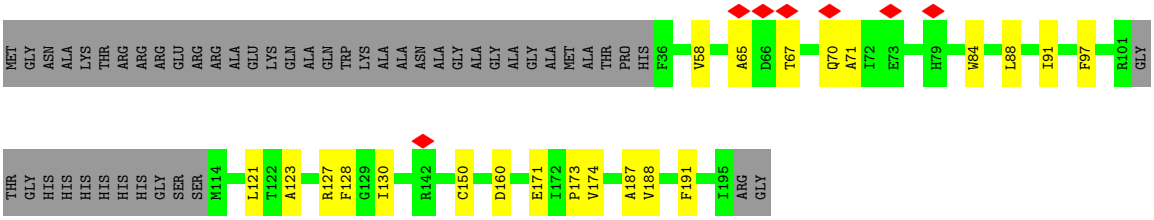
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JA:



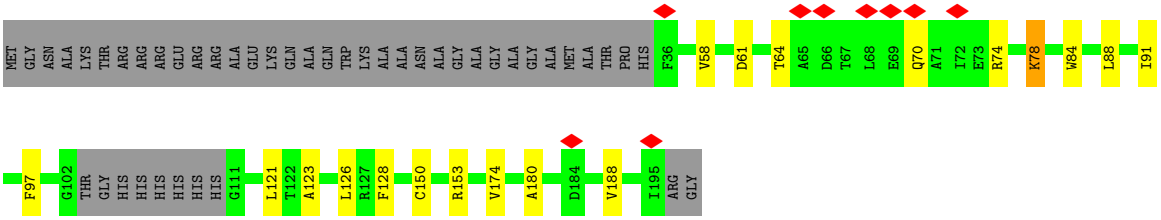
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JB:



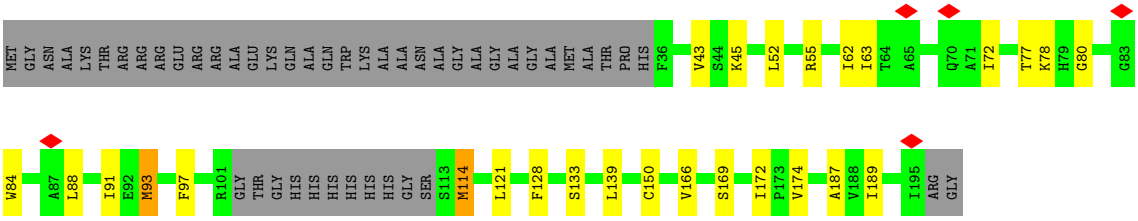
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JC:



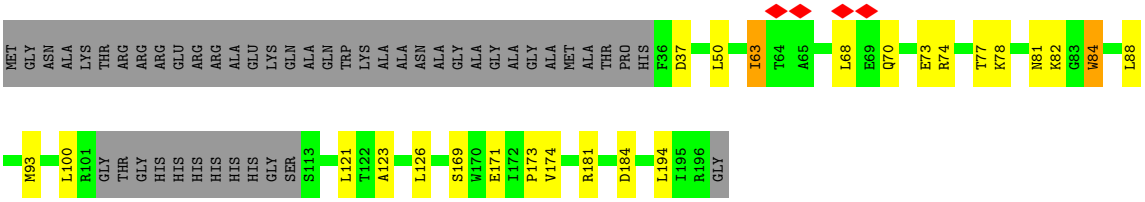
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JD:



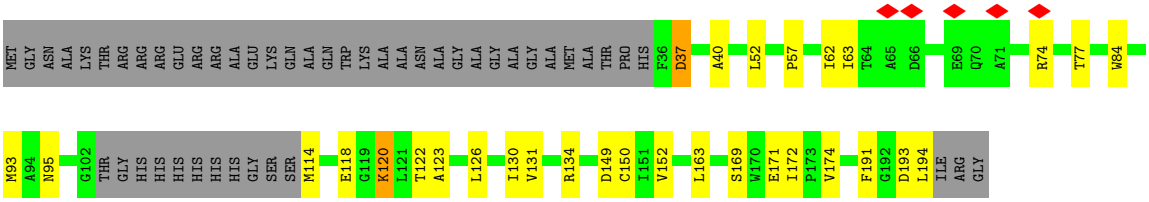
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JE:



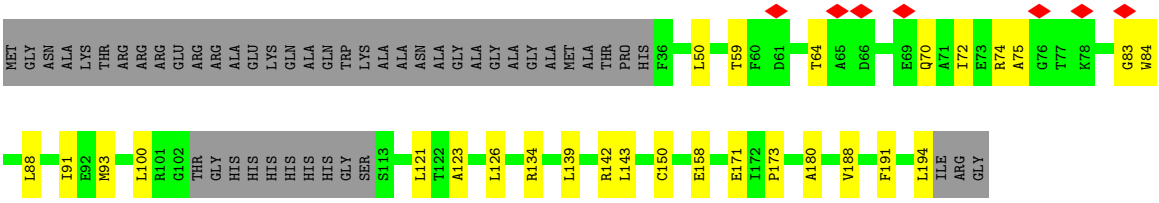
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JF:



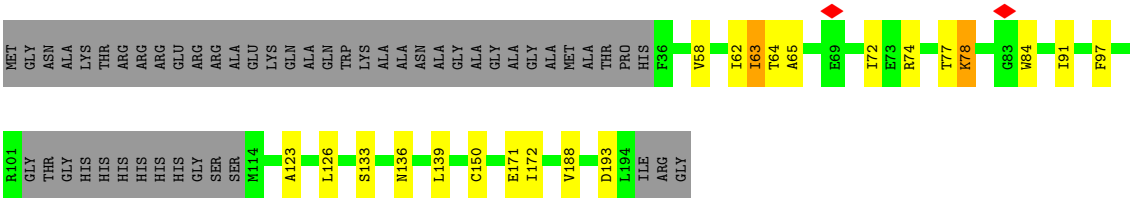
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JG:



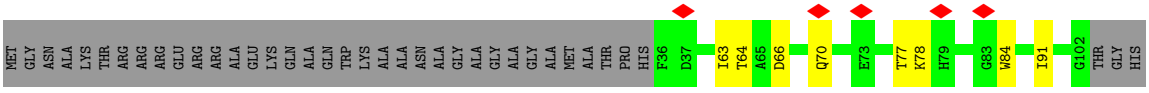
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JH:



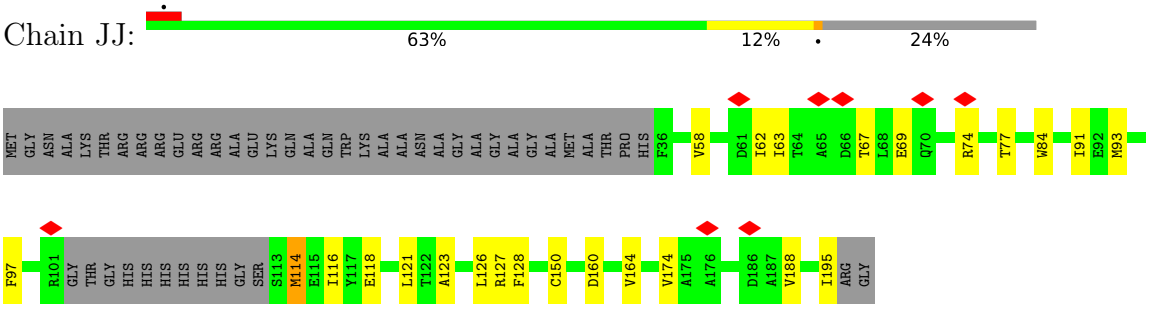
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JI:



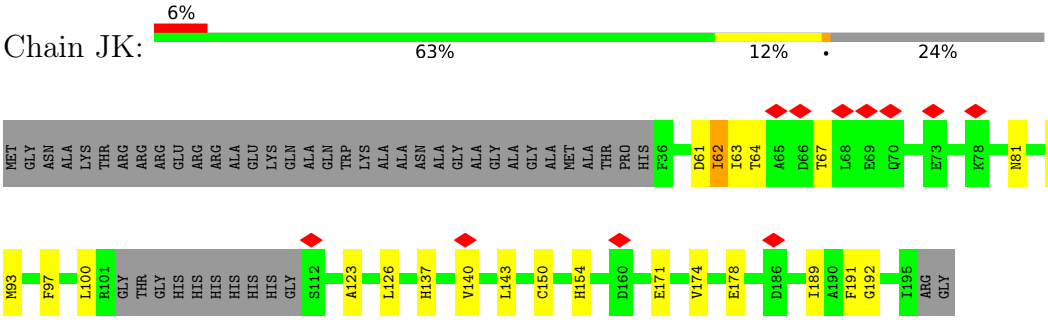
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JJ:



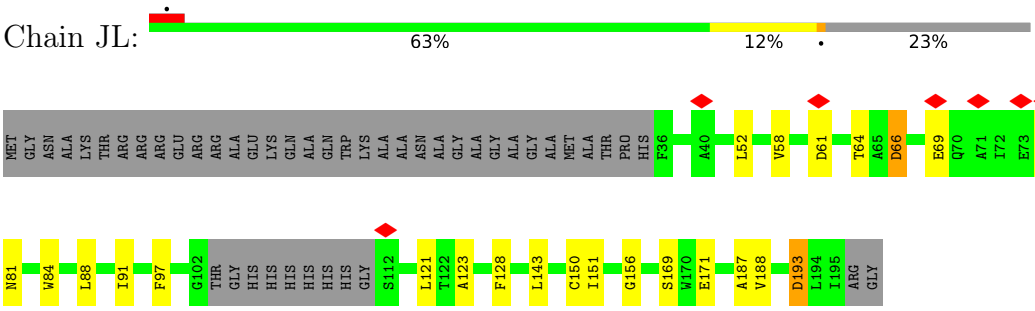
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JK:



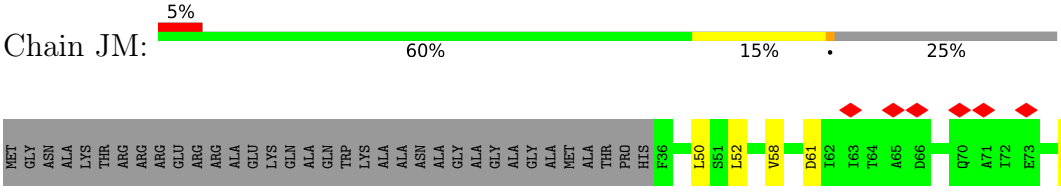
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

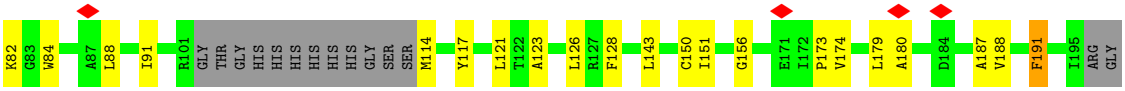
Chain JL:



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

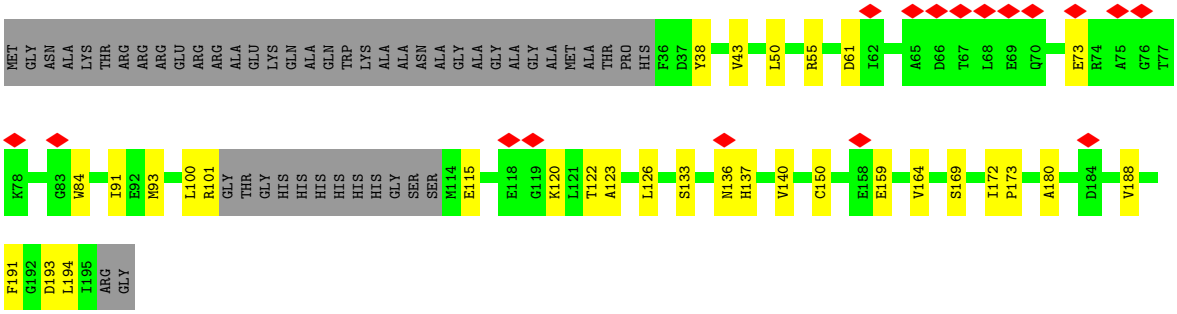
Chain JM:





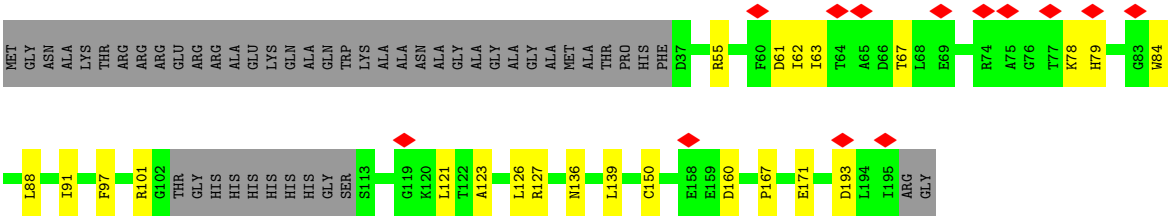
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JN:



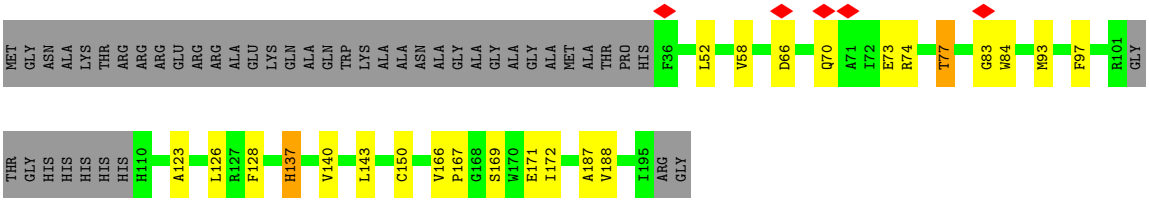
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JO:



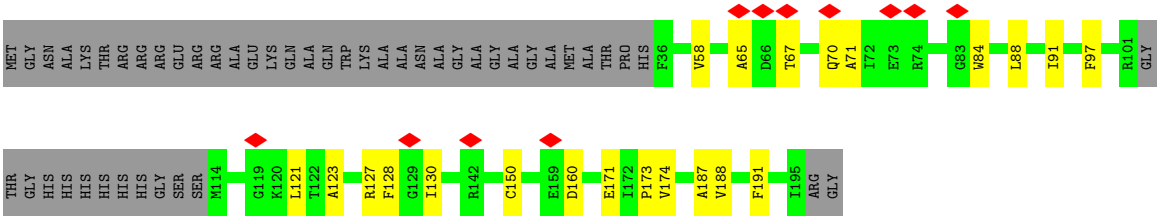
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KA:



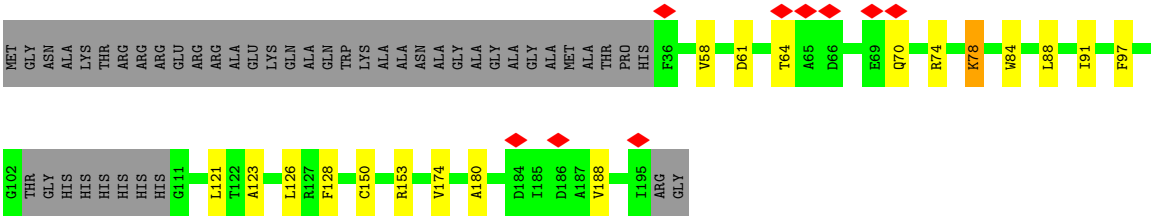
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KB:



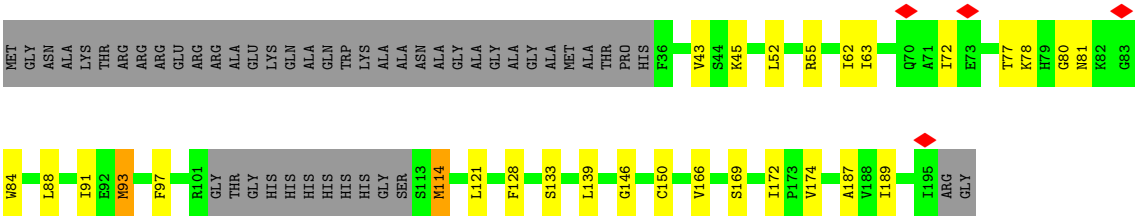
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KC:



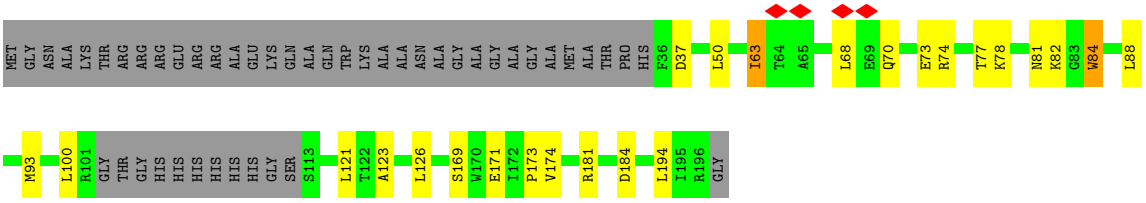
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KD:



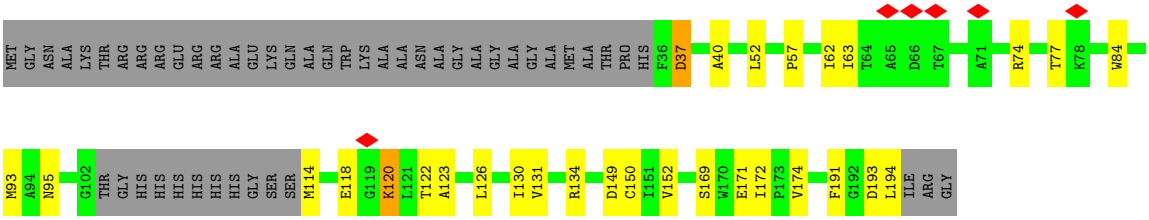
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KE:



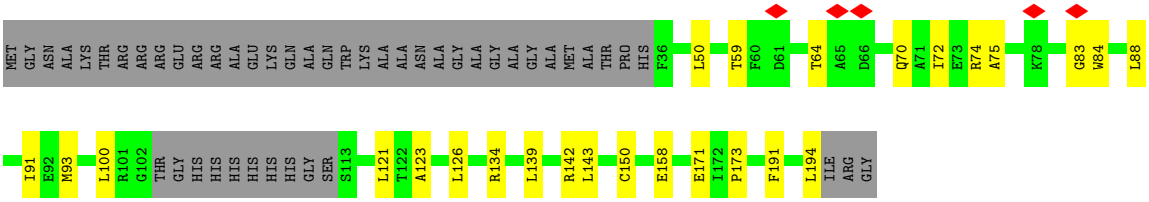
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KF:



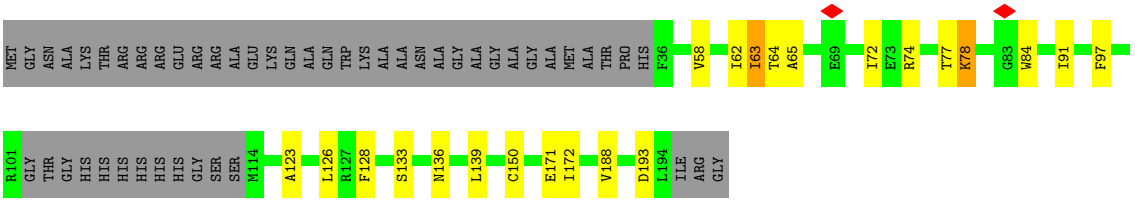
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KG:



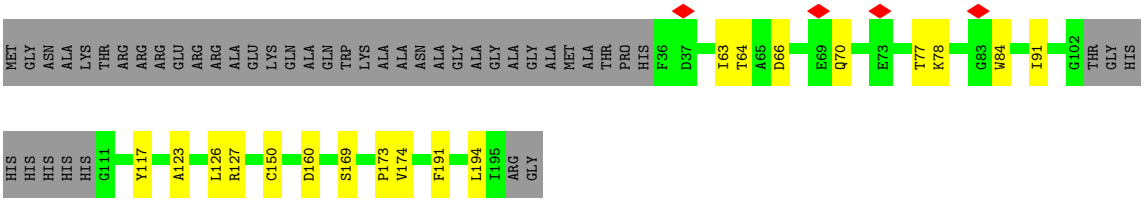
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KH:



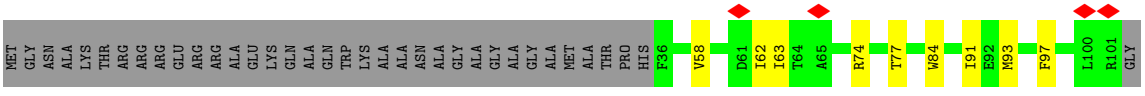
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

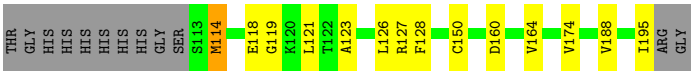
Chain KI:



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

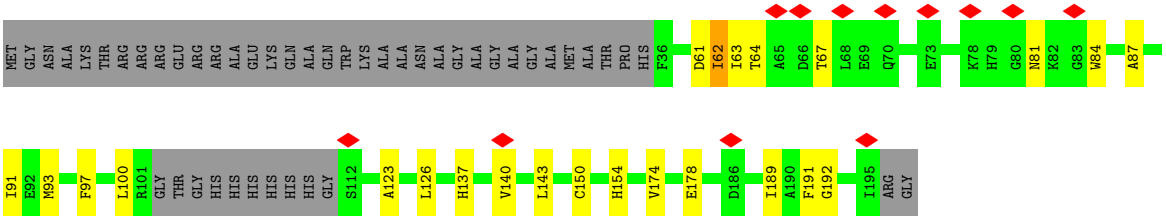
Chain KJ:





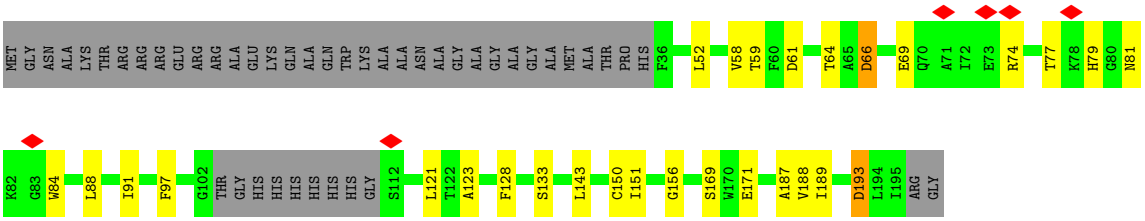
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KK:



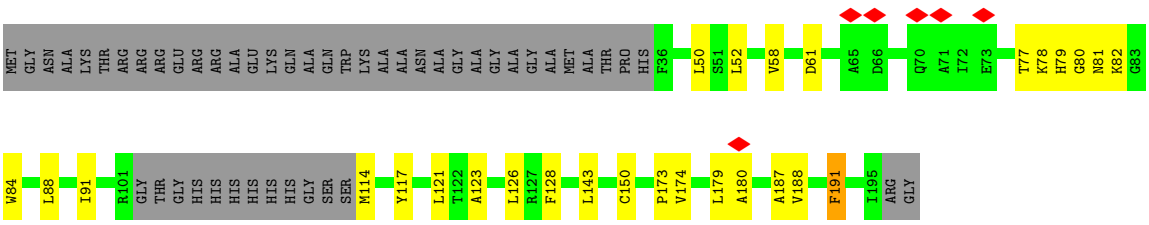
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KL:



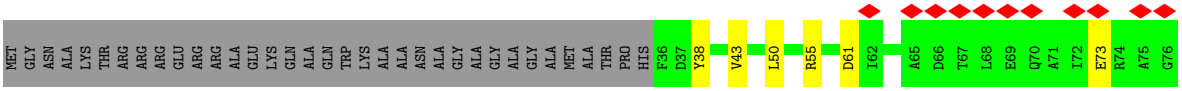
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

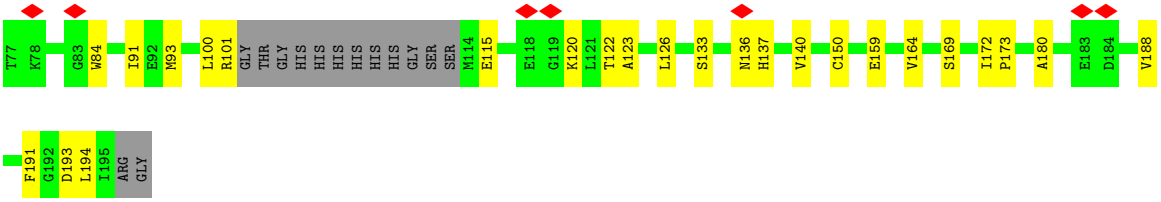
Chain KM:



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

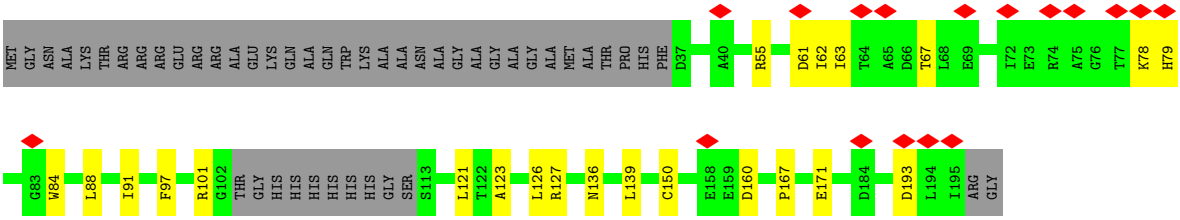
Chain KN:





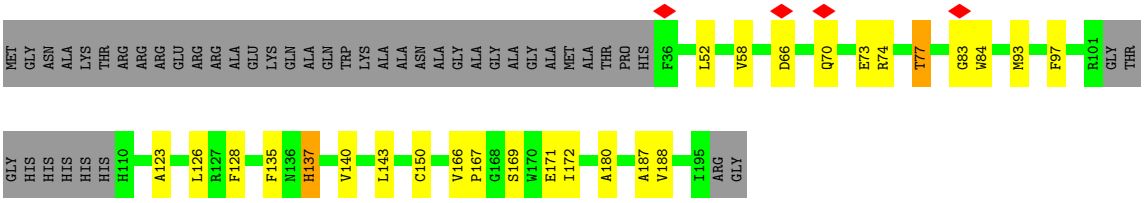
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KO:



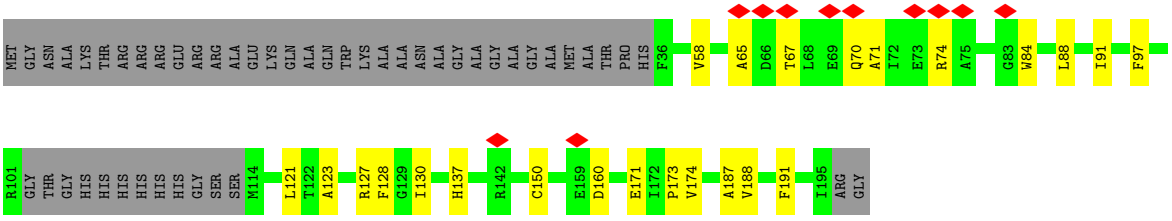
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LA:



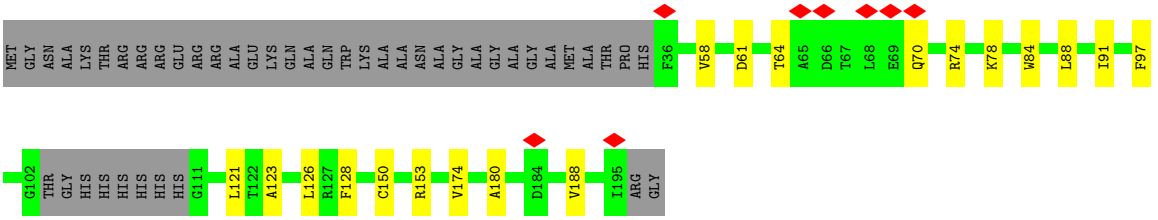
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LB:



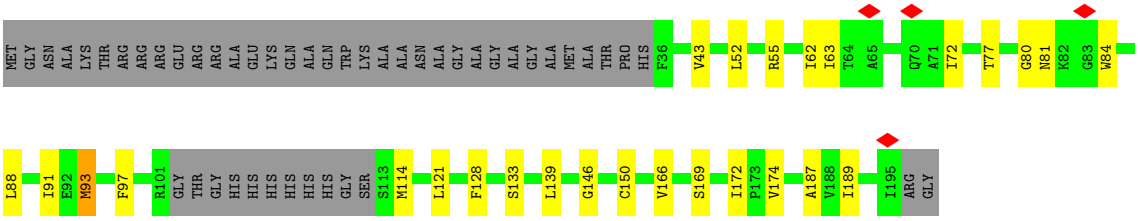
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LC:



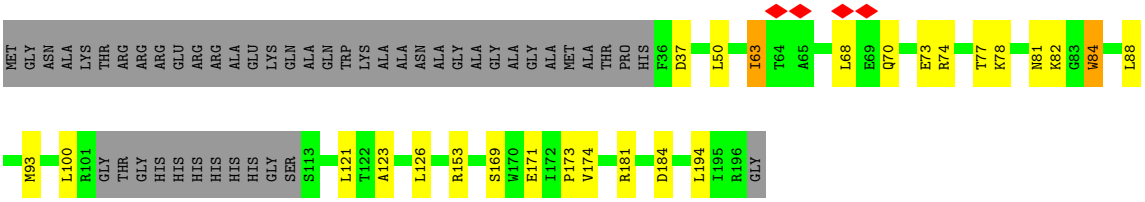
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LD:



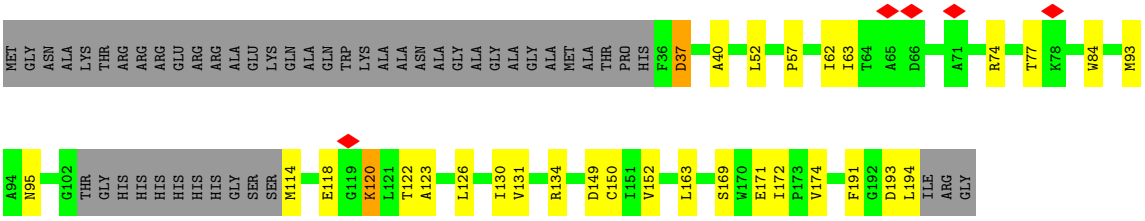
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LE:



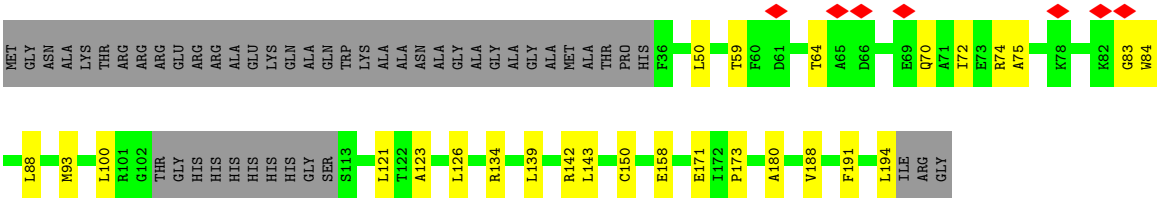
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LF:



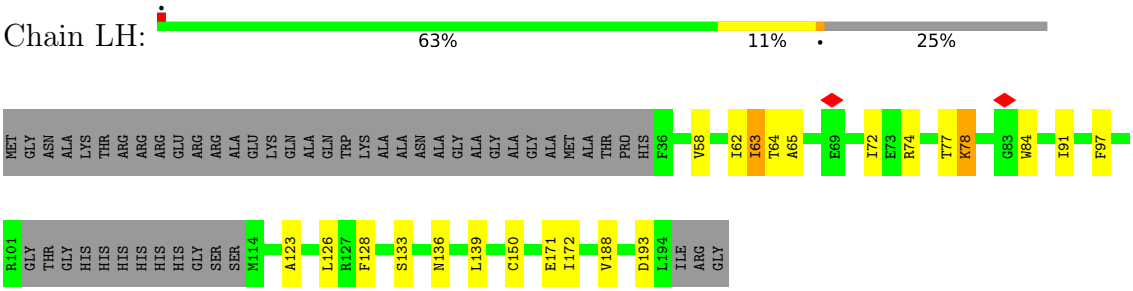
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LG:



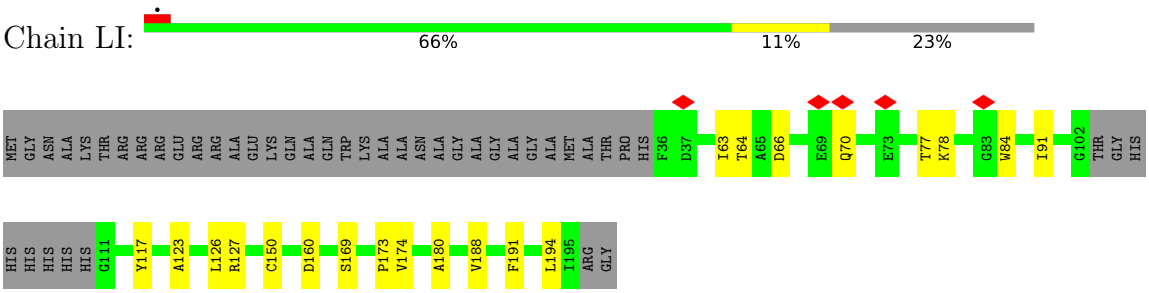
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LH:



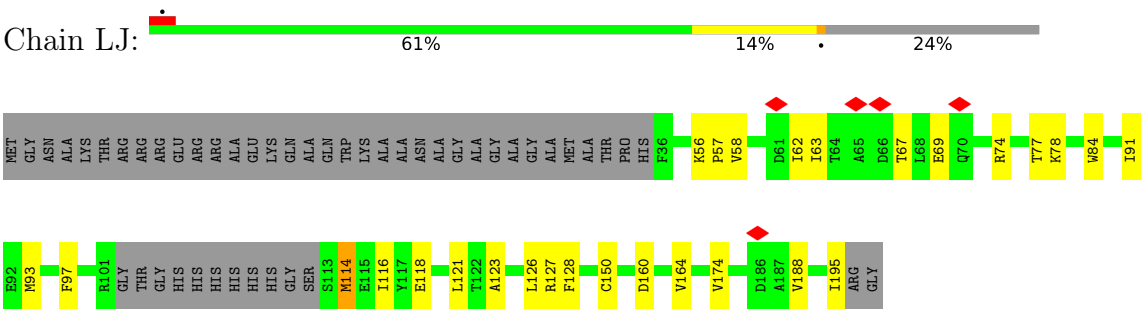
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LI:



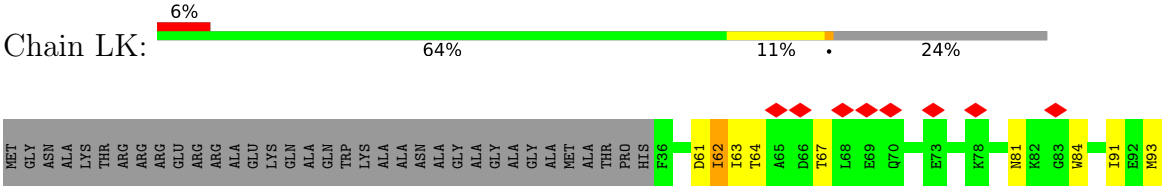
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

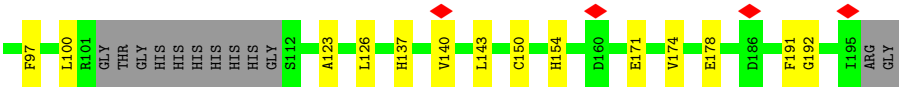
Chain LJ:



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

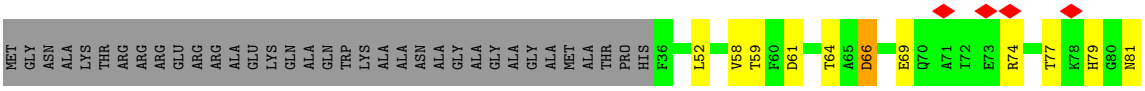
Chain LK:





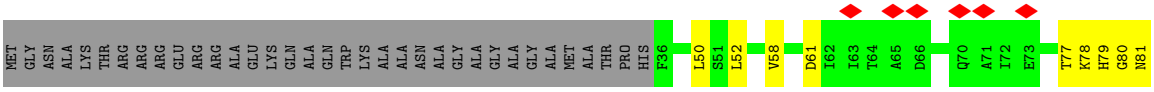
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

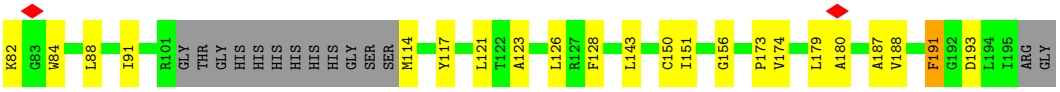
Chain LL:



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

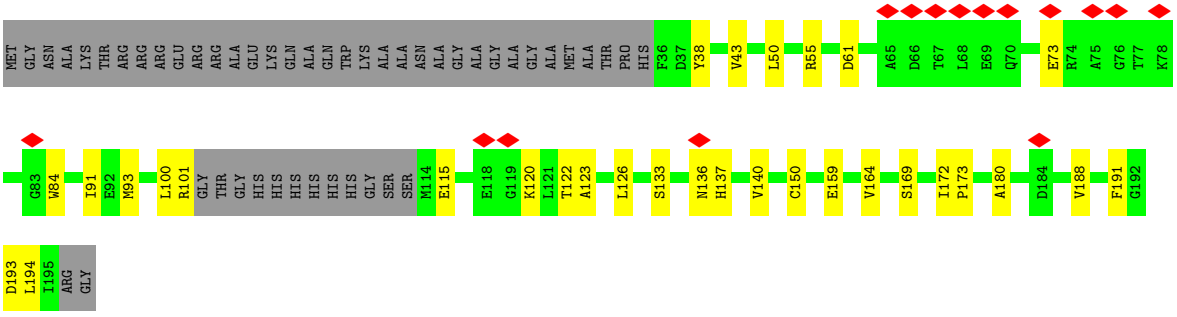
Chain LM:





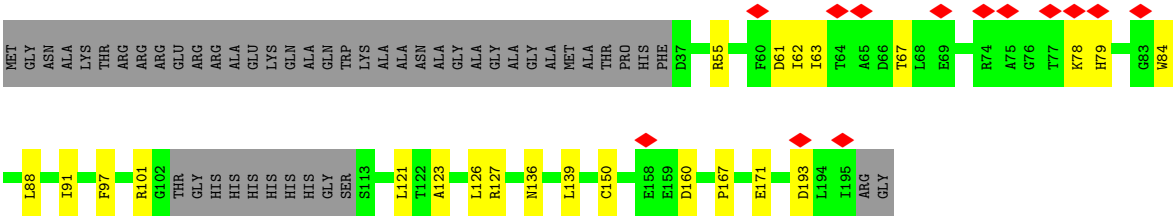
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LN:



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

Chain LO:


MET GLY ASN ALA LYS THR ARG ARG ARG GLU ARG ARG ALA GLU LYS GLN ALA GLN TRP LYS ALA ALA ASN ALA GLY ALA GLY ALA GLY ALA MET ALA THR PRO HIS PHE D37 R55 F60 D61 I62 I63 T64 A65 D66 T67 L68 E69 R74 A75 G76 T77 K78 H79 G83 W84
L88 I91 F97 R101 G102 THR GLY HIS HIS HIS HIS HIS HIS GLY SER S113 L121 T122 A123 L126 R127 N136 L139 C150 E158 E159 D160 P167 E171 D193 L194 I195 ARG GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	4037	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.231	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0265	Depositor
Map size (Å)	550.0, 550.0, 550.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.375, 1.375, 1.375	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AA	0.10	0/1165	0.25	0/1572
1	AB	0.10	0/1144	0.26	0/1544
1	AC	0.10	0/1164	0.26	0/1570
1	AD	0.11	0/1150	0.29	0/1552
1	AE	0.11	0/1155	0.32	0/1559
1	AF	0.11	0/1137	0.28	0/1535
1	AG	0.09	0/1149	0.25	0/1550
1	AH	0.10	0/1133	0.28	0/1530
1	AI	0.12	0/1164	0.27	0/1570
1	AJ	0.09	0/1150	0.25	0/1552
1	AK	0.12	0/1156	0.30	0/1560
1	AL	0.11	0/1160	0.28	0/1565
1	AM	0.10	0/1138	0.26	0/1537
1	AN	0.09	0/1144	0.25	0/1544
1	AO	0.10	0/1149	0.26	0/1550
1	BA	0.10	0/1165	0.25	0/1572
1	BB	0.10	0/1144	0.26	0/1544
1	BC	0.10	0/1164	0.26	0/1570
1	BD	0.11	0/1150	0.29	0/1552
1	BE	0.12	0/1155	0.32	0/1559
1	BF	0.12	0/1137	0.28	0/1535
1	BG	0.09	0/1149	0.25	0/1550
1	BH	0.11	0/1133	0.28	0/1530
1	BI	0.12	0/1164	0.27	0/1570
1	BJ	0.10	0/1150	0.26	0/1552
1	BK	0.12	0/1156	0.30	0/1560
1	BL	0.12	0/1160	0.28	0/1565
1	BM	0.11	0/1138	0.27	0/1537
1	BN	0.09	0/1144	0.25	0/1544
1	BO	0.10	0/1149	0.26	0/1550
1	CA	0.10	0/1165	0.25	0/1572
1	CB	0.10	0/1144	0.26	0/1544
1	CC	0.10	0/1164	0.26	0/1570
1	CD	0.11	0/1150	0.29	0/1552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	CE	0.12	0/1155	0.32	0/1559
1	CF	0.12	0/1137	0.28	0/1535
1	CG	0.10	0/1149	0.25	0/1550
1	CH	0.11	0/1133	0.28	0/1530
1	CI	0.12	0/1164	0.27	0/1570
1	CJ	0.10	0/1150	0.26	0/1552
1	CK	0.12	0/1156	0.30	0/1560
1	CL	0.11	0/1160	0.28	0/1565
1	CM	0.10	0/1138	0.26	0/1537
1	CN	0.09	0/1144	0.25	0/1544
1	CO	0.10	0/1149	0.26	0/1550
1	DA	0.10	0/1165	0.25	0/1572
1	DB	0.10	0/1144	0.26	0/1544
1	DC	0.10	0/1164	0.26	0/1570
1	DD	0.11	0/1150	0.29	0/1552
1	DE	0.12	0/1155	0.32	0/1559
1	DF	0.12	0/1137	0.28	0/1535
1	DG	0.09	0/1149	0.25	0/1550
1	DH	0.11	0/1133	0.28	0/1530
1	DI	0.12	0/1164	0.27	0/1570
1	DJ	0.10	0/1150	0.26	0/1552
1	DK	0.12	0/1156	0.30	0/1560
1	DL	0.11	0/1160	0.28	0/1565
1	DM	0.10	0/1138	0.27	0/1537
1	DN	0.09	0/1144	0.25	0/1544
1	DO	0.10	0/1149	0.26	0/1550
1	EA	0.10	0/1165	0.25	0/1572
1	EB	0.10	0/1144	0.26	0/1544
1	EC	0.10	0/1164	0.26	0/1570
1	ED	0.11	0/1150	0.29	0/1552
1	EE	0.11	0/1155	0.32	0/1559
1	EF	0.12	0/1137	0.28	0/1535
1	EG	0.09	0/1149	0.25	0/1550
1	EH	0.11	0/1133	0.28	0/1530
1	EI	0.12	0/1164	0.27	0/1570
1	EJ	0.10	0/1150	0.26	0/1552
1	EK	0.12	0/1156	0.30	0/1560
1	EL	0.11	0/1160	0.28	0/1565
1	EM	0.10	0/1138	0.26	0/1537
1	EN	0.09	0/1144	0.25	0/1544
1	EO	0.10	0/1149	0.26	0/1550
1	FA	0.10	0/1165	0.25	0/1572
1	FB	0.10	0/1144	0.26	0/1544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	FC	0.10	0/1164	0.26	0/1570
1	FD	0.11	0/1150	0.29	0/1552
1	FE	0.12	0/1155	0.32	0/1559
1	FF	0.12	0/1137	0.28	0/1535
1	FG	0.09	0/1149	0.25	0/1550
1	FH	0.11	0/1133	0.28	0/1530
1	FI	0.12	0/1164	0.27	0/1570
1	FJ	0.10	0/1150	0.26	0/1552
1	FK	0.12	0/1156	0.30	0/1560
1	FL	0.11	0/1160	0.28	0/1565
1	FM	0.11	0/1138	0.27	0/1537
1	FN	0.09	0/1144	0.25	0/1544
1	FO	0.10	0/1149	0.26	0/1550
1	GA	0.10	0/1165	0.25	0/1572
1	GB	0.10	0/1144	0.26	0/1544
1	GC	0.10	0/1164	0.26	0/1570
1	GD	0.11	0/1150	0.29	0/1552
1	GE	0.11	0/1155	0.32	0/1559
1	GF	0.12	0/1137	0.28	0/1535
1	GG	0.09	0/1149	0.25	0/1550
1	GH	0.11	0/1133	0.28	0/1530
1	GI	0.12	0/1164	0.27	0/1570
1	GJ	0.10	0/1150	0.26	0/1552
1	GK	0.12	0/1156	0.30	0/1560
1	GL	0.11	0/1160	0.28	0/1565
1	GM	0.11	0/1138	0.27	0/1537
1	GN	0.09	0/1144	0.25	0/1544
1	GO	0.10	0/1149	0.26	0/1550
1	HA	0.10	0/1165	0.25	0/1572
1	HB	0.10	0/1144	0.26	0/1544
1	HC	0.10	0/1164	0.27	0/1570
1	HD	0.11	0/1150	0.29	0/1552
1	HE	0.11	0/1155	0.32	0/1559
1	HF	0.12	0/1137	0.28	0/1535
1	HG	0.09	0/1149	0.25	0/1550
1	HH	0.11	0/1133	0.28	0/1530
1	HI	0.12	0/1164	0.27	0/1570
1	HJ	0.10	0/1150	0.26	0/1552
1	HK	0.12	0/1156	0.30	0/1560
1	HL	0.12	0/1160	0.28	0/1565
1	HM	0.11	0/1138	0.27	0/1537
1	HN	0.09	0/1144	0.24	0/1544
1	HO	0.10	0/1149	0.26	0/1550

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	IA	0.10	0/1165	0.25	0/1572
1	IB	0.10	0/1144	0.26	0/1544
1	IC	0.10	0/1164	0.26	0/1570
1	ID	0.11	0/1150	0.29	0/1552
1	IE	0.12	0/1155	0.32	0/1559
1	IF	0.12	0/1137	0.28	0/1535
1	IG	0.09	0/1149	0.25	0/1550
1	IH	0.11	0/1133	0.28	0/1530
1	II	0.12	0/1164	0.27	0/1570
1	IJ	0.10	0/1150	0.26	0/1552
1	IK	0.12	0/1156	0.30	0/1560
1	IL	0.12	0/1160	0.28	0/1565
1	IM	0.10	0/1138	0.27	0/1537
1	IN	0.09	0/1144	0.25	0/1544
1	IO	0.10	0/1149	0.26	0/1550
1	JA	0.10	0/1165	0.25	0/1572
1	JB	0.10	0/1144	0.26	0/1544
1	JC	0.10	0/1164	0.26	0/1570
1	JD	0.11	0/1150	0.29	0/1552
1	JE	0.12	0/1155	0.32	0/1559
1	JF	0.12	0/1137	0.28	0/1535
1	JG	0.10	0/1149	0.25	0/1550
1	JH	0.11	0/1133	0.28	0/1530
1	JI	0.12	0/1164	0.27	0/1570
1	JJ	0.10	0/1150	0.26	0/1552
1	JK	0.12	0/1156	0.30	0/1560
1	JL	0.11	0/1160	0.28	0/1565
1	JM	0.10	0/1138	0.27	0/1537
1	JN	0.09	0/1144	0.25	0/1544
1	JO	0.10	0/1149	0.26	0/1550
1	KA	0.10	0/1165	0.25	0/1572
1	KB	0.10	0/1144	0.26	0/1544
1	KC	0.10	0/1164	0.26	0/1570
1	KD	0.11	0/1150	0.29	0/1552
1	KE	0.11	0/1155	0.32	0/1559
1	KF	0.12	0/1137	0.28	0/1535
1	KG	0.09	0/1149	0.25	0/1550
1	KH	0.11	0/1133	0.28	0/1530
1	KI	0.12	0/1164	0.27	0/1570
1	KJ	0.10	0/1150	0.26	0/1552
1	KK	0.12	0/1156	0.30	0/1560
1	KL	0.11	0/1160	0.28	0/1565
1	KM	0.10	0/1138	0.26	0/1537

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	KN	0.09	0/1144	0.25	0/1544
1	KO	0.10	0/1149	0.26	0/1550
1	LA	0.10	0/1165	0.25	0/1572
1	LB	0.10	0/1144	0.26	0/1544
1	LC	0.10	0/1164	0.26	0/1570
1	LD	0.11	0/1150	0.29	0/1552
1	LE	0.12	0/1155	0.32	0/1559
1	LF	0.12	0/1137	0.28	0/1535
1	LG	0.09	0/1149	0.25	0/1550
1	LH	0.11	0/1133	0.28	0/1530
1	LI	0.12	0/1164	0.27	0/1570
1	LJ	0.10	0/1150	0.26	0/1552
1	LK	0.12	0/1156	0.30	0/1560
1	LL	0.11	0/1160	0.28	0/1565
1	LM	0.10	0/1138	0.27	0/1537
1	LN	0.09	0/1144	0.25	0/1544
1	LO	0.10	0/1149	0.26	0/1550
All	All	0.11	0/207096	0.27	0/279480

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)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1150	0	1151	16	0
1	AB	1129	0	1136	14	0
1	AC	1149	0	1152	13	0
1	AD	1135	0	1141	19	0
1	AE	1140	0	1143	20	0
1	AF	1122	0	1126	21	0
1	AG	1134	0	1142	17	0
1	AH	1118	0	1123	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AI	1149	0	1152	12	0
1	AJ	1135	0	1141	15	0
1	AK	1141	0	1146	16	0
1	AL	1145	0	1149	17	0
1	AM	1123	0	1125	20	0
1	AN	1129	0	1136	18	0
1	AO	1134	0	1142	11	0
1	BA	1150	0	1151	16	0
1	BB	1129	0	1136	15	0
1	BC	1149	0	1152	13	0
1	BD	1135	0	1141	18	0
1	BE	1140	0	1143	19	0
1	BF	1122	0	1126	22	0
1	BG	1134	0	1142	18	0
1	BH	1118	0	1123	16	0
1	BI	1149	0	1152	13	0
1	BJ	1135	0	1141	15	0
1	BK	1141	0	1146	17	0
1	BL	1145	0	1149	17	0
1	BM	1123	0	1125	18	0
1	BN	1129	0	1136	18	0
1	BO	1134	0	1142	12	0
1	CA	1150	0	1151	15	0
1	CB	1129	0	1136	15	0
1	CC	1149	0	1152	14	0
1	CD	1135	0	1141	20	0
1	CE	1140	0	1143	19	0
1	CF	1122	0	1126	22	0
1	CG	1134	0	1142	18	0
1	CH	1118	0	1123	17	0
1	CI	1149	0	1152	11	0
1	CJ	1135	0	1141	15	0
1	CK	1141	0	1146	17	0
1	CL	1145	0	1149	18	0
1	CM	1123	0	1125	19	0
1	CN	1129	0	1136	18	0
1	CO	1134	0	1142	12	0
1	DA	1150	0	1151	16	0
1	DB	1129	0	1136	14	0
1	DC	1149	0	1152	12	0
1	DD	1135	0	1141	20	0
1	DE	1140	0	1143	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DF	1122	0	1126	24	0
1	DG	1134	0	1142	17	0
1	DH	1118	0	1123	14	0
1	DI	1149	0	1152	11	0
1	DJ	1135	0	1141	16	0
1	DK	1141	0	1146	13	0
1	DL	1145	0	1149	16	0
1	DM	1123	0	1125	18	0
1	DN	1129	0	1136	18	0
1	DO	1134	0	1142	12	0
1	EA	1150	0	1151	16	0
1	EB	1129	0	1136	14	0
1	EC	1149	0	1152	13	0
1	ED	1135	0	1141	20	0
1	EE	1140	0	1143	20	0
1	EF	1122	0	1126	20	0
1	EG	1134	0	1142	18	0
1	EH	1118	0	1123	16	0
1	EI	1149	0	1152	12	0
1	EJ	1135	0	1141	16	0
1	EK	1141	0	1146	18	0
1	EL	1145	0	1149	17	0
1	EM	1123	0	1125	22	0
1	EN	1129	0	1136	18	0
1	EO	1134	0	1142	12	0
1	FA	1150	0	1151	18	0
1	FB	1129	0	1136	13	0
1	FC	1149	0	1152	14	0
1	FD	1135	0	1141	18	0
1	FE	1140	0	1143	18	0
1	FF	1122	0	1126	22	0
1	FG	1134	0	1142	17	0
1	FH	1118	0	1123	15	0
1	FI	1149	0	1152	11	0
1	FJ	1135	0	1141	15	0
1	FK	1141	0	1146	14	0
1	FL	1145	0	1149	17	0
1	FM	1123	0	1125	18	0
1	FN	1129	0	1136	18	0
1	FO	1134	0	1142	12	0
1	GA	1150	0	1151	18	0
1	GB	1129	0	1136	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GC	1149	0	1152	13	0
1	GD	1135	0	1141	19	0
1	GE	1140	0	1143	20	0
1	GF	1122	0	1126	21	0
1	GG	1134	0	1142	15	0
1	GH	1118	0	1123	15	0
1	GI	1149	0	1152	12	0
1	GJ	1135	0	1141	15	0
1	GK	1141	0	1146	16	0
1	GL	1145	0	1149	18	0
1	GM	1123	0	1125	21	0
1	GN	1129	0	1136	18	0
1	GO	1134	0	1142	11	0
1	HA	1150	0	1151	16	0
1	HB	1129	0	1136	14	0
1	HC	1149	0	1152	13	0
1	HD	1135	0	1141	19	0
1	HE	1140	0	1143	18	0
1	HF	1122	0	1126	21	0
1	HG	1134	0	1142	17	0
1	HH	1118	0	1123	15	0
1	HI	1149	0	1152	12	0
1	HJ	1135	0	1141	16	0
1	HK	1141	0	1146	14	0
1	HL	1145	0	1149	16	0
1	HM	1123	0	1125	19	0
1	HN	1129	0	1136	18	0
1	HO	1134	0	1142	12	0
1	IA	1150	0	1151	16	0
1	IB	1129	0	1136	14	0
1	IC	1149	0	1152	12	0
1	ID	1135	0	1141	20	0
1	IE	1140	0	1143	20	0
1	IF	1122	0	1126	22	0
1	IG	1134	0	1142	17	0
1	IH	1118	0	1123	12	0
1	II	1149	0	1152	12	0
1	IJ	1135	0	1141	15	0
1	IK	1141	0	1146	17	0
1	IL	1145	0	1149	17	0
1	IM	1123	0	1125	20	0
1	IN	1129	0	1136	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	IO	1134	0	1142	12	0
1	JA	1150	0	1151	21	0
1	JB	1129	0	1136	13	0
1	JC	1149	0	1152	13	0
1	JD	1135	0	1141	19	0
1	JE	1140	0	1143	19	0
1	JF	1122	0	1126	21	0
1	JG	1134	0	1142	17	0
1	JH	1118	0	1123	14	0
1	JI	1149	0	1152	12	0
1	JJ	1135	0	1141	15	0
1	JK	1141	0	1146	16	0
1	JL	1145	0	1149	15	0
1	JM	1123	0	1125	19	0
1	JN	1129	0	1136	18	0
1	JO	1134	0	1142	12	0
1	KA	1150	0	1151	17	0
1	KB	1129	0	1136	14	0
1	KC	1149	0	1152	13	0
1	KD	1135	0	1141	21	0
1	KE	1140	0	1143	21	0
1	KF	1122	0	1126	21	0
1	KG	1134	0	1142	15	0
1	KH	1118	0	1123	14	0
1	KI	1149	0	1152	11	0
1	KJ	1135	0	1141	14	0
1	KK	1141	0	1146	13	0
1	KL	1145	0	1149	17	0
1	KM	1123	0	1125	18	0
1	KN	1129	0	1136	18	0
1	KO	1134	0	1142	12	0
1	LA	1150	0	1151	20	0
1	LB	1129	0	1136	15	0
1	LC	1149	0	1152	12	0
1	LD	1135	0	1141	18	0
1	LE	1140	0	1143	23	0
1	LF	1122	0	1126	21	0
1	LG	1134	0	1142	15	0
1	LH	1118	0	1123	15	0
1	LI	1149	0	1152	12	0
1	LJ	1135	0	1141	17	0
1	LK	1141	0	1146	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	LL	1145	0	1149	18	0
1	LM	1123	0	1125	21	0
1	LN	1129	0	1136	18	0
1	LO	1134	0	1142	12	0
All	All	204396	0	205260	2498	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (2498) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GE:63:ILE:HG13	1:GE:70:GLN:HG2	1.73	0.71
1:LE:63:ILE:HG13	1:LE:70:GLN:HG2	1.73	0.70
1:KE:63:ILE:HG13	1:KE:70:GLN:HG2	1.73	0.70
1:BE:63:ILE:HG13	1:BE:70:GLN:HG2	1.73	0.70
1:EE:63:ILE:HG13	1:EE:70:GLN:HG2	1.73	0.70
1:FE:63:ILE:HG13	1:FE:70:GLN:HG2	1.73	0.70
1:JE:63:ILE:HG13	1:JE:70:GLN:HG2	1.73	0.70
1:DE:63:ILE:HG13	1:DE:70:GLN:HG2	1.74	0.70
1:HE:63:ILE:HG13	1:HE:70:GLN:HG2	1.73	0.70
1:IE:63:ILE:HG13	1:IE:70:GLN:HG2	1.73	0.70
1:AE:63:ILE:HG13	1:AE:70:GLN:HG2	1.73	0.70
1:CE:63:ILE:HG13	1:CE:70:GLN:HG2	1.73	0.69
1:HD:72:ILE:HD13	1:HD:139:LEU:HD21	1.76	0.68
1:CD:72:ILE:HD13	1:CD:139:LEU:HD21	1.76	0.68
1:LD:72:ILE:HD13	1:LD:139:LEU:HD21	1.76	0.68
1:BD:133:SER:HB3	1:BD:172:ILE:HD11	1.76	0.68
1:FD:72:ILE:HD13	1:FD:139:LEU:HD21	1.76	0.68
1:ID:133:SER:HB3	1:ID:172:ILE:HD11	1.76	0.68
1:JD:72:ILE:HD13	1:JD:139:LEU:HD21	1.76	0.67
1:AD:72:ILE:HD13	1:AD:139:LEU:HD21	1.76	0.67
1:ID:72:ILE:HD13	1:ID:139:LEU:HD21	1.76	0.67
1:JK:137:HIS:HA	1:JK:140:VAL:HB	1.77	0.67
1:BK:137:HIS:HA	1:BK:140:VAL:HB	1.77	0.67
1:AK:137:HIS:HA	1:AK:140:VAL:HB	1.77	0.67
1:ED:72:ILE:HD13	1:ED:139:LEU:HD21	1.76	0.67
1:GK:137:HIS:HA	1:GK:140:VAL:HB	1.77	0.67
1:KD:72:ILE:HD13	1:KD:139:LEU:HD21	1.76	0.67
1:CD:133:SER:HB3	1:CD:172:ILE:HD11	1.76	0.67
1:ED:133:SER:HB3	1:ED:172:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EK:137:HIS:HA	1:EK:140:VAL:HB	1.77	0.67
1:GD:72:ILE:HD13	1:GD:139:LEU:HD21	1.76	0.67
1:JD:133:SER:HB3	1:JD:172:ILE:HD11	1.76	0.67
1:KK:137:HIS:HA	1:KK:140:VAL:HB	1.77	0.67
1:HK:137:HIS:HA	1:HK:140:VAL:HB	1.77	0.66
1:LK:137:HIS:HA	1:LK:140:VAL:HB	1.77	0.66
1:KD:133:SER:HB3	1:KD:172:ILE:HD11	1.76	0.66
1:DK:137:HIS:HA	1:DK:140:VAL:HB	1.77	0.66
1:BD:72:ILE:HD13	1:BD:139:LEU:HD21	1.76	0.66
1:GD:133:SER:HB3	1:GD:172:ILE:HD11	1.76	0.66
1:CK:137:HIS:HA	1:CK:140:VAL:HB	1.77	0.66
1:DD:72:ILE:HD13	1:DD:139:LEU:HD21	1.76	0.66
1:FD:133:SER:HB3	1:FD:172:ILE:HD11	1.76	0.66
1:HD:133:SER:HB3	1:HD:172:ILE:HD11	1.76	0.66
1:JA:121:LEU:HG	1:LE:153:ARG:HG2	1.78	0.66
1:AD:133:SER:HB3	1:AD:172:ILE:HD11	1.76	0.65
1:LD:133:SER:HB3	1:LD:172:ILE:HD11	1.76	0.65
1:FK:137:HIS:HA	1:FK:140:VAL:HB	1.77	0.65
1:DD:133:SER:HB3	1:DD:172:ILE:HD11	1.76	0.65
1:II:64:THR:HB	1:II:194:LEU:HB3	1.79	0.65
1:IK:137:HIS:HA	1:IK:140:VAL:HB	1.77	0.65
1:CK:81:ASN:HD21	1:CK:143:LEU:HA	1.62	0.65
1:KI:64:THR:HB	1:KI:194:LEU:HB3	1.79	0.65
1:JK:81:ASN:HD21	1:JK:143:LEU:HA	1.62	0.65
1:JH:136:ASN:HD22	1:JH:193:ASP:HB2	1.63	0.64
1:CH:136:ASN:HD22	1:CH:193:ASP:HB2	1.63	0.64
1:BK:81:ASN:HD21	1:BK:143:LEU:HA	1.62	0.64
1:GI:64:THR:HB	1:GI:194:LEU:HB3	1.79	0.64
1:HK:81:ASN:HD21	1:HK:143:LEU:HA	1.62	0.64
1:IH:136:ASN:HD22	1:IH:193:ASP:HB2	1.63	0.64
1:DI:64:THR:HB	1:DI:194:LEU:HB3	1.79	0.64
1:FK:81:ASN:HD21	1:FK:143:LEU:HA	1.62	0.64
1:JI:64:THR:HB	1:JI:194:LEU:HB3	1.79	0.64
1:AH:136:ASN:HD22	1:AH:193:ASP:HB2	1.63	0.64
1:DH:136:ASN:HD22	1:DH:193:ASP:HB2	1.63	0.64
1:DK:81:ASN:HD21	1:DK:143:LEU:HA	1.62	0.64
1:LE:78:LYS:O	1:LE:81:ASN:ND2	2.31	0.64
1:BH:136:ASN:HD22	1:BH:193:ASP:HB2	1.63	0.64
1:DE:78:LYS:O	1:DE:81:ASN:ND2	2.31	0.64
1:EE:78:LYS:O	1:EE:81:ASN:ND2	2.31	0.64
1:LI:64:THR:HB	1:LI:194:LEU:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:78:LYS:O	1:CE:81:ASN:ND2	2.31	0.63
1:CI:64:THR:HB	1:CI:194:LEU:HB3	1.79	0.63
1:HE:78:LYS:O	1:HE:81:ASN:ND2	2.31	0.63
1:BE:78:LYS:O	1:BE:81:ASN:ND2	2.31	0.63
1:HI:64:THR:HB	1:HI:194:LEU:HB3	1.79	0.63
1:JE:78:LYS:O	1:JE:81:ASN:ND2	2.31	0.63
1:KK:81:ASN:HD21	1:KK:143:LEU:HA	1.62	0.63
1:EH:136:ASN:HD22	1:EH:193:ASP:HB2	1.63	0.63
1:EI:64:THR:HB	1:EI:194:LEU:HB3	1.79	0.63
1:IE:78:LYS:O	1:IE:81:ASN:ND2	2.31	0.63
1:AE:78:LYS:O	1:AE:81:ASN:ND2	2.31	0.63
1:EK:81:ASN:HD21	1:EK:143:LEU:HA	1.62	0.63
1:FL:58:VAL:HG22	1:FL:188:VAL:HB	1.81	0.63
1:IK:81:ASN:HD21	1:IK:143:LEU:HA	1.63	0.63
1:LK:81:ASN:HD21	1:LK:143:LEU:HA	1.62	0.63
1:BI:64:THR:HB	1:BI:194:LEU:HB3	1.79	0.63
1:BL:58:VAL:HG22	1:BL:188:VAL:HB	1.81	0.63
1:AI:64:THR:HB	1:AI:194:LEU:HB3	1.79	0.63
1:KE:78:LYS:O	1:KE:81:ASN:ND2	2.31	0.63
1:LH:136:ASN:HD22	1:LH:193:ASP:HB2	1.63	0.63
1:FI:64:THR:HB	1:FI:194:LEU:HB3	1.79	0.63
1:GE:78:LYS:O	1:GE:81:ASN:ND2	2.31	0.63
1:GK:81:ASN:HD21	1:GK:143:LEU:HA	1.63	0.63
1:DH:63:ILE:HG12	1:DH:65:ALA:H	1.64	0.63
1:LL:58:VAL:HG22	1:LL:188:VAL:HB	1.81	0.63
1:CL:58:VAL:HG22	1:CL:188:VAL:HB	1.81	0.63
1:GL:58:VAL:HG22	1:GL:188:VAL:HB	1.81	0.63
1:FH:63:ILE:HG12	1:FH:65:ALA:H	1.64	0.62
1:IL:58:VAL:HG22	1:IL:188:VAL:HB	1.81	0.62
1:AL:58:VAL:HG22	1:AL:188:VAL:HB	1.81	0.62
1:EJ:114:MET:N	1:EJ:114:MET:SD	2.72	0.62
1:GH:136:ASN:HD22	1:GH:193:ASP:HB2	1.63	0.62
1:BH:63:ILE:HG12	1:BH:65:ALA:H	1.64	0.62
1:AK:81:ASN:HD21	1:AK:143:LEU:HA	1.62	0.62
1:IH:63:ILE:HG12	1:IH:65:ALA:H	1.64	0.62
1:KH:136:ASN:HD22	1:KH:193:ASP:HB2	1.63	0.62
1:FH:136:ASN:HD22	1:FH:193:ASP:HB2	1.63	0.62
1:HH:63:ILE:HG12	1:HH:65:ALA:H	1.64	0.62
1:LH:63:ILE:HG12	1:LH:65:ALA:H	1.64	0.62
1:FE:78:LYS:O	1:FE:81:ASN:ND2	2.31	0.62
1:JL:58:VAL:HG22	1:JL:188:VAL:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EH:63:ILE:HG12	1:EH:65:ALA:H	1.64	0.62
1:HH:136:ASN:HD22	1:HH:193:ASP:HB2	1.63	0.62
1:AH:63:ILE:HG12	1:AH:65:ALA:H	1.64	0.62
1:HL:58:VAL:HG22	1:HL:188:VAL:HB	1.81	0.62
1:CJ:114:MET:SD	1:CJ:114:MET:N	2.72	0.62
1:EL:58:VAL:HG22	1:EL:188:VAL:HB	1.81	0.62
1:JH:63:ILE:HG12	1:JH:65:ALA:H	1.64	0.62
1:DJ:114:MET:N	1:DJ:114:MET:SD	2.72	0.62
1:EH:133:SER:HB3	1:EH:172:ILE:HD11	1.82	0.62
1:BO:55:ARG:HD2	1:BO:101:ARG:HH21	1.65	0.62
1:DH:133:SER:HB3	1:DH:172:ILE:HD11	1.82	0.62
1:GH:63:ILE:HG12	1:GH:65:ALA:H	1.64	0.61
1:GH:133:SER:HB3	1:GH:172:ILE:HD11	1.82	0.61
1:HH:133:SER:HB3	1:HH:172:ILE:HD11	1.82	0.61
1:CO:55:ARG:HD2	1:CO:101:ARG:HH21	1.65	0.61
1:IH:133:SER:HB3	1:IH:172:ILE:HD11	1.82	0.61
1:AJ:114:MET:N	1:AJ:114:MET:SD	2.72	0.61
1:FH:133:SER:HB3	1:FH:172:ILE:HD11	1.82	0.61
1:DL:58:VAL:HG22	1:DL:188:VAL:HB	1.81	0.61
1:EO:55:ARG:HD2	1:EO:101:ARG:HH21	1.65	0.61
1:FJ:114:MET:N	1:FJ:114:MET:SD	2.72	0.61
1:GO:55:ARG:HD2	1:GO:101:ARG:HH21	1.66	0.61
1:HO:55:ARG:HD2	1:HO:101:ARG:HH21	1.65	0.61
1:JO:55:ARG:HD2	1:JO:101:ARG:HH21	1.65	0.61
1:LO:55:ARG:HD2	1:LO:101:ARG:HH21	1.65	0.61
1:CH:63:ILE:HG12	1:CH:65:ALA:H	1.64	0.61
1:DO:55:ARG:HD2	1:DO:101:ARG:HH21	1.65	0.61
1:KH:63:ILE:HG12	1:KH:65:ALA:H	1.64	0.61
1:HJ:114:MET:SD	1:HJ:114:MET:N	2.72	0.61
1:JH:133:SER:HB3	1:JH:172:ILE:HD11	1.82	0.61
1:BJ:114:MET:N	1:BJ:114:MET:SD	2.72	0.60
1:FO:55:ARG:HD2	1:FO:101:ARG:HH21	1.65	0.60
1:KH:133:SER:HB3	1:KH:172:ILE:HD11	1.82	0.60
1:BH:133:SER:HB3	1:BH:172:ILE:HD11	1.82	0.60
1:GJ:114:MET:N	1:GJ:114:MET:SD	2.72	0.60
1:LH:133:SER:HB3	1:LH:172:ILE:HD11	1.82	0.60
1:KL:58:VAL:HG22	1:KL:188:VAL:HB	1.81	0.60
1:CA:171:GLU:HB3	1:CE:93:MET:HE3	1.84	0.60
1:KO:55:ARG:HD2	1:KO:101:ARG:HH21	1.65	0.60
1:AH:133:SER:HB3	1:AH:172:ILE:HD11	1.82	0.60
1:CH:133:SER:HB3	1:CH:172:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DI:123:ALA:HA	1:DI:126:LEU:HD12	1.84	0.60
1:LI:123:ALA:HA	1:LI:126:LEU:HD12	1.84	0.60
1:AO:55:ARG:HD2	1:AO:101:ARG:HH21	1.65	0.60
1:HA:171:GLU:HB3	1:HE:93:MET:HE3	1.84	0.60
1:HI:123:ALA:HA	1:HI:126:LEU:HD12	1.84	0.60
1:KI:123:ALA:HA	1:KI:126:LEU:HD12	1.84	0.60
1:FA:171:GLU:HB3	1:FE:93:MET:HE3	1.84	0.60
1:II:123:ALA:HA	1:II:126:LEU:HD12	1.84	0.59
1:KA:171:GLU:HB3	1:KE:93:MET:HE3	1.84	0.59
1:GI:123:ALA:HA	1:GI:126:LEU:HD12	1.84	0.59
1:GK:123:ALA:HA	1:GK:126:LEU:HD12	1.85	0.59
1:JI:123:ALA:HA	1:JI:126:LEU:HD12	1.84	0.59
1:LA:171:GLU:HB3	1:LE:93:MET:HE3	1.84	0.59
1:LJ:114:MET:N	1:LJ:114:MET:SD	2.72	0.59
1:LK:123:ALA:HA	1:LK:126:LEU:HD12	1.85	0.59
1:EI:123:ALA:HA	1:EI:126:LEU:HD12	1.84	0.59
1:JI:63:ILE:HG22	1:JI:194:LEU:HB2	1.85	0.59
1:KL:66:ASP:OD1	1:KL:66:ASP:N	2.33	0.59
1:FK:123:ALA:HA	1:FK:126:LEU:HD12	1.85	0.59
1:JK:123:ALA:HA	1:JK:126:LEU:HD12	1.85	0.59
1:KK:123:ALA:HA	1:KK:126:LEU:HD12	1.85	0.59
1:BI:123:ALA:HA	1:BI:126:LEU:HD12	1.84	0.59
1:AI:63:ILE:HG22	1:AI:194:LEU:HB2	1.85	0.59
1:AI:123:ALA:HA	1:AI:126:LEU:HD12	1.84	0.59
1:FI:63:ILE:HG22	1:FI:194:LEU:HB2	1.85	0.59
1:IA:171:GLU:HB3	1:IE:93:MET:HE3	1.84	0.59
1:II:63:ILE:HG22	1:II:194:LEU:HB2	1.85	0.59
1:AA:171:GLU:HB3	1:AE:93:MET:HE3	1.84	0.59
1:DK:123:ALA:HA	1:DK:126:LEU:HD12	1.84	0.59
1:FI:123:ALA:HA	1:FI:126:LEU:HD12	1.84	0.59
1:IO:55:ARG:HD2	1:IO:101:ARG:HH21	1.66	0.59
1:EI:63:ILE:HG22	1:EI:194:LEU:HB2	1.85	0.59
1:KG:123:ALA:HA	1:KG:126:LEU:HD12	1.85	0.59
1:KI:63:ILE:HG22	1:KI:194:LEU:HB2	1.85	0.59
1:LG:123:ALA:HA	1:LG:126:LEU:HD12	1.85	0.59
1:CI:63:ILE:HG22	1:CI:194:LEU:HB2	1.85	0.59
1:CI:123:ALA:HA	1:CI:126:LEU:HD12	1.84	0.59
1:DA:171:GLU:HB3	1:DE:93:MET:HE3	1.84	0.59
1:EG:123:ALA:HA	1:EG:126:LEU:HD12	1.85	0.59
1:HG:123:ALA:HA	1:HG:126:LEU:HD12	1.85	0.59
1:HI:63:ILE:HG22	1:HI:194:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HK:123:ALA:HA	1:HK:126:LEU:HD12	1.85	0.59
1:AG:123:ALA:HA	1:AG:126:LEU:HD12	1.85	0.59
1:FG:123:ALA:HA	1:FG:126:LEU:HD12	1.85	0.59
1:GG:123:ALA:HA	1:GG:126:LEU:HD12	1.85	0.59
1:JA:171:GLU:HB3	1:JE:93:MET:HE3	1.84	0.59
1:DI:63:ILE:HG22	1:DI:194:LEU:HB2	1.85	0.58
1:CK:123:ALA:HA	1:CK:126:LEU:HD12	1.85	0.58
1:DG:123:ALA:HA	1:DG:126:LEU:HD12	1.85	0.58
1:EA:171:GLU:HB3	1:EE:93:MET:HE3	1.84	0.58
1:FF:123:ALA:HA	1:FF:126:LEU:HD12	1.86	0.58
1:GF:123:ALA:HA	1:GF:126:LEU:HD12	1.86	0.58
1:EF:123:ALA:HA	1:EF:126:LEU:HD12	1.86	0.58
1:FO:127:ARG:HG2	1:FO:160:ASP:HB3	1.86	0.58
1:GA:171:GLU:HB3	1:GE:93:MET:HE3	1.84	0.58
1:IK:123:ALA:HA	1:IK:126:LEU:HD12	1.85	0.58
1:LI:63:ILE:HG22	1:LI:194:LEU:HB2	1.85	0.58
1:CG:123:ALA:HA	1:CG:126:LEU:HD12	1.85	0.58
1:IF:123:ALA:HA	1:IF:126:LEU:HD12	1.86	0.58
1:IO:127:ARG:HG2	1:IO:160:ASP:HB3	1.86	0.58
1:JG:123:ALA:HA	1:JG:126:LEU:HD12	1.85	0.58
1:BF:123:ALA:HA	1:BF:126:LEU:HD12	1.86	0.58
1:AF:123:ALA:HA	1:AF:126:LEU:HD12	1.86	0.58
1:GI:63:ILE:HG22	1:GI:194:LEU:HB2	1.85	0.58
1:DO:127:ARG:HG2	1:DO:160:ASP:HB3	1.86	0.58
1:EK:123:ALA:HA	1:EK:126:LEU:HD12	1.84	0.58
1:JO:127:ARG:HG2	1:JO:160:ASP:HB3	1.86	0.58
1:BI:63:ILE:HG22	1:BI:194:LEU:HB2	1.85	0.58
1:JF:123:ALA:HA	1:JF:126:LEU:HD12	1.86	0.58
1:AO:127:ARG:HG2	1:AO:160:ASP:HB3	1.86	0.58
1:FL:66:ASP:OD1	1:FL:66:ASP:N	2.33	0.58
1:JJ:114:MET:N	1:JJ:114:MET:SD	2.72	0.58
1:BA:171:GLU:HB3	1:BE:93:MET:HE3	1.84	0.57
1:DF:123:ALA:HA	1:DF:126:LEU:HD12	1.86	0.57
1:KF:123:ALA:HA	1:KF:126:LEU:HD12	1.86	0.57
1:AK:123:ALA:HA	1:AK:126:LEU:HD12	1.85	0.57
1:EO:127:ARG:HG2	1:EO:160:ASP:HB3	1.86	0.57
1:LF:123:ALA:HA	1:LF:126:LEU:HD12	1.86	0.57
1:CF:123:ALA:HA	1:CF:126:LEU:HD12	1.86	0.57
1:CO:127:ARG:HG2	1:CO:160:ASP:HB3	1.86	0.57
1:LM:84:TRP:CD1	1:LM:150:CYS:HB2	2.40	0.57
1:LO:127:ARG:HG2	1:LO:160:ASP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BO:127:ARG:HG2	1:BO:160:ASP:HB3	1.86	0.57
1:HF:123:ALA:HA	1:HF:126:LEU:HD12	1.86	0.57
1:IG:123:ALA:HA	1:IG:126:LEU:HD12	1.85	0.57
1:BG:123:ALA:HA	1:BG:126:LEU:HD12	1.85	0.57
1:DM:84:TRP:CD1	1:DM:150:CYS:HB2	2.40	0.57
1:GO:127:ARG:HG2	1:GO:160:ASP:HB3	1.86	0.57
1:HO:127:ARG:HG2	1:HO:160:ASP:HB3	1.86	0.57
1:KO:127:ARG:HG2	1:KO:160:ASP:HB3	1.86	0.57
1:BK:123:ALA:HA	1:BK:126:LEU:HD12	1.85	0.56
1:BM:84:TRP:CD1	1:BM:150:CYS:HB2	2.40	0.56
1:KJ:114:MET:SD	1:KJ:114:MET:N	2.72	0.56
1:AL:66:ASP:OD1	1:AL:66:ASP:N	2.33	0.56
1:IM:84:TRP:CD1	1:IM:150:CYS:HB2	2.40	0.56
1:AM:84:TRP:CD1	1:AM:150:CYS:HB2	2.40	0.56
1:CM:84:TRP:CD1	1:CM:150:CYS:HB2	2.40	0.56
1:GM:84:TRP:CD1	1:GM:150:CYS:HB2	2.40	0.56
1:HM:84:TRP:CD1	1:HM:150:CYS:HB2	2.40	0.56
1:JM:84:TRP:CD1	1:JM:150:CYS:HB2	2.40	0.56
1:KD:84:TRP:CD1	1:KD:150:CYS:HB2	2.41	0.56
1:KM:84:TRP:CD1	1:KM:150:CYS:HB2	2.40	0.56
1:AD:84:TRP:CD1	1:AD:150:CYS:HB2	2.41	0.56
1:CD:84:TRP:CD1	1:CD:150:CYS:HB2	2.41	0.56
1:ED:84:TRP:CD1	1:ED:150:CYS:HB2	2.41	0.56
1:EN:120:LYS:NZ	1:EN:122:THR:OG1	2.39	0.56
1:GD:84:TRP:CD1	1:GD:150:CYS:HB2	2.41	0.56
1:BD:84:TRP:CD1	1:BD:150:CYS:HB2	2.41	0.56
1:FM:84:TRP:CD1	1:FM:150:CYS:HB2	2.40	0.56
1:IJ:114:MET:N	1:IJ:114:MET:SD	2.72	0.56
1:HN:120:LYS:NZ	1:HN:122:THR:OG1	2.39	0.56
1:IM:78:LYS:HG3	1:IM:79:HIS:H	1.71	0.56
1:JD:84:TRP:CD1	1:JD:150:CYS:HB2	2.41	0.56
1:LD:84:TRP:CD1	1:LD:150:CYS:HB2	2.41	0.56
1:LN:120:LYS:NZ	1:LN:122:THR:OG1	2.39	0.56
1:BN:120:LYS:NZ	1:BN:122:THR:OG1	2.39	0.56
1:AD:55:ARG:HH12	1:AE:181:ARG:HG2	1.71	0.56
1:ED:55:ARG:HH12	1:EE:181:ARG:HG2	1.71	0.56
1:EM:84:TRP:CD1	1:EM:150:CYS:HB2	2.40	0.56
1:AM:78:LYS:HG3	1:AM:79:HIS:H	1.71	0.55
1:IN:120:LYS:NZ	1:IN:122:THR:OG1	2.39	0.55
1:BM:78:LYS:HG3	1:BM:79:HIS:H	1.71	0.55
1:DD:84:TRP:CD1	1:DD:150:CYS:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HM:78:LYS:HG3	1:HM:79:HIS:H	1.71	0.55
1:KM:78:LYS:HG3	1:KM:79:HIS:H	1.71	0.55
1:CD:55:ARG:HH12	1:CE:181:ARG:HG2	1.71	0.55
1:EG:93:MET:HE3	1:EH:171:GLU:HB3	1.89	0.55
1:JN:120:LYS:NZ	1:JN:122:THR:OG1	2.39	0.55
1:BD:55:ARG:HH12	1:BE:181:ARG:HG2	1.71	0.55
1:FM:78:LYS:HG3	1:FM:79:HIS:H	1.71	0.55
1:HD:55:ARG:HH12	1:HE:181:ARG:HG2	1.71	0.55
1:HD:84:TRP:CD1	1:HD:150:CYS:HB2	2.41	0.55
1:HG:93:MET:HE3	1:HH:171:GLU:HB3	1.89	0.55
1:GL:81:ASN:HB3	1:GL:143:LEU:HD23	1.89	0.55
1:LG:93:MET:HE3	1:LH:171:GLU:HB3	1.89	0.55
1:GG:93:MET:HE3	1:GH:171:GLU:HB3	1.89	0.55
1:IF:37:ASP:OD1	1:IF:37:ASP:N	2.33	0.55
1:JL:66:ASP:OD1	1:JL:66:ASP:N	2.33	0.55
1:FD:84:TRP:CD1	1:FD:150:CYS:HB2	2.41	0.55
1:JD:55:ARG:HH12	1:JE:181:ARG:HG2	1.71	0.55
1:JM:78:LYS:HG3	1:JM:79:HIS:H	1.71	0.55
1:KN:120:LYS:NZ	1:KN:122:THR:OG1	2.39	0.55
1:CG:93:MET:HE3	1:CH:171:GLU:HB3	1.89	0.55
1:EO:84:TRP:CD1	1:EO:150:CYS:HB2	2.42	0.55
1:LL:66:ASP:OD1	1:LL:66:ASP:N	2.33	0.55
1:BL:81:ASN:HB3	1:BL:143:LEU:HD23	1.89	0.55
1:CO:84:TRP:CD1	1:CO:150:CYS:HB2	2.42	0.55
1:ID:84:TRP:CD1	1:ID:150:CYS:HB2	2.41	0.55
1:JO:84:TRP:CD1	1:JO:150:CYS:HB2	2.42	0.55
1:KD:55:ARG:HH12	1:KE:181:ARG:HG2	1.71	0.55
1:GO:84:TRP:CD1	1:GO:150:CYS:HB2	2.42	0.55
1:HL:81:ASN:HB3	1:HL:143:LEU:HD23	1.89	0.55
1:IL:81:ASN:HB3	1:IL:143:LEU:HD23	1.89	0.55
1:JF:37:ASP:OD1	1:JF:37:ASP:N	2.33	0.55
1:BO:84:TRP:CD1	1:BO:150:CYS:HB2	2.42	0.54
1:CM:78:LYS:HG3	1:CM:79:HIS:H	1.71	0.54
1:IJ:123:ALA:HA	1:IJ:126:LEU:HD12	1.89	0.54
1:BG:93:MET:HE3	1:BH:171:GLU:HB3	1.89	0.54
1:BJ:123:ALA:HA	1:BJ:126:LEU:HD12	1.89	0.54
1:AL:81:ASN:HB3	1:AL:143:LEU:HD23	1.89	0.54
1:CJ:84:TRP:CD1	1:CJ:150:CYS:HB2	2.43	0.54
1:DD:55:ARG:HH12	1:DE:181:ARG:HG2	1.71	0.54
1:IB:84:TRP:CD1	1:IB:150:CYS:HB2	2.43	0.54
1:ID:55:ARG:HH12	1:IE:181:ARG:HG2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LD:55:ARG:HH12	1:LE:181:ARG:HG2	1.71	0.54
1:LL:81:ASN:HB3	1:LL:143:LEU:HD23	1.89	0.54
1:LM:78:LYS:HG3	1:LM:79:HIS:H	1.71	0.54
1:LO:84:TRP:CD1	1:LO:150:CYS:HB2	2.42	0.54
1:BJ:84:TRP:CD1	1:BJ:150:CYS:HB2	2.43	0.54
1:CL:81:ASN:HB3	1:CL:143:LEU:HD23	1.89	0.54
1:DG:93:MET:HE3	1:DH:171:GLU:HB3	1.89	0.54
1:DO:84:TRP:CD1	1:DO:150:CYS:HB2	2.42	0.54
1:EJ:84:TRP:CD1	1:EJ:150:CYS:HB2	2.43	0.54
1:FJ:84:TRP:CD1	1:FJ:150:CYS:HB2	2.43	0.54
1:GM:78:LYS:HG3	1:GM:79:HIS:H	1.71	0.54
1:KO:84:TRP:CD1	1:KO:150:CYS:HB2	2.42	0.54
1:LB:84:TRP:CD1	1:LB:150:CYS:HB2	2.43	0.54
1:DJ:84:TRP:CD1	1:DJ:150:CYS:HB2	2.43	0.54
1:FO:84:TRP:CD1	1:FO:150:CYS:HB2	2.42	0.54
1:HB:84:TRP:CD1	1:HB:150:CYS:HB2	2.43	0.54
1:AB:84:TRP:CD1	1:AB:150:CYS:HB2	2.43	0.54
1:KB:84:TRP:CD1	1:KB:150:CYS:HB2	2.43	0.54
1:AJ:84:TRP:CD1	1:AJ:150:CYS:HB2	2.43	0.54
1:AN:133:SER:HB3	1:AN:172:ILE:HD11	1.90	0.54
1:DB:84:TRP:CD1	1:DB:150:CYS:HB2	2.43	0.54
1:DN:93:MET:HE2	1:DO:167:PRO:HD2	1.90	0.54
1:EL:81:ASN:HB3	1:EL:143:LEU:HD23	1.89	0.54
1:GD:55:ARG:HH12	1:GE:181:ARG:HG2	1.71	0.54
1:GN:93:MET:HE2	1:GO:167:PRO:HD2	1.90	0.54
1:IN:93:MET:HE2	1:IO:167:PRO:HD2	1.90	0.54
1:KG:93:MET:HE3	1:KH:171:GLU:HB3	1.89	0.54
1:LA:93:MET:HE3	1:LB:171:GLU:HB3	1.90	0.54
1:BB:84:TRP:CD1	1:BB:150:CYS:HB2	2.43	0.54
1:CB:84:TRP:CD1	1:CB:150:CYS:HB2	2.43	0.54
1:CN:120:LYS:NZ	1:CN:122:THR:OG1	2.39	0.54
1:DM:78:LYS:HG3	1:DM:79:HIS:H	1.71	0.54
1:EJ:123:ALA:HA	1:EJ:126:LEU:HD12	1.89	0.54
1:FJ:123:ALA:HA	1:FJ:126:LEU:HD12	1.89	0.54
1:GJ:123:ALA:HA	1:GJ:126:LEU:HD12	1.89	0.54
1:GN:133:SER:HB3	1:GN:172:ILE:HD11	1.90	0.54
1:EA:74:ARG:O	1:EA:77:THR:OG1	2.26	0.54
1:EM:78:LYS:HG3	1:EM:79:HIS:H	1.71	0.54
1:EN:133:SER:HB3	1:EN:172:ILE:HD11	1.90	0.54
1:HJ:123:ALA:HA	1:HJ:126:LEU:HD12	1.89	0.54
1:HN:93:MET:HE2	1:HO:167:PRO:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IM:82:LYS:HB2	1:IM:143:LEU:HD22	1.90	0.54
1:JJ:84:TRP:CD1	1:JJ:150:CYS:HB2	2.43	0.54
1:CA:93:MET:HE3	1:CB:171:GLU:HB3	1.90	0.54
1:DN:133:SER:HB3	1:DN:172:ILE:HD11	1.90	0.54
1:EB:84:TRP:CD1	1:EB:150:CYS:HB2	2.43	0.54
1:GA:93:MET:HE3	1:GB:171:GLU:HB3	1.90	0.54
1:HM:82:LYS:HB2	1:HM:143:LEU:HD22	1.90	0.54
1:HO:84:TRP:CD1	1:HO:150:CYS:HB2	2.42	0.54
1:IG:93:MET:HE3	1:IH:171:GLU:HB3	1.89	0.54
1:JA:93:MET:HE3	1:JB:171:GLU:HB3	1.90	0.54
1:JG:93:MET:HE3	1:JH:171:GLU:HB3	1.89	0.54
1:JJ:123:ALA:HA	1:JJ:126:LEU:HD12	1.89	0.54
1:JL:81:ASN:HB3	1:JL:143:LEU:HD23	1.89	0.54
1:BN:133:SER:HB3	1:BN:172:ILE:HD11	1.90	0.54
1:CN:133:SER:HB3	1:CN:172:ILE:HD11	1.90	0.54
1:DA:93:MET:HE3	1:DB:171:GLU:HB3	1.90	0.54
1:DL:81:ASN:HB3	1:DL:143:LEU:HD23	1.89	0.54
1:FA:74:ARG:O	1:FA:77:THR:OG1	2.26	0.54
1:IO:84:TRP:CD1	1:IO:150:CYS:HB2	2.42	0.54
1:BA:93:MET:HE3	1:BB:171:GLU:HB3	1.90	0.53
1:AG:93:MET:HE3	1:AH:171:GLU:HB3	1.89	0.53
1:FC:84:TRP:CD1	1:FC:150:CYS:HB2	2.43	0.53
1:FG:93:MET:HE3	1:FH:171:GLU:HB3	1.89	0.53
1:GM:82:LYS:HB2	1:GM:143:LEU:HD22	1.90	0.53
1:HN:133:SER:HB3	1:HN:172:ILE:HD11	1.90	0.53
1:KA:93:MET:HE3	1:KB:171:GLU:HB3	1.90	0.53
1:LJ:84:TRP:CD1	1:LJ:150:CYS:HB2	2.43	0.53
1:AA:93:MET:HE3	1:AB:171:GLU:HB3	1.90	0.53
1:AO:84:TRP:CD1	1:AO:150:CYS:HB2	2.42	0.53
1:CM:82:LYS:HB2	1:CM:143:LEU:HD22	1.90	0.53
1:DM:82:LYS:HB2	1:DM:143:LEU:HD22	1.90	0.53
1:GJ:84:TRP:CD1	1:GJ:150:CYS:HB2	2.43	0.53
1:KJ:84:TRP:CD1	1:KJ:150:CYS:HB2	2.43	0.53
1:DN:120:LYS:NZ	1:DN:122:THR:OG1	2.39	0.53
1:FL:81:ASN:HB3	1:FL:143:LEU:HD23	1.89	0.53
1:GF:37:ASP:OD1	1:GF:37:ASP:N	2.33	0.53
1:IJ:84:TRP:CD1	1:IJ:150:CYS:HB2	2.43	0.53
1:JN:133:SER:HB3	1:JN:172:ILE:HD11	1.90	0.53
1:KJ:123:ALA:HA	1:KJ:126:LEU:HD12	1.89	0.53
1:LL:133:SER:OG	1:LL:193:ASP:OD2	2.26	0.53
1:LM:82:LYS:HB2	1:LM:143:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:84:TRP:CD1	1:BC:150:CYS:HB2	2.43	0.53
1:AJ:123:ALA:HA	1:AJ:126:LEU:HD12	1.89	0.53
1:EN:93:MET:HE2	1:EO:167:PRO:HD2	1.90	0.53
1:HJ:84:TRP:CD1	1:HJ:150:CYS:HB2	2.43	0.53
1:KE:68:LEU:HD23	1:KE:68:LEU:H	1.74	0.53
1:KN:133:SER:HB3	1:KN:172:ILE:HD11	1.90	0.53
1:LE:68:LEU:HD23	1:LE:68:LEU:H	1.74	0.53
1:AC:84:TRP:CD1	1:AC:150:CYS:HB2	2.43	0.53
1:KA:74:ARG:O	1:KA:77:THR:OG1	2.26	0.53
1:LA:74:ARG:O	1:LA:77:THR:OG1	2.26	0.53
1:LC:88:LEU:HD11	1:LC:121:LEU:HD13	1.91	0.53
1:LJ:123:ALA:HA	1:LJ:126:LEU:HD12	1.89	0.53
1:CJ:123:ALA:HA	1:CJ:126:LEU:HD12	1.89	0.53
1:DC:88:LEU:HD11	1:DC:121:LEU:HD13	1.91	0.53
1:GB:84:TRP:CD1	1:GB:150:CYS:HB2	2.43	0.53
1:GC:88:LEU:HD11	1:GC:121:LEU:HD13	1.91	0.53
1:HA:74:ARG:O	1:HA:77:THR:OG1	2.26	0.53
1:JB:84:TRP:CD1	1:JB:150:CYS:HB2	2.43	0.53
1:JE:68:LEU:HD23	1:JE:68:LEU:H	1.74	0.53
1:KL:81:ASN:HB3	1:KL:143:LEU:HD23	1.89	0.53
1:LN:133:SER:HB3	1:LN:172:ILE:HD11	1.90	0.53
1:BC:88:LEU:HD11	1:BC:121:LEU:HD13	1.91	0.53
1:AM:82:LYS:HB2	1:AM:143:LEU:HD22	1.90	0.53
1:AN:93:MET:HE2	1:AO:167:PRO:HD2	1.90	0.53
1:CN:93:MET:HE2	1:CO:167:PRO:HD2	1.90	0.53
1:DF:74:ARG:O	1:DF:77:THR:OG1	2.25	0.53
1:EC:84:TRP:CD1	1:EC:150:CYS:HB2	2.43	0.53
1:FB:84:TRP:CD1	1:FB:150:CYS:HB2	2.43	0.53
1:FD:55:ARG:HH12	1:FE:181:ARG:HG2	1.71	0.53
1:GL:133:SER:OG	1:GL:193:ASP:OD2	2.26	0.53
1:IC:88:LEU:HD11	1:IC:121:LEU:HD13	1.91	0.53
1:JC:88:LEU:HD11	1:JC:121:LEU:HD13	1.91	0.53
1:BE:74:ARG:HD3	1:BE:81:ASN:HA	1.91	0.53
1:EL:133:SER:OG	1:EL:193:ASP:OD2	2.26	0.53
1:FN:93:MET:HE2	1:FO:167:PRO:HD2	1.90	0.53
1:GC:84:TRP:CD1	1:GC:150:CYS:HB2	2.44	0.53
1:HC:84:TRP:CD1	1:HC:150:CYS:HB2	2.44	0.53
1:IC:84:TRP:CD1	1:IC:150:CYS:HB2	2.43	0.53
1:BN:93:MET:HE2	1:BO:167:PRO:HD2	1.90	0.53
1:AC:88:LEU:HD11	1:AC:121:LEU:HD13	1.91	0.53
1:AF:37:ASP:OD1	1:AF:37:ASP:N	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AN:120:LYS:NZ	1:AN:122:THR:OG1	2.39	0.53
1:EA:93:MET:HE3	1:EB:171:GLU:HB3	1.90	0.53
1:EE:74:ARG:HD3	1:EE:81:ASN:HA	1.91	0.53
1:EL:66:ASP:OD1	1:EL:66:ASP:N	2.33	0.53
1:FC:88:LEU:HD11	1:FC:121:LEU:HD13	1.91	0.53
1:LC:84:TRP:CD1	1:LC:150:CYS:HB2	2.44	0.53
1:CE:74:ARG:HD3	1:CE:81:ASN:HA	1.91	0.53
1:DC:84:TRP:CD1	1:DC:150:CYS:HB2	2.44	0.53
1:DE:74:ARG:HD3	1:DE:81:ASN:HA	1.91	0.53
1:EC:88:LEU:HD11	1:EC:121:LEU:HD13	1.91	0.53
1:EM:82:LYS:HB2	1:EM:143:LEU:HD22	1.90	0.53
1:KC:88:LEU:HD11	1:KC:121:LEU:HD13	1.91	0.53
1:KN:93:MET:HE2	1:KO:167:PRO:HD2	1.90	0.53
1:BE:68:LEU:HD23	1:BE:68:LEU:H	1.74	0.52
1:AE:68:LEU:HD23	1:AE:68:LEU:H	1.74	0.52
1:FA:93:MET:HE3	1:FB:171:GLU:HB3	1.90	0.52
1:FC:61:ASP:N	1:FC:61:ASP:OD1	2.42	0.52
1:FN:55:ARG:O	1:FN:101:ARG:NH2	2.43	0.52
1:GE:74:ARG:HD3	1:GE:81:ASN:HA	1.91	0.52
1:GL:66:ASP:OD1	1:GL:66:ASP:N	2.33	0.52
1:JA:74:ARG:O	1:JA:77:THR:OG1	2.26	0.52
1:JE:74:ARG:HD3	1:JE:81:ASN:HA	1.91	0.52
1:KL:133:SER:OG	1:KL:193:ASP:OD2	2.26	0.52
1:EN:55:ARG:O	1:EN:101:ARG:NH2	2.43	0.52
1:HC:88:LEU:HD11	1:HC:121:LEU:HD13	1.91	0.52
1:IN:133:SER:HB3	1:IN:172:ILE:HD11	1.90	0.52
1:JN:55:ARG:O	1:JN:101:ARG:NH2	2.43	0.52
1:KC:84:TRP:CD1	1:KC:150:CYS:HB2	2.43	0.52
1:BC:61:ASP:OD1	1:BC:61:ASP:N	2.42	0.52
1:DL:66:ASP:OD1	1:DL:66:ASP:N	2.33	0.52
1:FE:74:ARG:HD3	1:FE:81:ASN:HA	1.91	0.52
1:FM:82:LYS:HB2	1:FM:143:LEU:HD22	1.90	0.52
1:HC:61:ASP:N	1:HC:61:ASP:OD1	2.42	0.52
1:JC:84:TRP:CD1	1:JC:150:CYS:HB2	2.44	0.52
1:JN:93:MET:HE2	1:JO:167:PRO:HD2	1.90	0.52
1:KM:82:LYS:HB2	1:KM:143:LEU:HD22	1.90	0.52
1:LE:74:ARG:HD3	1:LE:81:ASN:HA	1.91	0.52
1:CC:84:TRP:CD1	1:CC:150:CYS:HB2	2.44	0.52
1:DG:84:TRP:CD1	1:DG:150:CYS:HB2	2.45	0.52
1:DJ:123:ALA:HA	1:DJ:126:LEU:HD12	1.89	0.52
1:EC:61:ASP:OD1	1:EC:61:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FN:133:SER:HB3	1:FN:172:ILE:HD11	1.90	0.52
1:GE:68:LEU:HD23	1:GE:68:LEU:H	1.74	0.52
1:GN:120:LYS:NZ	1:GN:122:THR:OG1	2.39	0.52
1:GN:123:ALA:HA	1:GN:126:LEU:HD12	1.92	0.52
1:HE:74:ARG:HD3	1:HE:81:ASN:HA	1.91	0.52
1:JM:82:LYS:HB2	1:JM:143:LEU:HD22	1.90	0.52
1:CE:68:LEU:HD23	1:CE:68:LEU:H	1.74	0.52
1:CN:55:ARG:O	1:CN:101:ARG:NH2	2.43	0.52
1:HA:93:MET:HE3	1:HB:171:GLU:HB3	1.90	0.52
1:IA:93:MET:HE3	1:IB:171:GLU:HB3	1.90	0.52
1:JC:61:ASP:OD1	1:JC:61:ASP:N	2.42	0.52
1:KG:84:TRP:CD1	1:KG:150:CYS:HB2	2.45	0.52
1:LN:55:ARG:O	1:LN:101:ARG:NH2	2.43	0.52
1:BM:82:LYS:HB2	1:BM:143:LEU:HD22	1.90	0.52
1:AC:61:ASP:N	1:AC:61:ASP:OD1	2.42	0.52
1:CL:133:SER:OG	1:CL:193:ASP:OD2	2.26	0.52
1:DC:61:ASP:OD1	1:DC:61:ASP:N	2.42	0.52
1:AG:84:TRP:CD1	1:AG:150:CYS:HB2	2.45	0.52
1:AN:123:ALA:HA	1:AN:126:LEU:HD12	1.92	0.52
1:CG:84:TRP:CD1	1:CG:150:CYS:HB2	2.45	0.52
1:DN:55:ARG:O	1:DN:101:ARG:NH2	2.43	0.52
1:GA:74:ARG:O	1:GA:77:THR:OG1	2.26	0.52
1:IN:123:ALA:HA	1:IN:126:LEU:HD12	1.92	0.52
1:JG:84:TRP:CD1	1:JG:150:CYS:HB2	2.45	0.52
1:JG:88:LEU:HD11	1:JG:121:LEU:HD13	1.92	0.52
1:BG:84:TRP:CD1	1:BG:150:CYS:HB2	2.45	0.52
1:AA:74:ARG:O	1:AA:77:THR:OG1	2.26	0.52
1:CC:61:ASP:N	1:CC:61:ASP:OD1	2.42	0.52
1:CL:66:ASP:OD1	1:CL:66:ASP:N	2.33	0.52
1:FN:120:LYS:NZ	1:FN:122:THR:OG1	2.39	0.52
1:KE:74:ARG:HD3	1:KE:81:ASN:HA	1.91	0.52
1:LC:61:ASP:OD1	1:LC:61:ASP:N	2.42	0.52
1:LN:93:MET:HE2	1:LO:167:PRO:HD2	1.90	0.52
1:EF:74:ARG:O	1:EF:77:THR:OG1	2.25	0.52
1:EG:84:TRP:CD1	1:EG:150:CYS:HB2	2.45	0.52
1:EG:88:LEU:HD11	1:EG:121:LEU:HD13	1.92	0.52
1:GN:55:ARG:O	1:GN:101:ARG:NH2	2.43	0.52
1:HE:68:LEU:H	1:HE:68:LEU:HD23	1.74	0.52
1:HN:55:ARG:O	1:HN:101:ARG:NH2	2.43	0.52
1:IG:88:LEU:HD11	1:IG:121:LEU:HD13	1.92	0.52
1:KC:61:ASP:N	1:KC:61:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LG:84:TRP:CD1	1:LG:150:CYS:HB2	2.45	0.52
1:LG:88:LEU:HD11	1:LG:121:LEU:HD13	1.92	0.52
1:CF:37:ASP:OD1	1:CF:37:ASP:N	2.33	0.52
1:FJ:58:VAL:HG22	1:FJ:188:VAL:HB	1.92	0.52
1:GC:61:ASP:OD1	1:GC:61:ASP:N	2.42	0.52
1:IE:68:LEU:HD23	1:IE:68:LEU:H	1.74	0.52
1:AJ:58:VAL:HG22	1:AJ:188:VAL:HB	1.92	0.51
1:EN:123:ALA:HA	1:EN:126:LEU:HD12	1.92	0.51
1:HJ:58:VAL:HG22	1:HJ:188:VAL:HB	1.92	0.51
1:BN:123:ALA:HA	1:BN:126:LEU:HD12	1.92	0.51
1:FG:88:LEU:HD11	1:FG:121:LEU:HD13	1.92	0.51
1:HG:84:TRP:CD1	1:HG:150:CYS:HB2	2.45	0.51
1:BJ:58:VAL:HG22	1:BJ:188:VAL:HB	1.92	0.51
1:AE:74:ARG:HD3	1:AE:81:ASN:HA	1.91	0.51
1:DI:127:ARG:HG2	1:DI:160:ASP:HB3	1.93	0.51
1:EI:127:ARG:HG2	1:EI:160:ASP:HB3	1.93	0.51
1:IC:61:ASP:N	1:IC:61:ASP:OD1	2.42	0.51
1:IO:136:ASN:HD22	1:IO:193:ASP:HB3	1.76	0.51
1:BA:74:ARG:O	1:BA:77:THR:OG1	2.26	0.51
1:AI:127:ARG:HG2	1:AI:160:ASP:HB3	1.93	0.51
1:AO:136:ASN:HD22	1:AO:193:ASP:HB3	1.76	0.51
1:CC:88:LEU:HD11	1:CC:121:LEU:HD13	1.91	0.51
1:EE:68:LEU:HD23	1:EE:68:LEU:H	1.74	0.51
1:FE:68:LEU:HD23	1:FE:68:LEU:H	1.74	0.51
1:FG:84:TRP:CD1	1:FG:150:CYS:HB2	2.45	0.51
1:IG:84:TRP:CD1	1:IG:150:CYS:HB2	2.45	0.51
1:KO:136:ASN:HD22	1:KO:193:ASP:HB3	1.76	0.51
1:AH:84:TRP:CD1	1:AH:150:CYS:HB2	2.46	0.51
1:AK:84:TRP:CD1	1:AK:150:CYS:HB2	2.46	0.51
1:DE:68:LEU:HD23	1:DE:68:LEU:H	1.74	0.51
1:DG:88:LEU:HD11	1:DG:121:LEU:HD13	1.92	0.51
1:EL:52:LEU:HD22	1:EM:50:LEU:HD11	1.93	0.51
1:EN:136:ASN:HD22	1:EN:193:ASP:HB3	1.76	0.51
1:FH:84:TRP:CD1	1:FH:150:CYS:HB2	2.46	0.51
1:FO:136:ASN:HD22	1:FO:193:ASP:HB3	1.76	0.51
1:GL:169:SER:OG	1:GL:193:ASP:OD1	2.29	0.51
1:IA:74:ARG:O	1:IA:77:THR:OG1	2.26	0.51
1:IN:55:ARG:O	1:IN:101:ARG:NH2	2.43	0.51
1:JJ:58:VAL:HG22	1:JJ:188:VAL:HB	1.92	0.51
1:KG:88:LEU:HD11	1:KG:121:LEU:HD13	1.92	0.51
1:KN:55:ARG:O	1:KN:101:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BH:84:TRP:CD1	1:BH:150:CYS:HB2	2.46	0.51
1:BN:55:ARG:O	1:BN:101:ARG:NH2	2.43	0.51
1:AH:77:THR:HB	1:AH:78:LYS:HD3	1.93	0.51
1:CG:88:LEU:HD11	1:CG:121:LEU:HD13	1.92	0.51
1:DJ:58:VAL:HG22	1:DJ:188:VAL:HB	1.92	0.51
1:DL:169:SER:OG	1:DL:193:ASP:OD1	2.29	0.51
1:DN:136:ASN:HD22	1:DN:193:ASP:HB3	1.76	0.51
1:EH:77:THR:HB	1:EH:78:LYS:HD3	1.93	0.51
1:GG:84:TRP:CD1	1:GG:150:CYS:HB2	2.45	0.51
1:HG:88:LEU:HD11	1:HG:121:LEU:HD13	1.92	0.51
1:DL:151:ILE:HG22	1:DL:156:GLY:HA3	1.93	0.51
1:DN:123:ALA:HA	1:DN:126:LEU:HD12	1.92	0.51
1:EJ:58:VAL:HG22	1:EJ:188:VAL:HB	1.92	0.51
1:EK:84:TRP:CD1	1:EK:150:CYS:HB2	2.46	0.51
1:GG:88:LEU:HD11	1:GG:121:LEU:HD13	1.92	0.51
1:GH:77:THR:HB	1:GH:78:LYS:HD3	1.93	0.51
1:HK:84:TRP:CD1	1:HK:150:CYS:HB2	2.46	0.51
1:IF:74:ARG:O	1:IF:77:THR:OG1	2.25	0.51
1:IH:77:THR:HB	1:IH:78:LYS:HD3	1.93	0.51
1:JI:127:ARG:HG2	1:JI:160:ASP:HB3	1.93	0.51
1:KL:52:LEU:HD22	1:KM:50:LEU:HD11	1.93	0.51
1:BD:93:MET:HE2	1:BE:171:GLU:HB3	1.93	0.51
1:BH:58:VAL:HG22	1:BH:188:VAL:HB	1.93	0.51
1:BL:84:TRP:CD1	1:BL:150:CYS:HB2	2.46	0.51
1:AM:123:ALA:HA	1:AM:126:LEU:HD12	1.93	0.51
1:CF:74:ARG:O	1:CF:77:THR:OG1	2.25	0.51
1:CH:77:THR:HB	1:CH:78:LYS:HD3	1.93	0.51
1:CL:169:SER:OG	1:CL:193:ASP:OD1	2.29	0.51
1:DH:77:THR:HB	1:DH:78:LYS:HD3	1.93	0.51
1:FK:84:TRP:CD1	1:FK:150:CYS:HB2	2.46	0.51
1:HF:37:ASP:OD1	1:HF:37:ASP:N	2.33	0.51
1:HL:169:SER:OG	1:HL:193:ASP:OD1	2.29	0.51
1:IL:169:SER:OG	1:IL:193:ASP:OD1	2.29	0.51
1:JH:84:TRP:CD1	1:JH:150:CYS:HB2	2.46	0.51
1:JN:136:ASN:HD22	1:JN:193:ASP:HB3	1.76	0.51
1:KN:123:ALA:HA	1:KN:126:LEU:HD12	1.92	0.51
1:KN:136:ASN:HD22	1:KN:193:ASP:HB3	1.76	0.51
1:LK:84:TRP:CD1	1:LK:150:CYS:HB2	2.46	0.51
1:LL:84:TRP:CD1	1:LL:150:CYS:HB2	2.46	0.51
1:BG:88:LEU:HD11	1:BG:121:LEU:HD13	1.92	0.51
1:BK:84:TRP:CD1	1:BK:150:CYS:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BL:151:ILE:HG22	1:BL:156:GLY:HA3	1.93	0.51
1:AD:93:MET:HE2	1:AE:171:GLU:HB3	1.93	0.51
1:AJ:63:ILE:HB	1:AJ:195:ILE:H	1.76	0.51
1:CL:151:ILE:HG22	1:CL:156:GLY:HA3	1.93	0.51
1:DK:84:TRP:CD1	1:DK:150:CYS:HB2	2.46	0.51
1:ED:93:MET:HE2	1:EE:171:GLU:HB3	1.93	0.51
1:EK:97:PHE:HA	1:EK:100:LEU:HB2	1.93	0.51
1:EL:84:TRP:CD1	1:EL:150:CYS:HB2	2.46	0.51
1:GF:74:ARG:O	1:GF:77:THR:OG1	2.25	0.51
1:GL:151:ILE:HG22	1:GL:156:GLY:HA3	1.93	0.51
1:HH:84:TRP:CD1	1:HH:150:CYS:HB2	2.46	0.51
1:HO:136:ASN:HD22	1:HO:193:ASP:HB3	1.76	0.51
1:JD:93:MET:HE2	1:JE:171:GLU:HB3	1.93	0.51
1:LH:84:TRP:CD1	1:LH:150:CYS:HB2	2.46	0.51
1:BH:77:THR:HB	1:BH:78:LYS:HD3	1.93	0.51
1:AN:55:ARG:O	1:AN:101:ARG:NH2	2.43	0.51
1:CI:127:ARG:HG2	1:CI:160:ASP:HB3	1.93	0.51
1:CL:84:TRP:CD1	1:CL:150:CYS:HB2	2.46	0.51
1:FI:127:ARG:HG2	1:FI:160:ASP:HB3	1.93	0.51
1:FL:84:TRP:CD1	1:FL:150:CYS:HB2	2.46	0.51
1:IE:74:ARG:HD3	1:IE:81:ASN:HA	1.91	0.51
1:IH:58:VAL:HG22	1:IH:188:VAL:HB	1.93	0.51
1:IH:84:TRP:CD1	1:IH:150:CYS:HB2	2.46	0.51
1:II:84:TRP:CD1	1:II:150:CYS:HB2	2.46	0.51
1:IL:84:TRP:CD1	1:IL:150:CYS:HB2	2.46	0.51
1:IO:61:ASP:OD1	1:IO:62:ILE:N	2.44	0.51
1:JH:58:VAL:HG22	1:JH:188:VAL:HB	1.93	0.51
1:JL:151:ILE:HG22	1:JL:156:GLY:HA3	1.93	0.51
1:KI:127:ARG:HG2	1:KI:160:ASP:HB3	1.93	0.51
1:KL:151:ILE:HG22	1:KL:156:GLY:HA3	1.93	0.51
1:LL:52:LEU:HD22	1:LM:50:LEU:HD11	1.93	0.51
1:LL:169:SER:OG	1:LL:193:ASP:OD1	2.29	0.51
1:BM:123:ALA:HA	1:BM:126:LEU:HD12	1.93	0.50
1:CL:52:LEU:HD22	1:CM:50:LEU:HD11	1.93	0.50
1:DA:74:ARG:O	1:DA:77:THR:OG1	2.26	0.50
1:DH:58:VAL:HG22	1:DH:188:VAL:HB	1.93	0.50
1:DL:52:LEU:HD22	1:DM:50:LEU:HD11	1.93	0.50
1:EM:123:ALA:HA	1:EM:126:LEU:HD12	1.93	0.50
1:FH:77:THR:HB	1:FH:78:LYS:HD3	1.93	0.50
1:GH:58:VAL:HG22	1:GH:188:VAL:HB	1.93	0.50
1:HI:84:TRP:CD1	1:HI:150:CYS:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JH:77:THR:HB	1:JH:78:LYS:HD3	1.93	0.50
1:JK:97:PHE:HA	1:JK:100:LEU:HB2	1.93	0.50
1:KL:169:SER:OG	1:KL:193:ASP:OD1	2.29	0.50
1:KO:61:ASP:OD1	1:KO:62:ILE:N	2.45	0.50
1:LJ:58:VAL:HG22	1:LJ:188:VAL:HB	1.92	0.50
1:LN:123:ALA:HA	1:LN:126:LEU:HD12	1.92	0.50
1:BL:52:LEU:HD22	1:BM:50:LEU:HD11	1.93	0.50
1:CO:136:ASN:HD22	1:CO:193:ASP:HB3	1.76	0.50
1:DM:123:ALA:HA	1:DM:126:LEU:HD12	1.93	0.50
1:EL:151:ILE:HG22	1:EL:156:GLY:HA3	1.93	0.50
1:FD:93:MET:HE2	1:FE:171:GLU:HB3	1.93	0.50
1:FH:58:VAL:HG22	1:FH:188:VAL:HB	1.93	0.50
1:HH:58:VAL:HG22	1:HH:188:VAL:HB	1.93	0.50
1:HH:77:THR:HB	1:HH:78:LYS:HD3	1.93	0.50
1:JN:123:ALA:HA	1:JN:126:LEU:HD12	1.92	0.50
1:JO:61:ASP:OD1	1:JO:62:ILE:N	2.44	0.50
1:JO:136:ASN:HD22	1:JO:193:ASP:HB3	1.76	0.50
1:KK:84:TRP:CD1	1:KK:150:CYS:HB2	2.46	0.50
1:LL:151:ILE:HG22	1:LL:156:GLY:HA3	1.93	0.50
1:LO:136:ASN:HD22	1:LO:193:ASP:HB3	1.76	0.50
1:BK:97:PHE:HA	1:BK:100:LEU:HB2	1.93	0.50
1:CA:74:ARG:O	1:CA:77:THR:OG1	2.26	0.50
1:CA:166:VAL:HG21	1:CA:172:ILE:HG12	1.94	0.50
1:CH:58:VAL:HG22	1:CH:188:VAL:HB	1.93	0.50
1:DL:84:TRP:CD1	1:DL:150:CYS:HB2	2.46	0.50
1:EH:62:ILE:HG12	1:EH:63:ILE:H	1.77	0.50
1:FA:166:VAL:HG21	1:FA:172:ILE:HG12	1.94	0.50
1:FH:62:ILE:HG12	1:FH:63:ILE:H	1.77	0.50
1:FL:52:LEU:HD22	1:FM:50:LEU:HD11	1.93	0.50
1:GL:84:TRP:CD1	1:GL:150:CYS:HB2	2.46	0.50
1:HM:123:ALA:HA	1:HM:126:LEU:HD12	1.93	0.50
1:HN:123:ALA:HA	1:HN:126:LEU:HD12	1.92	0.50
1:IK:97:PHE:HA	1:IK:100:LEU:HB2	1.93	0.50
1:KA:166:VAL:HG21	1:KA:172:ILE:HG12	1.94	0.50
1:BD:52:LEU:HD21	1:BE:173:PRO:HB2	1.94	0.50
1:AD:52:LEU:HD21	1:AE:173:PRO:HB2	1.94	0.50
1:AK:97:PHE:HA	1:AK:100:LEU:HB2	1.93	0.50
1:DH:84:TRP:CD1	1:DH:150:CYS:HB2	2.46	0.50
1:DN:93:MET:HE3	1:DO:171:GLU:HB3	1.94	0.50
1:EI:84:TRP:CD1	1:EI:150:CYS:HB2	2.47	0.50
1:EJ:63:ILE:HB	1:EJ:195:ILE:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GK:97:PHE:HA	1:GK:100:LEU:HB2	1.94	0.50
1:GM:123:ALA:HA	1:GM:126:LEU:HD12	1.93	0.50
1:GO:136:ASN:HD22	1:GO:193:ASP:HB3	1.76	0.50
1:JI:84:TRP:CD1	1:JI:150:CYS:HB2	2.46	0.50
1:KH:84:TRP:CD1	1:KH:150:CYS:HB2	2.46	0.50
1:KK:97:PHE:HA	1:KK:100:LEU:HB2	1.93	0.50
1:AL:151:ILE:HG22	1:AL:156:GLY:HA3	1.93	0.50
1:AN:136:ASN:HD22	1:AN:193:ASP:HB3	1.76	0.50
1:CM:123:ALA:HA	1:CM:126:LEU:HD12	1.93	0.50
1:CN:123:ALA:HA	1:CN:126:LEU:HD12	1.92	0.50
1:DA:166:VAL:HG21	1:DA:172:ILE:HG12	1.94	0.50
1:DE:37:ASP:N	1:DE:37:ASP:OD1	2.45	0.50
1:EA:166:VAL:HG21	1:EA:172:ILE:HG12	1.94	0.50
1:GJ:58:VAL:HG22	1:GJ:188:VAL:HB	1.92	0.50
1:HH:62:ILE:HG12	1:HH:63:ILE:H	1.77	0.50
1:HK:97:PHE:HA	1:HK:100:LEU:HB2	1.93	0.50
1:HL:52:LEU:HD22	1:HM:50:LEU:HD11	1.93	0.50
1:IA:166:VAL:HG21	1:IA:172:ILE:HG12	1.94	0.50
1:KD:52:LEU:HD21	1:KE:173:PRO:HB2	1.94	0.50
1:KJ:63:ILE:HB	1:KJ:195:ILE:H	1.76	0.50
1:LI:127:ARG:HG2	1:LI:160:ASP:HB3	1.93	0.50
1:AG:88:LEU:HD11	1:AG:121:LEU:HD13	1.92	0.50
1:AH:62:ILE:HG12	1:AH:63:ILE:H	1.77	0.50
1:AL:84:TRP:CD1	1:AL:150:CYS:HB2	2.46	0.50
1:CA:52:LEU:HD21	1:CB:173:PRO:HB2	1.94	0.50
1:CJ:58:VAL:HG22	1:CJ:188:VAL:HB	1.92	0.50
1:CN:93:MET:HE3	1:CO:171:GLU:HB3	1.94	0.50
1:EA:52:LEU:HD21	1:EB:173:PRO:HB2	1.94	0.50
1:EH:84:TRP:CD1	1:EH:150:CYS:HB2	2.46	0.50
1:FA:52:LEU:HD21	1:FB:173:PRO:HB2	1.94	0.50
1:FA:137:HIS:HA	1:FA:140:VAL:HG12	1.94	0.50
1:FN:136:ASN:HD22	1:FN:193:ASP:HB3	1.76	0.50
1:HD:52:LEU:HD21	1:HE:173:PRO:HB2	1.94	0.50
1:HI:127:ARG:HG2	1:HI:160:ASP:HB3	1.93	0.50
1:IN:136:ASN:HD22	1:IN:193:ASP:HB3	1.76	0.50
1:JA:52:LEU:HD21	1:JB:173:PRO:HB2	1.94	0.50
1:JF:74:ARG:O	1:JF:77:THR:OG1	2.25	0.50
1:LD:52:LEU:HD21	1:LE:173:PRO:HB2	1.94	0.50
1:LD:93:MET:HE2	1:LE:171:GLU:HB3	1.93	0.50
1:BA:137:HIS:HA	1:BA:140:VAL:HG12	1.94	0.50
1:DH:62:ILE:HG12	1:DH:63:ILE:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DO:136:ASN:HD22	1:DO:193:ASP:HB3	1.76	0.50
1:EE:37:ASP:OD1	1:EE:37:ASP:N	2.45	0.50
1:GJ:63:ILE:HB	1:GJ:195:ILE:H	1.76	0.50
1:GL:52:LEU:HD22	1:GM:50:LEU:HD11	1.93	0.50
1:IA:52:LEU:HD21	1:IB:173:PRO:HB2	1.94	0.50
1:LA:166:VAL:HG21	1:LA:172:ILE:HG12	1.94	0.50
1:LO:61:ASP:OD1	1:LO:62:ILE:N	2.45	0.50
1:BO:61:ASP:OD1	1:BO:62:ILE:N	2.45	0.50
1:AC:180:ALA:HB2	1:AC:188:VAL:HG21	1.94	0.50
1:AI:84:TRP:CD1	1:AI:150:CYS:HB2	2.47	0.50
1:AL:169:SER:OG	1:AL:193:ASP:OD1	2.29	0.50
1:CH:62:ILE:HG12	1:CH:63:ILE:H	1.77	0.50
1:DD:52:LEU:HD21	1:DE:173:PRO:HB2	1.94	0.50
1:EB:127:ARG:HG2	1:EB:160:ASP:HB3	1.94	0.50
1:EN:93:MET:HE3	1:EO:171:GLU:HB3	1.94	0.50
1:EO:61:ASP:OD1	1:EO:62:ILE:N	2.44	0.50
1:FD:52:LEU:HD21	1:FE:173:PRO:HB2	1.94	0.50
1:FF:37:ASP:OD1	1:FF:37:ASP:N	2.33	0.50
1:FN:93:MET:HE3	1:FO:171:GLU:HB3	1.94	0.50
1:FO:61:ASP:OD1	1:FO:62:ILE:N	2.44	0.50
1:IL:151:ILE:HG22	1:IL:156:GLY:HA3	1.93	0.50
1:JJ:63:ILE:HB	1:JJ:195:ILE:H	1.76	0.50
1:JK:84:TRP:CD1	1:JK:150:CYS:HB2	2.46	0.50
1:JM:123:ALA:HA	1:JM:126:LEU:HD12	1.93	0.50
1:KF:74:ARG:O	1:KF:77:THR:OG1	2.25	0.50
1:KH:58:VAL:HG22	1:KH:188:VAL:HB	1.93	0.50
1:KL:84:TRP:CD1	1:KL:150:CYS:HB2	2.46	0.50
1:KM:123:ALA:HA	1:KM:126:LEU:HD12	1.93	0.50
1:LJ:63:ILE:HB	1:LJ:195:ILE:H	1.76	0.50
1:BI:84:TRP:CD1	1:BI:150:CYS:HB2	2.47	0.50
1:BI:127:ARG:HG2	1:BI:160:ASP:HB3	1.93	0.50
1:BJ:63:ILE:HB	1:BJ:195:ILE:H	1.76	0.50
1:BL:169:SER:OG	1:BL:193:ASP:OD1	2.29	0.50
1:AL:52:LEU:HD22	1:AM:50:LEU:HD11	1.93	0.50
1:EC:180:ALA:HB2	1:EC:188:VAL:HG21	1.94	0.50
1:FE:37:ASP:N	1:FE:37:ASP:OD1	2.45	0.50
1:FI:84:TRP:CD1	1:FI:150:CYS:HB2	2.46	0.50
1:FN:123:ALA:HA	1:FN:126:LEU:HD12	1.92	0.50
1:HL:84:TRP:CD1	1:HL:150:CYS:HB2	2.46	0.50
1:JL:169:SER:OG	1:JL:193:ASP:OD1	2.29	0.50
1:KJ:58:VAL:HG22	1:KJ:188:VAL:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KN:93:MET:HE3	1:KO:171:GLU:HB3	1.94	0.50
1:LH:77:THR:HB	1:LH:78:LYS:HD3	1.93	0.50
1:CH:84:TRP:CD1	1:CH:150:CYS:HB2	2.46	0.49
1:CK:84:TRP:CD1	1:CK:150:CYS:HB2	2.46	0.49
1:DI:84:TRP:CD1	1:DI:150:CYS:HB2	2.47	0.49
1:ED:52:LEU:HD21	1:EE:173:PRO:HB2	1.94	0.49
1:EO:136:ASN:HD22	1:EO:193:ASP:HB3	1.76	0.49
1:GA:52:LEU:HD21	1:GB:173:PRO:HB2	1.94	0.49
1:GA:166:VAL:HG21	1:GA:172:ILE:HG12	1.94	0.49
1:GI:127:ARG:HG2	1:GI:160:ASP:HB3	1.93	0.49
1:GO:61:ASP:OD1	1:GO:62:ILE:N	2.45	0.49
1:HJ:63:ILE:HB	1:HJ:195:ILE:H	1.76	0.49
1:HL:66:ASP:OD1	1:HL:66:ASP:N	2.33	0.49
1:ID:52:LEU:HD21	1:IE:173:PRO:HB2	1.94	0.49
1:ID:93:MET:HE2	1:IE:171:GLU:HB3	1.93	0.49
1:JA:166:VAL:HG21	1:JA:172:ILE:HG12	1.94	0.49
1:JL:84:TRP:CD1	1:JL:150:CYS:HB2	2.46	0.49
1:KD:93:MET:HE2	1:KE:171:GLU:HB3	1.93	0.49
1:LK:97:PHE:HA	1:LK:100:LEU:HB2	1.93	0.49
1:AO:61:ASP:OD1	1:AO:62:ILE:N	2.44	0.49
1:CI:84:TRP:CD1	1:CI:150:CYS:HB2	2.46	0.49
1:CJ:63:ILE:HB	1:CJ:195:ILE:H	1.76	0.49
1:CM:58:VAL:HG22	1:CM:188:VAL:HB	1.94	0.49
1:DC:180:ALA:HB2	1:DC:188:VAL:HG21	1.94	0.49
1:DD:93:MET:HE2	1:DE:171:GLU:HB3	1.93	0.49
1:EH:123:ALA:HA	1:EH:126:LEU:HD12	1.95	0.49
1:EO:88:LEU:HD11	1:EO:121:LEU:HD13	1.95	0.49
1:FL:151:ILE:HG22	1:FL:156:GLY:HA3	1.93	0.49
1:GK:84:TRP:CD1	1:GK:150:CYS:HB2	2.46	0.49
1:GN:136:ASN:HD22	1:GN:193:ASP:HB3	1.76	0.49
1:IB:127:ARG:HG2	1:IB:160:ASP:HB3	1.94	0.49
1:JB:127:ARG:HG2	1:JB:160:ASP:HB3	1.94	0.49
1:JE:37:ASP:OD1	1:JE:37:ASP:N	2.45	0.49
1:JH:62:ILE:HG12	1:JH:63:ILE:H	1.77	0.49
1:KH:62:ILE:HG12	1:KH:63:ILE:H	1.77	0.49
1:KH:77:THR:HB	1:KH:78:LYS:HD3	1.93	0.49
1:LA:52:LEU:HD21	1:LB:173:PRO:HB2	1.94	0.49
1:LI:84:TRP:CD1	1:LI:150:CYS:HB2	2.47	0.49
1:BE:37:ASP:OD1	1:BE:37:ASP:N	2.45	0.49
1:BN:136:ASN:HD22	1:BN:193:ASP:HB3	1.76	0.49
1:BO:136:ASN:HD22	1:BO:193:ASP:HB3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:58:VAL:HG22	1:CA:188:VAL:HB	1.95	0.49
1:CD:52:LEU:HD21	1:CE:173:PRO:HB2	1.94	0.49
1:DA:137:HIS:HA	1:DA:140:VAL:HG12	1.94	0.49
1:DN:61:ASP:N	1:DN:61:ASP:OD1	2.46	0.49
1:EA:137:HIS:HA	1:EA:140:VAL:HG12	1.94	0.49
1:FH:123:ALA:HA	1:FH:126:LEU:HD12	1.95	0.49
1:FK:97:PHE:HA	1:FK:100:LEU:HB2	1.94	0.49
1:GH:84:TRP:CD1	1:GH:150:CYS:HB2	2.46	0.49
1:HL:151:ILE:HG22	1:HL:156:GLY:HA3	1.93	0.49
1:HN:136:ASN:HD22	1:HN:193:ASP:HB3	1.76	0.49
1:HO:61:ASP:OD1	1:HO:62:ILE:N	2.45	0.49
1:IH:123:ALA:HA	1:IH:126:LEU:HD12	1.94	0.49
1:II:127:ARG:HG2	1:II:160:ASP:HB3	1.93	0.49
1:IK:84:TRP:CD1	1:IK:150:CYS:HB2	2.46	0.49
1:JH:123:ALA:HA	1:JH:126:LEU:HD12	1.95	0.49
1:JN:61:ASP:OD1	1:JN:61:ASP:N	2.46	0.49
1:JN:93:MET:HE3	1:JO:171:GLU:HB3	1.94	0.49
1:LA:58:VAL:HG22	1:LA:188:VAL:HB	1.95	0.49
1:LC:180:ALA:HB2	1:LC:188:VAL:HG21	1.94	0.49
1:BC:180:ALA:HB2	1:BC:188:VAL:HG21	1.94	0.49
1:CO:61:ASP:OD1	1:CO:62:ILE:N	2.45	0.49
1:DK:97:PHE:HA	1:DK:100:LEU:HB2	1.93	0.49
1:DM:58:VAL:HG22	1:DM:188:VAL:HB	1.94	0.49
1:DO:88:LEU:HD11	1:DO:121:LEU:HD13	1.95	0.49
1:EL:169:SER:OG	1:EL:193:ASP:OD1	2.29	0.49
1:FL:169:SER:OG	1:FL:193:ASP:OD1	2.29	0.49
1:FM:123:ALA:HA	1:FM:126:LEU:HD12	1.93	0.49
1:GB:127:ARG:HG2	1:GB:160:ASP:HB3	1.94	0.49
1:HD:93:MET:HE2	1:HE:171:GLU:HB3	1.93	0.49
1:IJ:58:VAL:HG22	1:IJ:188:VAL:HB	1.92	0.49
1:IJ:63:ILE:HB	1:IJ:195:ILE:H	1.76	0.49
1:KC:180:ALA:HB2	1:KC:188:VAL:HG21	1.94	0.49
1:BH:123:ALA:HA	1:BH:126:LEU:HD12	1.95	0.49
1:CD:93:MET:HE2	1:CE:171:GLU:HB3	1.93	0.49
1:DA:52:LEU:HD21	1:DB:173:PRO:HB2	1.94	0.49
1:EH:58:VAL:HG22	1:EH:188:VAL:HB	1.93	0.49
1:FJ:63:ILE:HB	1:FJ:195:ILE:H	1.76	0.49
1:GD:93:MET:HE2	1:GE:171:GLU:HB3	1.93	0.49
1:JD:52:LEU:HD21	1:JE:173:PRO:HB2	1.94	0.49
1:KI:84:TRP:CD1	1:KI:150:CYS:HB2	2.46	0.49
1:LD:43:VAL:HG21	1:LD:169:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LM:123:ALA:HA	1:LM:126:LEU:HD12	1.93	0.49
1:BA:83:GLY:H	1:BA:143:LEU:HD22	1.78	0.49
1:BB:127:ARG:HG2	1:BB:160:ASP:HB3	1.94	0.49
1:BN:93:MET:HE3	1:BO:171:GLU:HB3	1.94	0.49
1:AE:37:ASP:N	1:AE:37:ASP:OD1	2.45	0.49
1:AH:123:ALA:HA	1:AH:126:LEU:HD12	1.95	0.49
1:CH:123:ALA:HA	1:CH:126:LEU:HD12	1.95	0.49
1:DA:58:VAL:HG22	1:DA:188:VAL:HB	1.95	0.49
1:DO:61:ASP:OD1	1:DO:62:ILE:N	2.45	0.49
1:FC:180:ALA:HB2	1:FC:188:VAL:HG21	1.94	0.49
1:GH:123:ALA:HA	1:GH:126:LEU:HD12	1.95	0.49
1:GI:84:TRP:CD1	1:GI:150:CYS:HB2	2.46	0.49
1:HA:83:GLY:H	1:HA:143:LEU:HD22	1.78	0.49
1:HE:37:ASP:OD1	1:HE:37:ASP:N	2.45	0.49
1:HH:123:ALA:HA	1:HH:126:LEU:HD12	1.95	0.49
1:KH:123:ALA:HA	1:KH:126:LEU:HD12	1.95	0.49
1:LH:123:ALA:HA	1:LH:126:LEU:HD12	1.95	0.49
1:LN:61:ASP:N	1:LN:61:ASP:OD1	2.46	0.49
1:AA:166:VAL:HG21	1:AA:172:ILE:HG12	1.94	0.49
1:CA:137:HIS:HA	1:CA:140:VAL:HG12	1.94	0.49
1:CN:61:ASP:N	1:CN:61:ASP:OD1	2.46	0.49
1:CN:136:ASN:HD22	1:CN:193:ASP:HB3	1.76	0.49
1:EM:58:VAL:HG22	1:EM:188:VAL:HB	1.94	0.49
1:GH:62:ILE:HG12	1:GH:63:ILE:H	1.77	0.49
1:HN:93:MET:HE3	1:HO:171:GLU:HB3	1.94	0.49
1:JA:58:VAL:HG22	1:JA:188:VAL:HB	1.95	0.49
1:JA:83:GLY:H	1:JA:143:LEU:HD22	1.78	0.49
1:JL:52:LEU:HD22	1:JM:50:LEU:HD11	1.93	0.49
1:KD:43:VAL:HG21	1:KD:169:SER:HB3	1.95	0.49
1:LH:62:ILE:HG12	1:LH:63:ILE:H	1.77	0.49
1:BA:52:LEU:HD21	1:BB:173:PRO:HB2	1.94	0.49
1:BH:62:ILE:HG12	1:BH:63:ILE:H	1.77	0.49
1:AF:130:ILE:HG23	1:AF:191:PHE:HE2	1.78	0.49
1:AM:58:VAL:HG22	1:AM:188:VAL:HB	1.94	0.49
1:AN:61:ASP:N	1:AN:61:ASP:OD1	2.46	0.49
1:CB:127:ARG:HG2	1:CB:160:ASP:HB3	1.94	0.49
1:CC:58:VAL:HA	1:CC:188:VAL:O	2.13	0.49
1:DJ:63:ILE:HB	1:DJ:195:ILE:H	1.76	0.49
1:FM:58:VAL:HG22	1:FM:188:VAL:HB	1.94	0.49
1:GN:93:MET:HE3	1:GO:171:GLU:HB3	1.94	0.49
1:HA:52:LEU:HD21	1:HB:173:PRO:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HI:66:ASP:HB2	1:HI:70:GLN:HB2	1.95	0.49
1:IA:137:HIS:HA	1:IA:140:VAL:HG12	1.94	0.49
1:ID:43:VAL:HG21	1:ID:169:SER:HB3	1.95	0.49
1:IM:123:ALA:HA	1:IM:126:LEU:HD12	1.93	0.49
1:JM:58:VAL:HG22	1:JM:188:VAL:HB	1.94	0.49
1:KF:130:ILE:HG23	1:KF:191:PHE:HE2	1.78	0.49
1:KM:58:VAL:HG22	1:KM:188:VAL:HB	1.94	0.49
1:LA:83:GLY:H	1:LA:143:LEU:HD22	1.78	0.49
1:LN:136:ASN:HD22	1:LN:193:ASP:HB3	1.76	0.49
1:BI:66:ASP:HB2	1:BI:70:GLN:HB2	1.95	0.49
1:AN:93:MET:HE3	1:AO:171:GLU:HB3	1.94	0.49
1:CK:97:PHE:HA	1:CK:100:LEU:HB2	1.93	0.49
1:DB:127:ARG:HG2	1:DB:160:ASP:HB3	1.94	0.49
1:HA:166:VAL:HG21	1:HA:172:ILE:HG12	1.94	0.49
1:IA:83:GLY:H	1:IA:143:LEU:HD22	1.78	0.49
1:IE:37:ASP:N	1:IE:37:ASP:OD1	2.45	0.49
1:LE:37:ASP:N	1:LE:37:ASP:OD1	2.45	0.49
1:LH:58:VAL:HG22	1:LH:188:VAL:HB	1.93	0.49
1:AA:137:HIS:HA	1:AA:140:VAL:HG12	1.94	0.49
1:AB:127:ARG:HG2	1:AB:160:ASP:HB3	1.94	0.49
1:FA:123:ALA:HA	1:FA:126:LEU:HD12	1.95	0.49
1:FF:130:ILE:HG23	1:FF:191:PHE:HE2	1.78	0.49
1:GD:52:LEU:HD21	1:GE:173:PRO:HB2	1.94	0.49
1:HA:58:VAL:HG22	1:HA:188:VAL:HB	1.95	0.49
1:HC:58:VAL:HA	1:HC:188:VAL:O	2.13	0.49
1:IC:180:ALA:HB2	1:IC:188:VAL:HG21	1.94	0.49
1:IF:130:ILE:HG23	1:IF:191:PHE:HE2	1.78	0.49
1:II:66:ASP:HB2	1:II:70:GLN:HB2	1.95	0.49
1:IL:52:LEU:HD22	1:IM:50:LEU:HD11	1.93	0.49
1:JC:58:VAL:HA	1:JC:188:VAL:O	2.13	0.49
1:KA:58:VAL:HG22	1:KA:188:VAL:HB	1.95	0.49
1:KA:83:GLY:H	1:KA:143:LEU:HD22	1.78	0.49
1:KI:66:ASP:HB2	1:KI:70:GLN:HB2	1.95	0.49
1:BA:123:ALA:HA	1:BA:126:LEU:HD12	1.95	0.48
1:BC:58:VAL:HA	1:BC:188:VAL:O	2.13	0.48
1:AA:83:GLY:H	1:AA:143:LEU:HD22	1.78	0.48
1:AH:58:VAL:HG22	1:AH:188:VAL:HB	1.93	0.48
1:AI:66:ASP:HB2	1:AI:70:GLN:HB2	1.95	0.48
1:CD:43:VAL:HG21	1:CD:169:SER:HB3	1.95	0.48
1:GC:58:VAL:HA	1:GC:188:VAL:O	2.13	0.48
1:HA:123:ALA:HA	1:HA:126:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HF:130:ILE:HG23	1:HF:191:PHE:HE2	1.78	0.48
1:IA:58:VAL:HG22	1:IA:188:VAL:HB	1.95	0.48
1:IC:58:VAL:HA	1:IC:188:VAL:O	2.13	0.48
1:KB:127:ARG:HG2	1:KB:160:ASP:HB3	1.94	0.48
1:BA:166:VAL:HG21	1:BA:172:ILE:HG12	1.94	0.48
1:BO:88:LEU:HD11	1:BO:121:LEU:HD13	1.95	0.48
1:CF:130:ILE:HG23	1:CF:191:PHE:HE2	1.78	0.48
1:DI:66:ASP:HB2	1:DI:70:GLN:HB2	1.95	0.48
1:GA:137:HIS:HA	1:GA:140:VAL:HG12	1.94	0.48
1:GC:180:ALA:HB2	1:GC:188:VAL:HG21	1.94	0.48
1:GE:37:ASP:OD1	1:GE:37:ASP:N	2.45	0.48
1:GF:134:ARG:HH22	1:GJ:118:GLU:HB3	1.79	0.48
1:IH:62:ILE:HG12	1:IH:63:ILE:H	1.77	0.48
1:LO:88:LEU:HD11	1:LO:121:LEU:HD13	1.95	0.48
1:BM:58:VAL:HG22	1:BM:188:VAL:HB	1.94	0.48
1:CA:123:ALA:HA	1:CA:126:LEU:HD12	1.95	0.48
1:DA:123:ALA:HA	1:DA:126:LEU:HD12	1.95	0.48
1:DF:134:ARG:HH22	1:DJ:118:GLU:HB3	1.79	0.48
1:EF:130:ILE:HG23	1:EF:191:PHE:HE2	1.78	0.48
1:EI:66:ASP:HB2	1:EI:70:GLN:HB2	1.95	0.48
1:FB:127:ARG:HG2	1:FB:160:ASP:HB3	1.94	0.48
1:FL:133:SER:OG	1:FL:193:ASP:OD2	2.26	0.48
1:GN:61:ASP:OD1	1:GN:61:ASP:N	2.46	0.48
1:IN:93:MET:HE3	1:IO:171:GLU:HB3	1.94	0.48
1:LA:137:HIS:HA	1:LA:140:VAL:HG12	1.94	0.48
1:LF:134:ARG:HH22	1:LJ:118:GLU:HB3	1.79	0.48
1:BD:43:VAL:HG21	1:BD:169:SER:HB3	1.95	0.48
1:AA:52:LEU:HD21	1:AB:173:PRO:HB2	1.94	0.48
1:AH:72:ILE:HA	1:AH:139:LEU:HD21	1.96	0.48
1:EH:72:ILE:HA	1:EH:139:LEU:HD21	1.96	0.48
1:FO:88:LEU:HD11	1:FO:121:LEU:HD13	1.95	0.48
1:JF:118:GLU:HB2	1:JG:134:ARG:HH22	1.79	0.48
1:LN:93:MET:HE3	1:LO:171:GLU:HB3	1.94	0.48
1:AO:88:LEU:HD11	1:AO:121:LEU:HD13	1.95	0.48
1:CA:83:GLY:H	1:CA:143:LEU:HD22	1.78	0.48
1:CF:134:ARG:HH22	1:CJ:118:GLU:HB3	1.79	0.48
1:CO:88:LEU:HD11	1:CO:121:LEU:HD13	1.95	0.48
1:EN:61:ASP:OD1	1:EN:61:ASP:N	2.46	0.48
1:FC:153:ARG:HG2	1:FJ:121:LEU:HG	1.96	0.48
1:FI:66:ASP:HB2	1:FI:70:GLN:HB2	1.95	0.48
1:GA:84:TRP:CD1	1:GA:150:CYS:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GM:58:VAL:HG22	1:GM:188:VAL:HB	1.94	0.48
1:HN:61:ASP:OD1	1:HN:61:ASP:N	2.46	0.48
1:JC:153:ARG:HG2	1:JJ:121:LEU:HG	1.96	0.48
1:KA:84:TRP:CD1	1:KA:150:CYS:HB2	2.49	0.48
1:KC:153:ARG:HG2	1:KJ:121:LEU:HG	1.96	0.48
1:KH:72:ILE:HA	1:KH:139:LEU:HD21	1.96	0.48
1:BA:58:VAL:HG22	1:BA:188:VAL:HB	1.95	0.48
1:DA:83:GLY:H	1:DA:143:LEU:HD22	1.78	0.48
1:DF:130:ILE:HG23	1:DF:191:PHE:HE2	1.78	0.48
1:ED:43:VAL:HG21	1:ED:169:SER:HB3	1.95	0.48
1:FD:43:VAL:HG21	1:FD:169:SER:HB3	1.95	0.48
1:FN:61:ASP:N	1:FN:61:ASP:OD1	2.46	0.48
1:GA:58:VAL:HG22	1:GA:188:VAL:HB	1.95	0.48
1:HC:180:ALA:HB2	1:HC:188:VAL:HG21	1.94	0.48
1:IF:118:GLU:HB2	1:IG:134:ARG:HH22	1.79	0.48
1:KC:58:VAL:HA	1:KC:188:VAL:O	2.13	0.48
1:LM:52:LEU:HD22	1:LN:50:LEU:HD11	1.96	0.48
1:BF:118:GLU:HB2	1:BG:134:ARG:HH22	1.79	0.48
1:BN:61:ASP:OD1	1:BN:61:ASP:N	2.46	0.48
1:AA:123:ALA:HA	1:AA:126:LEU:HD12	1.95	0.48
1:AL:133:SER:OG	1:AL:193:ASP:OD2	2.26	0.48
1:DA:84:TRP:CD1	1:DA:150:CYS:HB2	2.49	0.48
1:DC:58:VAL:HA	1:DC:188:VAL:O	2.13	0.48
1:DM:52:LEU:HD22	1:DN:50:LEU:HD11	1.96	0.48
1:EA:84:TRP:CD1	1:EA:150:CYS:HB2	2.49	0.48
1:HB:127:ARG:HG2	1:HB:160:ASP:HB3	1.94	0.48
1:HD:43:VAL:HG21	1:HD:169:SER:HB3	1.95	0.48
1:HM:58:VAL:HG22	1:HM:188:VAL:HB	1.94	0.48
1:HO:88:LEU:HD11	1:HO:121:LEU:HD13	1.95	0.48
1:IO:88:LEU:HD11	1:IO:121:LEU:HD13	1.95	0.48
1:JH:72:ILE:HA	1:JH:139:LEU:HD21	1.96	0.48
1:JO:88:LEU:HD11	1:JO:121:LEU:HD13	1.95	0.48
1:KA:52:LEU:HD21	1:KB:173:PRO:HB2	1.94	0.48
1:LB:127:ARG:HG2	1:LB:160:ASP:HB3	1.94	0.48
1:LI:66:ASP:HB2	1:LI:70:GLN:HB2	1.95	0.48
1:BH:97:PHE:HZ	1:BI:174:VAL:HG22	1.79	0.48
1:CA:84:TRP:CD1	1:CA:150:CYS:HB2	2.49	0.48
1:CE:37:ASP:N	1:CE:37:ASP:OD1	2.45	0.48
1:DD:43:VAL:HG21	1:DD:169:SER:HB3	1.95	0.48
1:EC:153:ARG:HG2	1:EJ:121:LEU:HG	1.96	0.48
1:EF:134:ARG:HH22	1:EJ:118:GLU:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:83:GLY:H	1:FA:143:LEU:HD22	1.78	0.48
1:HA:84:TRP:CD1	1:HA:150:CYS:HB2	2.49	0.48
1:KA:137:HIS:HA	1:KA:140:VAL:HG12	1.94	0.48
1:LM:58:VAL:HG22	1:LM:188:VAL:HB	1.94	0.48
1:AA:58:VAL:HG22	1:AA:188:VAL:HB	1.95	0.48
1:AF:134:ARG:HH22	1:AJ:118:GLU:HB3	1.79	0.48
1:AH:97:PHE:HZ	1:AI:174:VAL:HG22	1.79	0.48
1:CH:72:ILE:HA	1:CH:139:LEU:HD21	1.96	0.48
1:CM:52:LEU:HD22	1:CN:50:LEU:HD11	1.96	0.48
1:EA:123:ALA:HA	1:EA:126:LEU:HD12	1.95	0.48
1:FF:134:ARG:HH22	1:FJ:118:GLU:HB3	1.79	0.48
1:GA:123:ALA:HA	1:GA:126:LEU:HD12	1.95	0.48
1:GF:130:ILE:HG23	1:GF:191:PHE:HE2	1.78	0.48
1:HA:137:HIS:HA	1:HA:140:VAL:HG12	1.94	0.48
1:HF:118:GLU:HB2	1:HG:134:ARG:HH22	1.79	0.48
1:IN:61:ASP:N	1:IN:61:ASP:OD1	2.46	0.48
1:JD:43:VAL:HG21	1:JD:169:SER:HB3	1.95	0.48
1:KN:61:ASP:N	1:KN:61:ASP:OD1	2.46	0.48
1:KO:88:LEU:HD11	1:KO:121:LEU:HD13	1.95	0.48
1:BF:134:ARG:HH22	1:BJ:118:GLU:HB3	1.79	0.48
1:AC:58:VAL:HA	1:AC:188:VAL:O	2.13	0.48
1:AD:43:VAL:HG21	1:AD:169:SER:HB3	1.95	0.48
1:CC:180:ALA:HB2	1:CC:188:VAL:HG21	1.94	0.48
1:EA:83:GLY:H	1:EA:143:LEU:HD22	1.78	0.48
1:FC:58:VAL:HA	1:FC:188:VAL:O	2.13	0.48
1:FH:97:PHE:HZ	1:FI:174:VAL:HG22	1.79	0.48
1:GD:43:VAL:HG21	1:GD:169:SER:HB3	1.95	0.48
1:GH:72:ILE:HA	1:GH:139:LEU:HD21	1.96	0.48
1:IA:84:TRP:CD1	1:IA:150:CYS:HB2	2.49	0.48
1:JA:137:HIS:HA	1:JA:140:VAL:HG12	1.94	0.48
1:JI:66:ASP:HB2	1:JI:70:GLN:HB2	1.95	0.48
1:LA:84:TRP:CD1	1:LA:150:CYS:HB2	2.49	0.48
1:BA:84:TRP:CD1	1:BA:150:CYS:HB2	2.49	0.47
1:BF:130:ILE:HG23	1:BF:191:PHE:HE2	1.78	0.47
1:BM:52:LEU:HD22	1:BN:50:LEU:HD11	1.96	0.47
1:AF:118:GLU:HB2	1:AG:134:ARG:HH22	1.79	0.47
1:EA:58:VAL:HG22	1:EA:188:VAL:HB	1.95	0.47
1:EC:58:VAL:HA	1:EC:188:VAL:O	2.13	0.47
1:GM:52:LEU:HD22	1:GN:50:LEU:HD11	1.96	0.47
1:IM:52:LEU:HD22	1:IN:50:LEU:HD11	1.96	0.47
1:KM:80:GLY:HA3	1:KM:84:TRP:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LF:118:GLU:HB2	1:LG:134:ARG:HH22	1.79	0.47
1:BF:74:ARG:O	1:BF:77:THR:OG1	2.25	0.47
1:AM:88:LEU:HD11	1:AM:121:LEU:HD13	1.97	0.47
1:DF:114:MET:HB2	1:DG:158:GLU:HG2	1.97	0.47
1:DL:133:SER:OG	1:DL:193:ASP:OD2	2.26	0.47
1:DM:80:GLY:HA3	1:DM:84:TRP:CB	2.44	0.47
1:FA:58:VAL:HG22	1:FA:188:VAL:HB	1.95	0.47
1:FF:114:MET:HB2	1:FG:158:GLU:HG2	1.97	0.47
1:HF:74:ARG:O	1:HF:77:THR:OG1	2.25	0.47
1:HG:83:GLY:H	1:HG:143:LEU:HD22	1.80	0.47
1:IH:97:PHE:HZ	1:II:174:VAL:HG22	1.79	0.47
1:JC:180:ALA:HB2	1:JC:188:VAL:HG21	1.94	0.47
1:JF:131:VAL:HG12	1:JF:172:ILE:HD13	1.97	0.47
1:LF:114:MET:HB2	1:LG:158:GLU:HG2	1.97	0.47
1:BG:83:GLY:H	1:BG:143:LEU:HD22	1.80	0.47
1:AF:74:ARG:O	1:AF:77:THR:OG1	2.25	0.47
1:AF:114:MET:HB2	1:AG:158:GLU:HG2	1.97	0.47
1:CC:153:ARG:HG2	1:CJ:121:LEU:HG	1.96	0.47
1:CI:66:ASP:HB2	1:CI:70:GLN:HB2	1.95	0.47
1:DG:83:GLY:H	1:DG:143:LEU:HD22	1.80	0.47
1:DH:72:ILE:HA	1:DH:139:LEU:HD21	1.96	0.47
1:DM:88:LEU:HD11	1:DM:121:LEU:HD13	1.97	0.47
1:FA:84:TRP:CD1	1:FA:150:CYS:HB2	2.49	0.47
1:FM:80:GLY:HA3	1:FM:84:TRP:CB	2.44	0.47
1:GA:83:GLY:H	1:GA:143:LEU:HD22	1.78	0.47
1:GF:131:VAL:HG12	1:GF:172:ILE:HD13	1.97	0.47
1:IM:58:VAL:HG22	1:IM:188:VAL:HB	1.94	0.47
1:IM:80:GLY:HA3	1:IM:84:TRP:CB	2.44	0.47
1:JM:88:LEU:HD11	1:JM:121:LEU:HD13	1.97	0.47
1:KF:114:MET:HB2	1:KG:158:GLU:HG2	1.97	0.47
1:LC:58:VAL:HA	1:LC:188:VAL:O	2.13	0.47
1:AM:80:GLY:HA3	1:AM:84:TRP:CB	2.44	0.47
1:CM:80:GLY:HA3	1:CM:84:TRP:CB	2.44	0.47
1:DF:118:GLU:HB2	1:DG:134:ARG:HH22	1.79	0.47
1:DH:123:ALA:HA	1:DH:126:LEU:HD12	1.95	0.47
1:EF:131:VAL:HG12	1:EF:172:ILE:HD13	1.97	0.47
1:EM:80:GLY:HA3	1:EM:84:TRP:CB	2.44	0.47
1:FG:72:ILE:HD13	1:FG:139:LEU:HD21	1.97	0.47
1:FM:88:LEU:HD11	1:FM:121:LEU:HD13	1.97	0.47
1:GN:84:TRP:CD1	1:GN:150:CYS:HB2	2.50	0.47
1:HM:88:LEU:HD11	1:HM:121:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IF:134:ARG:HH22	1:IJ:118:GLU:HB3	1.79	0.47
1:IN:84:TRP:CD1	1:IN:150:CYS:HB2	2.50	0.47
1:JF:134:ARG:HH22	1:JJ:118:GLU:HB3	1.79	0.47
1:LC:153:ARG:HG2	1:LJ:121:LEU:HG	1.96	0.47
1:LF:130:ILE:HG23	1:LF:191:PHE:HE2	1.78	0.47
1:LG:72:ILE:HD13	1:LG:139:LEU:HD21	1.97	0.47
1:LM:88:LEU:HD11	1:LM:121:LEU:HD13	1.97	0.47
1:LN:180:ALA:HB2	1:LN:188:VAL:HG21	1.97	0.47
1:AK:63:ILE:O	1:AK:64:THR:HG22	2.15	0.47
1:AM:52:LEU:HD22	1:AN:50:LEU:HD11	1.96	0.47
1:CF:118:GLU:HB2	1:CG:134:ARG:HH22	1.79	0.47
1:DF:52:LEU:HD21	1:DG:173:PRO:HB2	1.97	0.47
1:DH:97:PHE:HZ	1:DI:174:VAL:HG22	1.79	0.47
1:EH:97:PHE:HZ	1:EI:174:VAL:HG22	1.79	0.47
1:GF:118:GLU:HB2	1:GG:134:ARG:HH22	1.79	0.47
1:GK:62:ILE:HA	1:GK:192:GLY:O	2.15	0.47
1:IA:123:ALA:HA	1:IA:126:LEU:HD12	1.95	0.47
1:IF:131:VAL:HG12	1:IF:172:ILE:HD13	1.97	0.47
1:JF:130:ILE:HG23	1:JF:191:PHE:HE2	1.78	0.47
1:JM:80:GLY:HA3	1:JM:84:TRP:CB	2.44	0.47
1:KF:118:GLU:HB2	1:KG:134:ARG:HH22	1.79	0.47
1:AK:62:ILE:HA	1:AK:192:GLY:O	2.15	0.47
1:CG:72:ILE:HD13	1:CG:139:LEU:HD21	1.97	0.47
1:EM:88:LEU:HD11	1:EM:121:LEU:HD13	1.97	0.47
1:EN:84:TRP:CD1	1:EN:150:CYS:HB2	2.50	0.47
1:GC:153:ARG:HG2	1:GJ:121:LEU:HG	1.96	0.47
1:GF:52:LEU:HD21	1:GG:173:PRO:HB2	1.97	0.47
1:HF:52:LEU:HD21	1:HG:173:PRO:HB2	1.97	0.47
1:HK:62:ILE:HA	1:HK:192:GLY:O	2.15	0.47
1:JG:72:ILE:HD13	1:JG:139:LEU:HD21	1.97	0.47
1:JM:52:LEU:HD22	1:JN:50:LEU:HD11	1.96	0.47
1:KA:123:ALA:HA	1:KA:126:LEU:HD12	1.95	0.47
1:LB:91:ILE:HD13	1:LB:123:ALA:HB2	1.97	0.47
1:LK:63:ILE:O	1:LK:64:THR:HG22	2.15	0.47
1:BC:153:ARG:HG2	1:BJ:121:LEU:HG	1.96	0.47
1:BK:63:ILE:O	1:BK:64:THR:HG22	2.15	0.47
1:BM:80:GLY:HA3	1:BM:84:TRP:CB	2.44	0.47
1:BM:88:LEU:HD11	1:BM:121:LEU:HD13	1.97	0.47
1:BN:180:ALA:HB2	1:BN:188:VAL:HG21	1.97	0.47
1:AA:84:TRP:CD1	1:AA:150:CYS:HB2	2.49	0.47
1:AB:91:ILE:HD13	1:AB:123:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CM:88:LEU:HD11	1:CM:121:LEU:HD13	1.97	0.47
1:DK:63:ILE:O	1:DK:64:THR:HG22	2.15	0.47
1:DN:84:TRP:CD1	1:DN:150:CYS:HB2	2.50	0.47
1:ED:114:MET:SD	1:ED:114:MET:N	2.84	0.47
1:EF:114:MET:HB2	1:EG:158:GLU:HG2	1.97	0.47
1:EF:118:GLU:HB2	1:EG:134:ARG:HH22	1.79	0.47
1:EG:72:ILE:HD13	1:EG:139:LEU:HD21	1.97	0.47
1:EK:63:ILE:O	1:EK:64:THR:HG22	2.15	0.47
1:FB:91:ILE:HD13	1:FB:123:ALA:HB2	1.97	0.47
1:FF:52:LEU:HD21	1:FG:173:PRO:HB2	1.97	0.47
1:FF:118:GLU:HB2	1:FG:134:ARG:HH22	1.79	0.47
1:FN:84:TRP:CD1	1:FN:150:CYS:HB2	2.50	0.47
1:GH:97:PHE:HZ	1:GI:174:VAL:HG22	1.79	0.47
1:GO:88:LEU:HD11	1:GO:121:LEU:HD13	1.95	0.47
1:HC:153:ARG:HG2	1:HJ:121:LEU:HG	1.96	0.47
1:HH:97:PHE:HZ	1:HI:174:VAL:HG22	1.79	0.47
1:IB:91:ILE:HD13	1:IB:123:ALA:HB2	1.97	0.47
1:IG:83:GLY:H	1:IG:143:LEU:HD22	1.80	0.47
1:JA:84:TRP:CD1	1:JA:150:CYS:HB2	2.49	0.47
1:JG:83:GLY:H	1:JG:143:LEU:HD22	1.80	0.47
1:KF:134:ARG:HH22	1:KJ:118:GLU:HB3	1.79	0.47
1:LH:97:PHE:HZ	1:LI:174:VAL:HG22	1.79	0.47
1:LM:80:GLY:HA3	1:LM:84:TRP:CB	2.44	0.47
1:BB:91:ILE:HD13	1:BB:123:ALA:HB2	1.97	0.47
1:BF:131:VAL:HG12	1:BF:172:ILE:HD13	1.97	0.47
1:AF:131:VAL:HG12	1:AF:172:ILE:HD13	1.97	0.47
1:CN:180:ALA:HB2	1:CN:188:VAL:HG21	1.96	0.47
1:GF:114:MET:HB2	1:GG:158:GLU:HG2	1.97	0.47
1:GM:88:LEU:HD11	1:GM:121:LEU:HD13	1.97	0.47
1:HF:114:MET:HB2	1:HG:158:GLU:HG2	1.96	0.47
1:HN:84:TRP:CD1	1:HN:150:CYS:HB2	2.50	0.47
1:JH:97:PHE:HZ	1:JI:174:VAL:HG22	1.79	0.47
1:KB:91:ILE:HD13	1:KB:123:ALA:HB2	1.97	0.47
1:KF:131:VAL:HG12	1:KF:172:ILE:HD13	1.97	0.47
1:KG:83:GLY:H	1:KG:143:LEU:HD22	1.80	0.47
1:KM:52:LEU:HD22	1:KN:50:LEU:HD11	1.96	0.47
1:KN:84:TRP:CD1	1:KN:150:CYS:HB2	2.50	0.47
1:LN:84:TRP:CD1	1:LN:150:CYS:HB2	2.50	0.47
1:DB:91:ILE:HD13	1:DB:123:ALA:HB2	1.97	0.47
1:DC:153:ARG:HG2	1:DJ:121:LEU:HG	1.96	0.47
1:EM:52:LEU:HD22	1:EN:50:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FH:72:ILE:HA	1:FH:139:LEU:HD21	1.96	0.47
1:GM:80:GLY:HA3	1:GM:84:TRP:CB	2.44	0.47
1:HM:80:GLY:HA3	1:HM:84:TRP:CB	2.44	0.47
1:JA:123:ALA:HA	1:JA:126:LEU:HD12	1.95	0.47
1:KK:63:ILE:O	1:KK:64:THR:HG22	2.15	0.47
1:KM:88:LEU:HD11	1:KM:121:LEU:HD13	1.97	0.47
1:LK:62:ILE:HA	1:LK:192:GLY:O	2.15	0.47
1:CK:63:ILE:O	1:CK:64:THR:HG22	2.15	0.47
1:FM:52:LEU:HD22	1:FN:50:LEU:HD11	1.96	0.47
1:GI:66:ASP:HB2	1:GI:70:GLN:HB2	1.95	0.47
1:JK:63:ILE:O	1:JK:64:THR:HG22	2.15	0.47
1:JN:84:TRP:CD1	1:JN:150:CYS:HB2	2.50	0.47
1:BH:72:ILE:HA	1:BH:139:LEU:HD21	1.96	0.46
1:AF:52:LEU:HD21	1:AG:173:PRO:HB2	1.97	0.46
1:AN:84:TRP:CD1	1:AN:150:CYS:HB2	2.50	0.46
1:CB:91:ILE:HD13	1:CB:123:ALA:HB2	1.97	0.46
1:CG:83:GLY:H	1:CG:143:LEU:HD22	1.80	0.46
1:FG:83:GLY:H	1:FG:143:LEU:HD22	1.80	0.46
1:JK:62:ILE:HA	1:JK:192:GLY:O	2.15	0.46
1:KE:37:ASP:N	1:KE:37:ASP:OD1	2.45	0.46
1:BG:72:ILE:HD13	1:BG:139:LEU:HD21	1.97	0.46
1:BN:137:HIS:HA	1:BN:140:VAL:HB	1.98	0.46
1:AC:153:ARG:HG2	1:AJ:121:LEU:HG	1.96	0.46
1:AG:83:GLY:H	1:AG:143:LEU:HD22	1.79	0.46
1:DG:72:ILE:HD13	1:DG:139:LEU:HD21	1.97	0.46
1:DK:62:ILE:HA	1:DK:192:GLY:O	2.15	0.46
1:EB:91:ILE:HD13	1:EB:123:ALA:HB2	1.97	0.46
1:HB:91:ILE:HD13	1:HB:123:ALA:HB2	1.97	0.46
1:HF:131:VAL:HG12	1:HF:172:ILE:HD13	1.97	0.46
1:HF:134:ARG:HH22	1:HJ:118:GLU:HB3	1.79	0.46
1:HH:72:ILE:HA	1:HH:139:LEU:HD21	1.96	0.46
1:HM:52:LEU:HD22	1:HN:50:LEU:HD11	1.96	0.46
1:IK:62:ILE:HA	1:IK:192:GLY:O	2.15	0.46
1:IM:88:LEU:HD11	1:IM:121:LEU:HD13	1.97	0.46
1:LA:123:ALA:HA	1:LA:126:LEU:HD12	1.95	0.46
1:LC:70:GLN:O	1:LC:74:ARG:HD3	2.16	0.46
1:AN:180:ALA:HB2	1:AN:188:VAL:HG21	1.96	0.46
1:CH:97:PHE:HZ	1:CI:174:VAL:HG22	1.79	0.46
1:DD:77:THR:HG23	1:DD:80:GLY:H	1.81	0.46
1:ED:77:THR:HG23	1:ED:80:GLY:H	1.81	0.46
1:EF:52:LEU:HD21	1:EG:173:PRO:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FD:77:THR:HG23	1:FD:80:GLY:H	1.81	0.46
1:HC:70:GLN:O	1:HC:74:ARG:HD3	2.16	0.46
1:HG:72:ILE:HD13	1:HG:139:LEU:HD21	1.97	0.46
1:IF:114:MET:HB2	1:IG:158:GLU:HG2	1.97	0.46
1:IL:91:ILE:HD13	1:IL:123:ALA:HB2	1.98	0.46
1:JC:70:GLN:O	1:JC:74:ARG:HD3	2.16	0.46
1:JN:180:ALA:HB2	1:JN:188:VAL:HG21	1.97	0.46
1:KN:180:ALA:HB2	1:KN:188:VAL:HG21	1.96	0.46
1:LG:83:GLY:H	1:LG:143:LEU:HD22	1.80	0.46
1:LN:137:HIS:HA	1:LN:140:VAL:HB	1.98	0.46
1:BN:84:TRP:CD1	1:BN:150:CYS:HB2	2.50	0.46
1:CK:62:ILE:HA	1:CK:192:GLY:O	2.15	0.46
1:FK:62:ILE:HA	1:FK:192:GLY:O	2.15	0.46
1:IF:52:LEU:HD21	1:IG:173:PRO:HB2	1.97	0.46
1:IH:72:ILE:HA	1:IH:139:LEU:HD21	1.96	0.46
1:JL:91:ILE:HD13	1:JL:123:ALA:HB2	1.98	0.46
1:BE:123:ALA:HA	1:BE:126:LEU:HD12	1.98	0.46
1:BK:62:ILE:HA	1:BK:192:GLY:O	2.15	0.46
1:AN:137:HIS:HA	1:AN:140:VAL:HB	1.98	0.46
1:CF:114:MET:HB2	1:CG:158:GLU:HG2	1.97	0.46
1:CN:84:TRP:CD1	1:CN:150:CYS:HB2	2.50	0.46
1:EG:83:GLY:H	1:EG:143:LEU:HD22	1.79	0.46
1:FB:67:THR:HB	1:FB:70:GLN:HB2	1.98	0.46
1:GB:91:ILE:HD13	1:GB:123:ALA:HB2	1.97	0.46
1:GK:63:ILE:O	1:GK:64:THR:HG22	2.15	0.46
1:GN:137:HIS:HA	1:GN:140:VAL:HB	1.98	0.46
1:GN:180:ALA:HB2	1:GN:188:VAL:HG21	1.96	0.46
1:HD:77:THR:HG23	1:HD:80:GLY:H	1.81	0.46
1:HK:63:ILE:O	1:HK:64:THR:HG22	2.15	0.46
1:IC:153:ARG:HG2	1:IJ:121:LEU:HG	1.96	0.46
1:ID:114:MET:SD	1:ID:114:MET:N	2.84	0.46
1:JB:91:ILE:HD13	1:JB:123:ALA:HB2	1.97	0.46
1:KF:52:LEU:HD21	1:KG:173:PRO:HB2	1.97	0.46
1:LD:77:THR:HG23	1:LD:80:GLY:H	1.81	0.46
1:LH:72:ILE:HA	1:LH:139:LEU:HD21	1.96	0.46
1:AD:77:THR:HG23	1:AD:80:GLY:H	1.81	0.46
1:CF:131:VAL:HG12	1:CF:172:ILE:HD13	1.97	0.46
1:DF:63:ILE:HG12	1:DF:74:ARG:HH21	1.81	0.46
1:FF:74:ARG:O	1:FF:77:THR:OG1	2.25	0.46
1:GG:83:GLY:H	1:GG:143:LEU:HD22	1.80	0.46
1:HN:180:ALA:HB2	1:HN:188:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:130:ILE:HG23	1:IB:191:PHE:HE2	1.81	0.46
1:IF:63:ILE:HG12	1:IF:74:ARG:HH21	1.81	0.46
1:JF:114:MET:HB2	1:JG:158:GLU:HG2	1.97	0.46
1:KG:72:ILE:HD13	1:KG:139:LEU:HD21	1.97	0.46
1:KK:62:ILE:HA	1:KK:192:GLY:O	2.15	0.46
1:LB:67:THR:HB	1:LB:70:GLN:HB2	1.98	0.46
1:BC:70:GLN:O	1:BC:74:ARG:HD3	2.16	0.46
1:BF:52:LEU:HD21	1:BG:173:PRO:HB2	1.97	0.46
1:AL:91:ILE:HD13	1:AL:123:ALA:HB2	1.98	0.46
1:FL:91:ILE:HD13	1:FL:123:ALA:HB2	1.98	0.46
1:FN:137:HIS:HA	1:FN:140:VAL:HB	1.98	0.46
1:FN:180:ALA:HB2	1:FN:188:VAL:HG21	1.97	0.46
1:HN:137:HIS:HA	1:HN:140:VAL:HB	1.98	0.46
1:IC:70:GLN:O	1:IC:74:ARG:HD3	2.16	0.46
1:KC:70:GLN:O	1:KC:74:ARG:HD3	2.16	0.46
1:LD:128:PHE:CD1	1:LD:187:ALA:HB3	2.51	0.46
1:AC:70:GLN:O	1:AC:74:ARG:HD3	2.16	0.46
1:AG:72:ILE:HD13	1:AG:139:LEU:HD21	1.97	0.46
1:EN:180:ALA:HB2	1:EN:188:VAL:HG21	1.97	0.46
1:GE:123:ALA:HA	1:GE:126:LEU:HD12	1.98	0.46
1:GG:72:ILE:HD13	1:GG:139:LEU:HD21	1.97	0.46
1:ID:128:PHE:CD1	1:ID:187:ALA:HB3	2.51	0.46
1:IN:137:HIS:HA	1:IN:140:VAL:HB	1.98	0.46
1:KD:77:THR:HG23	1:KD:80:GLY:H	1.81	0.46
1:KF:63:ILE:HG12	1:KF:74:ARG:HH21	1.81	0.46
1:LE:123:ALA:HA	1:LE:126:LEU:HD12	1.98	0.46
1:LF:52:LEU:HD21	1:LG:173:PRO:HB2	1.97	0.46
1:BL:133:SER:OG	1:BL:193:ASP:OD2	2.26	0.46
1:BM:128:PHE:HD1	1:BM:187:ALA:HB3	1.81	0.46
1:CD:77:THR:HG23	1:CD:80:GLY:H	1.81	0.46
1:DL:91:ILE:HD13	1:DL:123:ALA:HB2	1.98	0.46
1:FK:63:ILE:O	1:FK:64:THR:HG22	2.15	0.46
1:HE:123:ALA:HA	1:HE:126:LEU:HD12	1.98	0.46
1:IK:63:ILE:O	1:IK:64:THR:HG22	2.15	0.46
1:IN:180:ALA:HB2	1:IN:188:VAL:HG21	1.97	0.46
1:JD:114:MET:SD	1:JD:114:MET:N	2.84	0.46
1:JM:128:PHE:CD1	1:JM:187:ALA:HB3	2.51	0.46
1:JN:137:HIS:HA	1:JN:140:VAL:HB	1.98	0.46
1:LF:131:VAL:HG12	1:LF:172:ILE:HD13	1.97	0.46
1:BB:67:THR:HB	1:BB:70:GLN:HB2	1.98	0.46
1:AB:130:ILE:HG23	1:AB:191:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:70:GLN:O	1:CC:74:ARG:HD3	2.16	0.46
1:DB:130:ILE:HG23	1:DB:191:PHE:HE2	1.81	0.46
1:DF:131:VAL:HG12	1:DF:172:ILE:HD13	1.97	0.46
1:EF:193:ASP:OD1	1:EF:193:ASP:N	2.49	0.46
1:FM:128:PHE:CD1	1:FM:187:ALA:HB3	2.51	0.46
1:GM:117:TYR:HB2	1:GN:164:VAL:HG22	1.98	0.46
1:IL:66:ASP:OD1	1:IL:66:ASP:N	2.33	0.46
1:JD:77:THR:HG23	1:JD:80:GLY:H	1.81	0.46
1:JD:128:PHE:CD1	1:JD:187:ALA:HB3	2.51	0.46
1:LM:128:PHE:HD1	1:LM:187:ALA:HB3	1.81	0.46
1:BB:130:ILE:HG23	1:BB:191:PHE:HE2	1.81	0.45
1:BD:77:THR:HG23	1:BD:80:GLY:H	1.81	0.45
1:BL:91:ILE:HD13	1:BL:123:ALA:HB2	1.98	0.45
1:CM:193:ASP:OD1	1:CM:193:ASP:N	2.49	0.45
1:DM:117:TYR:HB2	1:DN:164:VAL:HG22	1.98	0.45
1:DM:128:PHE:HD1	1:DM:187:ALA:HB3	1.81	0.45
1:DN:137:HIS:HA	1:DN:140:VAL:HB	1.97	0.45
1:EM:128:PHE:HD1	1:EM:187:ALA:HB3	1.81	0.45
1:FF:131:VAL:HG12	1:FF:172:ILE:HD13	1.97	0.45
1:GD:114:MET:SD	1:GD:114:MET:N	2.84	0.45
1:GM:128:PHE:CD1	1:GM:187:ALA:HB3	2.51	0.45
1:GM:128:PHE:HD1	1:GM:187:ALA:HB3	1.81	0.45
1:JG:70:GLN:O	1:JG:74:ARG:HG2	2.17	0.45
1:KB:130:ILE:HG23	1:KB:191:PHE:HE2	1.81	0.45
1:KL:97:PHE:HZ	1:KM:174:VAL:HG22	1.81	0.45
1:LF:193:ASP:OD1	1:LF:193:ASP:N	2.49	0.45
1:LG:70:GLN:O	1:LG:74:ARG:HG2	2.17	0.45
1:CL:97:PHE:HZ	1:CM:174:VAL:HG22	1.81	0.45
1:CM:128:PHE:CD1	1:CM:187:ALA:HB3	2.51	0.45
1:DC:70:GLN:O	1:DC:74:ARG:HD3	2.16	0.45
1:EF:63:ILE:HG12	1:EF:74:ARG:HH21	1.81	0.45
1:EG:70:GLN:O	1:EG:74:ARG:HG2	2.16	0.45
1:EK:62:ILE:HA	1:EK:192:GLY:O	2.15	0.45
1:EM:117:TYR:HB2	1:EN:164:VAL:HG22	1.98	0.45
1:EM:128:PHE:CD1	1:EM:187:ALA:HB3	2.51	0.45
1:FB:130:ILE:HG23	1:FB:191:PHE:HE2	1.81	0.45
1:FF:63:ILE:HG12	1:FF:74:ARG:HH21	1.81	0.45
1:GB:67:THR:HB	1:GB:70:GLN:HB2	1.98	0.45
1:HG:70:GLN:O	1:HG:74:ARG:HG2	2.17	0.45
1:HL:97:PHE:HZ	1:HM:174:VAL:HG22	1.82	0.45
1:HM:128:PHE:HD1	1:HM:187:ALA:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IG:72:ILE:HD13	1:IG:139:LEU:HD21	1.97	0.45
1:IM:128:PHE:CD1	1:IM:187:ALA:HB3	2.51	0.45
1:JF:63:ILE:HG12	1:JF:74:ARG:HH21	1.81	0.45
1:KN:43:VAL:HG21	1:KN:169:SER:HB3	1.99	0.45
1:LB:130:ILE:HG23	1:LB:191:PHE:HE2	1.81	0.45
1:LF:63:ILE:HG12	1:LF:74:ARG:HH21	1.81	0.45
1:BD:128:PHE:CD1	1:BD:187:ALA:HB3	2.51	0.45
1:BF:114:MET:HB2	1:BG:158:GLU:HG2	1.97	0.45
1:AM:128:PHE:HD1	1:AM:187:ALA:HB3	1.81	0.45
1:CN:43:VAL:HG21	1:CN:169:SER:HB3	1.99	0.45
1:DN:43:VAL:HG21	1:DN:169:SER:HB3	1.99	0.45
1:DN:180:ALA:HB2	1:DN:188:VAL:HG21	1.97	0.45
1:EB:130:ILE:HG23	1:EB:191:PHE:HE2	1.81	0.45
1:FM:117:TYR:HB2	1:FN:164:VAL:HG22	1.98	0.45
1:HN:43:VAL:HG21	1:HN:169:SER:HB3	1.99	0.45
1:JM:128:PHE:HD1	1:JM:187:ALA:HB3	1.81	0.45
1:JN:43:VAL:HG21	1:JN:169:SER:HB3	1.99	0.45
1:KB:67:THR:HB	1:KB:70:GLN:HB2	1.98	0.45
1:LN:43:VAL:HG21	1:LN:169:SER:HB3	1.99	0.45
1:BM:128:PHE:CD1	1:BM:187:ALA:HB3	2.51	0.45
1:AG:75:ALA:HB1	1:AG:142:ARG:HG3	1.99	0.45
1:CB:130:ILE:HG23	1:CB:191:PHE:HE2	1.81	0.45
1:DD:128:PHE:CD1	1:DD:187:ALA:HB3	2.51	0.45
1:DM:128:PHE:CD1	1:DM:187:ALA:HB3	2.51	0.45
1:EC:70:GLN:O	1:EC:74:ARG:HD3	2.16	0.45
1:EL:97:PHE:HZ	1:EM:174:VAL:HG22	1.82	0.45
1:FG:70:GLN:O	1:FG:74:ARG:HG2	2.17	0.45
1:GD:77:THR:HG23	1:GD:80:GLY:H	1.81	0.45
1:IE:123:ALA:HA	1:IE:126:LEU:HD12	1.98	0.45
1:IM:128:PHE:HD1	1:IM:187:ALA:HB3	1.81	0.45
1:JB:130:ILE:HG23	1:JB:191:PHE:HE2	1.81	0.45
1:KD:128:PHE:CD1	1:KD:187:ALA:HB3	2.51	0.45
1:KM:128:PHE:CD1	1:KM:187:ALA:HB3	2.51	0.45
1:KO:79:HIS:ND1	1:KO:79:HIS:O	2.50	0.45
1:BF:63:ILE:HG12	1:BF:74:ARG:HH21	1.81	0.45
1:AD:128:PHE:CD1	1:AD:187:ALA:HB3	2.51	0.45
1:DF:193:ASP:OD1	1:DF:193:ASP:N	2.49	0.45
1:ED:128:PHE:CD1	1:ED:187:ALA:HB3	2.51	0.45
1:EE:123:ALA:HA	1:EE:126:LEU:HD12	1.98	0.45
1:EN:43:VAL:HG21	1:EN:169:SER:HB3	1.99	0.45
1:GB:130:ILE:HG23	1:GB:191:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GD:128:PHE:CD1	1:GD:187:ALA:HB3	2.51	0.45
1:GF:63:ILE:HG12	1:GF:74:ARG:HH21	1.81	0.45
1:GF:193:ASP:OD1	1:GF:193:ASP:N	2.49	0.45
1:HM:128:PHE:CD1	1:HM:187:ALA:HB3	2.51	0.45
1:JE:81:ASN:HD21	1:JE:84:TRP:HB2	1.82	0.45
1:JF:52:LEU:HD21	1:JG:173:PRO:HB2	1.97	0.45
1:KG:75:ALA:HB1	1:KG:142:ARG:HG3	1.99	0.45
1:KH:97:PHE:HZ	1:KI:174:VAL:HG22	1.79	0.45
1:KL:91:ILE:HD13	1:KL:123:ALA:HB2	1.98	0.45
1:KM:117:TYR:HB2	1:KN:164:VAL:HG22	1.98	0.45
1:LM:117:TYR:HB2	1:LN:164:VAL:HG22	1.98	0.45
1:LM:128:PHE:CD1	1:LM:187:ALA:HB3	2.51	0.45
1:BG:70:GLN:O	1:BG:74:ARG:HG2	2.17	0.45
1:AG:70:GLN:O	1:AG:74:ARG:HG2	2.17	0.45
1:CB:128:PHE:HD1	1:CB:187:ALA:HB3	1.82	0.45
1:CM:117:TYR:HB2	1:CN:164:VAL:HG22	1.98	0.45
1:DB:67:THR:HB	1:DB:70:GLN:HB2	1.98	0.45
1:DO:91:ILE:HD13	1:DO:123:ALA:HB2	1.99	0.45
1:EE:81:ASN:HD21	1:EE:84:TRP:HB2	1.82	0.45
1:GC:70:GLN:O	1:GC:74:ARG:HD3	2.16	0.45
1:GM:193:ASP:OD1	1:GM:193:ASP:N	2.49	0.45
1:GO:79:HIS:ND1	1:GO:79:HIS:O	2.50	0.45
1:JO:79:HIS:ND1	1:JO:79:HIS:O	2.50	0.45
1:KO:91:ILE:HD13	1:KO:123:ALA:HB2	1.99	0.45
1:LF:37:ASP:OD1	1:LF:37:ASP:N	2.33	0.45
1:CF:193:ASP:OD1	1:CF:193:ASP:N	2.49	0.45
1:CN:137:HIS:HA	1:CN:140:VAL:HB	1.98	0.45
1:DG:70:GLN:O	1:DG:74:ARG:HG2	2.17	0.45
1:FB:128:PHE:HD1	1:FB:187:ALA:HB3	1.82	0.45
1:FE:81:ASN:HD21	1:FE:84:TRP:HB2	1.82	0.45
1:FN:43:VAL:HG21	1:FN:169:SER:HB3	1.99	0.45
1:GN:43:VAL:HG21	1:GN:169:SER:HB3	1.99	0.45
1:IE:81:ASN:HD21	1:IE:84:TRP:HB2	1.82	0.45
1:JE:123:ALA:HA	1:JE:126:LEU:HD12	1.98	0.45
1:JM:117:TYR:HB2	1:JN:164:VAL:HG22	1.98	0.45
1:KM:128:PHE:HD1	1:KM:187:ALA:HB3	1.81	0.45
1:LO:79:HIS:O	1:LO:79:HIS:ND1	2.50	0.45
1:BD:114:MET:SD	1:BD:114:MET:N	2.84	0.45
1:BO:79:HIS:ND1	1:BO:79:HIS:O	2.50	0.45
1:AJ:78:LYS:HE3	1:AJ:78:LYS:HB2	1.81	0.45
1:CD:52:LEU:HD22	1:CE:50:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CF:52:LEU:HD21	1:CG:173:PRO:HB2	1.97	0.45
1:CG:70:GLN:O	1:CG:74:ARG:HG2	2.17	0.45
1:CL:91:ILE:HD13	1:CL:123:ALA:HB2	1.98	0.45
1:CM:128:PHE:HD1	1:CM:187:ALA:HB3	1.81	0.45
1:DG:75:ALA:HB1	1:DG:142:ARG:HG3	1.99	0.45
1:DO:79:HIS:O	1:DO:79:HIS:ND1	2.50	0.45
1:FC:70:GLN:O	1:FC:74:ARG:HD3	2.16	0.45
1:FD:128:PHE:CD1	1:FD:187:ALA:HB3	2.51	0.45
1:FL:97:PHE:HZ	1:FM:174:VAL:HG22	1.82	0.45
1:GF:84:TRP:CD1	1:GF:150:CYS:HB2	2.52	0.45
1:GL:91:ILE:HD13	1:GL:123:ALA:HB2	1.98	0.45
1:HE:81:ASN:HD21	1:HE:84:TRP:HB2	1.82	0.45
1:HF:63:ILE:HG12	1:HF:74:ARG:HH21	1.81	0.45
1:IN:43:VAL:HG21	1:IN:169:SER:HB3	1.99	0.45
1:KE:123:ALA:HA	1:KE:126:LEU:HD12	1.98	0.45
1:KN:137:HIS:HA	1:KN:140:VAL:HB	1.98	0.45
1:LL:97:PHE:HZ	1:LM:174:VAL:HG22	1.82	0.45
1:LO:91:ILE:HD13	1:LO:123:ALA:HB2	1.99	0.45
1:AB:67:THR:HB	1:AB:70:GLN:HB2	1.98	0.45
1:AF:63:ILE:HG12	1:AF:74:ARG:HH21	1.81	0.45
1:AN:43:VAL:HG21	1:AN:169:SER:HB3	1.99	0.45
1:CE:123:ALA:HA	1:CE:126:LEU:HD12	1.98	0.45
1:DE:123:ALA:HA	1:DE:126:LEU:HD12	1.98	0.45
1:DF:37:ASP:OD1	1:DF:37:ASP:N	2.33	0.45
1:FE:123:ALA:HA	1:FE:126:LEU:HD12	1.98	0.45
1:FM:114:MET:N	1:FN:159:GLU:HA	2.32	0.45
1:GL:97:PHE:HZ	1:GM:174:VAL:HG22	1.82	0.45
1:IB:128:PHE:HD1	1:IB:187:ALA:HB3	1.82	0.45
1:ID:52:LEU:HD22	1:IE:50:LEU:HD11	1.99	0.45
1:JB:67:THR:HB	1:JB:70:GLN:HB2	1.98	0.45
1:JB:128:PHE:HD1	1:JB:187:ALA:HB3	1.82	0.45
1:JD:52:LEU:HD22	1:JE:50:LEU:HD11	1.99	0.45
1:KE:81:ASN:HD21	1:KE:84:TRP:HB2	1.82	0.45
1:KG:70:GLN:O	1:KG:74:ARG:HG2	2.16	0.45
1:LD:52:LEU:HD22	1:LE:50:LEU:HD11	1.99	0.45
1:AF:84:TRP:CD1	1:AF:150:CYS:HB2	2.52	0.45
1:AL:97:PHE:HZ	1:AM:174:VAL:HG22	1.82	0.45
1:AM:128:PHE:CD1	1:AM:187:ALA:HB3	2.51	0.45
1:CF:84:TRP:CD1	1:CF:150:CYS:HB2	2.52	0.45
1:EL:91:ILE:HD13	1:EL:123:ALA:HB2	1.98	0.45
1:EO:91:ILE:HD13	1:EO:123:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IO:79:HIS:ND1	1:IO:79:HIS:O	2.50	0.45
1:JF:193:ASP:OD1	1:JF:193:ASP:N	2.49	0.45
1:LF:95:ASN:HB3	1:LF:120:LYS:HB2	1.99	0.45
1:LL:91:ILE:HD13	1:LL:123:ALA:HB2	1.98	0.45
1:BM:114:MET:N	1:BN:159:GLU:HA	2.32	0.44
1:AO:123:ALA:HA	1:AO:126:LEU:HD12	2.00	0.44
1:CB:67:THR:HB	1:CB:70:GLN:HB2	1.98	0.44
1:CD:128:PHE:HD1	1:CD:187:ALA:HB3	1.82	0.44
1:EF:84:TRP:CD1	1:EF:150:CYS:HB2	2.52	0.44
1:EN:137:HIS:HA	1:EN:140:VAL:HB	1.98	0.44
1:HB:130:ILE:HG23	1:HB:191:PHE:HE2	1.81	0.44
1:HF:95:ASN:HB3	1:HF:120:LYS:HB2	1.99	0.44
1:HM:117:TYR:HB2	1:HN:164:VAL:HG22	1.98	0.44
1:IB:67:THR:HB	1:IB:70:GLN:HB2	1.98	0.44
1:ID:77:THR:HG23	1:ID:80:GLY:H	1.81	0.44
1:IG:70:GLN:O	1:IG:74:ARG:HG2	2.17	0.44
1:IO:91:ILE:HD13	1:IO:123:ALA:HB2	1.99	0.44
1:JC:78:LYS:HE3	1:JC:78:LYS:HB2	1.88	0.44
1:JG:75:ALA:HB1	1:JG:142:ARG:HG3	1.99	0.44
1:LE:81:ASN:HD21	1:LE:84:TRP:HB2	1.82	0.44
1:BD:128:PHE:HD1	1:BD:187:ALA:HB3	1.82	0.44
1:BN:91:ILE:HD13	1:BN:123:ALA:HB2	1.99	0.44
1:CO:79:HIS:ND1	1:CO:79:HIS:O	2.50	0.44
1:EB:67:THR:HB	1:EB:70:GLN:HB2	1.98	0.44
1:EB:128:PHE:HD1	1:EB:187:ALA:HB3	1.82	0.44
1:ED:128:PHE:HD1	1:ED:187:ALA:HB3	1.82	0.44
1:EO:123:ALA:HA	1:EO:126:LEU:HD12	2.00	0.44
1:FD:128:PHE:HD1	1:FD:187:ALA:HB3	1.82	0.44
1:GD:128:PHE:HD1	1:GD:187:ALA:HB3	1.82	0.44
1:IL:97:PHE:HZ	1:IM:174:VAL:HG22	1.82	0.44
1:IM:117:TYR:HB2	1:IN:164:VAL:HG22	1.98	0.44
1:IO:123:ALA:HA	1:IO:126:LEU:HD12	2.00	0.44
1:JO:123:ALA:HA	1:JO:126:LEU:HD12	2.00	0.44
1:KN:91:ILE:HD13	1:KN:123:ALA:HB2	2.00	0.44
1:KO:123:ALA:HA	1:KO:126:LEU:HD12	1.99	0.44
1:LB:128:PHE:HD1	1:LB:187:ALA:HB3	1.82	0.44
1:LO:123:ALA:HA	1:LO:126:LEU:HD12	1.99	0.44
1:BF:193:ASP:OD1	1:BF:193:ASP:N	2.49	0.44
1:DM:114:MET:N	1:DN:159:GLU:HA	2.32	0.44
1:GF:95:ASN:HB3	1:GF:120:LYS:HB2	1.99	0.44
1:HB:128:PHE:HD1	1:HB:187:ALA:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HD:128:PHE:CD1	1:HD:187:ALA:HB3	2.51	0.44
1:HL:91:ILE:HD13	1:HL:123:ALA:HB2	1.98	0.44
1:HO:79:HIS:ND1	1:HO:79:HIS:O	2.50	0.44
1:HO:91:ILE:HD13	1:HO:123:ALA:HB2	1.99	0.44
1:IN:91:ILE:HD13	1:IN:123:ALA:HB2	2.00	0.44
1:JI:91:ILE:HD13	1:JI:123:ALA:HB2	2.00	0.44
1:KF:95:ASN:HB3	1:KF:120:LYS:HB2	1.99	0.44
1:LN:91:ILE:HD13	1:LN:123:ALA:HB2	2.00	0.44
1:BD:52:LEU:HD22	1:BE:50:LEU:HD11	1.99	0.44
1:BI:91:ILE:HD13	1:BI:123:ALA:HB2	2.00	0.44
1:BO:123:ALA:HA	1:BO:126:LEU:HD12	1.99	0.44
1:AE:123:ALA:HA	1:AE:126:LEU:HD12	1.98	0.44
1:CF:95:ASN:HB3	1:CF:120:LYS:HB2	1.99	0.44
1:EN:91:ILE:HD13	1:EN:123:ALA:HB2	2.00	0.44
1:FI:91:ILE:HD13	1:FI:123:ALA:HB2	2.00	0.44
1:FM:128:PHE:HD1	1:FM:187:ALA:HB3	1.81	0.44
1:FN:91:ILE:HD13	1:FN:123:ALA:HB2	2.00	0.44
1:GG:75:ALA:HB1	1:GG:142:ARG:HG3	1.99	0.44
1:GI:91:ILE:HD13	1:GI:123:ALA:HB2	2.00	0.44
1:GL:61:ASP:OD1	1:GL:61:ASP:N	2.51	0.44
1:HF:84:TRP:CD1	1:HF:150:CYS:HB2	2.52	0.44
1:JL:97:PHE:HZ	1:JM:174:VAL:HG22	1.82	0.44
1:KI:91:ILE:HD13	1:KI:123:ALA:HB2	2.00	0.44
1:KM:61:ASP:HB3	1:KM:191:PHE:HA	2.00	0.44
1:CD:128:PHE:CD1	1:CD:187:ALA:HB3	2.51	0.44
1:CG:75:ALA:HB1	1:CG:142:ARG:HG3	1.99	0.44
1:CI:91:ILE:HD13	1:CI:123:ALA:HB2	2.00	0.44
1:CM:114:MET:N	1:CN:159:GLU:HA	2.32	0.44
1:DD:52:LEU:HD22	1:DE:50:LEU:HD11	1.99	0.44
1:DF:95:ASN:HB3	1:DF:120:LYS:HB2	1.99	0.44
1:EG:75:ALA:HB1	1:EG:142:ARG:HG3	1.99	0.44
1:FF:193:ASP:OD1	1:FF:193:ASP:N	2.49	0.44
1:FO:91:ILE:HD13	1:FO:123:ALA:HB2	1.99	0.44
1:GG:70:GLN:O	1:GG:74:ARG:HG2	2.17	0.44
1:GN:91:ILE:HD13	1:GN:123:ALA:HB2	2.00	0.44
1:HF:193:ASP:OD1	1:HF:193:ASP:N	2.49	0.44
1:HG:75:ALA:HB1	1:HG:142:ARG:HG3	1.99	0.44
1:HO:123:ALA:HA	1:HO:126:LEU:HD12	2.00	0.44
1:IF:84:TRP:CD1	1:IF:150:CYS:HB2	2.52	0.44
1:IF:95:ASN:HB3	1:IF:120:LYS:HB2	1.99	0.44
1:IM:61:ASP:HB3	1:IM:191:PHE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IM:114:MET:N	1:IN:159:GLU:HA	2.32	0.44
1:JM:114:MET:N	1:JN:159:GLU:HA	2.32	0.44
1:KF:171:GLU:HB3	1:KJ:93:MET:HE3	2.00	0.44
1:KL:61:ASP:N	1:KL:61:ASP:OD1	2.51	0.44
1:BE:81:ASN:HD21	1:BE:84:TRP:HB2	1.82	0.44
1:BF:84:TRP:CD1	1:BF:150:CYS:HB2	2.52	0.44
1:BM:117:TYR:HB2	1:BN:164:VAL:HG22	1.98	0.44
1:AK:174:VAL:O	1:AK:178:GLU:HG2	2.18	0.44
1:AM:114:MET:N	1:AN:159:GLU:HA	2.32	0.44
1:AM:193:ASP:OD1	1:AM:193:ASP:N	2.49	0.44
1:DB:128:PHE:HD1	1:DB:187:ALA:HB3	1.82	0.44
1:DM:61:ASP:HB3	1:DM:191:PHE:HA	2.00	0.44
1:DN:91:ILE:HD13	1:DN:123:ALA:HB2	2.00	0.44
1:FB:65:ALA:HB3	1:FB:71:ALA:HB2	2.00	0.44
1:FK:174:VAL:O	1:FK:178:GLU:HG2	2.18	0.44
1:FO:79:HIS:ND1	1:FO:79:HIS:O	2.50	0.44
1:GB:128:PHE:HD1	1:GB:187:ALA:HB3	1.82	0.44
1:HL:128:PHE:HD1	1:HL:187:ALA:HB3	1.83	0.44
1:HN:91:ILE:HD13	1:HN:123:ALA:HB2	2.00	0.44
1:IL:61:ASP:OD1	1:IL:61:ASP:N	2.51	0.44
1:JB:65:ALA:HB3	1:JB:71:ALA:HB2	2.00	0.44
1:JF:95:ASN:HB3	1:JF:120:LYS:HB2	1.99	0.44
1:KD:52:LEU:HD22	1:KE:50:LEU:HD11	1.99	0.44
1:BG:75:ALA:HB1	1:BG:142:ARG:HG3	1.99	0.44
1:AE:81:ASN:HD21	1:AE:84:TRP:HB2	1.82	0.44
1:AF:193:ASP:OD1	1:AF:193:ASP:N	2.49	0.44
1:AM:61:ASP:HB3	1:AM:191:PHE:HA	2.00	0.44
1:AO:79:HIS:ND1	1:AO:79:HIS:O	2.50	0.44
1:CL:128:PHE:HD1	1:CL:187:ALA:HB3	1.83	0.44
1:DB:65:ALA:HB3	1:DB:71:ALA:HB2	2.00	0.44
1:DF:84:TRP:CD1	1:DF:150:CYS:HB2	2.52	0.44
1:EB:56:LYS:NZ	1:EB:180:ALA:O	2.39	0.44
1:ED:52:LEU:HD22	1:EE:50:LEU:HD11	1.99	0.44
1:EF:95:ASN:HB3	1:EF:120:LYS:HB2	1.99	0.44
1:EL:61:ASP:OD1	1:EL:61:ASP:N	2.51	0.44
1:EM:114:MET:N	1:EN:159:GLU:HA	2.32	0.44
1:EO:79:HIS:ND1	1:EO:79:HIS:O	2.50	0.44
1:GK:174:VAL:O	1:GK:178:GLU:HG2	2.18	0.44
1:GM:114:MET:N	1:GN:159:GLU:HA	2.32	0.44
1:GO:123:ALA:HA	1:GO:126:LEU:HD12	2.00	0.44
1:JD:128:PHE:HD1	1:JD:187:ALA:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JN:91:ILE:HD13	1:JN:123:ALA:HB2	2.00	0.44
1:LG:75:ALA:HB1	1:LG:142:ARG:HG3	1.99	0.44
1:BB:65:ALA:HB3	1:BB:71:ALA:HB2	2.00	0.44
1:AB:128:PHE:HD1	1:AB:187:ALA:HB3	1.82	0.44
1:AD:128:PHE:HD1	1:AD:187:ALA:HB3	1.82	0.44
1:AM:117:TYR:HB2	1:AN:164:VAL:HG22	1.98	0.44
1:CF:63:ILE:HG12	1:CF:74:ARG:HH21	1.81	0.44
1:DI:91:ILE:HD13	1:DI:123:ALA:HB2	2.00	0.44
1:DO:123:ALA:HA	1:DO:126:LEU:HD12	2.00	0.44
1:EI:91:ILE:HD13	1:EI:123:ALA:HB2	2.00	0.44
1:FK:171:GLU:OE1	1:FK:171:GLU:N	2.51	0.44
1:FO:123:ALA:HA	1:FO:126:LEU:HD12	1.99	0.44
1:GD:52:LEU:HD22	1:GE:50:LEU:HD11	1.99	0.44
1:HB:67:THR:HB	1:HB:70:GLN:HB2	1.98	0.44
1:HL:61:ASP:N	1:HL:61:ASP:OD1	2.51	0.44
1:IB:65:ALA:HB3	1:IB:71:ALA:HB2	2.00	0.44
1:II:91:ILE:HD13	1:II:123:ALA:HB2	2.00	0.44
1:KE:73:GLU:O	1:KE:77:THR:HG22	2.18	0.44
1:LB:65:ALA:HB3	1:LB:71:ALA:HB2	2.00	0.44
1:LF:84:TRP:CD1	1:LF:150:CYS:HB2	2.52	0.44
1:LL:128:PHE:HD1	1:LL:187:ALA:HB3	1.83	0.44
1:BF:171:GLU:HB3	1:BJ:93:MET:HE3	2.00	0.44
1:BL:128:PHE:HD1	1:BL:187:ALA:HB3	1.83	0.44
1:DB:58:VAL:HG22	1:DB:188:VAL:HB	2.00	0.44
1:DC:123:ALA:HA	1:DC:126:LEU:HD12	2.00	0.44
1:DL:97:PHE:HZ	1:DM:174:VAL:HG22	1.82	0.44
1:DM:193:ASP:OD1	1:DM:193:ASP:N	2.49	0.44
1:EB:65:ALA:HB3	1:EB:71:ALA:HB2	2.00	0.44
1:EC:123:ALA:HA	1:EC:126:LEU:HD12	2.00	0.44
1:FC:91:ILE:HD13	1:FC:123:ALA:HB2	2.00	0.44
1:GL:128:PHE:HD1	1:GL:187:ALA:HB3	1.83	0.44
1:GM:61:ASP:HB3	1:GM:191:PHE:HA	2.00	0.44
1:HB:65:ALA:HB3	1:HB:71:ALA:HB2	2.00	0.44
1:HF:171:GLU:HB3	1:HJ:93:MET:HE3	2.00	0.44
1:IF:149:ASP:HA	1:IF:152:VAL:HG12	2.00	0.44
1:JF:171:GLU:HB3	1:JJ:93:MET:HE3	2.00	0.44
1:JH:74:ARG:HH22	1:JH:78:LYS:HE2	1.83	0.44
1:KF:84:TRP:CD1	1:KF:150:CYS:HB2	2.52	0.44
1:KK:174:VAL:O	1:KK:178:GLU:HG2	2.18	0.44
1:KL:88:LEU:HD11	1:KL:121:LEU:HD13	2.00	0.44
1:KL:128:PHE:HD1	1:KL:187:ALA:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LF:149:ASP:HA	1:LF:152:VAL:HG12	2.00	0.44
1:LI:91:ILE:HD13	1:LI:123:ALA:HB2	2.00	0.44
1:LK:171:GLU:OE1	1:LK:171:GLU:N	2.51	0.44
1:LL:61:ASP:OD1	1:LL:61:ASP:N	2.51	0.44
1:LM:114:MET:N	1:LN:159:GLU:HA	2.32	0.44
1:BC:91:ILE:HD13	1:BC:123:ALA:HB2	2.00	0.43
1:BN:43:VAL:HG21	1:BN:169:SER:HB3	1.98	0.43
1:AE:73:GLU:O	1:AE:77:THR:HG22	2.18	0.43
1:CE:73:GLU:O	1:CE:77:THR:HG22	2.18	0.43
1:DL:88:LEU:HD11	1:DL:121:LEU:HD13	2.00	0.43
1:EK:56:LYS:NZ	1:EK:180:ALA:O	2.41	0.43
1:EK:174:VAL:O	1:EK:178:GLU:HG2	2.18	0.43
1:FB:58:VAL:HG22	1:FB:188:VAL:HB	2.00	0.43
1:FF:171:GLU:HB3	1:FJ:93:MET:HE3	2.00	0.43
1:FL:128:PHE:HD1	1:FL:187:ALA:HB3	1.83	0.43
1:GB:65:ALA:HB3	1:GB:71:ALA:HB2	2.00	0.43
1:GF:149:ASP:HA	1:GF:152:VAL:HG12	2.00	0.43
1:GF:171:GLU:HB3	1:GJ:93:MET:HE3	2.00	0.43
1:HC:91:ILE:HD13	1:HC:123:ALA:HB2	2.00	0.43
1:HD:52:LEU:HD22	1:HE:50:LEU:HD11	1.99	0.43
1:HL:88:LEU:HD11	1:HL:121:LEU:HD13	2.00	0.43
1:IK:93:MET:HE3	1:IL:171:GLU:HB3	2.00	0.43
1:IL:128:PHE:HD1	1:IL:187:ALA:HB3	1.83	0.43
1:JI:117:TYR:HB2	1:JJ:164:VAL:HG22	2.00	0.43
1:JL:61:ASP:N	1:JL:61:ASP:OD1	2.51	0.43
1:JL:128:PHE:HD1	1:JL:187:ALA:HB3	1.83	0.43
1:KB:65:ALA:HB3	1:KB:71:ALA:HB2	2.00	0.43
1:KM:91:ILE:HD13	1:KM:123:ALA:HB2	2.00	0.43
1:BF:95:ASN:HB3	1:BF:120:LYS:HB2	1.99	0.43
1:BF:149:ASP:HA	1:BF:152:VAL:HG12	2.00	0.43
1:BL:88:LEU:HD11	1:BL:121:LEU:HD13	2.00	0.43
1:AL:88:LEU:HD11	1:AL:121:LEU:HD13	2.00	0.43
1:AL:128:PHE:HD1	1:AL:187:ALA:HB3	1.83	0.43
1:AN:91:ILE:HD13	1:AN:123:ALA:HB2	2.00	0.43
1:AO:91:ILE:HD13	1:AO:123:ALA:HB2	1.99	0.43
1:CF:171:GLU:HB3	1:CJ:93:MET:HE3	2.00	0.43
1:CK:174:VAL:O	1:CK:178:GLU:HG2	2.18	0.43
1:CN:91:ILE:HD13	1:CN:123:ALA:HB2	2.00	0.43
1:DE:73:GLU:O	1:DE:77:THR:HG22	2.18	0.43
1:DE:81:ASN:HD21	1:DE:84:TRP:HB2	1.82	0.43
1:DI:117:TYR:HB2	1:DJ:164:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EF:171:GLU:HB3	1:EJ:93:MET:HE3	2.00	0.43
1:EI:117:TYR:HB2	1:EJ:164:VAL:HG22	2.00	0.43
1:EJ:78:LYS:HE3	1:EJ:78:LYS:HB2	1.81	0.43
1:GL:88:LEU:HD11	1:GL:121:LEU:HD13	2.00	0.43
1:GM:91:ILE:HD13	1:GM:123:ALA:HB2	2.01	0.43
1:HH:74:ARG:HH22	1:HH:78:LYS:HE2	1.83	0.43
1:HK:174:VAL:O	1:HK:178:GLU:HG2	2.18	0.43
1:HM:114:MET:N	1:HN:159:GLU:HA	2.32	0.43
1:KD:55:ARG:NH1	1:KE:181:ARG:HG2	2.33	0.43
1:KD:166:VAL:HG21	1:KD:172:ILE:HA	2.00	0.43
1:KH:74:ARG:HH22	1:KH:78:LYS:HE2	1.83	0.43
1:KM:114:MET:N	1:KN:159:GLU:HA	2.32	0.43
1:LI:117:TYR:HB2	1:LJ:164:VAL:HG22	2.00	0.43
1:BD:166:VAL:HG21	1:BD:172:ILE:HA	2.00	0.43
1:BE:73:GLU:O	1:BE:77:THR:HG22	2.18	0.43
1:BI:117:TYR:HB2	1:BJ:164:VAL:HG22	2.00	0.43
1:CK:93:MET:HE3	1:CL:171:GLU:HB3	2.00	0.43
1:DC:97:PHE:HZ	1:DD:174:VAL:HG22	1.84	0.43
1:DK:93:MET:HE3	1:DL:171:GLU:HB3	2.00	0.43
1:DK:174:VAL:O	1:DK:178:GLU:HG2	2.18	0.43
1:DL:128:PHE:HD1	1:DL:187:ALA:HB3	1.83	0.43
1:ED:166:VAL:HG21	1:ED:172:ILE:HA	2.00	0.43
1:FC:123:ALA:HA	1:FC:126:LEU:HD12	2.00	0.43
1:FF:84:TRP:CD1	1:FF:150:CYS:HB2	2.52	0.43
1:FM:61:ASP:HB3	1:FM:191:PHE:HA	2.00	0.43
1:GA:70:GLN:O	1:GA:74:ARG:HG2	2.19	0.43
1:GK:63:ILE:HD12	1:GK:63:ILE:HA	1.90	0.43
1:GO:91:ILE:HD13	1:GO:123:ALA:HB2	1.99	0.43
1:HD:128:PHE:HD1	1:HD:187:ALA:HB3	1.82	0.43
1:JA:70:GLN:O	1:JA:74:ARG:HG2	2.19	0.43
1:JB:58:VAL:HG22	1:JB:188:VAL:HB	2.00	0.43
1:JE:73:GLU:O	1:JE:77:THR:HG22	2.18	0.43
1:JO:91:ILE:HD13	1:JO:123:ALA:HB2	1.99	0.43
1:KB:58:VAL:HG22	1:KB:188:VAL:HB	2.00	0.43
1:KC:123:ALA:HA	1:KC:126:LEU:HD12	2.00	0.43
1:KD:128:PHE:HD1	1:KD:187:ALA:HB3	1.82	0.43
1:KF:149:ASP:HA	1:KF:152:VAL:HG12	2.00	0.43
1:KK:93:MET:HE3	1:KL:171:GLU:HB3	2.00	0.43
1:LD:128:PHE:HD1	1:LD:187:ALA:HB3	1.82	0.43
1:BL:97:PHE:HZ	1:BM:174:VAL:HG22	1.82	0.43
1:CA:167:PRO:HD2	1:CE:93:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:81:ASN:HD21	1:CE:84:TRP:HB2	1.82	0.43
1:DA:70:GLN:O	1:DA:74:ARG:HG2	2.19	0.43
1:DD:55:ARG:NH1	1:DE:181:ARG:HG2	2.33	0.43
1:DD:166:VAL:HG21	1:DD:172:ILE:HA	2.00	0.43
1:DF:171:GLU:HB3	1:DJ:93:MET:HE3	2.00	0.43
1:DL:61:ASP:OD1	1:DL:61:ASP:N	2.51	0.43
1:EF:52:LEU:HD22	1:EG:50:LEU:HD11	2.01	0.43
1:GK:56:LYS:NZ	1:GK:180:ALA:O	2.41	0.43
1:HA:70:GLN:O	1:HA:74:ARG:HG2	2.19	0.43
1:HI:117:TYR:HB2	1:HJ:164:VAL:HG22	2.00	0.43
1:IF:171:GLU:HB3	1:IJ:93:MET:HE3	2.00	0.43
1:IK:174:VAL:O	1:IK:178:GLU:HG2	2.18	0.43
1:JA:167:PRO:HD2	1:JE:93:MET:HE2	2.01	0.43
1:KA:97:PHE:HZ	1:KB:174:VAL:HG22	1.84	0.43
1:KF:193:ASP:OD1	1:KF:193:ASP:N	2.49	0.43
1:LA:167:PRO:HD2	1:LE:93:MET:HE2	2.01	0.43
1:LD:166:VAL:HG21	1:LD:172:ILE:HA	2.00	0.43
1:LF:74:ARG:O	1:LF:77:THR:OG1	2.25	0.43
1:LJ:78:LYS:HE3	1:LJ:78:LYS:HB2	1.81	0.43
1:LK:63:ILE:HD12	1:LK:63:ILE:HA	1.90	0.43
1:BC:97:PHE:HZ	1:BD:174:VAL:HG22	1.84	0.43
1:BK:174:VAL:O	1:BK:178:GLU:HG2	2.18	0.43
1:BL:61:ASP:OD1	1:BL:61:ASP:N	2.51	0.43
1:AC:91:ILE:HD13	1:AC:123:ALA:HB2	2.00	0.43
1:AF:52:LEU:HD22	1:AG:50:LEU:HD11	2.01	0.43
1:AI:91:ILE:HD13	1:AI:123:ALA:HB2	2.00	0.43
1:CC:123:ALA:HA	1:CC:126:LEU:HD12	2.00	0.43
1:CO:123:ALA:HA	1:CO:126:LEU:HD12	2.00	0.43
1:DD:128:PHE:HD1	1:DD:187:ALA:HB3	1.82	0.43
1:EB:58:VAL:HG22	1:EB:188:VAL:HB	2.00	0.43
1:FI:78:LYS:HA	1:FN:137:HIS:HE1	1.83	0.43
1:FJ:91:ILE:HG12	1:FJ:128:PHE:CZ	2.54	0.43
1:GF:52:LEU:HD22	1:GG:50:LEU:HD11	2.01	0.43
1:GJ:127:ARG:HG2	1:GJ:160:ASP:HB3	2.01	0.43
1:HD:166:VAL:HG21	1:HD:172:ILE:HA	2.00	0.43
1:HE:73:GLU:O	1:HE:77:THR:HG22	2.18	0.43
1:HN:169:SER:O	1:HN:173:PRO:HD3	2.19	0.43
1:KB:128:PHE:HD1	1:KB:187:ALA:HB3	1.82	0.43
1:LB:58:VAL:HG22	1:LB:188:VAL:HB	2.00	0.43
1:LF:52:LEU:HD22	1:LG:50:LEU:HD11	2.01	0.43
1:BB:128:PHE:HD1	1:BB:187:ALA:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BH:74:ARG:HH22	1:BH:78:LYS:HE2	1.83	0.43
1:BO:91:ILE:HD13	1:BO:123:ALA:HB2	1.99	0.43
1:AD:52:LEU:HD22	1:AE:50:LEU:HD11	1.99	0.43
1:AF:149:ASP:HA	1:AF:152:VAL:HG12	2.00	0.43
1:AH:74:ARG:HH22	1:AH:78:LYS:HE2	1.83	0.43
1:AJ:91:ILE:HG12	1:AJ:128:PHE:CZ	2.54	0.43
1:CB:58:VAL:HG22	1:CB:188:VAL:HB	2.00	0.43
1:CI:78:LYS:HA	1:CN:137:HIS:HE1	1.83	0.43
1:CJ:127:ARG:HG2	1:CJ:160:ASP:HB3	2.01	0.43
1:CL:77:THR:HG22	1:CL:79:HIS:H	1.84	0.43
1:CO:91:ILE:HD13	1:CO:123:ALA:HB2	1.99	0.43
1:EA:167:PRO:HD2	1:EE:93:MET:HE2	2.01	0.43
1:EC:97:PHE:HZ	1:ED:174:VAL:HG22	1.84	0.43
1:EE:73:GLU:O	1:EE:77:THR:HG22	2.18	0.43
1:EI:78:LYS:HA	1:EN:137:HIS:HE1	1.83	0.43
1:FA:97:PHE:HZ	1:FB:174:VAL:HG22	1.84	0.43
1:FE:73:GLU:O	1:FE:77:THR:HG22	2.18	0.43
1:FF:52:LEU:HD22	1:FG:50:LEU:HD11	2.01	0.43
1:FG:75:ALA:HB1	1:FG:142:ARG:HG3	1.99	0.43
1:FM:78:LYS:HD2	1:FM:78:LYS:HA	1.84	0.43
1:GD:55:ARG:NH1	1:GE:181:ARG:HG2	2.33	0.43
1:GI:117:TYR:HB2	1:GJ:164:VAL:HG22	2.00	0.43
1:GJ:91:ILE:HG12	1:GJ:128:PHE:CZ	2.54	0.43
1:HJ:78:LYS:HB2	1:HJ:78:LYS:HE3	1.81	0.43
1:HJ:91:ILE:HG12	1:HJ:128:PHE:CZ	2.54	0.43
1:HM:61:ASP:HB3	1:HM:191:PHE:HA	2.00	0.43
1:ID:166:VAL:HG21	1:ID:172:ILE:HA	2.00	0.43
1:IG:75:ALA:HB1	1:IG:142:ARG:HG3	1.99	0.43
1:JF:84:TRP:CD1	1:JF:150:CYS:HB2	2.52	0.43
1:JF:149:ASP:HA	1:JF:152:VAL:HG12	2.00	0.43
1:JJ:91:ILE:HG12	1:JJ:128:PHE:CZ	2.54	0.43
1:KF:174:VAL:HG22	1:KJ:97:PHE:HZ	1.84	0.43
1:KI:78:LYS:HA	1:KN:137:HIS:HE1	1.83	0.43
1:KJ:127:ARG:HG2	1:KJ:160:ASP:HB3	2.01	0.43
1:LJ:91:ILE:HG12	1:LJ:128:PHE:CZ	2.54	0.43
1:AF:174:VAL:HG22	1:AJ:97:PHE:HZ	1.84	0.43
1:CA:97:PHE:HZ	1:CB:174:VAL:HG22	1.84	0.43
1:CC:97:PHE:HZ	1:CD:174:VAL:HG22	1.84	0.43
1:CD:55:ARG:NH1	1:CE:181:ARG:HG2	2.33	0.43
1:CF:174:VAL:HG22	1:CJ:97:PHE:HZ	1.84	0.43
1:DC:91:ILE:HD13	1:DC:123:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DI:78:LYS:HA	1:DN:137:HIS:HE1	1.83	0.43
1:EL:128:PHE:HD1	1:EL:187:ALA:HB3	1.83	0.43
1:FC:97:PHE:HZ	1:FD:174:VAL:HG22	1.84	0.43
1:GB:58:VAL:HG22	1:GB:188:VAL:HB	2.00	0.43
1:GE:73:GLU:O	1:GE:77:THR:HG22	2.18	0.43
1:GL:77:THR:HG22	1:GL:79:HIS:H	1.84	0.43
1:HI:91:ILE:HD13	1:HI:123:ALA:HB2	2.00	0.43
1:IA:70:GLN:O	1:IA:74:ARG:HG2	2.19	0.43
1:ID:128:PHE:HD1	1:ID:187:ALA:HB3	1.82	0.43
1:IJ:91:ILE:HG12	1:IJ:128:PHE:CZ	2.54	0.43
1:IJ:127:ARG:HG2	1:IJ:160:ASP:HB3	2.01	0.43
1:JF:174:VAL:HG22	1:JJ:97:PHE:HZ	1.84	0.43
1:KC:97:PHE:HZ	1:KD:174:VAL:HG22	1.84	0.43
1:KI:117:TYR:HB2	1:KJ:164:VAL:HG22	2.00	0.43
1:KN:169:SER:O	1:KN:173:PRO:HD3	2.19	0.43
1:LA:70:GLN:O	1:LA:74:ARG:HG2	2.19	0.43
1:LC:91:ILE:HD13	1:LC:123:ALA:HB2	2.00	0.43
1:BC:123:ALA:HA	1:BC:126:LEU:HD12	2.00	0.43
1:BJ:91:ILE:HG12	1:BJ:128:PHE:CZ	2.54	0.43
1:BK:61:ASP:OD1	1:BK:191:PHE:HD1	2.02	0.43
1:BL:66:ASP:OD1	1:BL:66:ASP:N	2.33	0.43
1:BL:77:THR:HG22	1:BL:79:HIS:H	1.84	0.43
1:BM:61:ASP:HB3	1:BM:191:PHE:HA	2.00	0.43
1:AD:166:VAL:HG21	1:AD:172:ILE:HA	2.00	0.43
1:AL:61:ASP:OD1	1:AL:61:ASP:N	2.51	0.43
1:CJ:91:ILE:HG12	1:CJ:128:PHE:CZ	2.54	0.43
1:CN:169:SER:O	1:CN:173:PRO:HD3	2.19	0.43
1:DF:52:LEU:HD22	1:DG:50:LEU:HD11	2.01	0.43
1:DJ:91:ILE:HG12	1:DJ:128:PHE:CZ	2.54	0.43
1:DN:169:SER:O	1:DN:173:PRO:HD3	2.19	0.43
1:EA:97:PHE:HZ	1:EB:174:VAL:HG22	1.84	0.43
1:EF:40:ALA:HB2	1:EF:194:LEU:HD13	2.01	0.43
1:FD:52:LEU:HD22	1:FE:50:LEU:HD11	1.99	0.43
1:FI:117:TYR:HB2	1:FJ:164:VAL:HG22	2.00	0.43
1:FK:61:ASP:OD1	1:FK:191:PHE:HD1	2.02	0.43
1:FL:61:ASP:OD1	1:FL:61:ASP:N	2.51	0.43
1:HD:55:ARG:NH1	1:HE:181:ARG:HG2	2.33	0.43
1:HI:78:LYS:HA	1:HN:137:HIS:HE1	1.83	0.43
1:IC:91:ILE:HD13	1:IC:123:ALA:HB2	2.00	0.43
1:IF:193:ASP:OD1	1:IF:193:ASP:N	2.49	0.43
1:JI:78:LYS:HA	1:JN:137:HIS:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JK:174:VAL:O	1:JK:178:GLU:HG2	2.18	0.43
1:LE:73:GLU:O	1:LE:77:THR:HG22	2.18	0.43
1:LL:77:THR:HG22	1:LL:79:HIS:H	1.84	0.43
1:BA:167:PRO:HD2	1:BE:93:MET:HE2	2.01	0.43
1:BI:78:LYS:HA	1:BN:137:HIS:HE1	1.83	0.43
1:AB:65:ALA:HB3	1:AB:71:ALA:HB2	2.00	0.43
1:AC:97:PHE:HZ	1:AD:174:VAL:HG22	1.84	0.43
1:AF:40:ALA:HB2	1:AF:194:LEU:HD13	2.01	0.43
1:AF:95:ASN:HB3	1:AF:120:LYS:HB2	1.99	0.43
1:AJ:127:ARG:HG2	1:AJ:160:ASP:HB3	2.01	0.43
1:CA:70:GLN:O	1:CA:74:ARG:HG2	2.19	0.43
1:CL:88:LEU:HD11	1:CL:121:LEU:HD13	2.00	0.43
1:DF:40:ALA:HB2	1:DF:194:LEU:HD13	2.01	0.43
1:EK:93:MET:HE3	1:EL:171:GLU:HB3	2.00	0.43
1:EL:77:THR:HG22	1:EL:79:HIS:H	1.84	0.43
1:FD:55:ARG:NH1	1:FE:181:ARG:HG2	2.33	0.43
1:FD:166:VAL:HG21	1:FD:172:ILE:HA	2.00	0.43
1:GC:97:PHE:HZ	1:GD:174:VAL:HG22	1.84	0.43
1:GE:81:ASN:HD21	1:GE:84:TRP:HB2	1.82	0.43
1:GK:61:ASP:OD1	1:GK:191:PHE:HD1	2.02	0.43
1:HA:97:PHE:HZ	1:HB:174:VAL:HG22	1.84	0.43
1:HK:93:MET:HE3	1:HL:171:GLU:HB3	2.00	0.43
1:IA:97:PHE:HZ	1:IB:174:VAL:HG22	1.84	0.43
1:IH:74:ARG:HH22	1:IH:78:LYS:HE2	1.83	0.43
1:II:117:TYR:HB2	1:IJ:164:VAL:HG22	2.00	0.43
1:IM:91:ILE:HD13	1:IM:123:ALA:HB2	2.01	0.43
1:JK:171:GLU:OE1	1:JK:171:GLU:N	2.51	0.43
1:JL:88:LEU:HD11	1:JL:121:LEU:HD13	2.01	0.43
1:KJ:91:ILE:HG12	1:KJ:128:PHE:CZ	2.54	0.43
1:LD:55:ARG:NH1	1:LE:181:ARG:HG2	2.33	0.43
1:LM:61:ASP:HB3	1:LM:191:PHE:HA	2.00	0.43
1:LM:193:ASP:OD1	1:LM:193:ASP:N	2.49	0.43
1:AM:91:ILE:HD13	1:AM:123:ALA:HB2	2.01	0.43
1:CD:166:VAL:HG21	1:CD:172:ILE:HA	2.00	0.43
1:DM:91:ILE:HD13	1:DM:123:ALA:HB2	2.01	0.43
1:EF:149:ASP:HA	1:EF:152:VAL:HG12	2.00	0.43
1:FH:74:ARG:HH22	1:FH:78:LYS:HE2	1.83	0.43
1:GC:91:ILE:HD13	1:GC:123:ALA:HB2	2.00	0.43
1:GF:174:VAL:HG22	1:GJ:97:PHE:HZ	1.84	0.43
1:GK:93:MET:HE3	1:GL:171:GLU:HB3	2.00	0.43
1:HC:91:ILE:HG12	1:HC:128:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HC:97:PHE:HZ	1:HD:174:VAL:HG22	1.84	0.43
1:IE:73:GLU:O	1:IE:77:THR:HG22	2.18	0.43
1:IN:169:SER:O	1:IN:173:PRO:HD3	2.19	0.43
1:JC:123:ALA:HA	1:JC:126:LEU:HD12	2.00	0.43
1:JM:91:ILE:HD13	1:JM:123:ALA:HB2	2.01	0.43
1:KA:70:GLN:O	1:KA:74:ARG:HG2	2.19	0.43
1:KA:128:PHE:HD1	1:KA:187:ALA:HB3	1.84	0.43
1:KF:52:LEU:HD22	1:KG:50:LEU:HD11	2.01	0.43
1:LF:174:VAL:HG22	1:LJ:97:PHE:HZ	1.84	0.43
1:BL:52:LEU:HD21	1:BM:173:PRO:HB2	2.01	0.42
1:BM:91:ILE:HD13	1:BM:123:ALA:HB2	2.01	0.42
1:AA:70:GLN:O	1:AA:74:ARG:HG2	2.19	0.42
1:AI:78:LYS:HA	1:AN:137:HIS:HE1	1.83	0.42
1:AN:169:SER:O	1:AN:173:PRO:HD3	2.19	0.42
1:CC:91:ILE:HG12	1:CC:128:PHE:CZ	2.54	0.42
1:CC:91:ILE:HD13	1:CC:123:ALA:HB2	2.00	0.42
1:CI:117:TYR:HB2	1:CJ:164:VAL:HG22	2.00	0.42
1:EF:174:VAL:HG22	1:EJ:97:PHE:HZ	1.84	0.42
1:FC:91:ILE:HG12	1:FC:128:PHE:CZ	2.54	0.42
1:FF:95:ASN:HB3	1:FF:120:LYS:HB2	1.99	0.42
1:GA:167:PRO:HD2	1:GE:93:MET:HE2	2.01	0.42
1:GF:40:ALA:HB2	1:GF:194:LEU:HD13	2.01	0.42
1:HD:114:MET:SD	1:HD:114:MET:N	2.84	0.42
1:HF:40:ALA:HB2	1:HF:194:LEU:HD13	2.01	0.42
1:IA:128:PHE:HD1	1:IA:187:ALA:HB3	1.84	0.42
1:IB:58:VAL:HG22	1:IB:188:VAL:HB	2.00	0.42
1:JA:78:LYS:HD2	1:LA:135:PHE:CE1	2.54	0.42
1:JL:77:THR:HG22	1:JL:79:HIS:H	1.84	0.42
1:JM:61:ASP:HB3	1:JM:191:PHE:HA	2.00	0.42
1:KC:91:ILE:HG12	1:KC:128:PHE:CZ	2.54	0.42
1:KF:40:ALA:HB2	1:KF:194:LEU:HD13	2.01	0.42
1:LL:88:LEU:HD11	1:LL:121:LEU:HD13	2.00	0.42
1:BC:91:ILE:HG12	1:BC:128:PHE:CZ	2.54	0.42
1:AC:123:ALA:HA	1:AC:126:LEU:HD12	2.00	0.42
1:AF:171:GLU:HB3	1:AJ:93:MET:HE3	2.00	0.42
1:AI:117:TYR:HB2	1:AJ:164:VAL:HG22	2.00	0.42
1:AK:93:MET:HE3	1:AL:171:GLU:HB3	2.00	0.42
1:CF:52:LEU:HD22	1:CG:50:LEU:HD11	2.01	0.42
1:CF:149:ASP:HA	1:CF:152:VAL:HG12	2.00	0.42
1:CK:61:ASP:OD1	1:CK:191:PHE:HD1	2.02	0.42
1:DA:167:PRO:HD2	1:DE:93:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DH:74:ARG:HH22	1:DH:78:LYS:HE2	1.83	0.42
1:ED:55:ARG:NH1	1:EE:181:ARG:HG2	2.33	0.42
1:EM:61:ASP:HB3	1:EM:191:PHE:HA	2.00	0.42
1:EM:91:ILE:HD13	1:EM:123:ALA:HB2	2.01	0.42
1:FA:70:GLN:O	1:FA:74:ARG:HG2	2.19	0.42
1:FD:88:LEU:HD11	1:FD:121:LEU:HD13	2.01	0.42
1:FL:77:THR:HG22	1:FL:79:HIS:H	1.84	0.42
1:GA:128:PHE:HD1	1:GA:187:ALA:HB3	1.84	0.42
1:HA:167:PRO:HD2	1:HE:93:MET:HE2	2.01	0.42
1:HC:123:ALA:HA	1:HC:126:LEU:HD12	2.00	0.42
1:IC:123:ALA:HA	1:IC:126:LEU:HD12	2.00	0.42
1:JF:163:LEU:HD12	1:JJ:116:ILE:HG12	2.02	0.42
1:JJ:127:ARG:HG2	1:JJ:160:ASP:HB3	2.01	0.42
1:KD:97:PHE:HZ	1:KE:174:VAL:HG22	1.85	0.42
1:KL:77:THR:HG22	1:KL:79:HIS:H	1.84	0.42
1:LA:97:PHE:HZ	1:LB:174:VAL:HG22	1.84	0.42
1:LF:171:GLU:HB3	1:LJ:93:MET:HE3	2.00	0.42
1:LJ:127:ARG:HG2	1:LJ:160:ASP:HB3	2.01	0.42
1:BF:52:LEU:HD22	1:BG:50:LEU:HD11	2.01	0.42
1:BF:174:VAL:HG22	1:BJ:97:PHE:HZ	1.84	0.42
1:CH:74:ARG:HH22	1:CH:78:LYS:HE2	1.83	0.42
1:EJ:91:ILE:HG12	1:EJ:128:PHE:CZ	2.54	0.42
1:EK:61:ASP:OD1	1:EK:191:PHE:HD1	2.02	0.42
1:FJ:127:ARG:HG2	1:FJ:160:ASP:HB3	2.01	0.42
1:FL:88:LEU:HD11	1:FL:121:LEU:HD13	2.00	0.42
1:FM:91:ILE:HD13	1:FM:123:ALA:HB2	2.01	0.42
1:FN:169:SER:O	1:FN:173:PRO:HD3	2.19	0.42
1:GA:97:PHE:HZ	1:GB:174:VAL:HG22	1.84	0.42
1:GD:166:VAL:HG21	1:GD:172:ILE:HA	2.00	0.42
1:IA:167:PRO:HD2	1:IE:93:MET:HE2	2.01	0.42
1:IK:63:ILE:HD12	1:IK:63:ILE:HA	1.90	0.42
1:IL:77:THR:HG22	1:IL:79:HIS:H	1.84	0.42
1:JA:121:LEU:CG	1:LE:153:ARG:HG2	2.48	0.42
1:KJ:74:ARG:O	1:KJ:77:THR:HG22	2.20	0.42
1:KK:61:ASP:OD1	1:KK:191:PHE:HD1	2.02	0.42
1:KK:91:ILE:HD13	1:KK:123:ALA:HB2	2.02	0.42
1:LB:74:ARG:HA	1:LB:74:ARG:HD3	1.90	0.42
1:LC:123:ALA:HA	1:LC:126:LEU:HD12	2.00	0.42
1:LK:61:ASP:OD1	1:LK:191:PHE:HD1	2.02	0.42
1:LK:93:MET:HE3	1:LL:171:GLU:HB3	2.00	0.42
1:LK:174:VAL:O	1:LK:178:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:70:GLN:O	1:BA:74:ARG:HG2	2.19	0.42
1:BD:88:LEU:HD11	1:BD:121:LEU:HD13	2.01	0.42
1:BK:93:MET:HE3	1:BL:171:GLU:HB3	2.00	0.42
1:AD:88:LEU:HD11	1:AD:121:LEU:HD13	2.02	0.42
1:CJ:74:ARG:O	1:CJ:77:THR:HG22	2.20	0.42
1:CK:91:ILE:HD13	1:CK:123:ALA:HB2	2.02	0.42
1:CK:171:GLU:OE1	1:CK:171:GLU:N	2.51	0.42
1:CM:61:ASP:HB3	1:CM:191:PHE:HA	2.00	0.42
1:FL:52:LEU:HD21	1:FM:173:PRO:HB2	2.01	0.42
1:GL:52:LEU:HD21	1:GM:173:PRO:HB2	2.01	0.42
1:HF:149:ASP:HA	1:HF:152:VAL:HG12	2.00	0.42
1:IF:163:LEU:HD12	1:IJ:116:ILE:HG12	2.02	0.42
1:IK:91:ILE:HD13	1:IK:123:ALA:HB2	2.02	0.42
1:IL:52:LEU:HD21	1:IM:173:PRO:HB2	2.01	0.42
1:JC:91:ILE:HD13	1:JC:123:ALA:HB2	2.00	0.42
1:LC:91:ILE:HG12	1:LC:128:PHE:CZ	2.54	0.42
1:BF:163:LEU:HD12	1:BJ:116:ILE:HG12	2.02	0.42
1:AA:97:PHE:HZ	1:AB:174:VAL:HG22	1.84	0.42
1:AD:55:ARG:NH1	1:AE:181:ARG:HG2	2.33	0.42
1:CC:78:LYS:HE3	1:CC:78:LYS:HB2	1.88	0.42
1:DB:97:PHE:HZ	1:DC:174:VAL:HG22	1.85	0.42
1:DJ:74:ARG:O	1:DJ:77:THR:HG22	2.20	0.42
1:DK:61:ASP:OD1	1:DK:191:PHE:HD1	2.02	0.42
1:EC:91:ILE:HD13	1:EC:123:ALA:HB2	2.00	0.42
1:EJ:127:ARG:HG2	1:EJ:160:ASP:HB3	2.01	0.42
1:EL:88:LEU:HD11	1:EL:121:LEU:HD13	2.00	0.42
1:FF:149:ASP:HA	1:FF:152:VAL:HG12	2.00	0.42
1:GH:74:ARG:HH22	1:GH:78:LYS:HE2	1.83	0.42
1:HF:174:VAL:HG22	1:HJ:97:PHE:HZ	1.84	0.42
1:HL:77:THR:HG22	1:HL:79:HIS:H	1.84	0.42
1:IK:61:ASP:OD1	1:IK:191:PHE:HD1	2.02	0.42
1:JA:128:PHE:HD1	1:JA:187:ALA:HB3	1.84	0.42
1:JD:166:VAL:HG21	1:JD:172:ILE:HA	2.00	0.42
1:JF:52:LEU:HD22	1:JG:50:LEU:HD11	2.01	0.42
1:KB:97:PHE:HZ	1:KC:174:VAL:HG22	1.85	0.42
1:KL:52:LEU:HD21	1:KM:173:PRO:HB2	2.01	0.42
1:BB:74:ARG:HA	1:BB:74:ARG:HD3	1.90	0.42
1:AF:57:PRO:HB3	1:AF:93:MET:HB3	2.02	0.42
1:DC:91:ILE:HG12	1:DC:128:PHE:CZ	2.54	0.42
1:DD:114:MET:SD	1:DD:114:MET:N	2.84	0.42
1:EA:70:GLN:O	1:EA:74:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EL:52:LEU:HD21	1:EM:173:PRO:HB2	2.01	0.42
1:FA:128:PHE:HD1	1:FA:187:ALA:HB3	1.84	0.42
1:FB:97:PHE:HZ	1:FC:174:VAL:HG22	1.85	0.42
1:FF:163:LEU:HD12	1:FJ:116:ILE:HG12	2.02	0.42
1:FF:174:VAL:HG22	1:FJ:97:PHE:HZ	1.84	0.42
1:FK:91:ILE:HD13	1:FK:123:ALA:HB2	2.02	0.42
1:GC:91:ILE:HG12	1:GC:128:PHE:CZ	2.54	0.42
1:HF:52:LEU:HD22	1:HG:50:LEU:HD11	2.01	0.42
1:II:78:LYS:HA	1:IN:137:HIS:HE1	1.83	0.42
1:JD:97:PHE:HZ	1:JE:174:VAL:HG22	1.84	0.42
1:JK:93:MET:HE3	1:JL:171:GLU:HB3	2.00	0.42
1:JN:169:SER:O	1:JN:173:PRO:HD3	2.19	0.42
1:KC:91:ILE:HD13	1:KC:123:ALA:HB2	2.00	0.42
1:LI:78:LYS:HA	1:LN:137:HIS:HE1	1.83	0.42
1:AB:58:VAL:HG22	1:AB:188:VAL:HB	2.00	0.42
1:CB:65:ALA:HB3	1:CB:71:ALA:HB2	2.00	0.42
1:DA:97:PHE:HZ	1:DB:174:VAL:HG22	1.84	0.42
1:DD:97:PHE:HZ	1:DE:174:VAL:HG22	1.84	0.42
1:EC:91:ILE:HG12	1:EC:128:PHE:CZ	2.54	0.42
1:EM:78:LYS:HA	1:EM:78:LYS:HD2	1.84	0.42
1:FA:74:ARG:C	1:FA:77:THR:HG1	2.27	0.42
1:GI:78:LYS:HA	1:GN:137:HIS:HE1	1.83	0.42
1:HB:58:VAL:HG22	1:HB:188:VAL:HB	2.00	0.42
1:IF:40:ALA:HB2	1:IF:194:LEU:HD13	2.01	0.42
1:JA:97:PHE:HZ	1:JB:174:VAL:HG22	1.84	0.42
1:JB:97:PHE:HZ	1:JC:174:VAL:HG22	1.85	0.42
1:JF:169:SER:HA	1:JF:172:ILE:HG13	2.02	0.42
1:JK:61:ASP:OD1	1:JK:191:PHE:HD1	2.02	0.42
1:KA:167:PRO:HD2	1:KE:93:MET:HE2	2.01	0.42
1:LA:128:PHE:HD1	1:LA:187:ALA:HB3	1.84	0.42
1:LD:88:LEU:HD11	1:LD:121:LEU:HD13	2.02	0.42
1:BJ:127:ARG:HG2	1:BJ:160:ASP:HB3	2.01	0.42
1:BK:171:GLU:OE1	1:BK:171:GLU:N	2.51	0.42
1:BN:169:SER:O	1:BN:173:PRO:HD3	2.19	0.42
1:AC:91:ILE:HG12	1:AC:128:PHE:CZ	2.54	0.42
1:CF:169:SER:HA	1:CF:172:ILE:HG13	2.02	0.42
1:CL:52:LEU:HD21	1:CM:173:PRO:HB2	2.01	0.42
1:DF:149:ASP:HA	1:DF:152:VAL:HG12	2.00	0.42
1:DJ:127:ARG:HG2	1:DJ:160:ASP:HB3	2.01	0.42
1:DL:52:LEU:HD21	1:DM:173:PRO:HB2	2.01	0.42
1:EA:128:PHE:HD1	1:EA:187:ALA:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ED:91:ILE:HG12	1:ED:128:PHE:CZ	2.55	0.42
1:EF:57:PRO:HB3	1:EF:93:MET:HB3	2.02	0.42
1:FA:167:PRO:HD2	1:FE:93:MET:HE2	2.01	0.42
1:GI:169:SER:O	1:GI:173:PRO:HD3	2.20	0.42
1:HJ:127:ARG:HG2	1:HJ:160:ASP:HB3	2.01	0.42
1:HK:61:ASP:OD1	1:HK:191:PHE:HD1	2.02	0.42
1:IC:97:PHE:HZ	1:ID:174:VAL:HG22	1.84	0.42
1:ID:97:PHE:HZ	1:IE:174:VAL:HG22	1.84	0.42
1:IL:88:LEU:HD11	1:IL:121:LEU:HD13	2.00	0.42
1:KD:88:LEU:HD11	1:KD:121:LEU:HD13	2.02	0.42
1:KI:169:SER:O	1:KI:173:PRO:HD3	2.20	0.42
1:LN:169:SER:O	1:LN:173:PRO:HD3	2.19	0.42
1:BF:57:PRO:HB3	1:BF:93:MET:HB3	2.02	0.42
1:AD:91:ILE:HG12	1:AD:128:PHE:CZ	2.55	0.42
1:AD:97:PHE:HZ	1:AE:174:VAL:HG22	1.85	0.42
1:CL:61:ASP:OD1	1:CL:61:ASP:N	2.51	0.42
1:DF:57:PRO:HB3	1:DF:93:MET:HB3	2.02	0.42
1:DF:185:ILE:HD13	1:DF:185:ILE:HA	1.95	0.42
1:DI:169:SER:O	1:DI:173:PRO:HD3	2.20	0.42
1:DL:77:THR:HG22	1:DL:79:HIS:H	1.84	0.42
1:EH:74:ARG:HH22	1:EH:78:LYS:HE2	1.83	0.42
1:EH:91:ILE:HD13	1:EH:123:ALA:HB2	2.02	0.42
1:EI:169:SER:O	1:EI:173:PRO:HD3	2.20	0.42
1:EM:37:ASP:OD1	1:EM:37:ASP:N	2.48	0.42
1:FK:93:MET:HE3	1:FL:171:GLU:HB3	2.00	0.42
1:GF:163:LEU:HD12	1:GJ:116:ILE:HG12	2.02	0.42
1:GH:91:ILE:HD13	1:GH:123:ALA:HB2	2.02	0.42
1:HA:128:PHE:HD1	1:HA:187:ALA:HB3	1.84	0.42
1:HB:137:HIS:CE1	1:IE:78:LYS:HE3	2.55	0.42
1:HH:91:ILE:HD13	1:HH:123:ALA:HB2	2.02	0.42
1:IF:57:PRO:HB3	1:IF:93:MET:HB3	2.02	0.42
1:JD:88:LEU:HD11	1:JD:121:LEU:HD13	2.02	0.42
1:JF:40:ALA:HB2	1:JF:194:LEU:HD13	2.01	0.42
1:KH:91:ILE:HD13	1:KH:123:ALA:HB2	2.02	0.42
1:BB:58:VAL:HG22	1:BB:188:VAL:HB	2.00	0.42
1:BB:97:PHE:HZ	1:BC:174:VAL:HG22	1.85	0.42
1:BG:91:ILE:HD13	1:BG:123:ALA:HB2	2.02	0.42
1:BH:91:ILE:HD13	1:BH:123:ALA:HB2	2.02	0.42
1:AA:128:PHE:HD1	1:AA:187:ALA:HB3	1.84	0.42
1:AK:61:ASP:OD1	1:AK:191:PHE:HD1	2.02	0.42
1:AK:171:GLU:OE1	1:AK:171:GLU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:128:PHE:HD1	1:CA:187:ALA:HB3	1.84	0.42
1:CD:45:LYS:HE3	1:CD:45:LYS:HB3	1.90	0.42
1:CD:97:PHE:HZ	1:CE:174:VAL:HG22	1.84	0.42
1:CH:91:ILE:HD13	1:CH:123:ALA:HB2	2.02	0.42
1:CI:169:SER:O	1:CI:173:PRO:HD3	2.20	0.42
1:DA:128:PHE:HD1	1:DA:187:ALA:HB3	1.84	0.42
1:EN:169:SER:O	1:EN:173:PRO:HD3	2.19	0.42
1:FG:64:THR:HB	1:FG:194:LEU:HD23	2.02	0.42
1:FG:91:ILE:HD13	1:FG:123:ALA:HB2	2.02	0.42
1:GC:123:ALA:HA	1:GC:126:LEU:HD12	2.00	0.42
1:GM:78:LYS:HD2	1:GM:78:LYS:HA	1.84	0.42
1:GN:169:SER:O	1:GN:173:PRO:HD3	2.19	0.42
1:HB:88:LEU:HD11	1:HB:121:LEU:HD22	2.02	0.42
1:HB:97:PHE:HZ	1:HC:174:VAL:HG22	1.85	0.42
1:IC:91:ILE:HG12	1:IC:128:PHE:CZ	2.54	0.42
1:ID:91:ILE:HG12	1:ID:128:PHE:CZ	2.55	0.42
1:JA:121:LEU:HG	1:LE:153:ARG:CG	2.47	0.42
1:KE:78:LYS:HE3	1:LB:137:HIS:CE1	2.55	0.42
1:LD:91:ILE:HG12	1:LD:128:PHE:CZ	2.55	0.42
1:BA:128:PHE:HD1	1:BA:187:ALA:HB3	1.84	0.41
1:BD:55:ARG:NH1	1:BE:181:ARG:HG2	2.33	0.41
1:BF:37:ASP:OD1	1:BF:37:ASP:N	2.33	0.41
1:BJ:74:ARG:O	1:BJ:77:THR:HG22	2.20	0.41
1:BM:180:ALA:HB2	1:BM:188:VAL:HG21	2.03	0.41
1:AA:167:PRO:HD2	1:AE:93:MET:HE2	2.01	0.41
1:AE:88:LEU:HD11	1:AE:121:LEU:HD13	2.02	0.41
1:AL:77:THR:HG22	1:AL:79:HIS:H	1.84	0.41
1:CF:57:PRO:HB3	1:CF:93:MET:HB3	2.02	0.41
1:CG:64:THR:HB	1:CG:194:LEU:HD23	2.02	0.41
1:CG:180:ALA:HB2	1:CG:188:VAL:HG21	2.02	0.41
1:DG:91:ILE:HD13	1:DG:123:ALA:HB2	2.02	0.41
1:DG:180:ALA:HB2	1:DG:188:VAL:HG21	2.02	0.41
1:FB:88:LEU:HD11	1:FB:121:LEU:HD22	2.02	0.41
1:GF:169:SER:HA	1:GF:172:ILE:HG13	2.02	0.41
1:JF:57:PRO:HB3	1:JF:93:MET:HB3	2.02	0.41
1:JI:193:ASP:OD1	1:JI:193:ASP:N	2.53	0.41
1:JK:63:ILE:HD12	1:JK:63:ILE:HA	1.90	0.41
1:KD:91:ILE:HG12	1:KD:128:PHE:CZ	2.55	0.41
1:KD:114:MET:SD	1:KD:114:MET:N	2.84	0.41
1:LC:97:PHE:HZ	1:LD:174:VAL:HG22	1.84	0.41
1:LK:91:ILE:HD13	1:LK:123:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LL:52:LEU:HD21	1:LM:173:PRO:HB2	2.01	0.41
1:LM:91:ILE:HD13	1:LM:123:ALA:HB2	2.01	0.41
1:AB:88:LEU:HD11	1:AB:121:LEU:HD22	2.02	0.41
1:CF:40:ALA:HB2	1:CF:194:LEU:HD13	2.01	0.41
1:CO:63:ILE:HD13	1:CO:139:LEU:HB3	2.02	0.41
1:EG:83:GLY:HA2	1:EG:191:PHE:CE1	2.55	0.41
1:EG:180:ALA:HB2	1:EG:188:VAL:HG21	2.02	0.41
1:EM:77:THR:HB	1:EM:78:LYS:H	1.78	0.41
1:FD:91:ILE:HG12	1:FD:128:PHE:CZ	2.55	0.41
1:FF:57:PRO:HB3	1:FF:93:MET:HB3	2.02	0.41
1:FI:169:SER:O	1:FI:173:PRO:HD3	2.20	0.41
1:GB:97:PHE:HZ	1:GC:174:VAL:HG22	1.85	0.41
1:GD:91:ILE:HG12	1:GD:128:PHE:CZ	2.55	0.41
1:GK:150:CYS:O	1:GK:154:HIS:ND1	2.54	0.41
1:GM:180:ALA:HB2	1:GM:188:VAL:HG21	2.03	0.41
1:HD:91:ILE:HG12	1:HD:128:PHE:CZ	2.55	0.41
1:IF:52:LEU:HD22	1:IG:50:LEU:HD11	2.01	0.41
1:IG:180:ALA:HB2	1:IG:188:VAL:HG21	2.02	0.41
1:IM:78:LYS:HD2	1:IM:78:LYS:HA	1.84	0.41
1:IM:193:ASP:OD1	1:IM:193:ASP:N	2.49	0.41
1:JG:180:ALA:HB2	1:JG:188:VAL:HG21	2.02	0.41
1:JJ:74:ARG:O	1:JJ:77:THR:HG22	2.20	0.41
1:LF:40:ALA:HB2	1:LF:194:LEU:HD13	2.01	0.41
1:LI:169:SER:O	1:LI:173:PRO:HD3	2.20	0.41
1:BA:97:PHE:HZ	1:BB:174:VAL:HG22	1.84	0.41
1:BB:88:LEU:HD11	1:BB:121:LEU:HD22	2.02	0.41
1:BF:40:ALA:HB2	1:BF:194:LEU:HD13	2.01	0.41
1:BI:169:SER:O	1:BI:173:PRO:HD3	2.20	0.41
1:CA:169:SER:HA	1:CA:172:ILE:HG13	2.02	0.41
1:CB:97:PHE:HZ	1:CC:174:VAL:HG22	1.85	0.41
1:CD:88:LEU:HD11	1:CD:121:LEU:HD13	2.02	0.41
1:CD:91:ILE:HG12	1:CD:128:PHE:CZ	2.55	0.41
1:CM:180:ALA:HB2	1:CM:188:VAL:HG21	2.02	0.41
1:DB:88:LEU:HD11	1:DB:121:LEU:HD22	2.02	0.41
1:EK:150:CYS:O	1:EK:154:HIS:ND1	2.54	0.41
1:FG:180:ALA:HB2	1:FG:188:VAL:HG21	2.02	0.41
1:GE:88:LEU:HD11	1:GE:121:LEU:HD13	2.02	0.41
1:GF:57:PRO:HB3	1:GF:93:MET:HB3	2.02	0.41
1:HD:88:LEU:HD11	1:HD:121:LEU:HD13	2.01	0.41
1:HF:57:PRO:HB3	1:HF:93:MET:HB3	2.02	0.41
1:HI:169:SER:O	1:HI:173:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HL:133:SER:OG	1:HL:193:ASP:OD2	2.26	0.41
1:HM:91:ILE:HD13	1:HM:123:ALA:HB2	2.01	0.41
1:II:169:SER:O	1:II:173:PRO:HD3	2.20	0.41
1:JK:91:ILE:HD13	1:JK:123:ALA:HB2	2.02	0.41
1:KE:88:LEU:HD11	1:KE:121:LEU:HD13	2.02	0.41
1:LB:97:PHE:HZ	1:LC:174:VAL:HG22	1.85	0.41
1:LG:83:GLY:HA2	1:LG:191:PHE:CE1	2.55	0.41
1:LJ:74:ARG:O	1:LJ:77:THR:HG22	2.20	0.41
1:LM:78:LYS:HA	1:LM:78:LYS:HD2	1.84	0.41
1:AF:169:SER:HA	1:AF:172:ILE:HG13	2.02	0.41
1:AG:83:GLY:HA2	1:AG:191:PHE:CE1	2.55	0.41
1:AK:150:CYS:O	1:AK:154:HIS:ND1	2.54	0.41
1:CD:114:MET:SD	1:CD:114:MET:N	2.84	0.41
1:CF:163:LEU:HD12	1:CJ:116:ILE:HG12	2.02	0.41
1:CM:91:ILE:HD13	1:CM:123:ALA:HB2	2.01	0.41
1:DA:66:ASP:HB3	1:DA:70:GLN:HB3	2.03	0.41
1:DF:169:SER:HA	1:DF:172:ILE:HG13	2.02	0.41
1:EF:169:SER:HA	1:EF:172:ILE:HG13	2.02	0.41
1:FJ:74:ARG:O	1:FJ:77:THR:HG22	2.20	0.41
1:GB:74:ARG:HD3	1:GB:74:ARG:HA	1.90	0.41
1:GB:88:LEU:HD11	1:GB:121:LEU:HD22	2.02	0.41
1:GK:91:ILE:HD13	1:GK:123:ALA:HB2	2.02	0.41
1:HF:163:LEU:HD12	1:HJ:116:ILE:HG12	2.02	0.41
1:HF:169:SER:HA	1:HF:172:ILE:HG13	2.02	0.41
1:HJ:74:ARG:O	1:HJ:77:THR:HG22	2.20	0.41
1:IB:97:PHE:HZ	1:IC:174:VAL:HG22	1.85	0.41
1:IE:88:LEU:HD11	1:IE:121:LEU:HD13	2.02	0.41
1:IF:169:SER:HA	1:IF:172:ILE:HG13	2.02	0.41
1:IJ:74:ARG:O	1:IJ:77:THR:HG22	2.20	0.41
1:IM:180:ALA:HB2	1:IM:188:VAL:HG21	2.03	0.41
1:JC:91:ILE:HG12	1:JC:128:PHE:CZ	2.54	0.41
1:JK:150:CYS:O	1:JK:154:HIS:ND1	2.54	0.41
1:KD:45:LYS:HE3	1:KD:45:LYS:HB3	1.90	0.41
1:BG:83:GLY:HA2	1:BG:191:PHE:CE1	2.55	0.41
1:AG:91:ILE:HD13	1:AG:123:ALA:HB2	2.02	0.41
1:CG:91:ILE:HD13	1:CG:123:ALA:HB2	2.02	0.41
1:CK:150:CYS:O	1:CK:154:HIS:ND1	2.54	0.41
1:EF:163:LEU:HD12	1:EJ:116:ILE:HG12	2.02	0.41
1:EI:193:ASP:OD1	1:EI:193:ASP:N	2.53	0.41
1:FA:66:ASP:HB3	1:FA:70:GLN:HB3	2.03	0.41
1:GD:88:LEU:HD11	1:GD:121:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GD:97:PHE:HZ	1:GE:174:VAL:HG22	1.84	0.41
1:GI:169:SER:OG	1:GI:193:ASP:OD1	2.33	0.41
1:GK:87:ALA:HA	1:GK:189:ILE:HD13	2.03	0.41
1:HG:83:GLY:HA2	1:HG:191:PHE:CE1	2.55	0.41
1:HG:91:ILE:HD13	1:HG:123:ALA:HB2	2.02	0.41
1:HM:193:ASP:OD1	1:HM:193:ASP:N	2.49	0.41
1:JA:66:ASP:HB3	1:JA:70:GLN:HB3	2.03	0.41
1:JD:91:ILE:HG12	1:JD:128:PHE:CZ	2.55	0.41
1:JI:169:SER:O	1:JI:173:PRO:HD3	2.20	0.41
1:JL:52:LEU:HD21	1:JM:173:PRO:HB2	2.01	0.41
1:JM:180:ALA:HB2	1:JM:188:VAL:HG21	2.03	0.41
1:KB:88:LEU:HD11	1:KB:121:LEU:HD22	2.02	0.41
1:KE:184:ASP:OD1	1:KE:184:ASP:N	2.54	0.41
1:KF:57:PRO:HB3	1:KF:93:MET:HB3	2.02	0.41
1:KF:169:SER:HA	1:KF:172:ILE:HG13	2.02	0.41
1:LA:169:SER:HA	1:LA:172:ILE:HG13	2.03	0.41
1:LD:97:PHE:HZ	1:LE:174:VAL:HG22	1.84	0.41
1:LG:180:ALA:HB2	1:LG:188:VAL:HG21	2.02	0.41
1:LH:74:ARG:HH22	1:LH:78:LYS:HE2	1.83	0.41
1:LK:150:CYS:O	1:LK:154:HIS:ND1	2.54	0.41
1:LM:180:ALA:HB2	1:LM:188:VAL:HG21	2.02	0.41
1:LO:63:ILE:HD13	1:LO:139:LEU:HB3	2.02	0.41
1:BD:91:ILE:HG12	1:BD:128:PHE:CZ	2.55	0.41
1:BD:97:PHE:HZ	1:BE:174:VAL:HG22	1.85	0.41
1:BE:169:SER:HB2	1:BE:194:LEU:HD12	2.03	0.41
1:BO:63:ILE:HD13	1:BO:139:LEU:HB3	2.02	0.41
1:AC:78:LYS:HE3	1:AC:78:LYS:HB2	1.88	0.41
1:AF:163:LEU:HD12	1:AJ:116:ILE:HG12	2.02	0.41
1:AL:52:LEU:HD21	1:AM:173:PRO:HB2	2.01	0.41
1:CB:88:LEU:HD11	1:CB:121:LEU:HD22	2.02	0.41
1:CG:83:GLY:HA2	1:CG:191:PHE:CE1	2.55	0.41
1:DD:91:ILE:HG12	1:DD:128:PHE:CZ	2.55	0.41
1:DF:174:VAL:HG22	1:DJ:97:PHE:HZ	1.84	0.41
1:FK:87:ALA:HA	1:FK:189:ILE:HD13	2.03	0.41
1:FK:150:CYS:O	1:FK:154:HIS:ND1	2.54	0.41
1:FO:63:ILE:HD13	1:FO:139:LEU:HB3	2.02	0.41
1:GA:77:THR:H	1:GA:77:THR:HG1	1.59	0.41
1:HM:180:ALA:HB2	1:HM:188:VAL:HG21	2.02	0.41
1:ID:81:ASN:HD22	1:ID:146:GLY:HA3	1.86	0.41
1:JA:169:SER:HA	1:JA:172:ILE:HG13	2.02	0.41
1:KK:87:ALA:HA	1:KK:189:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BK:91:ILE:HD13	1:BK:123:ALA:HB2	2.02	0.41
1:AB:97:PHE:HZ	1:AC:174:VAL:HG22	1.85	0.41
1:AG:180:ALA:HB2	1:AG:188:VAL:HG21	2.02	0.41
1:CD:81:ASN:HD22	1:CD:146:GLY:HA3	1.86	0.41
1:DD:88:LEU:HD11	1:DD:121:LEU:HD13	2.02	0.41
1:DF:163:LEU:HD12	1:DJ:116:ILE:HG12	2.02	0.41
1:DK:171:GLU:OE1	1:DK:171:GLU:N	2.51	0.41
1:EE:88:LEU:HD11	1:EE:121:LEU:HD13	2.02	0.41
1:EK:91:ILE:HD13	1:EK:123:ALA:HB2	2.02	0.41
1:FE:184:ASP:OD1	1:FE:184:ASP:N	2.54	0.41
1:GH:74:ARG:NH2	1:GH:78:LYS:HE2	2.36	0.41
1:IE:81:ASN:H	1:IE:81:ASN:HD22	1.69	0.41
1:KG:64:THR:HB	1:KG:194:LEU:HD23	2.02	0.41
1:LG:64:THR:HB	1:LG:194:LEU:HD23	2.02	0.41
1:LH:74:ARG:NH2	1:LH:78:LYS:HE2	2.36	0.41
1:BG:64:THR:HB	1:BG:194:LEU:HD23	2.02	0.41
1:AE:81:ASN:HD22	1:AE:81:ASN:H	1.69	0.41
1:AK:61:ASP:OD1	1:AK:61:ASP:N	2.54	0.41
1:AK:91:ILE:HD13	1:AK:123:ALA:HB2	2.02	0.41
1:AK:97:PHE:HZ	1:AL:174:VAL:HG22	1.86	0.41
1:CH:74:ARG:NH2	1:CH:78:LYS:HE2	2.36	0.41
1:DO:63:ILE:HD13	1:DO:139:LEU:HB3	2.02	0.41
1:EG:91:ILE:HD13	1:EG:123:ALA:HB2	2.02	0.41
1:FG:83:GLY:HA2	1:FG:191:PHE:CE1	2.55	0.41
1:FH:74:ARG:NH2	1:FH:78:LYS:HE2	2.36	0.41
1:GE:169:SER:HB2	1:GE:194:LEU:HD12	2.03	0.41
1:GG:83:GLY:HA2	1:GG:191:PHE:CE1	2.55	0.41
1:HD:97:PHE:HZ	1:HE:174:VAL:HG22	1.85	0.41
1:HE:88:LEU:HD11	1:HE:121:LEU:HD13	2.02	0.41
1:HL:52:LEU:HD21	1:HM:173:PRO:HB2	2.01	0.41
1:IB:74:ARG:HD3	1:IB:74:ARG:HA	1.90	0.41
1:IB:88:LEU:HD11	1:IB:121:LEU:HD22	2.02	0.41
1:ID:88:LEU:HD11	1:ID:121:LEU:HD13	2.01	0.41
1:IK:97:PHE:HZ	1:IL:174:VAL:HG22	1.86	0.41
1:JK:61:ASP:OD1	1:JK:61:ASP:N	2.54	0.41
1:KO:63:ILE:HD13	1:KO:139:LEU:HB3	2.02	0.41
1:LH:91:ILE:HD13	1:LH:123:ALA:HB2	2.02	0.41
1:BA:180:ALA:HB2	1:BA:188:VAL:HG21	2.03	0.41
1:BJ:67:THR:HB	1:BJ:69:GLU:HG3	2.03	0.41
1:AE:78:LYS:HE3	1:CB:137:HIS:CE1	2.56	0.41
1:AE:184:ASP:OD1	1:AE:184:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:74:ARG:O	1:AJ:77:THR:HG22	2.20	0.41
1:AK:87:ALA:HA	1:AK:189:ILE:HD13	2.03	0.41
1:CE:81:ASN:HD22	1:CE:81:ASN:H	1.69	0.41
1:CG:114:MET:HB2	1:CH:158:GLU:HG2	2.03	0.41
1:CK:61:ASP:OD1	1:CK:61:ASP:N	2.54	0.41
1:CK:87:ALA:HA	1:CK:189:ILE:HD13	2.03	0.41
1:CK:97:PHE:HZ	1:CL:174:VAL:HG22	1.86	0.41
1:DE:184:ASP:OD1	1:DE:184:ASP:N	2.54	0.41
1:DG:83:GLY:HA2	1:DG:191:PHE:CE1	2.55	0.41
1:DH:74:ARG:NH2	1:DH:78:LYS:HE2	2.36	0.41
1:DK:91:ILE:HD13	1:DK:123:ALA:HB2	2.02	0.41
1:EB:97:PHE:HZ	1:EC:174:VAL:HG22	1.85	0.41
1:EE:169:SER:HB2	1:EE:194:LEU:HD12	2.03	0.41
1:EG:114:MET:HB2	1:EH:158:GLU:HG2	2.03	0.41
1:EJ:74:ARG:O	1:EJ:77:THR:HG22	2.20	0.41
1:EK:171:GLU:OE1	1:EK:171:GLU:N	2.51	0.41
1:FA:73:GLU:O	1:FA:77:THR:HG23	2.21	0.41
1:FC:78:LYS:HE3	1:FC:78:LYS:HB2	1.88	0.41
1:FE:81:ASN:H	1:FE:81:ASN:HD22	1.69	0.41
1:FF:40:ALA:HB2	1:FF:194:LEU:HD13	2.01	0.41
1:FH:91:ILE:HD13	1:FH:123:ALA:HB2	2.02	0.41
1:GJ:67:THR:HB	1:GJ:69:GLU:HG3	2.03	0.41
1:HC:58:VAL:HG23	1:HC:188:VAL:HB	2.03	0.41
1:HE:81:ASN:HD22	1:HE:81:ASN:H	1.69	0.41
1:HK:91:ILE:HD13	1:HK:123:ALA:HB2	2.02	0.41
1:HK:150:CYS:O	1:HK:154:HIS:ND1	2.53	0.41
1:IA:66:ASP:HB3	1:IA:70:GLN:HB3	2.03	0.41
1:ID:55:ARG:NH1	1:IE:181:ARG:HG2	2.33	0.41
1:IG:91:ILE:HD13	1:IG:123:ALA:HB2	2.02	0.41
1:IK:150:CYS:O	1:IK:154:HIS:ND1	2.54	0.41
1:IK:166:VAL:HB	1:IK:171:GLU:HB2	2.03	0.41
1:IL:133:SER:OG	1:IL:193:ASP:OD2	2.26	0.41
1:JB:88:LEU:HD11	1:JB:121:LEU:HD22	2.02	0.41
1:JC:97:PHE:HZ	1:JD:174:VAL:HG22	1.84	0.41
1:JE:88:LEU:HD11	1:JE:121:LEU:HD13	2.02	0.41
1:JG:83:GLY:HA2	1:JG:191:PHE:CE1	2.55	0.41
1:JJ:67:THR:HB	1:JJ:69:GLU:HG3	2.03	0.41
1:KC:78:LYS:HE3	1:KC:78:LYS:HB2	1.88	0.41
1:KG:83:GLY:HA2	1:KG:191:PHE:CE1	2.55	0.41
1:KK:150:CYS:O	1:KK:154:HIS:ND1	2.54	0.41
1:LF:163:LEU:HD12	1:LJ:116:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:73:GLU:O	1:BA:77:THR:HG23	2.21	0.41
1:BC:58:VAL:HG23	1:BC:188:VAL:HB	2.03	0.41
1:BF:169:SER:HA	1:BF:172:ILE:HG13	2.02	0.41
1:BK:87:ALA:HA	1:BK:189:ILE:HD13	2.03	0.41
1:AA:169:SER:HA	1:AA:172:ILE:HG13	2.03	0.41
1:AG:114:MET:HB2	1:AH:158:GLU:HG2	2.03	0.41
1:AM:151:ILE:HG22	1:AM:156:GLY:HA3	2.03	0.41
1:DE:88:LEU:HD11	1:DE:121:LEU:HD13	2.02	0.41
1:EA:180:ALA:HB2	1:EA:188:VAL:HG21	2.03	0.41
1:ED:97:PHE:HZ	1:EE:174:VAL:HG22	1.85	0.41
1:EH:74:ARG:NH2	1:EH:78:LYS:HE2	2.36	0.41
1:EK:87:ALA:HA	1:EK:189:ILE:HD13	2.03	0.41
1:EK:166:VAL:HB	1:EK:171:GLU:HB2	2.03	0.41
1:FF:169:SER:HA	1:FF:172:ILE:HG13	2.02	0.41
1:FG:84:TRP:HZ3	1:FG:88:LEU:HD22	1.86	0.41
1:GA:66:ASP:HB3	1:GA:70:GLN:HB3	2.03	0.41
1:GA:169:SER:HA	1:GA:172:ILE:HG13	2.02	0.41
1:GE:81:ASN:HD22	1:GE:81:ASN:H	1.69	0.41
1:HD:45:LYS:HE3	1:HD:45:LYS:HB3	1.90	0.41
1:HG:114:MET:HB2	1:HH:158:GLU:HG2	2.03	0.41
1:HK:61:ASP:OD1	1:HK:61:ASP:N	2.54	0.41
1:IF:174:VAL:HG22	1:IJ:97:PHE:HZ	1.84	0.41
1:IG:83:GLY:HA2	1:IG:191:PHE:CE1	2.55	0.41
1:IG:84:TRP:HZ3	1:IG:88:LEU:HD22	1.86	0.41
1:JH:74:ARG:NH2	1:JH:78:LYS:HE2	2.36	0.41
1:JK:87:ALA:HA	1:JK:189:ILE:HD13	2.03	0.41
1:JM:151:ILE:HG22	1:JM:156:GLY:HA3	2.03	0.41
1:KA:66:ASP:HB3	1:KA:70:GLN:HB3	2.03	0.41
1:KA:169:SER:HA	1:KA:172:ILE:HG13	2.02	0.41
1:KD:81:ASN:HD22	1:KD:146:GLY:HA3	1.86	0.41
1:LA:66:ASP:HB3	1:LA:70:GLN:HB3	2.03	0.41
1:LD:81:ASN:HD22	1:LD:146:GLY:HA3	1.86	0.41
1:LJ:67:THR:HB	1:LJ:69:GLU:HG3	2.03	0.41
1:BG:114:MET:HB2	1:BH:158:GLU:HG2	2.03	0.40
1:BG:180:ALA:HB2	1:BG:188:VAL:HG21	2.02	0.40
1:BK:150:CYS:O	1:BK:154:HIS:ND1	2.54	0.40
1:BK:166:VAL:HB	1:BK:171:GLU:HB2	2.03	0.40
1:AI:169:SER:O	1:AI:173:PRO:HD3	2.20	0.40
1:CB:91:ILE:HG12	1:CB:128:PHE:CZ	2.57	0.40
1:CE:184:ASP:OD1	1:CE:184:ASP:N	2.54	0.40
1:CG:84:TRP:HZ3	1:CG:88:LEU:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:169:SER:HA	1:DA:172:ILE:HG13	2.02	0.40
1:DD:77:THR:OG1	1:DD:78:LYS:N	2.54	0.40
1:ED:88:LEU:HD11	1:ED:121:LEU:HD13	2.02	0.40
1:EE:81:ASN:H	1:EE:81:ASN:HD22	1.69	0.40
1:EG:84:TRP:HZ3	1:EG:88:LEU:HD22	1.86	0.40
1:GG:180:ALA:HB2	1:GG:188:VAL:HG21	2.02	0.40
1:HA:180:ALA:HB2	1:HA:188:VAL:HG21	2.03	0.40
1:HG:64:THR:HB	1:HG:194:LEU:HD23	2.02	0.40
1:JD:45:LYS:HE3	1:JD:45:LYS:HB3	1.90	0.40
1:JG:91:ILE:HD13	1:JG:123:ALA:HB2	2.02	0.40
1:KE:81:ASN:HD22	1:KE:81:ASN:H	1.69	0.40
1:KM:180:ALA:HB2	1:KM:188:VAL:HG21	2.03	0.40
1:LF:57:PRO:HB3	1:LF:93:MET:HB3	2.02	0.40
1:LF:169:SER:HA	1:LF:172:ILE:HG13	2.02	0.40
1:LI:180:ALA:HB2	1:LI:188:VAL:HG21	2.04	0.40
1:LL:181:ARG:HD2	1:LL:181:ARG:HA	1.90	0.40
1:BE:88:LEU:HD11	1:BE:121:LEU:HD13	2.02	0.40
1:BH:74:ARG:NH2	1:BH:78:LYS:HE2	2.36	0.40
1:BH:91:ILE:HG12	1:BH:128:PHE:CZ	2.57	0.40
1:AA:180:ALA:HB2	1:AA:188:VAL:HG21	2.03	0.40
1:AG:84:TRP:HZ3	1:AG:88:LEU:HD22	1.86	0.40
1:CC:58:VAL:HG23	1:CC:188:VAL:HB	2.03	0.40
1:CF:50:LEU:HD11	1:CJ:52:LEU:HD22	2.04	0.40
1:CH:180:ALA:HB2	1:CH:188:VAL:HG21	2.04	0.40
1:CK:166:VAL:HB	1:CK:171:GLU:HB2	2.03	0.40
1:DB:91:ILE:HG12	1:DB:128:PHE:CZ	2.57	0.40
1:DG:84:TRP:HZ3	1:DG:88:LEU:HD22	1.86	0.40
1:DK:166:VAL:HB	1:DK:171:GLU:HB2	2.03	0.40
1:EG:64:THR:HB	1:EG:194:LEU:HD23	2.02	0.40
1:EJ:67:THR:HB	1:EJ:69:GLU:HG3	2.03	0.40
1:FE:88:LEU:HD11	1:FE:121:LEU:HD13	2.02	0.40
1:GD:77:THR:OG1	1:GD:78:LYS:N	2.54	0.40
1:GJ:74:ARG:O	1:GJ:77:THR:HG22	2.20	0.40
1:GL:181:ARG:HD2	1:GL:181:ARG:HA	1.90	0.40
1:HA:169:SER:HA	1:HA:172:ILE:HG13	2.03	0.40
1:II:169:SER:OG	1:II:193:ASP:OD1	2.33	0.40
1:JA:73:GLU:O	1:JA:77:THR:HG23	2.21	0.40
1:JE:169:SER:HB2	1:JE:194:LEU:HD12	2.03	0.40
1:JE:184:ASP:OD1	1:JE:184:ASP:N	2.54	0.40
1:KB:91:ILE:HG12	1:KB:128:PHE:CZ	2.57	0.40
1:LA:77:THR:H	1:LA:77:THR:HG1	1.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:180:ALA:HB2	1:LA:188:VAL:HG21	2.03	0.40
1:LH:91:ILE:HG12	1:LH:128:PHE:CZ	2.57	0.40
1:LM:151:ILE:HG22	1:LM:156:GLY:HA3	2.03	0.40
1:BB:91:ILE:HG12	1:BB:128:PHE:CZ	2.57	0.40
1:BG:84:TRP:HZ3	1:BG:88:LEU:HD22	1.87	0.40
1:AD:81:ASN:HD22	1:AD:146:GLY:HA3	1.86	0.40
1:AH:74:ARG:NH2	1:AH:78:LYS:HE2	2.36	0.40
1:AH:91:ILE:HD13	1:AH:123:ALA:HB2	2.02	0.40
1:EA:66:ASP:HB3	1:EA:70:GLN:HB3	2.03	0.40
1:ED:77:THR:OG1	1:ED:78:LYS:N	2.54	0.40
1:EK:97:PHE:HZ	1:EL:174:VAL:HG22	1.86	0.40
1:EM:180:ALA:HB2	1:EM:188:VAL:HG21	2.03	0.40
1:FA:169:SER:HA	1:FA:172:ILE:HG13	2.03	0.40
1:FC:58:VAL:HG23	1:FC:188:VAL:HB	2.03	0.40
1:FD:77:THR:OG1	1:FD:78:LYS:N	2.54	0.40
1:FH:91:ILE:HG12	1:FH:128:PHE:CZ	2.57	0.40
1:GK:97:PHE:HZ	1:GL:174:VAL:HG22	1.86	0.40
1:HH:91:ILE:HG12	1:HH:128:PHE:CZ	2.57	0.40
1:HJ:67:THR:HB	1:HJ:69:GLU:HG3	2.03	0.40
1:IO:63:ILE:HD13	1:IO:139:LEU:HB3	2.02	0.40
1:KE:169:SER:HB2	1:KE:194:LEU:HD12	2.03	0.40
1:KL:59:THR:OG1	1:KL:189:ILE:HG23	2.22	0.40
1:LA:73:GLU:O	1:LA:77:THR:HG23	2.21	0.40
1:LE:81:ASN:H	1:LE:81:ASN:HD22	1.69	0.40
1:LE:169:SER:HB2	1:LE:194:LEU:HD12	2.03	0.40
1:BE:81:ASN:H	1:BE:81:ASN:HD22	1.69	0.40
1:BF:73:GLU:O	1:BF:77:THR:HG23	2.22	0.40
1:BI:169:SER:OG	1:BI:193:ASP:OD1	2.33	0.40
1:BI:180:ALA:HB2	1:BI:188:VAL:HG21	2.04	0.40
1:AD:77:THR:OG1	1:AD:78:LYS:N	2.54	0.40
1:AI:87:ALA:HA	1:AI:189:ILE:HD13	2.04	0.40
1:DF:134:ARG:NH2	1:DJ:119:GLY:H	2.20	0.40
1:DH:91:ILE:HD13	1:DH:123:ALA:HB2	2.02	0.40
1:EB:91:ILE:HG12	1:EB:128:PHE:CZ	2.57	0.40
1:EC:58:VAL:HG23	1:EC:188:VAL:HB	2.03	0.40
1:ED:81:ASN:HD22	1:ED:146:GLY:HA3	1.86	0.40
1:EE:184:ASP:OD1	1:EE:184:ASP:N	2.54	0.40
1:EH:91:ILE:HG12	1:EH:128:PHE:CZ	2.57	0.40
1:EK:61:ASP:OD1	1:EK:61:ASP:N	2.54	0.40
1:EO:63:ILE:HD13	1:EO:139:LEU:HB3	2.02	0.40
1:FD:81:ASN:HD22	1:FD:146:GLY:HA3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FF:73:GLU:O	1:FF:77:THR:HG23	2.22	0.40
1:GA:73:GLU:O	1:GA:77:THR:HG23	2.21	0.40
1:GC:58:VAL:HG23	1:GC:188:VAL:HB	2.03	0.40
1:GM:56:LYS:HA	1:GM:57:PRO:HD3	1.96	0.40
1:HK:171:GLU:OE1	1:HK:171:GLU:N	2.51	0.40
1:ID:77:THR:OG1	1:ID:78:LYS:N	2.54	0.40
1:IE:169:SER:HB2	1:IE:194:LEU:HD12	2.03	0.40
1:IF:134:ARG:NH2	1:IJ:119:GLY:H	2.20	0.40
1:IK:61:ASP:OD1	1:IK:61:ASP:N	2.54	0.40
1:IK:87:ALA:HA	1:IK:189:ILE:HD13	2.03	0.40
1:JG:84:TRP:HZ3	1:JG:88:LEU:HD22	1.86	0.40
1:JH:91:ILE:HD13	1:JH:123:ALA:HB2	2.02	0.40
1:JO:63:ILE:HD13	1:JO:139:LEU:HB3	2.02	0.40
1:KD:77:THR:OG1	1:KD:78:LYS:N	2.54	0.40
1:KF:37:ASP:OD1	1:KF:37:ASP:N	2.33	0.40
1:KH:91:ILE:HG12	1:KH:128:PHE:CZ	2.57	0.40
1:LE:184:ASP:OD1	1:LE:184:ASP:N	2.54	0.40
1:BK:61:ASP:OD1	1:BK:61:ASP:N	2.54	0.40
1:BK:97:PHE:HZ	1:BL:174:VAL:HG22	1.86	0.40
1:AB:91:ILE:HG12	1:AB:128:PHE:CZ	2.57	0.40
1:AH:91:ILE:HG12	1:AH:128:PHE:CZ	2.57	0.40
1:AM:180:ALA:HB2	1:AM:188:VAL:HG21	2.03	0.40
1:CE:88:LEU:HD11	1:CE:121:LEU:HD13	2.02	0.40
1:CH:91:ILE:HG12	1:CH:128:PHE:CZ	2.57	0.40
1:CL:59:THR:OG1	1:CL:189:ILE:HG23	2.22	0.40
1:DD:179:LEU:HD23	1:DD:179:LEU:HA	1.95	0.40
1:DF:73:GLU:O	1:DF:77:THR:HG23	2.22	0.40
1:DG:64:THR:HB	1:DG:194:LEU:HD23	2.02	0.40
1:DJ:67:THR:HB	1:DJ:69:GLU:HG3	2.03	0.40
1:EM:151:ILE:HG22	1:EM:156:GLY:HA3	2.03	0.40
1:FJ:78:LYS:HB2	1:FJ:78:LYS:HE3	1.81	0.40
1:FL:59:THR:OG1	1:FL:189:ILE:HG23	2.22	0.40
1:GE:184:ASP:OD1	1:GE:184:ASP:N	2.54	0.40
1:GG:64:THR:HB	1:GG:194:LEU:HD23	2.02	0.40
1:GH:91:ILE:HG12	1:GH:128:PHE:CZ	2.57	0.40
1:HG:84:TRP:HZ3	1:HG:88:LEU:HD22	1.86	0.40
1:HI:87:ALA:HA	1:HI:189:ILE:HD13	2.04	0.40
1:HO:63:ILE:HD13	1:HO:139:LEU:HB3	2.02	0.40
1:IA:169:SER:HA	1:IA:172:ILE:HG13	2.02	0.40
1:IG:64:THR:HB	1:IG:194:LEU:HD23	2.02	0.40
1:JD:77:THR:OG1	1:JD:78:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JE:81:ASN:H	1:JE:81:ASN:HD22	1.69	0.40
1:JG:64:THR:HB	1:JG:194:LEU:HD23	2.02	0.40
1:KA:73:GLU:O	1:KA:77:THR:HG23	2.21	0.40
1:KF:134:ARG:NH2	1:KJ:119:GLY:H	2.20	0.40
1:KG:91:ILE:HD13	1:KG:123:ALA:HB2	2.02	0.40
1:LB:88:LEU:HD11	1:LB:121:LEU:HD22	2.02	0.40
1:LE:88:LEU:HD11	1:LE:121:LEU:HD13	2.02	0.40
1:LJ:56:LYS:HA	1:LJ:57:PRO:HD3	1.97	0.40
1:LL:59:THR:OG1	1:LL:189:ILE:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	AB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	AC	148/197 (75%)	147 (99%)	1 (1%)	0	100	100
1	AD	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	AE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	AF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	AG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	AH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	AI	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	AJ	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	AK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	AL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	AM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100
1	AO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100
1	BA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	BB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	BC	148/197 (75%)	147 (99%)	1 (1%)	0	100	100
1	BD	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	BE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	BF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	BG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	BH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	BI	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	BJ	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	BK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	BL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	BM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100
1	BN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100
1	BO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100
1	CA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	CB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	CC	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	CD	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	CE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	CF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	CG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	CH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	CI	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	CJ	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	CK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	CL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	CM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100
1	CN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100
1	DA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	DB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	DC	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	DD	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	DE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	DF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	DG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	DH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	DI	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	DJ	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	DK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	DL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	DM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100
1	DN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100
1	DO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100
1	EA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	EB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	EC	148/197 (75%)	147 (99%)	1 (1%)	0	100	100
1	ED	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	EE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	EF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	EG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	EH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	EI	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	EJ	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	EK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	EL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	EM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100
1	EN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100
1	EO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	FB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	FC	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	FD	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	FE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	FF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	FG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	FH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	FI	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	FJ	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	FK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	FL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	FM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100
1	FN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100
1	FO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100
1	GA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	GB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	GC	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	GD	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	GE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	GF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	GG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	GH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	GI	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	GJ	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	GK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	GL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	GM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100
1	GN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100
1	GO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100
1	HA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	HC	148/197 (75%)	147 (99%)	1 (1%)	0	100	100
1	HD	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	HE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	HF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	HG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	HH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	HI	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	HJ	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	HK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	HL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	HM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100
1	HN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100
1	HO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100
1	IA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	IB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	IC	148/197 (75%)	147 (99%)	1 (1%)	0	100	100
1	ID	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	IE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	IF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	IG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	IH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	II	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	IJ	145/197 (74%)	142 (98%)	3 (2%)	0	100	100
1	IK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	IL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	IM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100
1	IN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100
1	IO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100
1	JA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	JB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JC	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	JD	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	JE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	JF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	JG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	JH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	JI	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	JJ	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	JK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	JL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	JM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100
1	JN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100
1	JO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100
1	KA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	KB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	KC	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	KD	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	KE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	KF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	KG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	KH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	KI	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	KJ	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	KK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	KL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	KM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100
1	KN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100
1	KO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100
1	LA	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	LB	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	LC	148/197 (75%)	147 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LD	145/197 (74%)	140 (97%)	5 (3%)	0	100	100
1	LE	146/197 (74%)	143 (98%)	3 (2%)	0	100	100
1	LF	144/197 (73%)	143 (99%)	1 (1%)	0	100	100
1	LG	145/197 (74%)	144 (99%)	1 (1%)	0	100	100
1	LH	143/197 (73%)	139 (97%)	4 (3%)	0	100	100
1	LI	148/197 (75%)	146 (99%)	2 (1%)	0	100	100
1	LJ	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	LK	146/197 (74%)	142 (97%)	4 (3%)	0	100	100
1	LL	147/197 (75%)	145 (99%)	2 (1%)	0	100	100
1	LM	144/197 (73%)	139 (96%)	5 (4%)	0	100	100
1	LN	144/197 (73%)	142 (99%)	2 (1%)	0	100	100
1	LO	145/197 (74%)	143 (99%)	2 (1%)	0	100	100
All	All	26184/35460 (74%)	25711 (98%)	473 (2%)	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	AA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	AB	115/148 (78%)	115 (100%)	0	100	100
1	AC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	AD	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	AE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	AF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	AG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	AH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	AI	117/148 (79%)	115 (98%)	2 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AJ	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	AK	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	AL	117/148 (79%)	112 (96%)	5 (4%)	26	48
1	AM	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	AN	115/148 (78%)	109 (95%)	6 (5%)	21	43
1	AO	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	BA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	BB	115/148 (78%)	115 (100%)	0	100	100
1	BC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	BD	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	BE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	BF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	BG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	BH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	BI	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	BJ	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	BK	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	BL	117/148 (79%)	112 (96%)	5 (4%)	26	48
1	BM	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	BN	115/148 (78%)	109 (95%)	6 (5%)	21	43
1	BO	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	CA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	CB	115/148 (78%)	115 (100%)	0	100	100
1	CC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	CD	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	CE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	CF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	CG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	CH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	CI	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	CJ	116/148 (78%)	113 (97%)	3 (3%)	40	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CK	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	CL	117/148 (79%)	112 (96%)	5 (4%)	26	48
1	CM	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	CN	115/148 (78%)	109 (95%)	6 (5%)	21	43
1	CO	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	DA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	DB	115/148 (78%)	115 (100%)	0	100	100
1	DC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	DD	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	DE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	DF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	DG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	DH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	DI	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	DJ	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	DK	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	DL	117/148 (79%)	112 (96%)	5 (4%)	26	48
1	DM	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	DN	115/148 (78%)	109 (95%)	6 (5%)	21	43
1	DO	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	EA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	EB	115/148 (78%)	115 (100%)	0	100	100
1	EC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	ED	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	EE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	EF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	EG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	EH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	EI	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	EJ	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	EK	117/148 (79%)	115 (98%)	2 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EL	117/148 (79%)	112 (96%)	5 (4%)	26	48
1	EM	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	EN	115/148 (78%)	109 (95%)	6 (5%)	21	43
1	EO	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	FA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	FB	115/148 (78%)	115 (100%)	0	100	100
1	FC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	FD	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	FE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	FF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	FG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	FH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	FI	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	FJ	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	FK	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	FL	117/148 (79%)	112 (96%)	5 (4%)	26	48
1	FM	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	FN	115/148 (78%)	109 (95%)	6 (5%)	21	43
1	FO	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	GA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	GB	115/148 (78%)	115 (100%)	0	100	100
1	GC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	GD	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	GE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	GF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	GG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	GH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	GI	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	GJ	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	GK	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	GL	117/148 (79%)	112 (96%)	5 (4%)	26	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GM	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	GN	115/148 (78%)	109 (95%)	6 (5%)	21	43
1	GO	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	HA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	HB	115/148 (78%)	115 (100%)	0	100	100
1	HC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	HD	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	HE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	HF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	HG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	HH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	HI	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	HJ	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	HK	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	HL	117/148 (79%)	112 (96%)	5 (4%)	26	48
1	HM	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	HN	115/148 (78%)	109 (95%)	6 (5%)	21	43
1	HO	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	IA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	IB	115/148 (78%)	115 (100%)	0	100	100
1	IC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	ID	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	IE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	IF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	IG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	IH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	II	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	IJ	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	IK	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	IL	117/148 (79%)	112 (96%)	5 (4%)	26	48
1	IM	114/148 (77%)	110 (96%)	4 (4%)	32	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IN	115/148 (78%)	109 (95%)	6 (5%)	21	43
1	IO	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	JA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	JB	115/148 (78%)	115 (100%)	0	100	100
1	JC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	JD	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	JE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	JF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	JG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	JH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	JI	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	JJ	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	JK	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	JL	117/148 (79%)	112 (96%)	5 (4%)	26	48
1	JM	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	JN	115/148 (78%)	109 (95%)	6 (5%)	21	43
1	JO	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	KA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	KB	115/148 (78%)	115 (100%)	0	100	100
1	KC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	KD	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	KE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	KF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	KG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	KH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	KI	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	KJ	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	KK	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	KL	117/148 (79%)	112 (96%)	5 (4%)	26	48
1	KM	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	KN	115/148 (78%)	109 (95%)	6 (5%)	21	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	KO	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	LA	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	LB	115/148 (78%)	115 (100%)	0	100	100
1	LC	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	LD	116/148 (78%)	111 (96%)	5 (4%)	26	48
1	LE	116/148 (78%)	112 (97%)	4 (3%)	32	54
1	LF	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	LG	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	LH	114/148 (77%)	111 (97%)	3 (3%)	40	60
1	LI	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	LJ	116/148 (78%)	113 (97%)	3 (3%)	40	60
1	LK	117/148 (79%)	115 (98%)	2 (2%)	53	67
1	LL	117/148 (79%)	112 (96%)	5 (4%)	26	48
1	LM	114/148 (77%)	110 (96%)	4 (4%)	32	53
1	LN	115/148 (78%)	109 (95%)	6 (5%)	21	43
1	LO	116/148 (78%)	113 (97%)	3 (3%)	40	60
All	All	20844/26640 (78%)	20268 (97%)	576 (3%)	38	59

All (576) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BA	77	THR
1	BA	137	HIS
1	BC	64	THR
1	BC	78	LYS
1	BD	62	ILE
1	BD	63	ILE
1	BD	93	MET
1	BD	114	MET
1	BD	189	ILE
1	BE	63	ILE
1	BE	82	LYS
1	BE	84	TRP
1	BE	100	LEU
1	BF	37	ASP
1	BF	62	ILE

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Mol	Chain	Res	Type
1	BF	120	LYS
1	BF	122	THR
1	BG	59	THR
1	BG	100	LEU
1	BG	171	GLU
1	BH	63	ILE
1	BH	64	THR
1	BH	78	LYS
1	BI	77	THR
1	BI	191	PHE
1	BJ	62	ILE
1	BJ	114	MET
1	BJ	174	VAL
1	BK	62	ILE
1	BK	67	THR
1	BL	64	THR
1	BL	66	ASP
1	BL	69	GLU
1	BL	74	ARG
1	BL	193	ASP
1	BM	77	THR
1	BM	81	ASN
1	BM	179	LEU
1	BM	191	PHE
1	BN	38	TYR
1	BN	73	GLU
1	BN	100	LEU
1	BN	115	GLU
1	BN	191	PHE
1	BN	194	LEU
1	BO	67	THR
1	BO	78	LYS
1	BO	97	PHE
1	AA	77	THR
1	AA	137	HIS
1	AC	64	THR
1	AC	78	LYS
1	AD	62	ILE
1	AD	63	ILE
1	AD	93	MET
1	AD	114	MET
1	AD	189	ILE

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Mol	Chain	Res	Type
1	AE	63	ILE
1	AE	82	LYS
1	AE	84	TRP
1	AE	100	LEU
1	AF	37	ASP
1	AF	62	ILE
1	AF	120	LYS
1	AF	122	THR
1	AG	59	THR
1	AG	100	LEU
1	AG	171	GLU
1	AH	63	ILE
1	AH	64	THR
1	AH	78	LYS
1	AI	77	THR
1	AI	191	PHE
1	AJ	62	ILE
1	AJ	114	MET
1	AJ	174	VAL
1	AK	62	ILE
1	AK	67	THR
1	AL	64	THR
1	AL	66	ASP
1	AL	69	GLU
1	AL	74	ARG
1	AL	193	ASP
1	AM	77	THR
1	AM	81	ASN
1	AM	179	LEU
1	AM	191	PHE
1	AN	38	TYR
1	AN	73	GLU
1	AN	100	LEU
1	AN	115	GLU
1	AN	191	PHE
1	AN	194	LEU
1	AO	67	THR
1	AO	78	LYS
1	AO	97	PHE
1	CA	77	THR
1	CA	137	HIS
1	CC	64	THR

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Mol	Chain	Res	Type
1	CC	78	LYS
1	CD	62	ILE
1	CD	63	ILE
1	CD	93	MET
1	CD	114	MET
1	CD	189	ILE
1	CE	63	ILE
1	CE	82	LYS
1	CE	84	TRP
1	CE	100	LEU
1	CF	37	ASP
1	CF	62	ILE
1	CF	120	LYS
1	CF	122	THR
1	CG	59	THR
1	CG	100	LEU
1	CG	171	GLU
1	CH	63	ILE
1	CH	64	THR
1	CH	78	LYS
1	CI	77	THR
1	CI	191	PHE
1	CJ	62	ILE
1	CJ	114	MET
1	CJ	174	VAL
1	CK	62	ILE
1	CK	67	THR
1	CL	64	THR
1	CL	66	ASP
1	CL	69	GLU
1	CL	74	ARG
1	CL	193	ASP
1	CM	77	THR
1	CM	81	ASN
1	CM	179	LEU
1	CM	191	PHE
1	CN	38	TYR
1	CN	73	GLU
1	CN	100	LEU
1	CN	115	GLU
1	CN	191	PHE
1	CN	194	LEU

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Mol	Chain	Res	Type
1	CO	67	THR
1	CO	78	LYS
1	CO	97	PHE
1	DA	77	THR
1	DA	137	HIS
1	DC	64	THR
1	DC	78	LYS
1	DD	62	ILE
1	DD	63	ILE
1	DD	93	MET
1	DD	114	MET
1	DD	189	ILE
1	DE	63	ILE
1	DE	82	LYS
1	DE	84	TRP
1	DE	100	LEU
1	DF	37	ASP
1	DF	62	ILE
1	DF	120	LYS
1	DF	122	THR
1	DG	59	THR
1	DG	100	LEU
1	DG	171	GLU
1	DH	63	ILE
1	DH	64	THR
1	DH	78	LYS
1	DI	77	THR
1	DI	191	PHE
1	DJ	62	ILE
1	DJ	114	MET
1	DJ	174	VAL
1	DK	62	ILE
1	DK	67	THR
1	DL	64	THR
1	DL	66	ASP
1	DL	69	GLU
1	DL	74	ARG
1	DL	193	ASP
1	DM	77	THR
1	DM	81	ASN
1	DM	179	LEU
1	DM	191	PHE

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Mol	Chain	Res	Type
1	DN	38	TYR
1	DN	73	GLU
1	DN	100	LEU
1	DN	115	GLU
1	DN	191	PHE
1	DN	194	LEU
1	DO	67	THR
1	DO	78	LYS
1	DO	97	PHE
1	EA	77	THR
1	EA	137	HIS
1	EC	64	THR
1	EC	78	LYS
1	ED	62	ILE
1	ED	63	ILE
1	ED	93	MET
1	ED	114	MET
1	ED	189	ILE
1	EE	63	ILE
1	EE	82	LYS
1	EE	84	TRP
1	EE	100	LEU
1	EF	37	ASP
1	EF	62	ILE
1	EF	120	LYS
1	EF	122	THR
1	EG	59	THR
1	EG	100	LEU
1	EG	171	GLU
1	EH	63	ILE
1	EH	64	THR
1	EH	78	LYS
1	EI	77	THR
1	EI	191	PHE
1	EJ	62	ILE
1	EJ	114	MET
1	EJ	174	VAL
1	EK	62	ILE
1	EK	67	THR
1	EL	64	THR
1	EL	66	ASP
1	EL	69	GLU

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Mol	Chain	Res	Type
1	EL	74	ARG
1	EL	193	ASP
1	EM	77	THR
1	EM	81	ASN
1	EM	179	LEU
1	EM	191	PHE
1	EN	38	TYR
1	EN	73	GLU
1	EN	100	LEU
1	EN	115	GLU
1	EN	191	PHE
1	EN	194	LEU
1	EO	67	THR
1	EO	78	LYS
1	EO	97	PHE
1	FA	77	THR
1	FA	137	HIS
1	FC	64	THR
1	FC	78	LYS
1	FD	62	ILE
1	FD	63	ILE
1	FD	93	MET
1	FD	114	MET
1	FD	189	ILE
1	FE	63	ILE
1	FE	82	LYS
1	FE	84	TRP
1	FE	100	LEU
1	FF	37	ASP
1	FF	62	ILE
1	FF	120	LYS
1	FF	122	THR
1	FG	59	THR
1	FG	100	LEU
1	FG	171	GLU
1	FH	63	ILE
1	FH	64	THR
1	FH	78	LYS
1	FI	77	THR
1	FI	191	PHE
1	FJ	62	ILE
1	FJ	114	MET

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Mol	Chain	Res	Type
1	FJ	174	VAL
1	FK	62	ILE
1	FK	67	THR
1	FL	64	THR
1	FL	66	ASP
1	FL	69	GLU
1	FL	74	ARG
1	FL	193	ASP
1	FM	77	THR
1	FM	81	ASN
1	FM	179	LEU
1	FM	191	PHE
1	FN	38	TYR
1	FN	73	GLU
1	FN	100	LEU
1	FN	115	GLU
1	FN	191	PHE
1	FN	194	LEU
1	FO	67	THR
1	FO	78	LYS
1	FO	97	PHE
1	GA	77	THR
1	GA	137	HIS
1	GC	64	THR
1	GC	78	LYS
1	GD	62	ILE
1	GD	63	ILE
1	GD	93	MET
1	GD	114	MET
1	GD	189	ILE
1	GE	63	ILE
1	GE	82	LYS
1	GE	84	TRP
1	GE	100	LEU
1	GF	37	ASP
1	GF	62	ILE
1	GF	120	LYS
1	GF	122	THR
1	GG	59	THR
1	GG	100	LEU
1	GG	171	GLU
1	GH	63	ILE

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Mol	Chain	Res	Type
1	GH	64	THR
1	GH	78	LYS
1	GI	77	THR
1	GI	191	PHE
1	GJ	62	ILE
1	GJ	114	MET
1	GJ	174	VAL
1	GK	62	ILE
1	GK	67	THR
1	GL	64	THR
1	GL	66	ASP
1	GL	69	GLU
1	GL	74	ARG
1	GL	193	ASP
1	GM	77	THR
1	GM	81	ASN
1	GM	179	LEU
1	GM	191	PHE
1	GN	38	TYR
1	GN	73	GLU
1	GN	100	LEU
1	GN	115	GLU
1	GN	191	PHE
1	GN	194	LEU
1	GO	67	THR
1	GO	78	LYS
1	GO	97	PHE
1	HA	77	THR
1	HA	137	HIS
1	HC	64	THR
1	HC	78	LYS
1	HD	62	ILE
1	HD	63	ILE
1	HD	93	MET
1	HD	114	MET
1	HD	189	ILE
1	HE	63	ILE
1	HE	82	LYS
1	HE	84	TRP
1	HE	100	LEU
1	HF	37	ASP
1	HF	62	ILE

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Mol	Chain	Res	Type
1	HF	120	LYS
1	HF	122	THR
1	HG	59	THR
1	HG	100	LEU
1	HG	171	GLU
1	HH	63	ILE
1	HH	64	THR
1	HH	78	LYS
1	HI	77	THR
1	HI	191	PHE
1	HJ	62	ILE
1	HJ	114	MET
1	HJ	174	VAL
1	HK	62	ILE
1	HK	67	THR
1	HL	64	THR
1	HL	66	ASP
1	HL	69	GLU
1	HL	74	ARG
1	HL	193	ASP
1	HM	77	THR
1	HM	81	ASN
1	HM	179	LEU
1	HM	191	PHE
1	HN	38	TYR
1	HN	73	GLU
1	HN	100	LEU
1	HN	115	GLU
1	HN	191	PHE
1	HN	194	LEU
1	HO	67	THR
1	HO	78	LYS
1	HO	97	PHE
1	IA	77	THR
1	IA	137	HIS
1	IC	64	THR
1	IC	78	LYS
1	ID	62	ILE
1	ID	63	ILE
1	ID	93	MET
1	ID	114	MET
1	ID	189	ILE

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Mol	Chain	Res	Type
1	IE	63	ILE
1	IE	82	LYS
1	IE	84	TRP
1	IE	100	LEU
1	IF	37	ASP
1	IF	62	ILE
1	IF	120	LYS
1	IF	122	THR
1	IG	59	THR
1	IG	100	LEU
1	IG	171	GLU
1	IH	63	ILE
1	IH	64	THR
1	IH	78	LYS
1	II	77	THR
1	II	191	PHE
1	IJ	62	ILE
1	IJ	114	MET
1	IJ	174	VAL
1	IK	62	ILE
1	IK	67	THR
1	IL	64	THR
1	IL	66	ASP
1	IL	69	GLU
1	IL	74	ARG
1	IL	193	ASP
1	IM	77	THR
1	IM	81	ASN
1	IM	179	LEU
1	IM	191	PHE
1	IN	38	TYR
1	IN	73	GLU
1	IN	100	LEU
1	IN	115	GLU
1	IN	191	PHE
1	IN	194	LEU
1	IO	67	THR
1	IO	78	LYS
1	IO	97	PHE
1	JA	77	THR
1	JA	137	HIS
1	JC	64	THR

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Mol	Chain	Res	Type
1	JC	78	LYS
1	JD	62	ILE
1	JD	63	ILE
1	JD	93	MET
1	JD	114	MET
1	JD	189	ILE
1	JE	63	ILE
1	JE	82	LYS
1	JE	84	TRP
1	JE	100	LEU
1	JF	37	ASP
1	JF	62	ILE
1	JF	120	LYS
1	JF	122	THR
1	JG	59	THR
1	JG	100	LEU
1	JG	171	GLU
1	JH	63	ILE
1	JH	64	THR
1	JH	78	LYS
1	JI	77	THR
1	JI	191	PHE
1	JJ	62	ILE
1	JJ	114	MET
1	JJ	174	VAL
1	JK	62	ILE
1	JK	67	THR
1	JL	64	THR
1	JL	66	ASP
1	JL	69	GLU
1	JL	74	ARG
1	JL	193	ASP
1	JM	77	THR
1	JM	81	ASN
1	JM	179	LEU
1	JM	191	PHE
1	JN	38	TYR
1	JN	73	GLU
1	JN	100	LEU
1	JN	115	GLU
1	JN	191	PHE
1	JN	194	LEU

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Mol	Chain	Res	Type
1	JO	67	THR
1	JO	78	LYS
1	JO	97	PHE
1	KA	77	THR
1	KA	137	HIS
1	KC	64	THR
1	KC	78	LYS
1	KD	62	ILE
1	KD	63	ILE
1	KD	93	MET
1	KD	114	MET
1	KD	189	ILE
1	KE	63	ILE
1	KE	82	LYS
1	KE	84	TRP
1	KE	100	LEU
1	KF	37	ASP
1	KF	62	ILE
1	KF	120	LYS
1	KF	122	THR
1	KG	59	THR
1	KG	100	LEU
1	KG	171	GLU
1	KH	63	ILE
1	KH	64	THR
1	KH	78	LYS
1	KI	77	THR
1	KI	191	PHE
1	KJ	62	ILE
1	KJ	114	MET
1	KJ	174	VAL
1	KK	62	ILE
1	KK	67	THR
1	KL	64	THR
1	KL	66	ASP
1	KL	69	GLU
1	KL	74	ARG
1	KL	193	ASP
1	KM	77	THR
1	KM	81	ASN
1	KM	179	LEU
1	KM	191	PHE

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Mol	Chain	Res	Type
1	KN	38	TYR
1	KN	73	GLU
1	KN	100	LEU
1	KN	115	GLU
1	KN	191	PHE
1	KN	194	LEU
1	KO	67	THR
1	KO	78	LYS
1	KO	97	PHE
1	LA	77	THR
1	LA	137	HIS
1	LC	64	THR
1	LC	78	LYS
1	LD	62	ILE
1	LD	63	ILE
1	LD	93	MET
1	LD	114	MET
1	LD	189	ILE
1	LE	63	ILE
1	LE	82	LYS
1	LE	84	TRP
1	LE	100	LEU
1	LF	37	ASP
1	LF	62	ILE
1	LF	120	LYS
1	LF	122	THR
1	LG	59	THR
1	LG	100	LEU
1	LG	171	GLU
1	LH	63	ILE
1	LH	64	THR
1	LH	78	LYS
1	LI	77	THR
1	LI	191	PHE
1	LJ	62	ILE
1	LJ	114	MET
1	LJ	174	VAL
1	LK	62	ILE
1	LK	67	THR
1	LL	64	THR
1	LL	66	ASP
1	LL	69	GLU

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Mol	Chain	Res	Type
1	LL	74	ARG
1	LL	193	ASP
1	LM	77	THR
1	LM	81	ASN
1	LM	179	LEU
1	LM	191	PHE
1	LN	38	TYR
1	LN	73	GLU
1	LN	100	LEU
1	LN	115	GLU
1	LN	191	PHE
1	LN	194	LEU
1	LO	67	THR
1	LO	78	LYS
1	LO	97	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (331) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	95	ASN
1	BB	137	HIS
1	BC	95	ASN
1	BD	95	ASN
1	BD	154	HIS
1	BE	79	HIS
1	BE	81	ASN
1	BE	95	ASN
1	BE	154	HIS
1	BF	95	ASN
1	BG	95	ASN
1	BH	95	ASN
1	BH	136	ASN
1	BI	95	ASN
1	BJ	70	GLN
1	BJ	81	ASN
1	BJ	95	ASN
1	BJ	154	HIS
1	BK	81	ASN
1	BK	95	ASN
1	BL	95	ASN
1	BM	95	ASN
1	BM	154	HIS

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Mol	Chain	Res	Type
1	BN	95	ASN
1	BN	136	ASN
1	BN	137	HIS
1	BO	95	ASN
1	BO	136	ASN
1	AA	95	ASN
1	AB	137	HIS
1	AC	95	ASN
1	AD	95	ASN
1	AD	154	HIS
1	AE	79	HIS
1	AE	81	ASN
1	AE	95	ASN
1	AE	154	HIS
1	AF	95	ASN
1	AG	95	ASN
1	AH	95	ASN
1	AH	136	ASN
1	AI	95	ASN
1	AJ	70	GLN
1	AJ	81	ASN
1	AJ	154	HIS
1	AK	81	ASN
1	AK	95	ASN
1	AL	95	ASN
1	AM	95	ASN
1	AM	154	HIS
1	AN	95	ASN
1	AN	136	ASN
1	AN	137	HIS
1	AO	95	ASN
1	AO	136	ASN
1	CA	95	ASN
1	CB	137	HIS
1	CC	95	ASN
1	CD	95	ASN
1	CD	154	HIS
1	CE	79	HIS
1	CE	81	ASN
1	CE	95	ASN
1	CE	154	HIS
1	CF	95	ASN

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Mol	Chain	Res	Type
1	CG	95	ASN
1	CH	95	ASN
1	CH	136	ASN
1	CI	95	ASN
1	CJ	70	GLN
1	CJ	81	ASN
1	CJ	95	ASN
1	CJ	154	HIS
1	CK	81	ASN
1	CK	95	ASN
1	CL	95	ASN
1	CM	95	ASN
1	CM	154	HIS
1	CN	95	ASN
1	CN	136	ASN
1	CN	137	HIS
1	CO	95	ASN
1	CO	136	ASN
1	DA	95	ASN
1	DC	95	ASN
1	DD	95	ASN
1	DD	154	HIS
1	DE	81	ASN
1	DE	95	ASN
1	DE	154	HIS
1	DF	79	HIS
1	DF	95	ASN
1	DG	95	ASN
1	DH	136	ASN
1	DI	95	ASN
1	DJ	70	GLN
1	DJ	81	ASN
1	DJ	95	ASN
1	DJ	154	HIS
1	DK	81	ASN
1	DK	95	ASN
1	DL	95	ASN
1	DM	95	ASN
1	DM	154	HIS
1	DN	95	ASN
1	DN	136	ASN
1	DN	137	HIS

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Mol	Chain	Res	Type
1	DO	95	ASN
1	DO	136	ASN
1	EA	95	ASN
1	EC	95	ASN
1	ED	95	ASN
1	ED	154	HIS
1	EE	79	HIS
1	EE	81	ASN
1	EE	95	ASN
1	EE	154	HIS
1	EF	95	ASN
1	EG	95	ASN
1	EH	136	ASN
1	EI	95	ASN
1	EJ	70	GLN
1	EJ	81	ASN
1	EJ	95	ASN
1	EJ	154	HIS
1	EK	81	ASN
1	EK	95	ASN
1	EL	95	ASN
1	EM	95	ASN
1	EM	154	HIS
1	EN	95	ASN
1	EN	136	ASN
1	EN	137	HIS
1	EO	95	ASN
1	EO	136	ASN
1	FA	95	ASN
1	FC	81	ASN
1	FC	95	ASN
1	FD	95	ASN
1	FD	154	HIS
1	FE	81	ASN
1	FE	95	ASN
1	FE	154	HIS
1	FF	95	ASN
1	FG	95	ASN
1	FH	95	ASN
1	FH	136	ASN
1	FI	95	ASN
1	FJ	70	GLN

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Mol	Chain	Res	Type
1	FJ	81	ASN
1	FJ	154	HIS
1	FK	81	ASN
1	FK	95	ASN
1	FL	95	ASN
1	FM	95	ASN
1	FM	154	HIS
1	FN	95	ASN
1	FN	136	ASN
1	FN	137	HIS
1	FO	95	ASN
1	FO	136	ASN
1	GA	70	GLN
1	GA	95	ASN
1	GC	95	ASN
1	GD	95	ASN
1	GD	154	HIS
1	GE	79	HIS
1	GE	81	ASN
1	GE	95	ASN
1	GE	154	HIS
1	GF	95	ASN
1	GG	95	ASN
1	GH	95	ASN
1	GH	136	ASN
1	GI	95	ASN
1	GJ	70	GLN
1	GJ	81	ASN
1	GJ	154	HIS
1	GK	81	ASN
1	GK	95	ASN
1	GL	95	ASN
1	GM	95	ASN
1	GM	154	HIS
1	GN	95	ASN
1	GN	136	ASN
1	GN	137	HIS
1	GO	95	ASN
1	GO	136	ASN
1	HA	70	GLN
1	HA	95	ASN
1	HC	95	ASN

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Mol	Chain	Res	Type
1	HD	95	ASN
1	HD	154	HIS
1	HE	79	HIS
1	HE	81	ASN
1	HE	95	ASN
1	HE	154	HIS
1	HF	95	ASN
1	HG	95	ASN
1	HH	95	ASN
1	HH	136	ASN
1	HI	95	ASN
1	HI	137	HIS
1	HJ	70	GLN
1	HJ	81	ASN
1	HJ	154	HIS
1	HK	81	ASN
1	HK	95	ASN
1	HL	95	ASN
1	HM	95	ASN
1	HM	154	HIS
1	HN	95	ASN
1	HN	136	ASN
1	HN	137	HIS
1	HO	95	ASN
1	HO	136	ASN
1	IA	70	GLN
1	IA	95	ASN
1	IC	95	ASN
1	ID	95	ASN
1	ID	154	HIS
1	IE	79	HIS
1	IE	81	ASN
1	IE	95	ASN
1	IE	154	HIS
1	IF	95	ASN
1	IG	70	GLN
1	IG	95	ASN
1	IH	136	ASN
1	II	95	ASN
1	IJ	70	GLN
1	IJ	81	ASN
1	IJ	154	HIS

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Mol	Chain	Res	Type
1	IK	81	ASN
1	IK	95	ASN
1	IL	70	GLN
1	IL	95	ASN
1	IM	95	ASN
1	IM	154	HIS
1	IN	95	ASN
1	IN	136	ASN
1	IN	137	HIS
1	IO	95	ASN
1	IO	136	ASN
1	JA	70	GLN
1	JA	95	ASN
1	JB	137	HIS
1	JC	81	ASN
1	JC	95	ASN
1	JD	95	ASN
1	JD	154	HIS
1	JE	79	HIS
1	JE	81	ASN
1	JE	95	ASN
1	JE	154	HIS
1	JF	95	ASN
1	JG	95	ASN
1	JG	136	ASN
1	JH	95	ASN
1	JH	136	ASN
1	JI	95	ASN
1	JJ	70	GLN
1	JJ	81	ASN
1	JJ	154	HIS
1	JK	81	ASN
1	JK	95	ASN
1	JL	95	ASN
1	JM	95	ASN
1	JM	154	HIS
1	JN	95	ASN
1	JN	136	ASN
1	JN	137	HIS
1	JO	95	ASN
1	JO	136	ASN
1	KA	95	ASN

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Mol	Chain	Res	Type
1	KC	95	ASN
1	KD	95	ASN
1	KD	154	HIS
1	KE	79	HIS
1	KE	81	ASN
1	KE	95	ASN
1	KE	154	HIS
1	KF	95	ASN
1	KG	95	ASN
1	KG	154	HIS
1	KH	95	ASN
1	KH	136	ASN
1	KI	95	ASN
1	KJ	70	GLN
1	KJ	81	ASN
1	KJ	95	ASN
1	KJ	154	HIS
1	KK	81	ASN
1	KK	95	ASN
1	KL	95	ASN
1	KL	136	ASN
1	KM	95	ASN
1	KM	154	HIS
1	KN	95	ASN
1	KN	136	ASN
1	KN	137	HIS
1	KO	95	ASN
1	KO	136	ASN
1	LA	70	GLN
1	LA	95	ASN
1	LB	137	HIS
1	LC	95	ASN
1	LD	95	ASN
1	LD	154	HIS
1	LE	79	HIS
1	LE	81	ASN
1	LE	95	ASN
1	LE	154	HIS
1	LF	95	ASN
1	LG	95	ASN
1	LH	95	ASN
1	LH	136	ASN

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Mol	Chain	Res	Type
1	LI	95	ASN
1	LJ	70	GLN
1	LJ	81	ASN
1	LJ	154	HIS
1	LK	81	ASN
1	LK	95	ASN
1	LL	95	ASN
1	LM	95	ASN
1	LM	154	HIS
1	LN	95	ASN
1	LN	136	ASN
1	LN	137	HIS
1	LO	95	ASN
1	LO	136	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

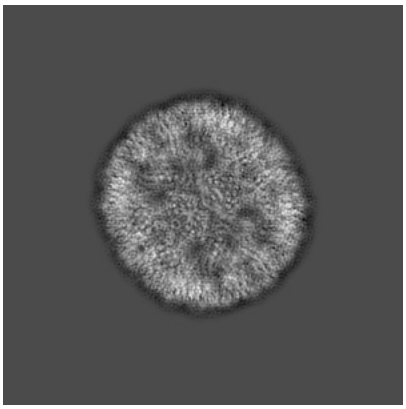
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11633. These allow visual inspection of the internal detail of the map and identification of artifacts.

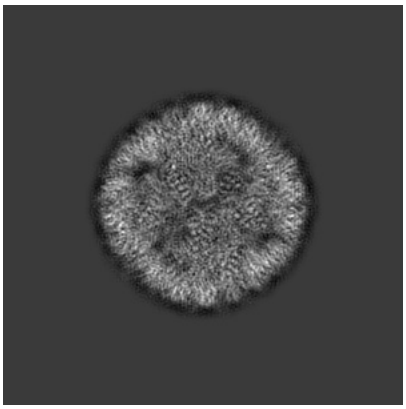
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

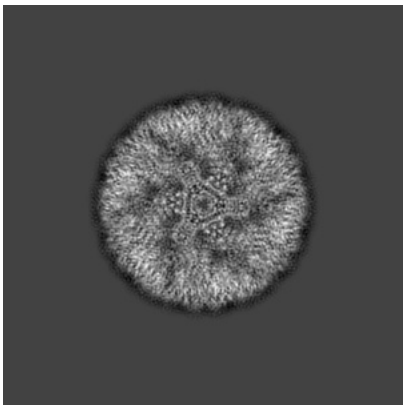
6.1.1 Primary map



X

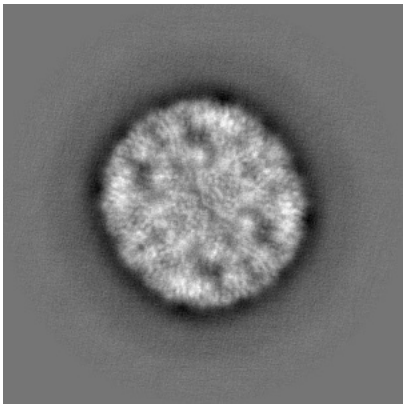


Y

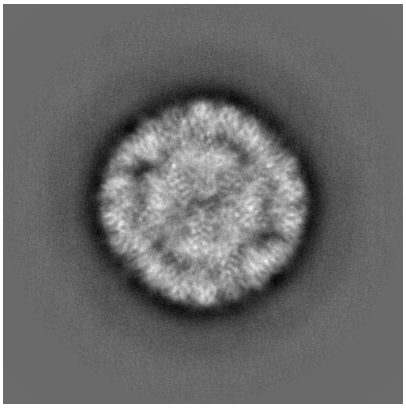


Z

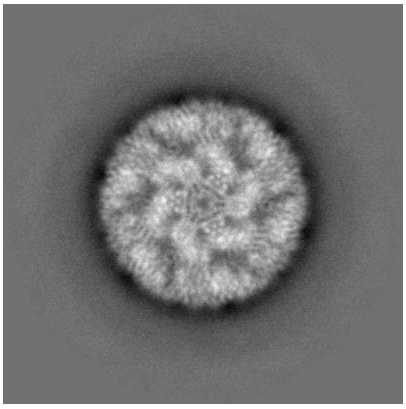
6.1.2 Raw map



X



Y

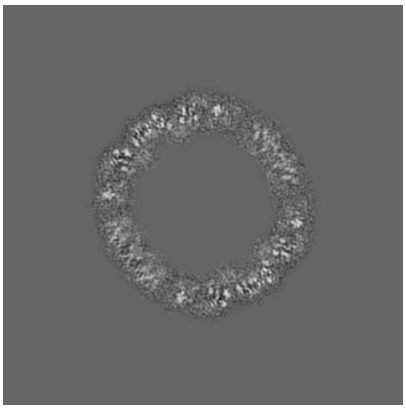


Z

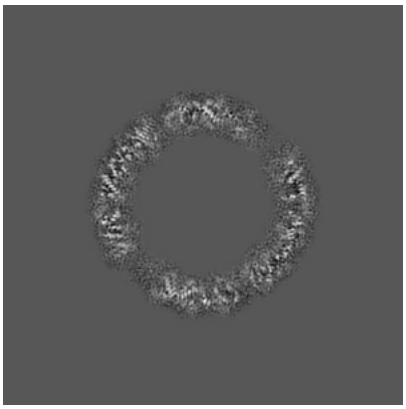
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

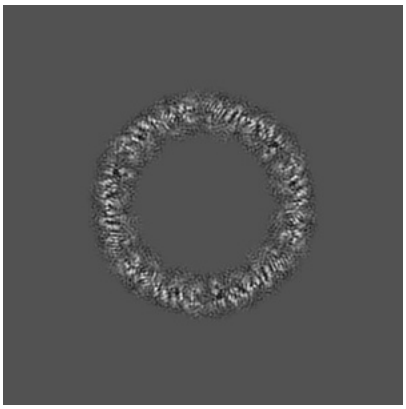
6.2.1 Primary map



X Index: 200

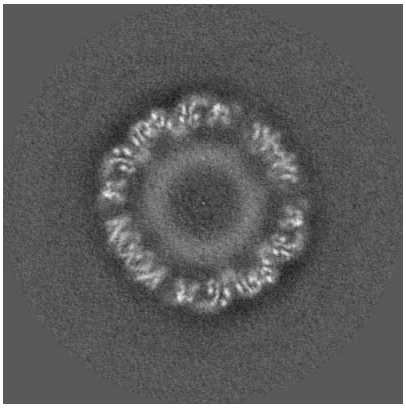


Y Index: 200

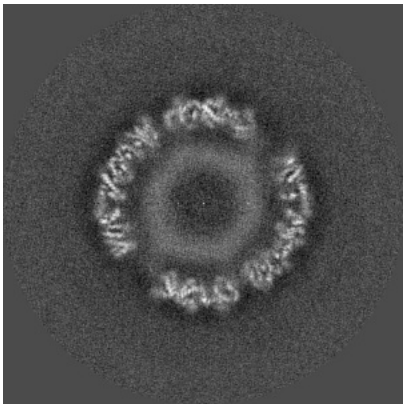


Z Index: 200

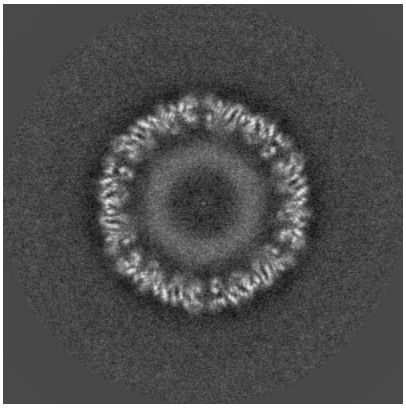
6.2.2 Raw map



X Index: 200



Y Index: 200

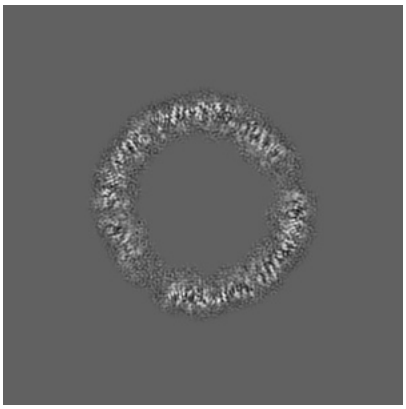


Z Index: 200

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

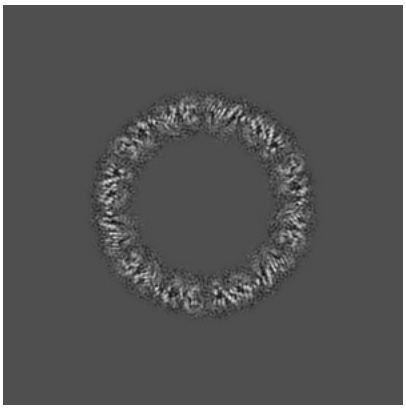
6.3 Largest variance slices (i)

6.3.1 Primary map



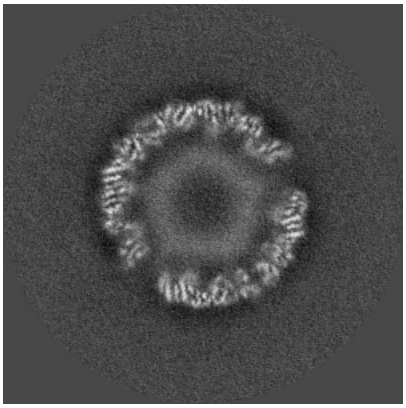
X Index: 211

Y Index: 233

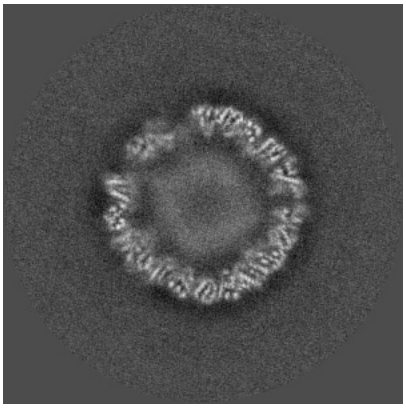


Z Index: 199

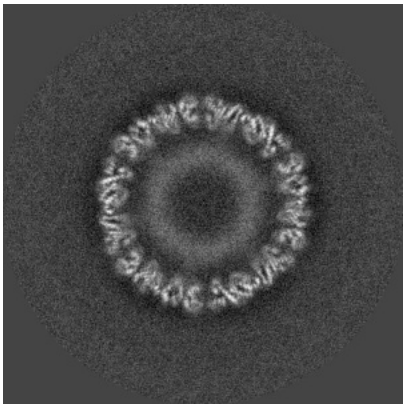
6.3.2 Raw map



X Index: 218



Y Index: 233

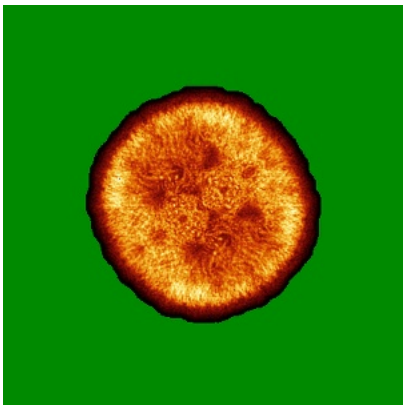


Z Index: 199

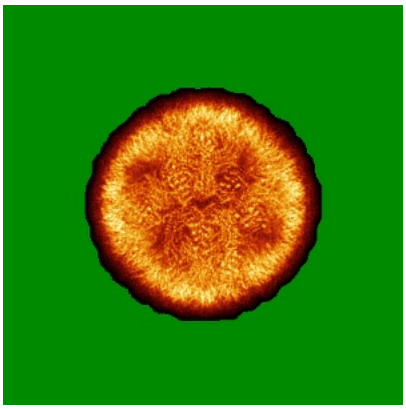
The images above show the largest variance slices of the map in three orthogonal directions.

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

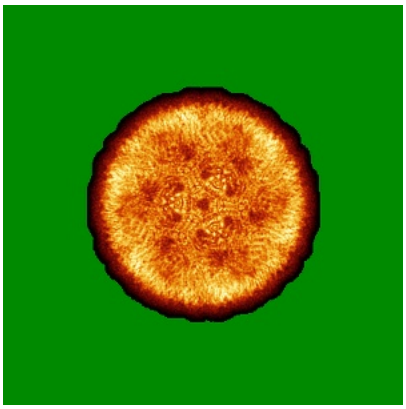
6.4.1 Primary map



X

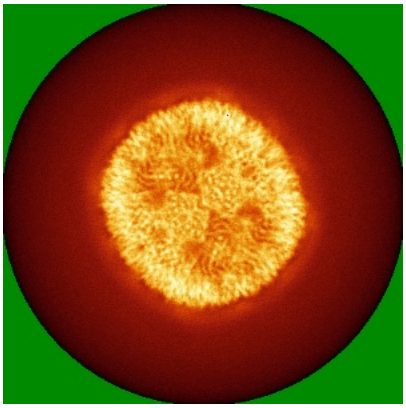


Y

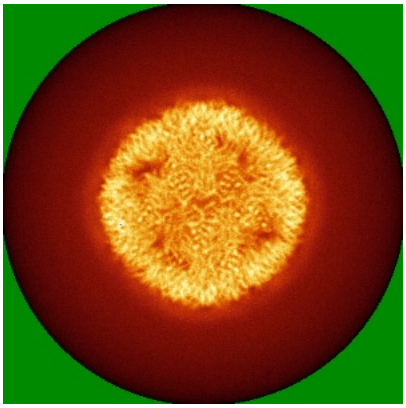


Z

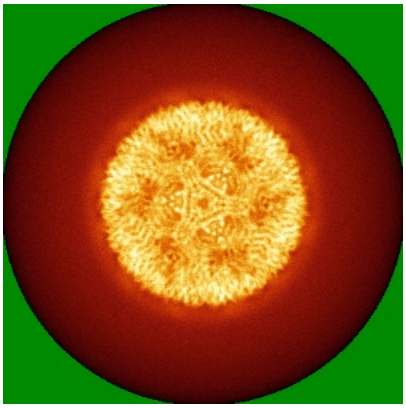
6.4.2 Raw map



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 0.0265. 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.

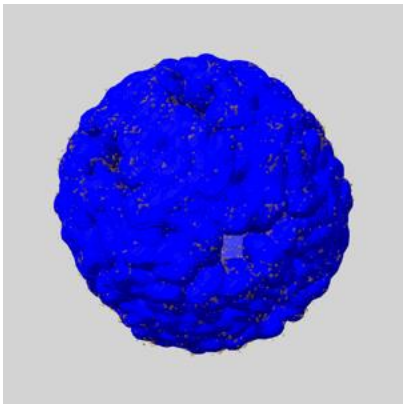
6.6 Mask visualisation

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

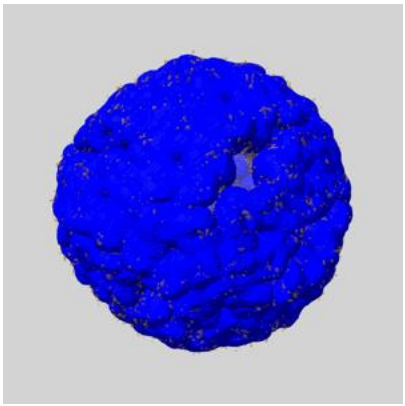
A mask typically either:

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

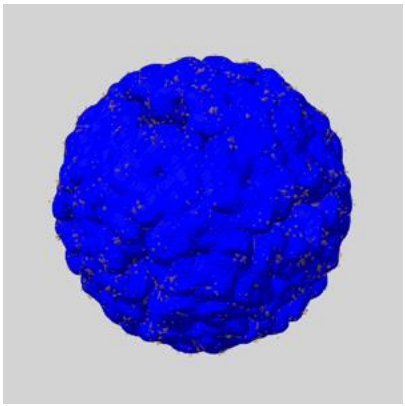
6.6.1 emd_11633_msk_1.map



X



Y

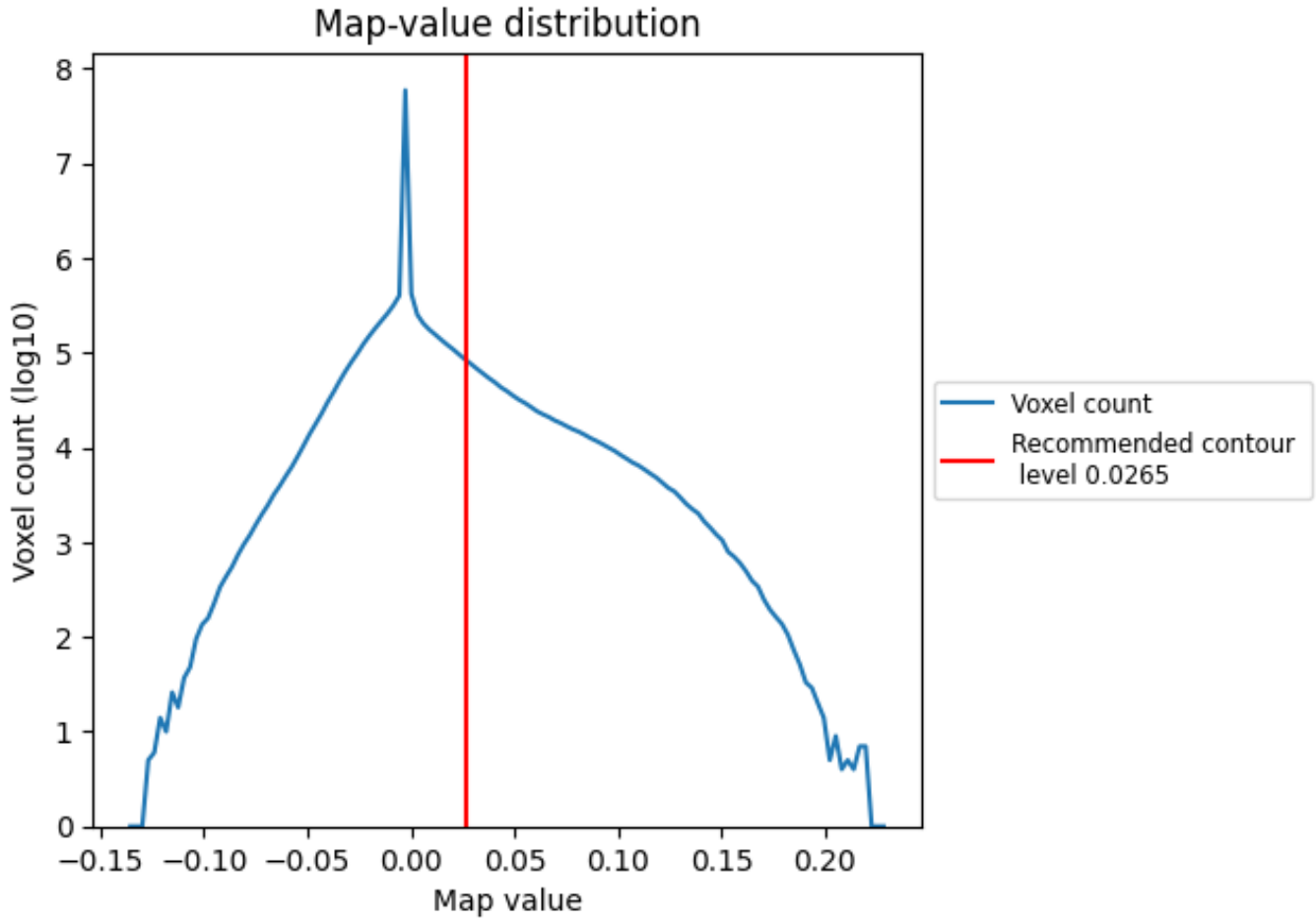


Z

7 Map analysis

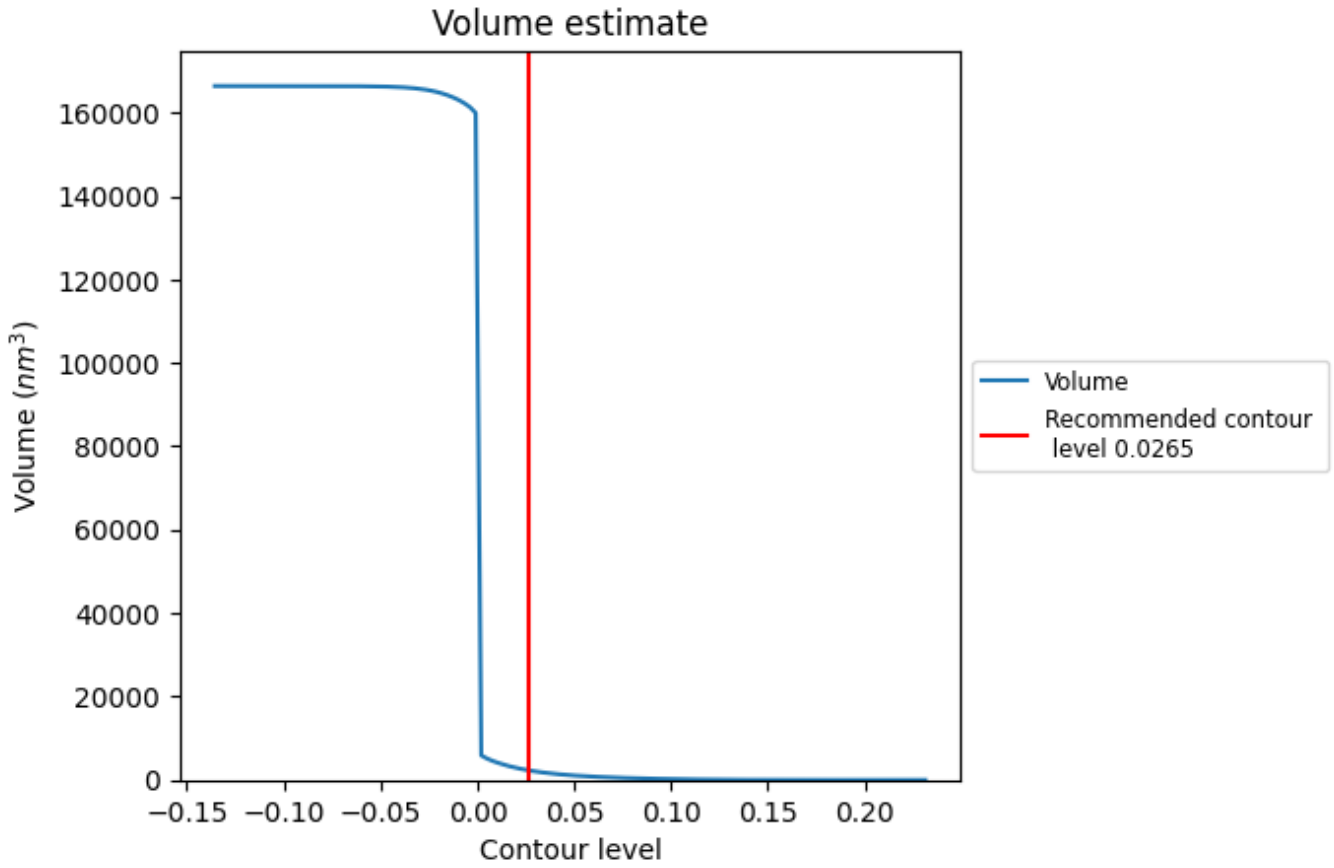
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

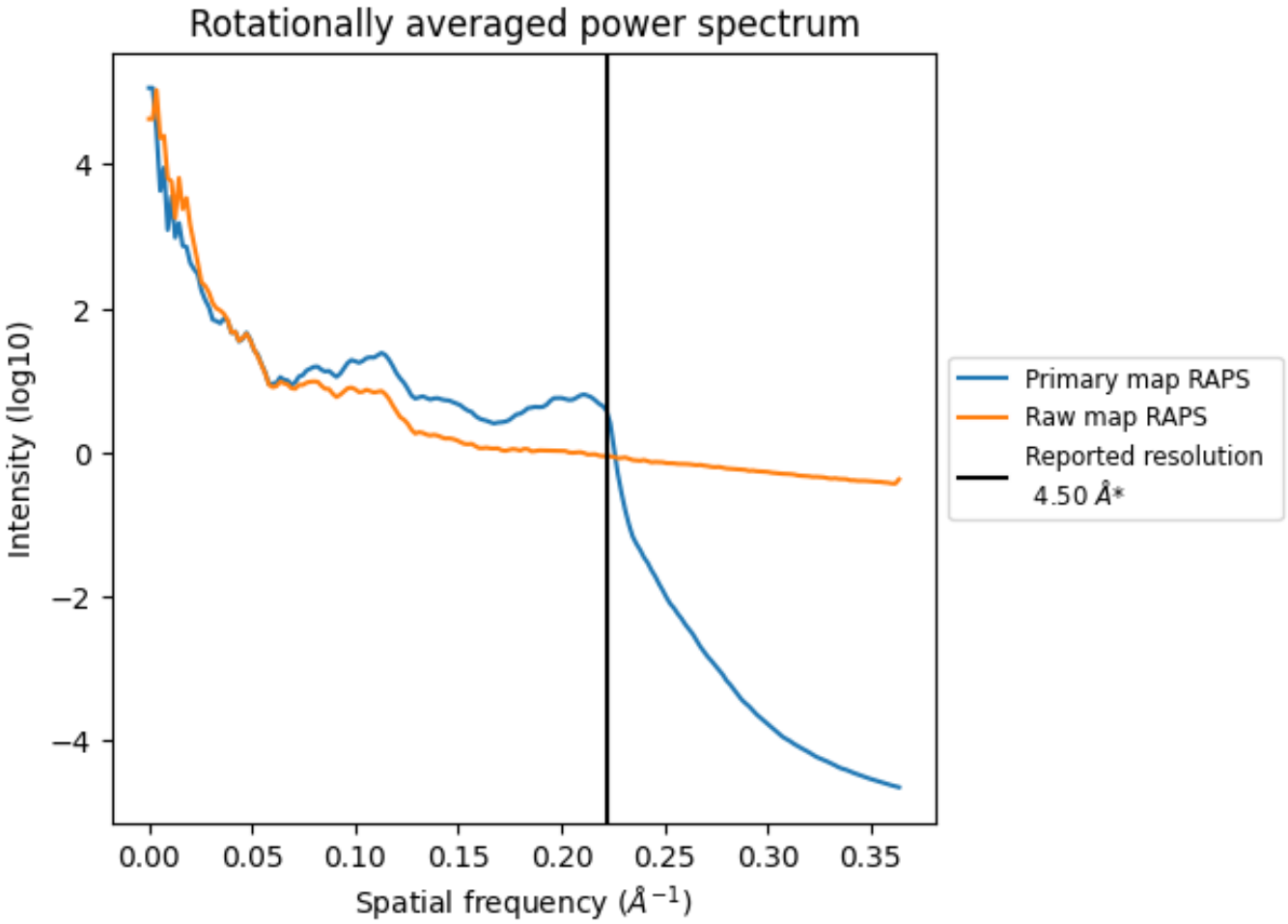
7.2 Volume estimate



The volume at the recommended contour level is 2304 nm^3; this corresponds to an approximate mass of 2081 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)

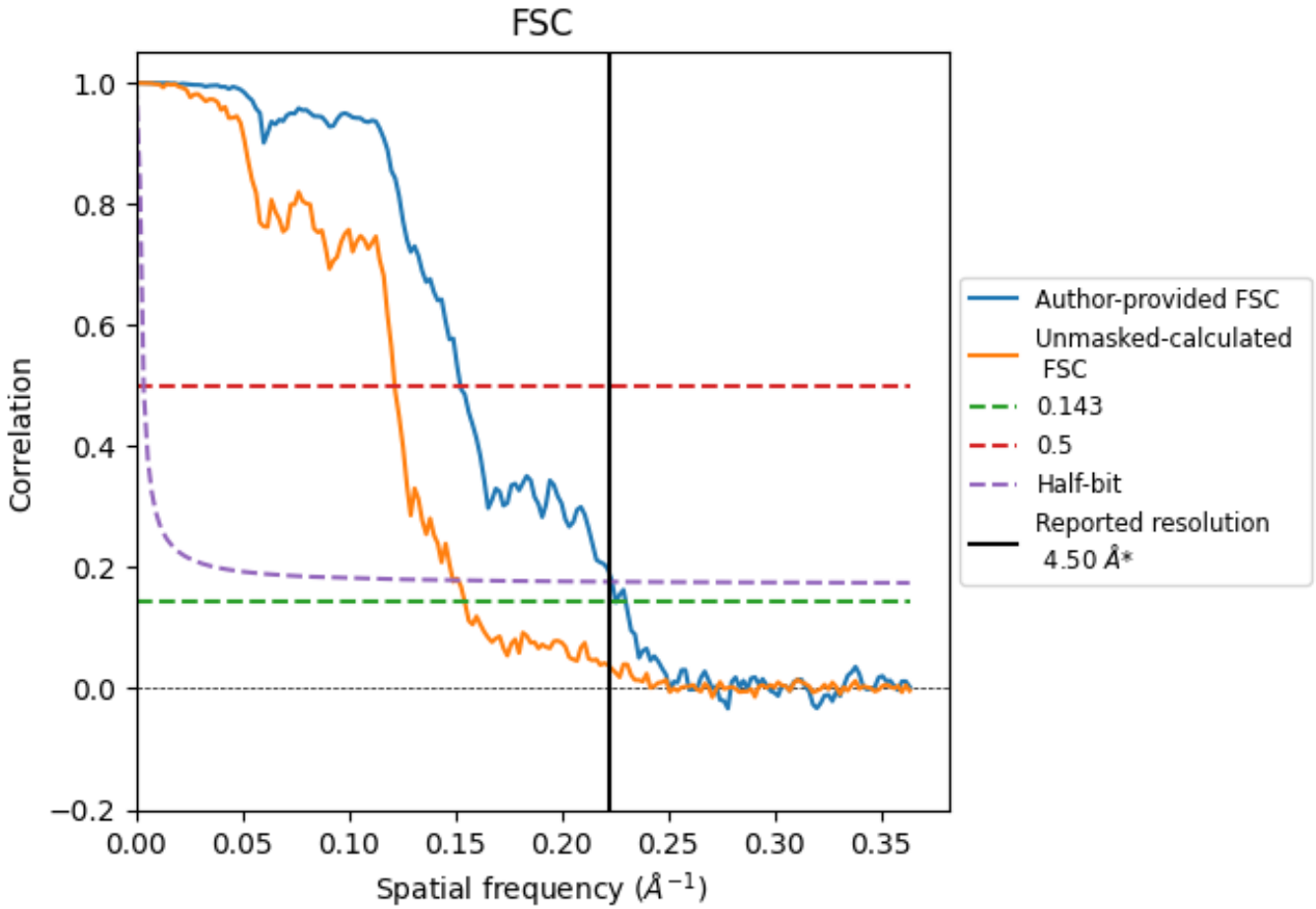


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8.2 Resolution estimates (i)

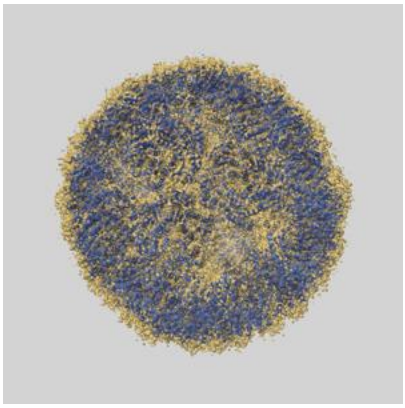
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.44	6.56	4.47
Unmasked-calculated*	6.47	8.22	6.72

*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 6.47 differs from the reported value 4.5 by more than 10 %

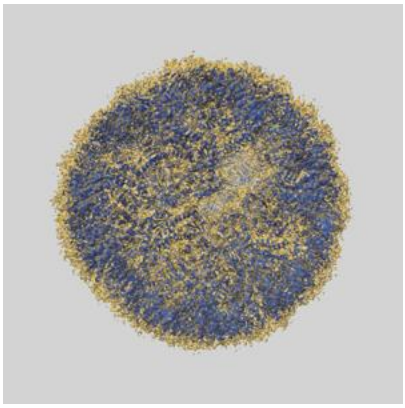
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11633 and PDB model 7A4H. Per-residue inclusion information can be found in section 3 on page 162.

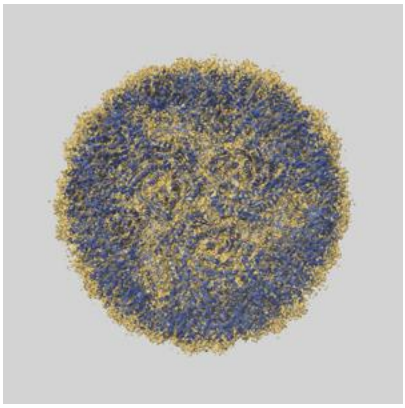
9.1 Map-model overlay



X



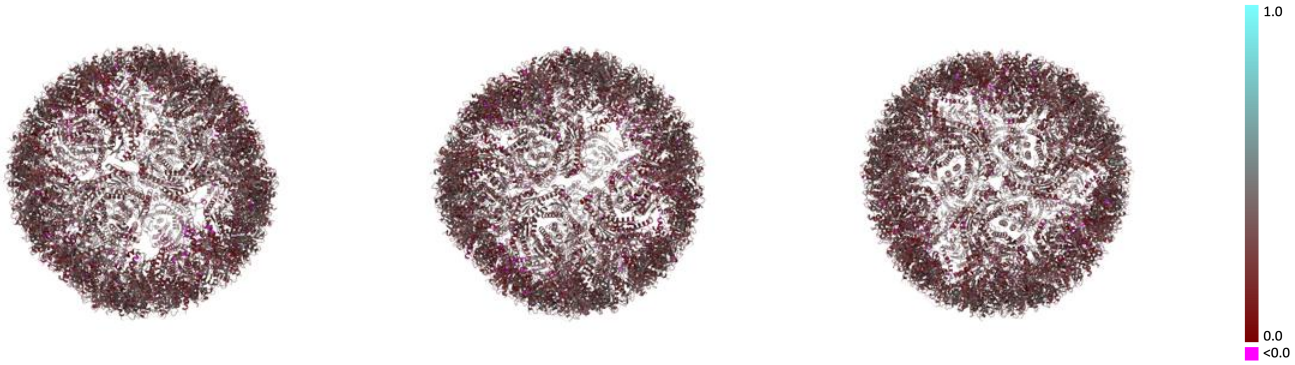
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0265 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.

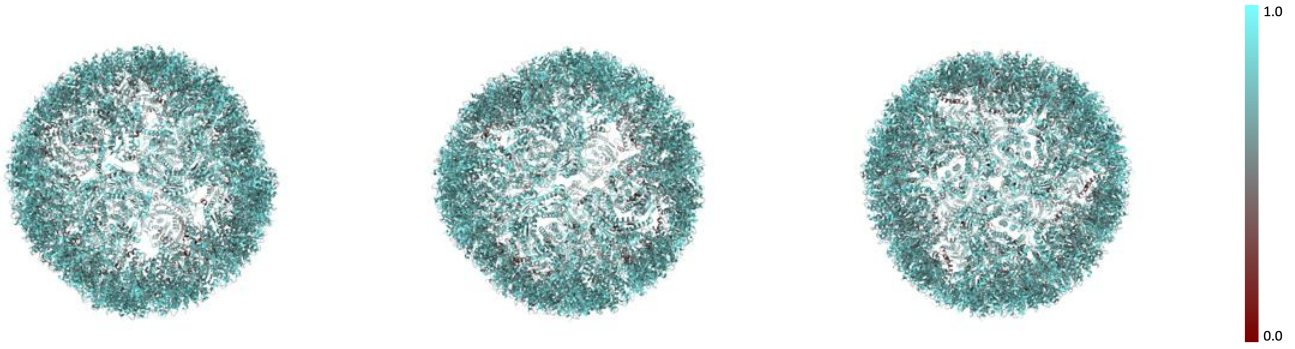
9.2 Q-score mapped to coordinate model (i)



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.

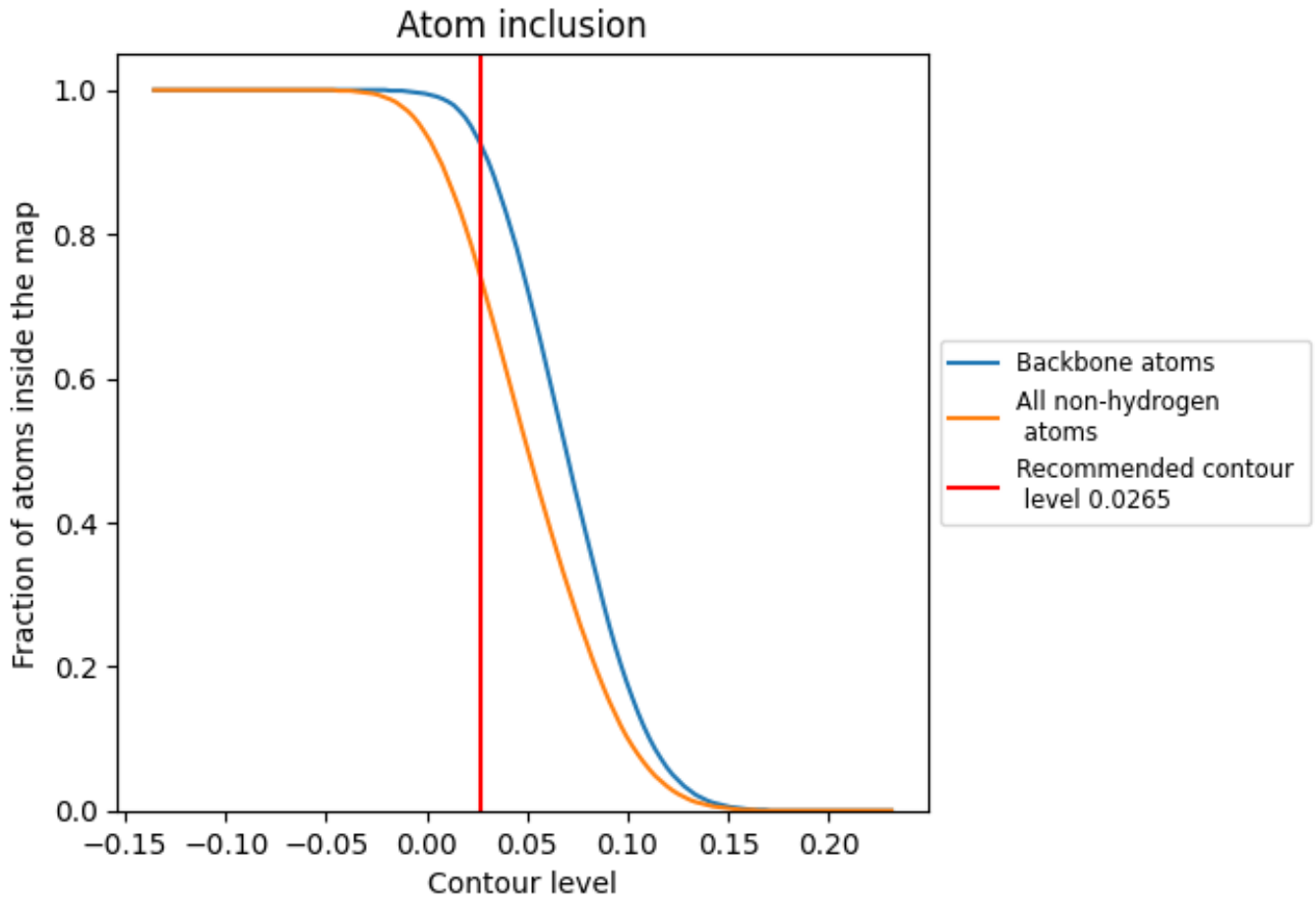
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0265).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0265) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.2900
AA	0.7680	0.3220
AB	0.7290	0.2680
AC	0.7520	0.2980
AD	0.7790	0.3170
AE	0.7800	0.3230
AF	0.7420	0.2770
AG	0.7560	0.2950
AH	0.7940	0.3360
AI	0.7730	0.3190
AJ	0.7620	0.3030
AK	0.7040	0.2450
AL	0.7280	0.2910
AM	0.7490	0.3100
AN	0.6820	0.2480
AO	0.6860	0.2390
BA	0.7660	0.3180
BB	0.7300	0.2690
BC	0.7560	0.2980
BD	0.7800	0.3160
BE	0.7740	0.3250
BF	0.7460	0.2800
BG	0.7540	0.3030
BH	0.7960	0.3380
BI	0.7720	0.3180
BJ	0.7600	0.2990
BK	0.6980	0.2430
BL	0.7310	0.2910
BM	0.7560	0.3100
BN	0.6900	0.2480
BO	0.6860	0.2420
CA	0.7730	0.3170
CB	0.7290	0.2680
CC	0.7540	0.2960
CD	0.7730	0.3150

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Chain	Atom inclusion	Q-score
CE	0.7760	0.3240
CF	0.7350	0.2770
CG	0.7590	0.2940
CH	0.7860	0.3340
CI	0.7670	0.3110
CJ	0.7680	0.2970
CK	0.7060	0.2480
CL	0.7350	0.2890
CM	0.7450	0.3070
CN	0.6870	0.2450
CO	0.6860	0.2410
DA	0.7660	0.3150
DB	0.7280	0.2640
DC	0.7560	0.2890
DD	0.7730	0.3130
DE	0.7790	0.3170
DF	0.7470	0.2780
DG	0.7630	0.2970
DH	0.7970	0.3340
DI	0.7720	0.3190
DJ	0.7580	0.2980
DK	0.6930	0.2440
DL	0.7290	0.2890
DM	0.7510	0.3050
DN	0.6800	0.2450
DO	0.6870	0.2390
EA	0.7590	0.3040
EB	0.7310	0.2580
EC	0.7490	0.2830
ED	0.7630	0.3030
EE	0.7620	0.3090
EF	0.7410	0.2720
EG	0.7520	0.2940
EH	0.7940	0.3340
EI	0.7760	0.3120
EJ	0.7460	0.2930
EK	0.6930	0.2380
EL	0.7280	0.2840
EM	0.7480	0.2980
EN	0.6820	0.2400
EO	0.6870	0.2360
FA	0.7640	0.3140

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Chain	Atom inclusion	Q-score
FB	0.7270	0.2610
FC	0.7460	0.2870
FD	0.7690	0.3080
FE	0.7670	0.3160
FF	0.7440	0.2740
FG	0.7550	0.2980
FH	0.7900	0.3350
FI	0.7720	0.3130
FJ	0.7520	0.2960
FK	0.6990	0.2390
FL	0.7290	0.2870
FM	0.7420	0.3030
FN	0.6820	0.2420
FO	0.6900	0.2400
GA	0.7690	0.3190
GB	0.7300	0.2630
GC	0.7540	0.2950
GD	0.7740	0.3170
GE	0.7740	0.3230
GF	0.7380	0.2760
GG	0.7590	0.2990
GH	0.7930	0.3380
GI	0.7720	0.3200
GJ	0.7600	0.3030
GK	0.7010	0.2440
GL	0.7310	0.2900
GM	0.7500	0.3100
GN	0.6780	0.2480
GO	0.6870	0.2410
HA	0.7700	0.3150
HB	0.7310	0.2700
HC	0.7560	0.2970
HD	0.7680	0.3180
HE	0.7800	0.3210
HF	0.7460	0.2780
HG	0.7470	0.2910
HH	0.7820	0.3310
HI	0.7630	0.3130
HJ	0.7630	0.2980
HK	0.6950	0.2430
HL	0.7300	0.2850
HM	0.7500	0.3030

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Chain	Atom inclusion	Q-score
HN	0.6780	0.2410
HO	0.6670	0.2330
IA	0.7750	0.3180
IB	0.7280	0.2640
IC	0.7620	0.2940
ID	0.7760	0.3180
IE	0.7750	0.3200
IF	0.7500	0.2770
IG	0.7560	0.2990
IH	0.7900	0.3370
II	0.7720	0.3160
IJ	0.7670	0.2960
IK	0.6980	0.2400
IL	0.7280	0.2890
IM	0.7520	0.3110
IN	0.6850	0.2460
IO	0.6890	0.2400
JA	0.7810	0.3040
JB	0.7290	0.2550
JC	0.7440	0.2900
JD	0.7740	0.3110
JE	0.7740	0.3160
JF	0.7470	0.2780
JG	0.7540	0.2970
JH	0.7820	0.3300
JI	0.7680	0.3100
JJ	0.7610	0.2900
JK	0.6960	0.2390
JL	0.7160	0.2790
JM	0.7350	0.3000
JN	0.6800	0.2430
JO	0.6830	0.2350
KA	0.7650	0.3210
KB	0.7310	0.2680
KC	0.7570	0.2960
KD	0.7790	0.3170
KE	0.7710	0.3230
KF	0.7440	0.2740
KG	0.7590	0.3020
KH	0.7960	0.3390
KI	0.7710	0.3200
KJ	0.7610	0.3030

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Chain	Atom inclusion	Q-score
KK	0.6990	0.2430
KL	0.7270	0.2900
KM	0.7510	0.3120
KN	0.6800	0.2420
KO	0.6840	0.2380
LA	0.7710	0.3180
LB	0.7320	0.2640
LC	0.7590	0.2940
LD	0.7800	0.3170
LE	0.7740	0.3230
LF	0.7430	0.2740
LG	0.7560	0.2960
LH	0.7930	0.3310
LI	0.7660	0.3150
LJ	0.7680	0.2950
LK	0.7080	0.2430
LL	0.7290	0.2900
LM	0.7470	0.3110
LN	0.6920	0.2460
LO	0.6860	0.2420