Full wwPDB EM Validation Report ⓘ

Apr 23, 2024 – 02:17 pm BST

PDB ID	:	7A4F
EMDB ID	:	EMD-11631
Title	:	Aquifex aeolicus lumazine synthase-derived nucleocapsid variant NC-1 (120-mer)
Authors	:	Tetter, S.; Hilvert, D.
Deposited on	:	2020-08-19
Resolution	:	3.50 Å(reported)
Based on initial model	:	1HQK

The following versions of software and data (see references ⓘ) were used in the production of this report:

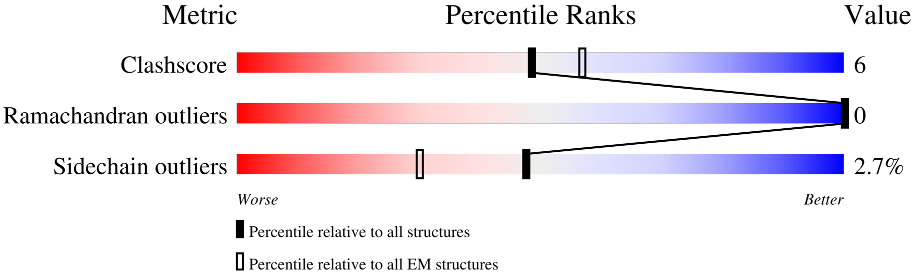
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

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

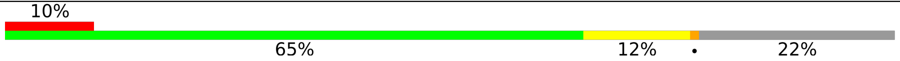
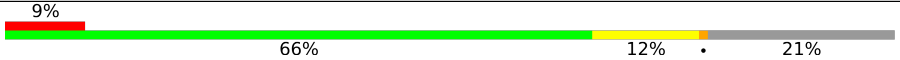
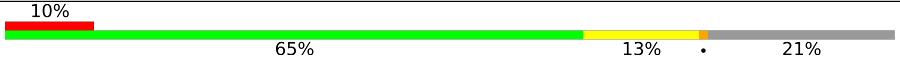
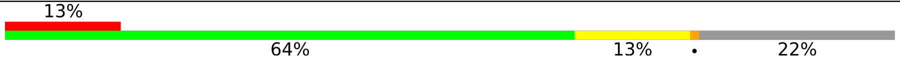
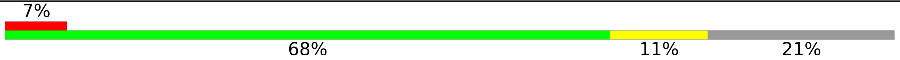
The reported resolution of this entry is 3.50 Å.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	AA	197	
1	AB	197	
1	AC	197	
1	AD	197	
1	AE	197	
1	AF	197	
1	AG	197	
1	AH	197	

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Mol	Chain	Length	Quality of chain
1	AI	197	6% 67% 12% • 21%
1	AJ	197	9% 66% 11% • 22%
1	BA	197	9% 66% 12% 22%
1	BB	197	11% 65% 12% • 22%
1	BC	197	9% 65% 13% • 21%
1	BD	197	9% 65% 13% • 21%
1	BE	197	12% 64% 13% • 22%
1	BF	197	8% 66% 12% • 21%
1	BG	197	• 61% 16% • 21%
1	BH	197	• 65% 12% • 21%
1	BI	197	5% 68% 11% • 21%
1	BJ	197	11% 66% 11% • 22%
1	CA	197	10% 66% 12% 22%
1	CB	197	10% 65% 12% • 22%
1	CC	197	8% 66% 12% • 21%
1	CD	197	10% 65% 13% • 21%
1	CE	197	13% 63% 14% • 22%
1	CF	197	7% 68% 10% • 21%
1	CG	197	• 60% 17% • 21%
1	CH	197	• 65% 11% • 21%
1	CI	197	7% 68% 11% • 21%
1	CJ	197	9% 66% 11% • 22%
1	DA	197	9% 66% 12% 22%
1	DB	197	10% 65% 12% • 22%
1	DC	197	9% 66% 12% • 21%

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Mol	Chain	Length	Quality of chain
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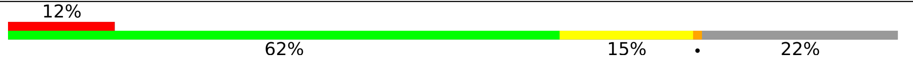
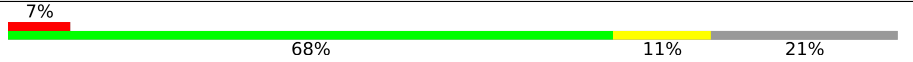
1	DE	197	
1	DF	197	
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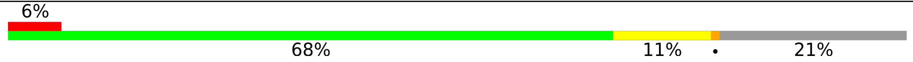
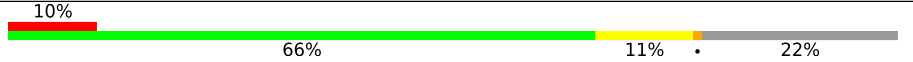
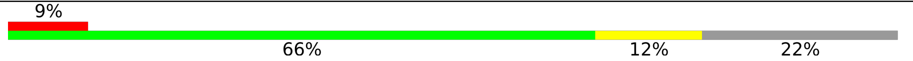
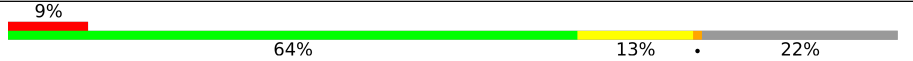
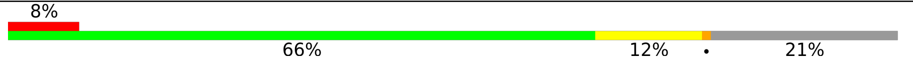
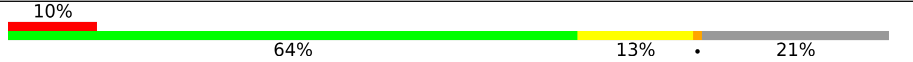
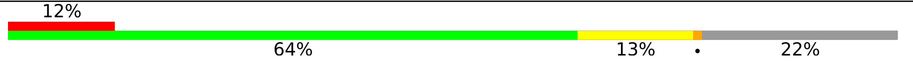
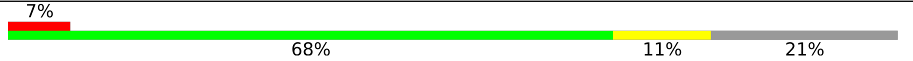
1	DI	197	
1	DJ	197	
1	EA	197	
1	EB	197	
1	EC	197	
1	ED	197	
1	EE	197	
1	EF	197	
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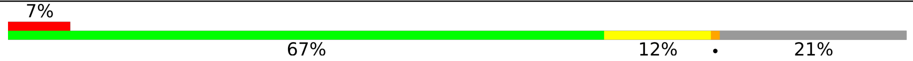
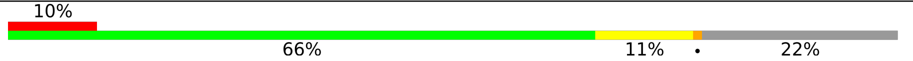
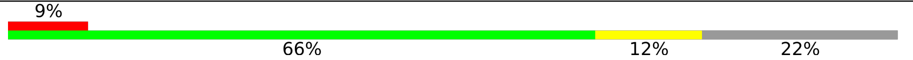
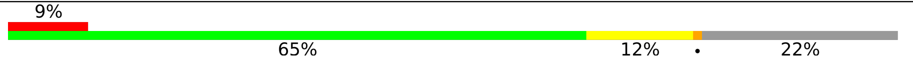
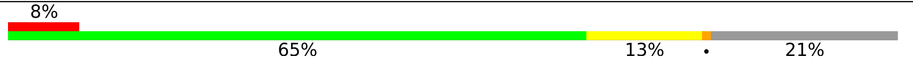
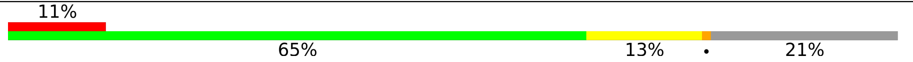
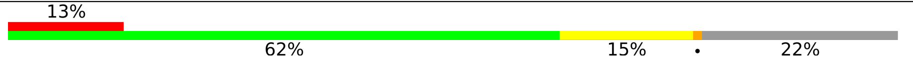
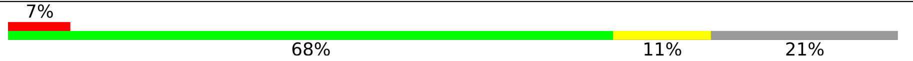
1	EH	197	
1	EI	197	
1	EJ	197	
1	FA	197	
1	FB	197	
1	FC	197	
1	FD	197	
1	FE	197	
1	FF	197	
1	FG	197	
1	FH	197	

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Mol	Chain	Length	Quality of chain
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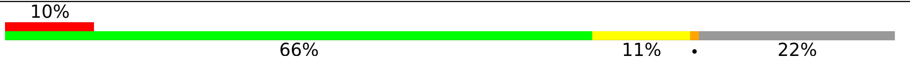
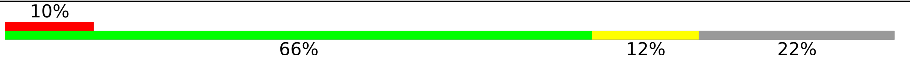
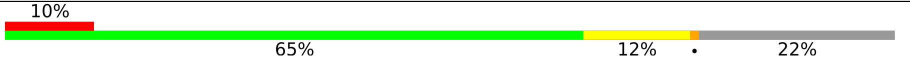
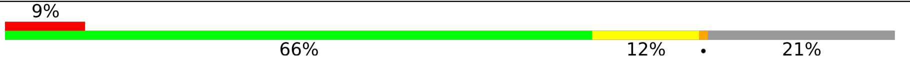
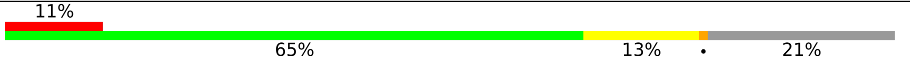
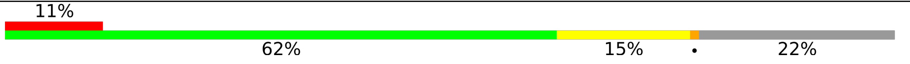
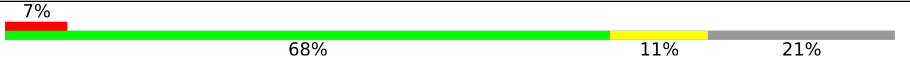
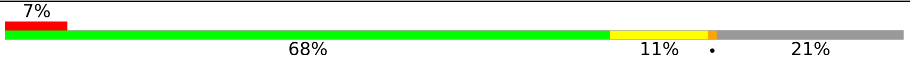
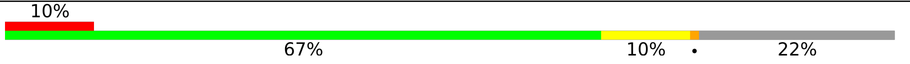
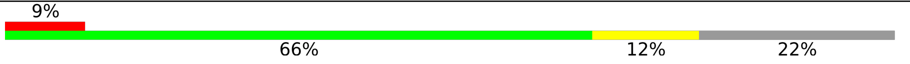
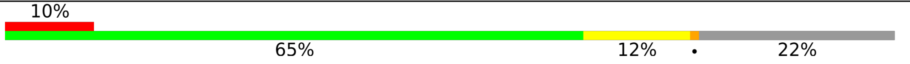
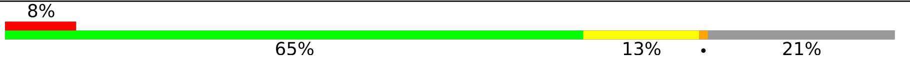
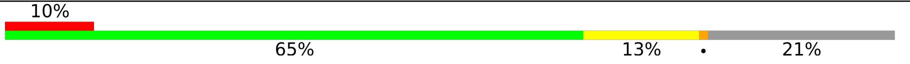
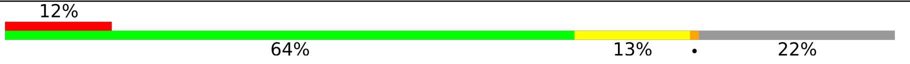
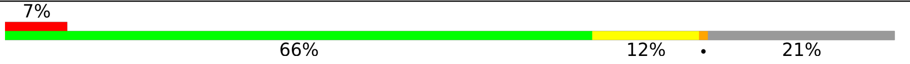
1	FJ	197	
1	GA	197	
1	GB	197	
1	GC	197	
1	GD	197	
1	GE	197	
1	GF	197	
1	GG	197	
1	GH	197	
1	GI	197	
1	GJ	197	
1	HA	197	
1	HB	197	
1	HC	197	
1	HD	197	
1	HE	197	
1	HF	197	
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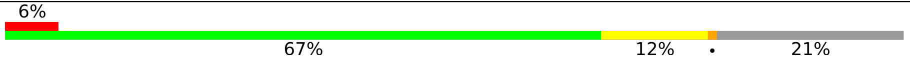
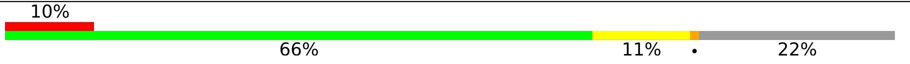
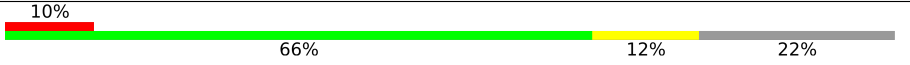
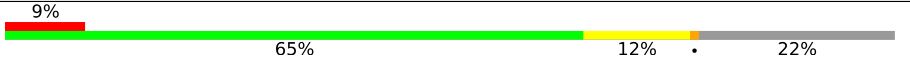
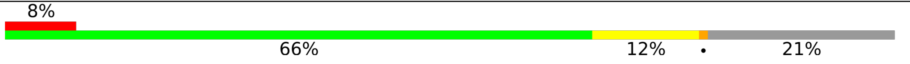
1	HI	197	
1	HJ	197	
1	IA	197	
1	IB	197	
1	IC	197	

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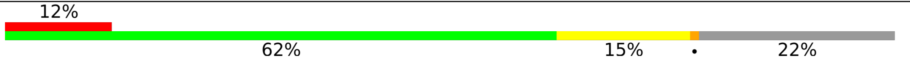
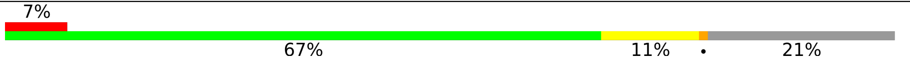
Mol	Chain	Length	Quality of chain
1	ID	197	
1	IE	197	
1	IF	197	
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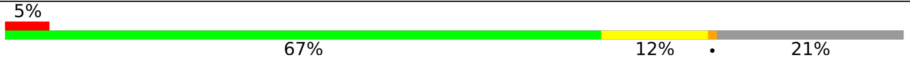
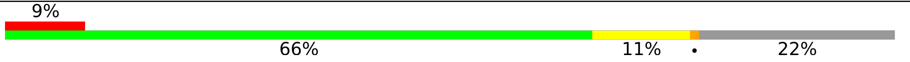
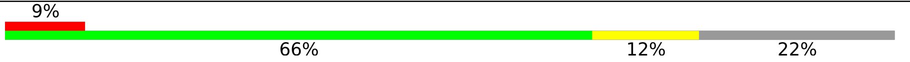
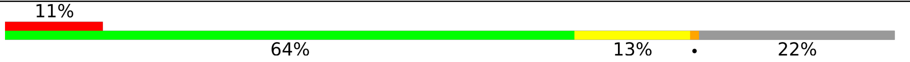
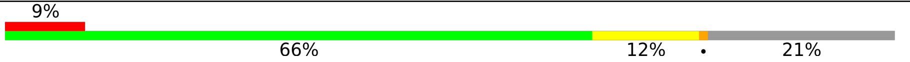
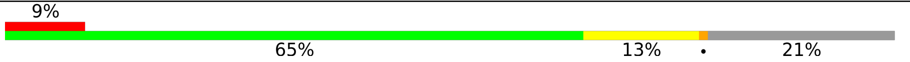
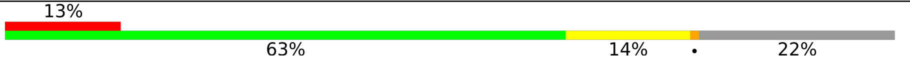
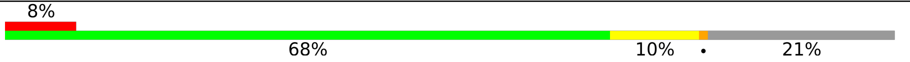
1	IH	197	
1	II	197	
1	IJ	197	
1	JA	197	
1	JB	197	
1	JC	197	
1	JD	197	
1	JE	197	
1	JF	197	
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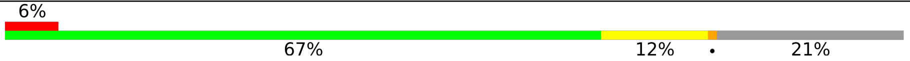
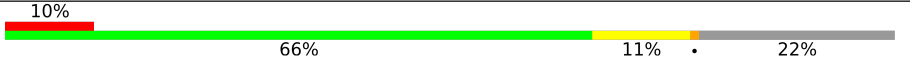
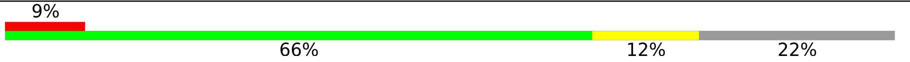
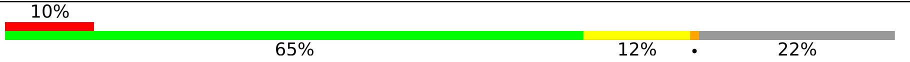
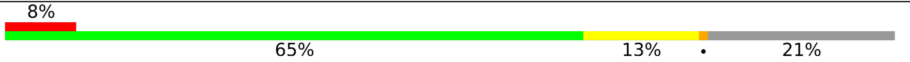
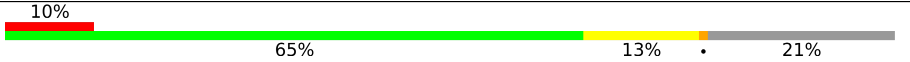
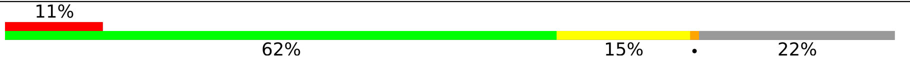
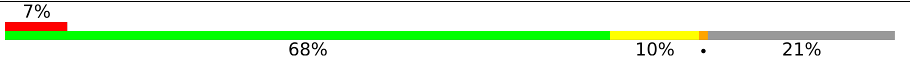
1	JH	197	
1	JI	197	
1	JJ	197	
1	KA	197	
1	KB	197	
1	KC	197	
1	KD	197	
1	KE	197	
1	KF	197	
1	KG	197	
1	KH	197	

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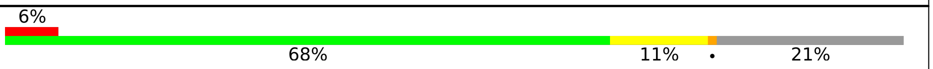
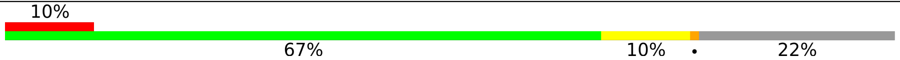
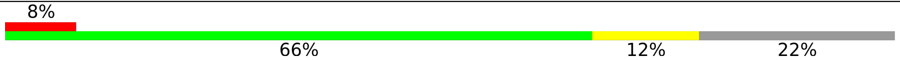
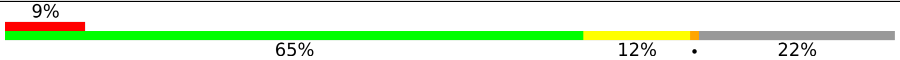
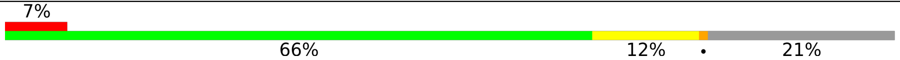
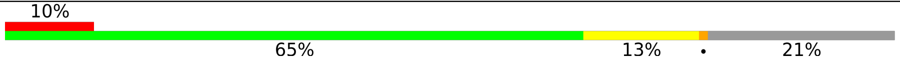
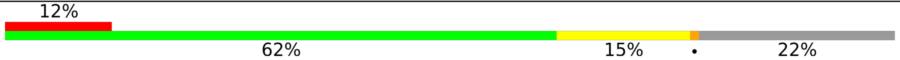
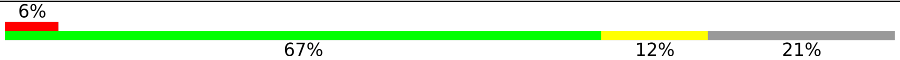
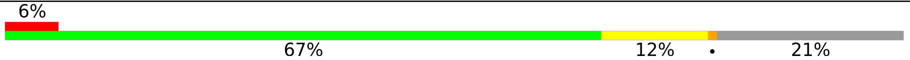
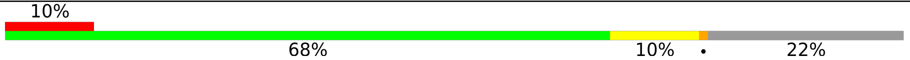
Mol	Chain	Length	Quality of chain
1	KI	197	
1	KJ	197	
1	LA	197	
1	LB	197	
1	LC	197	
1	LD	197	
1	LE	197	
1	LF	197	
1	LG	197	
1	LH	197	
1	LI	197	
1	LJ	197	

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 141432 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	AA	154	Total 1174	C 743	N 209	O 219	S 3	0	0
1	AB	154	Total 1174	C 743	N 209	O 219	S 3	0	0
1	AC	155	Total 1182	C 748	N 210	O 221	S 3	0	0
1	AD	155	Total 1182	C 748	N 210	O 221	S 3	0	0
1	AE	153	Total 1170	C 741	N 208	O 218	S 3	0	0
1	AF	155	Total 1182	C 748	N 210	O 221	S 3	0	0
1	AG	155	Total 1182	C 748	N 210	O 221	S 3	0	0
1	AH	155	Total 1182	C 748	N 210	O 221	S 3	0	0
1	AI	156	Total 1188	C 751	N 211	O 223	S 3	0	0
1	AJ	153	Total 1170	C 741	N 208	O 218	S 3	0	0
1	BA	154	Total 1174	C 743	N 209	O 219	S 3	0	0
1	BB	154	Total 1174	C 743	N 209	O 219	S 3	0	0
1	BC	155	Total 1182	C 748	N 210	O 221	S 3	0	0
1	BD	155	Total 1182	C 748	N 210	O 221	S 3	0	0
1	BE	153	Total 1170	C 741	N 208	O 218	S 3	0	0
1	BF	155	Total 1182	C 748	N 210	O 221	S 3	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	BG	155	Total C N O S 1182 748 210 221 3	0	0
1	BH	155	Total C N O S 1182 748 210 221 3	0	0
1	BI	156	Total C N O S 1188 751 211 223 3	0	0
1	BJ	153	Total C N O S 1170 741 208 218 3	0	0
1	CA	154	Total C N O S 1174 743 209 219 3	0	0
1	CB	154	Total C N O S 1174 743 209 219 3	0	0
1	CC	155	Total C N O S 1182 748 210 221 3	0	0
1	CD	155	Total C N O S 1182 748 210 221 3	0	0
1	CE	153	Total C N O S 1170 741 208 218 3	0	0
1	CF	155	Total C N O S 1182 748 210 221 3	0	0
1	CG	155	Total C N O S 1182 748 210 221 3	0	0
1	CH	155	Total C N O S 1182 748 210 221 3	0	0
1	CI	156	Total C N O S 1188 751 211 223 3	0	0
1	CJ	153	Total C N O S 1170 741 208 218 3	0	0
1	DA	154	Total C N O S 1174 743 209 219 3	0	0
1	DB	154	Total C N O S 1174 743 209 219 3	0	0
1	DC	155	Total C N O S 1182 748 210 221 3	0	0
1	DD	155	Total C N O S 1182 748 210 221 3	0	0
1	DE	153	Total C N O S 1170 741 208 218 3	0	0
1	DF	155	Total C N O S 1182 748 210 221 3	0	0
1	DG	155	Total C N O S 1182 748 210 221 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	DH	155	1182	748	210	221	3	0	0
1	DI	156	1188	751	211	223	3	0	0
1	DJ	153	1170	741	208	218	3	0	0
1	EA	154	1174	743	209	219	3	0	0
1	EB	154	1174	743	209	219	3	0	0
1	EC	155	1182	748	210	221	3	0	0
1	ED	155	1182	748	210	221	3	0	0
1	EE	153	1170	741	208	218	3	0	0
1	EF	155	1182	748	210	221	3	0	0
1	EG	155	1182	748	210	221	3	0	0
1	EH	155	1182	748	210	221	3	0	0
1	EI	156	1188	751	211	223	3	0	0
1	EJ	153	1170	741	208	218	3	0	0
1	FA	154	1174	743	209	219	3	0	0
1	FB	154	1174	743	209	219	3	0	0
1	FC	155	1182	748	210	221	3	0	0
1	FD	155	1182	748	210	221	3	0	0
1	FE	153	1170	741	208	218	3	0	0
1	FF	155	1182	748	210	221	3	0	0
1	FG	155	1182	748	210	221	3	0	0
1	FH	155	1182	748	210	221	3	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	FI	156	Total C N O S 1188 751 211 223 3	0	0
1	FJ	153	Total C N O S 1170 741 208 218 3	0	0
1	GA	154	Total C N O S 1174 743 209 219 3	0	0
1	GB	154	Total C N O S 1174 743 209 219 3	0	0
1	GC	155	Total C N O S 1182 748 210 221 3	0	0
1	GD	155	Total C N O S 1182 748 210 221 3	0	0
1	GE	153	Total C N O S 1170 741 208 218 3	0	0
1	GF	155	Total C N O S 1182 748 210 221 3	0	0
1	GG	155	Total C N O S 1182 748 210 221 3	0	0
1	GH	155	Total C N O S 1182 748 210 221 3	0	0
1	GI	156	Total C N O S 1188 751 211 223 3	0	0
1	GJ	153	Total C N O S 1170 741 208 218 3	0	0
1	HA	154	Total C N O S 1174 743 209 219 3	0	0
1	HB	154	Total C N O S 1174 743 209 219 3	0	0
1	HC	155	Total C N O S 1182 748 210 221 3	0	0
1	HD	155	Total C N O S 1182 748 210 221 3	0	0
1	HE	153	Total C N O S 1170 741 208 218 3	0	0
1	HF	155	Total C N O S 1182 748 210 221 3	0	0
1	HG	155	Total C N O S 1182 748 210 221 3	0	0
1	HH	155	Total C N O S 1182 748 210 221 3	0	0
1	HI	156	Total C N O S 1188 751 211 223 3	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	HJ	153	Total C N O S 1170 741 208 218 3	0	0
1	IA	154	Total C N O S 1174 743 209 219 3	0	0
1	IB	154	Total C N O S 1174 743 209 219 3	0	0
1	IC	155	Total C N O S 1182 748 210 221 3	0	0
1	ID	155	Total C N O S 1182 748 210 221 3	0	0
1	IE	153	Total C N O S 1170 741 208 218 3	0	0
1	IF	155	Total C N O S 1182 748 210 221 3	0	0
1	IG	155	Total C N O S 1182 748 210 221 3	0	0
1	IH	155	Total C N O S 1182 748 210 221 3	0	0
1	II	156	Total C N O S 1188 751 211 223 3	0	0
1	IJ	153	Total C N O S 1170 741 208 218 3	0	0
1	JA	154	Total C N O S 1174 743 209 219 3	0	0
1	JB	154	Total C N O S 1174 743 209 219 3	0	0
1	JC	155	Total C N O S 1182 748 210 221 3	0	0
1	JD	155	Total C N O S 1182 748 210 221 3	0	0
1	JE	153	Total C N O S 1170 741 208 218 3	0	0
1	JF	155	Total C N O S 1182 748 210 221 3	0	0
1	JG	155	Total C N O S 1182 748 210 221 3	0	0
1	JH	155	Total C N O S 1182 748 210 221 3	0	0
1	JI	156	Total C N O S 1188 751 211 223 3	0	0
1	JJ	153	Total C N O S 1170 741 208 218 3	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	KA	154	Total C N O S 1174 743 209 219 3	0	0
1	KB	154	Total C N O S 1174 743 209 219 3	0	0
1	KC	155	Total C N O S 1182 748 210 221 3	0	0
1	KD	155	Total C N O S 1182 748 210 221 3	0	0
1	KE	153	Total C N O S 1170 741 208 218 3	0	0
1	KF	155	Total C N O S 1182 748 210 221 3	0	0
1	KG	155	Total C N O S 1182 748 210 221 3	0	0
1	KH	155	Total C N O S 1182 748 210 221 3	0	0
1	KI	156	Total C N O S 1188 751 211 223 3	0	0
1	KJ	153	Total C N O S 1170 741 208 218 3	0	0
1	LA	154	Total C N O S 1174 743 209 219 3	0	0
1	LB	154	Total C N O S 1174 743 209 219 3	0	0
1	LC	155	Total C N O S 1182 748 210 221 3	0	0
1	LD	155	Total C N O S 1182 748 210 221 3	0	0
1	LE	153	Total C N O S 1170 741 208 218 3	0	0
1	LF	155	Total C N O S 1182 748 210 221 3	0	0
1	LG	155	Total C N O S 1182 748 210 221 3	0	0
1	LH	155	Total C N O S 1182 748 210 221 3	0	0
1	LI	156	Total C N O S 1188 751 211 223 3	0	0
1	LJ	153	Total C N O S 1170 741 208 218 3	0	0

There are 3240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1	MET	-	cloning artifact	UNP P03045
AA	2	GLY	-	cloning artifact	UNP P03045
AA	3	ASN	-	cloning artifact	UNP P03045
AA	4	ALA	-	cloning artifact	UNP P03045
AA	5	LYS	-	cloning artifact	UNP P03045
AA	6	THR	-	cloning artifact	UNP P03045
AA	24	ALA	-	linker	UNP P03045
AA	25	GLY	-	linker	UNP P03045
AA	26	ALA	-	linker	UNP P03045
AA	27	GLY	-	linker	UNP P03045
AA	28	ALA	-	linker	UNP P03045
AA	29	GLY	-	linker	UNP P03045
AA	30	ALA	-	linker	UNP P03045
AA	31	MET	-	linker	UNP P03045
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
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	102	GLY	-	linker	UNP O66529
AB	103	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
AB	104	GLY	-	linker	UNP O66529
AB	105	HIS	-	linker	UNP O66529
AB	106	HIS	-	linker	UNP O66529
AB	107	HIS	-	linker	UNP O66529
AB	108	HIS	-	linker	UNP O66529
AB	109	HIS	-	linker	UNP O66529
AB	110	HIS	-	linker	UNP O66529
AB	111	GLY	-	linker	UNP O66529
AB	112	SER	-	linker	UNP O66529
AB	113	SER	-	linker	UNP O66529
AB	115	GLU	GLN	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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
AI	1	MET	-	cloning artifact	UNP P03045
AI	2	GLY	-	cloning artifact	UNP P03045
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
AJ	28	ALA	-	linker	UNP P03045
AJ	29	GLY	-	linker	UNP P03045
AJ	30	ALA	-	linker	UNP P03045
AJ	31	MET	-	linker	UNP P03045
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
BA	1	MET	-	cloning artifact	UNP P03045
BA	2	GLY	-	cloning artifact	UNP P03045
BA	3	ASN	-	cloning artifact	UNP P03045
BA	4	ALA	-	cloning artifact	UNP P03045
BA	5	LYS	-	cloning artifact	UNP P03045
BA	6	THR	-	cloning artifact	UNP P03045
BA	24	ALA	-	linker	UNP P03045
BA	25	GLY	-	linker	UNP P03045
BA	26	ALA	-	linker	UNP P03045
BA	27	GLY	-	linker	UNP P03045
BA	28	ALA	-	linker	UNP P03045
BA	29	GLY	-	linker	UNP P03045
BA	30	ALA	-	linker	UNP P03045
BA	31	MET	-	linker	UNP P03045
BA	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

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Chain	Residue	Modelled	Actual	Comment	Reference
BA	113	SER	-	linker	UNP O66529
BA	115	GLU	GLN	engineered mutation	UNP O66529
BB	1	MET	-	cloning artifact	UNP P03045
BB	2	GLY	-	cloning artifact	UNP P03045
BB	3	ASN	-	cloning artifact	UNP P03045
BB	4	ALA	-	cloning artifact	UNP P03045
BB	5	LYS	-	cloning artifact	UNP P03045
BB	6	THR	-	cloning artifact	UNP P03045
BB	24	ALA	-	linker	UNP P03045
BB	25	GLY	-	linker	UNP P03045
BB	26	ALA	-	linker	UNP P03045
BB	27	GLY	-	linker	UNP P03045
BB	28	ALA	-	linker	UNP P03045
BB	29	GLY	-	linker	UNP P03045
BB	30	ALA	-	linker	UNP P03045
BB	31	MET	-	linker	UNP P03045
BB	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
BC	31	MET	-	linker	UNP P03045
BC	102	GLY	-	linker	UNP O66529
BC	103	THR	-	linker	UNP O66529
BC	104	GLY	-	linker	UNP O66529
BC	105	HIS	-	linker	UNP O66529
BC	106	HIS	-	linker	UNP O66529
BC	107	HIS	-	linker	UNP O66529
BC	108	HIS	-	linker	UNP O66529
BC	109	HIS	-	linker	UNP O66529
BC	110	HIS	-	linker	UNP O66529
BC	111	GLY	-	linker	UNP O66529
BC	112	SER	-	linker	UNP O66529
BC	113	SER	-	linker	UNP O66529
BC	115	GLU	GLN	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	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
BE	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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
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	102	GLY	-	linker	UNP O66529
BF	103	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
BJ	1	MET	-	cloning artifact	UNP P03045
BJ	2	GLY	-	cloning artifact	UNP P03045
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	102	GLY	-	linker	UNP O66529
CA	103	THR	-	linker	UNP O66529
CA	104	GLY	-	linker	UNP O66529
CA	105	HIS	-	linker	UNP O66529
CA	106	HIS	-	linker	UNP O66529
CA	107	HIS	-	linker	UNP O66529
CA	108	HIS	-	linker	UNP O66529
CA	109	HIS	-	linker	UNP O66529
CA	110	HIS	-	linker	UNP O66529
CA	111	GLY	-	linker	UNP O66529
CA	112	SER	-	linker	UNP O66529
CA	113	SER	-	linker	UNP O66529
CA	115	GLU	GLN	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	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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
CE	113	SER	-	linker	UNP O66529
CE	115	GLU	GLN	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	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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
CG	31	MET	-	linker	UNP P03045
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
CH	1	MET	-	cloning artifact	UNP P03045
CH	2	GLY	-	cloning artifact	UNP P03045
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	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
CI	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
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
CI	29	GLY	-	linker	UNP P03045
CI	30	ALA	-	linker	UNP P03045
CI	31	MET	-	linker	UNP P03045
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
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	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
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
DC	1	MET	-	cloning artifact	UNP P03045
DC	2	GLY	-	cloning artifact	UNP P03045
DC	3	ASN	-	cloning artifact	UNP P03045
DC	4	ALA	-	cloning artifact	UNP P03045
DC	5	LYS	-	cloning artifact	UNP P03045
DC	6	THR	-	cloning artifact	UNP P03045
DC	24	ALA	-	linker	UNP P03045
DC	25	GLY	-	linker	UNP P03045
DC	26	ALA	-	linker	UNP P03045
DC	27	GLY	-	linker	UNP P03045
DC	28	ALA	-	linker	UNP P03045
DC	29	GLY	-	linker	UNP P03045
DC	30	ALA	-	linker	UNP P03045
DC	31	MET	-	linker	UNP P03045
DC	102	GLY	-	linker	UNP O66529
DC	103	THR	-	linker	UNP O66529
DC	104	GLY	-	linker	UNP O66529
DC	105	HIS	-	linker	UNP O66529
DC	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
DC	107	HIS	-	linker	UNP O66529
DC	108	HIS	-	linker	UNP O66529
DC	109	HIS	-	linker	UNP O66529
DC	110	HIS	-	linker	UNP O66529
DC	111	GLY	-	linker	UNP O66529
DC	112	SER	-	linker	UNP O66529
DC	113	SER	-	linker	UNP O66529
DC	115	GLU	GLN	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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
DG	1	MET	-	cloning artifact	UNP P03045
DG	2	GLY	-	cloning artifact	UNP P03045
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
DH	28	ALA	-	linker	UNP P03045
DH	29	GLY	-	linker	UNP P03045
DH	30	ALA	-	linker	UNP P03045
DH	31	MET	-	linker	UNP P03045
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
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	102	GLY	-	linker	UNP O66529
DI	103	THR	-	linker	UNP O66529
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

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Chain	Residue	Modelled	Actual	Comment	Reference
DI	113	SER	-	linker	UNP O66529
DI	115	GLU	GLN	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	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
DJ	113	SER	-	linker	UNP O66529
DJ	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
EA	31	MET	-	linker	UNP P03045
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
EB	1	MET	-	cloning artifact	UNP P03045
EB	2	GLY	-	cloning artifact	UNP P03045
EB	3	ASN	-	cloning artifact	UNP P03045
EB	4	ALA	-	cloning artifact	UNP P03045
EB	5	LYS	-	cloning artifact	UNP P03045
EB	6	THR	-	cloning artifact	UNP P03045
EB	24	ALA	-	linker	UNP P03045
EB	25	GLY	-	linker	UNP P03045
EB	26	ALA	-	linker	UNP P03045
EB	27	GLY	-	linker	UNP P03045
EB	28	ALA	-	linker	UNP P03045
EB	29	GLY	-	linker	UNP P03045
EB	30	ALA	-	linker	UNP P03045
EB	31	MET	-	linker	UNP P03045
EB	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
EC	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
EC	2	GLY	-	cloning artifact	UNP P03045
EC	3	ASN	-	cloning artifact	UNP P03045
EC	4	ALA	-	cloning artifact	UNP P03045
EC	5	LYS	-	cloning artifact	UNP P03045
EC	6	THR	-	cloning artifact	UNP P03045
EC	24	ALA	-	linker	UNP P03045
EC	25	GLY	-	linker	UNP P03045
EC	26	ALA	-	linker	UNP P03045
EC	27	GLY	-	linker	UNP P03045
EC	28	ALA	-	linker	UNP P03045
EC	29	GLY	-	linker	UNP P03045
EC	30	ALA	-	linker	UNP P03045
EC	31	MET	-	linker	UNP P03045
EC	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
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	102	GLY	-	linker	UNP O66529
ED	103	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
ED	104	GLY	-	linker	UNP O66529
ED	105	HIS	-	linker	UNP O66529
ED	106	HIS	-	linker	UNP O66529
ED	107	HIS	-	linker	UNP O66529
ED	108	HIS	-	linker	UNP O66529
ED	109	HIS	-	linker	UNP O66529
ED	110	HIS	-	linker	UNP O66529
ED	111	GLY	-	linker	UNP O66529
ED	112	SER	-	linker	UNP O66529
ED	113	SER	-	linker	UNP O66529
ED	115	GLU	GLN	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	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
EF	1	MET	-	cloning artifact	UNP P03045
EF	2	GLY	-	cloning artifact	UNP P03045
EF	3	ASN	-	cloning artifact	UNP P03045
EF	4	ALA	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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
EG	29	GLY	-	linker	UNP P03045
EG	30	ALA	-	linker	UNP P03045
EG	31	MET	-	linker	UNP P03045
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	102	GLY	-	linker	UNP O66529
EH	103	THR	-	linker	UNP O66529
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
EI	113	SER	-	linker	UNP O66529
EI	115	GLU	GLN	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	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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	102	GLY	-	linker	UNP O66529
FC	103	THR	-	linker	UNP O66529
FC	104	GLY	-	linker	UNP O66529
FC	105	HIS	-	linker	UNP O66529
FC	106	HIS	-	linker	UNP O66529
FC	107	HIS	-	linker	UNP O66529
FC	108	HIS	-	linker	UNP O66529
FC	109	HIS	-	linker	UNP O66529
FC	110	HIS	-	linker	UNP O66529
FC	111	GLY	-	linker	UNP O66529
FC	112	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
FC	113	SER	-	linker	UNP O66529
FC	115	GLU	GLN	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	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
FE	1	MET	-	cloning artifact	UNP P03045
FE	2	GLY	-	cloning artifact	UNP P03045
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

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Chain	Residue	Modelled	Actual	Comment	Reference
FE	31	MET	-	linker	UNP P03045
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
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
FF	29	GLY	-	linker	UNP P03045
FF	30	ALA	-	linker	UNP P03045
FF	31	MET	-	linker	UNP P03045
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
FG	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
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	102	GLY	-	linker	UNP O66529
FG	103	THR	-	linker	UNP O66529
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
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	102	GLY	-	linker	UNP O66529
FH	103	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
FH	113	SER	-	linker	UNP O66529
FH	115	GLU	GLN	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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
FJ	5	LYS	-	cloning artifact	UNP P03045
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	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
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	102	GLY	-	linker	UNP O66529
GA	103	THR	-	linker	UNP O66529
GA	104	GLY	-	linker	UNP O66529
GA	105	HIS	-	linker	UNP O66529
GA	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
GA	107	HIS	-	linker	UNP O66529
GA	108	HIS	-	linker	UNP O66529
GA	109	HIS	-	linker	UNP O66529
GA	110	HIS	-	linker	UNP O66529
GA	111	GLY	-	linker	UNP O66529
GA	112	SER	-	linker	UNP O66529
GA	113	SER	-	linker	UNP O66529
GA	115	GLU	GLN	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	102	GLY	-	linker	UNP O66529
GB	103	THR	-	linker	UNP O66529
GB	104	GLY	-	linker	UNP O66529
GB	105	HIS	-	linker	UNP O66529
GB	106	HIS	-	linker	UNP O66529
GB	107	HIS	-	linker	UNP O66529
GB	108	HIS	-	linker	UNP O66529
GB	109	HIS	-	linker	UNP O66529
GB	110	HIS	-	linker	UNP O66529
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
GD	1	MET	-	cloning artifact	UNP P03045
GD	2	GLY	-	cloning artifact	UNP P03045
GD	3	ASN	-	cloning artifact	UNP P03045
GD	4	ALA	-	cloning artifact	UNP P03045
GD	5	LYS	-	cloning artifact	UNP P03045
GD	6	THR	-	cloning artifact	UNP P03045
GD	24	ALA	-	linker	UNP P03045
GD	25	GLY	-	linker	UNP P03045
GD	26	ALA	-	linker	UNP P03045
GD	27	GLY	-	linker	UNP P03045
GD	28	ALA	-	linker	UNP P03045
GD	29	GLY	-	linker	UNP P03045
GD	30	ALA	-	linker	UNP P03045
GD	31	MET	-	linker	UNP P03045
GD	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
GE	29	GLY	-	linker	UNP P03045
GE	30	ALA	-	linker	UNP P03045
GE	31	MET	-	linker	UNP P03045
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	102	GLY	-	linker	UNP O66529
GF	103	THR	-	linker	UNP O66529
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
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	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
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	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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
GI	31	MET	-	linker	UNP P03045
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
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
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
HA	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
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	102	GLY	-	linker	UNP O66529
HA	103	THR	-	linker	UNP O66529
HA	104	GLY	-	linker	UNP O66529
HA	105	HIS	-	linker	UNP O66529
HA	106	HIS	-	linker	UNP O66529
HA	107	HIS	-	linker	UNP O66529
HA	108	HIS	-	linker	UNP O66529
HA	109	HIS	-	linker	UNP O66529
HA	110	HIS	-	linker	UNP O66529
HA	111	GLY	-	linker	UNP O66529
HA	112	SER	-	linker	UNP O66529
HA	113	SER	-	linker	UNP O66529
HA	115	GLU	GLN	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	102	GLY	-	linker	UNP O66529
HB	103	THR	-	linker	UNP O66529

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
HD	29	GLY	-	linker	UNP P03045
HD	30	ALA	-	linker	UNP P03045
HD	31	MET	-	linker	UNP P03045
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
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	102	GLY	-	linker	UNP O66529
HE	103	THR	-	linker	UNP O66529
HE	104	GLY	-	linker	UNP O66529
HE	105	HIS	-	linker	UNP O66529
HE	106	HIS	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	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
HF	113	SER	-	linker	UNP O66529
HF	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
IA	113	SER	-	linker	UNP O66529
IA	115	GLU	GLN	engineered mutation	UNP O66529
IB	1	MET	-	cloning artifact	UNP P03045
IB	2	GLY	-	cloning artifact	UNP P03045
IB	3	ASN	-	cloning artifact	UNP P03045
IB	4	ALA	-	cloning artifact	UNP P03045
IB	5	LYS	-	cloning artifact	UNP P03045
IB	6	THR	-	cloning artifact	UNP P03045
IB	24	ALA	-	linker	UNP P03045
IB	25	GLY	-	linker	UNP P03045
IB	26	ALA	-	linker	UNP P03045
IB	27	GLY	-	linker	UNP P03045
IB	28	ALA	-	linker	UNP P03045
IB	29	GLY	-	linker	UNP P03045
IB	30	ALA	-	linker	UNP P03045
IB	31	MET	-	linker	UNP P03045
IB	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
IC	1	MET	-	cloning artifact	UNP P03045
IC	2	GLY	-	cloning artifact	UNP P03045
IC	3	ASN	-	cloning artifact	UNP P03045
IC	4	ALA	-	cloning artifact	UNP P03045
IC	5	LYS	-	cloning artifact	UNP P03045
IC	6	THR	-	cloning artifact	UNP P03045
IC	24	ALA	-	linker	UNP P03045
IC	25	GLY	-	linker	UNP P03045
IC	26	ALA	-	linker	UNP P03045
IC	27	GLY	-	linker	UNP P03045
IC	28	ALA	-	linker	UNP P03045
IC	29	GLY	-	linker	UNP P03045
IC	30	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
IC	31	MET	-	linker	UNP P03045
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
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	102	GLY	-	linker	UNP O66529
ID	103	THR	-	linker	UNP O66529
ID	104	GLY	-	linker	UNP O66529
ID	105	HIS	-	linker	UNP O66529
ID	106	HIS	-	linker	UNP O66529
ID	107	HIS	-	linker	UNP O66529
ID	108	HIS	-	linker	UNP O66529
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
IE	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
IE	113	SER	-	linker	UNP O66529
IE	115	GLU	GLN	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	102	GLY	-	linker	UNP O66529
IF	103	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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	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
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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
JB	1	MET	-	cloning artifact	UNP P03045
JB	2	GLY	-	cloning artifact	UNP P03045
JB	3	ASN	-	cloning artifact	UNP P03045
JB	4	ALA	-	cloning artifact	UNP P03045
JB	5	LYS	-	cloning artifact	UNP P03045
JB	6	THR	-	cloning artifact	UNP P03045
JB	24	ALA	-	linker	UNP P03045
JB	25	GLY	-	linker	UNP P03045
JB	26	ALA	-	linker	UNP P03045
JB	27	GLY	-	linker	UNP P03045
JB	28	ALA	-	linker	UNP P03045
JB	29	GLY	-	linker	UNP P03045
JB	30	ALA	-	linker	UNP P03045
JB	31	MET	-	linker	UNP P03045
JB	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	102	GLY	-	linker	UNP O66529
JC	103	THR	-	linker	UNP O66529
JC	104	GLY	-	linker	UNP O66529
JC	105	HIS	-	linker	UNP O66529
JC	106	HIS	-	linker	UNP O66529
JC	107	HIS	-	linker	UNP O66529
JC	108	HIS	-	linker	UNP O66529
JC	109	HIS	-	linker	UNP O66529
JC	110	HIS	-	linker	UNP O66529
JC	111	GLY	-	linker	UNP O66529
JC	112	SER	-	linker	UNP O66529
JC	113	SER	-	linker	UNP O66529
JC	115	GLU	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	102	GLY	-	linker	UNP O66529
JD	103	THR	-	linker	UNP O66529
JD	104	GLY	-	linker	UNP O66529
JD	105	HIS	-	linker	UNP O66529
JD	106	HIS	-	linker	UNP O66529
JD	107	HIS	-	linker	UNP O66529
JD	108	HIS	-	linker	UNP O66529
JD	109	HIS	-	linker	UNP O66529
JD	110	HIS	-	linker	UNP O66529
JD	111	GLY	-	linker	UNP O66529
JD	112	SER	-	linker	UNP O66529
JD	113	SER	-	linker	UNP O66529
JD	115	GLU	GLN	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
JE	113	SER	-	linker	UNP O66529
JE	115	GLU	GLN	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
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
JG	31	MET	-	linker	UNP P03045
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
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	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
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
JI	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	102	GLY	-	linker	UNP O66529
JJ	103	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
KA	1	MET	-	cloning artifact	UNP P03045
KA	2	GLY	-	cloning artifact	UNP P03045
KA	3	ASN	-	cloning artifact	UNP P03045
KA	4	ALA	-	cloning artifact	UNP P03045
KA	5	LYS	-	cloning artifact	UNP P03045
KA	6	THR	-	cloning artifact	UNP P03045
KA	24	ALA	-	linker	UNP P03045
KA	25	GLY	-	linker	UNP P03045
KA	26	ALA	-	linker	UNP P03045
KA	27	GLY	-	linker	UNP P03045
KA	28	ALA	-	linker	UNP P03045
KA	29	GLY	-	linker	UNP P03045
KA	30	ALA	-	linker	UNP P03045
KA	31	MET	-	linker	UNP P03045
KA	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	102	GLY	-	linker	UNP O66529
KB	103	THR	-	linker	UNP O66529
KB	104	GLY	-	linker	UNP O66529
KB	105	HIS	-	linker	UNP O66529
KB	106	HIS	-	linker	UNP O66529
KB	107	HIS	-	linker	UNP O66529
KB	108	HIS	-	linker	UNP O66529
KB	109	HIS	-	linker	UNP O66529
KB	110	HIS	-	linker	UNP O66529
KB	111	GLY	-	linker	UNP O66529
KB	112	SER	-	linker	UNP O66529
KB	113	SER	-	linker	UNP O66529
KB	115	GLU	GLN	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
KC	107	HIS	-	linker	UNP O66529
KC	108	HIS	-	linker	UNP O66529
KC	109	HIS	-	linker	UNP O66529
KC	110	HIS	-	linker	UNP O66529
KC	111	GLY	-	linker	UNP O66529
KC	112	SER	-	linker	UNP O66529
KC	113	SER	-	linker	UNP O66529
KC	115	GLU	GLN	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	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
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
KE	6	THR	-	cloning artifact	UNP P03045
KE	24	ALA	-	linker	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
KI	113	SER	-	linker	UNP O66529
KI	115	GLU	GLN	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
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
LA	31	MET	-	linker	UNP P03045
LA	102	GLY	-	linker	UNP O66529
LA	103	THR	-	linker	UNP O66529
LA	104	GLY	-	linker	UNP O66529
LA	105	HIS	-	linker	UNP O66529
LA	106	HIS	-	linker	UNP O66529
LA	107	HIS	-	linker	UNP O66529
LA	108	HIS	-	linker	UNP O66529
LA	109	HIS	-	linker	UNP O66529
LA	110	HIS	-	linker	UNP O66529
LA	111	GLY	-	linker	UNP O66529
LA	112	SER	-	linker	UNP O66529
LA	113	SER	-	linker	UNP O66529
LA	115	GLU	GLN	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	102	GLY	-	linker	UNP O66529
LB	103	THR	-	linker	UNP O66529
LB	104	GLY	-	linker	UNP O66529
LB	105	HIS	-	linker	UNP O66529
LB	106	HIS	-	linker	UNP O66529
LB	107	HIS	-	linker	UNP O66529
LB	108	HIS	-	linker	UNP O66529
LB	109	HIS	-	linker	UNP O66529
LB	110	HIS	-	linker	UNP O66529
LB	111	GLY	-	linker	UNP O66529
LB	112	SER	-	linker	UNP O66529
LB	113	SER	-	linker	UNP O66529
LB	115	GLU	GLN	engineered mutation	UNP O66529
LC	1	MET	-	cloning artifact	UNP P03045

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Chain	Residue	Modelled	Actual	Comment	Reference
LC	2	GLY	-	cloning artifact	UNP P03045
LC	3	ASN	-	cloning artifact	UNP P03045
LC	4	ALA	-	cloning artifact	UNP P03045
LC	5	LYS	-	cloning artifact	UNP P03045
LC	6	THR	-	cloning artifact	UNP P03045
LC	24	ALA	-	linker	UNP P03045
LC	25	GLY	-	linker	UNP P03045
LC	26	ALA	-	linker	UNP P03045
LC	27	GLY	-	linker	UNP P03045
LC	28	ALA	-	linker	UNP P03045
LC	29	GLY	-	linker	UNP P03045
LC	30	ALA	-	linker	UNP P03045
LC	31	MET	-	linker	UNP P03045
LC	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
LD	1	MET	-	cloning artifact	UNP P03045
LD	2	GLY	-	cloning artifact	UNP P03045
LD	3	ASN	-	cloning artifact	UNP P03045
LD	4	ALA	-	cloning artifact	UNP P03045
LD	5	LYS	-	cloning artifact	UNP P03045
LD	6	THR	-	cloning artifact	UNP P03045
LD	24	ALA	-	linker	UNP P03045
LD	25	GLY	-	linker	UNP P03045
LD	26	ALA	-	linker	UNP P03045
LD	27	GLY	-	linker	UNP P03045
LD	28	ALA	-	linker	UNP P03045
LD	29	GLY	-	linker	UNP P03045
LD	30	ALA	-	linker	UNP P03045
LD	31	MET	-	linker	UNP P03045
LD	102	GLY	-	linker	UNP O66529
LD	103	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
LI	25	GLY	-	linker	UNP P03045
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	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
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	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

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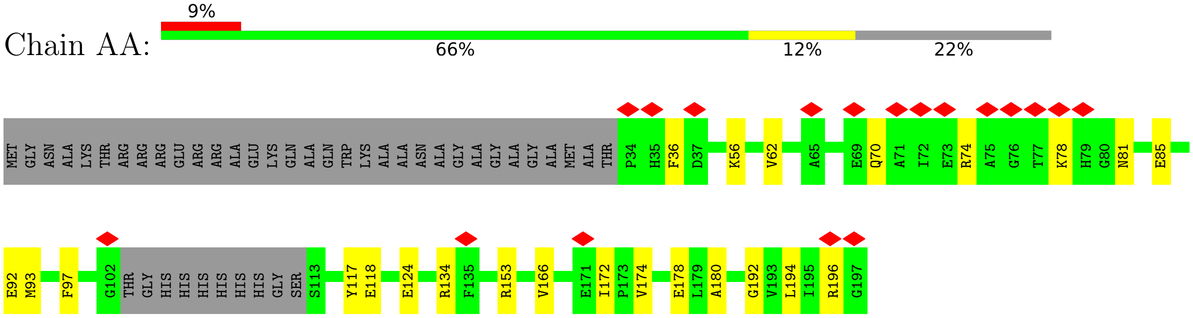
Chain	Residue	Modelled	Actual	Comment	Reference
LJ	110	HIS	-	linker	UNP O66529
LJ	111	GLY	-	linker	UNP O66529
LJ	112	SER	-	linker	UNP O66529
LJ	113	SER	-	linker	UNP O66529
LJ	115	GLU	GLN	engineered mutation	UNP O66529

3 Residue-property plots ⓘ

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

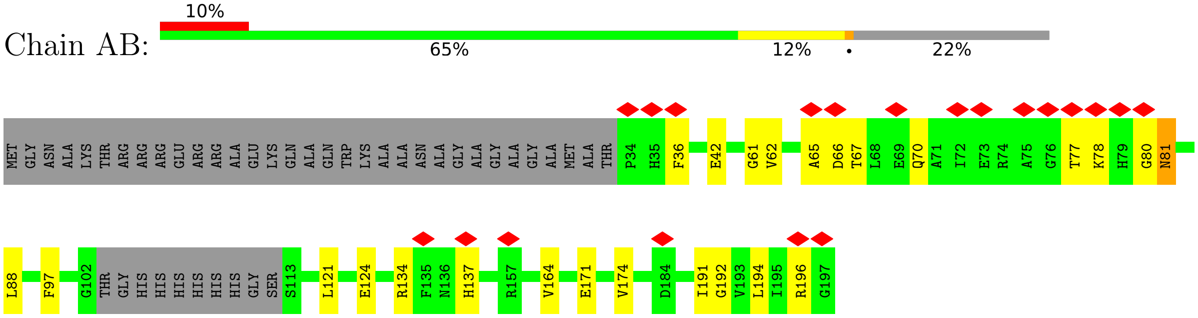
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AA:



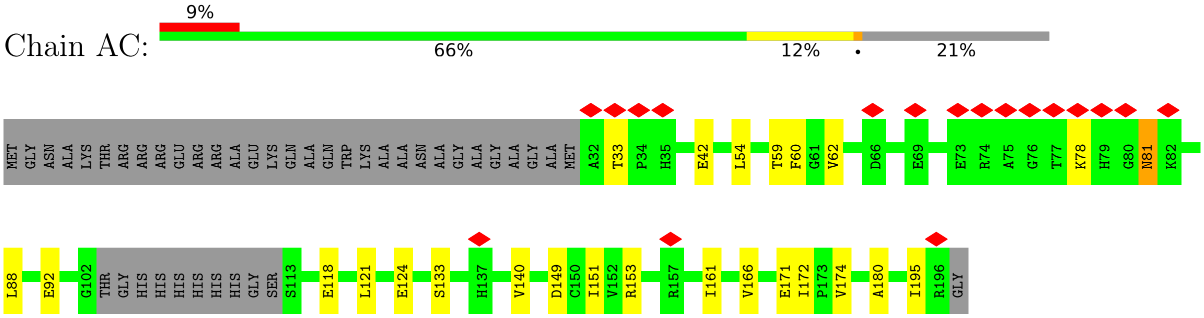
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AB:

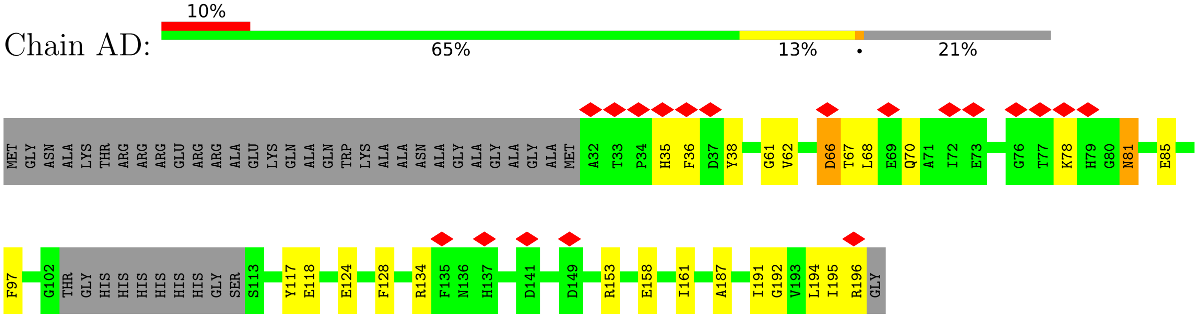


- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

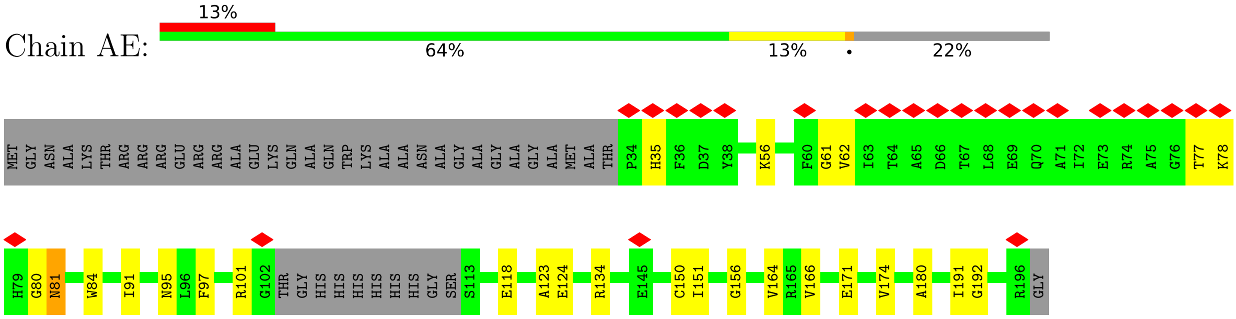
Chain AC:



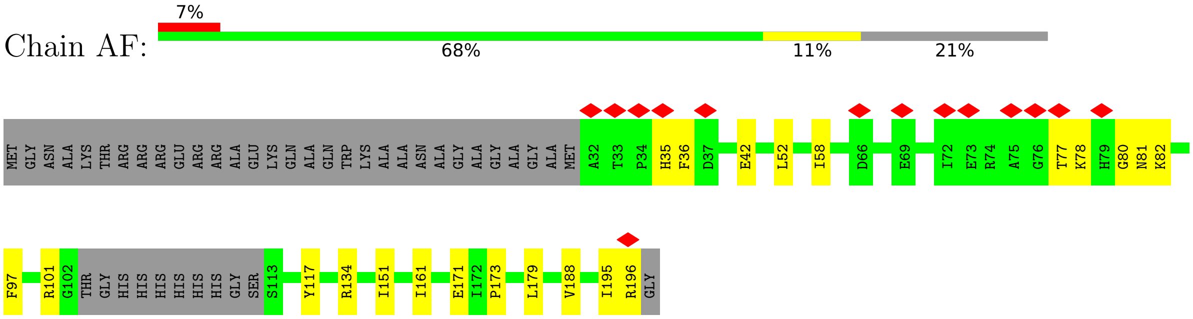
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase



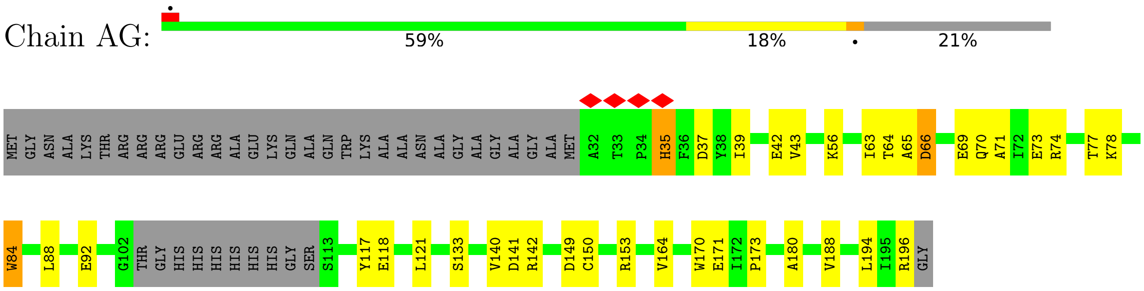
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase



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

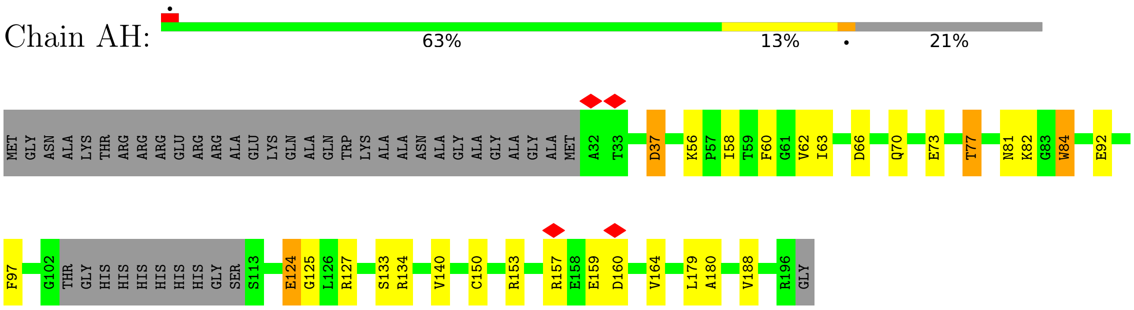


- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase



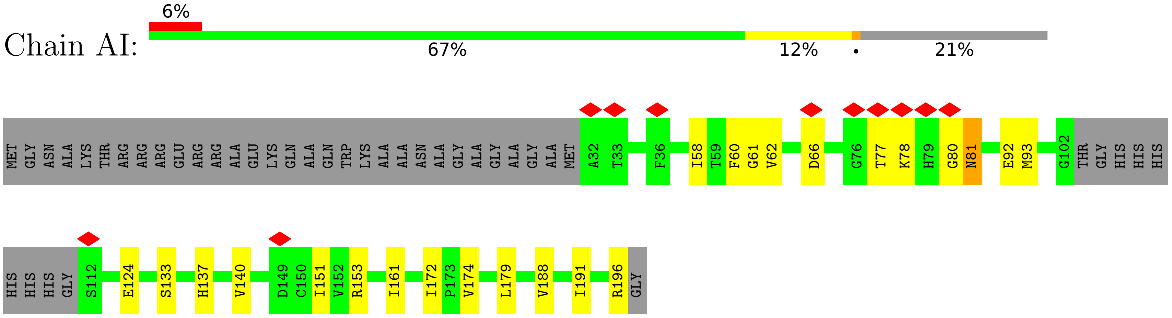
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AH:



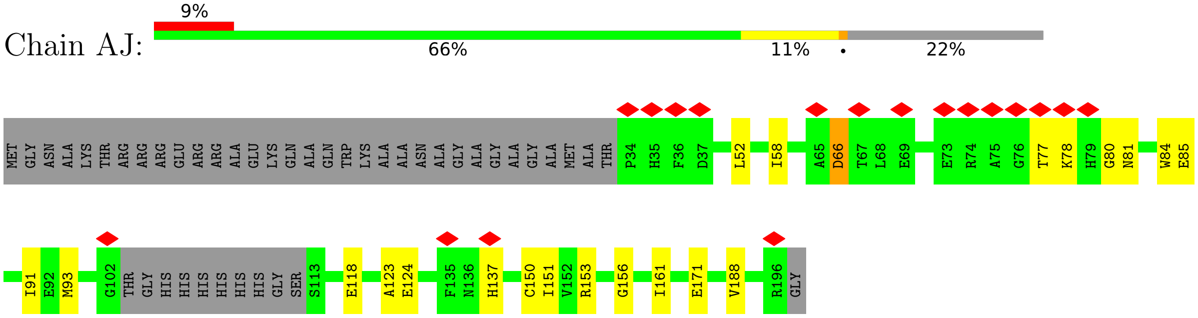
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AI:



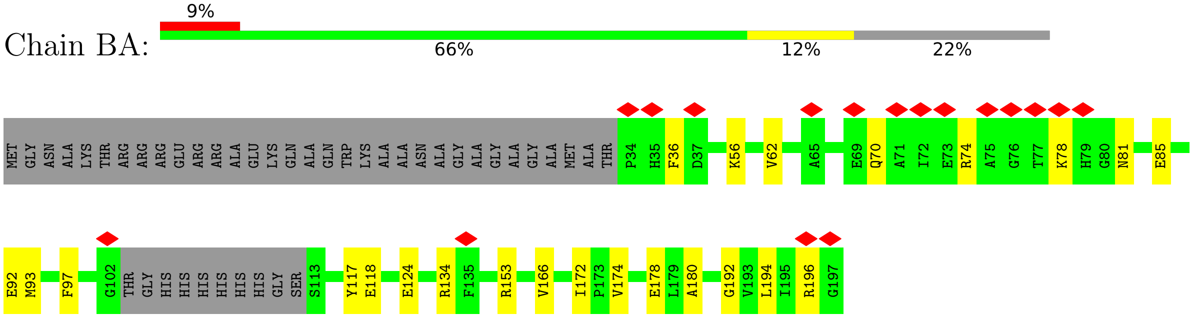
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain AJ:



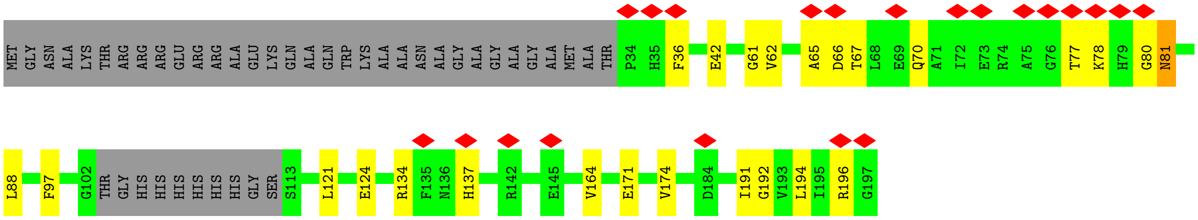
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BA:



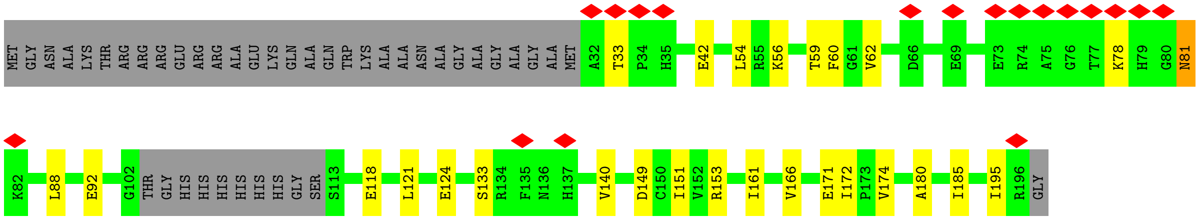
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BB:



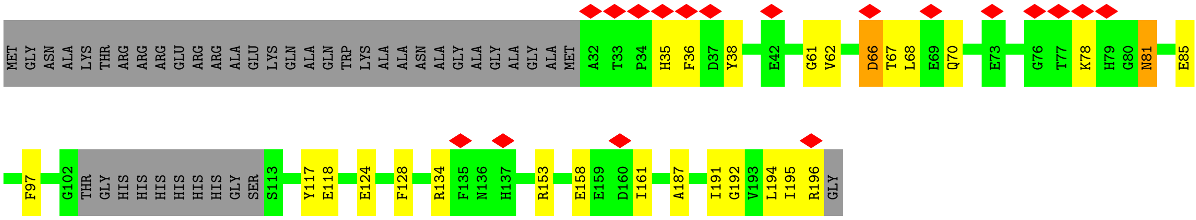
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BC:



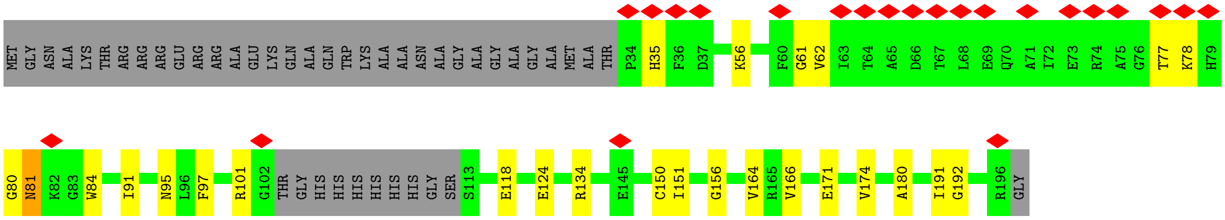
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BD:



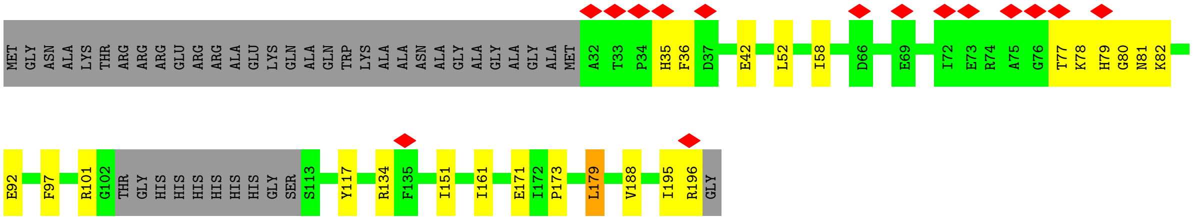
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BE:



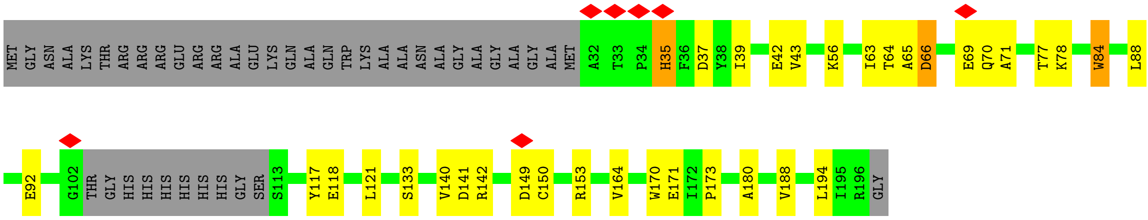
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BF:



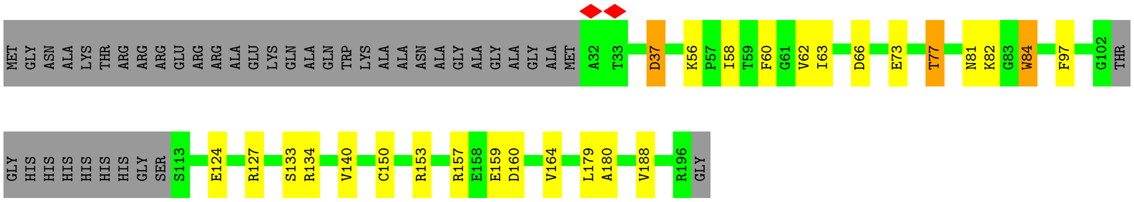
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BG:



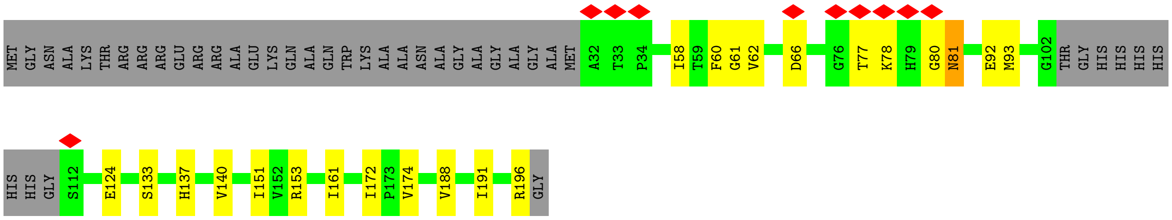
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BH:



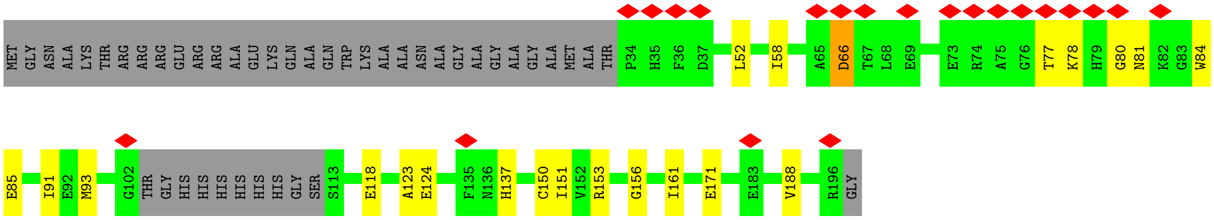
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BI:



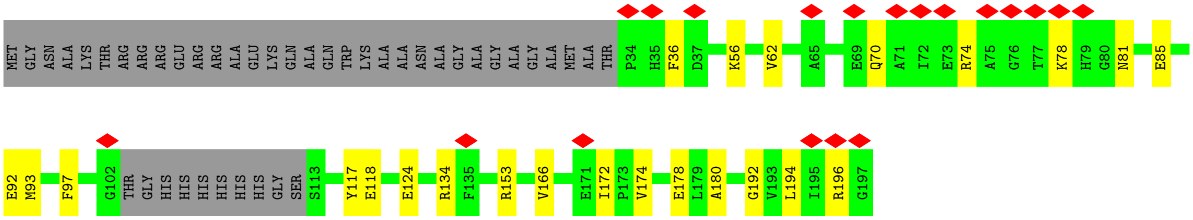
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain BJ:



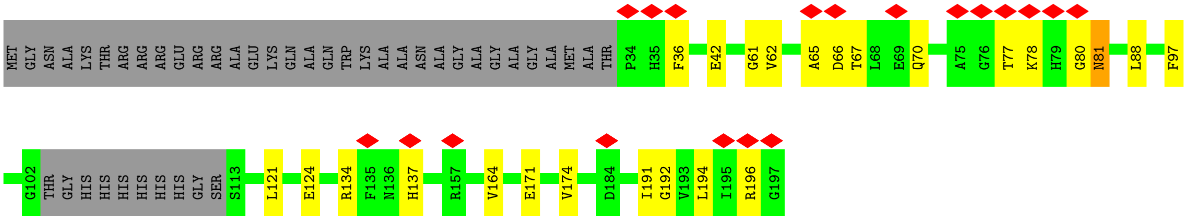
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CA:



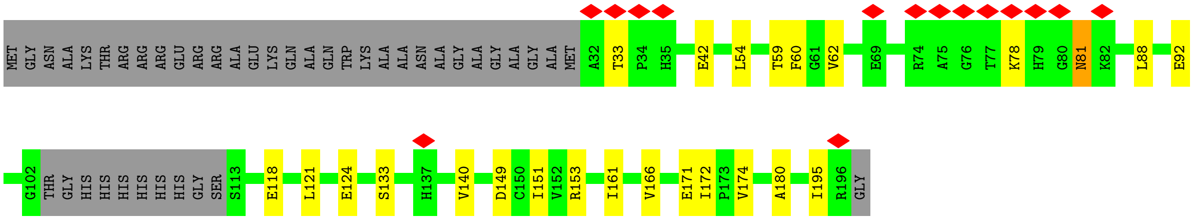
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CB:



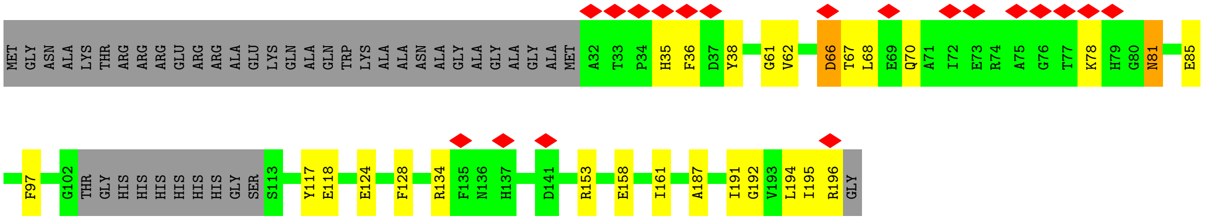
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CC:



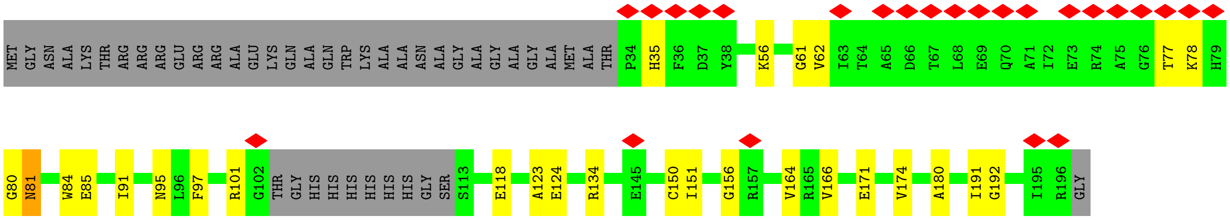
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CD:



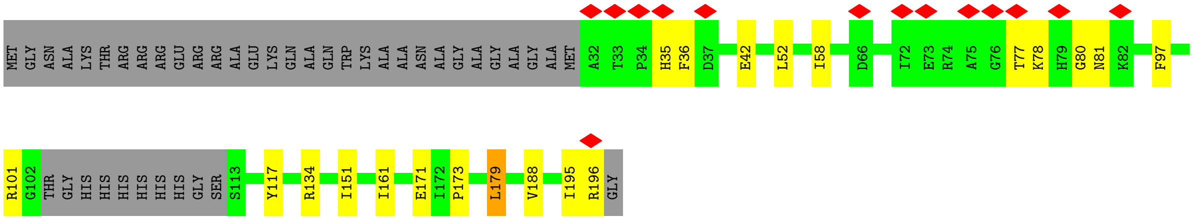
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CE:



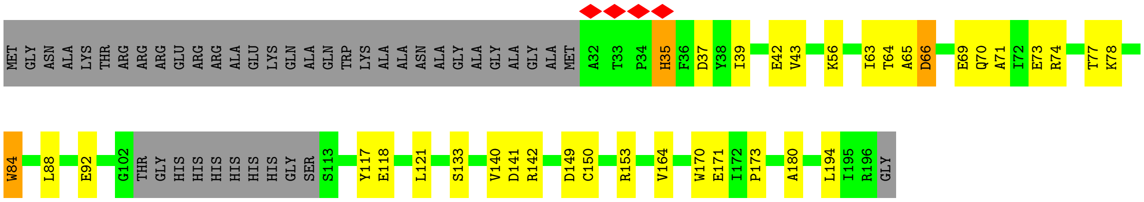
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CF:



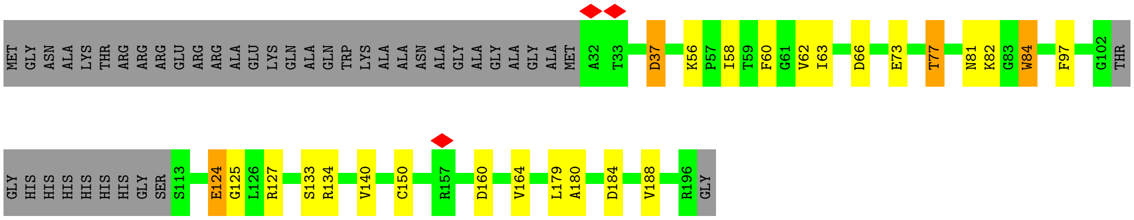
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CG:



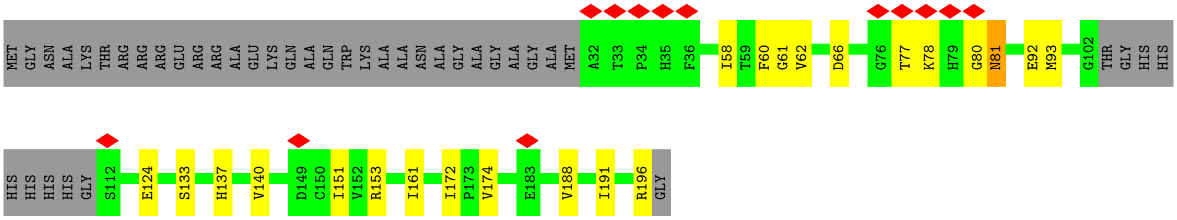
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain CH:



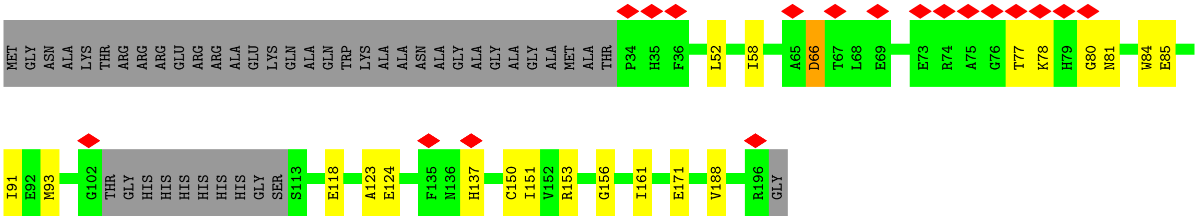
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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

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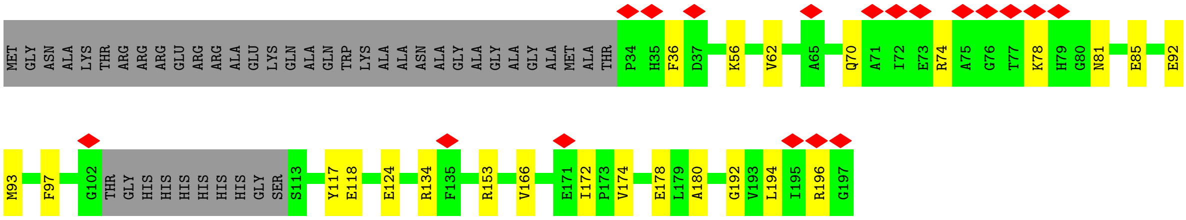
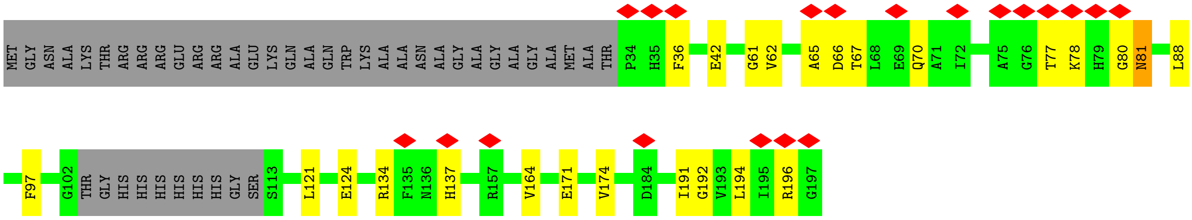


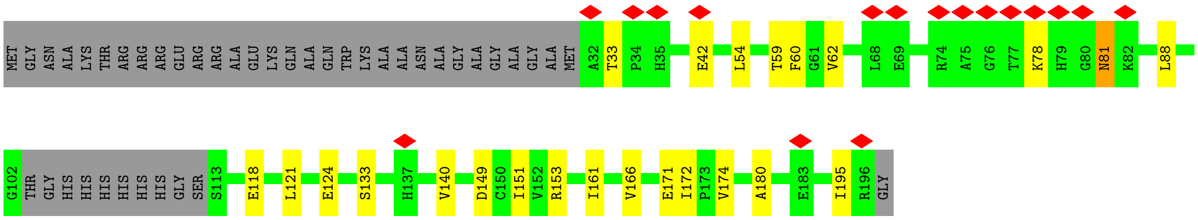
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DB:



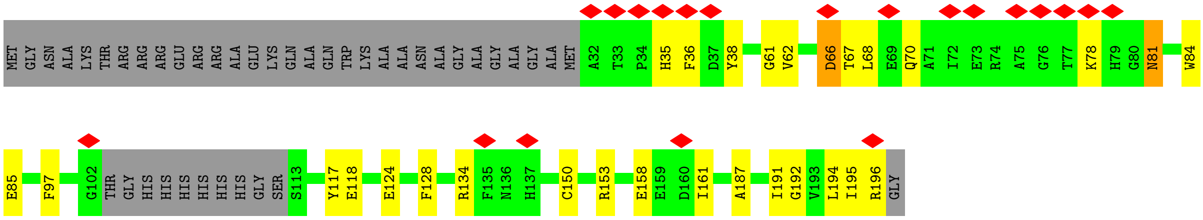
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DC:



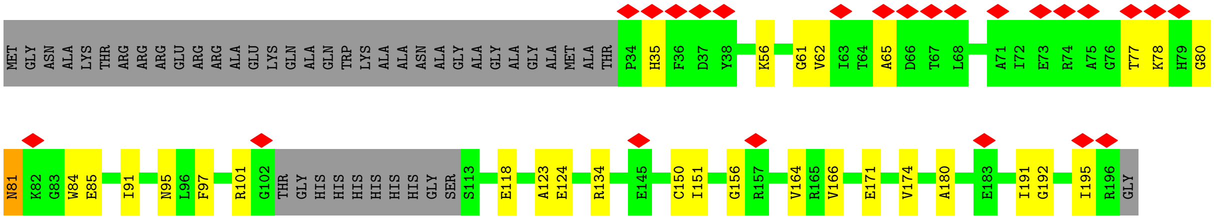
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DD:



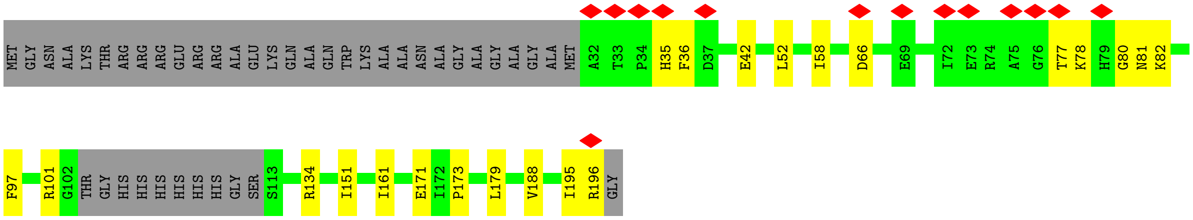
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DE:



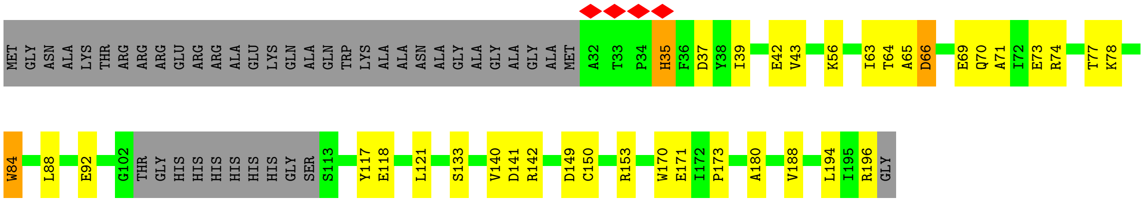
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DF:



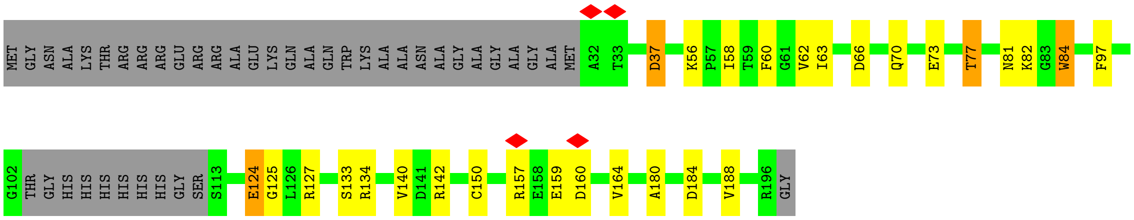
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DG:



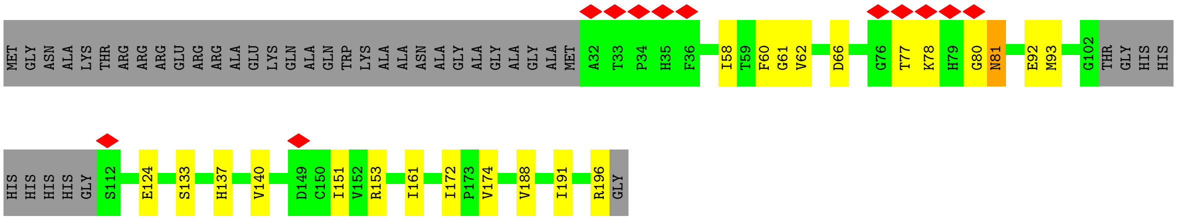
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DH:



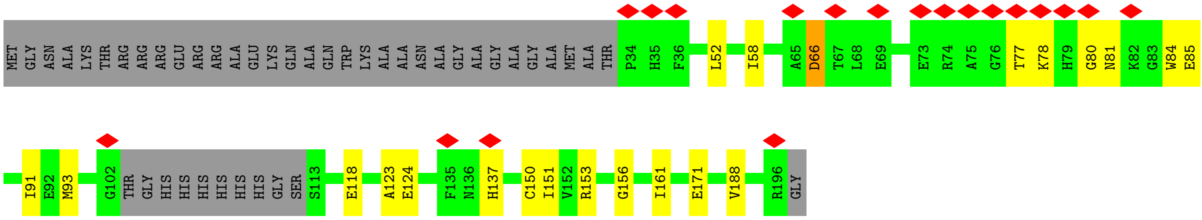
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DI:



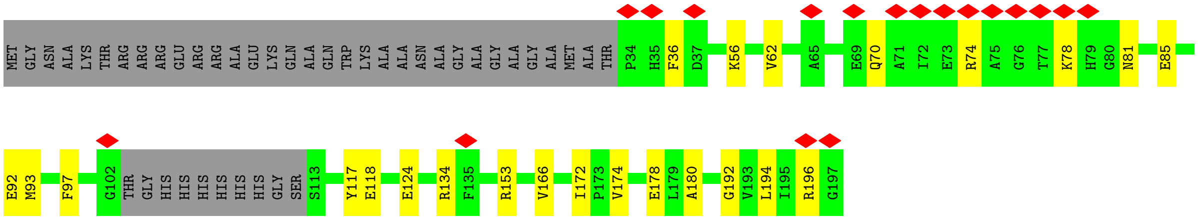
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain DJ:



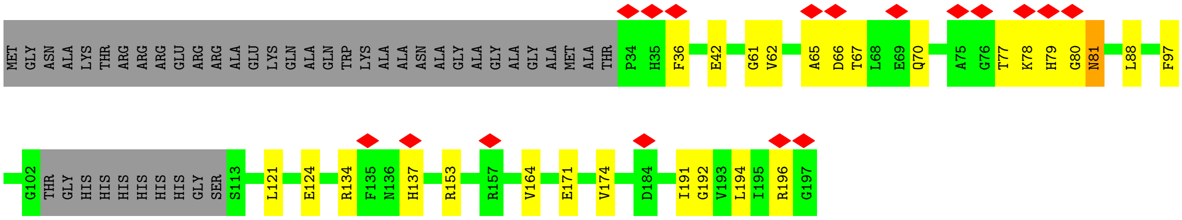
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EA:



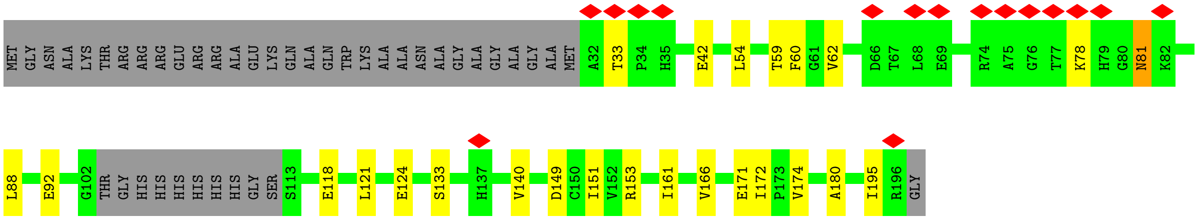
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EB:



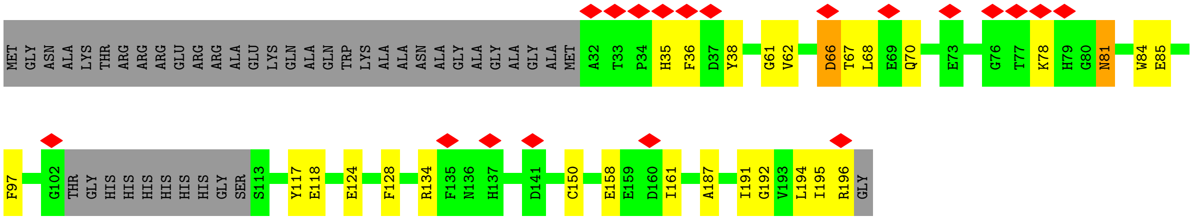
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EC:



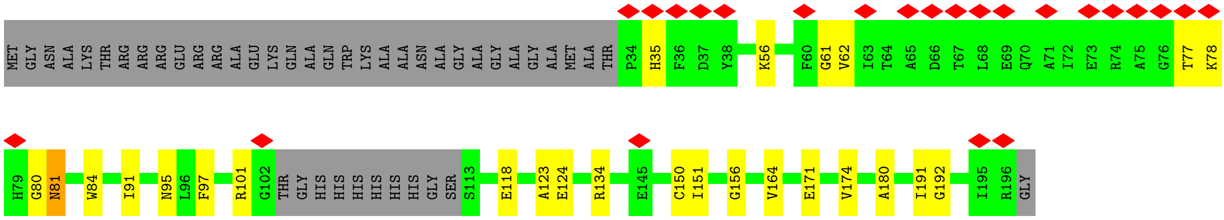
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain ED:



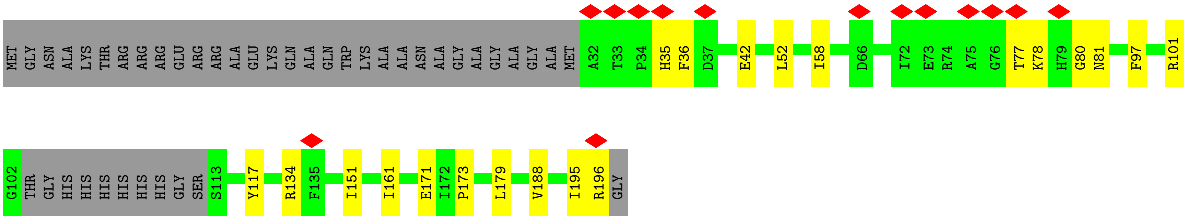
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EE:



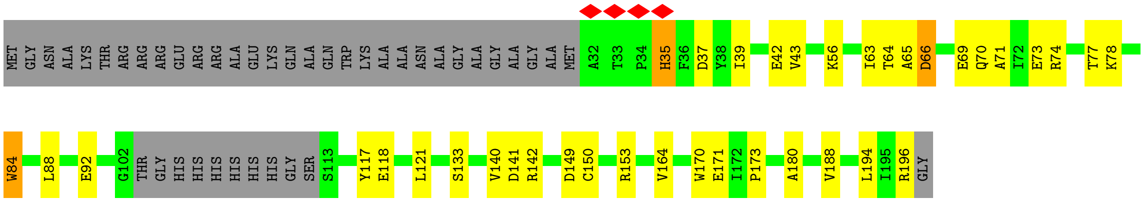
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EF:



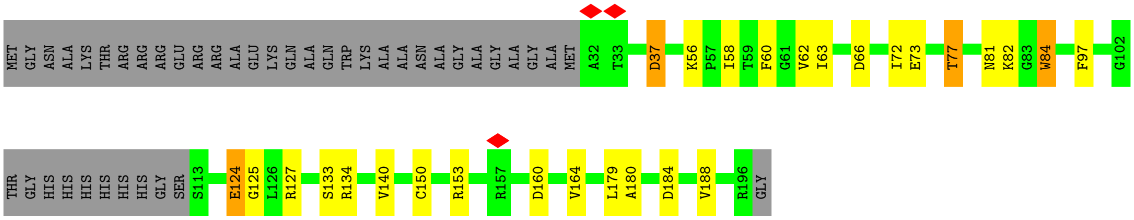
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EG:



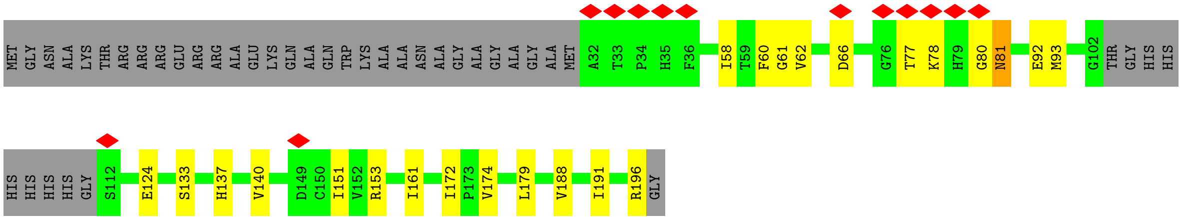
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain EH:



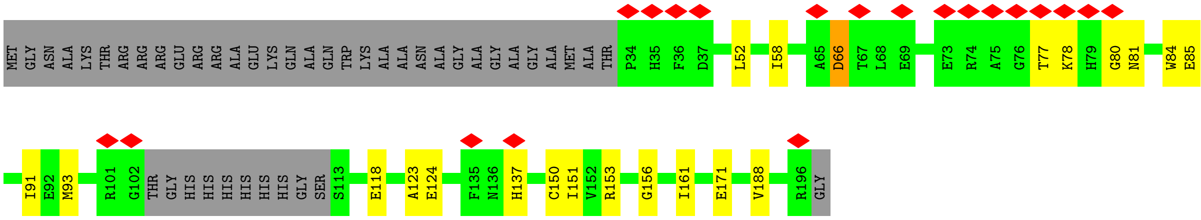
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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

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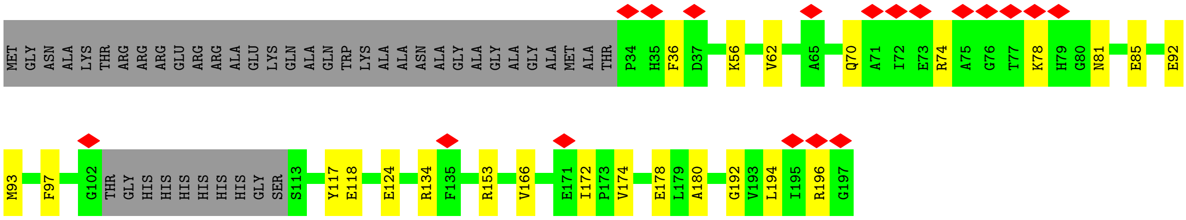

• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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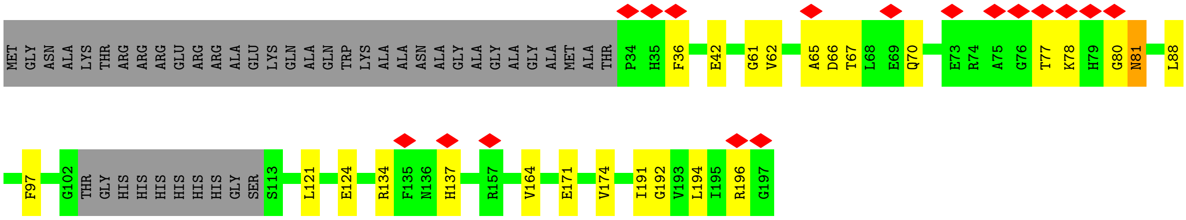
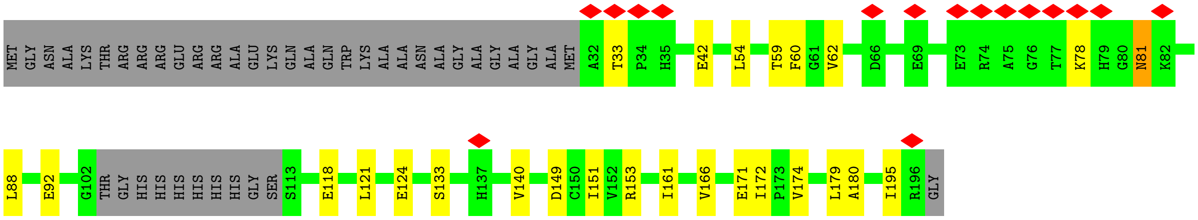


• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FC:



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

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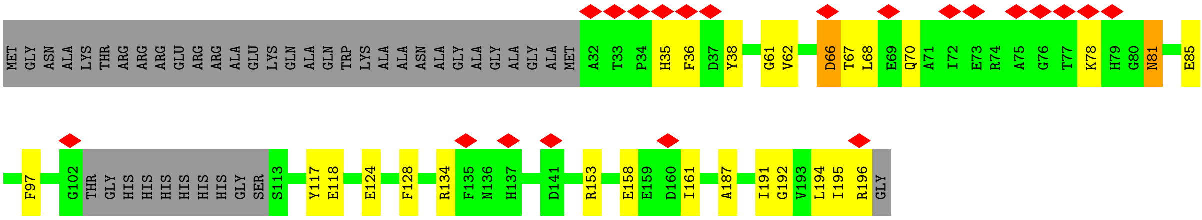

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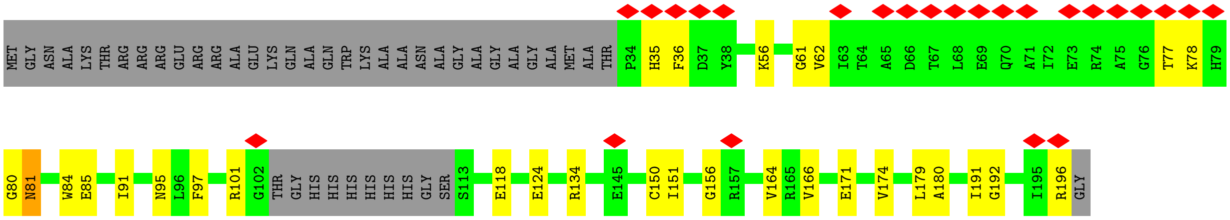

• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

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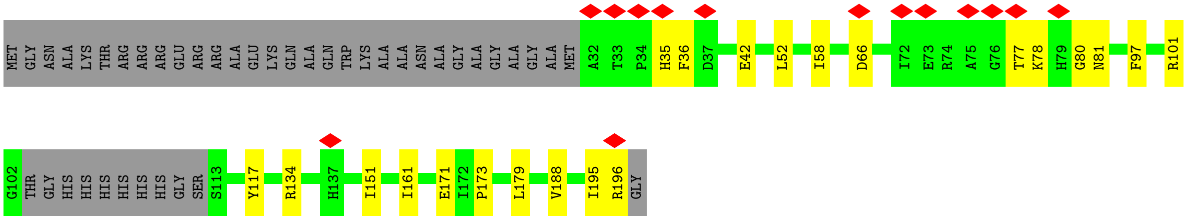
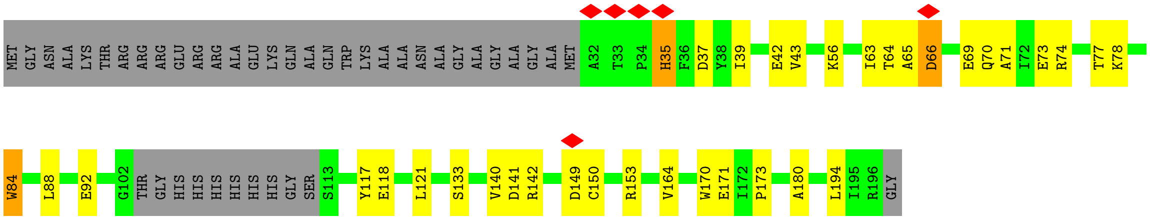


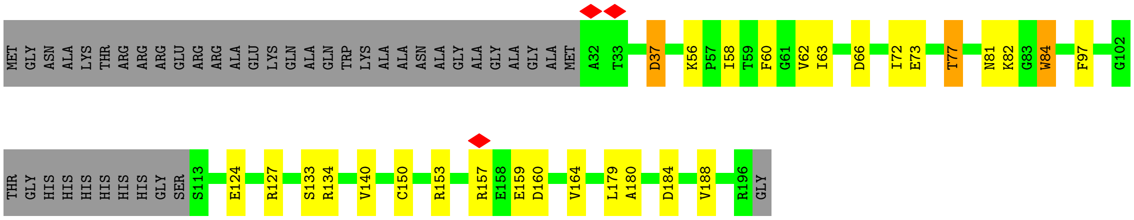
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FG:



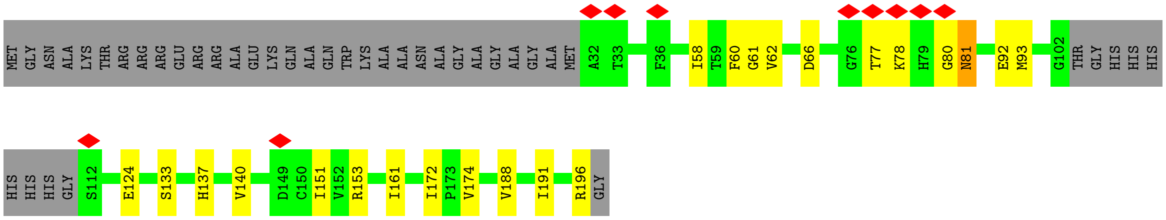
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FH:



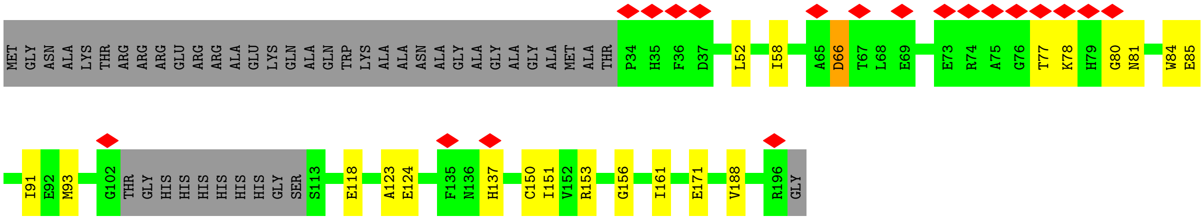
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain FI:



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

Chain FJ:



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

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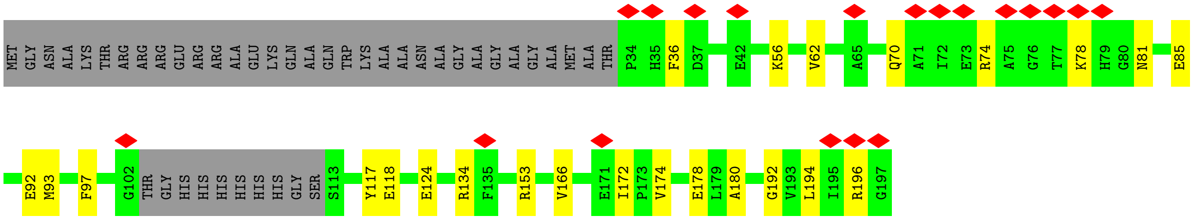
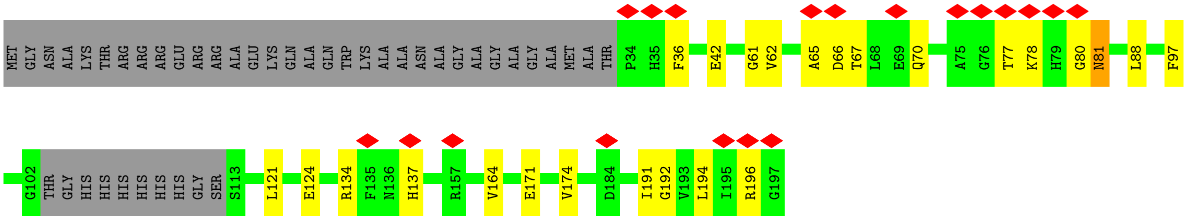


- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain GB:



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

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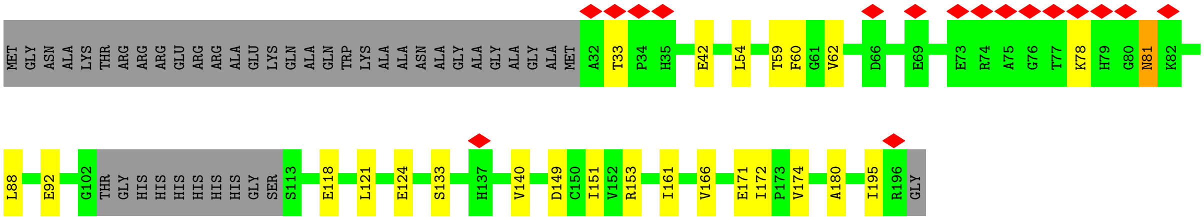

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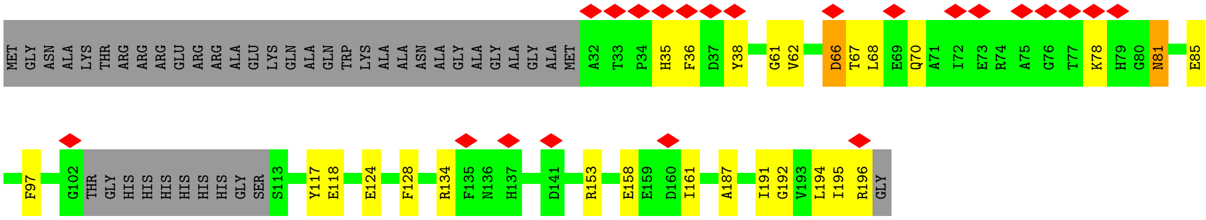
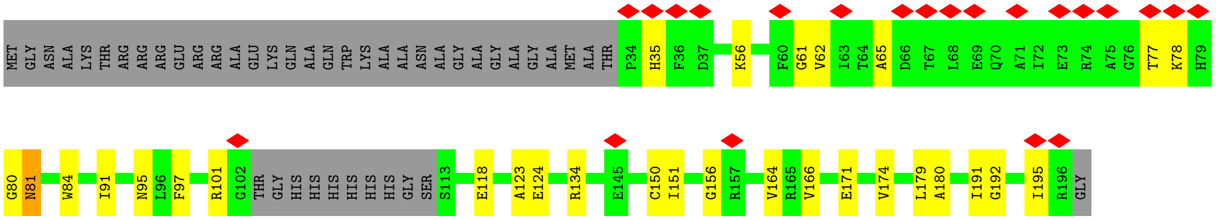


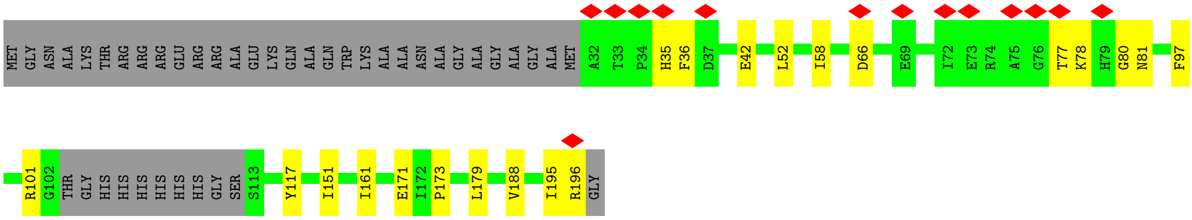
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain GE:



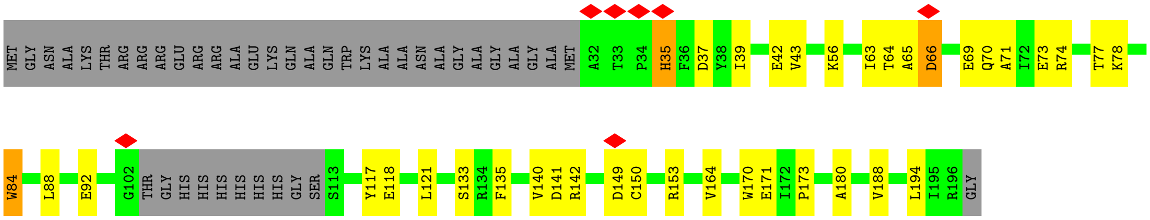
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain GF:



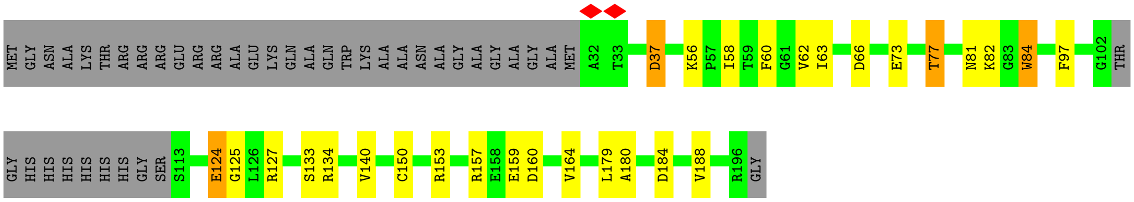
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain GG:



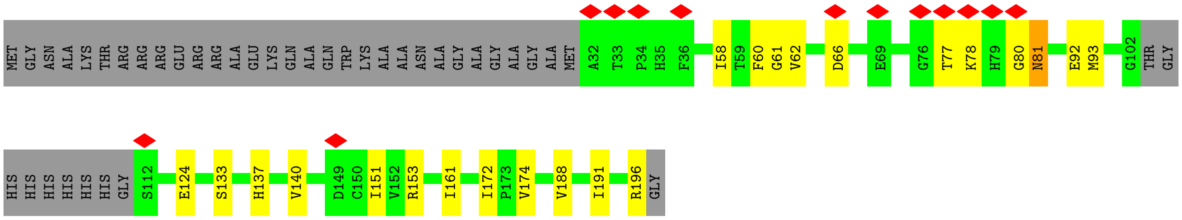
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain GH:



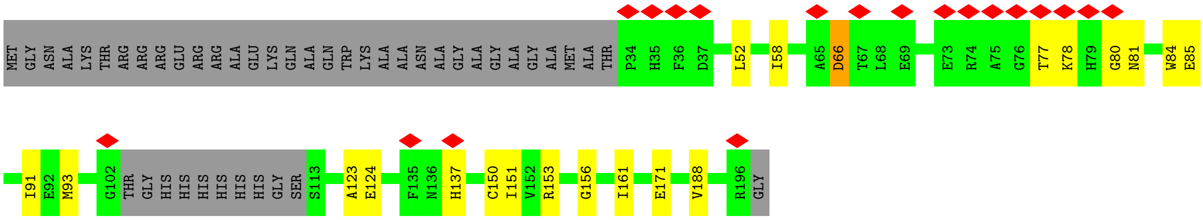
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain GI:



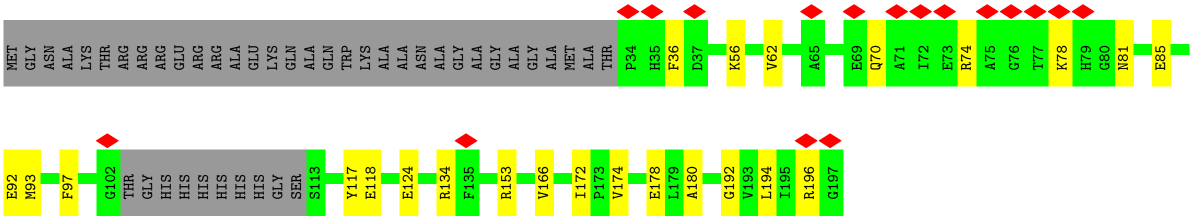
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain GJ:



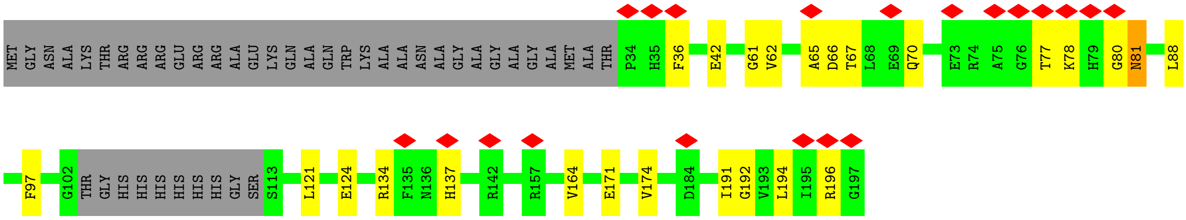
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HA:



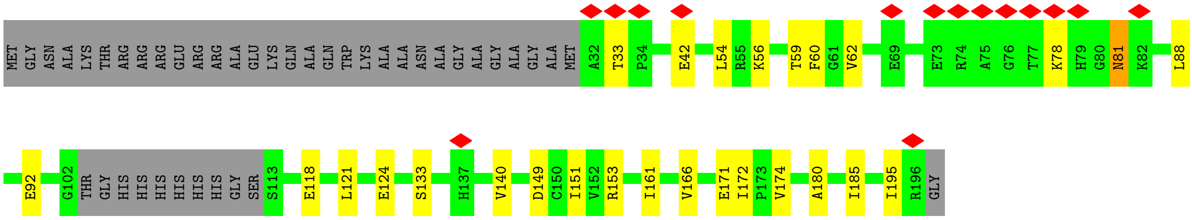
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HB:



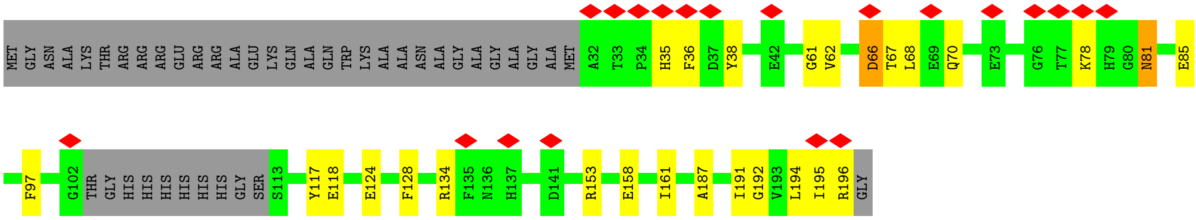
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HC:



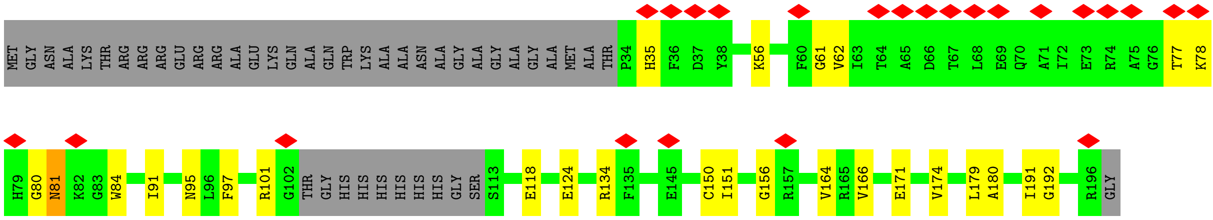
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HD:



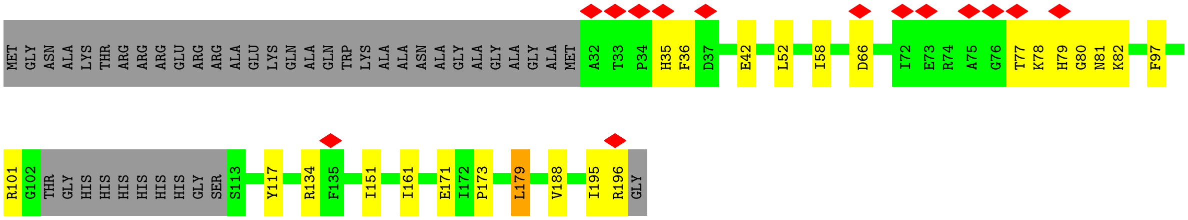
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HE:



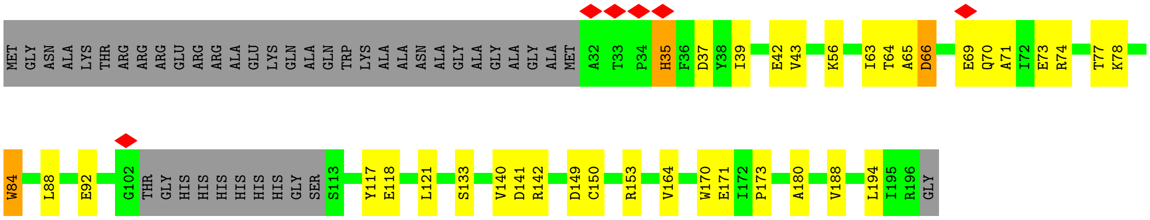
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HF:



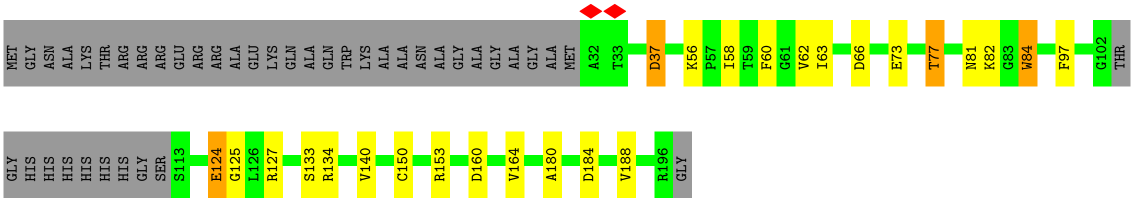
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HG:



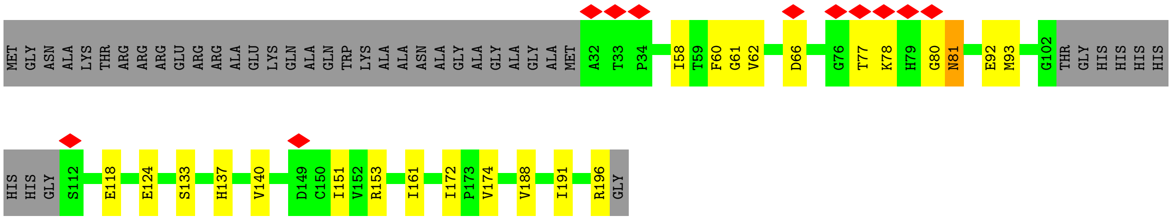
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HH:



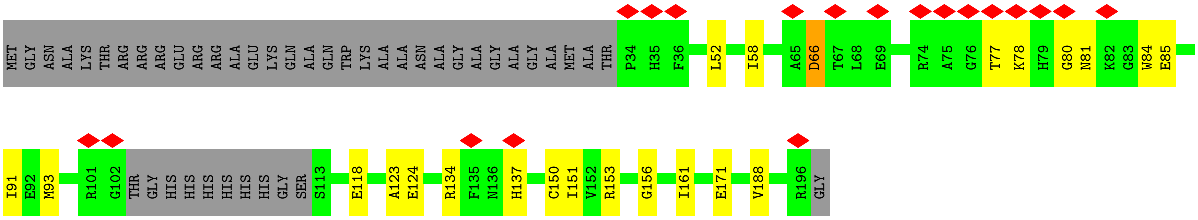
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HI:



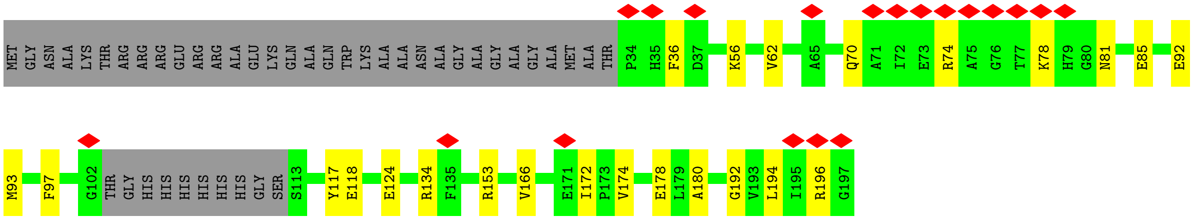
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain HJ:



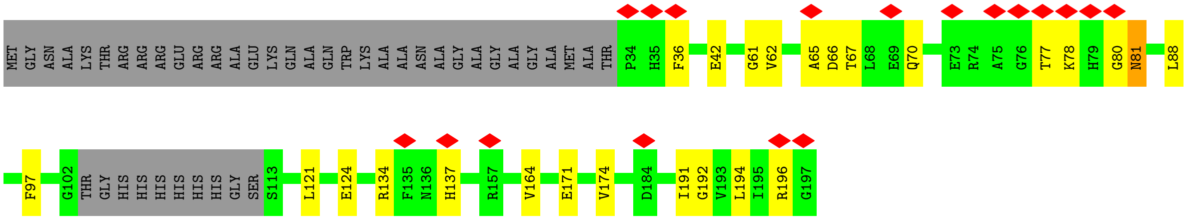
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IA:



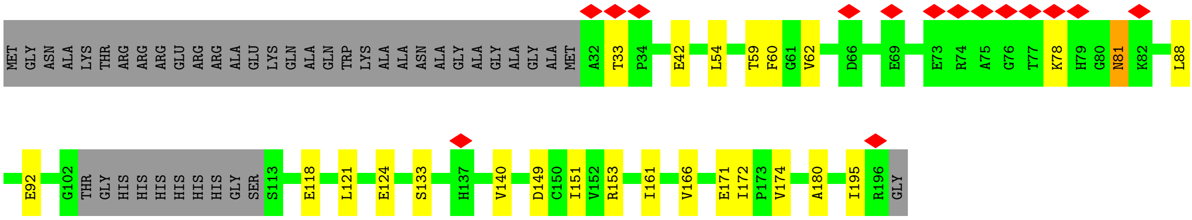
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IB:



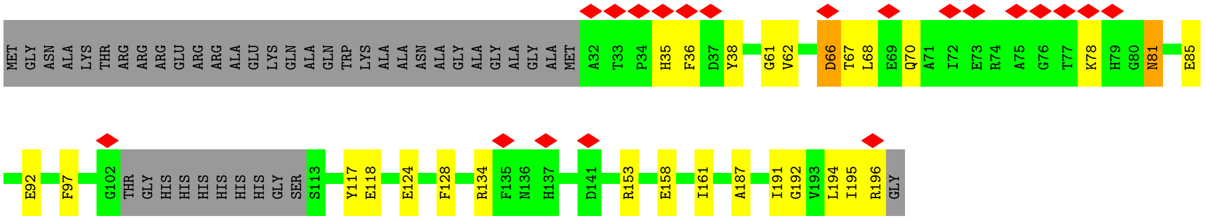
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IC:



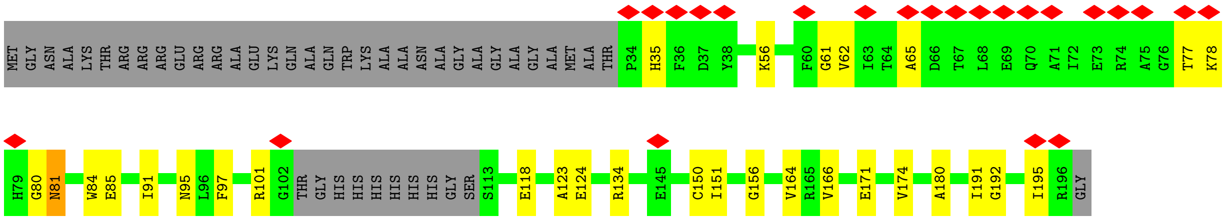
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain ID:



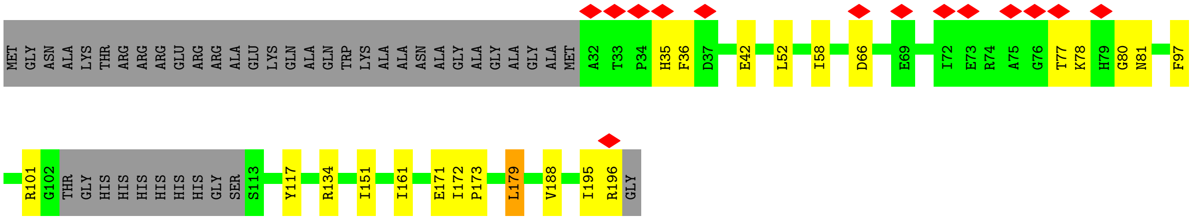
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IE:



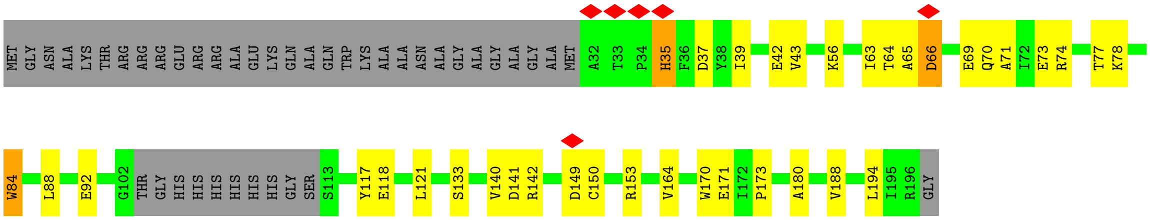
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IF:



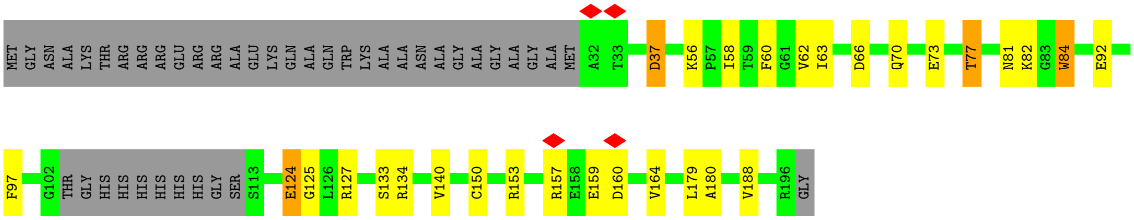
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IG:



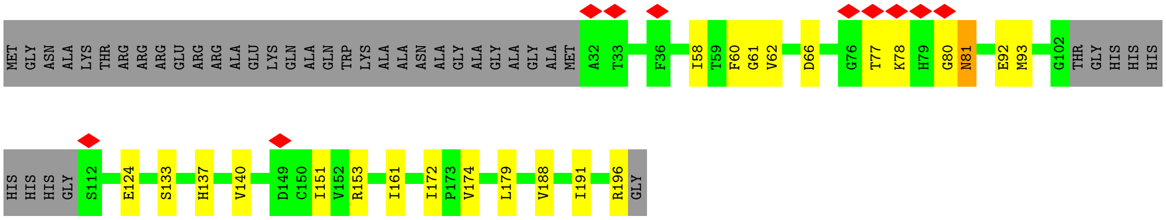
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IH:



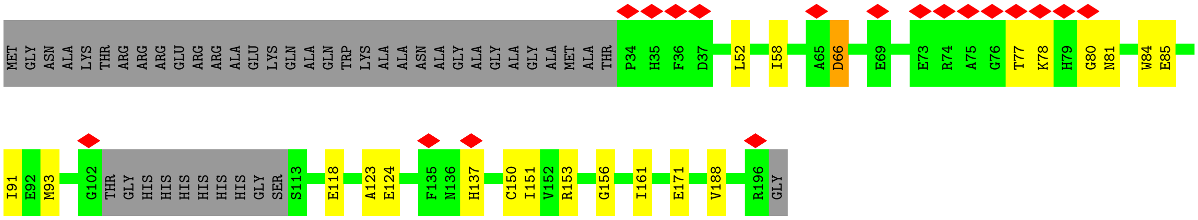
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain II:



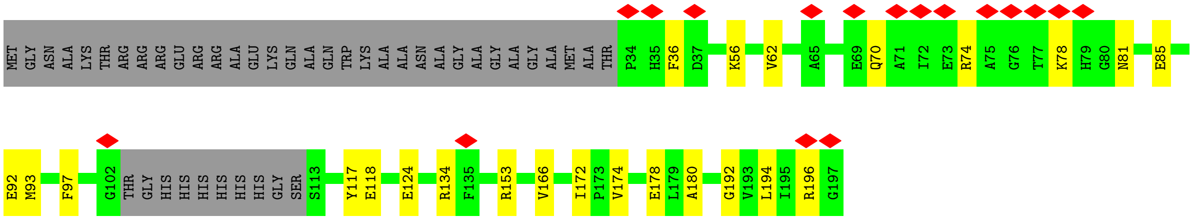
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain IJ:



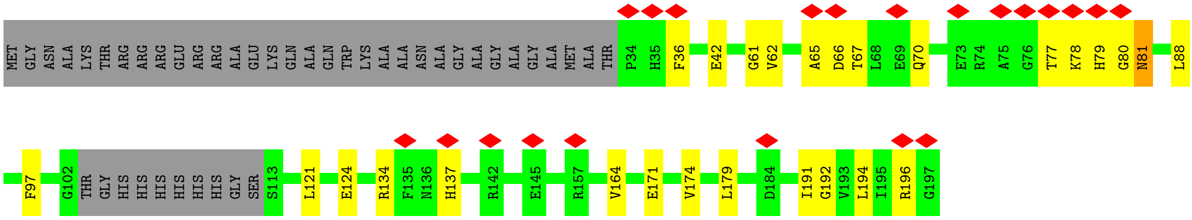
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JA:



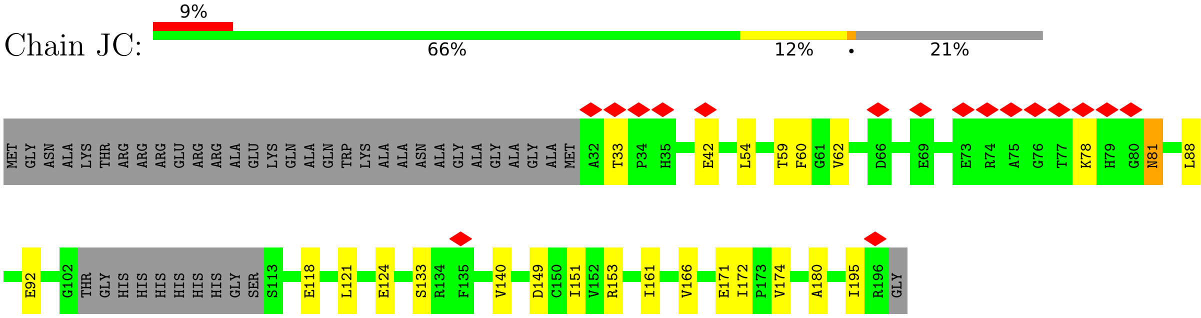
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JB:



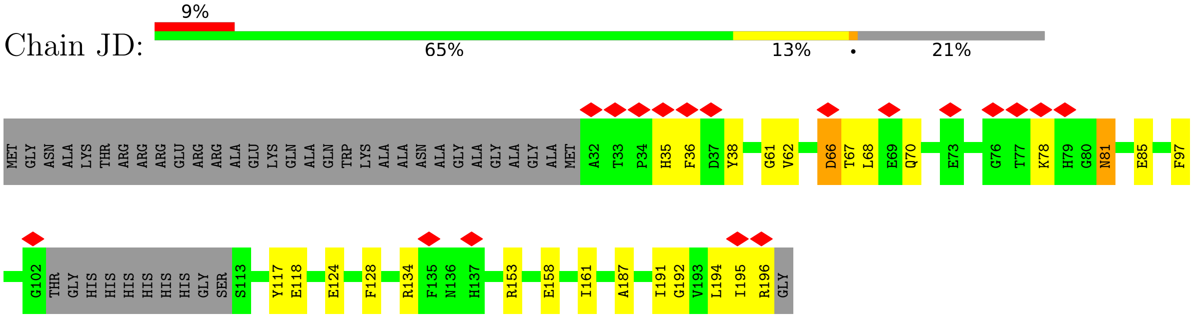
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JC:



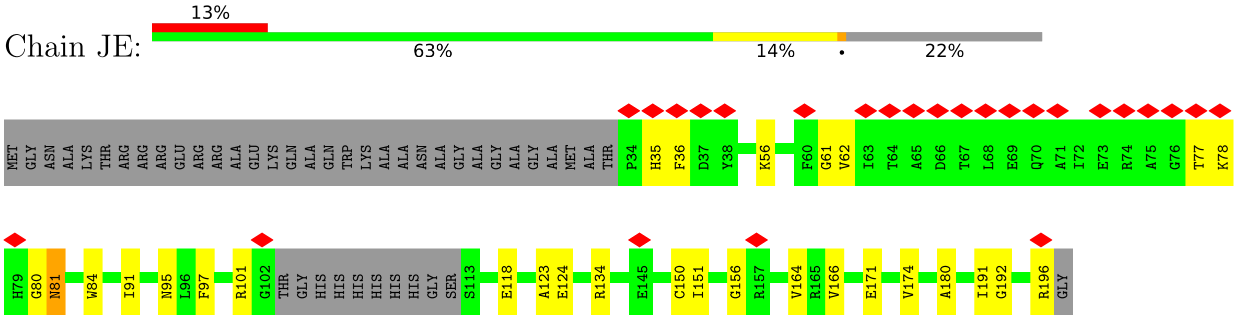
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JD:



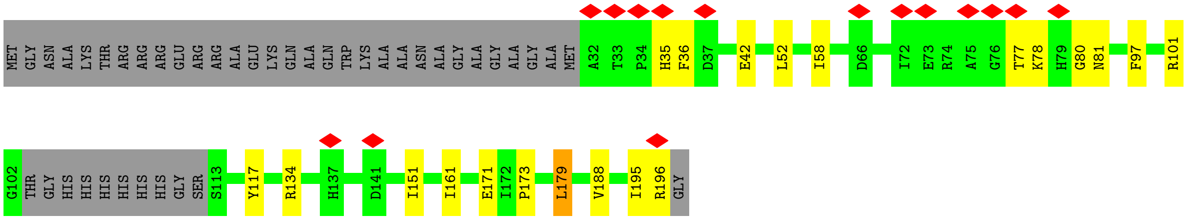
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JE:



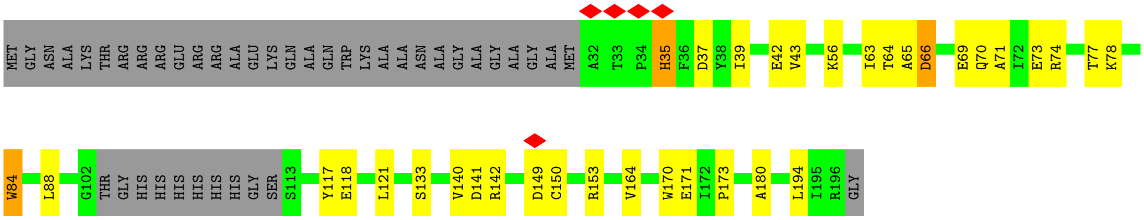
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JF:



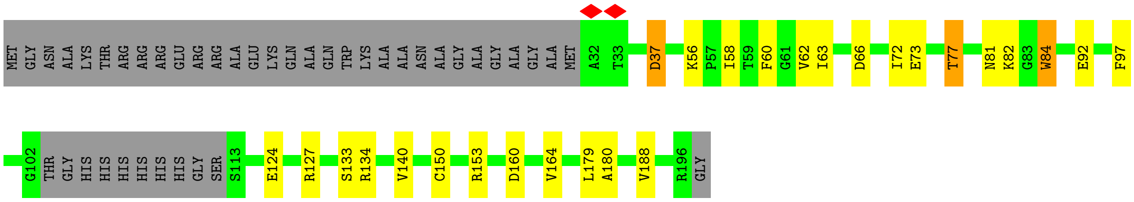
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JG:



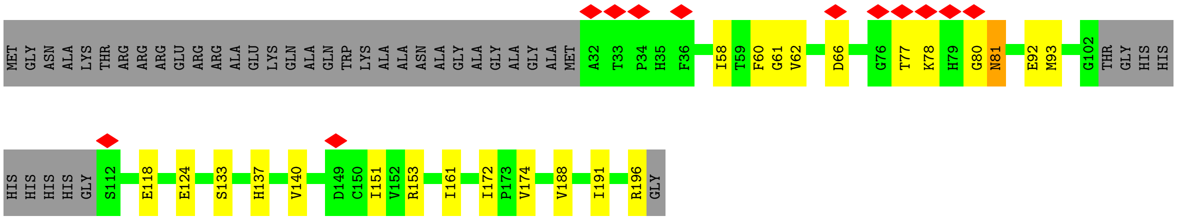
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JH:



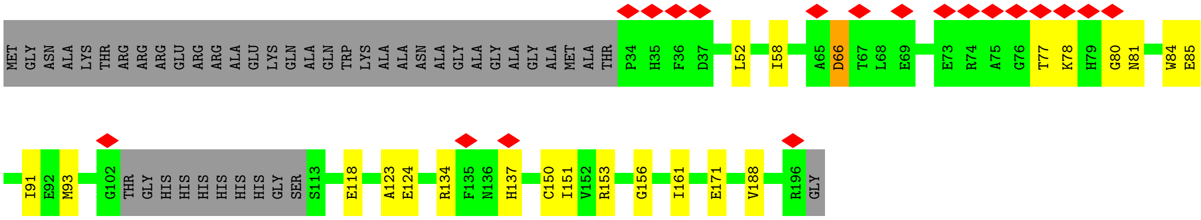
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JI:



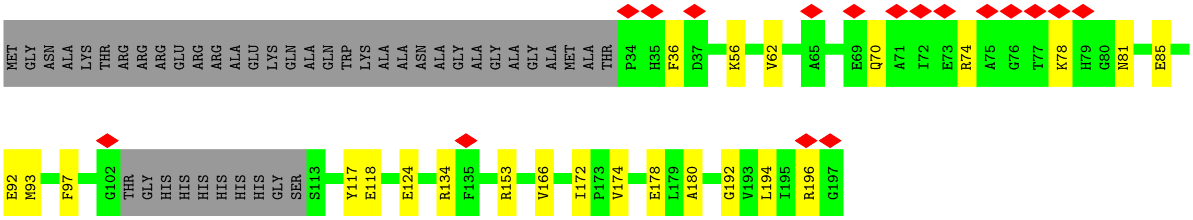
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain JJ:



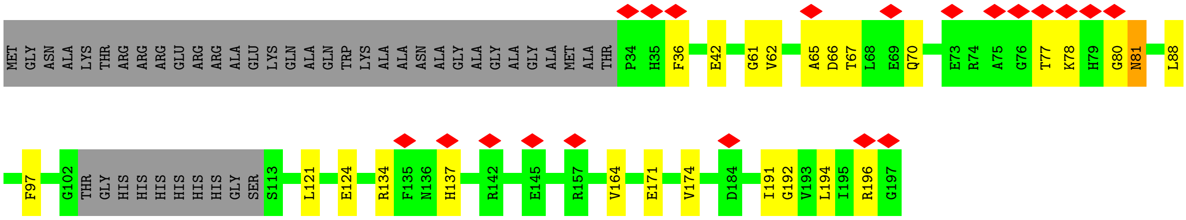
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KA:



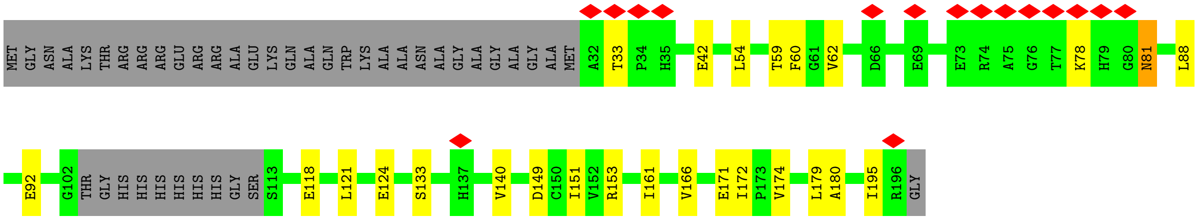
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KB:



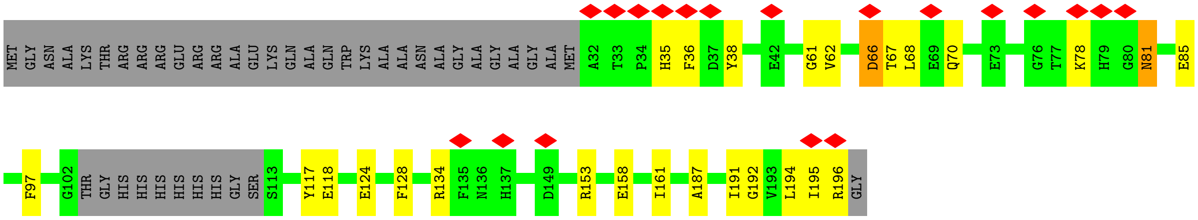
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KC:



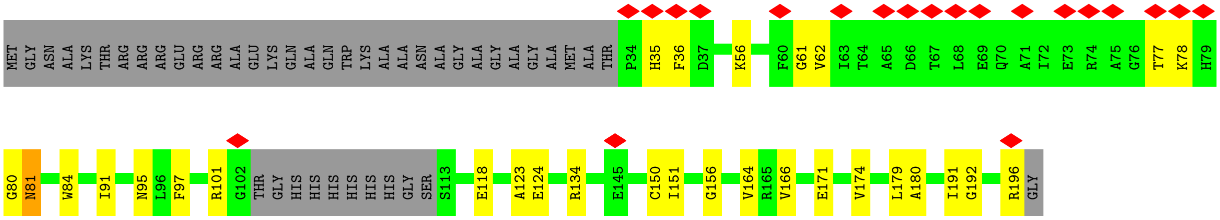
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KD:



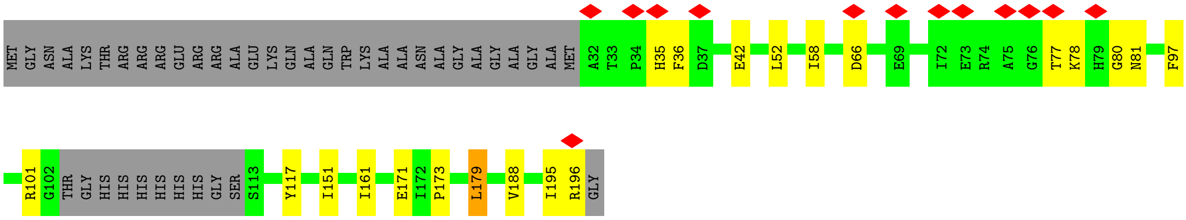
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KE:



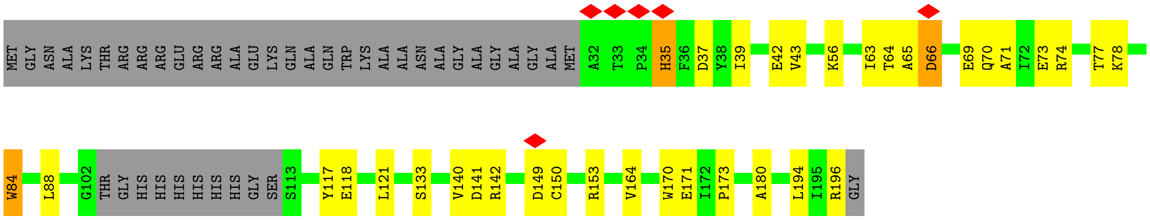
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KF:



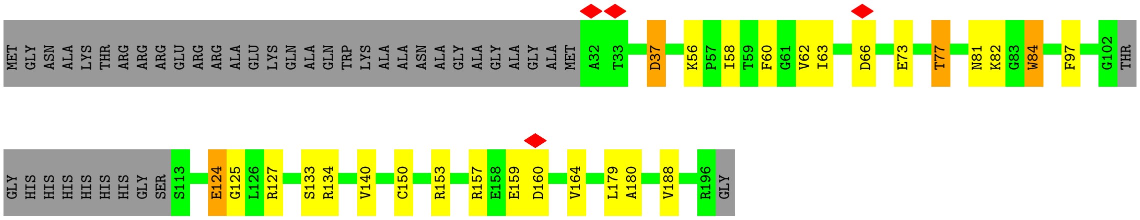
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KG:



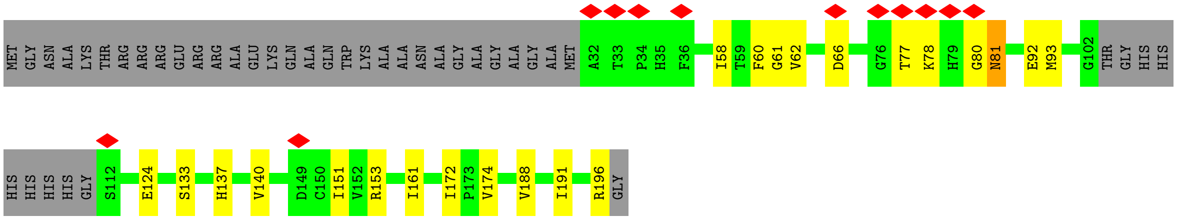
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KH:



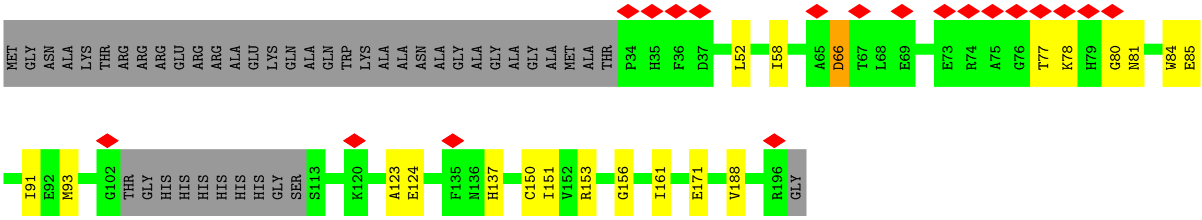
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KI:



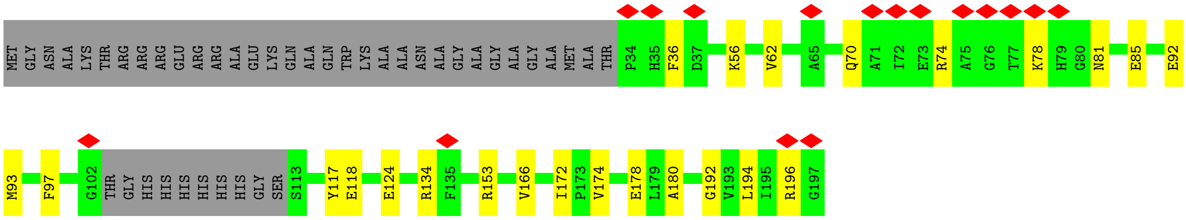
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain KJ:



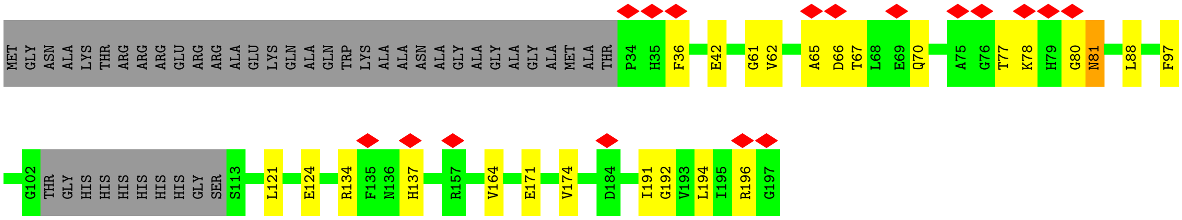
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LA:



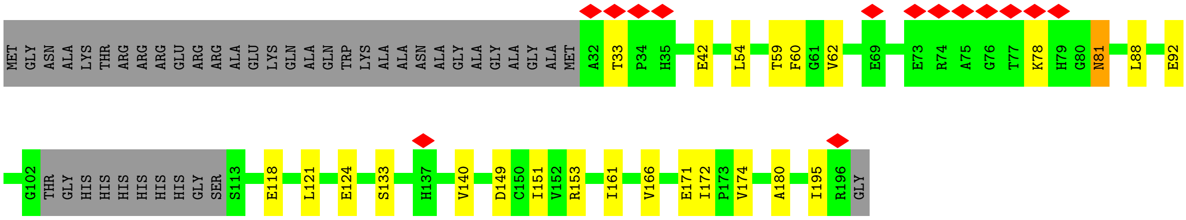
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LB:



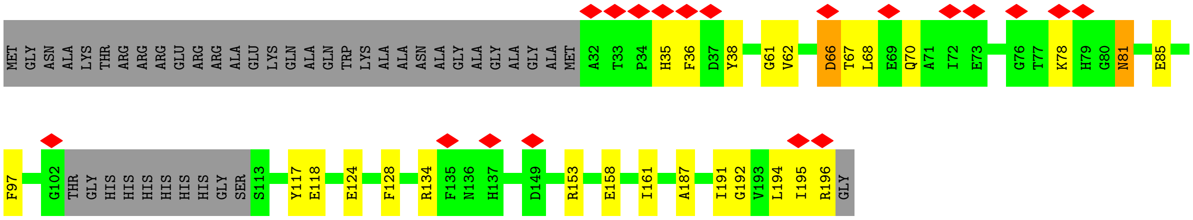
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LC:

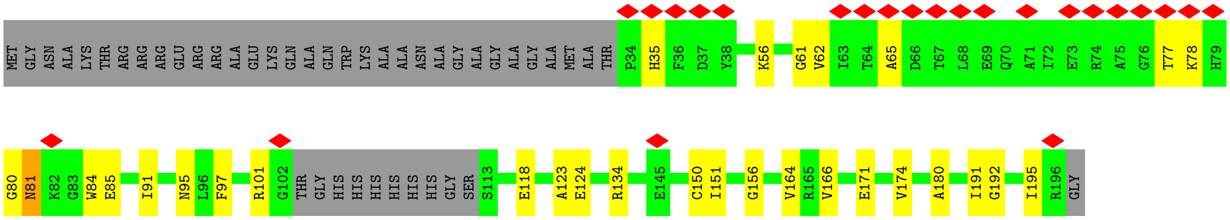
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LD:

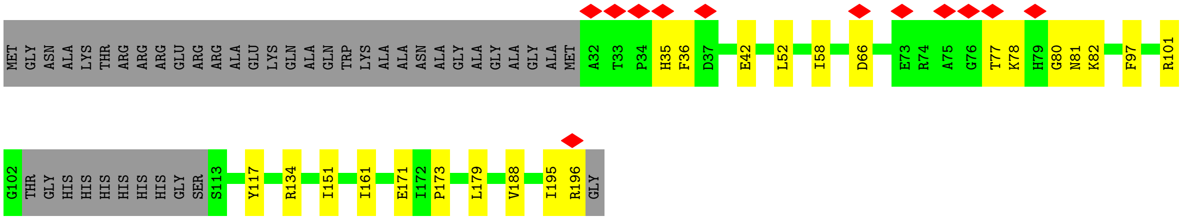
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LE:

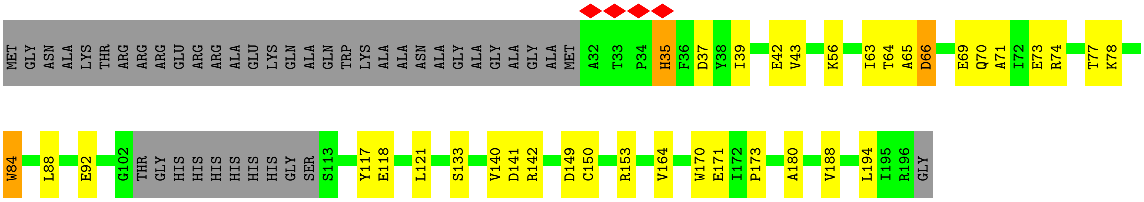
- Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LF:

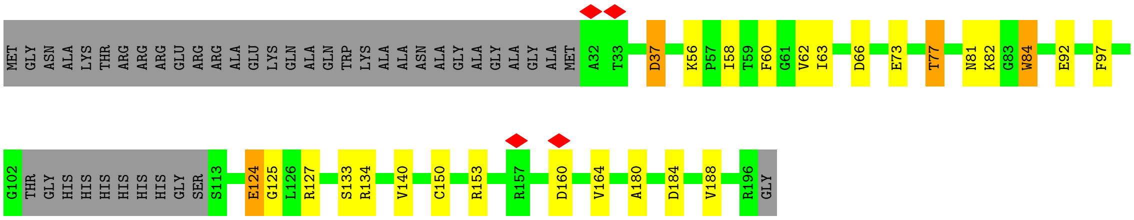
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LG:



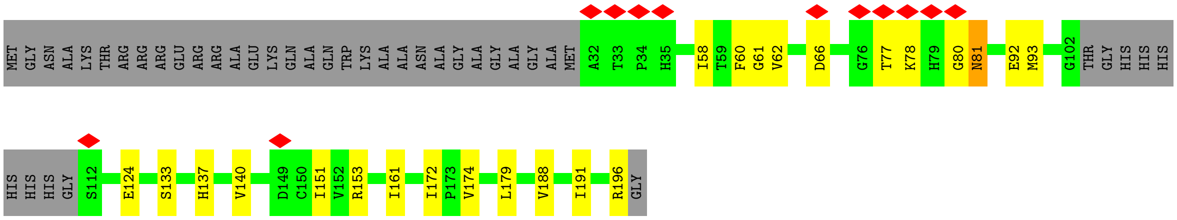
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LH:



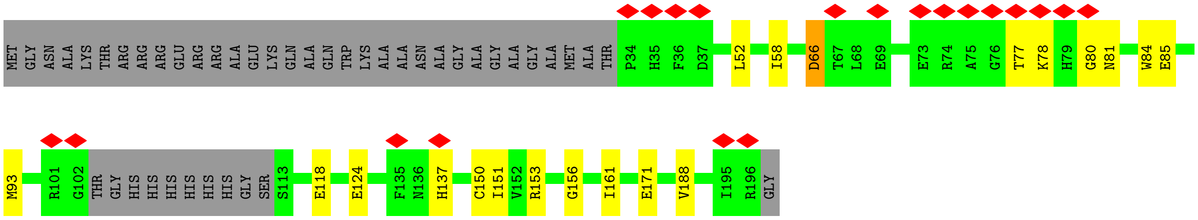
• Molecule 1: Antitermination protein N,6,7-dimethyl-8-ribityllumazine synthase,6,7-dimethyl-8-ribityllumazine synthase

Chain LI:



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

Chain LJ:


MET
GLY
ASN
ALA
LYS
THR
ARG
ARG
ARG
GLU
ARG
ARG
ALA
GLU
LYS
GLN
ALA
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TRP
LYS
ALA
ALA
ASN
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ALA
GLY
ALA
GLY
ALA
MET
ALA
THR
P34
H35
F36
D37
L52
I58
D66
T67
L68
E69
E73
R74
A75
G76
T77
K78
H79
G80
N81
W84
E85
M93
R101
G102
THR
GLY
HIS
HIS
HIS
HIS
HIS
HIS
GLY
SER
S113
E118
E124
F135
N136
H137
C150
I151
V152
R153
G156
I161
E171
V188
I195
R196
GLY

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	5257	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	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	23.398	Depositor
Minimum map value	-11.367	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.85	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	0.24	0/1191	0.39	0/1605
1	AB	0.24	0/1191	0.40	0/1605
1	AC	0.24	0/1199	0.40	0/1618
1	AD	0.24	0/1199	0.40	0/1618
1	AE	0.24	0/1187	0.39	0/1600
1	AF	0.24	0/1199	0.41	0/1618
1	AG	0.24	0/1199	0.41	0/1618
1	AH	0.24	0/1199	0.40	0/1618
1	AI	0.24	0/1205	0.40	0/1626
1	AJ	0.24	0/1187	0.39	0/1600
1	BA	0.24	0/1191	0.39	0/1605
1	BB	0.24	0/1191	0.40	0/1605
1	BC	0.24	0/1199	0.40	0/1618
1	BD	0.24	0/1199	0.40	0/1618
1	BE	0.24	0/1187	0.39	0/1600
1	BF	0.24	0/1199	0.41	0/1618
1	BG	0.24	0/1199	0.41	0/1618
1	BH	0.24	0/1199	0.40	0/1618
1	BI	0.25	0/1205	0.40	0/1626
1	BJ	0.24	0/1187	0.39	0/1600
1	CA	0.24	0/1191	0.39	0/1605
1	CB	0.24	0/1191	0.40	0/1605
1	CC	0.24	0/1199	0.40	0/1618
1	CD	0.24	0/1199	0.40	0/1618
1	CE	0.24	0/1187	0.39	0/1600
1	CF	0.24	0/1199	0.41	0/1618
1	CG	0.24	0/1199	0.41	0/1618
1	CH	0.24	0/1199	0.40	0/1618
1	CI	0.25	0/1205	0.40	0/1626
1	CJ	0.24	0/1187	0.39	0/1600
1	DA	0.24	0/1191	0.39	0/1605
1	DB	0.24	0/1191	0.40	0/1605
1	DC	0.24	0/1199	0.40	0/1618
1	DD	0.24	0/1199	0.40	0/1618

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	DE	0.24	0/1187	0.39	0/1600
1	DF	0.25	0/1199	0.41	0/1618
1	DG	0.24	0/1199	0.41	0/1618
1	DH	0.24	0/1199	0.40	0/1618
1	DI	0.24	0/1205	0.40	0/1626
1	DJ	0.24	0/1187	0.39	0/1600
1	EA	0.24	0/1191	0.39	0/1605
1	EB	0.24	0/1191	0.40	0/1605
1	EC	0.24	0/1199	0.40	0/1618
1	ED	0.24	0/1199	0.40	0/1618
1	EE	0.24	0/1187	0.39	0/1600
1	EF	0.24	0/1199	0.41	0/1618
1	EG	0.24	0/1199	0.41	0/1618
1	EH	0.24	0/1199	0.40	0/1618
1	EI	0.24	0/1205	0.40	0/1626
1	EJ	0.24	0/1187	0.39	0/1600
1	FA	0.24	0/1191	0.39	0/1605
1	FB	0.24	0/1191	0.40	0/1605
1	FC	0.24	0/1199	0.40	0/1618
1	FD	0.24	0/1199	0.40	0/1618
1	FE	0.24	0/1187	0.39	0/1600
1	FF	0.25	0/1199	0.41	0/1618
1	FG	0.24	0/1199	0.41	0/1618
1	FH	0.24	0/1199	0.40	0/1618
1	FI	0.24	0/1205	0.40	0/1626
1	FJ	0.24	0/1187	0.39	0/1600
1	GA	0.24	0/1191	0.39	0/1605
1	GB	0.24	0/1191	0.40	0/1605
1	GC	0.24	0/1199	0.40	0/1618
1	GD	0.24	0/1199	0.40	0/1618
1	GE	0.24	0/1187	0.39	0/1600
1	GF	0.25	0/1199	0.41	0/1618
1	GG	0.24	0/1199	0.41	0/1618
1	GH	0.24	0/1199	0.40	0/1618
1	GI	0.24	0/1205	0.40	0/1626
1	GJ	0.24	0/1187	0.39	0/1600
1	HA	0.24	0/1191	0.39	0/1605
1	HB	0.24	0/1191	0.40	0/1605
1	HC	0.24	0/1199	0.40	0/1618
1	HD	0.24	0/1199	0.40	0/1618
1	HE	0.24	0/1187	0.39	0/1600
1	HF	0.24	0/1199	0.41	0/1618
1	HG	0.24	0/1199	0.41	0/1618

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	HH	0.24	0/1199	0.40	0/1618
1	HI	0.25	0/1205	0.40	0/1626
1	HJ	0.24	0/1187	0.39	0/1600
1	IA	0.24	0/1191	0.39	0/1605
1	IB	0.24	0/1191	0.40	0/1605
1	IC	0.24	0/1199	0.40	0/1618
1	ID	0.24	0/1199	0.40	0/1618
1	IE	0.24	0/1187	0.39	0/1600
1	IF	0.25	0/1199	0.41	0/1618
1	IG	0.24	0/1199	0.41	0/1618
1	IH	0.24	0/1199	0.40	0/1618
1	II	0.24	0/1205	0.40	0/1626
1	IJ	0.24	0/1187	0.39	0/1600
1	JA	0.24	0/1191	0.39	0/1605
1	JB	0.24	0/1191	0.40	0/1605
1	JC	0.24	0/1199	0.40	0/1618
1	JD	0.24	0/1199	0.40	0/1618
1	JE	0.24	0/1187	0.39	0/1600
1	JF	0.24	0/1199	0.41	0/1618
1	JG	0.24	0/1199	0.41	0/1618
1	JH	0.24	0/1199	0.40	0/1618
1	JI	0.24	0/1205	0.40	0/1626
1	JJ	0.24	0/1187	0.39	0/1600
1	KA	0.24	0/1191	0.39	0/1605
1	KB	0.24	0/1191	0.40	0/1605
1	KC	0.24	0/1199	0.40	0/1618
1	KD	0.24	0/1199	0.40	0/1618
1	KE	0.24	0/1187	0.39	0/1600
1	KF	0.25	0/1199	0.41	0/1618
1	KG	0.24	0/1199	0.41	0/1618
1	KH	0.24	0/1199	0.40	0/1618
1	KI	0.24	0/1205	0.40	0/1626
1	KJ	0.24	0/1187	0.39	0/1600
1	LA	0.24	0/1191	0.39	0/1605
1	LB	0.24	0/1191	0.40	0/1605
1	LC	0.24	0/1199	0.40	0/1618
1	LD	0.24	0/1199	0.40	0/1618
1	LE	0.24	0/1187	0.39	0/1600
1	LF	0.25	0/1199	0.41	0/1618
1	LG	0.24	0/1199	0.41	0/1618
1	LH	0.24	0/1199	0.40	0/1618
1	LI	0.25	0/1205	0.40	0/1626
1	LJ	0.24	0/1187	0.39	0/1600

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.24	0/143472	0.40	0/193512

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1174	0	1194	17	0
1	AB	1174	0	1194	17	0
1	AC	1182	0	1202	13	0
1	AD	1182	0	1202	21	0
1	AE	1170	0	1191	18	0
1	AF	1182	0	1202	14	0
1	AG	1182	0	1202	28	0
1	AH	1182	0	1202	21	0
1	AI	1188	0	1207	17	0
1	AJ	1170	0	1191	15	0
1	BA	1174	0	1194	17	0
1	BB	1174	0	1194	18	0
1	BC	1182	0	1202	14	0
1	BD	1182	0	1202	21	0
1	BE	1170	0	1191	17	0
1	BF	1182	0	1202	19	0
1	BG	1182	0	1202	26	0
1	BH	1182	0	1202	18	0
1	BI	1188	0	1207	16	0
1	BJ	1170	0	1191	15	0
1	CA	1174	0	1194	17	0
1	CB	1174	0	1194	16	0
1	CC	1182	0	1202	13	0
1	CD	1182	0	1202	20	0
1	CE	1170	0	1191	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CF	1182	0	1202	14	0
1	CG	1182	0	1202	26	0
1	CH	1182	0	1202	18	0
1	CI	1188	0	1207	15	0
1	CJ	1170	0	1191	15	0
1	DA	1174	0	1194	17	0
1	DB	1174	0	1194	16	0
1	DC	1182	0	1202	12	0
1	DD	1182	0	1202	20	0
1	DE	1170	0	1191	20	0
1	DF	1182	0	1202	14	0
1	DG	1182	0	1202	27	0
1	DH	1182	0	1202	20	0
1	DI	1188	0	1207	16	0
1	DJ	1170	0	1191	15	0
1	EA	1174	0	1194	17	0
1	EB	1174	0	1194	19	0
1	EC	1182	0	1202	13	0
1	ED	1182	0	1202	20	0
1	EE	1170	0	1191	17	0
1	EF	1182	0	1202	13	0
1	EG	1182	0	1202	28	0
1	EH	1182	0	1202	20	0
1	EI	1188	0	1207	15	0
1	EJ	1170	0	1191	15	0
1	FA	1174	0	1194	17	0
1	FB	1174	0	1194	15	0
1	FC	1182	0	1202	14	0
1	FD	1182	0	1202	20	0
1	FE	1170	0	1191	20	0
1	FF	1182	0	1202	14	0
1	FG	1182	0	1202	26	0
1	FH	1182	0	1202	20	0
1	FI	1188	0	1207	14	0
1	FJ	1170	0	1191	15	0
1	GA	1174	0	1194	17	0
1	GB	1174	0	1194	15	0
1	GC	1182	0	1202	13	0
1	GD	1182	0	1202	20	0
1	GE	1170	0	1191	20	0
1	GF	1182	0	1202	13	0
1	GG	1182	0	1202	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GH	1182	0	1202	20	0
1	GI	1188	0	1207	15	0
1	GJ	1170	0	1191	14	0
1	HA	1174	0	1194	17	0
1	HB	1174	0	1194	16	0
1	HC	1182	0	1202	15	0
1	HD	1182	0	1202	20	0
1	HE	1170	0	1191	18	0
1	HF	1182	0	1202	17	0
1	HG	1182	0	1202	28	0
1	HH	1182	0	1202	18	0
1	HI	1188	0	1207	17	0
1	HJ	1170	0	1191	16	0
1	IA	1174	0	1194	17	0
1	IB	1174	0	1194	15	0
1	IC	1182	0	1202	13	0
1	ID	1182	0	1202	20	0
1	IE	1170	0	1191	20	0
1	IF	1182	0	1202	16	0
1	IG	1182	0	1202	27	0
1	IH	1182	0	1202	21	0
1	II	1188	0	1207	16	0
1	IJ	1170	0	1191	15	0
1	JA	1174	0	1194	17	0
1	JB	1174	0	1194	18	0
1	JC	1182	0	1202	14	0
1	JD	1182	0	1202	21	0
1	JE	1170	0	1191	19	0
1	JF	1182	0	1202	14	0
1	JG	1182	0	1202	24	0
1	JH	1182	0	1202	19	0
1	JI	1188	0	1207	16	0
1	JJ	1170	0	1191	16	0
1	KA	1174	0	1194	17	0
1	KB	1174	0	1194	15	0
1	KC	1182	0	1202	14	0
1	KD	1182	0	1202	20	0
1	KE	1170	0	1191	20	0
1	KF	1182	0	1202	14	0
1	KG	1182	0	1202	25	0
1	KH	1182	0	1202	19	0
1	KI	1188	0	1207	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	KJ	1170	0	1191	14	0
1	LA	1174	0	1194	17	0
1	LB	1174	0	1194	16	0
1	LC	1182	0	1202	13	0
1	LD	1182	0	1202	19	0
1	LE	1170	0	1191	19	0
1	LF	1182	0	1202	15	0
1	LG	1182	0	1202	28	0
1	LH	1182	0	1202	19	0
1	LI	1188	0	1207	16	0
1	LJ	1170	0	1191	14	0
All	All	141432	0	143844	1767	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 (1767) 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:AG:77:THR:HG22	1:AG:78:LYS:H	1.08	1.13
1:GG:77:THR:HG22	1:GG:78:LYS:H	1.08	1.11
1:DG:77:THR:HG22	1:DG:78:LYS:H	1.08	1.10
1:EG:77:THR:HG22	1:EG:78:LYS:H	1.08	1.09
1:CG:77:THR:HG22	1:CG:78:LYS:H	1.08	1.08
1:LG:77:THR:HG22	1:LG:78:LYS:H	1.08	1.08
1:FG:77:THR:HG22	1:FG:78:LYS:H	1.08	1.07
1:JG:77:THR:HG22	1:JG:78:LYS:H	1.08	1.07
1:IG:77:THR:HG22	1:IG:78:LYS:H	1.08	1.07
1:KG:77:THR:HG22	1:KG:78:LYS:H	1.08	1.06
1:BG:77:THR:HG22	1:BG:78:LYS:H	1.08	1.05
1:HG:77:THR:HG22	1:HG:78:LYS:H	1.08	1.05
1:BG:77:THR:HG22	1:BG:78:LYS:N	1.88	0.89
1:DG:77:THR:HG22	1:DG:78:LYS:N	1.88	0.89
1:JG:77:THR:HG22	1:JG:78:LYS:N	1.88	0.89
1:CG:77:THR:HG22	1:CG:78:LYS:N	1.88	0.89
1:LG:77:THR:HG22	1:LG:78:LYS:N	1.88	0.89
1:KG:77:THR:HG22	1:KG:78:LYS:N	1.88	0.88
1:IG:77:THR:HG22	1:IG:78:LYS:N	1.88	0.88
1:FG:77:THR:HG22	1:FG:78:LYS:N	1.88	0.88
1:GG:77:THR:HG22	1:GG:78:LYS:N	1.87	0.88
1:HG:77:THR:HG22	1:HG:78:LYS:N	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EG:77:THR:HG22	1:EG:78:LYS:N	1.88	0.88
1:FG:77:THR:CG2	1:FG:78:LYS:H	1.89	0.86
1:AG:77:THR:HG22	1:AG:78:LYS:N	1.88	0.86
1:EG:77:THR:CG2	1:EG:78:LYS:H	1.89	0.86
1:GG:77:THR:CG2	1:GG:78:LYS:H	1.89	0.86
1:KG:77:THR:CG2	1:KG:78:LYS:H	1.89	0.86
1:HG:77:THR:CG2	1:HG:78:LYS:H	1.89	0.86
1:BG:77:THR:CG2	1:BG:78:LYS:H	1.89	0.86
1:CG:77:THR:CG2	1:CG:78:LYS:H	1.89	0.86
1:DG:77:THR:CG2	1:DG:78:LYS:H	1.89	0.86
1:LG:77:THR:CG2	1:LG:78:LYS:H	1.89	0.85
1:IG:77:THR:CG2	1:IG:78:LYS:H	1.89	0.83
1:JG:77:THR:CG2	1:JG:78:LYS:H	1.89	0.83
1:AG:77:THR:CG2	1:AG:78:LYS:H	1.89	0.82
1:CI:78:LYS:O	1:CI:81:ASN:ND2	2.21	0.74
1:HI:78:LYS:O	1:HI:81:ASN:ND2	2.21	0.74
1:GI:78:LYS:O	1:GI:81:ASN:ND2	2.21	0.73
1:KI:78:LYS:O	1:KI:81:ASN:ND2	2.21	0.73
1:BI:78:LYS:O	1:BI:81:ASN:ND2	2.21	0.73
1:FI:78:LYS:O	1:FI:81:ASN:ND2	2.21	0.73
1:AI:78:LYS:O	1:AI:81:ASN:ND2	2.21	0.73
1:DI:78:LYS:O	1:DI:81:ASN:ND2	2.21	0.73
1:EI:78:LYS:O	1:EI:81:ASN:ND2	2.21	0.72
1:II:78:LYS:O	1:II:81:ASN:ND2	2.21	0.72
1:ID:153:ARG:NH2	1:JC:92:GLU:OE2	2.23	0.72
1:LI:78:LYS:O	1:LI:81:ASN:ND2	2.21	0.72
1:DJ:78:LYS:O	1:DJ:81:ASN:ND2	2.23	0.72
1:GJ:78:LYS:O	1:GJ:81:ASN:ND2	2.23	0.72
1:JI:78:LYS:O	1:JI:81:ASN:ND2	2.21	0.72
1:KJ:78:LYS:O	1:KJ:81:ASN:ND2	2.23	0.72
1:LJ:78:LYS:O	1:LJ:81:ASN:ND2	2.23	0.72
1:HJ:78:LYS:O	1:HJ:81:ASN:ND2	2.23	0.71
1:AJ:78:LYS:O	1:AJ:81:ASN:ND2	2.23	0.71
1:FJ:78:LYS:O	1:FJ:81:ASN:ND2	2.23	0.71
1:CJ:78:LYS:O	1:CJ:81:ASN:ND2	2.23	0.71
1:EJ:78:LYS:O	1:EJ:81:ASN:ND2	2.23	0.71
1:IJ:78:LYS:O	1:IJ:81:ASN:ND2	2.23	0.71
1:JD:78:LYS:O	1:JD:81:ASN:ND2	2.24	0.71
1:JJ:78:LYS:O	1:JJ:81:ASN:ND2	2.23	0.71
1:LD:78:LYS:O	1:LD:81:ASN:ND2	2.24	0.71
1:DD:78:LYS:O	1:DD:81:ASN:ND2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FD:78:LYS:O	1:FD:81:ASN:ND2	2.24	0.70
1:HD:78:LYS:O	1:HD:81:ASN:ND2	2.24	0.70
1:BJ:78:LYS:O	1:BJ:81:ASN:ND2	2.23	0.70
1:KD:78:LYS:O	1:KD:81:ASN:ND2	2.24	0.70
1:GD:78:LYS:O	1:GD:81:ASN:ND2	2.24	0.70
1:AD:78:LYS:O	1:AD:81:ASN:ND2	2.24	0.70
1:CD:78:LYS:O	1:CD:81:ASN:ND2	2.24	0.70
1:ED:78:LYS:O	1:ED:81:ASN:ND2	2.24	0.70
1:ID:78:LYS:O	1:ID:81:ASN:ND2	2.24	0.70
1:BD:78:LYS:O	1:BD:81:ASN:ND2	2.24	0.69
1:GF:78:LYS:O	1:GF:81:ASN:ND2	2.26	0.69
1:HF:78:LYS:O	1:HF:81:ASN:ND2	2.26	0.69
1:CF:78:LYS:O	1:CF:81:ASN:ND2	2.26	0.69
1:JF:78:LYS:O	1:JF:81:ASN:ND2	2.26	0.69
1:KF:78:LYS:O	1:KF:81:ASN:ND2	2.26	0.69
1:LF:78:LYS:O	1:LF:81:ASN:ND2	2.26	0.68
1:BF:78:LYS:O	1:BF:81:ASN:ND2	2.26	0.68
1:EF:78:LYS:O	1:EF:81:ASN:ND2	2.26	0.68
1:FF:78:LYS:O	1:FF:81:ASN:ND2	2.26	0.68
1:DF:78:LYS:O	1:DF:81:ASN:ND2	2.26	0.68
1:IF:78:LYS:O	1:IF:81:ASN:ND2	2.26	0.68
1:AF:78:LYS:O	1:AF:81:ASN:ND2	2.26	0.67
1:HJ:151:ILE:HG22	1:HJ:156:GLY:HA3	1.77	0.67
1:EJ:151:ILE:HG22	1:EJ:156:GLY:HA3	1.77	0.67
1:LJ:151:ILE:HG22	1:LJ:156:GLY:HA3	1.77	0.67
1:IJ:151:ILE:HG22	1:IJ:156:GLY:HA3	1.76	0.67
1:KJ:151:ILE:HG22	1:KJ:156:GLY:HA3	1.77	0.67
1:BJ:151:ILE:HG22	1:BJ:156:GLY:HA3	1.77	0.67
1:GJ:151:ILE:HG22	1:GJ:156:GLY:HA3	1.77	0.67
1:JJ:151:ILE:HG22	1:JJ:156:GLY:HA3	1.77	0.67
1:GF:52:LEU:HD21	1:GG:173:PRO:HB2	1.78	0.66
1:BF:52:LEU:HD21	1:BG:173:PRO:HB2	1.78	0.66
1:DF:52:LEU:HD21	1:DG:173:PRO:HB2	1.78	0.66
1:CF:52:LEU:HD21	1:CG:173:PRO:HB2	1.78	0.66
1:HF:52:LEU:HD21	1:HG:173:PRO:HB2	1.78	0.66
1:IF:52:LEU:HD21	1:IG:173:PRO:HB2	1.78	0.66
1:AF:52:LEU:HD21	1:AG:173:PRO:HB2	1.78	0.66
1:DJ:151:ILE:HG22	1:DJ:156:GLY:HA3	1.77	0.66
1:FF:52:LEU:HD21	1:FG:173:PRO:HB2	1.78	0.66
1:FJ:151:ILE:HG22	1:FJ:156:GLY:HA3	1.77	0.66
1:JF:52:LEU:HD21	1:JG:173:PRO:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:118:GLU:OE2	1:AB:134:ARG:NH1	2.28	0.66
1:KA:118:GLU:OE2	1:KB:134:ARG:NH1	2.28	0.66
1:KF:52:LEU:HD21	1:KG:173:PRO:HB2	1.78	0.66
1:LF:52:LEU:HD21	1:LG:173:PRO:HB2	1.78	0.66
1:LC:78:LYS:O	1:LC:81:ASN:ND2	2.29	0.66
1:AJ:151:ILE:HG22	1:AJ:156:GLY:HA3	1.77	0.65
1:FA:118:GLU:OE2	1:FB:134:ARG:NH1	2.28	0.65
1:CC:78:LYS:O	1:CC:81:ASN:ND2	2.30	0.65
1:GA:118:GLU:OE2	1:GB:134:ARG:NH1	2.28	0.65
1:AC:92:GLU:OE2	1:KD:153:ARG:NH2	2.30	0.65
1:CJ:151:ILE:HG22	1:CJ:156:GLY:HA3	1.77	0.65
1:FC:78:LYS:O	1:FC:81:ASN:ND2	2.30	0.65
1:GC:78:LYS:O	1:GC:81:ASN:ND2	2.29	0.65
1:BC:78:LYS:O	1:BC:81:ASN:ND2	2.30	0.65
1:EB:77:THR:O	1:EB:80:GLY:N	2.30	0.65
1:CA:118:GLU:OE2	1:CB:134:ARG:NH1	2.28	0.65
1:IA:118:GLU:OE2	1:IB:134:ARG:NH1	2.28	0.65
1:IC:78:LYS:O	1:IC:81:ASN:ND2	2.30	0.65
1:AC:78:LYS:O	1:AC:81:ASN:ND2	2.29	0.65
1:BA:118:GLU:OE2	1:BB:134:ARG:NH1	2.28	0.65
1:BB:77:THR:O	1:BB:80:GLY:N	2.30	0.65
1:LA:118:GLU:OE2	1:LB:134:ARG:NH1	2.28	0.65
1:EF:52:LEU:HD21	1:EG:173:PRO:HB2	1.78	0.65
1:EC:78:LYS:O	1:EC:81:ASN:ND2	2.30	0.65
1:HC:78:LYS:O	1:HC:81:ASN:ND2	2.29	0.65
1:FB:77:THR:O	1:FB:80:GLY:N	2.30	0.64
1:GI:58:ILE:HG12	1:GI:188:VAL:HB	1.79	0.64
1:HB:77:THR:O	1:HB:80:GLY:N	2.30	0.64
1:JC:78:LYS:O	1:JC:81:ASN:ND2	2.29	0.64
1:AD:36:PHE:HZ	1:AD:194:LEU:HB3	1.63	0.64
1:DB:77:THR:O	1:DB:80:GLY:N	2.30	0.64
1:LB:77:THR:O	1:LB:80:GLY:N	2.30	0.64
1:DC:78:LYS:O	1:DC:81:ASN:ND2	2.30	0.64
1:KB:77:THR:O	1:KB:80:GLY:N	2.30	0.64
1:AI:58:ILE:HG12	1:AI:188:VAL:HB	1.79	0.64
1:ED:36:PHE:HZ	1:ED:194:LEU:HB3	1.63	0.64
1:EI:58:ILE:HG12	1:EI:188:VAL:HB	1.79	0.64
1:GD:36:PHE:HZ	1:GD:194:LEU:HB3	1.63	0.64
1:HI:58:ILE:HG12	1:HI:188:VAL:HB	1.79	0.64
1:IB:77:THR:O	1:IB:80:GLY:N	2.30	0.64
1:ID:36:PHE:HZ	1:ID:194:LEU:HB3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KC:78:LYS:O	1:KC:81:ASN:ND2	2.29	0.64
1:CB:77:THR:O	1:CB:80:GLY:N	2.30	0.64
1:DD:36:PHE:HZ	1:DD:194:LEU:HB3	1.63	0.64
1:JB:77:THR:O	1:JB:80:GLY:N	2.30	0.64
1:CA:117:TYR:HB2	1:CB:164:VAL:HG22	1.80	0.64
1:DA:118:GLU:OE2	1:DB:134:ARG:NH1	2.28	0.64
1:KB:67:THR:H	1:KB:70:GLN:HE21	1.46	0.64
1:CD:36:PHE:HZ	1:CD:194:LEU:HB3	1.63	0.64
1:GB:77:THR:O	1:GB:80:GLY:N	2.30	0.64
1:LD:36:PHE:HZ	1:LD:194:LEU:HB3	1.63	0.64
1:BA:117:TYR:HB2	1:BB:164:VAL:HG22	1.80	0.63
1:DI:58:ILE:HG12	1:DI:188:VAL:HB	1.79	0.63
1:EA:117:TYR:HB2	1:EB:164:VAL:HG22	1.80	0.63
1:FD:36:PHE:HZ	1:FD:194:LEU:HB3	1.63	0.63
1:GB:67:THR:H	1:GB:70:GLN:HE21	1.46	0.63
1:HA:117:TYR:HB2	1:HB:164:VAL:HG22	1.80	0.63
1:HD:36:PHE:HZ	1:HD:194:LEU:HB3	1.63	0.63
1:JD:36:PHE:HZ	1:JD:194:LEU:HB3	1.63	0.63
1:KD:36:PHE:HZ	1:KD:194:LEU:HB3	1.63	0.63
1:FB:67:THR:H	1:FB:70:GLN:HE21	1.46	0.63
1:HB:67:THR:H	1:HB:70:GLN:HE21	1.46	0.63
1:AB:77:THR:O	1:AB:80:GLY:N	2.30	0.63
1:CB:67:THR:H	1:CB:70:GLN:HE21	1.46	0.63
1:DA:117:TYR:HB2	1:DB:164:VAL:HG22	1.80	0.63
1:KI:58:ILE:HG12	1:KI:188:VAL:HB	1.79	0.63
1:LI:58:ILE:HG12	1:LI:188:VAL:HB	1.79	0.63
1:JI:58:ILE:HG12	1:JI:188:VAL:HB	1.79	0.63
1:BI:58:ILE:HG12	1:BI:188:VAL:HB	1.79	0.63
1:FI:58:ILE:HG12	1:FI:188:VAL:HB	1.79	0.63
1:BD:36:PHE:HZ	1:BD:194:LEU:HB3	1.63	0.63
1:FA:117:TYR:HB2	1:FB:164:VAL:HG22	1.80	0.63
1:HA:118:GLU:OE2	1:HB:134:ARG:NH1	2.28	0.63
1:II:58:ILE:HG12	1:II:188:VAL:HB	1.79	0.63
1:IB:67:THR:H	1:IB:70:GLN:HE21	1.46	0.62
1:CE:151:ILE:HG22	1:CE:156:GLY:HA3	1.81	0.62
1:DB:67:THR:H	1:DB:70:GLN:HE21	1.46	0.62
1:EA:118:GLU:OE2	1:EB:134:ARG:NH1	2.28	0.62
1:HE:151:ILE:HG22	1:HE:156:GLY:HA3	1.82	0.62
1:JA:117:TYR:HB2	1:JB:164:VAL:HG22	1.80	0.62
1:JE:151:ILE:HG22	1:JE:156:GLY:HA3	1.82	0.62
1:LA:117:TYR:HB2	1:LB:164:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:117:TYR:HB2	1:AB:164:VAL:HG22	1.80	0.62
1:DE:151:ILE:HG22	1:DE:156:GLY:HA3	1.82	0.62
1:KA:117:TYR:HB2	1:KB:164:VAL:HG22	1.80	0.62
1:AB:67:THR:H	1:AB:70:GLN:HE21	1.46	0.62
1:JB:67:THR:H	1:JB:70:GLN:HE21	1.46	0.62
1:CI:58:ILE:HG12	1:CI:188:VAL:HB	1.79	0.62
1:GA:117:TYR:HB2	1:GB:164:VAL:HG22	1.80	0.62
1:GD:153:ARG:NH2	1:IC:92:GLU:OE2	2.33	0.62
1:BB:67:THR:H	1:BB:70:GLN:HE21	1.46	0.62
1:CA:92:GLU:OE2	1:CI:153:ARG:NH2	2.33	0.62
1:EB:67:THR:H	1:EB:70:GLN:HE21	1.46	0.62
1:JA:118:GLU:OE2	1:JB:134:ARG:NH1	2.28	0.62
1:AA:92:GLU:OE2	1:AI:153:ARG:NH2	2.33	0.61
1:EA:92:GLU:OE2	1:EI:153:ARG:NH2	2.33	0.61
1:LE:151:ILE:HG22	1:LE:156:GLY:HA3	1.82	0.61
1:AB:61:GLY:O	1:AB:191:ILE:HA	2.01	0.61
1:DA:92:GLU:OE2	1:DI:153:ARG:NH2	2.33	0.61
1:IA:92:GLU:OE2	1:II:153:ARG:NH2	2.33	0.61
1:IE:151:ILE:HG22	1:IE:156:GLY:HA3	1.81	0.61
1:DB:61:GLY:O	1:DB:191:ILE:HA	2.01	0.61
1:FA:92:GLU:OE2	1:FI:153:ARG:NH2	2.33	0.61
1:GE:151:ILE:HG22	1:GE:156:GLY:HA3	1.82	0.61
1:HB:61:GLY:O	1:HB:191:ILE:HA	2.00	0.61
1:JA:92:GLU:OE2	1:JI:153:ARG:NH2	2.33	0.61
1:CG:170:TRP:HD1	1:CG:171:GLU:HG3	1.66	0.61
1:EG:170:TRP:HD1	1:EG:171:GLU:HG3	1.66	0.61
1:DG:170:TRP:HD1	1:DG:171:GLU:HG3	1.66	0.61
1:FG:170:TRP:HD1	1:FG:171:GLU:HG3	1.66	0.61
1:HG:170:TRP:HD1	1:HG:171:GLU:HG3	1.66	0.61
1:IG:170:TRP:HD1	1:IG:171:GLU:HG3	1.66	0.61
1:BD:153:ARG:NH2	1:KC:92:GLU:OE2	2.34	0.61
1:IA:117:TYR:HB2	1:IB:164:VAL:HG22	1.80	0.61
1:LA:92:GLU:OE2	1:LI:153:ARG:NH2	2.33	0.61
1:BE:151:ILE:HG22	1:BE:156:GLY:HA3	1.82	0.61
1:IB:61:GLY:O	1:IB:191:ILE:HA	2.01	0.61
1:JB:61:GLY:O	1:JB:191:ILE:HA	2.01	0.61
1:LB:67:THR:H	1:LB:70:GLN:HE21	1.46	0.61
1:LG:170:TRP:HD1	1:LG:171:GLU:HG3	1.66	0.61
1:AG:170:TRP:HD1	1:AG:171:GLU:HG3	1.66	0.61
1:BA:92:GLU:OE2	1:BI:153:ARG:NH2	2.33	0.61
1:JG:170:TRP:HD1	1:JG:171:GLU:HG3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KB:61:GLY:O	1:KB:191:ILE:HA	2.01	0.61
1:AE:151:ILE:HG22	1:AE:156:GLY:HA3	1.82	0.61
1:BB:61:GLY:O	1:BB:191:ILE:HA	2.01	0.61
1:FE:151:ILE:HG22	1:FE:156:GLY:HA3	1.81	0.61
1:GG:170:TRP:HD1	1:GG:171:GLU:HG3	1.66	0.61
1:HG:92:GLU:OE2	1:JH:153:ARG:NH2	2.34	0.61
1:KA:92:GLU:OE2	1:KI:153:ARG:NH2	2.33	0.61
1:KE:151:ILE:HG22	1:KE:156:GLY:HA3	1.81	0.60
1:KG:170:TRP:HD1	1:KG:171:GLU:HG3	1.66	0.60
1:GB:61:GLY:O	1:GB:191:ILE:HA	2.01	0.60
1:LE:91:ILE:O	1:LE:95:ASN:ND2	2.33	0.60
1:HA:92:GLU:OE2	1:HI:153:ARG:NH2	2.33	0.60
1:CB:61:GLY:O	1:CB:191:ILE:HA	2.01	0.60
1:EB:61:GLY:O	1:EB:191:ILE:HA	2.01	0.60
1:FB:61:GLY:O	1:FB:191:ILE:HA	2.01	0.60
1:GA:92:GLU:OE2	1:GI:153:ARG:NH2	2.33	0.60
1:EE:151:ILE:HG22	1:EE:156:GLY:HA3	1.82	0.60
1:EE:91:ILE:O	1:EE:95:ASN:ND2	2.33	0.60
1:IE:91:ILE:O	1:IE:95:ASN:ND2	2.33	0.60
1:IG:56:LYS:HD2	1:IG:180:ALA:HB1	1.84	0.60
1:AA:70:GLN:HG3	1:AA:74:ARG:HH12	1.67	0.60
1:AE:91:ILE:O	1:AE:95:ASN:ND2	2.33	0.60
1:AG:56:LYS:HD2	1:AG:180:ALA:HB1	1.84	0.60
1:FA:70:GLN:HG3	1:FA:74:ARG:HH12	1.67	0.60
1:LG:56:LYS:HD2	1:LG:180:ALA:HB1	1.84	0.60
1:BG:170:TRP:HD1	1:BG:171:GLU:HG3	1.66	0.59
1:EG:56:LYS:HD2	1:EG:180:ALA:HB1	1.84	0.59
1:FG:56:LYS:HD2	1:FG:180:ALA:HB1	1.84	0.59
1:KG:56:LYS:HD2	1:KG:180:ALA:HB1	1.84	0.59
1:BA:70:GLN:HG3	1:BA:74:ARG:HH12	1.67	0.59
1:CA:70:GLN:HG3	1:CA:74:ARG:HH12	1.67	0.59
1:EA:70:GLN:HG3	1:EA:74:ARG:HH12	1.67	0.59
1:DG:56:LYS:HD2	1:DG:180:ALA:HB1	1.84	0.59
1:LB:61:GLY:O	1:LB:191:ILE:HA	2.01	0.59
1:BF:77:THR:O	1:BF:81:ASN:ND2	2.35	0.59
1:DC:118:GLU:OE1	1:DD:134:ARG:NH2	2.35	0.59
1:GC:118:GLU:OE1	1:GD:134:ARG:NH2	2.35	0.59
1:GA:70:GLN:HG3	1:GA:74:ARG:HH12	1.67	0.59
1:HG:56:LYS:HD2	1:HG:180:ALA:HB1	1.84	0.59
1:BG:56:LYS:HD2	1:BG:180:ALA:HB1	1.84	0.59
1:CF:77:THR:O	1:CF:81:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CG:56:LYS:HD2	1:CG:180:ALA:HB1	1.84	0.59
1:DB:88:LEU:HD11	1:DB:121:LEU:HD13	1.85	0.59
1:GF:77:THR:O	1:GF:81:ASN:ND2	2.35	0.59
1:IA:70:GLN:HG3	1:IA:74:ARG:HH12	1.67	0.59
1:JE:91:ILE:O	1:JE:95:ASN:ND2	2.33	0.59
1:JG:56:LYS:HD2	1:JG:180:ALA:HB1	1.84	0.59
1:CC:118:GLU:OE1	1:CD:134:ARG:NH2	2.35	0.58
1:EC:118:GLU:OE1	1:ED:134:ARG:NH2	2.35	0.58
1:JA:56:LYS:HD2	1:JA:180:ALA:HB1	1.85	0.58
1:FC:118:GLU:OE1	1:FD:134:ARG:NH2	2.35	0.58
1:FF:77:THR:O	1:FF:81:ASN:ND2	2.35	0.58
1:HA:70:GLN:HG3	1:HA:74:ARG:HH12	1.67	0.58
1:JA:70:GLN:HG3	1:JA:74:ARG:HH12	1.67	0.58
1:JB:88:LEU:HD11	1:JB:121:LEU:HD13	1.85	0.58
1:KC:118:GLU:OE1	1:KD:134:ARG:NH2	2.35	0.58
1:BA:56:LYS:HD2	1:BA:180:ALA:HB1	1.85	0.58
1:IC:118:GLU:OE1	1:ID:134:ARG:NH2	2.35	0.58
1:LA:70:GLN:HG3	1:LA:74:ARG:HH12	1.67	0.58
1:AA:56:LYS:HD2	1:AA:180:ALA:HB1	1.85	0.58
1:GG:56:LYS:HD2	1:GG:180:ALA:HB1	1.84	0.58
1:DA:70:GLN:HG3	1:DA:74:ARG:HH12	1.67	0.58
1:FA:56:LYS:HD2	1:FA:180:ALA:HB1	1.85	0.58
1:KB:88:LEU:HD11	1:KB:121:LEU:HD13	1.85	0.58
1:DA:56:LYS:HD2	1:DA:180:ALA:HB1	1.85	0.58
1:GA:56:LYS:HD2	1:GA:180:ALA:HB1	1.85	0.58
1:IA:56:LYS:HD2	1:IA:180:ALA:HB1	1.85	0.58
1:EB:88:LEU:HD11	1:EB:121:LEU:HD13	1.85	0.58
1:GB:88:LEU:HD11	1:GB:121:LEU:HD13	1.85	0.58
1:KA:56:LYS:HD2	1:KA:180:ALA:HB1	1.85	0.58
1:KA:70:GLN:HG3	1:KA:74:ARG:HH12	1.67	0.58
1:CB:88:LEU:HD11	1:CB:121:LEU:HD13	1.85	0.58
1:FB:88:LEU:HD11	1:FB:121:LEU:HD13	1.85	0.58
1:LG:118:GLU:HG3	1:LH:134:ARG:HH22	1.69	0.58
1:BE:56:LYS:HD2	1:BE:180:ALA:HB1	1.86	0.58
1:CA:56:LYS:HD2	1:CA:180:ALA:HB1	1.85	0.58
1:DE:56:LYS:HD2	1:DE:180:ALA:HB1	1.86	0.58
1:HE:56:LYS:HD2	1:HE:180:ALA:HB1	1.86	0.58
1:AE:56:LYS:HD2	1:AE:180:ALA:HB1	1.86	0.57
1:CE:56:LYS:HD2	1:CE:180:ALA:HB1	1.86	0.57
1:FE:56:LYS:HD2	1:FE:180:ALA:HB1	1.86	0.57
1:LA:56:LYS:HD2	1:LA:180:ALA:HB1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:66:ASP:HA	1:EB:196:ARG:HB3	1.87	0.57
1:HB:66:ASP:HA	1:HB:196:ARG:HB3	1.86	0.57
1:IB:88:LEU:HD11	1:IB:121:LEU:HD13	1.85	0.57
1:LB:88:LEU:HD11	1:LB:121:LEU:HD13	1.85	0.57
1:EG:118:GLU:HG3	1:EH:134:ARG:HH22	1.69	0.57
1:GE:56:LYS:HD2	1:GE:180:ALA:HB1	1.86	0.57
1:HA:56:LYS:HD2	1:HA:180:ALA:HB1	1.85	0.57
1:IE:56:LYS:HD2	1:IE:180:ALA:HB1	1.86	0.57
1:JE:56:LYS:HD2	1:JE:180:ALA:HB1	1.86	0.57
1:CG:118:GLU:HG3	1:CH:134:ARG:HH22	1.69	0.57
1:HF:77:THR:O	1:HF:81:ASN:ND2	2.35	0.57
1:AB:88:LEU:HD11	1:AB:121:LEU:HD13	1.85	0.57
1:EE:56:LYS:HD2	1:EE:180:ALA:HB1	1.86	0.57
1:FD:81:ASN:H	1:FD:81:ASN:HD22	1.53	0.57
1:KE:56:LYS:HD2	1:KE:180:ALA:HB1	1.86	0.57
1:FB:66:ASP:HA	1:FB:196:ARG:HB3	1.87	0.57
1:LF:77:THR:O	1:LF:81:ASN:ND2	2.35	0.57
1:AG:65:ALA:HB1	1:AG:70:GLN:HG3	1.87	0.57
1:EA:56:LYS:HD2	1:EA:180:ALA:HB1	1.85	0.57
1:EF:77:THR:O	1:EF:81:ASN:ND2	2.35	0.57
1:HD:153:ARG:NH2	1:LC:92:GLU:OE2	2.37	0.57
1:LB:66:ASP:HA	1:LB:196:ARG:HB3	1.87	0.57
1:EG:65:ALA:HB1	1:EG:70:GLN:HG3	1.87	0.57
1:HD:81:ASN:H	1:HD:81:ASN:HD22	1.53	0.57
1:IG:118:GLU:HG3	1:IH:134:ARG:HH22	1.69	0.57
1:BC:118:GLU:OE1	1:BD:134:ARG:NH2	2.35	0.57
1:DG:65:ALA:HB1	1:DG:70:GLN:HG3	1.87	0.57
1:JD:81:ASN:HD22	1:JD:81:ASN:H	1.53	0.57
1:JG:65:ALA:HB1	1:JG:70:GLN:HG3	1.87	0.57
1:KG:65:ALA:HB1	1:KG:70:GLN:HG3	1.87	0.57
1:BB:88:LEU:HD11	1:BB:121:LEU:HD13	1.85	0.57
1:GG:118:GLU:HG3	1:GH:134:ARG:HH22	1.69	0.57
1:IG:65:ALA:HB1	1:IG:70:GLN:HG3	1.87	0.57
1:HB:88:LEU:HD11	1:HB:121:LEU:HD13	1.85	0.56
1:KD:81:ASN:H	1:KD:81:ASN:HD22	1.53	0.56
1:LD:81:ASN:HD22	1:LD:81:ASN:H	1.53	0.56
1:LE:56:LYS:HD2	1:LE:180:ALA:HB1	1.86	0.56
1:JG:118:GLU:HG3	1:JH:134:ARG:HH22	1.69	0.56
1:KG:118:GLU:HG3	1:KH:134:ARG:HH22	1.69	0.56
1:AD:81:ASN:HD22	1:AD:81:ASN:H	1.53	0.56
1:CG:65:ALA:HB1	1:CG:70:GLN:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:66:ASP:HA	1:GB:196:ARG:HB3	1.87	0.56
1:IB:66:ASP:HA	1:IB:196:ARG:HB3	1.87	0.56
1:CB:66:ASP:HA	1:CB:196:ARG:HB3	1.87	0.56
1:DG:118:GLU:HG3	1:DH:134:ARG:HH22	1.69	0.56
1:ED:81:ASN:H	1:ED:81:ASN:HD22	1.53	0.56
1:GG:65:ALA:HB1	1:GG:70:GLN:HG3	1.87	0.56
1:AC:118:GLU:OE1	1:AD:134:ARG:NH2	2.35	0.56
1:GD:81:ASN:HD22	1:GD:81:ASN:H	1.53	0.56
1:DD:81:ASN:HD22	1:DD:81:ASN:H	1.53	0.56
1:HG:65:ALA:HB1	1:HG:70:GLN:HG3	1.87	0.56
1:AJ:151:ILE:HG21	1:AJ:161:ILE:HD11	1.88	0.56
1:BB:66:ASP:HA	1:BB:196:ARG:HB3	1.87	0.56
1:HG:118:GLU:HG3	1:HH:134:ARG:HH22	1.69	0.56
1:JB:66:ASP:HA	1:JB:196:ARG:HB3	1.87	0.56
1:AB:66:ASP:HA	1:AB:196:ARG:HB3	1.87	0.56
1:AD:153:ARG:NH2	1:BC:92:GLU:OE2	2.39	0.56
1:BG:118:GLU:HG3	1:BH:134:ARG:HH22	1.69	0.56
1:GE:91:ILE:O	1:GE:95:ASN:ND2	2.33	0.56
1:KB:66:ASP:HA	1:KB:196:ARG:HB3	1.87	0.56
1:KJ:151:ILE:HG21	1:KJ:161:ILE:HD11	1.88	0.56
1:AG:118:GLU:HG3	1:AH:134:ARG:HH22	1.69	0.56
1:BJ:151:ILE:HG21	1:BJ:161:ILE:HD11	1.88	0.56
1:HC:118:GLU:OE1	1:HD:134:ARG:NH2	2.35	0.56
1:ID:81:ASN:HD22	1:ID:81:ASN:H	1.53	0.56
1:KD:66:ASP:N	1:KD:66:ASP:OD1	2.39	0.56
1:LC:118:GLU:OE1	1:LD:134:ARG:NH2	2.35	0.56
1:CE:91:ILE:O	1:CE:95:ASN:ND2	2.33	0.56
1:JD:66:ASP:OD1	1:JD:66:ASP:N	2.39	0.56
1:LD:66:ASP:N	1:LD:66:ASP:OD1	2.39	0.56
1:AG:92:GLU:OE2	1:IH:153:ARG:NH2	2.39	0.55
1:CD:81:ASN:H	1:CD:81:ASN:HD22	1.53	0.55
1:FG:118:GLU:HG3	1:FH:134:ARG:HH22	1.69	0.55
1:IG:153:ARG:HH22	1:LH:92:GLU:CD	2.09	0.55
1:KE:91:ILE:O	1:KE:95:ASN:ND2	2.33	0.55
1:LG:65:ALA:HB1	1:LG:70:GLN:HG3	1.87	0.55
1:AD:66:ASP:N	1:AD:66:ASP:OD1	2.39	0.55
1:CJ:151:ILE:HG21	1:CJ:161:ILE:HD11	1.88	0.55
1:IH:37:ASP:N	1:IH:37:ASP:OD1	2.39	0.55
1:JF:77:THR:O	1:JF:81:ASN:ND2	2.35	0.55
1:BG:92:GLU:OE2	1:EH:153:ARG:NH2	2.40	0.55
1:LJ:151:ILE:HG21	1:LJ:161:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BG:65:ALA:HB1	1:BG:70:GLN:HG3	1.87	0.55
1:DB:66:ASP:HA	1:DB:196:ARG:HB3	1.87	0.55
1:DH:37:ASP:OD1	1:DH:37:ASP:N	2.39	0.55
1:ED:66:ASP:OD1	1:ED:66:ASP:N	2.39	0.55
1:FE:91:ILE:O	1:FE:95:ASN:ND2	2.33	0.55
1:EH:37:ASP:OD1	1:EH:37:ASP:N	2.40	0.55
1:IF:77:THR:O	1:IF:81:ASN:ND2	2.35	0.55
1:AF:77:THR:O	1:AF:81:ASN:ND2	2.35	0.55
1:BD:66:ASP:OD1	1:BD:66:ASP:N	2.39	0.55
1:FG:65:ALA:HB1	1:FG:70:GLN:HG3	1.87	0.55
1:BD:81:ASN:HD22	1:BD:81:ASN:H	1.53	0.55
1:ED:118:GLU:HG3	1:EE:134:ARG:HH22	1.72	0.55
1:EJ:151:ILE:HG21	1:EJ:161:ILE:HD11	1.88	0.55
1:HH:37:ASP:N	1:HH:37:ASP:OD1	2.39	0.55
1:KD:118:GLU:HG3	1:KE:134:ARG:HH22	1.72	0.55
1:FJ:151:ILE:HG21	1:FJ:161:ILE:HD11	1.88	0.55
1:GJ:151:ILE:HG21	1:GJ:161:ILE:HD11	1.88	0.55
1:BF:92:GLU:OE2	1:EB:153:ARG:NH2	2.32	0.55
1:DC:151:ILE:HG21	1:DC:161:ILE:HD11	1.89	0.55
1:GD:66:ASP:OD1	1:GD:66:ASP:N	2.39	0.55
1:HJ:151:ILE:HG21	1:HJ:161:ILE:HD11	1.88	0.55
1:ID:118:GLU:HG3	1:IE:134:ARG:HH22	1.72	0.55
1:BE:91:ILE:O	1:BE:95:ASN:ND2	2.33	0.55
1:CD:118:GLU:HG3	1:CE:134:ARG:HH22	1.72	0.55
1:FD:118:GLU:HG3	1:FE:134:ARG:HH22	1.72	0.55
1:BC:151:ILE:HG21	1:BC:161:ILE:HD11	1.89	0.54
1:CH:37:ASP:N	1:CH:37:ASP:OD1	2.39	0.54
1:GH:37:ASP:OD1	1:GH:37:ASP:N	2.39	0.54
1:HD:118:GLU:HG3	1:HE:134:ARG:HH22	1.72	0.54
1:HH:81:ASN:HB3	1:HH:84:TRP:HB2	1.89	0.54
1:IG:92:GLU:OE2	1:LH:153:ARG:NH2	2.40	0.54
1:IJ:151:ILE:HG21	1:IJ:161:ILE:HD11	1.88	0.54
1:LD:118:GLU:HG3	1:LE:134:ARG:HH22	1.72	0.54
1:AH:81:ASN:HB3	1:AH:84:TRP:HB2	1.89	0.54
1:DJ:151:ILE:HG21	1:DJ:161:ILE:HD11	1.88	0.54
1:FH:81:ASN:HB3	1:FH:84:TRP:HB2	1.89	0.54
1:HE:91:ILE:O	1:HE:95:ASN:ND2	2.33	0.54
1:ID:66:ASP:N	1:ID:66:ASP:OD1	2.39	0.54
1:JJ:151:ILE:HG21	1:JJ:161:ILE:HD11	1.88	0.54
1:KH:37:ASP:N	1:KH:37:ASP:OD1	2.39	0.54
1:EG:43:VAL:HG23	1:EG:173:PRO:HD3	1.90	0.54

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:FC:151:ILE:HG21	1:FC:161:ILE:HD11	1.89	0.54
1:FH:63:ILE:HG12	1:FH:82:LYS:HD3	1.90	0.54
1:IH:63:ILE:HG12	1:IH:82:LYS:HD3	1.90	0.54
1:IH:81:ASN:HB3	1:IH:84:TRP:HB2	1.89	0.54
1:JD:118:GLU:HG3	1:JE:134:ARG:HH22	1.72	0.54
1:JH:63:ILE:HG12	1:JH:82:LYS:HD3	1.90	0.54
1:KC:151:ILE:HG21	1:KC:161:ILE:HD11	1.89	0.54
1:KE:171:GLU:N	1:KE:171:GLU:OE2	2.41	0.54
1:AC:151:ILE:HG21	1:AC:161:ILE:HD11	1.89	0.54
1:BF:79:HIS:HB3	1:EB:79:HIS:CE1	2.41	0.54
1:CH:63:ILE:HG12	1:CH:82:LYS:HD3	1.90	0.54
1:CH:81:ASN:HB3	1:CH:84:TRP:HB2	1.89	0.54
1:DD:118:GLU:HG3	1:DE:134:ARG:HH22	1.72	0.54
1:EC:151:ILE:HG21	1:EC:161:ILE:HD11	1.89	0.54
1:GH:63:ILE:HG12	1:GH:82:LYS:HD3	1.90	0.54
1:JE:171:GLU:N	1:JE:171:GLU:OE2	2.41	0.54
1:JH:37:ASP:OD1	1:JH:37:ASP:N	2.39	0.54
1:BH:81:ASN:HB3	1:BH:84:TRP:HB2	1.89	0.54
1:LG:43:VAL:HG23	1:LG:173:PRO:HD3	1.90	0.54
1:DG:43:VAL:HG23	1:DG:173:PRO:HD3	1.90	0.54
1:DH:63:ILE:HG12	1:DH:82:LYS:HD3	1.90	0.54
1:DH:81:ASN:HB3	1:DH:84:TRP:HB2	1.89	0.54
1:LC:151:ILE:HG21	1:LC:161:ILE:HD11	1.89	0.54
1:AG:43:VAL:HG23	1:AG:173:PRO:HD3	1.90	0.54
1:BD:118:GLU:HG3	1:BE:134:ARG:HH22	1.72	0.54
1:CC:151:ILE:HG21	1:CC:161:ILE:HD11	1.89	0.54
1:FG:43:VAL:HG23	1:FG:173:PRO:HD3	1.90	0.54
1:GD:118:GLU:HG3	1:GE:134:ARG:HH22	1.72	0.54
1:HD:66:ASP:N	1:HD:66:ASP:OD1	2.39	0.54
1:IC:151:ILE:HG21	1:IC:161:ILE:HD11	1.89	0.54
1:JC:151:ILE:HG21	1:JC:161:ILE:HD11	1.89	0.54
1:AD:118:GLU:HG3	1:AE:134:ARG:HH22	1.72	0.54
1:HC:151:ILE:HG21	1:HC:161:ILE:HD11	1.89	0.54
1:HE:171:GLU:N	1:HE:171:GLU:OE2	2.41	0.54
1:IE:171:GLU:N	1:IE:171:GLU:OE2	2.41	0.54
1:JG:43:VAL:HG23	1:JG:173:PRO:HD3	1.90	0.54
1:AE:171:GLU:N	1:AE:171:GLU:OE2	2.41	0.54
1:BG:43:VAL:HG23	1:BG:173:PRO:HD3	1.90	0.54
1:BH:63:ILE:HG12	1:BH:82:LYS:HD3	1.90	0.54
1:EE:171:GLU:N	1:EE:171:GLU:OE2	2.41	0.54
1:GH:81:ASN:HB3	1:GH:84:TRP:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HG:43:VAL:HG23	1:HG:173:PRO:HD3	1.90	0.54
1:DD:66:ASP:OD1	1:DD:66:ASP:N	2.39	0.54
1:LH:37:ASP:OD1	1:LH:37:ASP:N	2.39	0.54
1:AH:37:ASP:N	1:AH:37:ASP:OD1	2.39	0.53
1:FI:93:MET:HG3	1:FJ:171:GLU:HG2	1.90	0.53
1:GE:171:GLU:N	1:GE:171:GLU:OE2	2.41	0.53
1:HG:66:ASP:N	1:HG:66:ASP:OD1	2.42	0.53
1:JI:93:MET:HG3	1:JJ:171:GLU:HG2	1.91	0.53
1:CG:43:VAL:HG23	1:CG:173:PRO:HD3	1.90	0.53
1:FD:66:ASP:N	1:FD:66:ASP:OD1	2.39	0.53
1:IG:43:VAL:HG23	1:IG:173:PRO:HD3	1.90	0.53
1:JC:118:GLU:OE1	1:JD:134:ARG:NH2	2.35	0.53
1:KF:77:THR:O	1:KF:81:ASN:ND2	2.35	0.53
1:KI:93:MET:HG3	1:KJ:171:GLU:HG2	1.91	0.53
1:LE:171:GLU:OE2	1:LE:171:GLU:N	2.41	0.53
1:DG:66:ASP:OD1	1:DG:66:ASP:N	2.42	0.53
1:GC:151:ILE:HG21	1:GC:161:ILE:HD11	1.89	0.53
1:IG:66:ASP:N	1:IG:66:ASP:OD1	2.42	0.53
1:LH:81:ASN:HB3	1:LH:84:TRP:HB2	1.89	0.53
1:BE:171:GLU:N	1:BE:171:GLU:OE2	2.41	0.53
1:EG:66:ASP:OD1	1:EG:66:ASP:N	2.42	0.53
1:HH:63:ILE:HG12	1:HH:82:LYS:HD3	1.90	0.53
1:KH:63:ILE:HG12	1:KH:82:LYS:HD3	1.90	0.53
1:CC:92:GLU:OE2	1:LD:153:ARG:NH2	2.42	0.53
1:CD:66:ASP:N	1:CD:66:ASP:OD1	2.39	0.53
1:CE:171:GLU:N	1:CE:171:GLU:OE2	2.41	0.53
1:EH:81:ASN:HB3	1:EH:84:TRP:HB2	1.89	0.53
1:FH:37:ASP:N	1:FH:37:ASP:OD1	2.39	0.53
1:CD:153:ARG:NH2	1:HC:92:GLU:OE2	2.42	0.53
1:EI:93:MET:HG3	1:EJ:171:GLU:HG2	1.91	0.53
1:DF:151:ILE:HG21	1:DF:161:ILE:HD11	1.91	0.53
1:FE:171:GLU:N	1:FE:171:GLU:OE2	2.41	0.53
1:GF:151:ILE:HG21	1:GF:161:ILE:HD11	1.91	0.53
1:GG:43:VAL:HG23	1:GG:173:PRO:HD3	1.90	0.53
1:CF:151:ILE:HG21	1:CF:161:ILE:HD11	1.91	0.53
1:HE:78:LYS:O	1:HE:81:ASN:ND2	2.29	0.53
1:KG:43:VAL:HG23	1:KG:173:PRO:HD3	1.90	0.53
1:LG:66:ASP:OD1	1:LG:66:ASP:N	2.42	0.53
1:LH:63:ILE:HG12	1:LH:82:LYS:HD3	1.90	0.53
1:LI:93:MET:HG3	1:LJ:171:GLU:HG2	1.91	0.53
1:AH:63:ILE:HG12	1:AH:82:LYS:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CG:66:ASP:N	1:CG:66:ASP:OD1	2.41	0.53
1:DE:171:GLU:OE2	1:DE:171:GLU:N	2.41	0.53
1:DF:77:THR:O	1:DF:81:ASN:ND2	2.35	0.53
1:EF:151:ILE:HG21	1:EF:161:ILE:HD11	1.91	0.53
1:EH:63:ILE:HG12	1:EH:82:LYS:HD3	1.90	0.53
1:CH:84:TRP:CD1	1:CH:150:CYS:HB2	2.45	0.52
1:KH:81:ASN:HB3	1:KH:84:TRP:HB2	1.89	0.52
1:IH:84:TRP:CD1	1:IH:150:CYS:HB2	2.45	0.52
1:KF:151:ILE:HG21	1:KF:161:ILE:HD11	1.91	0.52
1:BF:151:ILE:HG21	1:BF:161:ILE:HD11	1.91	0.52
1:EH:84:TRP:CD1	1:EH:150:CYS:HB2	2.45	0.52
1:FH:84:TRP:CD1	1:FH:150:CYS:HB2	2.45	0.52
1:GG:66:ASP:OD1	1:GG:66:ASP:N	2.42	0.52
1:GI:93:MET:HG3	1:GJ:171:GLU:HG2	1.91	0.52
1:II:93:MET:HG3	1:IJ:171:GLU:HG2	1.90	0.52
1:AG:141:ASP:OD1	1:AG:142:ARG:N	2.43	0.52
1:AH:84:TRP:CD1	1:AH:150:CYS:HB2	2.45	0.52
1:BH:84:TRP:CD1	1:BH:150:CYS:HB2	2.44	0.52
1:FG:141:ASP:OD1	1:FG:142:ARG:N	2.43	0.52
1:JH:81:ASN:HB3	1:JH:84:TRP:HB2	1.89	0.52
1:LF:151:ILE:HG21	1:LF:161:ILE:HD11	1.91	0.52
1:AF:151:ILE:HG21	1:AF:161:ILE:HD11	1.91	0.52
1:BG:66:ASP:OD1	1:BG:66:ASP:N	2.42	0.52
1:CI:93:MET:HG3	1:CJ:171:GLU:HG2	1.91	0.52
1:DI:93:MET:HG3	1:DJ:171:GLU:HG2	1.90	0.52
1:FF:151:ILE:HG21	1:FF:161:ILE:HD11	1.91	0.52
1:GH:84:TRP:CD1	1:GH:150:CYS:HB2	2.45	0.52
1:HF:151:ILE:HG21	1:HF:161:ILE:HD11	1.91	0.52
1:HI:93:MET:HG3	1:HJ:171:GLU:HG2	1.91	0.52
1:EC:92:GLU:OE2	1:FD:153:ARG:NH2	2.43	0.52
1:CG:141:ASP:OD1	1:CG:142:ARG:N	2.43	0.52
1:DE:91:ILE:O	1:DE:95:ASN:ND2	2.33	0.52
1:HG:141:ASP:OD1	1:HG:142:ARG:N	2.43	0.52
1:DG:92:GLU:OE2	1:HH:153:ARG:NH2	2.42	0.52
1:GD:67:THR:H	1:GD:70:GLN:HE21	1.58	0.52
1:KH:56:LYS:HD2	1:KH:180:ALA:HB1	1.92	0.52
1:LD:67:THR:H	1:LD:70:GLN:HE21	1.58	0.52
1:BH:56:LYS:HD2	1:BH:180:ALA:HB1	1.92	0.52
1:DH:84:TRP:CD1	1:DH:150:CYS:HB2	2.45	0.52
1:FD:67:THR:H	1:FD:70:GLN:HE21	1.58	0.52
1:IH:56:LYS:HD2	1:IH:180:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KH:84:TRP:CD1	1:KH:150:CYS:HB2	2.45	0.52
1:LH:84:TRP:CD1	1:LH:150:CYS:HB2	2.45	0.52
1:AH:56:LYS:HD2	1:AH:180:ALA:HB1	1.92	0.52
1:EG:141:ASP:OD1	1:EG:142:ARG:N	2.43	0.52
1:ID:67:THR:H	1:ID:70:GLN:HE21	1.58	0.52
1:BI:93:MET:HG3	1:BJ:171:GLU:HG2	1.91	0.51
1:DG:141:ASP:OD1	1:DG:142:ARG:N	2.43	0.51
1:FF:36:PHE:CG	1:FF:196:ARG:HG2	2.45	0.51
1:GH:133:SER:O	1:GH:140:VAL:HG11	2.10	0.51
1:HD:67:THR:H	1:HD:70:GLN:HE21	1.58	0.51
1:IB:65:ALA:HB1	1:IB:70:GLN:HG3	1.93	0.51
1:IF:36:PHE:CG	1:IF:196:ARG:HG2	2.46	0.51
1:IG:141:ASP:OD1	1:IG:142:ARG:N	2.43	0.51
1:JD:67:THR:H	1:JD:70:GLN:HE21	1.58	0.51
1:JH:133:SER:O	1:JH:140:VAL:HG11	2.11	0.51
1:LG:141:ASP:OD1	1:LG:142:ARG:N	2.43	0.51
1:LH:133:SER:O	1:LH:140:VAL:HG11	2.11	0.51
1:AB:65:ALA:HB1	1:AB:70:GLN:HG3	1.93	0.51
1:AI:93:MET:HG3	1:AJ:171:GLU:HG2	1.91	0.51
1:BD:67:THR:H	1:BD:70:GLN:HE21	1.58	0.51
1:CD:67:THR:H	1:CD:70:GLN:HE21	1.58	0.51
1:CF:36:PHE:CG	1:CF:196:ARG:HG2	2.46	0.51
1:DD:153:ARG:NH2	1:FC:92:GLU:OE2	2.43	0.51
1:ED:67:THR:H	1:ED:70:GLN:HE21	1.58	0.51
1:EI:66:ASP:HA	1:EI:196:ARG:HB2	1.93	0.51
1:GG:141:ASP:OD1	1:GG:142:ARG:N	2.43	0.51
1:HH:84:TRP:CD1	1:HH:150:CYS:HB2	2.45	0.51
1:KD:67:THR:H	1:KD:70:GLN:HE21	1.58	0.51
1:AD:67:THR:H	1:AD:70:GLN:HE21	1.58	0.51
1:BG:141:ASP:OD1	1:BG:142:ARG:N	2.43	0.51
1:CI:66:ASP:HA	1:CI:196:ARG:HB2	1.93	0.51
1:EF:36:PHE:CG	1:EF:196:ARG:HG2	2.46	0.51
1:EG:92:GLU:OE2	1:GH:153:ARG:NH2	2.43	0.51
1:FJ:66:ASP:N	1:FJ:66:ASP:OD1	2.44	0.51
1:HB:65:ALA:HB1	1:HB:70:GLN:HG3	1.93	0.51
1:KE:78:LYS:O	1:KE:81:ASN:ND2	2.29	0.51
1:DH:56:LYS:HD2	1:DH:180:ALA:HB1	1.92	0.51
1:FI:66:ASP:HA	1:FI:196:ARG:HB2	1.93	0.51
1:HF:36:PHE:CG	1:HF:196:ARG:HG2	2.46	0.51
1:IF:151:ILE:HG21	1:IF:161:ILE:HD11	1.91	0.51
1:JF:151:ILE:HG21	1:JF:161:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BH:37:ASP:OD1	1:BH:37:ASP:N	2.39	0.51
1:CH:133:SER:O	1:CH:140:VAL:HG11	2.10	0.51
1:DF:36:PHE:CG	1:DF:196:ARG:HG2	2.46	0.51
1:DJ:66:ASP:OD1	1:DJ:66:ASP:N	2.44	0.51
1:EI:151:ILE:HG21	1:EI:161:ILE:HD11	1.93	0.51
1:GF:36:PHE:CG	1:GF:196:ARG:HG2	2.46	0.51
1:GI:66:ASP:HA	1:GI:196:ARG:HB2	1.93	0.51
1:IH:133:SER:O	1:IH:140:VAL:HG11	2.10	0.51
1:AF:36:PHE:CG	1:AF:196:ARG:HG2	2.46	0.51
1:AG:66:ASP:N	1:AG:66:ASP:OD1	2.42	0.51
1:BB:65:ALA:HB1	1:BB:70:GLN:HG3	1.93	0.51
1:CH:56:LYS:HD2	1:CH:180:ALA:HB1	1.92	0.51
1:DD:67:THR:H	1:DD:70:GLN:HE21	1.58	0.51
1:JB:65:ALA:HB1	1:JB:70:GLN:HG3	1.93	0.51
1:KF:171:GLU:OE2	1:KF:171:GLU:N	2.44	0.51
1:KJ:66:ASP:N	1:KJ:66:ASP:OD1	2.44	0.51
1:AH:133:SER:O	1:AH:140:VAL:HG11	2.11	0.51
1:BI:66:ASP:HA	1:BI:196:ARG:HB2	1.93	0.51
1:DF:171:GLU:N	1:DF:171:GLU:OE2	2.44	0.51
1:DH:133:SER:O	1:DH:140:VAL:HG11	2.10	0.51
1:FF:171:GLU:N	1:FF:171:GLU:OE2	2.44	0.51
1:HF:171:GLU:N	1:HF:171:GLU:OE2	2.44	0.51
1:HH:133:SER:O	1:HH:140:VAL:HG11	2.10	0.51
1:JG:37:ASP:N	1:JG:37:ASP:OD1	2.44	0.51
1:KG:37:ASP:OD1	1:KG:37:ASP:N	2.44	0.51
1:LF:171:GLU:N	1:LF:171:GLU:OE2	2.44	0.51
1:LG:37:ASP:N	1:LG:37:ASP:OD1	2.44	0.51
1:AF:171:GLU:N	1:AF:171:GLU:OE2	2.44	0.51
1:BF:36:PHE:CG	1:BF:196:ARG:HG2	2.46	0.51
1:CD:61:GLY:O	1:CD:191:ILE:HA	2.11	0.51
1:EF:171:GLU:N	1:EF:171:GLU:OE2	2.44	0.51
1:HI:66:ASP:HA	1:HI:196:ARG:HB2	1.92	0.51
1:HI:151:ILE:HG21	1:HI:161:ILE:HD11	1.93	0.51
1:IE:78:LYS:O	1:IE:81:ASN:ND2	2.29	0.51
1:II:151:ILE:HG21	1:II:161:ILE:HD11	1.93	0.51
1:JF:171:GLU:N	1:JF:171:GLU:OE2	2.44	0.51
1:LD:61:GLY:O	1:LD:191:ILE:HA	2.11	0.51
1:BE:78:LYS:O	1:BE:81:ASN:ND2	2.29	0.51
1:FB:65:ALA:HB1	1:FB:70:GLN:HG3	1.93	0.51
1:IF:171:GLU:N	1:IF:171:GLU:OE2	2.44	0.51
1:JG:141:ASP:OD1	1:JG:142:ARG:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JH:84:TRP:CD1	1:JH:150:CYS:HB2	2.45	0.51
1:KF:36:PHE:CG	1:KF:196:ARG:HG2	2.46	0.51
1:KG:141:ASP:OD1	1:KG:142:ARG:N	2.43	0.51
1:KI:151:ILE:HG21	1:KI:161:ILE:HD11	1.93	0.51
1:LB:65:ALA:HB1	1:LB:70:GLN:HG3	1.93	0.51
1:LF:36:PHE:CG	1:LF:196:ARG:HG2	2.46	0.51
1:LI:66:ASP:HA	1:LI:196:ARG:HB2	1.93	0.51
1:LI:151:ILE:HG21	1:LI:161:ILE:HD11	1.93	0.51
1:BD:61:GLY:O	1:BD:191:ILE:HA	2.11	0.51
1:EH:56:LYS:HD2	1:EH:180:ALA:HB1	1.92	0.51
1:GB:65:ALA:HB1	1:GB:70:GLN:HG3	1.93	0.51
1:GG:37:ASP:N	1:GG:37:ASP:OD1	2.44	0.51
1:JF:36:PHE:CG	1:JF:196:ARG:HG2	2.46	0.51
1:KG:66:ASP:N	1:KG:66:ASP:OD1	2.42	0.51
1:KH:133:SER:O	1:KH:140:VAL:HG11	2.10	0.51
1:LJ:66:ASP:OD1	1:LJ:66:ASP:N	2.44	0.51
1:CB:65:ALA:HB1	1:CB:70:GLN:HG3	1.93	0.50
1:GF:171:GLU:N	1:GF:171:GLU:OE2	2.44	0.50
1:GI:151:ILE:HG21	1:GI:161:ILE:HD11	1.93	0.50
1:ID:61:GLY:O	1:ID:191:ILE:HA	2.11	0.50
1:KI:66:ASP:HA	1:KI:196:ARG:HB2	1.93	0.50
1:DG:37:ASP:N	1:DG:37:ASP:OD1	2.44	0.50
1:DI:66:ASP:HA	1:DI:196:ARG:HB2	1.93	0.50
1:JJ:66:ASP:OD1	1:JJ:66:ASP:N	2.44	0.50
1:AI:151:ILE:HG21	1:AI:161:ILE:HD11	1.93	0.50
1:BI:151:ILE:HG21	1:BI:161:ILE:HD11	1.93	0.50
1:CF:171:GLU:OE2	1:CF:171:GLU:N	2.44	0.50
1:DB:65:ALA:HB1	1:DB:70:GLN:HG3	1.93	0.50
1:HD:61:GLY:O	1:HD:191:ILE:HA	2.11	0.50
1:HG:37:ASP:OD1	1:HG:37:ASP:N	2.44	0.50
1:HG:77:THR:CG2	1:HG:78:LYS:N	2.59	0.50
1:II:66:ASP:HA	1:II:196:ARG:HB2	1.93	0.50
1:LG:77:THR:CG2	1:LG:78:LYS:N	2.59	0.50
1:AH:153:ARG:NH2	1:LG:92:GLU:OE2	2.45	0.50
1:AJ:84:TRP:CD2	1:AJ:150:CYS:HB2	2.47	0.50
1:CG:37:ASP:OD1	1:CG:37:ASP:N	2.44	0.50
1:EB:65:ALA:HB1	1:EB:70:GLN:HG3	1.93	0.50
1:FH:56:LYS:HD2	1:FH:180:ALA:HB1	1.92	0.50
1:FH:133:SER:O	1:FH:140:VAL:HG11	2.11	0.50
1:GD:61:GLY:O	1:GD:191:ILE:HA	2.11	0.50
1:AG:37:ASP:N	1:AG:37:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:171:GLU:N	1:BF:171:GLU:OE2	2.44	0.50
1:CI:151:ILE:HG21	1:CI:161:ILE:HD11	1.93	0.50
1:EJ:84:TRP:CD2	1:EJ:150:CYS:HB2	2.47	0.50
1:FJ:84:TRP:CD2	1:FJ:150:CYS:HB2	2.47	0.50
1:KJ:84:TRP:CD2	1:KJ:150:CYS:HB2	2.47	0.50
1:AD:61:GLY:O	1:AD:191:ILE:HA	2.11	0.50
1:AG:84:TRP:CD1	1:AG:150:CYS:HB2	2.47	0.50
1:ED:61:GLY:O	1:ED:191:ILE:HA	2.11	0.50
1:FD:61:GLY:O	1:FD:191:ILE:HA	2.11	0.50
1:GA:97:PHE:HZ	1:GB:174:VAL:HG22	1.77	0.50
1:LG:84:TRP:CD1	1:LG:150:CYS:HB2	2.47	0.50
1:CG:84:TRP:CD1	1:CG:150:CYS:HB2	2.47	0.50
1:CJ:66:ASP:N	1:CJ:66:ASP:OD1	2.44	0.50
1:DA:97:PHE:HZ	1:DB:174:VAL:HG22	1.77	0.50
1:EH:133:SER:O	1:EH:140:VAL:HG11	2.10	0.50
1:GH:56:LYS:HD2	1:GH:180:ALA:HB1	1.92	0.50
1:JG:84:TRP:CD1	1:JG:150:CYS:HB2	2.47	0.50
1:JI:66:ASP:HA	1:JI:196:ARG:HB2	1.93	0.50
1:DI:151:ILE:HG21	1:DI:161:ILE:HD11	1.93	0.50
1:FG:37:ASP:OD1	1:FG:37:ASP:N	2.44	0.50
1:HH:56:LYS:HD2	1:HH:180:ALA:HB1	1.92	0.50
1:IG:37:ASP:N	1:IG:37:ASP:OD1	2.44	0.50
1:KA:97:PHE:HZ	1:KB:174:VAL:HG22	1.77	0.50
1:KB:78:LYS:HA	1:KB:81:ASN:HB3	1.94	0.50
1:AI:66:ASP:HA	1:AI:196:ARG:HB2	1.93	0.50
1:DD:61:GLY:O	1:DD:191:ILE:HA	2.11	0.50
1:DG:84:TRP:CD1	1:DG:150:CYS:HB2	2.47	0.50
1:FI:151:ILE:HG21	1:FI:161:ILE:HD11	1.93	0.50
1:JB:78:LYS:HA	1:JB:81:ASN:HB3	1.94	0.50
1:JH:56:LYS:HD2	1:JH:180:ALA:HB1	1.92	0.50
1:KB:65:ALA:HB1	1:KB:70:GLN:HG3	1.93	0.50
1:BB:78:LYS:HA	1:BB:81:ASN:HB3	1.94	0.49
1:CB:78:LYS:HA	1:CB:81:ASN:HB3	1.94	0.49
1:DJ:84:TRP:CD2	1:DJ:150:CYS:HB2	2.47	0.49
1:EG:37:ASP:OD1	1:EG:37:ASP:N	2.44	0.49
1:FE:61:GLY:O	1:FE:191:ILE:HA	2.12	0.49
1:GE:61:GLY:O	1:GE:191:ILE:HA	2.12	0.49
1:IG:84:TRP:CD1	1:IG:150:CYS:HB2	2.47	0.49
1:KD:61:GLY:O	1:KD:191:ILE:HA	2.11	0.49
1:BJ:84:TRP:CD2	1:BJ:150:CYS:HB2	2.47	0.49
1:CA:97:PHE:HZ	1:CB:174:VAL:HG22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DE:61:GLY:O	1:DE:191:ILE:HA	2.12	0.49
1:GB:78:LYS:HA	1:GB:81:ASN:HB3	1.94	0.49
1:GJ:66:ASP:OD1	1:GJ:66:ASP:N	2.44	0.49
1:HG:84:TRP:CD1	1:HG:150:CYS:HB2	2.47	0.49
1:HJ:66:ASP:N	1:HJ:66:ASP:OD1	2.44	0.49
1:JF:58:ILE:HG12	1:JF:188:VAL:HB	1.94	0.49
1:JI:151:ILE:HG21	1:JI:161:ILE:HD11	1.93	0.49
1:KE:61:GLY:O	1:KE:191:ILE:HA	2.13	0.49
1:LE:78:LYS:O	1:LE:81:ASN:ND2	2.29	0.49
1:BC:171:GLU:N	1:BC:171:GLU:OE2	2.46	0.49
1:CJ:84:TRP:CD2	1:CJ:150:CYS:HB2	2.47	0.49
1:DB:78:LYS:HA	1:DB:81:ASN:HB3	1.94	0.49
1:DF:58:ILE:HG12	1:DF:188:VAL:HB	1.94	0.49
1:HE:61:GLY:O	1:HE:191:ILE:HA	2.13	0.49
1:HF:58:ILE:HG12	1:HF:188:VAL:HB	1.94	0.49
1:HJ:84:TRP:CD2	1:HJ:150:CYS:HB2	2.47	0.49
1:IJ:84:TRP:CD2	1:IJ:150:CYS:HB2	2.47	0.49
1:JA:97:PHE:HZ	1:JB:174:VAL:HG22	1.77	0.49
1:JE:61:GLY:O	1:JE:191:ILE:HA	2.12	0.49
1:EE:61:GLY:O	1:EE:191:ILE:HA	2.12	0.49
1:EE:78:LYS:O	1:EE:81:ASN:ND2	2.29	0.49
1:FG:66:ASP:N	1:FG:66:ASP:OD1	2.42	0.49
1:HA:97:PHE:HZ	1:HB:174:VAL:HG22	1.77	0.49
1:LJ:84:TRP:CD2	1:LJ:150:CYS:HB2	2.47	0.49
1:BA:97:PHE:HZ	1:BB:174:VAL:HG22	1.77	0.49
1:BH:133:SER:O	1:BH:140:VAL:HG11	2.10	0.49
1:CE:61:GLY:O	1:CE:191:ILE:HA	2.13	0.49
1:EG:84:TRP:CD1	1:EG:150:CYS:HB2	2.47	0.49
1:LA:97:PHE:HZ	1:LB:174:VAL:HG22	1.77	0.49
1:LB:78:LYS:HA	1:LB:81:ASN:HB3	1.94	0.49
1:LF:58:ILE:HG12	1:LF:188:VAL:HB	1.94	0.49
1:LI:77:THR:HG22	1:LI:80:GLY:H	1.78	0.49
1:CE:84:TRP:CD2	1:CE:150:CYS:HB2	2.48	0.49
1:DI:77:THR:HG22	1:DI:80:GLY:H	1.78	0.49
1:FG:84:TRP:CD1	1:FG:150:CYS:HB2	2.47	0.49
1:FI:77:THR:HG22	1:FI:80:GLY:H	1.78	0.49
1:GJ:84:TRP:CD2	1:GJ:150:CYS:HB2	2.47	0.49
1:HE:84:TRP:CD2	1:HE:150:CYS:HB2	2.48	0.49
1:JD:61:GLY:O	1:JD:191:ILE:HA	2.11	0.49
1:KF:58:ILE:HG12	1:KF:188:VAL:HB	1.94	0.49
1:AE:84:TRP:CD2	1:AE:150:CYS:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:66:ASP:OD1	1:AJ:66:ASP:N	2.44	0.49
1:BE:61:GLY:O	1:BE:191:ILE:HA	2.12	0.49
1:BG:37:ASP:N	1:BG:37:ASP:OD1	2.44	0.49
1:FG:77:THR:CG2	1:FG:78:LYS:N	2.59	0.49
1:JE:84:TRP:CD2	1:JE:150:CYS:HB2	2.48	0.49
1:LH:56:LYS:HD2	1:LH:180:ALA:HB1	1.92	0.49
1:CF:58:ILE:HG12	1:CF:188:VAL:HB	1.94	0.49
1:FC:171:GLU:N	1:FC:171:GLU:OE2	2.46	0.49
1:GG:84:TRP:CD1	1:GG:150:CYS:HB2	2.47	0.49
1:IA:97:PHE:HZ	1:IB:174:VAL:HG22	1.77	0.49
1:IC:88:LEU:HD11	1:IC:121:LEU:HD13	1.95	0.49
1:IE:61:GLY:O	1:IE:191:ILE:HA	2.12	0.49
1:IF:58:ILE:HG12	1:IF:188:VAL:HB	1.94	0.49
1:JJ:84:TRP:CD2	1:JJ:150:CYS:HB2	2.47	0.49
1:KE:84:TRP:CD2	1:KE:150:CYS:HB2	2.48	0.49
1:BE:84:TRP:CD2	1:BE:150:CYS:HB2	2.48	0.49
1:BG:84:TRP:CD1	1:BG:150:CYS:HB2	2.47	0.49
1:CE:62:VAL:HA	1:CE:192:GLY:O	2.13	0.49
1:DC:171:GLU:N	1:DC:171:GLU:OE2	2.46	0.49
1:EA:97:PHE:HZ	1:EB:174:VAL:HG22	1.77	0.49
1:EE:84:TRP:CD2	1:EE:150:CYS:HB2	2.48	0.49
1:EF:58:ILE:HG12	1:EF:188:VAL:HB	1.95	0.49
1:EJ:66:ASP:N	1:EJ:66:ASP:OD1	2.44	0.49
1:GC:171:GLU:N	1:GC:171:GLU:OE2	2.46	0.49
1:IC:171:GLU:N	1:IC:171:GLU:OE2	2.46	0.49
1:JC:171:GLU:N	1:JC:171:GLU:OE2	2.46	0.49
1:LE:62:VAL:HA	1:LE:192:GLY:O	2.13	0.49
1:LE:84:TRP:CD2	1:LE:150:CYS:HB2	2.48	0.49
1:AE:61:GLY:O	1:AE:191:ILE:HA	2.12	0.49
1:AF:58:ILE:HG12	1:AF:188:VAL:HB	1.94	0.49
1:HC:171:GLU:N	1:HC:171:GLU:OE2	2.46	0.49
1:IB:78:LYS:HA	1:IB:81:ASN:HB3	1.94	0.49
1:KI:77:THR:HG22	1:KI:80:GLY:H	1.78	0.49
1:AD:68:LEU:HB2	1:AD:195:ILE:HD12	1.95	0.48
1:BD:68:LEU:HB2	1:BD:195:ILE:HD12	1.95	0.48
1:BF:58:ILE:HG12	1:BF:188:VAL:HB	1.95	0.48
1:CC:171:GLU:OE2	1:CC:171:GLU:N	2.46	0.48
1:DD:68:LEU:HB2	1:DD:195:ILE:HD12	1.95	0.48
1:FB:78:LYS:HA	1:FB:81:ASN:HB3	1.94	0.48
1:ID:68:LEU:HB2	1:ID:195:ILE:HD12	1.95	0.48
1:KG:84:TRP:CD1	1:KG:150:CYS:HB2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:171:GLU:N	1:AC:171:GLU:OE2	2.46	0.48
1:AE:62:VAL:HA	1:AE:192:GLY:O	2.13	0.48
1:BC:88:LEU:HD11	1:BC:121:LEU:HD13	1.95	0.48
1:BJ:66:ASP:OD1	1:BJ:66:ASP:N	2.44	0.48
1:EC:171:GLU:N	1:EC:171:GLU:OE2	2.46	0.48
1:HC:88:LEU:HD11	1:HC:121:LEU:HD13	1.95	0.48
1:JG:63:ILE:HD11	1:JG:71:ALA:HA	1.96	0.48
1:KD:68:LEU:HB2	1:KD:195:ILE:HD12	1.95	0.48
1:KE:62:VAL:HA	1:KE:192:GLY:O	2.13	0.48
1:KF:173:PRO:HB2	1:KJ:52:LEU:HD21	1.95	0.48
1:CG:63:ILE:HD11	1:CG:71:ALA:HA	1.96	0.48
1:DE:62:VAL:HA	1:DE:192:GLY:O	2.13	0.48
1:DE:84:TRP:CD2	1:DE:150:CYS:HB2	2.48	0.48
1:EE:62:VAL:HA	1:EE:192:GLY:O	2.13	0.48
1:GF:173:PRO:HB2	1:GJ:52:LEU:HD21	1.95	0.48
1:HG:170:TRP:CD1	1:HG:171:GLU:HG3	2.48	0.48
1:IF:173:PRO:HB2	1:IJ:52:LEU:HD21	1.95	0.48
1:JF:173:PRO:HB2	1:JJ:52:LEU:HD21	1.95	0.48
1:LC:171:GLU:N	1:LC:171:GLU:OE2	2.46	0.48
1:FD:68:LEU:HB2	1:FD:195:ILE:HD12	1.95	0.48
1:GA:36:PHE:CE2	1:GA:194:LEU:HB3	2.49	0.48
1:GA:178:GLU:OE2	1:GE:101:ARG:NH2	2.47	0.48
1:GE:62:VAL:HA	1:GE:192:GLY:O	2.13	0.48
1:GE:84:TRP:CD2	1:GE:150:CYS:HB2	2.48	0.48
1:IE:84:TRP:CD2	1:IE:150:CYS:HB2	2.48	0.48
1:II:77:THR:HG22	1:II:80:GLY:H	1.78	0.48
1:JD:68:LEU:HB2	1:JD:195:ILE:HD12	1.95	0.48
1:JG:66:ASP:OD1	1:JG:66:ASP:N	2.42	0.48
1:KA:78:LYS:HG2	1:KJ:137:HIS:CE1	2.49	0.48
1:KC:171:GLU:N	1:KC:171:GLU:OE2	2.46	0.48
1:AA:97:PHE:HZ	1:AB:174:VAL:HG22	1.77	0.48
1:BA:178:GLU:OE2	1:BE:101:ARG:NH2	2.47	0.48
1:BI:77:THR:HG22	1:BI:80:GLY:H	1.78	0.48
1:CA:36:PHE:CE2	1:CA:194:LEU:HB3	2.49	0.48
1:EA:78:LYS:HG2	1:EJ:137:HIS:CE1	2.49	0.48
1:EB:78:LYS:HA	1:EB:81:ASN:HB3	1.94	0.48
1:EH:72:ILE:O	1:EH:77:THR:OG1	2.22	0.48
1:FA:78:LYS:HG2	1:FJ:137:HIS:CE1	2.49	0.48
1:GF:58:ILE:HG12	1:GF:188:VAL:HB	1.94	0.48
1:IE:62:VAL:HA	1:IE:192:GLY:O	2.13	0.48
1:IG:170:TRP:CD1	1:IG:171:GLU:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:36:PHE:CE2	1:JA:194:LEU:HB3	2.49	0.48
1:KA:178:GLU:OE2	1:KE:101:ARG:NH2	2.47	0.48
1:LA:178:GLU:OE2	1:LE:101:ARG:NH2	2.47	0.48
1:AA:36:PHE:CE2	1:AA:194:LEU:HB3	2.49	0.48
1:CG:92:GLU:OE2	1:FH:153:ARG:NH2	2.46	0.48
1:EA:36:PHE:CE2	1:EA:194:LEU:HB3	2.49	0.48
1:EI:77:THR:HG22	1:EI:80:GLY:H	1.78	0.48
1:FA:97:PHE:HZ	1:FB:174:VAL:HG22	1.77	0.48
1:FF:58:ILE:HG12	1:FF:188:VAL:HB	1.94	0.48
1:GD:68:LEU:HB2	1:GD:195:ILE:HD12	1.95	0.48
1:HA:78:LYS:HG2	1:HJ:137:HIS:CE1	2.49	0.48
1:IA:178:GLU:OE2	1:IE:101:ARG:NH2	2.47	0.48
1:JE:62:VAL:HA	1:JE:192:GLY:O	2.13	0.48
1:KA:36:PHE:CE2	1:KA:194:LEU:HB3	2.49	0.48
1:LA:36:PHE:CE2	1:LA:194:LEU:HB3	2.49	0.48
1:LG:63:ILE:HD11	1:LG:71:ALA:HA	1.96	0.48
1:AA:178:GLU:OE2	1:AE:101:ARG:NH2	2.47	0.48
1:AI:77:THR:HG22	1:AI:80:GLY:H	1.78	0.48
1:FA:178:GLU:OE2	1:FE:101:ARG:NH2	2.47	0.48
1:FE:84:TRP:CD2	1:FE:150:CYS:HB2	2.48	0.48
1:GA:78:LYS:HG2	1:GJ:137:HIS:CE1	2.49	0.48
1:JC:88:LEU:HD11	1:JC:121:LEU:HD13	1.95	0.48
1:KI:61:GLY:O	1:KI:191:ILE:HA	2.14	0.48
1:LJ:85:GLU:OE1	1:LJ:85:GLU:N	2.47	0.48
1:AF:171:GLU:HG2	1:AJ:93:MET:HG3	1.96	0.48
1:CD:68:LEU:HB2	1:CD:195:ILE:HD12	1.95	0.48
1:CJ:85:GLU:N	1:CJ:85:GLU:OE1	2.47	0.48
1:DG:77:THR:CG2	1:DG:78:LYS:N	2.59	0.48
1:EJ:85:GLU:OE1	1:EJ:85:GLU:N	2.47	0.48
1:FF:171:GLU:HG2	1:FJ:93:MET:HG3	1.96	0.48
1:GF:171:GLU:HG2	1:GJ:93:MET:HG3	1.96	0.48
1:GJ:85:GLU:OE1	1:GJ:85:GLU:N	2.47	0.48
1:JA:78:LYS:HG2	1:JJ:137:HIS:CE1	2.49	0.48
1:LF:173:PRO:HB2	1:LJ:52:LEU:HD21	1.95	0.48
1:AB:78:LYS:HA	1:AB:81:ASN:HB3	1.94	0.48
1:AG:63:ILE:HD11	1:AG:71:ALA:HA	1.96	0.48
1:BF:79:HIS:ND1	1:EB:79:HIS:HB2	2.29	0.48
1:EA:178:GLU:OE2	1:EE:101:ARG:NH2	2.47	0.48
1:FF:173:PRO:HB2	1:FJ:52:LEU:HD21	1.95	0.48
1:HF:173:PRO:HB2	1:HJ:52:LEU:HD21	1.95	0.48
1:KF:171:GLU:HG2	1:KJ:93:MET:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LE:61:GLY:O	1:LE:191:ILE:HA	2.13	0.48
1:AB:36:PHE:HE1	1:AB:194:LEU:HB3	1.79	0.48
1:AC:88:LEU:HD11	1:AC:121:LEU:HD13	1.95	0.48
1:AJ:85:GLU:OE1	1:AJ:85:GLU:N	2.47	0.48
1:BE:62:VAL:HA	1:BE:192:GLY:O	2.13	0.48
1:BJ:85:GLU:OE1	1:BJ:85:GLU:N	2.47	0.48
1:DA:36:PHE:CE2	1:DA:194:LEU:HB3	2.49	0.48
1:DF:171:GLU:HG2	1:DJ:93:MET:HG3	1.96	0.48
1:FA:36:PHE:CE2	1:FA:194:LEU:HB3	2.49	0.48
1:FE:62:VAL:HA	1:FE:192:GLY:O	2.13	0.48
1:FG:170:TRP:CD1	1:FG:171:GLU:HG3	2.48	0.48
1:GG:63:ILE:HD11	1:GG:71:ALA:HA	1.96	0.48
1:HI:77:THR:HG22	1:HI:80:GLY:H	1.78	0.48
1:HJ:85:GLU:OE1	1:HJ:85:GLU:N	2.47	0.48
1:JI:77:THR:HG22	1:JI:80:GLY:H	1.78	0.48
1:KA:166:VAL:HG21	1:KA:172:ILE:HG12	1.96	0.48
1:KG:63:ILE:HD11	1:KG:71:ALA:HA	1.96	0.48
1:AJ:77:THR:HB	1:AJ:80:GLY:HA3	1.96	0.47
1:BA:36:PHE:CE2	1:BA:194:LEU:HB3	2.49	0.47
1:BF:173:PRO:HB2	1:BJ:52:LEU:HD21	1.95	0.47
1:BG:118:GLU:OE2	1:BH:134:ARG:NH1	2.44	0.47
1:DA:178:GLU:OE2	1:DE:101:ARG:NH2	2.47	0.47
1:DI:61:GLY:O	1:DI:191:ILE:HA	2.14	0.47
1:EG:63:ILE:HD11	1:EG:71:ALA:HA	1.96	0.47
1:FJ:77:THR:HB	1:FJ:80:GLY:HA3	1.96	0.47
1:HB:78:LYS:HA	1:HB:81:ASN:HB3	1.94	0.47
1:HE:62:VAL:HA	1:HE:192:GLY:O	2.13	0.47
1:ID:35:HIS:HA	1:ID:38:TYR:HD1	1.79	0.47
1:LC:88:LEU:HD11	1:LC:121:LEU:HD13	1.95	0.47
1:AA:78:LYS:HG2	1:AJ:137:HIS:CE1	2.49	0.47
1:BI:137:HIS:HA	1:BI:140:VAL:HB	1.97	0.47
1:FB:36:PHE:HE1	1:FB:194:LEU:HB3	1.79	0.47
1:FG:63:ILE:HD11	1:FG:71:ALA:HA	1.96	0.47
1:HA:166:VAL:HG21	1:HA:172:ILE:HG12	1.96	0.47
1:HA:178:GLU:OE2	1:HE:101:ARG:NH2	2.47	0.47
1:HJ:77:THR:HB	1:HJ:80:GLY:HA3	1.96	0.47
1:IG:63:ILE:HD11	1:IG:71:ALA:HA	1.96	0.47
1:JI:61:GLY:O	1:JI:191:ILE:HA	2.14	0.47
1:KB:36:PHE:HE1	1:KB:194:LEU:HB3	1.79	0.47
1:KJ:85:GLU:N	1:KJ:85:GLU:OE1	2.47	0.47
1:LI:61:GLY:O	1:LI:191:ILE:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:78:LYS:HG2	1:CJ:137:HIS:CE1	2.49	0.47
1:CF:173:PRO:HB2	1:CJ:52:LEU:HD21	1.95	0.47
1:DH:66:ASP:OD1	1:DH:66:ASP:N	2.48	0.47
1:ED:68:LEU:HB2	1:ED:195:ILE:HD12	1.95	0.47
1:EI:61:GLY:O	1:EI:191:ILE:HA	2.14	0.47
1:FJ:85:GLU:N	1:FJ:85:GLU:OE1	2.47	0.47
1:GI:137:HIS:HA	1:GI:140:VAL:HB	1.96	0.47
1:HG:118:GLU:OE2	1:HH:134:ARG:NH1	2.44	0.47
1:HG:153:ARG:HH22	1:JH:92:GLU:CD	2.18	0.47
1:HI:61:GLY:O	1:HI:191:ILE:HA	2.14	0.47
1:IB:36:PHE:HE1	1:IB:194:LEU:HB3	1.79	0.47
1:JG:118:GLU:OE2	1:JH:134:ARG:NH1	2.44	0.47
1:KH:66:ASP:OD1	1:KH:66:ASP:N	2.48	0.47
1:BD:35:HIS:HA	1:BD:38:TYR:HD1	1.79	0.47
1:CA:178:GLU:OE2	1:CE:101:ARG:NH2	2.47	0.47
1:CH:179:LEU:HD23	1:CH:179:LEU:HA	1.80	0.47
1:DA:166:VAL:HG21	1:DA:172:ILE:HG12	1.96	0.47
1:DB:36:PHE:HE1	1:DB:194:LEU:HB3	1.79	0.47
1:DC:88:LEU:HD11	1:DC:121:LEU:HD13	1.95	0.47
1:DF:173:PRO:HB2	1:DJ:52:LEU:HD21	1.95	0.47
1:DG:63:ILE:HD11	1:DG:71:ALA:HA	1.96	0.47
1:DI:137:HIS:HA	1:DI:140:VAL:HB	1.97	0.47
1:DJ:85:GLU:OE1	1:DJ:85:GLU:N	2.47	0.47
1:FH:66:ASP:OD1	1:FH:66:ASP:N	2.48	0.47
1:GB:36:PHE:HE1	1:GB:194:LEU:HB3	1.79	0.47
1:JA:178:GLU:OE2	1:JE:101:ARG:NH2	2.47	0.47
1:JJ:85:GLU:OE1	1:JJ:85:GLU:N	2.47	0.47
1:KC:88:LEU:HD11	1:KC:121:LEU:HD13	1.95	0.47
1:LD:68:LEU:HB2	1:LD:195:ILE:HD12	1.95	0.47
1:AF:173:PRO:HB2	1:AJ:52:LEU:HD21	1.95	0.47
1:BA:166:VAL:HG21	1:BA:172:ILE:HG12	1.96	0.47
1:BG:170:TRP:CD1	1:BG:171:GLU:HG3	2.48	0.47
1:CC:88:LEU:HD11	1:CC:121:LEU:HD13	1.95	0.47
1:CI:77:THR:HG22	1:CI:80:GLY:H	1.78	0.47
1:CI:137:HIS:HA	1:CI:140:VAL:HB	1.97	0.47
1:DD:35:HIS:HA	1:DD:38:TYR:HD1	1.80	0.47
1:EA:166:VAL:HG21	1:EA:172:ILE:HG12	1.96	0.47
1:GC:54:LEU:HD13	1:GC:180:ALA:HB3	1.97	0.47
1:GI:77:THR:HG22	1:GI:80:GLY:H	1.78	0.47
1:HB:36:PHE:HE1	1:HB:194:LEU:HB3	1.79	0.47
1:IC:54:LEU:HD13	1:IC:180:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IF:171:GLU:HG2	1:IJ:93:MET:HG3	1.96	0.47
1:IG:35:HIS:O	1:IG:39:ILE:HG12	2.15	0.47
1:IJ:66:ASP:OD1	1:IJ:66:ASP:N	2.44	0.47
1:JF:171:GLU:HG2	1:JJ:93:MET:HG3	1.96	0.47
1:JJ:77:THR:HB	1:JJ:80:GLY:HA3	1.96	0.47
1:KI:137:HIS:HA	1:KI:140:VAL:HB	1.97	0.47
1:CC:54:LEU:HD13	1:CC:180:ALA:HB3	1.97	0.47
1:EC:88:LEU:HD11	1:EC:121:LEU:HD13	1.95	0.47
1:EF:171:GLU:HG2	1:EJ:93:MET:HG3	1.96	0.47
1:GC:88:LEU:HD11	1:GC:121:LEU:HD13	1.95	0.47
1:JD:35:HIS:HA	1:JD:38:TYR:HD1	1.80	0.47
1:KH:179:LEU:HD23	1:KH:179:LEU:HA	1.80	0.47
1:LA:78:LYS:HG2	1:LJ:137:HIS:CE1	2.49	0.47
1:LA:166:VAL:HG21	1:LA:172:ILE:HG12	1.96	0.47
1:LH:97:PHE:HZ	1:LI:174:VAL:HG22	1.80	0.47
1:AI:61:GLY:O	1:AI:191:ILE:HA	2.14	0.47
1:BC:54:LEU:HD13	1:BC:180:ALA:HB3	1.97	0.47
1:BJ:77:THR:HB	1:BJ:80:GLY:HA3	1.96	0.47
1:CF:171:GLU:HG2	1:CJ:93:MET:HG3	1.96	0.47
1:CG:35:HIS:O	1:CG:39:ILE:HG12	2.15	0.47
1:CI:61:GLY:O	1:CI:191:ILE:HA	2.14	0.47
1:EB:36:PHE:HE1	1:EB:194:LEU:HB3	1.79	0.47
1:EG:35:HIS:O	1:EG:39:ILE:HG12	2.15	0.47
1:EH:97:PHE:HZ	1:EI:174:VAL:HG22	1.80	0.47
1:FD:35:HIS:HA	1:FD:38:TYR:HD1	1.80	0.47
1:GA:166:VAL:HG21	1:GA:172:ILE:HG12	1.96	0.47
1:GD:35:HIS:HA	1:GD:38:TYR:HD1	1.79	0.47
1:HA:36:PHE:CE2	1:HA:194:LEU:HB3	2.49	0.47
1:HG:35:HIS:O	1:HG:39:ILE:HG12	2.15	0.47
1:HH:97:PHE:HZ	1:HI:174:VAL:HG22	1.80	0.47
1:HI:137:HIS:HA	1:HI:140:VAL:HB	1.97	0.47
1:IA:36:PHE:CE2	1:IA:194:LEU:HB3	2.49	0.47
1:IJ:58:ILE:HG12	1:IJ:188:VAL:HB	1.97	0.47
1:IJ:85:GLU:N	1:IJ:85:GLU:OE1	2.47	0.47
1:JB:36:PHE:HE1	1:JB:194:LEU:HB3	1.79	0.47
1:KG:170:TRP:CD1	1:KG:171:GLU:HG3	2.48	0.47
1:LG:35:HIS:O	1:LG:39:ILE:HG12	2.15	0.47
1:LI:137:HIS:HA	1:LI:140:VAL:HB	1.97	0.47
1:AH:97:PHE:HZ	1:AI:174:VAL:HG22	1.80	0.47
1:BA:78:LYS:HG2	1:BJ:137:HIS:CE1	2.49	0.47
1:BF:77:THR:HB	1:BF:80:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BG:35:HIS:O	1:BG:39:ILE:HG12	2.15	0.47
1:BG:88:LEU:HD11	1:BG:121:LEU:HD13	1.97	0.47
1:BI:61:GLY:O	1:BI:191:ILE:HA	2.14	0.47
1:DG:35:HIS:O	1:DG:39:ILE:HG12	2.15	0.47
1:FA:166:VAL:HG21	1:FA:172:ILE:HG12	1.96	0.47
1:FI:137:HIS:HA	1:FI:140:VAL:HB	1.97	0.47
1:GI:61:GLY:O	1:GI:191:ILE:HA	2.14	0.47
1:HC:54:LEU:HD13	1:HC:180:ALA:HB3	1.97	0.47
1:HD:68:LEU:HB2	1:HD:195:ILE:HD12	1.95	0.47
1:II:61:GLY:O	1:II:191:ILE:HA	2.14	0.47
1:IJ:77:THR:HB	1:IJ:80:GLY:HA3	1.96	0.47
1:KD:35:HIS:HA	1:KD:38:TYR:HD1	1.80	0.47
1:AA:166:VAL:HG21	1:AA:172:ILE:HG12	1.96	0.47
1:AG:88:LEU:HD11	1:AG:121:LEU:HD13	1.97	0.47
1:CE:78:LYS:O	1:CE:81:ASN:ND2	2.29	0.47
1:CH:97:PHE:HZ	1:CI:174:VAL:HG22	1.80	0.47
1:CJ:58:ILE:HG12	1:CJ:188:VAL:HB	1.97	0.47
1:DA:78:LYS:HG2	1:DJ:137:HIS:CE1	2.49	0.47
1:EF:77:THR:HB	1:EF:80:GLY:HA3	1.97	0.47
1:EH:66:ASP:N	1:EH:66:ASP:OD1	2.48	0.47
1:FG:88:LEU:HD11	1:FG:121:LEU:HD13	1.97	0.47
1:FI:61:GLY:O	1:FI:191:ILE:HA	2.14	0.47
1:GG:77:THR:CG2	1:GG:78:LYS:N	2.59	0.47
1:HF:77:THR:HB	1:HF:80:GLY:HA3	1.97	0.47
1:HG:88:LEU:HD11	1:HG:121:LEU:HD13	1.97	0.47
1:IA:78:LYS:HG2	1:IJ:137:HIS:CE1	2.49	0.47
1:JG:35:HIS:O	1:JG:39:ILE:HG12	2.15	0.47
1:KF:77:THR:HB	1:KF:80:GLY:HA3	1.97	0.47
1:KJ:77:THR:HB	1:KJ:80:GLY:HA3	1.96	0.47
1:LD:35:HIS:HA	1:LD:38:TYR:HD1	1.79	0.47
1:LG:170:TRP:CD1	1:LG:171:GLU:HG3	2.48	0.47
1:LH:66:ASP:OD1	1:LH:66:ASP:N	2.48	0.47
1:BI:133:SER:HB3	1:BI:172:ILE:HD11	1.97	0.47
1:CH:66:ASP:OD1	1:CH:66:ASP:N	2.48	0.47
1:DG:170:TRP:CD1	1:DG:171:GLU:HG3	2.48	0.47
1:EF:173:PRO:HB2	1:EJ:52:LEU:HD21	1.95	0.47
1:GG:35:HIS:O	1:GG:39:ILE:HG12	2.15	0.47
1:GJ:77:THR:HB	1:GJ:80:GLY:HA3	1.96	0.47
1:HG:63:ILE:HD11	1:HG:71:ALA:HA	1.96	0.47
1:IA:166:VAL:HG21	1:IA:172:ILE:HG12	1.96	0.47
1:IG:88:LEU:HD11	1:IG:121:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JF:77:THR:HB	1:JF:80:GLY:HA3	1.97	0.47
1:KG:88:LEU:HD11	1:KG:121:LEU:HD13	1.97	0.47
1:LF:77:THR:HB	1:LF:80:GLY:HA3	1.97	0.47
1:AI:133:SER:HB3	1:AI:172:ILE:HD11	1.98	0.46
1:BF:171:GLU:HG2	1:BJ:93:MET:HG3	1.96	0.46
1:CB:36:PHE:HE1	1:CB:194:LEU:HB3	1.79	0.46
1:FC:88:LEU:HD11	1:FC:121:LEU:HD13	1.95	0.46
1:LG:88:LEU:HD11	1:LG:121:LEU:HD13	1.97	0.46
1:AG:35:HIS:O	1:AG:39:ILE:HG12	2.15	0.46
1:AI:137:HIS:HA	1:AI:140:VAL:HB	1.96	0.46
1:DH:97:PHE:HZ	1:DI:174:VAL:HG22	1.80	0.46
1:DJ:77:THR:HB	1:DJ:80:GLY:HA3	1.96	0.46
1:ED:35:HIS:HA	1:ED:38:TYR:HD1	1.80	0.46
1:GG:88:LEU:HD11	1:GG:121:LEU:HD13	1.97	0.46
1:HD:35:HIS:HA	1:HD:38:TYR:HD1	1.80	0.46
1:HH:58:ILE:HG12	1:HH:188:VAL:HB	1.98	0.46
1:LJ:77:THR:HB	1:LJ:80:GLY:HA3	1.96	0.46
1:AD:35:HIS:HA	1:AD:38:TYR:HD1	1.79	0.46
1:CJ:77:THR:HB	1:CJ:80:GLY:HA3	1.96	0.46
1:DC:54:LEU:HD13	1:DC:180:ALA:HB3	1.97	0.46
1:EJ:77:THR:HB	1:EJ:80:GLY:HA3	1.96	0.46
1:FH:97:PHE:HZ	1:FI:174:VAL:HG22	1.80	0.46
1:FJ:58:ILE:HG12	1:FJ:188:VAL:HB	1.97	0.46
1:JG:170:TRP:CD1	1:JG:171:GLU:HG3	2.48	0.46
1:JI:137:HIS:HA	1:JI:140:VAL:HB	1.96	0.46
1:KG:35:HIS:O	1:KG:39:ILE:HG12	2.15	0.46
1:LB:36:PHE:HE1	1:LB:194:LEU:HB3	1.79	0.46
1:BG:63:ILE:HD11	1:BG:71:ALA:HA	1.96	0.46
1:CF:77:THR:HB	1:CF:80:GLY:HA3	1.97	0.46
1:EJ:58:ILE:HG12	1:EJ:188:VAL:HB	1.97	0.46
1:GI:133:SER:HB3	1:GI:172:ILE:HD11	1.97	0.46
1:JI:133:SER:HB3	1:JI:172:ILE:HD11	1.98	0.46
1:KH:97:PHE:HZ	1:KI:174:VAL:HG22	1.80	0.46
1:LC:54:LEU:HD13	1:LC:180:ALA:HB3	1.97	0.46
1:LH:58:ILE:HG12	1:LH:188:VAL:HB	1.98	0.46
1:AC:54:LEU:HD13	1:AC:180:ALA:HB3	1.97	0.46
1:BB:36:PHE:HE1	1:BB:194:LEU:HB3	1.79	0.46
1:BJ:58:ILE:HG12	1:BJ:188:VAL:HB	1.97	0.46
1:CD:35:HIS:HA	1:CD:38:TYR:HD1	1.80	0.46
1:EI:133:SER:HB3	1:EI:172:ILE:HD11	1.98	0.46
1:GF:77:THR:HB	1:GF:80:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GH:66:ASP:N	1:GH:66:ASP:OD1	2.48	0.46
1:HF:171:GLU:HG2	1:HJ:93:MET:HG3	1.96	0.46
1:HI:133:SER:HB3	1:HI:172:ILE:HD11	1.97	0.46
1:IF:77:THR:HB	1:IF:80:GLY:HA3	1.97	0.46
1:LD:62:VAL:HA	1:LD:192:GLY:O	2.16	0.46
1:BH:97:PHE:HZ	1:BI:174:VAL:HG22	1.80	0.46
1:HH:66:ASP:N	1:HH:66:ASP:OD1	2.48	0.46
1:IH:58:ILE:HG12	1:IH:188:VAL:HB	1.98	0.46
1:II:133:SER:HB3	1:II:172:ILE:HD11	1.98	0.46
1:BH:58:ILE:HG12	1:BH:188:VAL:HB	1.98	0.46
1:FC:54:LEU:HD13	1:FC:180:ALA:HB3	1.97	0.46
1:FD:62:VAL:HA	1:FD:192:GLY:O	2.16	0.46
1:FE:78:LYS:O	1:FE:81:ASN:ND2	2.29	0.46
1:JG:88:LEU:HD11	1:JG:121:LEU:HD13	1.97	0.46
1:LF:171:GLU:HG2	1:LJ:93:MET:HG3	1.96	0.46
1:GH:58:ILE:HG12	1:GH:188:VAL:HB	1.98	0.46
1:GH:97:PHE:HZ	1:GI:174:VAL:HG22	1.80	0.46
1:II:137:HIS:HA	1:II:140:VAL:HB	1.96	0.46
1:JC:54:LEU:HD13	1:JC:180:ALA:HB3	1.97	0.46
1:KC:54:LEU:HD13	1:KC:180:ALA:HB3	1.97	0.46
1:KJ:58:ILE:HG12	1:KJ:188:VAL:HB	1.97	0.46
1:BA:174:VAL:HG22	1:BE:97:PHE:HZ	1.81	0.46
1:EG:88:LEU:HD11	1:EG:121:LEU:HD13	1.97	0.46
1:FA:174:VAL:HG22	1:FE:97:PHE:HZ	1.81	0.46
1:FG:35:HIS:O	1:FG:39:ILE:HG12	2.15	0.46
1:JH:58:ILE:HG12	1:JH:188:VAL:HB	1.98	0.46
1:JH:66:ASP:N	1:JH:66:ASP:OD1	2.48	0.46
1:LJ:58:ILE:HG12	1:LJ:188:VAL:HB	1.97	0.46
1:CA:166:VAL:HG21	1:CA:172:ILE:HG12	1.96	0.46
1:DA:174:VAL:HG22	1:DE:97:PHE:HZ	1.81	0.46
1:DJ:58:ILE:HG12	1:DJ:188:VAL:HB	1.97	0.46
1:JA:166:VAL:HG21	1:JA:172:ILE:HG12	1.96	0.46
1:JH:97:PHE:HZ	1:JI:174:VAL:HG22	1.80	0.46
1:KA:174:VAL:HG22	1:KE:97:PHE:HZ	1.81	0.46
1:AA:174:VAL:HG22	1:AE:97:PHE:HZ	1.81	0.45
1:AB:62:VAL:HA	1:AB:192:GLY:O	2.17	0.45
1:BB:62:VAL:HA	1:BB:192:GLY:O	2.16	0.45
1:BF:134:ARG:NH1	1:BJ:118:GLU:OE2	2.42	0.45
1:DG:88:LEU:HD11	1:DG:121:LEU:HD13	1.97	0.45
1:GD:62:VAL:HA	1:GD:192:GLY:O	2.16	0.45
1:GJ:58:ILE:HG12	1:GJ:188:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HB:137:HIS:HB2	1:HI:78:LYS:HB2	1.99	0.45
1:JA:174:VAL:HG22	1:JE:97:PHE:HZ	1.81	0.45
1:DD:62:VAL:HA	1:DD:192:GLY:O	2.16	0.45
1:DF:77:THR:HB	1:DF:80:GLY:HA3	1.97	0.45
1:DI:133:SER:HB3	1:DI:172:ILE:HD11	1.98	0.45
1:EI:137:HIS:HA	1:EI:140:VAL:HB	1.97	0.45
1:HD:117:TYR:HB2	1:HE:164:VAL:HG22	1.99	0.45
1:KB:62:VAL:HA	1:KB:192:GLY:O	2.17	0.45
1:BH:66:ASP:N	1:BH:66:ASP:OD1	2.48	0.45
1:EG:170:TRP:CD1	1:EG:171:GLU:HG3	2.48	0.45
1:FF:77:THR:HB	1:FF:80:GLY:HA3	1.97	0.45
1:HA:174:VAL:HG22	1:HE:97:PHE:HZ	1.81	0.45
1:LG:64:THR:HG22	1:LG:194:LEU:HD12	1.98	0.45
1:CB:62:VAL:HA	1:CB:192:GLY:O	2.17	0.45
1:CG:88:LEU:HD11	1:CG:121:LEU:HD13	1.97	0.45
1:EA:174:VAL:HG22	1:EE:97:PHE:HZ	1.81	0.45
1:GB:137:HIS:HB2	1:GI:78:LYS:HB2	1.99	0.45
1:HD:62:VAL:HA	1:HD:192:GLY:O	2.16	0.45
1:ID:117:TYR:HB2	1:IE:164:VAL:HG22	1.99	0.45
1:JD:62:VAL:HA	1:JD:192:GLY:O	2.16	0.45
1:JD:117:TYR:HB2	1:JE:164:VAL:HG22	1.99	0.45
1:KG:118:GLU:OE2	1:KH:134:ARG:NH1	2.44	0.45
1:LA:174:VAL:HG22	1:LE:97:PHE:HZ	1.81	0.45
1:LI:133:SER:HB3	1:LI:172:ILE:HD11	1.98	0.45
1:CA:174:VAL:HG22	1:CE:97:PHE:HZ	1.81	0.45
1:CB:137:HIS:HB2	1:CI:78:LYS:HB2	1.99	0.45
1:DB:62:VAL:HA	1:DB:192:GLY:O	2.17	0.45
1:DD:117:TYR:HB2	1:DE:164:VAL:HG22	1.99	0.45
1:EB:62:VAL:HA	1:EB:192:GLY:O	2.17	0.45
1:EG:64:THR:HG22	1:EG:194:LEU:HD12	1.98	0.45
1:EG:117:TYR:HB2	1:EH:164:VAL:HG22	1.99	0.45
1:FB:137:HIS:HB2	1:FI:78:LYS:HB2	1.99	0.45
1:GB:62:VAL:HA	1:GB:192:GLY:O	2.17	0.45
1:GG:170:TRP:CD1	1:GG:171:GLU:HG3	2.48	0.45
1:HB:62:VAL:HA	1:HB:192:GLY:O	2.17	0.45
1:IA:174:VAL:HG22	1:IE:97:PHE:HZ	1.81	0.45
1:IG:118:GLU:OE2	1:IH:134:ARG:NH1	2.44	0.45
1:KD:62:VAL:HA	1:KD:192:GLY:O	2.16	0.45
1:AD:62:VAL:HA	1:AD:192:GLY:O	2.16	0.45
1:AF:77:THR:HB	1:AF:80:GLY:HA3	1.97	0.45
1:AG:64:THR:HG22	1:AG:194:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:58:ILE:HG12	1:AJ:188:VAL:HB	1.97	0.45
1:BF:79:HIS:HB3	1:EB:79:HIS:CG	2.52	0.45
1:GH:127:ARG:NE	1:GH:184:ASP:O	2.39	0.45
1:HG:64:THR:HG22	1:HG:194:LEU:HD12	1.98	0.45
1:HJ:58:ILE:HG12	1:HJ:188:VAL:HB	1.97	0.45
1:IC:60:PHE:CZ	1:IC:62:VAL:HB	2.52	0.45
1:KD:117:TYR:HB2	1:KE:164:VAL:HG22	1.99	0.45
1:LB:137:HIS:HB2	1:LI:78:LYS:HB2	1.99	0.45
1:AC:60:PHE:CZ	1:AC:62:VAL:HB	2.52	0.45
1:AG:117:TYR:HB2	1:AH:164:VAL:HG22	1.99	0.45
1:BD:62:VAL:HA	1:BD:192:GLY:O	2.16	0.45
1:DH:58:ILE:HG12	1:DH:188:VAL:HB	1.98	0.45
1:EC:60:PHE:CZ	1:EC:62:VAL:HB	2.52	0.45
1:ED:62:VAL:HA	1:ED:192:GLY:O	2.16	0.45
1:EH:58:ILE:HG12	1:EH:188:VAL:HB	1.97	0.45
1:HG:117:TYR:HB2	1:HH:164:VAL:HG22	1.99	0.45
1:IB:62:VAL:HA	1:IB:192:GLY:O	2.17	0.45
1:ID:62:VAL:HA	1:ID:192:GLY:O	2.16	0.45
1:JG:117:TYR:HB2	1:JH:164:VAL:HG22	1.99	0.45
1:JJ:58:ILE:HG12	1:JJ:188:VAL:HB	1.97	0.45
1:KG:117:TYR:HB2	1:KH:164:VAL:HG22	1.99	0.45
1:AH:66:ASP:OD1	1:AH:66:ASP:N	2.48	0.45
1:AH:179:LEU:HD23	1:AH:179:LEU:HA	1.80	0.45
1:BD:117:TYR:HB2	1:BE:164:VAL:HG22	1.99	0.45
1:CG:117:TYR:HB2	1:CH:164:VAL:HG22	1.99	0.45
1:DA:153:ARG:NH2	1:DI:92:GLU:OE2	2.50	0.45
1:EC:54:LEU:HD13	1:EC:180:ALA:HB3	1.97	0.45
1:FH:127:ARG:NE	1:FH:184:ASP:O	2.39	0.45
1:IH:66:ASP:OD1	1:IH:66:ASP:N	2.48	0.45
1:KA:153:ARG:NH2	1:KI:92:GLU:OE2	2.50	0.45
1:KI:133:SER:HB3	1:KI:172:ILE:HD11	1.98	0.45
1:LG:117:TYR:HB2	1:LH:164:VAL:HG22	1.99	0.45
1:AH:58:ILE:HG12	1:AH:188:VAL:HB	1.98	0.45
1:CI:133:SER:HB3	1:CI:172:ILE:HD11	1.98	0.45
1:DB:137:HIS:HB2	1:DI:78:LYS:HB2	1.99	0.45
1:EA:153:ARG:NH2	1:EI:92:GLU:OE2	2.50	0.45
1:ED:117:TYR:HB2	1:EE:164:VAL:HG22	1.99	0.45
1:GC:60:PHE:CZ	1:GC:62:VAL:HB	2.52	0.45
1:IH:60:PHE:CZ	1:IH:62:VAL:HB	2.52	0.45
1:LA:153:ARG:NH2	1:LI:92:GLU:OE2	2.50	0.45
1:AH:60:PHE:CZ	1:AH:62:VAL:HB	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CH:58:ILE:HG12	1:CH:188:VAL:HB	1.98	0.45
1:CH:60:PHE:CZ	1:CH:62:VAL:HB	2.52	0.45
1:DB:97:PHE:HZ	1:DC:174:VAL:HG22	1.82	0.45
1:FC:60:PHE:CZ	1:FC:62:VAL:HB	2.52	0.45
1:FH:72:ILE:O	1:FH:77:THR:OG1	2.22	0.45
1:GA:174:VAL:HG22	1:GE:97:PHE:HZ	1.81	0.45
1:GH:60:PHE:CZ	1:GH:62:VAL:HB	2.52	0.45
1:HC:60:PHE:CZ	1:HC:62:VAL:HB	2.52	0.45
1:IA:153:ARG:NH2	1:II:92:GLU:OE2	2.50	0.45
1:IG:64:THR:HG22	1:IG:194:LEU:HD12	1.98	0.45
1:IG:117:TYR:HB2	1:IH:164:VAL:HG22	1.99	0.45
1:IH:97:PHE:HZ	1:II:174:VAL:HG22	1.80	0.45
1:JB:62:VAL:HA	1:JB:192:GLY:O	2.17	0.45
1:JB:97:PHE:HZ	1:JC:174:VAL:HG22	1.82	0.45
1:KG:64:THR:HG22	1:KG:194:LEU:HD12	1.98	0.45
1:KH:58:ILE:HG12	1:KH:188:VAL:HB	1.98	0.45
1:LB:62:VAL:HA	1:LB:192:GLY:O	2.17	0.45
1:AA:36:PHE:HB3	1:AA:196:ARG:HD3	1.99	0.44
1:BG:64:THR:HG22	1:BG:194:LEU:HD12	1.98	0.44
1:BH:60:PHE:CZ	1:BH:62:VAL:HB	2.52	0.44
1:FH:60:PHE:CZ	1:FH:62:VAL:HB	2.52	0.44
1:GA:153:ARG:NH2	1:GI:92:GLU:OE2	2.50	0.44
1:HA:36:PHE:HB3	1:HA:196:ARG:HD3	1.99	0.44
1:KB:97:PHE:HZ	1:KC:174:VAL:HG22	1.82	0.44
1:AA:153:ARG:NH2	1:AI:92:GLU:OE2	2.50	0.44
1:AE:78:LYS:O	1:AE:81:ASN:ND2	2.29	0.44
1:BF:179:LEU:HD23	1:BF:179:LEU:HA	1.85	0.44
1:CC:60:PHE:CZ	1:CC:62:VAL:HB	2.52	0.44
1:DD:85:GLU:OE1	1:DD:85:GLU:N	2.51	0.44
1:DH:127:ARG:HA	1:DH:160:ASP:HB3	2.00	0.44
1:FA:153:ARG:NH2	1:FI:92:GLU:OE2	2.50	0.44
1:FB:62:VAL:HA	1:FB:192:GLY:O	2.16	0.44
1:FD:85:GLU:N	1:FD:85:GLU:OE1	2.51	0.44
1:FG:64:THR:HG22	1:FG:194:LEU:HD12	1.98	0.44
1:FI:133:SER:HB3	1:FI:172:ILE:HD11	1.98	0.44
1:HD:85:GLU:OE1	1:HD:85:GLU:N	2.51	0.44
1:IB:97:PHE:HZ	1:IC:174:VAL:HG22	1.82	0.44
1:JD:85:GLU:OE1	1:JD:85:GLU:N	2.51	0.44
1:JJ:84:TRP:HH2	1:JJ:153:ARG:HD2	1.83	0.44
1:AD:117:TYR:HB2	1:AE:164:VAL:HG22	1.99	0.44
1:BA:153:ARG:NH2	1:BI:92:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:153:ARG:NH2	1:CI:92:GLU:OE2	2.50	0.44
1:CD:62:VAL:HA	1:CD:192:GLY:O	2.16	0.44
1:JA:36:PHE:HB3	1:JA:196:ARG:HD3	1.99	0.44
1:JA:153:ARG:NH2	1:JI:92:GLU:OE2	2.50	0.44
1:KH:127:ARG:HA	1:KH:160:ASP:HB3	2.00	0.44
1:BC:60:PHE:CZ	1:BC:62:VAL:HB	2.52	0.44
1:CD:85:GLU:OE1	1:CD:85:GLU:N	2.51	0.44
1:EG:118:GLU:OE2	1:EH:134:ARG:NH1	2.44	0.44
1:EH:60:PHE:CZ	1:EH:62:VAL:HB	2.52	0.44
1:FD:36:PHE:CZ	1:FD:194:LEU:HB3	2.50	0.44
1:FH:179:LEU:HD23	1:FH:179:LEU:HA	1.80	0.44
1:GD:85:GLU:OE1	1:GD:85:GLU:N	2.51	0.44
1:GG:64:THR:HG22	1:GG:194:LEU:HD12	1.98	0.44
1:JC:60:PHE:CZ	1:JC:62:VAL:HB	2.52	0.44
1:LB:97:PHE:HZ	1:LC:174:VAL:HG22	1.82	0.44
1:LD:85:GLU:N	1:LD:85:GLU:OE1	2.51	0.44
1:AB:97:PHE:HZ	1:AC:174:VAL:HG22	1.82	0.44
1:AH:157:ARG:NH1	1:AH:159:GLU:OE1	2.44	0.44
1:BB:97:PHE:HZ	1:BC:174:VAL:HG22	1.82	0.44
1:CG:64:THR:HG22	1:CG:194:LEU:HD12	1.98	0.44
1:CH:127:ARG:HA	1:CH:160:ASP:HB3	2.00	0.44
1:GG:118:GLU:OE2	1:GH:134:ARG:NH1	2.44	0.44
1:HA:153:ARG:NH2	1:HI:92:GLU:OE2	2.50	0.44
1:HJ:84:TRP:HH2	1:HJ:153:ARG:HD2	1.83	0.44
1:IA:36:PHE:HB3	1:IA:196:ARG:HD3	1.99	0.44
1:IJ:84:TRP:HH2	1:IJ:153:ARG:HD2	1.83	0.44
1:LC:60:PHE:CZ	1:LC:62:VAL:HB	2.52	0.44
1:LD:117:TYR:HB2	1:LE:164:VAL:HG22	1.99	0.44
1:LG:118:GLU:OE2	1:LH:134:ARG:NH1	2.44	0.44
1:AB:137:HIS:HB2	1:AI:78:LYS:HB2	1.99	0.44
1:CJ:84:TRP:HH2	1:CJ:153:ARG:HD2	1.83	0.44
1:DG:64:THR:HG22	1:DG:194:LEU:HD12	1.98	0.44
1:JB:137:HIS:HB2	1:JI:78:LYS:HB2	1.99	0.44
1:KA:36:PHE:HB3	1:KA:196:ARG:HD3	1.99	0.44
1:AG:170:TRP:CD1	1:AG:171:GLU:HG3	2.48	0.44
1:CD:117:TYR:HB2	1:CE:164:VAL:HG22	1.99	0.44
1:CF:134:ARG:NH1	1:CJ:118:GLU:OE2	2.42	0.44
1:CH:73:GLU:HA	1:CH:77:THR:HB	2.00	0.44
1:DG:117:TYR:HB2	1:DH:164:VAL:HG22	1.99	0.44
1:DH:73:GLU:HA	1:DH:77:THR:HB	2.00	0.44
1:DH:127:ARG:NE	1:DH:184:ASP:O	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:36:PHE:HB3	1:FA:196:ARG:HD3	1.99	0.44
1:JH:127:ARG:HA	1:JH:160:ASP:HB3	2.00	0.44
1:LJ:84:TRP:HH2	1:LJ:153:ARG:HD2	1.83	0.44
1:BB:137:HIS:HB2	1:BI:78:LYS:HB2	1.99	0.44
1:BG:117:TYR:HB2	1:BH:164:VAL:HG22	1.99	0.44
1:CI:60:PHE:CZ	1:CI:62:VAL:HB	2.53	0.44
1:ED:85:GLU:OE1	1:ED:85:GLU:N	2.51	0.44
1:FG:117:TYR:HB2	1:FH:164:VAL:HG22	1.99	0.44
1:FH:58:ILE:HG12	1:FH:188:VAL:HB	1.98	0.44
1:HH:73:GLU:HA	1:HH:77:THR:HB	2.00	0.44
1:JH:60:PHE:CZ	1:JH:62:VAL:HB	2.52	0.44
1:LH:73:GLU:HA	1:LH:77:THR:HB	2.00	0.44
1:BD:85:GLU:OE1	1:BD:85:GLU:N	2.51	0.44
1:DA:36:PHE:HB3	1:DA:196:ARG:HD3	1.99	0.44
1:EB:137:HIS:HB2	1:EI:78:LYS:HB2	1.99	0.44
1:IH:127:ARG:HA	1:IH:160:ASP:HB3	2.00	0.44
1:JG:64:THR:HG22	1:JG:194:LEU:HD12	1.98	0.44
1:JH:73:GLU:HA	1:JH:77:THR:HB	2.00	0.44
1:KC:60:PHE:CZ	1:KC:62:VAL:HB	2.52	0.44
1:CA:85:GLU:OE1	1:CA:85:GLU:N	2.51	0.43
1:DJ:84:TRP:HH2	1:DJ:153:ARG:HD2	1.83	0.43
1:EA:85:GLU:OE1	1:EA:85:GLU:N	2.51	0.43
1:EH:127:ARG:HA	1:EH:160:ASP:HB3	2.00	0.43
1:HB:97:PHE:HZ	1:HC:174:VAL:HG22	1.82	0.43
1:IH:179:LEU:HD23	1:IH:179:LEU:HA	1.80	0.43
1:BI:60:PHE:CZ	1:BI:62:VAL:HB	2.53	0.43
1:BJ:84:TRP:HH2	1:BJ:153:ARG:HD2	1.83	0.43
1:CB:97:PHE:HZ	1:CC:174:VAL:HG22	1.82	0.43
1:GD:36:PHE:CZ	1:GD:194:LEU:HB3	2.50	0.43
1:GH:127:ARG:HA	1:GH:160:ASP:HB3	2.00	0.43
1:JI:60:PHE:CZ	1:JI:62:VAL:HB	2.53	0.43
1:KC:179:LEU:HD23	1:KC:179:LEU:HA	1.85	0.43
1:KH:60:PHE:CZ	1:KH:62:VAL:HB	2.52	0.43
1:LA:85:GLU:N	1:LA:85:GLU:OE1	2.51	0.43
1:LI:60:PHE:CZ	1:LI:62:VAL:HB	2.53	0.43
1:AD:85:GLU:N	1:AD:85:GLU:OE1	2.51	0.43
1:AG:133:SER:O	1:AG:140:VAL:HG11	2.19	0.43
1:AI:60:PHE:CZ	1:AI:62:VAL:HB	2.53	0.43
1:BA:36:PHE:HB3	1:BA:196:ARG:HD3	1.99	0.43
1:BF:97:PHE:O	1:BF:101:ARG:HG2	2.19	0.43
1:BG:133:SER:O	1:BG:140:VAL:HG11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DH:60:PHE:CZ	1:DH:62:VAL:HB	2.52	0.43
1:EH:73:GLU:HA	1:EH:77:THR:HB	2.00	0.43
1:FH:127:ARG:HA	1:FH:160:ASP:HB3	2.00	0.43
1:GA:85:GLU:OE1	1:GA:85:GLU:N	2.51	0.43
1:GB:97:PHE:HZ	1:GC:174:VAL:HG22	1.82	0.43
1:GG:133:SER:O	1:GG:140:VAL:HG11	2.18	0.43
1:HI:60:PHE:CZ	1:HI:62:VAL:HB	2.53	0.43
1:IA:134:ARG:HH12	1:IE:118:GLU:HG3	1.84	0.43
1:IF:97:PHE:O	1:IF:101:ARG:HG2	2.19	0.43
1:KA:85:GLU:OE1	1:KA:85:GLU:N	2.51	0.43
1:KB:137:HIS:HB2	1:KI:78:LYS:HB2	1.99	0.43
1:BH:73:GLU:HA	1:BH:77:THR:HB	2.00	0.43
1:CG:77:THR:CG2	1:CG:78:LYS:N	2.59	0.43
1:CH:127:ARG:NE	1:CH:184:ASP:O	2.39	0.43
1:DC:60:PHE:CZ	1:DC:62:VAL:HB	2.52	0.43
1:DG:133:SER:O	1:DG:140:VAL:HG11	2.19	0.43
1:FF:97:PHE:O	1:FF:101:ARG:HG2	2.19	0.43
1:GI:60:PHE:CZ	1:GI:62:VAL:HB	2.53	0.43
1:HF:97:PHE:O	1:HF:101:ARG:HG2	2.19	0.43
1:IB:137:HIS:HB2	1:II:78:LYS:HB2	1.99	0.43
1:KI:60:PHE:CZ	1:KI:62:VAL:HB	2.53	0.43
1:LA:36:PHE:HB3	1:LA:196:ARG:HD3	1.99	0.43
1:LH:127:ARG:HA	1:LH:160:ASP:HB3	2.00	0.43
1:AH:92:GLU:CD	1:LG:153:ARG:HH22	2.20	0.43
1:BF:82:LYS:HD3	1:BF:82:LYS:HA	1.85	0.43
1:BH:127:ARG:HA	1:BH:160:ASP:HB3	2.00	0.43
1:BH:179:LEU:HD23	1:BH:179:LEU:HA	1.79	0.43
1:CA:134:ARG:HH12	1:CE:118:GLU:HG3	1.84	0.43
1:DI:60:PHE:CZ	1:DI:62:VAL:HB	2.53	0.43
1:EB:97:PHE:HZ	1:EC:174:VAL:HG22	1.82	0.43
1:EI:60:PHE:CZ	1:EI:62:VAL:HB	2.53	0.43
1:EJ:84:TRP:HH2	1:EJ:153:ARG:HD2	1.83	0.43
1:FD:117:TYR:HB2	1:FE:164:VAL:HG22	1.99	0.43
1:FF:134:ARG:NH1	1:FJ:118:GLU:OE2	2.42	0.43
1:FG:133:SER:O	1:FG:140:VAL:HG11	2.19	0.43
1:GD:117:TYR:HB2	1:GE:164:VAL:HG22	1.99	0.43
1:GH:73:GLU:HA	1:GH:77:THR:HB	2.00	0.43
1:HG:133:SER:O	1:HG:140:VAL:HG11	2.19	0.43
1:JF:97:PHE:O	1:JF:101:ARG:HG2	2.19	0.43
1:KF:97:PHE:O	1:KF:101:ARG:HG2	2.19	0.43
1:LF:134:ARG:NH1	1:LJ:118:GLU:OE2	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:73:GLU:HA	1:AH:77:THR:HB	2.00	0.43
1:BE:77:THR:HG22	1:BE:80:GLY:H	1.84	0.43
1:FA:85:GLU:OE1	1:FA:85:GLU:N	2.51	0.43
1:GA:36:PHE:HB3	1:GA:196:ARG:HD3	1.99	0.43
1:JA:134:ARG:HH12	1:JE:118:GLU:HG3	1.84	0.43
1:JG:133:SER:O	1:JG:140:VAL:HG11	2.19	0.43
1:KH:73:GLU:HA	1:KH:77:THR:HB	2.00	0.43
1:LH:60:PHE:CZ	1:LH:62:VAL:HB	2.52	0.43
1:CA:36:PHE:HB3	1:CA:196:ARG:HD3	1.99	0.43
1:CE:77:THR:HG22	1:CE:80:GLY:H	1.84	0.43
1:FC:33:THR:N	1:FC:195:ILE:O	2.52	0.43
1:GC:33:THR:N	1:GC:195:ILE:O	2.52	0.43
1:GG:117:TYR:HB2	1:GH:164:VAL:HG22	1.99	0.43
1:GH:179:LEU:HA	1:GH:179:LEU:HD23	1.80	0.43
1:HB:134:ARG:HE	1:HI:78:LYS:HZ2	1.66	0.43
1:HF:82:LYS:HD3	1:HF:82:LYS:HA	1.85	0.43
1:HH:60:PHE:CZ	1:HH:62:VAL:HB	2.52	0.43
1:KD:85:GLU:OE1	1:KD:85:GLU:N	2.51	0.43
1:AG:153:ARG:HH22	1:IH:92:GLU:CD	2.21	0.43
1:AJ:84:TRP:HH2	1:AJ:153:ARG:HD2	1.83	0.43
1:BA:85:GLU:OE1	1:BA:85:GLU:N	2.51	0.43
1:DC:33:THR:N	1:DC:195:ILE:O	2.52	0.43
1:EA:36:PHE:HB3	1:EA:196:ARG:HD3	2.00	0.43
1:EA:134:ARG:HH12	1:EE:118:GLU:HG3	1.84	0.43
1:EF:97:PHE:O	1:EF:101:ARG:HG2	2.19	0.43
1:FD:158:GLU:O	1:FD:161:ILE:HG22	2.19	0.43
1:FG:118:GLU:OE2	1:FH:134:ARG:NH1	2.44	0.43
1:FH:73:GLU:HA	1:FH:77:THR:HB	2.00	0.43
1:HA:85:GLU:OE1	1:HA:85:GLU:N	2.51	0.43
1:HA:134:ARG:HH12	1:HE:118:GLU:HG3	1.84	0.43
1:ID:85:GLU:N	1:ID:85:GLU:OE1	2.51	0.43
1:KF:179:LEU:HD23	1:KF:179:LEU:HA	1.85	0.43
1:LD:36:PHE:CZ	1:LD:194:LEU:HB3	2.50	0.43
1:AF:97:PHE:O	1:AF:101:ARG:HG2	2.19	0.43
1:CG:118:GLU:OE2	1:CH:134:ARG:NH1	2.44	0.43
1:DE:77:THR:HG22	1:DE:80:GLY:H	1.84	0.43
1:FB:97:PHE:HZ	1:FC:174:VAL:HG22	1.82	0.43
1:HD:158:GLU:O	1:HD:161:ILE:HG22	2.19	0.43
1:HE:77:THR:HG22	1:HE:80:GLY:H	1.84	0.43
1:KD:128:PHE:CD2	1:KD:187:ALA:HB3	2.54	0.43
1:LF:97:PHE:O	1:LF:101:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LG:133:SER:O	1:LG:140:VAL:HG11	2.19	0.43
1:AA:85:GLU:N	1:AA:85:GLU:OE1	2.51	0.43
1:DF:97:PHE:O	1:DF:101:ARG:HG2	2.19	0.43
1:EG:133:SER:O	1:EG:140:VAL:HG11	2.19	0.43
1:FD:128:PHE:CD2	1:FD:187:ALA:HB3	2.54	0.43
1:FE:77:THR:HG22	1:FE:80:GLY:H	1.84	0.43
1:ID:158:GLU:O	1:ID:161:ILE:HG22	2.19	0.43
1:IE:77:THR:HG22	1:IE:80:GLY:H	1.84	0.43
1:II:60:PHE:CZ	1:II:62:VAL:HB	2.53	0.43
1:JA:93:MET:HG3	1:JB:171:GLU:HG2	2.01	0.43
1:LC:33:THR:N	1:LC:195:ILE:O	2.52	0.43
1:LD:158:GLU:O	1:LD:161:ILE:HG22	2.19	0.43
1:AC:33:THR:N	1:AC:195:ILE:O	2.52	0.42
1:CC:33:THR:N	1:CC:195:ILE:O	2.52	0.42
1:CF:97:PHE:O	1:CF:101:ARG:HG2	2.19	0.42
1:CG:133:SER:O	1:CG:140:VAL:HG11	2.19	0.42
1:DD:128:PHE:CD2	1:DD:187:ALA:HB3	2.54	0.42
1:FJ:84:TRP:HH2	1:FJ:153:ARG:HD2	1.83	0.42
1:JA:85:GLU:OE1	1:JA:85:GLU:N	2.51	0.42
1:JC:33:THR:N	1:JC:195:ILE:O	2.52	0.42
1:JD:158:GLU:O	1:JD:161:ILE:HG22	2.19	0.42
1:JF:134:ARG:NH1	1:JJ:118:GLU:OE2	2.42	0.42
1:KJ:84:TRP:HH2	1:KJ:153:ARG:HD2	1.83	0.42
1:LA:93:MET:HG3	1:LB:171:GLU:HG2	2.01	0.42
1:LF:82:LYS:HA	1:LF:82:LYS:HD3	1.85	0.42
1:AA:62:VAL:HA	1:AA:192:GLY:O	2.20	0.42
1:BG:77:THR:CG2	1:BG:78:LYS:N	2.59	0.42
1:BG:149:ASP:O	1:BG:153:ARG:HG3	2.19	0.42
1:CD:158:GLU:O	1:CD:161:ILE:HG22	2.19	0.42
1:DA:85:GLU:N	1:DA:85:GLU:OE1	2.51	0.42
1:DD:158:GLU:O	1:DD:161:ILE:HG22	2.19	0.42
1:DF:82:LYS:HD3	1:DF:82:LYS:HA	1.85	0.42
1:FI:60:PHE:CZ	1:FI:62:VAL:HB	2.53	0.42
1:GD:158:GLU:O	1:GD:161:ILE:HG22	2.19	0.42
1:GG:149:ASP:O	1:GG:153:ARG:HG3	2.20	0.42
1:HA:62:VAL:HA	1:HA:192:GLY:O	2.20	0.42
1:HD:128:PHE:CD2	1:HD:187:ALA:HB3	2.54	0.42
1:ID:128:PHE:CD2	1:ID:187:ALA:HB3	2.54	0.42
1:AD:158:GLU:O	1:AD:161:ILE:HG22	2.19	0.42
1:DH:157:ARG:NH1	1:DH:159:GLU:OE1	2.44	0.42
1:HF:134:ARG:NH1	1:HJ:118:GLU:OE2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HH:127:ARG:HA	1:HH:160:ASP:HB3	2.00	0.42
1:IC:33:THR:N	1:IC:195:ILE:O	2.52	0.42
1:IF:179:LEU:HD23	1:IF:179:LEU:HA	1.85	0.42
1:IG:149:ASP:O	1:IG:153:ARG:HG3	2.20	0.42
1:JD:36:PHE:CZ	1:JD:194:LEU:HB3	2.50	0.42
1:KA:62:VAL:HA	1:KA:192:GLY:O	2.20	0.42
1:KG:133:SER:O	1:KG:140:VAL:HG11	2.19	0.42
1:LA:134:ARG:HH12	1:LE:118:GLU:HG3	1.84	0.42
1:LE:77:THR:HG22	1:LE:80:GLY:H	1.84	0.42
1:BC:149:ASP:O	1:BC:153:ARG:HG3	2.20	0.42
1:BC:166:VAL:HG21	1:BC:172:ILE:HG12	2.02	0.42
1:CG:149:ASP:O	1:CG:153:ARG:HG3	2.20	0.42
1:DA:93:MET:HG3	1:DB:171:GLU:HG2	2.01	0.42
1:DE:78:LYS:O	1:DE:81:ASN:ND2	2.29	0.42
1:DG:149:ASP:O	1:DG:153:ARG:HG3	2.20	0.42
1:ED:158:GLU:O	1:ED:161:ILE:HG22	2.19	0.42
1:GA:62:VAL:HA	1:GA:192:GLY:O	2.20	0.42
1:GC:133:SER:O	1:GC:140:VAL:HG11	2.20	0.42
1:GE:77:THR:HG22	1:GE:80:GLY:H	1.84	0.42
1:GJ:84:TRP:HH2	1:GJ:153:ARG:HD2	1.83	0.42
1:IC:166:VAL:HG21	1:IC:172:ILE:HG12	2.02	0.42
1:KC:149:ASP:O	1:KC:153:ARG:HG3	2.20	0.42
1:KC:166:VAL:HG21	1:KC:172:ILE:HG12	2.02	0.42
1:LD:128:PHE:CD2	1:LD:187:ALA:HB3	2.54	0.42
1:AA:134:ARG:HH12	1:AE:118:GLU:HG3	1.84	0.42
1:AH:127:ARG:HA	1:AH:160:ASP:HB3	2.00	0.42
1:EC:166:VAL:HG21	1:EC:172:ILE:HG12	2.02	0.42
1:FC:133:SER:O	1:FC:140:VAL:HG11	2.20	0.42
1:FC:166:VAL:HG21	1:FC:172:ILE:HG12	2.02	0.42
1:GA:93:MET:HG3	1:GB:171:GLU:HG2	2.01	0.42
1:GF:97:PHE:O	1:GF:101:ARG:HG2	2.19	0.42
1:HC:166:VAL:HG21	1:HC:172:ILE:HG12	2.02	0.42
1:IA:85:GLU:N	1:IA:85:GLU:OE1	2.51	0.42
1:IC:133:SER:O	1:IC:140:VAL:HG11	2.20	0.42
1:JB:134:ARG:HE	1:JI:78:LYS:HZ2	1.67	0.42
1:JC:149:ASP:O	1:JC:153:ARG:HG3	2.20	0.42
1:KD:158:GLU:O	1:KD:161:ILE:HG22	2.19	0.42
1:BD:128:PHE:CD2	1:BD:187:ALA:HB3	2.54	0.42
1:EA:62:VAL:HA	1:EA:192:GLY:O	2.20	0.42
1:EE:77:THR:HG22	1:EE:80:GLY:H	1.84	0.42
1:EG:77:THR:CG2	1:EG:78:LYS:N	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GD:128:PHE:CD2	1:GD:187:ALA:HB3	2.54	0.42
1:GE:78:LYS:O	1:GE:81:ASN:ND2	2.29	0.42
1:HC:133:SER:O	1:HC:140:VAL:HG11	2.20	0.42
1:IG:133:SER:O	1:IG:140:VAL:HG11	2.19	0.42
1:LC:149:ASP:O	1:LC:153:ARG:HG3	2.20	0.42
1:AC:149:ASP:O	1:AC:153:ARG:HG3	2.20	0.42
1:AD:128:PHE:CD2	1:AD:187:ALA:HB3	2.54	0.42
1:AG:149:ASP:O	1:AG:153:ARG:HG3	2.20	0.42
1:BC:33:THR:N	1:BC:195:ILE:O	2.52	0.42
1:FA:134:ARG:HH12	1:FE:118:GLU:HG3	1.84	0.42
1:FG:149:ASP:O	1:FG:153:ARG:HG3	2.20	0.42
1:HF:79:HIS:HB3	1:JB:79:HIS:CG	2.55	0.42
1:JA:62:VAL:HA	1:JA:192:GLY:O	2.20	0.42
1:JD:97:PHE:HZ	1:JE:174:VAL:HG22	1.85	0.42
1:JD:128:PHE:CD2	1:JD:187:ALA:HB3	2.54	0.42
1:AC:166:VAL:HG21	1:AC:172:ILE:HG12	2.02	0.42
1:BA:62:VAL:HA	1:BA:192:GLY:O	2.20	0.42
1:CA:93:MET:HG3	1:CB:171:GLU:HG2	2.01	0.42
1:CC:133:SER:O	1:CC:140:VAL:HG11	2.20	0.42
1:CD:128:PHE:CD2	1:CD:187:ALA:HB3	2.54	0.42
1:DC:149:ASP:O	1:DC:153:ARG:HG3	2.20	0.42
1:DD:97:PHE:CZ	1:DE:174:VAL:HG22	2.55	0.42
1:ED:128:PHE:CD2	1:ED:187:ALA:HB3	2.54	0.42
1:FJ:91:ILE:HD13	1:FJ:123:ALA:HB2	2.02	0.42
1:GA:134:ARG:HH12	1:GE:118:GLU:HG3	1.84	0.42
1:GD:97:PHE:HZ	1:GE:174:VAL:HG22	1.85	0.42
1:HA:93:MET:HG3	1:HB:171:GLU:HG2	2.01	0.42
1:HI:118:GLU:OE2	1:HJ:134:ARG:NH1	2.39	0.42
1:IH:73:GLU:HA	1:IH:77:THR:HB	2.00	0.42
1:JE:77:THR:HG22	1:JE:80:GLY:H	1.84	0.42
1:CD:97:PHE:HZ	1:CE:174:VAL:HG22	1.85	0.42
1:CD:97:PHE:CZ	1:CE:174:VAL:HG22	2.55	0.42
1:CG:170:TRP:CD1	1:CG:171:GLU:HG3	2.48	0.42
1:DB:134:ARG:HE	1:DI:78:LYS:HZ2	1.67	0.42
1:DG:118:GLU:OE2	1:DH:134:ARG:NH1	2.44	0.42
1:EA:93:MET:HG3	1:EB:171:GLU:HG2	2.01	0.42
1:EC:133:SER:O	1:EC:140:VAL:HG11	2.20	0.42
1:FC:149:ASP:O	1:FC:153:ARG:HG3	2.20	0.42
1:IC:149:ASP:O	1:IC:153:ARG:HG3	2.20	0.42
1:IE:91:ILE:HD13	1:IE:123:ALA:HB2	2.02	0.42
1:KA:134:ARG:HH12	1:KE:118:GLU:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KC:33:THR:N	1:KC:195:ILE:O	2.52	0.42
1:KD:97:PHE:HZ	1:KE:174:VAL:HG22	1.85	0.42
1:LC:166:VAL:HG21	1:LC:172:ILE:HG12	2.02	0.42
1:BD:97:PHE:HZ	1:BE:174:VAL:HG22	1.85	0.42
1:EC:33:THR:N	1:EC:195:ILE:O	2.52	0.42
1:ED:36:PHE:CZ	1:ED:194:LEU:HB3	2.50	0.42
1:EE:91:ILE:HD13	1:EE:123:ALA:HB2	2.02	0.42
1:FD:97:PHE:HZ	1:FE:174:VAL:HG22	1.85	0.42
1:GC:149:ASP:O	1:GC:153:ARG:HG3	2.20	0.42
1:GJ:91:ILE:HD13	1:GJ:123:ALA:HB2	2.02	0.42
1:HC:33:THR:N	1:HC:195:ILE:O	2.52	0.42
1:HE:134:ARG:HG3	1:HE:166:VAL:O	2.20	0.42
1:HF:179:LEU:HD23	1:HF:179:LEU:HA	1.85	0.42
1:IH:157:ARG:NH1	1:IH:159:GLU:OE1	2.44	0.42
1:LE:85:GLU:H	1:LE:85:GLU:HG3	1.69	0.42
1:AJ:91:ILE:HD13	1:AJ:123:ALA:HB2	2.02	0.41
1:BA:134:ARG:HH12	1:BE:118:GLU:HG3	1.84	0.41
1:BD:97:PHE:CZ	1:BE:174:VAL:HG22	2.55	0.41
1:CA:62:VAL:HA	1:CA:192:GLY:O	2.20	0.41
1:DA:62:VAL:HA	1:DA:192:GLY:O	2.20	0.41
1:DE:91:ILE:HD13	1:DE:123:ALA:HB2	2.02	0.41
1:EC:149:ASP:O	1:EC:153:ARG:HG3	2.20	0.41
1:FA:62:VAL:HA	1:FA:192:GLY:O	2.20	0.41
1:FA:93:MET:HG3	1:FB:171:GLU:HG2	2.01	0.41
1:GC:166:VAL:HG21	1:GC:172:ILE:HG12	2.02	0.41
1:ID:92:GLU:OE2	1:JC:153:ARG:NH2	2.45	0.41
1:IH:70:GLN:H	1:IH:70:GLN:HG2	1.69	0.41
1:KE:77:THR:HG22	1:KE:80:GLY:H	1.84	0.41
1:KH:157:ARG:NH1	1:KH:159:GLU:OE1	2.44	0.41
1:LC:133:SER:O	1:LC:140:VAL:HG11	2.20	0.41
1:DA:134:ARG:HH12	1:DE:118:GLU:HG3	1.84	0.41
1:EF:117:TYR:HB2	1:EG:164:VAL:HG22	2.03	0.41
1:ID:36:PHE:CD1	1:ID:196:ARG:HG2	2.56	0.41
1:IJ:91:ILE:HD13	1:IJ:123:ALA:HB2	2.02	0.41
1:JC:166:VAL:HG21	1:JC:172:ILE:HG12	2.02	0.41
1:JE:134:ARG:HG3	1:JE:166:VAL:O	2.20	0.41
1:KD:36:PHE:CD1	1:KD:196:ARG:HG2	2.56	0.41
1:KD:97:PHE:CZ	1:KE:174:VAL:HG22	2.55	0.41
1:LG:149:ASP:O	1:LG:153:ARG:HG3	2.20	0.41
1:AA:93:MET:HG3	1:AB:171:GLU:HG2	2.01	0.41
1:AD:97:PHE:CZ	1:AE:174:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:77:THR:HG22	1:AE:80:GLY:H	1.84	0.41
1:BB:78:LYS:HE3	1:GG:135:PHE:HE1	1.85	0.41
1:CJ:91:ILE:HD13	1:CJ:123:ALA:HB2	2.02	0.41
1:FD:97:PHE:CZ	1:FE:174:VAL:HG22	2.55	0.41
1:FH:157:ARG:NH1	1:FH:159:GLU:OE1	2.44	0.41
1:HG:149:ASP:O	1:HG:153:ARG:HG3	2.20	0.41
1:HG:180:ALA:HB2	1:HG:188:VAL:HG21	2.03	0.41
1:ID:97:PHE:CZ	1:IE:174:VAL:HG22	2.55	0.41
1:JC:133:SER:O	1:JC:140:VAL:HG11	2.20	0.41
1:JG:149:ASP:O	1:JG:153:ARG:HG3	2.20	0.41
1:JH:179:LEU:HA	1:JH:179:LEU:HD23	1.80	0.41
1:JI:118:GLU:OE2	1:JJ:134:ARG:NH1	2.39	0.41
1:KA:93:MET:HG3	1:KB:171:GLU:HG2	2.01	0.41
1:AE:134:ARG:HG3	1:AE:166:VAL:O	2.20	0.41
1:BC:133:SER:O	1:BC:140:VAL:HG11	2.20	0.41
1:DJ:91:ILE:HD13	1:DJ:123:ALA:HB2	2.02	0.41
1:EH:127:ARG:NE	1:EH:184:ASP:O	2.39	0.41
1:EI:179:LEU:HD23	1:EI:179:LEU:HA	1.90	0.41
1:GD:97:PHE:CZ	1:GE:174:VAL:HG22	2.55	0.41
1:ID:97:PHE:HZ	1:IE:174:VAL:HG22	1.85	0.41
1:IF:117:TYR:HB2	1:IG:164:VAL:HG22	2.03	0.41
1:KJ:91:ILE:HD13	1:KJ:123:ALA:HB2	2.02	0.41
1:LE:91:ILE:HD13	1:LE:123:ALA:HB2	2.02	0.41
1:LF:117:TYR:HB2	1:LG:164:VAL:HG22	2.02	0.41
1:AG:180:ALA:HB2	1:AG:188:VAL:HG21	2.03	0.41
1:BD:158:GLU:O	1:BD:161:ILE:HG22	2.19	0.41
1:BF:117:TYR:HB2	1:BG:164:VAL:HG22	2.03	0.41
1:DD:97:PHE:HZ	1:DE:174:VAL:HG22	1.85	0.41
1:DE:134:ARG:HG3	1:DE:166:VAL:O	2.21	0.41
1:DH:142:ARG:HD3	1:DH:142:ARG:HA	1.91	0.41
1:ED:36:PHE:CD1	1:ED:196:ARG:HG2	2.56	0.41
1:FE:179:LEU:HD23	1:FE:179:LEU:HA	1.85	0.41
1:GG:180:ALA:HB2	1:GG:188:VAL:HG21	2.03	0.41
1:GH:157:ARG:NH1	1:GH:159:GLU:OE1	2.44	0.41
1:JE:91:ILE:HD13	1:JE:123:ALA:HB2	2.02	0.41
1:KD:36:PHE:CZ	1:KD:194:LEU:HB3	2.50	0.41
1:KG:149:ASP:O	1:KG:153:ARG:HG3	2.20	0.41
1:LG:180:ALA:HB2	1:LG:188:VAL:HG21	2.03	0.41
1:AC:133:SER:O	1:AC:140:VAL:HG11	2.20	0.41
1:AD:81:ASN:ND2	1:AD:81:ASN:H	2.19	0.41
1:BD:81:ASN:ND2	1:BD:81:ASN:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BG:180:ALA:HB2	1:BG:188:VAL:HG21	2.03	0.41
1:BH:153:ARG:NH2	1:GG:92:GLU:OE2	2.53	0.41
1:DH:70:GLN:H	1:DH:70:GLN:HG2	1.69	0.41
1:EG:149:ASP:O	1:EG:153:ARG:HG3	2.20	0.41
1:HD:36:PHE:CD1	1:HD:196:ARG:HG2	2.56	0.41
1:IA:93:MET:HG3	1:IB:171:GLU:HG2	2.01	0.41
1:JD:36:PHE:CD1	1:JD:196:ARG:HG2	2.56	0.41
1:JF:117:TYR:HB2	1:JG:164:VAL:HG22	2.03	0.41
1:KE:179:LEU:HD23	1:KE:179:LEU:HA	1.85	0.41
1:AD:36:PHE:CD1	1:AD:196:ARG:HG2	2.56	0.41
1:CC:149:ASP:O	1:CC:153:ARG:HG3	2.20	0.41
1:DD:36:PHE:CD1	1:DD:196:ARG:HG2	2.56	0.41
1:DF:134:ARG:NH1	1:DJ:118:GLU:OE2	2.42	0.41
1:EH:179:LEU:HD23	1:EH:179:LEU:HA	1.80	0.41
1:GE:134:ARG:HG3	1:GE:166:VAL:O	2.21	0.41
1:GF:117:TYR:HB2	1:GG:164:VAL:HG22	2.02	0.41
1:IA:62:VAL:HA	1:IA:192:GLY:O	2.20	0.41
1:JD:81:ASN:ND2	1:JD:81:ASN:H	2.19	0.41
1:KF:117:TYR:HB2	1:KG:164:VAL:HG22	2.02	0.41
1:LA:62:VAL:HA	1:LA:192:GLY:O	2.20	0.41
1:AI:133:SER:O	1:AI:140:VAL:HG11	2.21	0.41
1:CF:117:TYR:HB2	1:CG:164:VAL:HG22	2.02	0.41
1:DE:85:GLU:H	1:DE:85:GLU:HG3	1.69	0.41
1:FE:85:GLU:H	1:FE:85:GLU:HG3	1.69	0.41
1:HF:117:TYR:HB2	1:HG:164:VAL:HG22	2.02	0.41
1:HJ:91:ILE:HD13	1:HJ:123:ALA:HB2	2.02	0.41
1:IE:85:GLU:H	1:IE:85:GLU:HG3	1.69	0.41
1:IG:180:ALA:HB2	1:IG:188:VAL:HG21	2.03	0.41
1:II:133:SER:O	1:II:140:VAL:HG11	2.21	0.41
1:JJ:91:ILE:HD13	1:JJ:123:ALA:HB2	2.02	0.41
1:LD:97:PHE:CZ	1:LE:174:VAL:HG22	2.55	0.41
1:LH:124:GLU:OE1	1:LH:125:GLY:N	2.54	0.41
1:AD:36:PHE:CZ	1:AD:194:LEU:HB3	2.50	0.41
1:AD:97:PHE:HZ	1:AE:174:VAL:HG22	1.85	0.41
1:AF:82:LYS:HA	1:AF:82:LYS:HD3	1.85	0.41
1:AG:118:GLU:OE2	1:AH:134:ARG:NH1	2.44	0.41
1:BC:56:LYS:NZ	1:BC:185:ILE:O	2.52	0.41
1:BD:36:PHE:CZ	1:BD:194:LEU:HB3	2.50	0.41
1:BE:134:ARG:HG3	1:BE:166:VAL:O	2.21	0.41
1:BI:133:SER:O	1:BI:140:VAL:HG11	2.21	0.41
1:BJ:91:ILE:HD13	1:BJ:123:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:166:VAL:HG21	1:CC:172:ILE:HG12	2.02	0.41
1:CE:85:GLU:H	1:CE:85:GLU:HG3	1.69	0.41
1:CG:73:GLU:OE2	1:CG:74:ARG:NH1	2.54	0.41
1:DC:133:SER:O	1:DC:140:VAL:HG11	2.20	0.41
1:DC:166:VAL:HG21	1:DC:172:ILE:HG12	2.02	0.41
1:DG:73:GLU:OE2	1:DG:74:ARG:NH1	2.54	0.41
1:DG:180:ALA:HB2	1:DG:188:VAL:HG21	2.03	0.41
1:DI:133:SER:O	1:DI:140:VAL:HG11	2.21	0.41
1:ED:97:PHE:CZ	1:EE:174:VAL:HG22	2.55	0.41
1:EF:134:ARG:NH1	1:EJ:118:GLU:OE2	2.42	0.41
1:FG:92:GLU:OE2	1:KH:153:ARG:NH2	2.54	0.41
1:GD:36:PHE:CD1	1:GD:196:ARG:HG2	2.56	0.41
1:GI:133:SER:O	1:GI:140:VAL:HG11	2.21	0.41
1:HD:36:PHE:CZ	1:HD:194:LEU:HB3	2.50	0.41
1:HD:97:PHE:HZ	1:HE:174:VAL:HG22	1.85	0.41
1:HF:66:ASP:HA	1:HF:196:ARG:HB2	2.03	0.41
1:IF:134:ARG:NH1	1:IJ:118:GLU:OE2	2.42	0.41
1:JB:179:LEU:HD23	1:JB:179:LEU:HA	1.92	0.41
1:JD:97:PHE:CZ	1:JE:174:VAL:HG22	2.55	0.41
1:KC:133:SER:O	1:KC:140:VAL:HG11	2.20	0.41
1:KG:73:GLU:OE2	1:KG:74:ARG:NH1	2.54	0.41
1:KH:124:GLU:OE1	1:KH:125:GLY:N	2.54	0.41
1:LD:36:PHE:CD1	1:LD:196:ARG:HG2	2.55	0.41
1:LE:134:ARG:HG3	1:LE:166:VAL:O	2.20	0.41
1:LH:127:ARG:NE	1:LH:184:ASP:O	2.39	0.41
1:AE:91:ILE:HD13	1:AE:123:ALA:HB2	2.02	0.41
1:BH:157:ARG:NH1	1:BH:159:GLU:OE1	2.44	0.41
1:CE:91:ILE:HD13	1:CE:123:ALA:HB2	2.02	0.41
1:EH:124:GLU:OE1	1:EH:125:GLY:N	2.54	0.41
1:FD:36:PHE:CD1	1:FD:196:ARG:HG2	2.56	0.41
1:FE:134:ARG:HG3	1:FE:166:VAL:O	2.20	0.41
1:FF:117:TYR:HB2	1:FG:164:VAL:HG22	2.02	0.41
1:GE:179:LEU:HD23	1:GE:179:LEU:HA	1.85	0.41
1:GH:124:GLU:OE1	1:GH:125:GLY:N	2.54	0.41
1:HC:149:ASP:O	1:HC:153:ARG:HG3	2.20	0.41
1:HH:124:GLU:OE1	1:HH:125:GLY:N	2.54	0.41
1:KE:91:ILE:HD13	1:KE:123:ALA:HB2	2.02	0.41
1:AF:134:ARG:NH1	1:AJ:118:GLU:OE2	2.42	0.40
1:DF:66:ASP:HA	1:DF:196:ARG:HB2	2.03	0.40
1:DH:124:GLU:OE1	1:DH:125:GLY:N	2.54	0.40
1:EG:66:ASP:HA	1:EG:196:ARG:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EG:73:GLU:OE2	1:EG:74:ARG:NH1	2.54	0.40
1:FC:179:LEU:HD23	1:FC:179:LEU:HA	1.85	0.40
1:GE:91:ILE:HD13	1:GE:123:ALA:HB2	2.02	0.40
1:HC:88:LEU:HD12	1:HC:88:LEU:HA	1.97	0.40
1:II:179:LEU:HD23	1:II:179:LEU:HA	1.90	0.40
1:JH:72:ILE:O	1:JH:77:THR:OG1	2.22	0.40
1:KI:133:SER:O	1:KI:140:VAL:HG11	2.21	0.40
1:LG:73:GLU:OE2	1:LG:74:ARG:NH1	2.54	0.40
1:AF:117:TYR:HB2	1:AG:164:VAL:HG22	2.02	0.40
1:BA:93:MET:HG3	1:BB:171:GLU:HG2	2.01	0.40
1:CD:36:PHE:CZ	1:CD:194:LEU:HB3	2.50	0.40
1:CD:36:PHE:CD1	1:CD:196:ARG:HG2	2.55	0.40
1:CF:179:LEU:HD23	1:CF:179:LEU:HA	1.85	0.40
1:DE:65:ALA:O	1:DE:195:ILE:HA	2.22	0.40
1:DG:66:ASP:HA	1:DG:196:ARG:HG2	2.04	0.40
1:ED:97:PHE:HZ	1:EE:174:VAL:HG22	1.85	0.40
1:EJ:91:ILE:HD13	1:EJ:123:ALA:HB2	2.02	0.40
1:FG:73:GLU:OE2	1:FG:74:ARG:NH1	2.54	0.40
1:GG:73:GLU:OE2	1:GG:74:ARG:NH1	2.54	0.40
1:HG:73:GLU:OE2	1:HG:74:ARG:NH1	2.54	0.40
1:HH:127:ARG:NE	1:HH:184:ASP:O	2.39	0.40
1:HI:133:SER:O	1:HI:140:VAL:HG11	2.21	0.40
1:IF:66:ASP:HA	1:IF:196:ARG:HB2	2.03	0.40
1:IG:73:GLU:OE2	1:IG:74:ARG:NH1	2.54	0.40
1:JE:78:LYS:O	1:JE:81:ASN:ND2	2.29	0.40
1:JG:73:GLU:OE2	1:JG:74:ARG:NH1	2.54	0.40
1:LI:179:LEU:HD23	1:LI:179:LEU:HA	1.90	0.40
1:AH:124:GLU:OE1	1:AH:125:GLY:N	2.54	0.40
1:AI:179:LEU:HD23	1:AI:179:LEU:HA	1.90	0.40
1:BD:36:PHE:CD1	1:BD:196:ARG:HG2	2.55	0.40
1:CE:134:ARG:HG3	1:CE:166:VAL:O	2.21	0.40
1:ED:84:TRP:CE3	1:ED:150:CYS:HB2	2.57	0.40
1:FE:36:PHE:HB2	1:FE:196:ARG:HG2	2.04	0.40
1:GC:92:GLU:OE2	1:JD:153:ARG:NH2	2.54	0.40
1:HE:179:LEU:HD23	1:HE:179:LEU:HA	1.86	0.40
1:JF:179:LEU:HD23	1:JF:179:LEU:HA	1.85	0.40
1:KE:134:ARG:HG3	1:KE:166:VAL:O	2.20	0.40
1:KG:66:ASP:HA	1:KG:196:ARG:HG2	2.04	0.40
1:LB:134:ARG:HE	1:LI:78:LYS:NZ	2.19	0.40
1:LE:65:ALA:O	1:LE:195:ILE:HA	2.22	0.40
1:AB:134:ARG:HE	1:AI:78:LYS:NZ	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:73:GLU:OE2	1:AG:74:ARG:NH1	2.54	0.40
1:EG:180:ALA:HB2	1:EG:188:VAL:HG21	2.03	0.40
1:FF:66:ASP:HA	1:FF:196:ARG:HB2	2.03	0.40
1:GF:66:ASP:HA	1:GF:196:ARG:HB2	2.03	0.40
1:HD:97:PHE:CZ	1:HE:174:VAL:HG22	2.55	0.40
1:IE:65:ALA:O	1:IE:195:ILE:HA	2.22	0.40
1:IF:172:ILE:HB	1:IF:173:PRO:HD3	2.04	0.40
1:IH:124:GLU:OE1	1:IH:125:GLY:N	2.54	0.40
1:JE:36:PHE:HB2	1:JE:196:ARG:HG2	2.04	0.40
1:KE:36:PHE:HB2	1:KE:196:ARG:HG2	2.04	0.40
1:KF:66:ASP:HA	1:KF:196:ARG:HB2	2.03	0.40
1:AB:36:PHE:CE1	1:AB:194:LEU:HB3	2.57	0.40
1:AG:66:ASP:HA	1:AG:196:ARG:HG2	2.04	0.40
1:AH:70:GLN:H	1:AH:70:GLN:HG2	1.68	0.40
1:BB:36:PHE:CE1	1:BB:194:LEU:HB3	2.57	0.40
1:BB:134:ARG:HE	1:BI:78:LYS:NZ	2.19	0.40
1:CB:134:ARG:HE	1:CI:78:LYS:NZ	2.19	0.40
1:CH:124:GLU:OE1	1:CH:125:GLY:N	2.54	0.40
1:DD:84:TRP:CE3	1:DD:150:CYS:HB2	2.57	0.40
1:GE:65:ALA:O	1:GE:195:ILE:HA	2.22	0.40
1:HC:56:LYS:NZ	1:HC:185:ILE:O	2.52	0.40
1:IE:134:ARG:HG3	1:IE:166:VAL:O	2.21	0.40
1:LF:66:ASP:HA	1:LF:196:ARG:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	150/197 (76%)	147 (98%)	3 (2%)	0	100	100
1	AB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	AD	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	AE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100
1	AF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	AG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	AH	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	AI	152/197 (77%)	150 (99%)	2 (1%)	0	100	100
1	AJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
1	BA	150/197 (76%)	147 (98%)	3 (2%)	0	100	100
1	BB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100
1	BC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	BD	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	BE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100
1	BF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	BG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	BH	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	BI	152/197 (77%)	150 (99%)	2 (1%)	0	100	100
1	BJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
1	CA	150/197 (76%)	147 (98%)	3 (2%)	0	100	100
1	CB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100
1	CC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	CD	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	CE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100
1	CF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	CG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	CH	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	CI	152/197 (77%)	150 (99%)	2 (1%)	0	100	100
1	CJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
1	DA	150/197 (76%)	147 (98%)	3 (2%)	0	100	100
1	DB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100
1	DC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DD	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	DE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100
1	DF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	DG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	DH	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	DI	152/197 (77%)	149 (98%)	3 (2%)	0	100	100
1	DJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
1	EA	150/197 (76%)	148 (99%)	2 (1%)	0	100	100
1	EB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100
1	EC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	ED	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	EE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100
1	EF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	EG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	EH	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	EI	152/197 (77%)	150 (99%)	2 (1%)	0	100	100
1	EJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
1	FA	150/197 (76%)	147 (98%)	3 (2%)	0	100	100
1	FB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100
1	FC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	FD	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	FE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100
1	FF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	FG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	FH	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	FI	152/197 (77%)	150 (99%)	2 (1%)	0	100	100
1	FJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
1	GA	150/197 (76%)	147 (98%)	3 (2%)	0	100	100
1	GB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100
1	GC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	GD	151/197 (77%)	148 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100
1	GF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	GG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	GH	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	GI	152/197 (77%)	150 (99%)	2 (1%)	0	100	100
1	GJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
1	HA	150/197 (76%)	148 (99%)	2 (1%)	0	100	100
1	HB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100
1	HC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	HD	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	HE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100
1	HF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	HG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	HH	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	HI	152/197 (77%)	150 (99%)	2 (1%)	0	100	100
1	HJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
1	IA	150/197 (76%)	147 (98%)	3 (2%)	0	100	100
1	IB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100
1	IC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	ID	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	IE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100
1	IF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	IG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	IH	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	II	152/197 (77%)	150 (99%)	2 (1%)	0	100	100
1	IJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
1	JA	150/197 (76%)	147 (98%)	3 (2%)	0	100	100
1	JB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100
1	JC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	JD	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	JE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	JG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	JH	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	JI	152/197 (77%)	150 (99%)	2 (1%)	0	100	100
1	JJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
1	KA	150/197 (76%)	148 (99%)	2 (1%)	0	100	100
1	KB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100
1	KC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	KD	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	KE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100
1	KF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	KG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	KH	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	KI	152/197 (77%)	150 (99%)	2 (1%)	0	100	100
1	KJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
1	LA	150/197 (76%)	147 (98%)	3 (2%)	0	100	100
1	LB	150/197 (76%)	146 (97%)	4 (3%)	0	100	100
1	LC	151/197 (77%)	149 (99%)	2 (1%)	0	100	100
1	LD	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	LE	149/197 (76%)	146 (98%)	3 (2%)	0	100	100
1	LF	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	LG	151/197 (77%)	145 (96%)	6 (4%)	0	100	100
1	LH	151/197 (77%)	148 (98%)	3 (2%)	0	100	100
1	LI	152/197 (77%)	150 (99%)	2 (1%)	0	100	100
1	LJ	149/197 (76%)	145 (97%)	4 (3%)	0	100	100
All	All	18060/23640 (76%)	17633 (98%)	427 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	AB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	AC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	AD	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	AE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	AF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	AG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	AH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	AI	122/147 (83%)	120 (98%)	2 (2%)	62	83
1	AJ	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	BA	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	BB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	BC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	BD	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	BE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	BF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	BG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	BH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	BI	122/147 (83%)	120 (98%)	2 (2%)	62	83
1	BJ	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	CA	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	CB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	CC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	CD	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	CE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	CF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	CG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	CH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	CI	122/147 (83%)	120 (98%)	2 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CJ	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	DA	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	DB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	DC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	DD	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	DE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	DF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	DG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	DH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	DI	122/147 (83%)	120 (98%)	2 (2%)	62	83
1	DJ	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	EA	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	EB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	EC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	ED	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	EE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	EF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	EG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	EH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	EI	122/147 (83%)	120 (98%)	2 (2%)	62	83
1	EJ	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	FA	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	FB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	FC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	FD	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	FE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	FF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	FG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	FH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	FI	122/147 (83%)	120 (98%)	2 (2%)	62	83
1	FJ	120/147 (82%)	118 (98%)	2 (2%)	60	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GA	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	GB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	GC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	GD	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	GE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	GF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	GG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	GH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	GI	122/147 (83%)	120 (98%)	2 (2%)	62	83
1	GJ	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	HA	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	HB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	HC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	HD	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	HE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	HF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	HG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	HH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	HI	122/147 (83%)	120 (98%)	2 (2%)	62	83
1	HJ	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	IA	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	IB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	IC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	ID	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	IE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	IF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	IG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	IH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	II	122/147 (83%)	120 (98%)	2 (2%)	62	83
1	IJ	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	JA	120/147 (82%)	118 (98%)	2 (2%)	60	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	JC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	JD	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	JE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	JF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	JG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	JH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	JI	122/147 (83%)	120 (98%)	2 (2%)	62	83
1	JJ	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	KA	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	KB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	KC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	KD	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	KE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	KF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	KG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	KH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	KI	122/147 (83%)	120 (98%)	2 (2%)	62	83
1	KJ	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	LA	120/147 (82%)	118 (98%)	2 (2%)	60	82
1	LB	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	LC	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	LD	121/147 (82%)	118 (98%)	3 (2%)	47	75
1	LE	120/147 (82%)	117 (98%)	3 (2%)	47	75
1	LF	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	LG	121/147 (82%)	116 (96%)	5 (4%)	30	63
1	LH	121/147 (82%)	117 (97%)	4 (3%)	38	68
1	LI	122/147 (83%)	120 (98%)	2 (2%)	62	83
1	LJ	120/147 (82%)	118 (98%)	2 (2%)	60	82
All	All	14484/17640 (82%)	14100 (97%)	384 (3%)	48	73

All (384) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	81	ASN
1	AA	124	GLU
1	AB	42	GLU
1	AB	81	ASN
1	AB	124	GLU
1	AC	42	GLU
1	AC	59	THR
1	AC	81	ASN
1	AC	124	GLU
1	AD	66	ASP
1	AD	81	ASN
1	AD	124	GLU
1	AE	35	HIS
1	AE	81	ASN
1	AE	124	GLU
1	AF	35	HIS
1	AF	42	GLU
1	AF	179	LEU
1	AF	195	ILE
1	AG	35	HIS
1	AG	42	GLU
1	AG	66	ASP
1	AG	69	GLU
1	AG	84	TRP
1	AH	37	ASP
1	AH	77	THR
1	AH	84	TRP
1	AH	124	GLU
1	AI	81	ASN
1	AI	124	GLU
1	AJ	66	ASP
1	AJ	124	GLU
1	BA	81	ASN
1	BA	124	GLU
1	BB	42	GLU
1	BB	81	ASN
1	BB	124	GLU
1	BC	42	GLU
1	BC	59	THR
1	BC	81	ASN
1	BC	124	GLU
1	BD	66	ASP
1	BD	81	ASN

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Mol	Chain	Res	Type
1	BD	124	GLU
1	BE	35	HIS
1	BE	81	ASN
1	BE	124	GLU
1	BF	35	HIS
1	BF	42	GLU
1	BF	179	LEU
1	BF	195	ILE
1	BG	35	HIS
1	BG	42	GLU
1	BG	66	ASP
1	BG	69	GLU
1	BG	84	TRP
1	BH	37	ASP
1	BH	77	THR
1	BH	84	TRP
1	BH	124	GLU
1	BI	81	ASN
1	BI	124	GLU
1	BJ	66	ASP
1	BJ	124	GLU
1	CA	81	ASN
1	CA	124	GLU
1	CB	42	GLU
1	CB	81	ASN
1	CB	124	GLU
1	CC	42	GLU
1	CC	59	THR
1	CC	81	ASN
1	CC	124	GLU
1	CD	66	ASP
1	CD	81	ASN
1	CD	124	GLU
1	CE	35	HIS
1	CE	81	ASN
1	CE	124	GLU
1	CF	35	HIS
1	CF	42	GLU
1	CF	179	LEU
1	CF	195	ILE
1	CG	35	HIS
1	CG	42	GLU

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Mol	Chain	Res	Type
1	CG	66	ASP
1	CG	69	GLU
1	CG	84	TRP
1	CH	37	ASP
1	CH	77	THR
1	CH	84	TRP
1	CH	124	GLU
1	CI	81	ASN
1	CI	124	GLU
1	CJ	66	ASP
1	CJ	124	GLU
1	DA	81	ASN
1	DA	124	GLU
1	DB	42	GLU
1	DB	81	ASN
1	DB	124	GLU
1	DC	42	GLU
1	DC	59	THR
1	DC	81	ASN
1	DC	124	GLU
1	DD	66	ASP
1	DD	81	ASN
1	DD	124	GLU
1	DE	35	HIS
1	DE	81	ASN
1	DE	124	GLU
1	DF	35	HIS
1	DF	42	GLU
1	DF	179	LEU
1	DF	195	ILE
1	DG	35	HIS
1	DG	42	GLU
1	DG	66	ASP
1	DG	69	GLU
1	DG	84	TRP
1	DH	37	ASP
1	DH	77	THR
1	DH	84	TRP
1	DH	124	GLU
1	DI	81	ASN
1	DI	124	GLU
1	DJ	66	ASP

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Mol	Chain	Res	Type
1	DJ	124	GLU
1	EA	81	ASN
1	EA	124	GLU
1	EB	42	GLU
1	EB	81	ASN
1	EB	124	GLU
1	EC	42	GLU
1	EC	59	THR
1	EC	81	ASN
1	EC	124	GLU
1	ED	66	ASP
1	ED	81	ASN
1	ED	124	GLU
1	EE	35	HIS
1	EE	81	ASN
1	EE	124	GLU
1	EF	35	HIS
1	EF	42	GLU
1	EF	179	LEU
1	EF	195	ILE
1	EG	35	HIS
1	EG	42	GLU
1	EG	66	ASP
1	EG	69	GLU
1	EG	84	TRP
1	EH	37	ASP
1	EH	77	THR
1	EH	84	TRP
1	EH	124	GLU
1	EI	81	ASN
1	EI	124	GLU
1	EJ	66	ASP
1	EJ	124	GLU
1	FA	81	ASN
1	FA	124	GLU
1	FB	42	GLU
1	FB	81	ASN
1	FB	124	GLU
1	FC	42	GLU
1	FC	59	THR
1	FC	81	ASN
1	FC	124	GLU

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Mol	Chain	Res	Type
1	FD	66	ASP
1	FD	81	ASN
1	FD	124	GLU
1	FE	35	HIS
1	FE	81	ASN
1	FE	124	GLU
1	FF	35	HIS
1	FF	42	GLU
1	FF	179	LEU
1	FF	195	ILE
1	FG	35	HIS
1	FG	42	GLU
1	FG	66	ASP
1	FG	69	GLU
1	FG	84	TRP
1	FH	37	ASP
1	FH	77	THR
1	FH	84	TRP
1	FH	124	GLU
1	FI	81	ASN
1	FI	124	GLU
1	FJ	66	ASP
1	FJ	124	GLU
1	GA	81	ASN
1	GA	124	GLU
1	GB	42	GLU
1	GB	81	ASN
1	GB	124	GLU
1	GC	42	GLU
1	GC	59	THR
1	GC	81	ASN
1	GC	124	GLU
1	GD	66	ASP
1	GD	81	ASN
1	GD	124	GLU
1	GE	35	HIS
1	GE	81	ASN
1	GE	124	GLU
1	GF	35	HIS
1	GF	42	GLU
1	GF	179	LEU
1	GF	195	ILE

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Mol	Chain	Res	Type
1	GG	35	HIS
1	GG	42	GLU
1	GG	66	ASP
1	GG	69	GLU
1	GG	84	TRP
1	GH	37	ASP
1	GH	77	THR
1	GH	84	TRP
1	GH	124	GLU
1	GI	81	ASN
1	GI	124	GLU
1	GJ	66	ASP
1	GJ	124	GLU
1	HA	81	ASN
1	HA	124	GLU
1	HB	42	GLU
1	HB	81	ASN
1	HB	124	GLU
1	HC	42	GLU
1	HC	59	THR
1	HC	81	ASN
1	HC	124	GLU
1	HD	66	ASP
1	HD	81	ASN
1	HD	124	GLU
1	HE	35	HIS
1	HE	81	ASN
1	HE	124	GLU
1	HF	35	HIS
1	HF	42	GLU
1	HF	179	LEU
1	HF	195	ILE
1	HG	35	HIS
1	HG	42	GLU
1	HG	66	ASP
1	HG	69	GLU
1	HG	84	TRP
1	HH	37	ASP
1	HH	77	THR
1	HH	84	TRP
1	HH	124	GLU
1	HI	81	ASN

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Mol	Chain	Res	Type
1	HI	124	GLU
1	HJ	66	ASP
1	HJ	124	GLU
1	IA	81	ASN
1	IA	124	GLU
1	IB	42	GLU
1	IB	81	ASN
1	IB	124	GLU
1	IC	42	GLU
1	IC	59	THR
1	IC	81	ASN
1	IC	124	GLU
1	ID	66	ASP
1	ID	81	ASN
1	ID	124	GLU
1	IE	35	HIS
1	IE	81	ASN
1	IE	124	GLU
1	IF	35	HIS
1	IF	42	GLU
1	IF	179	LEU
1	IF	195	ILE
1	IG	35	HIS
1	IG	42	GLU
1	IG	66	ASP
1	IG	69	GLU
1	IG	84	TRP
1	IH	37	ASP
1	IH	77	THR
1	IH	84	TRP
1	IH	124	GLU
1	II	81	ASN
1	II	124	GLU
1	IJ	66	ASP
1	IJ	124	GLU
1	JA	81	ASN
1	JA	124	GLU
1	JB	42	GLU
1	JB	81	ASN
1	JB	124	GLU
1	JC	42	GLU
1	JC	59	THR

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Mol	Chain	Res	Type
1	JC	81	ASN
1	JC	124	GLU
1	JD	66	ASP
1	JD	81	ASN
1	JD	124	GLU
1	JE	35	HIS
1	JE	81	ASN
1	JE	124	GLU
1	JF	35	HIS
1	JF	42	GLU
1	JF	179	LEU
1	JF	195	ILE
1	JG	35	HIS
1	JG	42	GLU
1	JG	66	ASP
1	JG	69	GLU
1	JG	84	TRP
1	JH	37	ASP
1	JH	77	THR
1	JH	84	TRP
1	JH	124	GLU
1	JI	81	ASN
1	JI	124	GLU
1	JJ	66	ASP
1	JJ	124	GLU
1	KA	81	ASN
1	KA	124	GLU
1	KB	42	GLU
1	KB	81	ASN
1	KB	124	GLU
1	KC	42	GLU
1	KC	59	THR
1	KC	81	ASN
1	KC	124	GLU
1	KD	66	ASP
1	KD	81	ASN
1	KD	124	GLU
1	KE	35	HIS
1	KE	81	ASN
1	KE	124	GLU
1	KF	35	HIS
1	KF	42	GLU

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Mol	Chain	Res	Type
1	KF	179	LEU
1	KF	195	ILE
1	KG	35	HIS
1	KG	42	GLU
1	KG	66	ASP
1	KG	69	GLU
1	KG	84	TRP
1	KH	37	ASP
1	KH	77	THR
1	KH	84	TRP
1	KH	124	GLU
1	KI	81	ASN
1	KI	124	GLU
1	KJ	66	ASP
1	KJ	124	GLU
1	LA	81	ASN
1	LA	124	GLU
1	LB	42	GLU
1	LB	81	ASN
1	LB	124	GLU
1	LC	42	GLU
1	LC	59	THR
1	LC	81	ASN
1	LC	124	GLU
1	LD	66	ASP
1	LD	81	ASN
1	LD	124	GLU
1	LE	35	HIS
1	LE	81	ASN
1	LE	124	GLU
1	LF	35	HIS
1	LF	42	GLU
1	LF	179	LEU
1	LF	195	ILE
1	LG	35	HIS
1	LG	42	GLU
1	LG	66	ASP
1	LG	69	GLU
1	LG	84	TRP
1	LH	37	ASP
1	LH	77	THR
1	LH	84	TRP

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Mol	Chain	Res	Type
1	LH	124	GLU
1	LI	81	ASN
1	LI	124	GLU
1	LJ	66	ASP
1	LJ	124	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	70	GLN
1	AC	81	ASN
1	AD	81	ASN
1	AI	81	ASN
1	AJ	70	GLN
1	BB	70	GLN
1	BC	81	ASN
1	BD	81	ASN
1	BI	81	ASN
1	BJ	70	GLN
1	CB	70	GLN
1	CC	81	ASN
1	CD	81	ASN
1	CI	81	ASN
1	CJ	70	GLN
1	DB	70	GLN
1	DC	81	ASN
1	DD	81	ASN
1	DI	81	ASN
1	DJ	70	GLN
1	EB	70	GLN
1	EC	81	ASN
1	ED	81	ASN
1	EI	81	ASN
1	EI	137	HIS
1	EJ	70	GLN
1	FB	70	GLN
1	FC	81	ASN
1	FD	81	ASN
1	FI	81	ASN
1	FJ	70	GLN
1	GB	70	GLN
1	GC	81	ASN

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Mol	Chain	Res	Type
1	GD	81	ASN
1	GI	81	ASN
1	GJ	70	GLN
1	HB	70	GLN
1	HC	81	ASN
1	HD	81	ASN
1	HI	81	ASN
1	HJ	70	GLN
1	IB	70	GLN
1	IC	81	ASN
1	ID	81	ASN
1	II	81	ASN
1	IJ	70	GLN
1	JB	70	GLN
1	JC	81	ASN
1	JD	81	ASN
1	JI	81	ASN
1	JJ	70	GLN
1	KB	70	GLN
1	KC	81	ASN
1	KD	81	ASN
1	KI	81	ASN
1	KJ	70	GLN
1	LB	70	GLN
1	LC	81	ASN
1	LD	81	ASN
1	LI	81	ASN
1	LJ	70	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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.

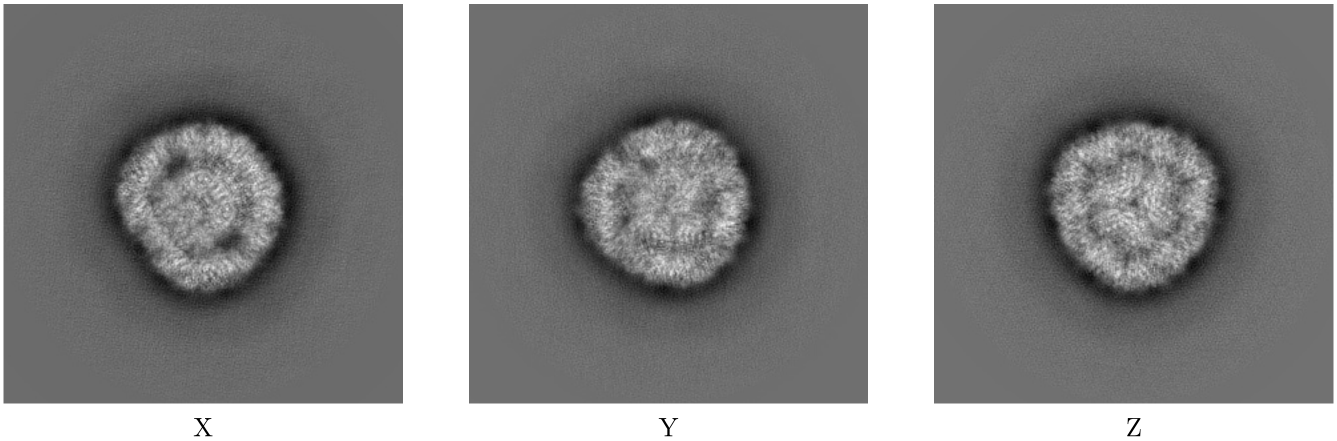
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11631. These allow visual inspection of the internal detail of the map and identification of artifacts.

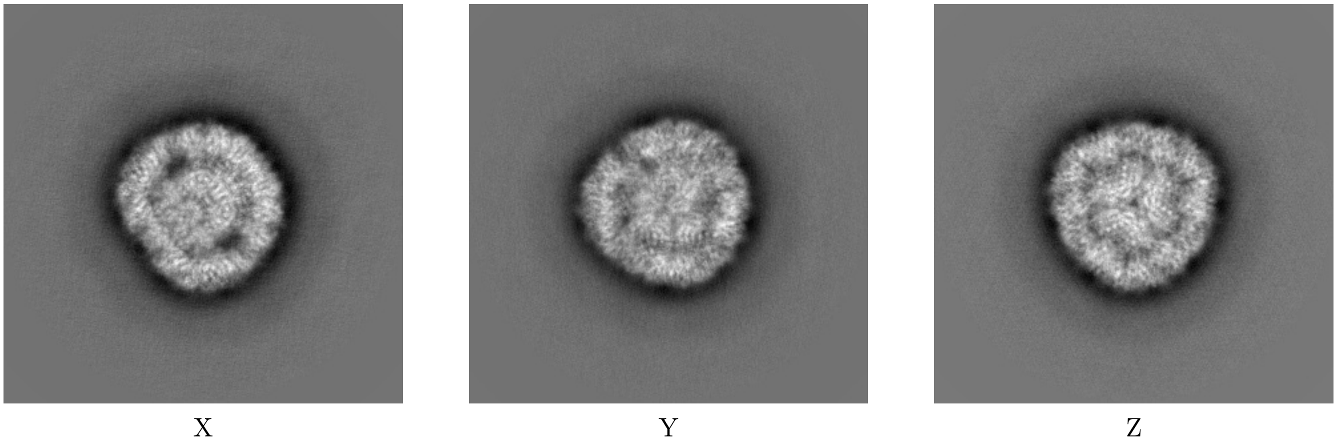
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X Y Z

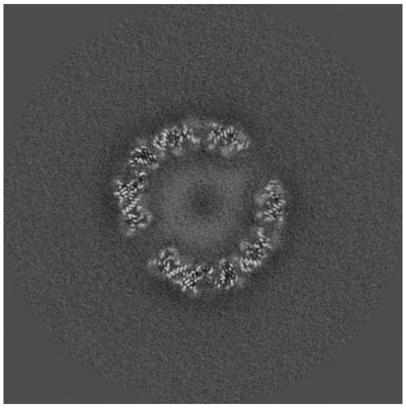
6.1.2 Raw map


X Y Z

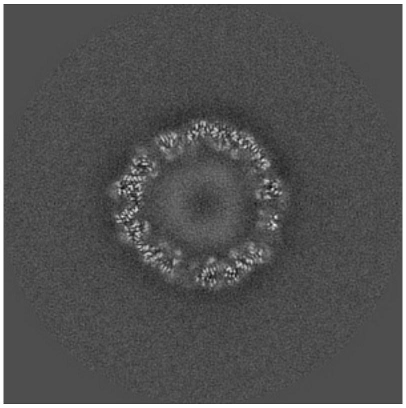
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

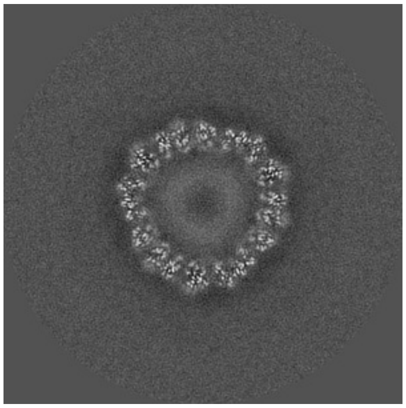
6.2.1 Primary map



X Index: 200

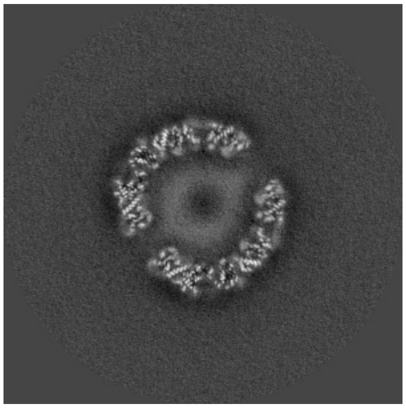


Y Index: 200

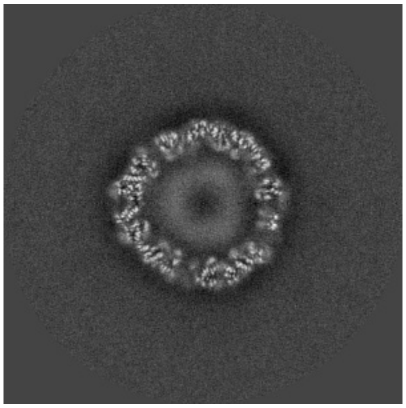


Z Index: 200

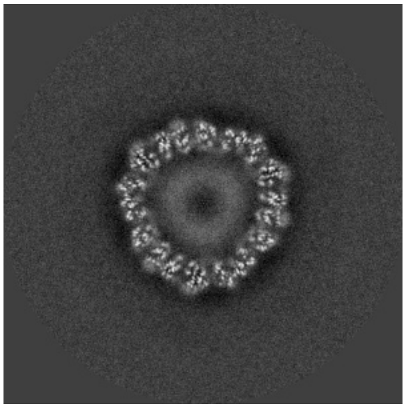
6.2.2 Raw map



X Index: 200



Y Index: 200

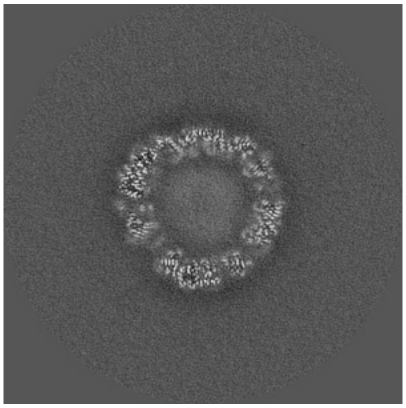


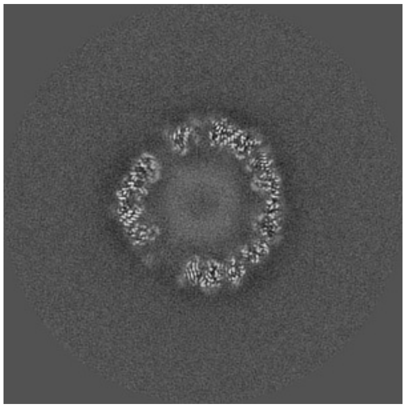
Z Index: 200

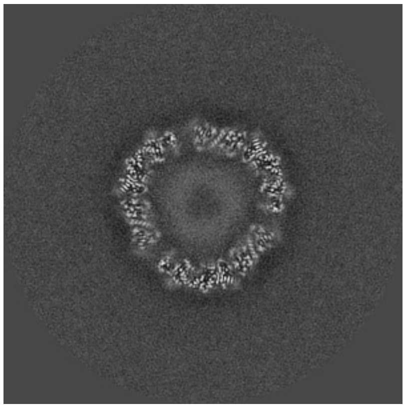
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

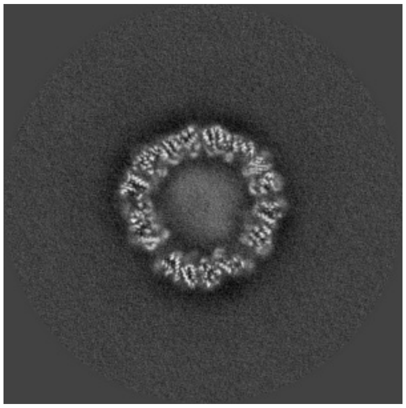
6.3.1 Primary map

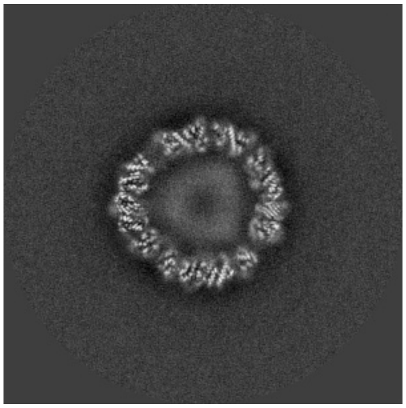

X Index: 180

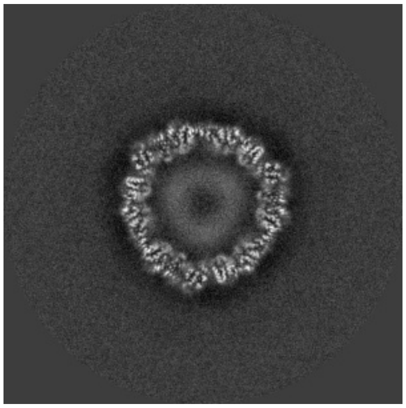

Y Index: 215


Z Index: 209

6.3.2 Raw map


X Index: 175

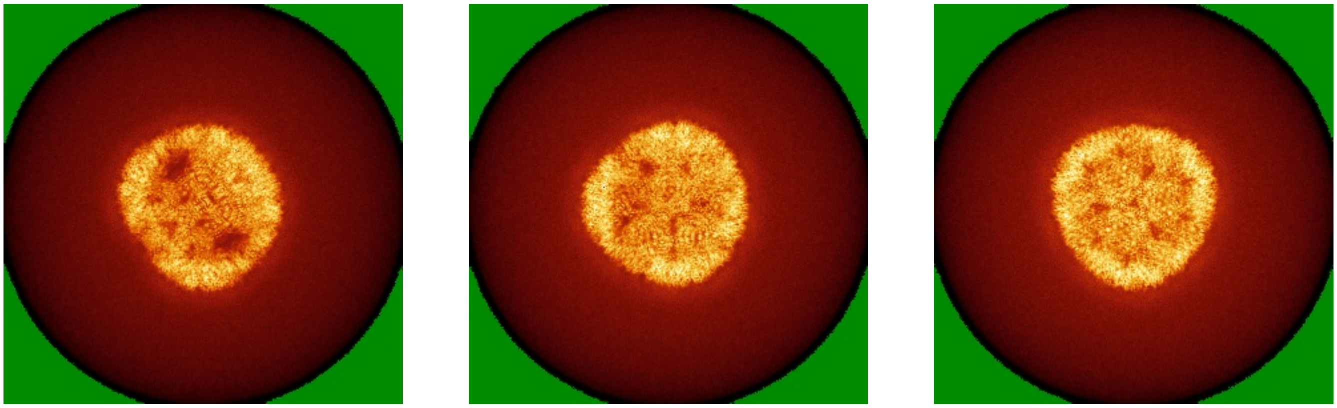

Y Index: 189


Z Index: 195

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

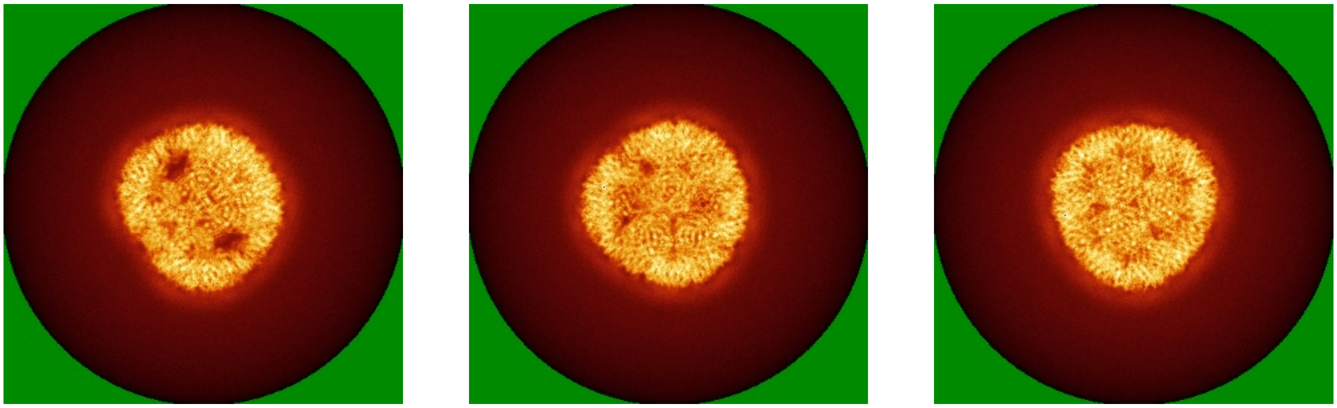
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

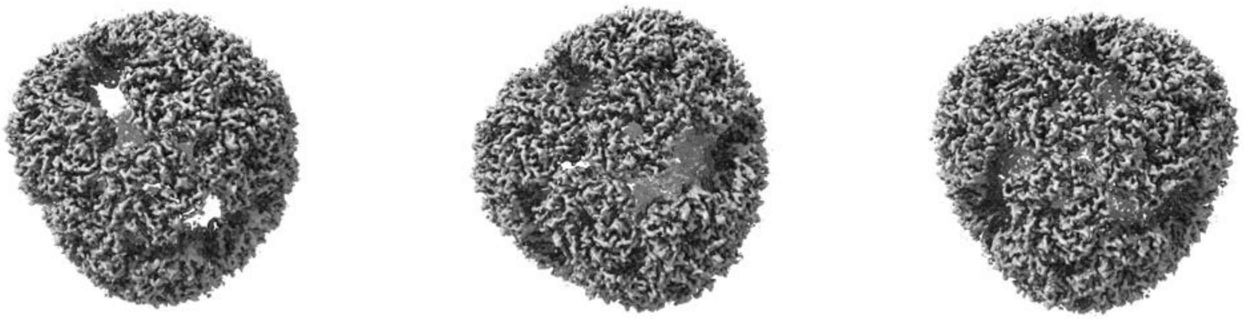


X Y Z

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

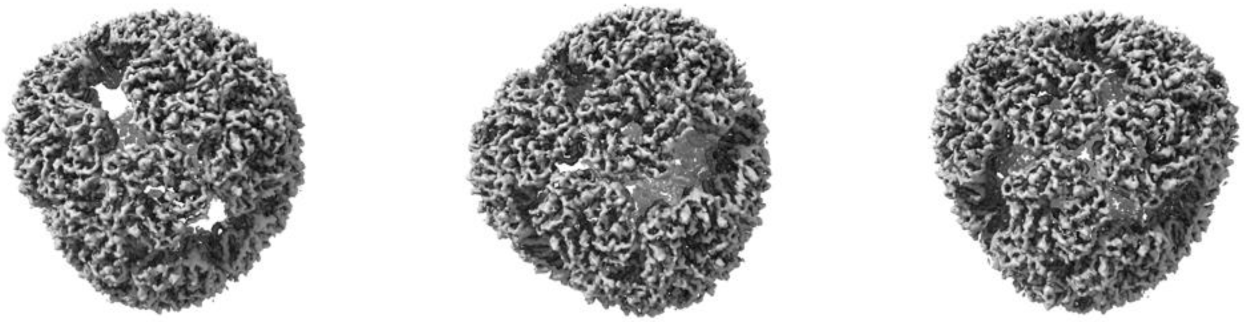
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.85. 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.

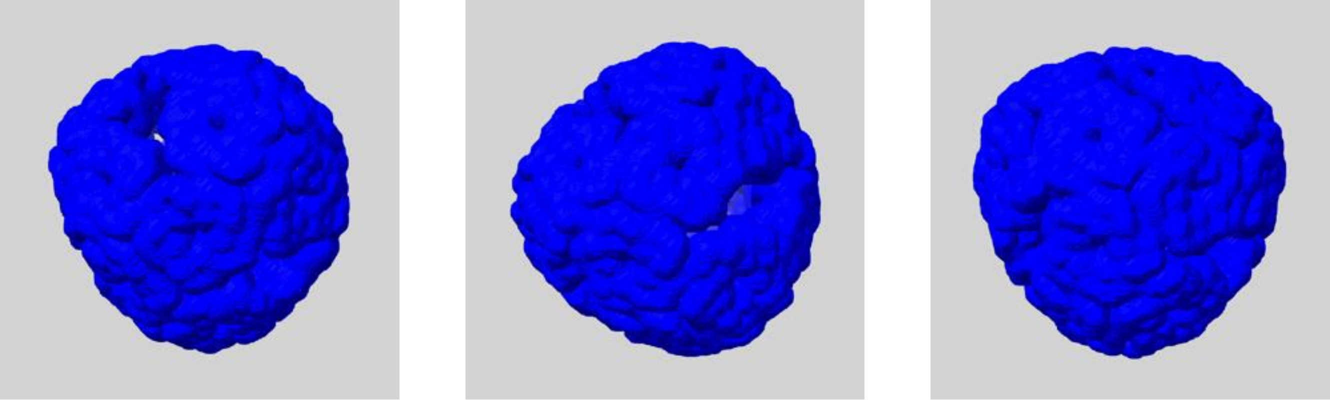
6.6 Mask visualisation ⓘ

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_11631_msk_1.map ⓘ

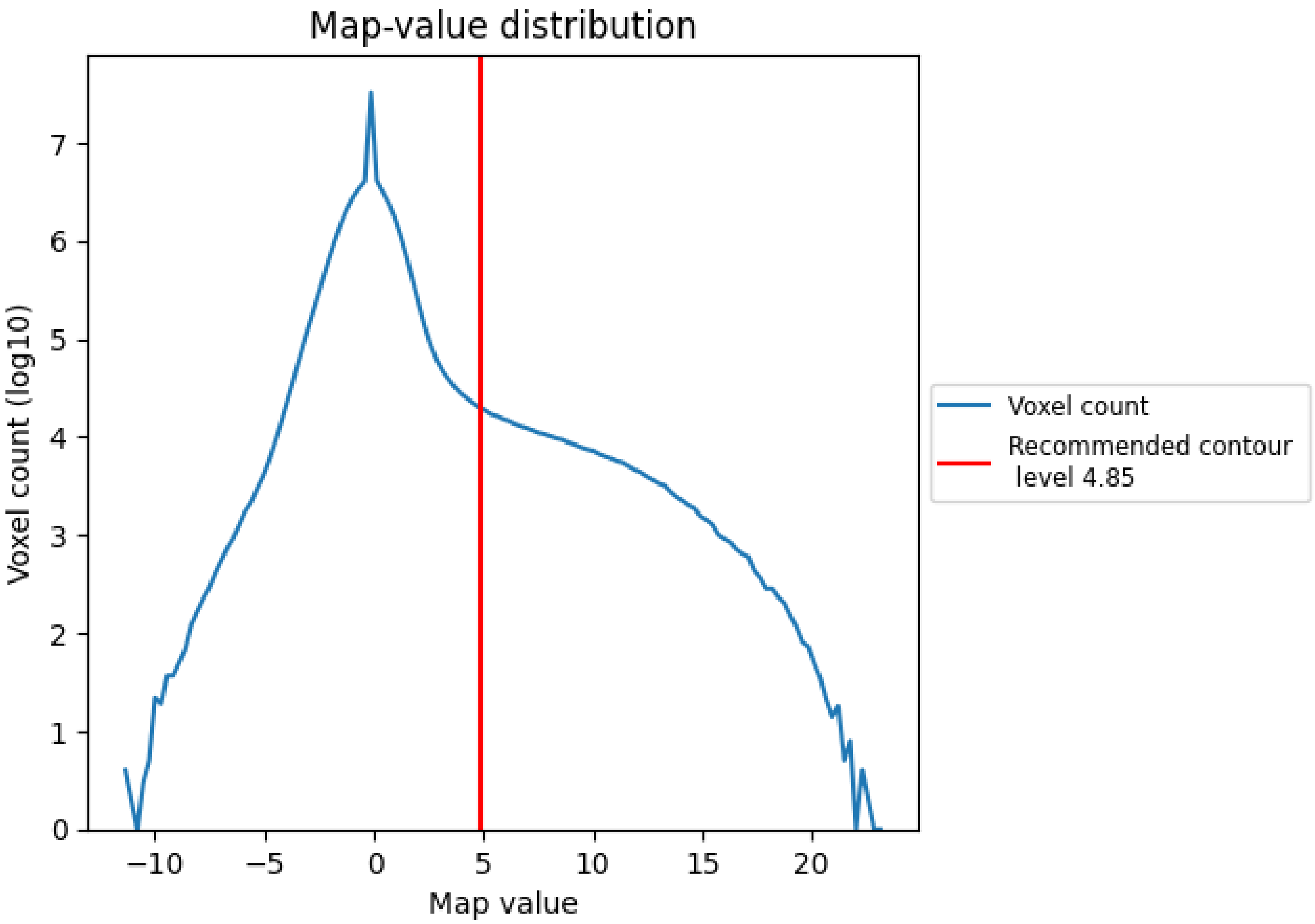


X Y Z

7 Map analysis ⓘ

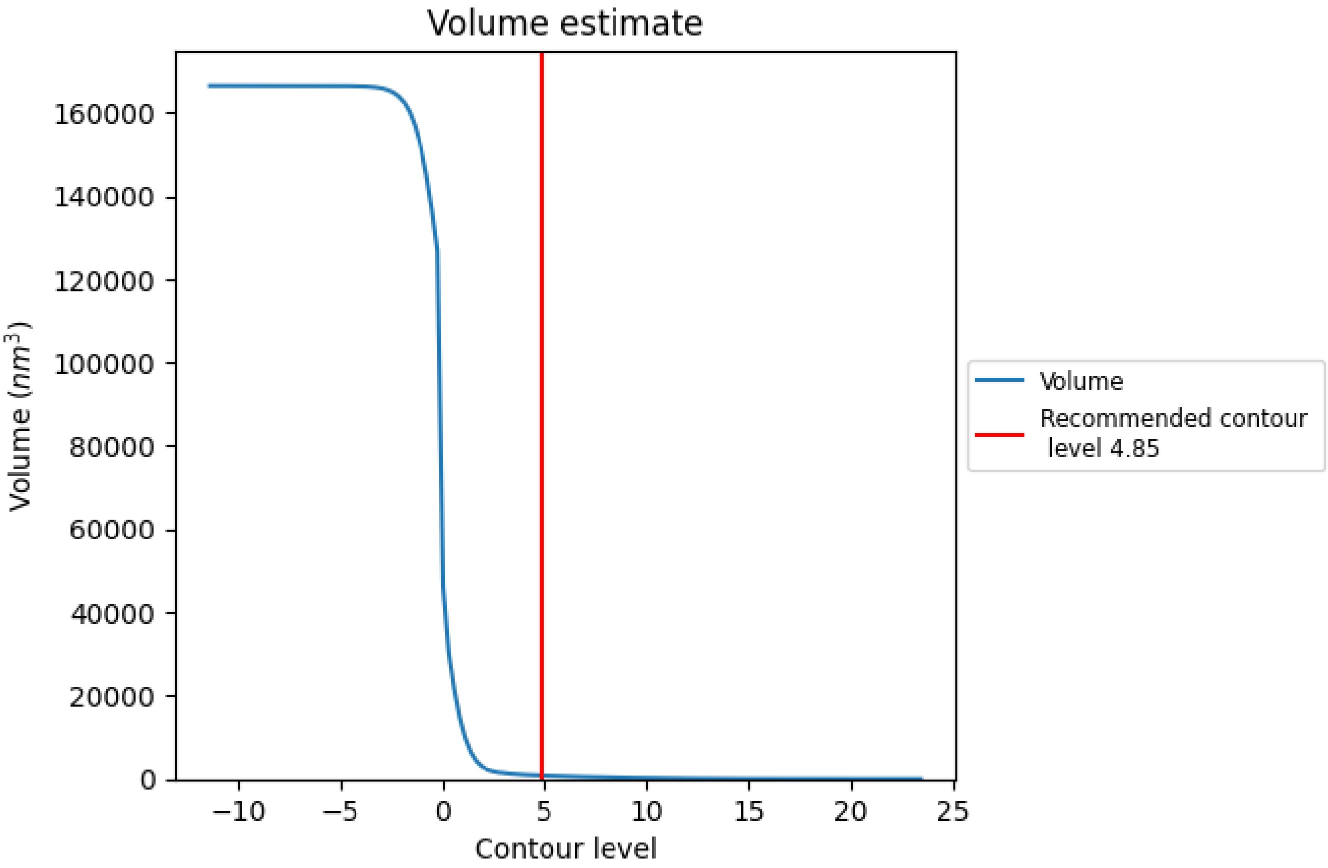
This section contains the results of statistical analysis of the map.

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.

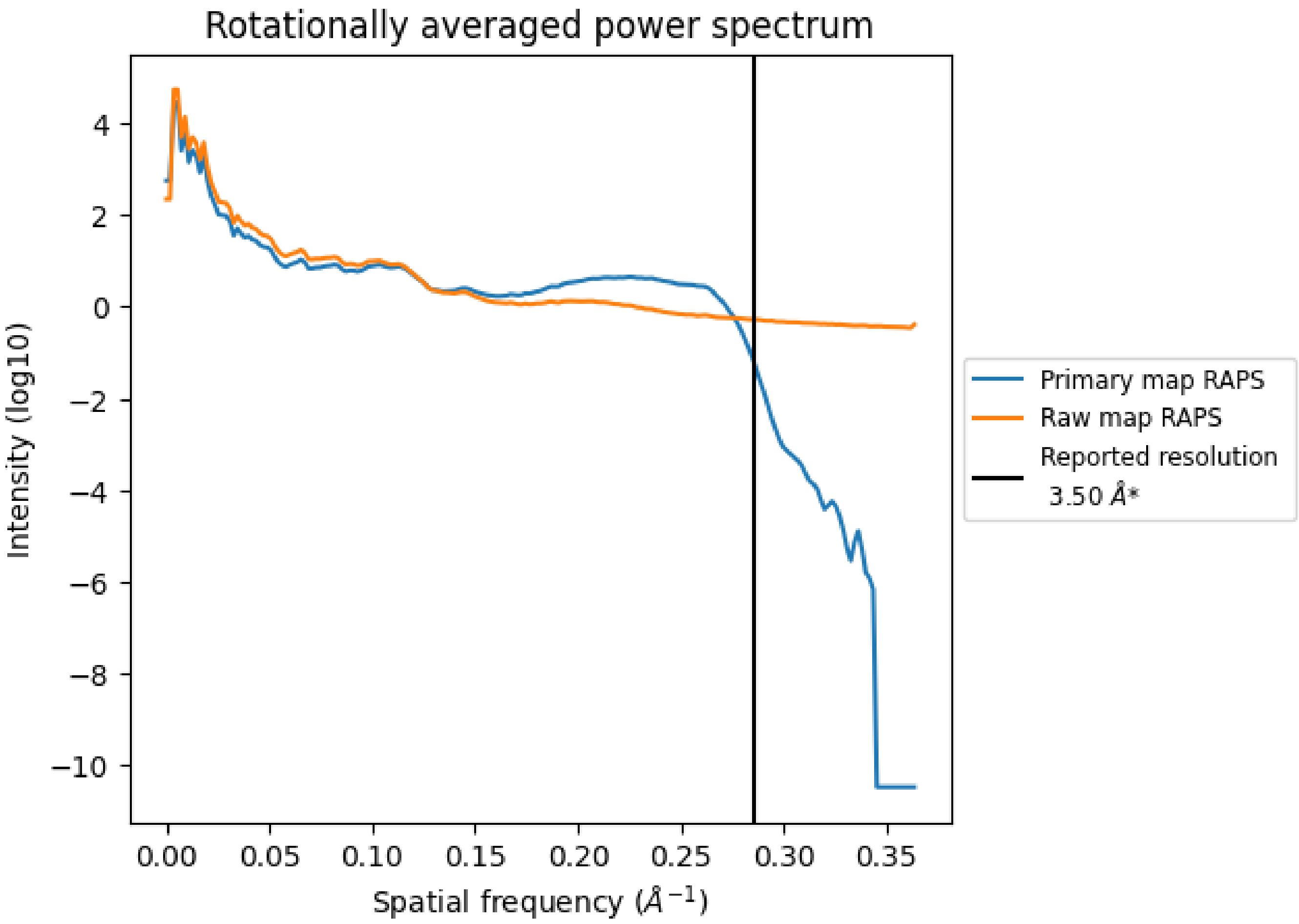
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 832 nm^3; this corresponds to an approximate mass of 752 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

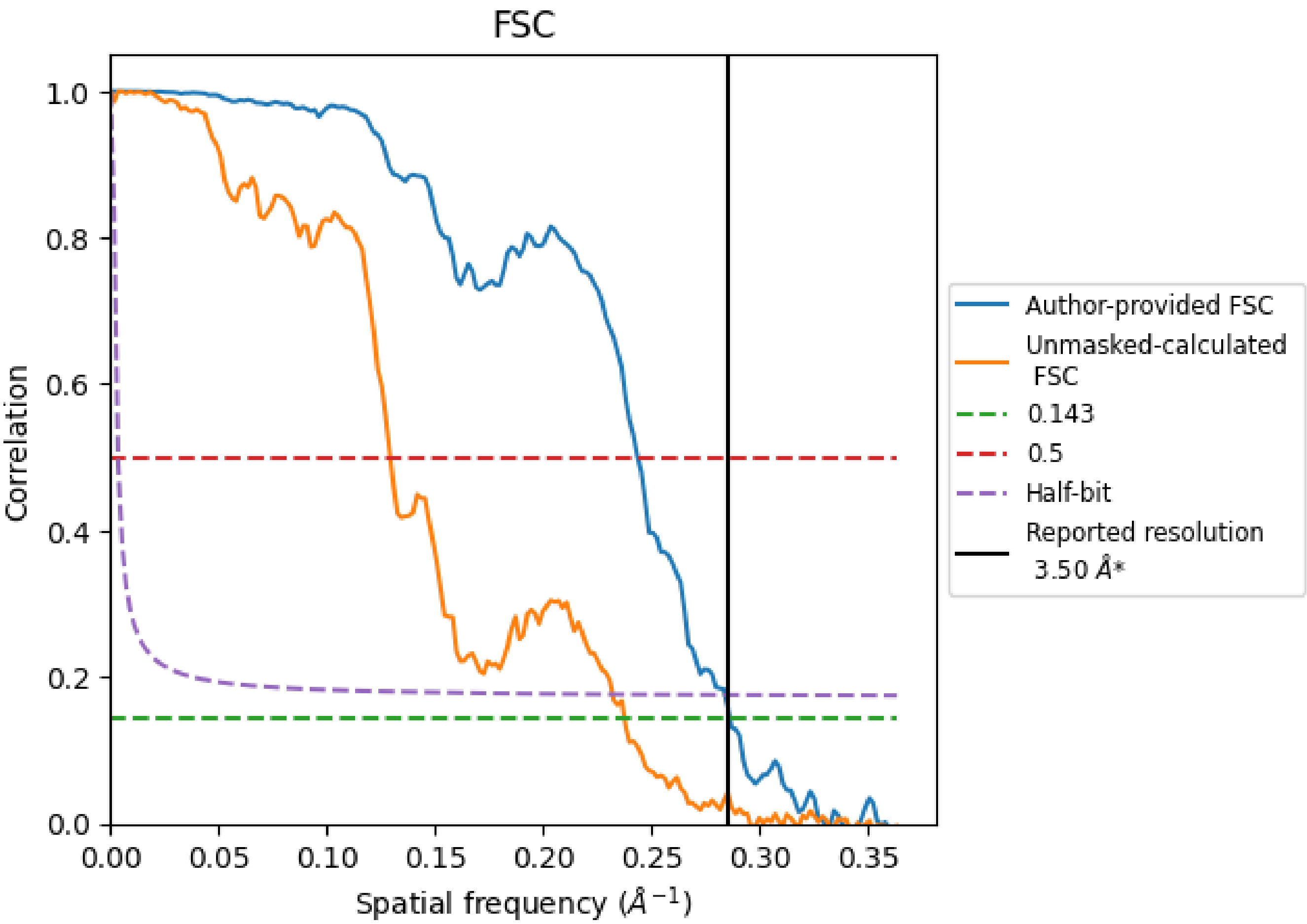


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates ⓘ

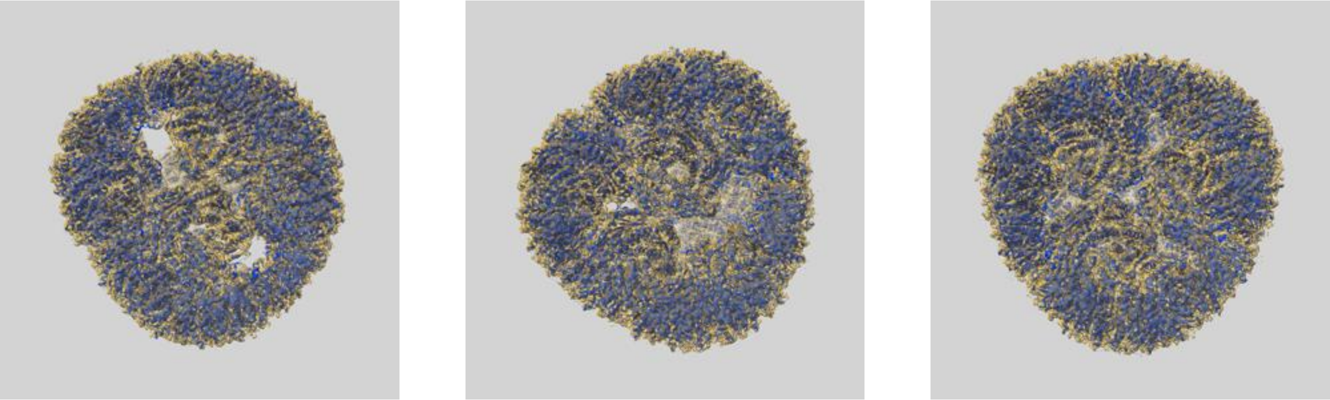
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.10	3.52
Unmasked-calculated*	4.21	7.73	4.31

*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 4.21 differs from the reported value 3.5 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11631 and PDB model 7A4F. Per-residue inclusion information can be found in section 3 on page 92.

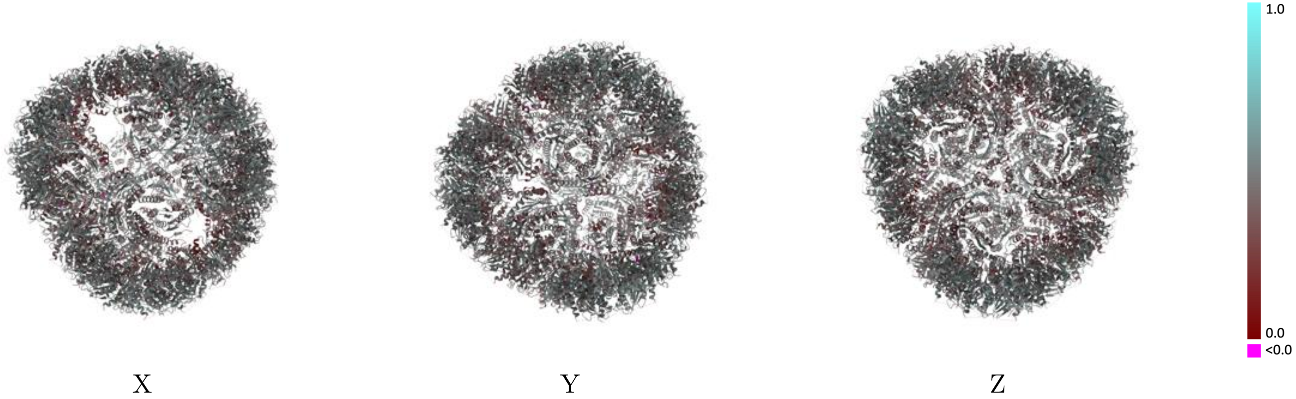
9.1 Map-model overlay (i)



X Y Z

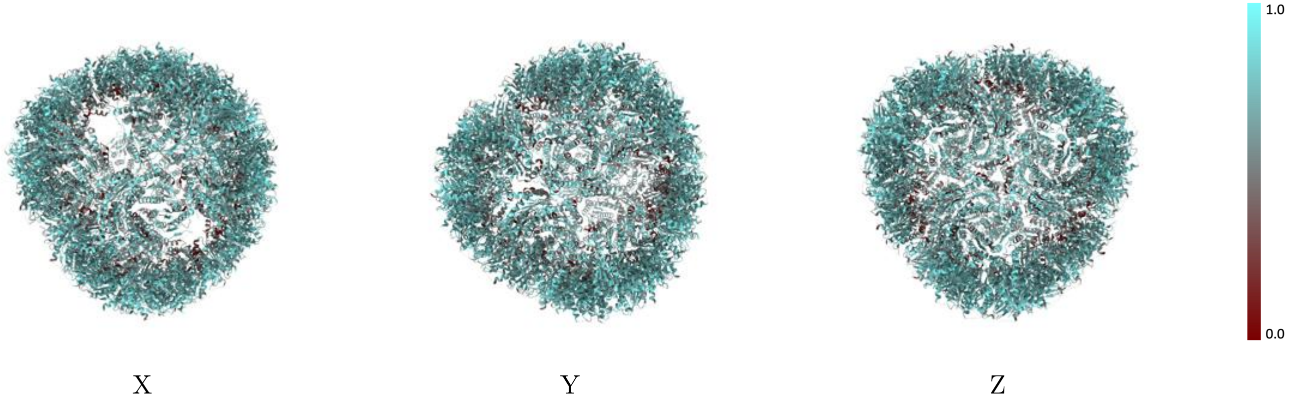
The images above show the 3D surface view of the map at the recommended contour level 4.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



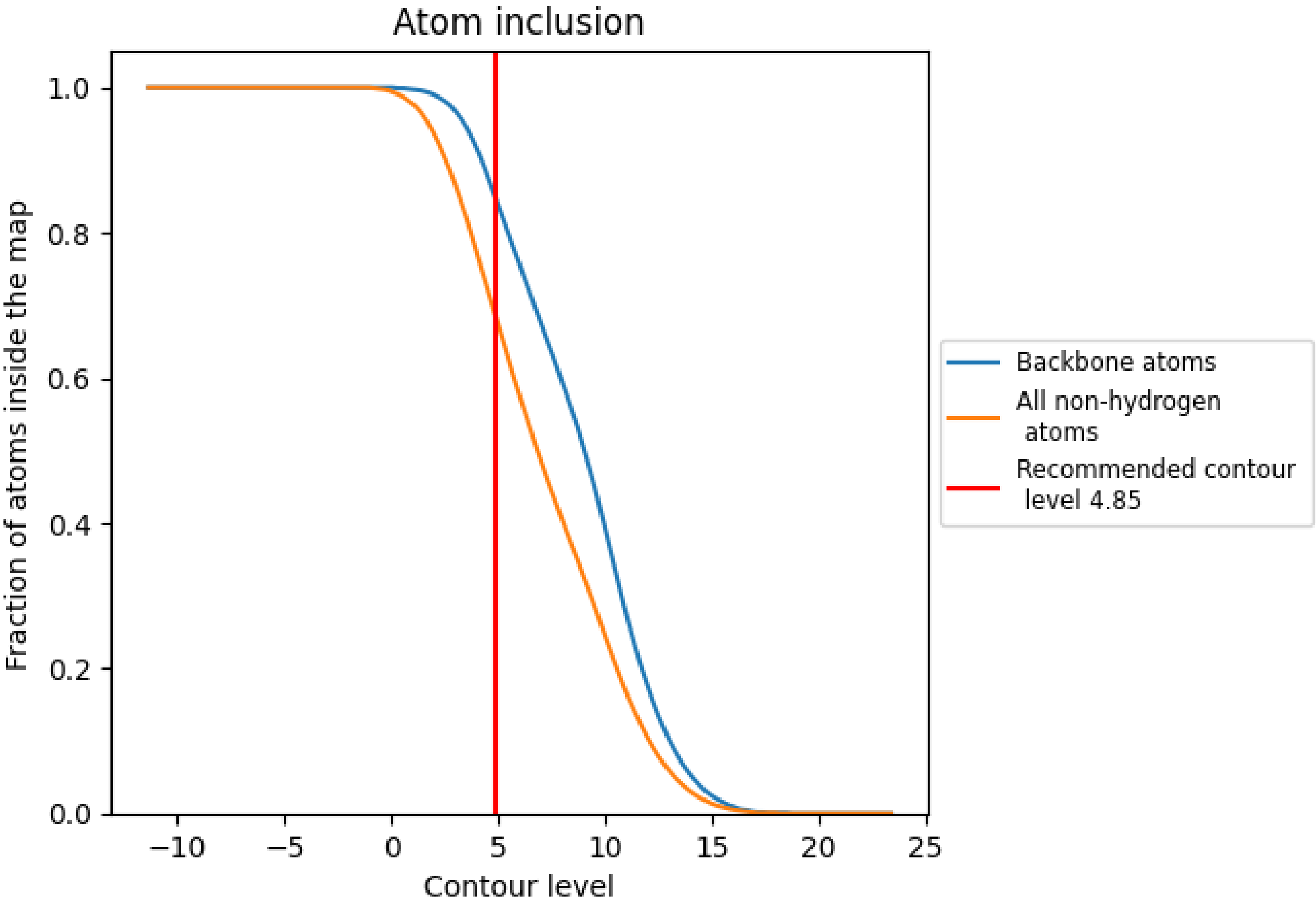
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (4.85).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 69% 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 (4.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.4460
AA	0.6680	0.4320
AB	0.6600	0.4330
AC	0.6840	0.4590
AD	0.6720	0.4350
AE	0.6310	0.4150
AF	0.6990	0.4500
AG	0.7450	0.4780
AH	0.7680	0.4950
AI	0.7040	0.4670
AJ	0.6630	0.4170
BA	0.6590	0.4240
BB	0.6650	0.4330
BC	0.7020	0.4590
BD	0.6700	0.4350
BE	0.6350	0.4100
BF	0.6940	0.4430
BG	0.7340	0.4700
BH	0.7770	0.4890
BI	0.7160	0.4650
BJ	0.6560	0.4160
CA	0.6580	0.4260
CB	0.6590	0.4340
CC	0.6970	0.4580
CD	0.6680	0.4370
CE	0.6310	0.4120
CF	0.6950	0.4470
CG	0.7440	0.4750
CH	0.7650	0.4960
CI	0.7070	0.4650
CJ	0.6530	0.4190
DA	0.6550	0.4210
DB	0.6580	0.4310
DC	0.6890	0.4480
DD	0.6440	0.4220

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Chain	Atom inclusion	Q-score
DE	0.6210	0.4040
DF	0.6930	0.4470
DG	0.7410	0.4780
DH	0.7690	0.4930
DI	0.7050	0.4670
DJ	0.6550	0.4200
EA	0.6620	0.4250
EB	0.6660	0.4330
EC	0.6990	0.4580
ED	0.6620	0.4340
EE	0.6280	0.4110
EF	0.6940	0.4410
EG	0.7350	0.4740
EH	0.7660	0.4900
EI	0.7020	0.4630
EJ	0.6640	0.4180
FA	0.6640	0.4290
FB	0.6600	0.4350
FC	0.6960	0.4600
FD	0.6630	0.4340
FE	0.6310	0.4140
FF	0.6910	0.4490
FG	0.7340	0.4800
FH	0.7700	0.4960
FI	0.7090	0.4670
FJ	0.6590	0.4160
GA	0.6590	0.4250
GB	0.6640	0.4360
GC	0.6910	0.4570
GD	0.6610	0.4270
GE	0.6290	0.4090
GF	0.6920	0.4500
GG	0.7510	0.4790
GH	0.7810	0.4910
GI	0.7150	0.4670
GJ	0.6570	0.4220
HA	0.6630	0.4280
HB	0.6580	0.4340
HC	0.7020	0.4590
HD	0.6670	0.4330
HE	0.6330	0.4090
HF	0.6960	0.4410

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Chain	Atom inclusion	Q-score
HG	0.7350	0.4770
HH	0.7550	0.4900
HI	0.7150	0.4640
HJ	0.6530	0.4180
IA	0.6600	0.4300
IB	0.6610	0.4340
IC	0.6960	0.4590
ID	0.6660	0.4370
IE	0.6330	0.4110
IF	0.6920	0.4500
IG	0.7400	0.4780
IH	0.7800	0.4950
II	0.7030	0.4680
IJ	0.6560	0.4200
JA	0.6690	0.4300
JB	0.6580	0.4360
JC	0.6950	0.4610
JD	0.6650	0.4380
JE	0.6280	0.4150
JF	0.6870	0.4480
JG	0.7450	0.4820
JH	0.7780	0.4950
JI	0.7100	0.4690
JJ	0.6490	0.4140
KA	0.6690	0.4260
KB	0.6580	0.4350
KC	0.6930	0.4600
KD	0.6660	0.4350
KE	0.6380	0.4150
KF	0.6900	0.4470
KG	0.7480	0.4770
KH	0.7700	0.4950
KI	0.7070	0.4640
KJ	0.6590	0.4190
LA	0.6610	0.4250
LB	0.6620	0.4300
LC	0.6920	0.4570
LD	0.6700	0.4360
LE	0.6330	0.4100
LF	0.6960	0.4470
LG	0.7380	0.4730
LH	0.7480	0.4930

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Chain	**Atom inclusion**	**Q-score**
LI	▬ 0.7070	▬ 0.4630
LJ	▬ 0.6590	▬ 0.4190