Full wwPDB EM Validation Report

Mar 25, 2026 – 01:59 AM UTC

PDB ID	:	9G3J / pdb_00009g3j
EMDB ID	:	EMD-51001
Title	:	Circularly permuted lumazine synthase twisted tube with 28 Angstrom gap between double strands
Authors	:	Koziej, L.; Azuma, Y.
Deposited on	:	2024-07-12
Resolution	:	3.10 Å(reported)
Based on initial model	:	1HQK

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

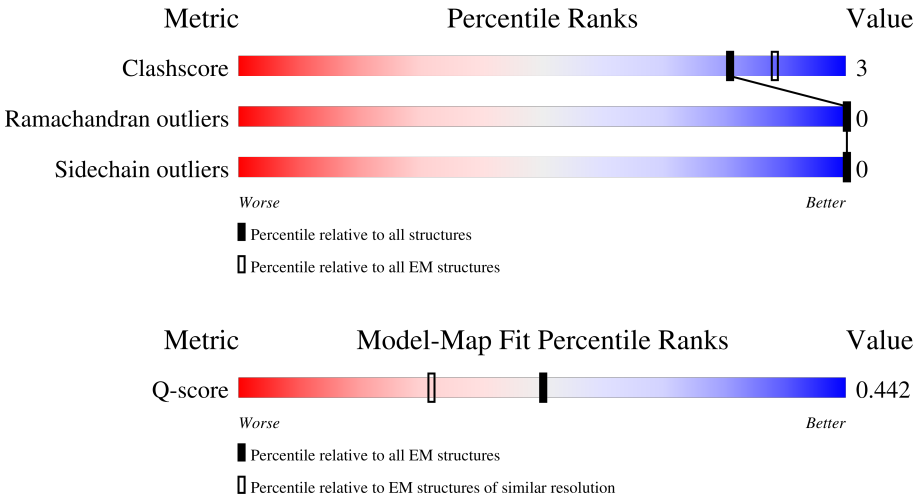
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	A	163	89% 8%
1	AA	163	87% 5% 9%
1	AB	163	87% 12%
1	AC	163	87% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	B	163	86% 6% 9%
1	BA	163	89% 9%
1	BB	163	87% 10%
1	BC	163	84% 7% 9%
1	C	163	87% 11%
1	CA	163	87% 10%
1	CB	163	84% 7% 9%
1	CC	163	88% 9%
1	D	163	88% 10%
1	DA	163	85% 7% 9%
1	DB	163	90% 7%
1	DC	163	87% 9%
1	E	163	84% 7% 9%
1	EA	163	86% 11%
1	EB	163	86% 6% 9%
1	EC	163	88% 10%
1	F	163	90% 7%
1	FA	163	87% 5% 9%
1	FB	163	87% 12%
1	FC	163	87% 10%
1	G	163	87% 9%
1	GA	163	88% 10%
1	GB	163	88% 10%
1	GC	163	84% 7% 9%
1	H	163	87% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	HA	163	87% 10%
1	HB	163	84% 7% 9%
1	HC	163	88% 9%
1	I	163	87% 10%
1	IA	163	83% 8% 9%
1	IB	163	90% 7%
1	IC	163	87% 5% 9%
1	J	163	83% 8% 9%
1	JA	163	88% 9%
1	JB	163	87% 9%
1	JC	163	88% 10%
1	K	163	88% 9%
1	KA	163	86% 6% 9%
1	KB	163	88% 10%
1	KC	163	88% 10%
1	L	163	87% 5% 9%
1	LA	163	87% 11%
1	LB	163	87% 10%
1	LC	163	85% 7% 9%
1	M	163	88% 10%
1	MA	163	87% 10%
1	MB	163	84% 7% 9%
1	MC	163	88% 9%
1	N	163	87% 10%
1	NA	163	83% 8% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	NB	163	88% 9%
1	NC	163	87% 5% 9%
1	O	163	84% 7% 9%
1	OA	163	88% 9%
1	OB	163	87% 9%
1	OC	163	88% 10%
1	P	163	88% 9%
1	PA	163	87% 9%
1	PB	163	88% 10%
1	PC	163	87% 10%
1	Q	163	87% 5% 9%
1	QA	163	87% 11%
1	QB	163	88% 10%
1	QC	163	85% 7% 9%
1	R	163	88% 10%
1	RA	163	87% 10%
1	RB	163	84% 7% 9%
1	RC	163	89% 8%
1	S	163	87% 10%
1	SA	163	84% 7% 9%
1	SB	163	87% 10%
1	SC	163	86% 6% 9%
1	T	163	85% 7% 9%
1	TA	163	89% 8%
1	TB	163	87% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	TC	163	88% 10%
1	U	163	88% 9%
1	UA	163	86% 6% 9%
1	UB	163	90% 9%
1	UC	163	88% 10%
1	V	163	87% 5% 9%
1	VA	163	88% 10%
1	VB	163	87% 10%
1	VC	163	83% 8% 9%
1	W	163	88% 10%
1	WA	163	88% 10%
1	WB	163	84% 7% 9%
1	X	163	88% 10%
1	XA	163	84% 7% 9%
1	XB	163	87% 10%
1	Y	163	85% 7% 9%
1	YA	163	88% 9%
1	YB	163	87% 5% 9%
1	Z	163	88% 9%
1	ZA	163	87% 5% 9%
1	ZB	163	87% 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 114640 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 6,7-dimethyl-8-ribityllumazine synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	B	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	C	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	D	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	E	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	F	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	G	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	H	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	I	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	J	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	K	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	L	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	M	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	N	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	O	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	P	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	Q	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	S	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	T	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	U	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	V	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	W	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	X	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	Y	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	Z	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	AA	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	BA	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	CA	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	DA	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	EA	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	FA	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	GA	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	HA	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	IA	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	JA	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	KA	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	LA	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	MA	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	NA	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	OA	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	PA	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	QA	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	RA	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	SA	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	TA	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	UA	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	VA	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	WA	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	XA	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	YA	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	ZA	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	AB	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	BB	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	CB	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	DB	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	EB	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	FB	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	GB	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	HB	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	IB	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	JB	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	KB	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	LB	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	MB	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	NB	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	OB	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	PB	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	QB	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	RB	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	SB	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	TB	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	UB	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	VB	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	WB	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	XB	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	YB	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	ZB	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	AC	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	BC	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CC	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	DC	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	EC	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	FC	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	GC	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	HC	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	IC	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	JC	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	KC	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	LC	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	MC	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	NC	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	OC	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	PC	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	QC	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	RC	158	Total	C	N	O	S	0	0
			1186	747	213	223	3		
1	SC	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		
1	TC	160	Total	C	N	O	S	0	0
			1203	758	215	227	3		
1	UC	147	Total	C	N	O	S	0	0
			1105	699	195	208	3		
1	VC	149	Total	C	N	O	S	0	0
			1119	707	199	210	3		

There are 1300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O66529
A	37	GLY	-	linker	UNP O66529
A	38	THR	-	linker	UNP O66529
A	39	GLY	-	linker	UNP O66529
A	40	GLY	-	linker	UNP O66529
A	41	SER	-	linker	UNP O66529
A	42	GLY	-	linker	UNP O66529
A	43	SER	-	linker	UNP O66529
A	44	SER	-	linker	UNP O66529
A	45	MET	-	linker	UNP O66529
A	46	GLU	-	linker	UNP O66529
A	81	SER	CYS	engineered mutation	UNP O66529
A	129	CYS	ALA	engineered mutation	UNP O66529
B	1	MET	-	initiating methionine	UNP O66529
B	37	GLY	-	linker	UNP O66529
B	38	THR	-	linker	UNP O66529
B	39	GLY	-	linker	UNP O66529
B	40	GLY	-	linker	UNP O66529
B	41	SER	-	linker	UNP O66529
B	42	GLY	-	linker	UNP O66529
B	43	SER	-	linker	UNP O66529
B	44	SER	-	linker	UNP O66529
B	45	MET	-	linker	UNP O66529
B	46	GLU	-	linker	UNP O66529
B	81	SER	CYS	engineered mutation	UNP O66529
B	129	CYS	ALA	engineered mutation	UNP O66529
C	1	MET	-	initiating methionine	UNP O66529
C	37	GLY	-	linker	UNP O66529
C	38	THR	-	linker	UNP O66529
C	39	GLY	-	linker	UNP O66529
C	40	GLY	-	linker	UNP O66529
C	41	SER	-	linker	UNP O66529
C	42	GLY	-	linker	UNP O66529
C	43	SER	-	linker	UNP O66529
C	44	SER	-	linker	UNP O66529
C	45	MET	-	linker	UNP O66529
C	46	GLU	-	linker	UNP O66529
C	81	SER	CYS	engineered mutation	UNP O66529
C	129	CYS	ALA	engineered mutation	UNP O66529
D	1	MET	-	initiating methionine	UNP O66529
D	37	GLY	-	linker	UNP O66529
D	38	THR	-	linker	UNP O66529
D	39	GLY	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	40	GLY	-	linker	UNP O66529
D	41	SER	-	linker	UNP O66529
D	42	GLY	-	linker	UNP O66529
D	43	SER	-	linker	UNP O66529
D	44	SER	-	linker	UNP O66529
D	45	MET	-	linker	UNP O66529
D	46	GLU	-	linker	UNP O66529
D	81	SER	CYS	engineered mutation	UNP O66529
D	129	CYS	ALA	engineered mutation	UNP O66529
E	1	MET	-	initiating methionine	UNP O66529
E	37	GLY	-	linker	UNP O66529
E	38	THR	-	linker	UNP O66529
E	39	GLY	-	linker	UNP O66529
E	40	GLY	-	linker	UNP O66529
E	41	SER	-	linker	UNP O66529
E	42	GLY	-	linker	UNP O66529
E	43	SER	-	linker	UNP O66529
E	44	SER	-	linker	UNP O66529
E	45	MET	-	linker	UNP O66529
E	46	GLU	-	linker	UNP O66529
E	81	SER	CYS	engineered mutation	UNP O66529
E	129	CYS	ALA	engineered mutation	UNP O66529
F	1	MET	-	initiating methionine	UNP O66529
F	37	GLY	-	linker	UNP O66529
F	38	THR	-	linker	UNP O66529
F	39	GLY	-	linker	UNP O66529
F	40	GLY	-	linker	UNP O66529
F	41	SER	-	linker	UNP O66529
F	42	GLY	-	linker	UNP O66529
F	43	SER	-	linker	UNP O66529
F	44	SER	-	linker	UNP O66529
F	45	MET	-	linker	UNP O66529
F	46	GLU	-	linker	UNP O66529
F	81	SER	CYS	engineered mutation	UNP O66529
F	129	CYS	ALA	engineered mutation	UNP O66529
G	1	MET	-	initiating methionine	UNP O66529
G	37	GLY	-	linker	UNP O66529
G	38	THR	-	linker	UNP O66529
G	39	GLY	-	linker	UNP O66529
G	40	GLY	-	linker	UNP O66529
G	41	SER	-	linker	UNP O66529
G	42	GLY	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	43	SER	-	linker	UNP O66529
G	44	SER	-	linker	UNP O66529
G	45	MET	-	linker	UNP O66529
G	46	GLU	-	linker	UNP O66529
G	81	SER	CYS	engineered mutation	UNP O66529
G	129	CYS	ALA	engineered mutation	UNP O66529
H	1	MET	-	initiating methionine	UNP O66529
H	37	GLY	-	linker	UNP O66529
H	38	THR	-	linker	UNP O66529
H	39	GLY	-	linker	UNP O66529
H	40	GLY	-	linker	UNP O66529
H	41	SER	-	linker	UNP O66529
H	42	GLY	-	linker	UNP O66529
H	43	SER	-	linker	UNP O66529
H	44	SER	-	linker	UNP O66529
H	45	MET	-	linker	UNP O66529
H	46	GLU	-	linker	UNP O66529
H	81	SER	CYS	engineered mutation	UNP O66529
H	129	CYS	ALA	engineered mutation	UNP O66529
I	1	MET	-	initiating methionine	UNP O66529
I	37	GLY	-	linker	UNP O66529
I	38	THR	-	linker	UNP O66529
I	39	GLY	-	linker	UNP O66529
I	40	GLY	-	linker	UNP O66529
I	41	SER	-	linker	UNP O66529
I	42	GLY	-	linker	UNP O66529
I	43	SER	-	linker	UNP O66529
I	44	SER	-	linker	UNP O66529
I	45	MET	-	linker	UNP O66529
I	46	GLU	-	linker	UNP O66529
I	81	SER	CYS	engineered mutation	UNP O66529
I	129	CYS	ALA	engineered mutation	UNP O66529
J	1	MET	-	initiating methionine	UNP O66529
J	37	GLY	-	linker	UNP O66529
J	38	THR	-	linker	UNP O66529
J	39	GLY	-	linker	UNP O66529
J	40	GLY	-	linker	UNP O66529
J	41	SER	-	linker	UNP O66529
J	42	GLY	-	linker	UNP O66529
J	43	SER	-	linker	UNP O66529
J	44	SER	-	linker	UNP O66529
J	45	MET	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	46	GLU	-	linker	UNP O66529
J	81	SER	CYS	engineered mutation	UNP O66529
J	129	CYS	ALA	engineered mutation	UNP O66529
K	1	MET	-	initiating methionine	UNP O66529
K	37	GLY	-	linker	UNP O66529
K	38	THR	-	linker	UNP O66529
K	39	GLY	-	linker	UNP O66529
K	40	GLY	-	linker	UNP O66529
K	41	SER	-	linker	UNP O66529
K	42	GLY	-	linker	UNP O66529
K	43	SER	-	linker	UNP O66529
K	44	SER	-	linker	UNP O66529
K	45	MET	-	linker	UNP O66529
K	46	GLU	-	linker	UNP O66529
K	81	SER	CYS	engineered mutation	UNP O66529
K	129	CYS	ALA	engineered mutation	UNP O66529
L	1	MET	-	initiating methionine	UNP O66529
L	37	GLY	-	linker	UNP O66529
L	38	THR	-	linker	UNP O66529
L	39	GLY	-	linker	UNP O66529
L	40	GLY	-	linker	UNP O66529
L	41	SER	-	linker	UNP O66529
L	42	GLY	-	linker	UNP O66529
L	43	SER	-	linker	UNP O66529
L	44	SER	-	linker	UNP O66529
L	45	MET	-	linker	UNP O66529
L	46	GLU	-	linker	UNP O66529
L	81	SER	CYS	engineered mutation	UNP O66529
L	129	CYS	ALA	engineered mutation	UNP O66529
M	1	MET	-	initiating methionine	UNP O66529
M	37	GLY	-	linker	UNP O66529
M	38	THR	-	linker	UNP O66529
M	39	GLY	-	linker	UNP O66529
M	40	GLY	-	linker	UNP O66529
M	41	SER	-	linker	UNP O66529
M	42	GLY	-	linker	UNP O66529
M	43	SER	-	linker	UNP O66529
M	44	SER	-	linker	UNP O66529
M	45	MET	-	linker	UNP O66529
M	46	GLU	-	linker	UNP O66529
M	81	SER	CYS	engineered mutation	UNP O66529
M	129	CYS	ALA	engineered mutation	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	1	MET	-	initiating methionine	UNP O66529
N	37	GLY	-	linker	UNP O66529
N	38	THR	-	linker	UNP O66529
N	39	GLY	-	linker	UNP O66529
N	40	GLY	-	linker	UNP O66529
N	41	SER	-	linker	UNP O66529
N	42	GLY	-	linker	UNP O66529
N	43	SER	-	linker	UNP O66529
N	44	SER	-	linker	UNP O66529
N	45	MET	-	linker	UNP O66529
N	46	GLU	-	linker	UNP O66529
N	81	SER	CYS	engineered mutation	UNP O66529
N	129	CYS	ALA	engineered mutation	UNP O66529
O	1	MET	-	initiating methionine	UNP O66529
O	37	GLY	-	linker	UNP O66529
O	38	THR	-	linker	UNP O66529
O	39	GLY	-	linker	UNP O66529
O	40	GLY	-	linker	UNP O66529
O	41	SER	-	linker	UNP O66529
O	42	GLY	-	linker	UNP O66529
O	43	SER	-	linker	UNP O66529
O	44	SER	-	linker	UNP O66529
O	45	MET	-	linker	UNP O66529
O	46	GLU	-	linker	UNP O66529
O	81	SER	CYS	engineered mutation	UNP O66529
O	129	CYS	ALA	engineered mutation	UNP O66529
P	1	MET	-	initiating methionine	UNP O66529
P	37	GLY	-	linker	UNP O66529
P	38	THR	-	linker	UNP O66529
P	39	GLY	-	linker	UNP O66529
P	40	GLY	-	linker	UNP O66529
P	41	SER	-	linker	UNP O66529
P	42	GLY	-	linker	UNP O66529
P	43	SER	-	linker	UNP O66529
P	44	SER	-	linker	UNP O66529
P	45	MET	-	linker	UNP O66529
P	46	GLU	-	linker	UNP O66529
P	81	SER	CYS	engineered mutation	UNP O66529
P	129	CYS	ALA	engineered mutation	UNP O66529
Q	1	MET	-	initiating methionine	UNP O66529
Q	37	GLY	-	linker	UNP O66529
Q	38	THR	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Q	39	GLY	-	linker	UNP O66529
Q	40	GLY	-	linker	UNP O66529
Q	41	SER	-	linker	UNP O66529
Q	42	GLY	-	linker	UNP O66529
Q	43	SER	-	linker	UNP O66529
Q	44	SER	-	linker	UNP O66529
Q	45	MET	-	linker	UNP O66529
Q	46	GLU	-	linker	UNP O66529
Q	81	SER	CYS	engineered mutation	UNP O66529
Q	129	CYS	ALA	engineered mutation	UNP O66529
R	1	MET	-	initiating methionine	UNP O66529
R	37	GLY	-	linker	UNP O66529
R	38	THR	-	linker	UNP O66529
R	39	GLY	-	linker	UNP O66529
R	40	GLY	-	linker	UNP O66529
R	41	SER	-	linker	UNP O66529
R	42	GLY	-	linker	UNP O66529
R	43	SER	-	linker	UNP O66529
R	44	SER	-	linker	UNP O66529
R	45	MET	-	linker	UNP O66529
R	46	GLU	-	linker	UNP O66529
R	81	SER	CYS	engineered mutation	UNP O66529
R	129	CYS	ALA	engineered mutation	UNP O66529
S	1	MET	-	initiating methionine	UNP O66529
S	37	GLY	-	linker	UNP O66529
S	38	THR	-	linker	UNP O66529
S	39	GLY	-	linker	UNP O66529
S	40	GLY	-	linker	UNP O66529
S	41	SER	-	linker	UNP O66529
S	42	GLY	-	linker	UNP O66529
S	43	SER	-	linker	UNP O66529
S	44	SER	-	linker	UNP O66529
S	45	MET	-	linker	UNP O66529
S	46	GLU	-	linker	UNP O66529
S	81	SER	CYS	engineered mutation	UNP O66529
S	129	CYS	ALA	engineered mutation	UNP O66529
T	1	MET	-	initiating methionine	UNP O66529
T	37	GLY	-	linker	UNP O66529
T	38	THR	-	linker	UNP O66529
T	39	GLY	-	linker	UNP O66529
T	40	GLY	-	linker	UNP O66529
T	41	SER	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
T	42	GLY	-	linker	UNP O66529
T	43	SER	-	linker	UNP O66529
T	44	SER	-	linker	UNP O66529
T	45	MET	-	linker	UNP O66529
T	46	GLU	-	linker	UNP O66529
T	81	SER	CYS	engineered mutation	UNP O66529
T	129	CYS	ALA	engineered mutation	UNP O66529
U	1	MET	-	initiating methionine	UNP O66529
U	37	GLY	-	linker	UNP O66529
U	38	THR	-	linker	UNP O66529
U	39	GLY	-	linker	UNP O66529
U	40	GLY	-	linker	UNP O66529
U	41	SER	-	linker	UNP O66529
U	42	GLY	-	linker	UNP O66529
U	43	SER	-	linker	UNP O66529
U	44	SER	-	linker	UNP O66529
U	45	MET	-	linker	UNP O66529
U	46	GLU	-	linker	UNP O66529
U	81	SER	CYS	engineered mutation	UNP O66529
U	129	CYS	ALA	engineered mutation	UNP O66529
V	1	MET	-	initiating methionine	UNP O66529
V	37	GLY	-	linker	UNP O66529
V	38	THR	-	linker	UNP O66529
V	39	GLY	-	linker	UNP O66529
V	40	GLY	-	linker	UNP O66529
V	41	SER	-	linker	UNP O66529
V	42	GLY	-	linker	UNP O66529
V	43	SER	-	linker	UNP O66529
V	44	SER	-	linker	UNP O66529
V	45	MET	-	linker	UNP O66529
V	46	GLU	-	linker	UNP O66529
V	81	SER	CYS	engineered mutation	UNP O66529
V	129	CYS	ALA	engineered mutation	UNP O66529
W	1	MET	-	initiating methionine	UNP O66529
W	37	GLY	-	linker	UNP O66529
W	38	THR	-	linker	UNP O66529
W	39	GLY	-	linker	UNP O66529
W	40	GLY	-	linker	UNP O66529
W	41	SER	-	linker	UNP O66529
W	42	GLY	-	linker	UNP O66529
W	43	SER	-	linker	UNP O66529
W	44	SER	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
W	45	MET	-	linker	UNP O66529
W	46	GLU	-	linker	UNP O66529
W	81	SER	CYS	engineered mutation	UNP O66529
W	129	CYS	ALA	engineered mutation	UNP O66529
X	1	MET	-	initiating methionine	UNP O66529
X	37	GLY	-	linker	UNP O66529
X	38	THR	-	linker	UNP O66529
X	39	GLY	-	linker	UNP O66529
X	40	GLY	-	linker	UNP O66529
X	41	SER	-	linker	UNP O66529
X	42	GLY	-	linker	UNP O66529
X	43	SER	-	linker	UNP O66529
X	44	SER	-	linker	UNP O66529
X	45	MET	-	linker	UNP O66529
X	46	GLU	-	linker	UNP O66529
X	81	SER	CYS	engineered mutation	UNP O66529
X	129	CYS	ALA	engineered mutation	UNP O66529
Y	1	MET	-	initiating methionine	UNP O66529
Y	37	GLY	-	linker	UNP O66529
Y	38	THR	-	linker	UNP O66529
Y	39	GLY	-	linker	UNP O66529
Y	40	GLY	-	linker	UNP O66529
Y	41	SER	-	linker	UNP O66529
Y	42	GLY	-	linker	UNP O66529
Y	43	SER	-	linker	UNP O66529
Y	44	SER	-	linker	UNP O66529
Y	45	MET	-	linker	UNP O66529
Y	46	GLU	-	linker	UNP O66529
Y	81	SER	CYS	engineered mutation	UNP O66529
Y	129	CYS	ALA	engineered mutation	UNP O66529
Z	1	MET	-	initiating methionine	UNP O66529
Z	37	GLY	-	linker	UNP O66529
Z	38	THR	-	linker	UNP O66529
Z	39	GLY	-	linker	UNP O66529
Z	40	GLY	-	linker	UNP O66529
Z	41	SER	-	linker	UNP O66529
Z	42	GLY	-	linker	UNP O66529
Z	43	SER	-	linker	UNP O66529
Z	44	SER	-	linker	UNP O66529
Z	45	MET	-	linker	UNP O66529
Z	46	GLU	-	linker	UNP O66529
Z	81	SER	CYS	engineered mutation	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Z	129	CYS	ALA	engineered mutation	UNP O66529
AA	1	MET	-	initiating methionine	UNP O66529
AA	37	GLY	-	linker	UNP O66529
AA	38	THR	-	linker	UNP O66529
AA	39	GLY	-	linker	UNP O66529
AA	40	GLY	-	linker	UNP O66529
AA	41	SER	-	linker	UNP O66529
AA	42	GLY	-	linker	UNP O66529
AA	43	SER	-	linker	UNP O66529
AA	44	SER	-	linker	UNP O66529
AA	45	MET	-	linker	UNP O66529
AA	46	GLU	-	linker	UNP O66529
AA	81	SER	CYS	engineered mutation	UNP O66529
AA	129	CYS	ALA	engineered mutation	UNP O66529
BA	1	MET	-	initiating methionine	UNP O66529
BA	37	GLY	-	linker	UNP O66529
BA	38	THR	-	linker	UNP O66529
BA	39	GLY	-	linker	UNP O66529
BA	40	GLY	-	linker	UNP O66529
BA	41	SER	-	linker	UNP O66529
BA	42	GLY	-	linker	UNP O66529
BA	43	SER	-	linker	UNP O66529
BA	44	SER	-	linker	UNP O66529
BA	45	MET	-	linker	UNP O66529
BA	46	GLU	-	linker	UNP O66529
BA	81	SER	CYS	engineered mutation	UNP O66529
BA	129	CYS	ALA	engineered mutation	UNP O66529
CA	1	MET	-	initiating methionine	UNP O66529
CA	37	GLY	-	linker	UNP O66529
CA	38	THR	-	linker	UNP O66529
CA	39	GLY	-	linker	UNP O66529
CA	40	GLY	-	linker	UNP O66529
CA	41	SER	-	linker	UNP O66529
CA	42	GLY	-	linker	UNP O66529
CA	43	SER	-	linker	UNP O66529
CA	44	SER	-	linker	UNP O66529
CA	45	MET	-	linker	UNP O66529
CA	46	GLU	-	linker	UNP O66529
CA	81	SER	CYS	engineered mutation	UNP O66529
CA	129	CYS	ALA	engineered mutation	UNP O66529
DA	1	MET	-	initiating methionine	UNP O66529
DA	37	GLY	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DA	38	THR	-	linker	UNP O66529
DA	39	GLY	-	linker	UNP O66529
DA	40	GLY	-	linker	UNP O66529
DA	41	SER	-	linker	UNP O66529
DA	42	GLY	-	linker	UNP O66529
DA	43	SER	-	linker	UNP O66529
DA	44	SER	-	linker	UNP O66529
DA	45	MET	-	linker	UNP O66529
DA	46	GLU	-	linker	UNP O66529
DA	81	SER	CYS	engineered mutation	UNP O66529
DA	129	CYS	ALA	engineered mutation	UNP O66529
EA	1	MET	-	initiating methionine	UNP O66529
EA	37	GLY	-	linker	UNP O66529
EA	38	THR	-	linker	UNP O66529
EA	39	GLY	-	linker	UNP O66529
EA	40	GLY	-	linker	UNP O66529
EA	41	SER	-	linker	UNP O66529
EA	42	GLY	-	linker	UNP O66529
EA	43	SER	-	linker	UNP O66529
EA	44	SER	-	linker	UNP O66529
EA	45	MET	-	linker	UNP O66529
EA	46	GLU	-	linker	UNP O66529
EA	81	SER	CYS	engineered mutation	UNP O66529
EA	129	CYS	ALA	engineered mutation	UNP O66529
FA	1	MET	-	initiating methionine	UNP O66529
FA	37	GLY	-	linker	UNP O66529
FA	38	THR	-	linker	UNP O66529
FA	39	GLY	-	linker	UNP O66529
FA	40	GLY	-	linker	UNP O66529
FA	41	SER	-	linker	UNP O66529
FA	42	GLY	-	linker	UNP O66529
FA	43	SER	-	linker	UNP O66529
FA	44	SER	-	linker	UNP O66529
FA	45	MET	-	linker	UNP O66529
FA	46	GLU	-	linker	UNP O66529
FA	81	SER	CYS	engineered mutation	UNP O66529
FA	129	CYS	ALA	engineered mutation	UNP O66529
GA	1	MET	-	initiating methionine	UNP O66529
GA	37	GLY	-	linker	UNP O66529
GA	38	THR	-	linker	UNP O66529
GA	39	GLY	-	linker	UNP O66529
GA	40	GLY	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
GA	41	SER	-	linker	UNP O66529
GA	42	GLY	-	linker	UNP O66529
GA	43	SER	-	linker	UNP O66529
GA	44	SER	-	linker	UNP O66529
GA	45	MET	-	linker	UNP O66529
GA	46	GLU	-	linker	UNP O66529
GA	81	SER	CYS	engineered mutation	UNP O66529
GA	129	CYS	ALA	engineered mutation	UNP O66529
HA	1	MET	-	initiating methionine	UNP O66529
HA	37	GLY	-	linker	UNP O66529
HA	38	THR	-	linker	UNP O66529
HA	39	GLY	-	linker	UNP O66529
HA	40	GLY	-	linker	UNP O66529
HA	41	SER	-	linker	UNP O66529
HA	42	GLY	-	linker	UNP O66529
HA	43	SER	-	linker	UNP O66529
HA	44	SER	-	linker	UNP O66529
HA	45	MET	-	linker	UNP O66529
HA	46	GLU	-	linker	UNP O66529
HA	81	SER	CYS	engineered mutation	UNP O66529
HA	129	CYS	ALA	engineered mutation	UNP O66529
IA	1	MET	-	initiating methionine	UNP O66529
IA	37	GLY	-	linker	UNP O66529
IA	38	THR	-	linker	UNP O66529
IA	39	GLY	-	linker	UNP O66529
IA	40	GLY	-	linker	UNP O66529
IA	41	SER	-	linker	UNP O66529
IA	42	GLY	-	linker	UNP O66529
IA	43	SER	-	linker	UNP O66529
IA	44	SER	-	linker	UNP O66529
IA	45	MET	-	linker	UNP O66529
IA	46	GLU	-	linker	UNP O66529
IA	81	SER	CYS	engineered mutation	UNP O66529
IA	129	CYS	ALA	engineered mutation	UNP O66529
JA	1	MET	-	initiating methionine	UNP O66529
JA	37	GLY	-	linker	UNP O66529
JA	38	THR	-	linker	UNP O66529
JA	39	GLY	-	linker	UNP O66529
JA	40	GLY	-	linker	UNP O66529
JA	41	SER	-	linker	UNP O66529
JA	42	GLY	-	linker	UNP O66529
JA	43	SER	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JA	44	SER	-	linker	UNP O66529
JA	45	MET	-	linker	UNP O66529
JA	46	GLU	-	linker	UNP O66529
JA	81	SER	CYS	engineered mutation	UNP O66529
JA	129	CYS	ALA	engineered mutation	UNP O66529
KA	1	MET	-	initiating methionine	UNP O66529
KA	37	GLY	-	linker	UNP O66529
KA	38	THR	-	linker	UNP O66529
KA	39	GLY	-	linker	UNP O66529
KA	40	GLY	-	linker	UNP O66529
KA	41	SER	-	linker	UNP O66529
KA	42	GLY	-	linker	UNP O66529
KA	43	SER	-	linker	UNP O66529
KA	44	SER	-	linker	UNP O66529
KA	45	MET	-	linker	UNP O66529
KA	46	GLU	-	linker	UNP O66529
KA	81	SER	CYS	engineered mutation	UNP O66529
KA	129	CYS	ALA	engineered mutation	UNP O66529
LA	1	MET	-	initiating methionine	UNP O66529
LA	37	GLY	-	linker	UNP O66529
LA	38	THR	-	linker	UNP O66529
LA	39	GLY	-	linker	UNP O66529
LA	40	GLY	-	linker	UNP O66529
LA	41	SER	-	linker	UNP O66529
LA	42	GLY	-	linker	UNP O66529
LA	43	SER	-	linker	UNP O66529
LA	44	SER	-	linker	UNP O66529
LA	45	MET	-	linker	UNP O66529
LA	46	GLU	-	linker	UNP O66529
LA	81	SER	CYS	engineered mutation	UNP O66529
LA	129	CYS	ALA	engineered mutation	UNP O66529
MA	1	MET	-	initiating methionine	UNP O66529
MA	37	GLY	-	linker	UNP O66529
MA	38	THR	-	linker	UNP O66529
MA	39	GLY	-	linker	UNP O66529
MA	40	GLY	-	linker	UNP O66529
MA	41	SER	-	linker	UNP O66529
MA	42	GLY	-	linker	UNP O66529
MA	43	SER	-	linker	UNP O66529
MA	44	SER	-	linker	UNP O66529
MA	45	MET	-	linker	UNP O66529
MA	46	GLU	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
MA	81	SER	CYS	engineered mutation	UNP O66529
MA	129	CYS	ALA	engineered mutation	UNP O66529
NA	1	MET	-	initiating methionine	UNP O66529
NA	37	GLY	-	linker	UNP O66529
NA	38	THR	-	linker	UNP O66529
NA	39	GLY	-	linker	UNP O66529
NA	40	GLY	-	linker	UNP O66529
NA	41	SER	-	linker	UNP O66529
NA	42	GLY	-	linker	UNP O66529
NA	43	SER	-	linker	UNP O66529
NA	44	SER	-	linker	UNP O66529
NA	45	MET	-	linker	UNP O66529
NA	46	GLU	-	linker	UNP O66529
NA	81	SER	CYS	engineered mutation	UNP O66529
NA	129	CYS	ALA	engineered mutation	UNP O66529
OA	1	MET	-	initiating methionine	UNP O66529
OA	37	GLY	-	linker	UNP O66529
OA	38	THR	-	linker	UNP O66529
OA	39	GLY	-	linker	UNP O66529
OA	40	GLY	-	linker	UNP O66529
OA	41	SER	-	linker	UNP O66529
OA	42	GLY	-	linker	UNP O66529
OA	43	SER	-	linker	UNP O66529
OA	44	SER	-	linker	UNP O66529
OA	45	MET	-	linker	UNP O66529
OA	46	GLU	-	linker	UNP O66529
OA	81	SER	CYS	engineered mutation	UNP O66529
OA	129	CYS	ALA	engineered mutation	UNP O66529
PA	1	MET	-	initiating methionine	UNP O66529
PA	37	GLY	-	linker	UNP O66529
PA	38	THR	-	linker	UNP O66529
PA	39	GLY	-	linker	UNP O66529
PA	40	GLY	-	linker	UNP O66529
PA	41	SER	-	linker	UNP O66529
PA	42	GLY	-	linker	UNP O66529
PA	43	SER	-	linker	UNP O66529
PA	44	SER	-	linker	UNP O66529
PA	45	MET	-	linker	UNP O66529
PA	46	GLU	-	linker	UNP O66529
PA	81	SER	CYS	engineered mutation	UNP O66529
PA	129	CYS	ALA	engineered mutation	UNP O66529
QA	1	MET	-	initiating methionine	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
QA	37	GLY	-	linker	UNP O66529
QA	38	THR	-	linker	UNP O66529
QA	39	GLY	-	linker	UNP O66529
QA	40	GLY	-	linker	UNP O66529
QA	41	SER	-	linker	UNP O66529
QA	42	GLY	-	linker	UNP O66529
QA	43	SER	-	linker	UNP O66529
QA	44	SER	-	linker	UNP O66529
QA	45	MET	-	linker	UNP O66529
QA	46	GLU	-	linker	UNP O66529
QA	81	SER	CYS	engineered mutation	UNP O66529
QA	129	CYS	ALA	engineered mutation	UNP O66529
RA	1	MET	-	initiating methionine	UNP O66529
RA	37	GLY	-	linker	UNP O66529
RA	38	THR	-	linker	UNP O66529
RA	39	GLY	-	linker	UNP O66529
RA	40	GLY	-	linker	UNP O66529
RA	41	SER	-	linker	UNP O66529
RA	42	GLY	-	linker	UNP O66529
RA	43	SER	-	linker	UNP O66529
RA	44	SER	-	linker	UNP O66529
RA	45	MET	-	linker	UNP O66529
RA	46	GLU	-	linker	UNP O66529
RA	81	SER	CYS	engineered mutation	UNP O66529
RA	129	CYS	ALA	engineered mutation	UNP O66529
SA	1	MET	-	initiating methionine	UNP O66529
SA	37	GLY	-	linker	UNP O66529
SA	38	THR	-	linker	UNP O66529
SA	39	GLY	-	linker	UNP O66529
SA	40	GLY	-	linker	UNP O66529
SA	41	SER	-	linker	UNP O66529
SA	42	GLY	-	linker	UNP O66529
SA	43	SER	-	linker	UNP O66529
SA	44	SER	-	linker	UNP O66529
SA	45	MET	-	linker	UNP O66529
SA	46	GLU	-	linker	UNP O66529
SA	81	SER	CYS	engineered mutation	UNP O66529
SA	129	CYS	ALA	engineered mutation	UNP O66529
TA	1	MET	-	initiating methionine	UNP O66529
TA	37	GLY	-	linker	UNP O66529
TA	38	THR	-	linker	UNP O66529
TA	39	GLY	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
TA	40	GLY	-	linker	UNP O66529
TA	41	SER	-	linker	UNP O66529
TA	42	GLY	-	linker	UNP O66529
TA	43	SER	-	linker	UNP O66529
TA	44	SER	-	linker	UNP O66529
TA	45	MET	-	linker	UNP O66529
TA	46	GLU	-	linker	UNP O66529
TA	81	SER	CYS	engineered mutation	UNP O66529
TA	129	CYS	ALA	engineered mutation	UNP O66529
UA	1	MET	-	initiating methionine	UNP O66529
UA	37	GLY	-	linker	UNP O66529
UA	38	THR	-	linker	UNP O66529
UA	39	GLY	-	linker	UNP O66529
UA	40	GLY	-	linker	UNP O66529
UA	41	SER	-	linker	UNP O66529
UA	42	GLY	-	linker	UNP O66529
UA	43	SER	-	linker	UNP O66529
UA	44	SER	-	linker	UNP O66529
UA	45	MET	-	linker	UNP O66529
UA	46	GLU	-	linker	UNP O66529
UA	81	SER	CYS	engineered mutation	UNP O66529
UA	129	CYS	ALA	engineered mutation	UNP O66529
VA	1	MET	-	initiating methionine	UNP O66529
VA	37	GLY	-	linker	UNP O66529
VA	38	THR	-	linker	UNP O66529
VA	39	GLY	-	linker	UNP O66529
VA	40	GLY	-	linker	UNP O66529
VA	41	SER	-	linker	UNP O66529
VA	42	GLY	-	linker	UNP O66529
VA	43	SER	-	linker	UNP O66529
VA	44	SER	-	linker	UNP O66529
VA	45	MET	-	linker	UNP O66529
VA	46	GLU	-	linker	UNP O66529
VA	81	SER	CYS	engineered mutation	UNP O66529
VA	129	CYS	ALA	engineered mutation	UNP O66529
WA	1	MET	-	initiating methionine	UNP O66529
WA	37	GLY	-	linker	UNP O66529
WA	38	THR	-	linker	UNP O66529
WA	39	GLY	-	linker	UNP O66529
WA	40	GLY	-	linker	UNP O66529
WA	41	SER	-	linker	UNP O66529
WA	42	GLY	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
WA	43	SER	-	linker	UNP O66529
WA	44	SER	-	linker	UNP O66529
WA	45	MET	-	linker	UNP O66529
WA	46	GLU	-	linker	UNP O66529
WA	81	SER	CYS	engineered mutation	UNP O66529
WA	129	CYS	ALA	engineered mutation	UNP O66529
XA	1	MET	-	initiating methionine	UNP O66529
XA	37	GLY	-	linker	UNP O66529
XA	38	THR	-	linker	UNP O66529
XA	39	GLY	-	linker	UNP O66529
XA	40	GLY	-	linker	UNP O66529
XA	41	SER	-	linker	UNP O66529
XA	42	GLY	-	linker	UNP O66529
XA	43	SER	-	linker	UNP O66529
XA	44	SER	-	linker	UNP O66529
XA	45	MET	-	linker	UNP O66529
XA	46	GLU	-	linker	UNP O66529
XA	81	SER	CYS	engineered mutation	UNP O66529
XA	129	CYS	ALA	engineered mutation	UNP O66529
YA	1	MET	-	initiating methionine	UNP O66529
YA	37	GLY	-	linker	UNP O66529
YA	38	THR	-	linker	UNP O66529
YA	39	GLY	-	linker	UNP O66529
YA	40	GLY	-	linker	UNP O66529
YA	41	SER	-	linker	UNP O66529
YA	42	GLY	-	linker	UNP O66529
YA	43	SER	-	linker	UNP O66529
YA	44	SER	-	linker	UNP O66529
YA	45	MET	-	linker	UNP O66529
YA	46	GLU	-	linker	UNP O66529
YA	81	SER	CYS	engineered mutation	UNP O66529
YA	129	CYS	ALA	engineered mutation	UNP O66529
ZA	1	MET	-	initiating methionine	UNP O66529
ZA	37	GLY	-	linker	UNP O66529
ZA	38	THR	-	linker	UNP O66529
ZA	39	GLY	-	linker	UNP O66529
ZA	40	GLY	-	linker	UNP O66529
ZA	41	SER	-	linker	UNP O66529
ZA	42	GLY	-	linker	UNP O66529
ZA	43	SER	-	linker	UNP O66529
ZA	44	SER	-	linker	UNP O66529
ZA	45	MET	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZA	46	GLU	-	linker	UNP O66529
ZA	81	SER	CYS	engineered mutation	UNP O66529
ZA	129	CYS	ALA	engineered mutation	UNP O66529
AB	1	MET	-	initiating methionine	UNP O66529
AB	37	GLY	-	linker	UNP O66529
AB	38	THR	-	linker	UNP O66529
AB	39	GLY	-	linker	UNP O66529
AB	40	GLY	-	linker	UNP O66529
AB	41	SER	-	linker	UNP O66529
AB	42	GLY	-	linker	UNP O66529
AB	43	SER	-	linker	UNP O66529
AB	44	SER	-	linker	UNP O66529
AB	45	MET	-	linker	UNP O66529
AB	46	GLU	-	linker	UNP O66529
AB	81	SER	CYS	engineered mutation	UNP O66529
AB	129	CYS	ALA	engineered mutation	UNP O66529
BB	1	MET	-	initiating methionine	UNP O66529
BB	37	GLY	-	linker	UNP O66529
BB	38	THR	-	linker	UNP O66529
BB	39	GLY	-	linker	UNP O66529
BB	40	GLY	-	linker	UNP O66529
BB	41	SER	-	linker	UNP O66529
BB	42	GLY	-	linker	UNP O66529
BB	43	SER	-	linker	UNP O66529
BB	44	SER	-	linker	UNP O66529
BB	45	MET	-	linker	UNP O66529
BB	46	GLU	-	linker	UNP O66529
BB	81	SER	CYS	engineered mutation	UNP O66529
BB	129	CYS	ALA	engineered mutation	UNP O66529
CB	1	MET	-	initiating methionine	UNP O66529
CB	37	GLY	-	linker	UNP O66529
CB	38	THR	-	linker	UNP O66529
CB	39	GLY	-	linker	UNP O66529
CB	40	GLY	-	linker	UNP O66529
CB	41	SER	-	linker	UNP O66529
CB	42	GLY	-	linker	UNP O66529
CB	43	SER	-	linker	UNP O66529
CB	44	SER	-	linker	UNP O66529
CB	45	MET	-	linker	UNP O66529
CB	46	GLU	-	linker	UNP O66529
CB	81	SER	CYS	engineered mutation	UNP O66529
CB	129	CYS	ALA	engineered mutation	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DB	1	MET	-	initiating methionine	UNP O66529
DB	37	GLY	-	linker	UNP O66529
DB	38	THR	-	linker	UNP O66529
DB	39	GLY	-	linker	UNP O66529
DB	40	GLY	-	linker	UNP O66529
DB	41	SER	-	linker	UNP O66529
DB	42	GLY	-	linker	UNP O66529
DB	43	SER	-	linker	UNP O66529
DB	44	SER	-	linker	UNP O66529
DB	45	MET	-	linker	UNP O66529
DB	46	GLU	-	linker	UNP O66529
DB	81	SER	CYS	engineered mutation	UNP O66529
DB	129	CYS	ALA	engineered mutation	UNP O66529
EB	1	MET	-	initiating methionine	UNP O66529
EB	37	GLY	-	linker	UNP O66529
EB	38	THR	-	linker	UNP O66529
EB	39	GLY	-	linker	UNP O66529
EB	40	GLY	-	linker	UNP O66529
EB	41	SER	-	linker	UNP O66529
EB	42	GLY	-	linker	UNP O66529
EB	43	SER	-	linker	UNP O66529
EB	44	SER	-	linker	UNP O66529
EB	45	MET	-	linker	UNP O66529
EB	46	GLU	-	linker	UNP O66529
EB	81	SER	CYS	engineered mutation	UNP O66529
EB	129	CYS	ALA	engineered mutation	UNP O66529
FB	1	MET	-	initiating methionine	UNP O66529
FB	37	GLY	-	linker	UNP O66529
FB	38	THR	-	linker	UNP O66529
FB	39	GLY	-	linker	UNP O66529
FB	40	GLY	-	linker	UNP O66529
FB	41	SER	-	linker	UNP O66529
FB	42	GLY	-	linker	UNP O66529
FB	43	SER	-	linker	UNP O66529
FB	44	SER	-	linker	UNP O66529
FB	45	MET	-	linker	UNP O66529
FB	46	GLU	-	linker	UNP O66529
FB	81	SER	CYS	engineered mutation	UNP O66529
FB	129	CYS	ALA	engineered mutation	UNP O66529
GB	1	MET	-	initiating methionine	UNP O66529
GB	37	GLY	-	linker	UNP O66529
GB	38	THR	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
GB	39	GLY	-	linker	UNP O66529
GB	40	GLY	-	linker	UNP O66529
GB	41	SER	-	linker	UNP O66529
GB	42	GLY	-	linker	UNP O66529
GB	43	SER	-	linker	UNP O66529
GB	44	SER	-	linker	UNP O66529
GB	45	MET	-	linker	UNP O66529
GB	46	GLU	-	linker	UNP O66529
GB	81	SER	CYS	engineered mutation	UNP O66529
GB	129	CYS	ALA	engineered mutation	UNP O66529
HB	1	MET	-	initiating methionine	UNP O66529
HB	37	GLY	-	linker	UNP O66529
HB	38	THR	-	linker	UNP O66529
HB	39	GLY	-	linker	UNP O66529
HB	40	GLY	-	linker	UNP O66529
HB	41	SER	-	linker	UNP O66529
HB	42	GLY	-	linker	UNP O66529
HB	43	SER	-	linker	UNP O66529
HB	44	SER	-	linker	UNP O66529
HB	45	MET	-	linker	UNP O66529
HB	46	GLU	-	linker	UNP O66529
HB	81	SER	CYS	engineered mutation	UNP O66529
HB	129	CYS	ALA	engineered mutation	UNP O66529
IB	1	MET	-	initiating methionine	UNP O66529
IB	37	GLY	-	linker	UNP O66529
IB	38	THR	-	linker	UNP O66529
IB	39	GLY	-	linker	UNP O66529
IB	40	GLY	-	linker	UNP O66529
IB	41	SER	-	linker	UNP O66529
IB	42	GLY	-	linker	UNP O66529
IB	43	SER	-	linker	UNP O66529
IB	44	SER	-	linker	UNP O66529
IB	45	MET	-	linker	UNP O66529
IB	46	GLU	-	linker	UNP O66529
IB	81	SER	CYS	engineered mutation	UNP O66529
IB	129	CYS	ALA	engineered mutation	UNP O66529
JB	1	MET	-	initiating methionine	UNP O66529
JB	37	GLY	-	linker	UNP O66529
JB	38	THR	-	linker	UNP O66529
JB	39	GLY	-	linker	UNP O66529
JB	40	GLY	-	linker	UNP O66529
JB	41	SER	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JB	42	GLY	-	linker	UNP O66529
JB	43	SER	-	linker	UNP O66529
JB	44	SER	-	linker	UNP O66529
JB	45	MET	-	linker	UNP O66529
JB	46	GLU	-	linker	UNP O66529
JB	81	SER	CYS	engineered mutation	UNP O66529
JB	129	CYS	ALA	engineered mutation	UNP O66529
KB	1	MET	-	initiating methionine	UNP O66529
KB	37	GLY	-	linker	UNP O66529
KB	38	THR	-	linker	UNP O66529
KB	39	GLY	-	linker	UNP O66529
KB	40	GLY	-	linker	UNP O66529
KB	41	SER	-	linker	UNP O66529
KB	42	GLY	-	linker	UNP O66529
KB	43	SER	-	linker	UNP O66529
KB	44	SER	-	linker	UNP O66529
KB	45	MET	-	linker	UNP O66529
KB	46	GLU	-	linker	UNP O66529
KB	81	SER	CYS	engineered mutation	UNP O66529
KB	129	CYS	ALA	engineered mutation	UNP O66529
LB	1	MET	-	initiating methionine	UNP O66529
LB	37	GLY	-	linker	UNP O66529
LB	38	THR	-	linker	UNP O66529
LB	39	GLY	-	linker	UNP O66529
LB	40	GLY	-	linker	UNP O66529
LB	41	SER	-	linker	UNP O66529
LB	42	GLY	-	linker	UNP O66529
LB	43	SER	-	linker	UNP O66529
LB	44	SER	-	linker	UNP O66529
LB	45	MET	-	linker	UNP O66529
LB	46	GLU	-	linker	UNP O66529
LB	81	SER	CYS	engineered mutation	UNP O66529
LB	129	CYS	ALA	engineered mutation	UNP O66529
MB	1	MET	-	initiating methionine	UNP O66529
MB	37	GLY	-	linker	UNP O66529
MB	38	THR	-	linker	UNP O66529
MB	39	GLY	-	linker	UNP O66529
MB	40	GLY	-	linker	UNP O66529
MB	41	SER	-	linker	UNP O66529
MB	42	GLY	-	linker	UNP O66529
MB	43	SER	-	linker	UNP O66529
MB	44	SER	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
MB	45	MET	-	linker	UNP O66529
MB	46	GLU	-	linker	UNP O66529
MB	81	SER	CYS	engineered mutation	UNP O66529
MB	129	CYS	ALA	engineered mutation	UNP O66529
NB	1	MET	-	initiating methionine	UNP O66529
NB	37	GLY	-	linker	UNP O66529
NB	38	THR	-	linker	UNP O66529
NB	39	GLY	-	linker	UNP O66529
NB	40	GLY	-	linker	UNP O66529
NB	41	SER	-	linker	UNP O66529
NB	42	GLY	-	linker	UNP O66529
NB	43	SER	-	linker	UNP O66529
NB	44	SER	-	linker	UNP O66529
NB	45	MET	-	linker	UNP O66529
NB	46	GLU	-	linker	UNP O66529
NB	81	SER	CYS	engineered mutation	UNP O66529
NB	129	CYS	ALA	engineered mutation	UNP O66529
OB	1	MET	-	initiating methionine	UNP O66529
OB	37	GLY	-	linker	UNP O66529
OB	38	THR	-	linker	UNP O66529
OB	39	GLY	-	linker	UNP O66529
OB	40	GLY	-	linker	UNP O66529
OB	41	SER	-	linker	UNP O66529
OB	42	GLY	-	linker	UNP O66529
OB	43	SER	-	linker	UNP O66529
OB	44	SER	-	linker	UNP O66529
OB	45	MET	-	linker	UNP O66529
OB	46	GLU	-	linker	UNP O66529
OB	81	SER	CYS	engineered mutation	UNP O66529
OB	129	CYS	ALA	engineered mutation	UNP O66529
PB	1	MET	-	initiating methionine	UNP O66529
PB	37	GLY	-	linker	UNP O66529
PB	38	THR	-	linker	UNP O66529
PB	39	GLY	-	linker	UNP O66529
PB	40	GLY	-	linker	UNP O66529
PB	41	SER	-	linker	UNP O66529
PB	42	GLY	-	linker	UNP O66529
PB	43	SER	-	linker	UNP O66529
PB	44	SER	-	linker	UNP O66529
PB	45	MET	-	linker	UNP O66529
PB	46	GLU	-	linker	UNP O66529
PB	81	SER	CYS	engineered mutation	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
PB	129	CYS	ALA	engineered mutation	UNP O66529
QB	1	MET	-	initiating methionine	UNP O66529
QB	37	GLY	-	linker	UNP O66529
QB	38	THR	-	linker	UNP O66529
QB	39	GLY	-	linker	UNP O66529
QB	40	GLY	-	linker	UNP O66529
QB	41	SER	-	linker	UNP O66529
QB	42	GLY	-	linker	UNP O66529
QB	43	SER	-	linker	UNP O66529
QB	44	SER	-	linker	UNP O66529
QB	45	MET	-	linker	UNP O66529
QB	46	GLU	-	linker	UNP O66529
QB	81	SER	CYS	engineered mutation	UNP O66529
QB	129	CYS	ALA	engineered mutation	UNP O66529
RB	1	MET	-	initiating methionine	UNP O66529
RB	37	GLY	-	linker	UNP O66529
RB	38	THR	-	linker	UNP O66529
RB	39	GLY	-	linker	UNP O66529
RB	40	GLY	-	linker	UNP O66529
RB	41	SER	-	linker	UNP O66529
RB	42	GLY	-	linker	UNP O66529
RB	43	SER	-	linker	UNP O66529
RB	44	SER	-	linker	UNP O66529
RB	45	MET	-	linker	UNP O66529
RB	46	GLU	-	linker	UNP O66529
RB	81	SER	CYS	engineered mutation	UNP O66529
RB	129	CYS	ALA	engineered mutation	UNP O66529
SB	1	MET	-	initiating methionine	UNP O66529
SB	37	GLY	-	linker	UNP O66529
SB	38	THR	-	linker	UNP O66529
SB	39	GLY	-	linker	UNP O66529
SB	40	GLY	-	linker	UNP O66529
SB	41	SER	-	linker	UNP O66529
SB	42	GLY	-	linker	UNP O66529
SB	43	SER	-	linker	UNP O66529
SB	44	SER	-	linker	UNP O66529
SB	45	MET	-	linker	UNP O66529
SB	46	GLU	-	linker	UNP O66529
SB	81	SER	CYS	engineered mutation	UNP O66529
SB	129	CYS	ALA	engineered mutation	UNP O66529
TB	1	MET	-	initiating methionine	UNP O66529
TB	37	GLY	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
TB	38	THR	-	linker	UNP O66529
TB	39	GLY	-	linker	UNP O66529
TB	40	GLY	-	linker	UNP O66529
TB	41	SER	-	linker	UNP O66529
TB	42	GLY	-	linker	UNP O66529
TB	43	SER	-	linker	UNP O66529
TB	44	SER	-	linker	UNP O66529
TB	45	MET	-	linker	UNP O66529
TB	46	GLU	-	linker	UNP O66529
TB	81	SER	CYS	engineered mutation	UNP O66529
TB	129	CYS	ALA	engineered mutation	UNP O66529
UB	1	MET	-	initiating methionine	UNP O66529
UB	37	GLY	-	linker	UNP O66529
UB	38	THR	-	linker	UNP O66529
UB	39	GLY	-	linker	UNP O66529
UB	40	GLY	-	linker	UNP O66529
UB	41	SER	-	linker	UNP O66529
UB	42	GLY	-	linker	UNP O66529
UB	43	SER	-	linker	UNP O66529
UB	44	SER	-	linker	UNP O66529
UB	45	MET	-	linker	UNP O66529
UB	46	GLU	-	linker	UNP O66529
UB	81	SER	CYS	engineered mutation	UNP O66529
UB	129	CYS	ALA	engineered mutation	UNP O66529
VB	1	MET	-	initiating methionine	UNP O66529
VB	37	GLY	-	linker	UNP O66529
VB	38	THR	-	linker	UNP O66529
VB	39	GLY	-	linker	UNP O66529
VB	40	GLY	-	linker	UNP O66529
VB	41	SER	-	linker	UNP O66529
VB	42	GLY	-	linker	UNP O66529
VB	43	SER	-	linker	UNP O66529
VB	44	SER	-	linker	UNP O66529
VB	45	MET	-	linker	UNP O66529
VB	46	GLU	-	linker	UNP O66529
VB	81	SER	CYS	engineered mutation	UNP O66529
VB	129	CYS	ALA	engineered mutation	UNP O66529
WB	1	MET	-	initiating methionine	UNP O66529
WB	37	GLY	-	linker	UNP O66529
WB	38	THR	-	linker	UNP O66529
WB	39	GLY	-	linker	UNP O66529
WB	40	GLY	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
WB	41	SER	-	linker	UNP O66529
WB	42	GLY	-	linker	UNP O66529
WB	43	SER	-	linker	UNP O66529
WB	44	SER	-	linker	UNP O66529
WB	45	MET	-	linker	UNP O66529
WB	46	GLU	-	linker	UNP O66529
WB	81	SER	CYS	engineered mutation	UNP O66529
WB	129	CYS	ALA	engineered mutation	UNP O66529
XB	1	MET	-	initiating methionine	UNP O66529
XB	37	GLY	-	linker	UNP O66529
XB	38	THR	-	linker	UNP O66529
XB	39	GLY	-	linker	UNP O66529
XB	40	GLY	-	linker	UNP O66529
XB	41	SER	-	linker	UNP O66529
XB	42	GLY	-	linker	UNP O66529
XB	43	SER	-	linker	UNP O66529
XB	44	SER	-	linker	UNP O66529
XB	45	MET	-	linker	UNP O66529
XB	46	GLU	-	linker	UNP O66529
XB	81	SER	CYS	engineered mutation	UNP O66529
XB	129	CYS	ALA	engineered mutation	UNP O66529
YB	1	MET	-	initiating methionine	UNP O66529
YB	37	GLY	-	linker	UNP O66529
YB	38	THR	-	linker	UNP O66529
YB	39	GLY	-	linker	UNP O66529
YB	40	GLY	-	linker	UNP O66529
YB	41	SER	-	linker	UNP O66529
YB	42	GLY	-	linker	UNP O66529
YB	43	SER	-	linker	UNP O66529
YB	44	SER	-	linker	UNP O66529
YB	45	MET	-	linker	UNP O66529
YB	46	GLU	-	linker	UNP O66529
YB	81	SER	CYS	engineered mutation	UNP O66529
YB	129	CYS	ALA	engineered mutation	UNP O66529
ZB	1	MET	-	initiating methionine	UNP O66529
ZB	37	GLY	-	linker	UNP O66529
ZB	38	THR	-	linker	UNP O66529
ZB	39	GLY	-	linker	UNP O66529
ZB	40	GLY	-	linker	UNP O66529
ZB	41	SER	-	linker	UNP O66529
ZB	42	GLY	-	linker	UNP O66529
ZB	43	SER	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZB	44	SER	-	linker	UNP O66529
ZB	45	MET	-	linker	UNP O66529
ZB	46	GLU	-	linker	UNP O66529
ZB	81	SER	CYS	engineered mutation	UNP O66529
ZB	129	CYS	ALA	engineered mutation	UNP O66529
AC	1	MET	-	initiating methionine	UNP O66529
AC	37	GLY	-	linker	UNP O66529
AC	38	THR	-	linker	UNP O66529
AC	39	GLY	-	linker	UNP O66529
AC	40	GLY	-	linker	UNP O66529
AC	41	SER	-	linker	UNP O66529
AC	42	GLY	-	linker	UNP O66529
AC	43	SER	-	linker	UNP O66529
AC	44	SER	-	linker	UNP O66529
AC	45	MET	-	linker	UNP O66529
AC	46	GLU	-	linker	UNP O66529
AC	81	SER	CYS	engineered mutation	UNP O66529
AC	129	CYS	ALA	engineered mutation	UNP O66529
BC	1	MET	-	initiating methionine	UNP O66529
BC	37	GLY	-	linker	UNP O66529
BC	38	THR	-	linker	UNP O66529
BC	39	GLY	-	linker	UNP O66529
BC	40	GLY	-	linker	UNP O66529
BC	41	SER	-	linker	UNP O66529
BC	42	GLY	-	linker	UNP O66529
BC	43	SER	-	linker	UNP O66529
BC	44	SER	-	linker	UNP O66529
BC	45	MET	-	linker	UNP O66529
BC	46	GLU	-	linker	UNP O66529
BC	81	SER	CYS	engineered mutation	UNP O66529
BC	129	CYS	ALA	engineered mutation	UNP O66529
CC	1	MET	-	initiating methionine	UNP O66529
CC	37	GLY	-	linker	UNP O66529
CC	38	THR	-	linker	UNP O66529
CC	39	GLY	-	linker	UNP O66529
CC	40	GLY	-	linker	UNP O66529
CC	41	SER	-	linker	UNP O66529
CC	42	GLY	-	linker	UNP O66529
CC	43	SER	-	linker	UNP O66529
CC	44	SER	-	linker	UNP O66529
CC	45	MET	-	linker	UNP O66529
CC	46	GLU	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CC	81	SER	CYS	engineered mutation	UNP O66529
CC	129	CYS	ALA	engineered mutation	UNP O66529
DC	1	MET	-	initiating methionine	UNP O66529
DC	37	GLY	-	linker	UNP O66529
DC	38	THR	-	linker	UNP O66529
DC	39	GLY	-	linker	UNP O66529
DC	40	GLY	-	linker	UNP O66529
DC	41	SER	-	linker	UNP O66529
DC	42	GLY	-	linker	UNP O66529
DC	43	SER	-	linker	UNP O66529
DC	44	SER	-	linker	UNP O66529
DC	45	MET	-	linker	UNP O66529
DC	46	GLU	-	linker	UNP O66529
DC	81	SER	CYS	engineered mutation	UNP O66529
DC	129	CYS	ALA	engineered mutation	UNP O66529
EC	1	MET	-	initiating methionine	UNP O66529
EC	37	GLY	-	linker	UNP O66529
EC	38	THR	-	linker	UNP O66529
EC	39	GLY	-	linker	UNP O66529
EC	40	GLY	-	linker	UNP O66529
EC	41	SER	-	linker	UNP O66529
EC	42	GLY	-	linker	UNP O66529
EC	43	SER	-	linker	UNP O66529
EC	44	SER	-	linker	UNP O66529
EC	45	MET	-	linker	UNP O66529
EC	46	GLU	-	linker	UNP O66529
EC	81	SER	CYS	engineered mutation	UNP O66529
EC	129	CYS	ALA	engineered mutation	UNP O66529
FC	1	MET	-	initiating methionine	UNP O66529
FC	37	GLY	-	linker	UNP O66529
FC	38	THR	-	linker	UNP O66529
FC	39	GLY	-	linker	UNP O66529
FC	40	GLY	-	linker	UNP O66529
FC	41	SER	-	linker	UNP O66529
FC	42	GLY	-	linker	UNP O66529
FC	43	SER	-	linker	UNP O66529
FC	44	SER	-	linker	UNP O66529
FC	45	MET	-	linker	UNP O66529
FC	46	GLU	-	linker	UNP O66529
FC	81	SER	CYS	engineered mutation	UNP O66529
FC	129	CYS	ALA	engineered mutation	UNP O66529
GC	1	MET	-	initiating methionine	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
GC	37	GLY	-	linker	UNP O66529
GC	38	THR	-	linker	UNP O66529
GC	39	GLY	-	linker	UNP O66529
GC	40	GLY	-	linker	UNP O66529
GC	41	SER	-	linker	UNP O66529
GC	42	GLY	-	linker	UNP O66529
GC	43	SER	-	linker	UNP O66529
GC	44	SER	-	linker	UNP O66529
GC	45	MET	-	linker	UNP O66529
GC	46	GLU	-	linker	UNP O66529
GC	81	SER	CYS	engineered mutation	UNP O66529
GC	129	CYS	ALA	engineered mutation	UNP O66529
HC	1	MET	-	initiating methionine	UNP O66529
HC	37	GLY	-	linker	UNP O66529
HC	38	THR	-	linker	UNP O66529
HC	39	GLY	-	linker	UNP O66529
HC	40	GLY	-	linker	UNP O66529
HC	41	SER	-	linker	UNP O66529
HC	42	GLY	-	linker	UNP O66529
HC	43	SER	-	linker	UNP O66529
HC	44	SER	-	linker	UNP O66529
HC	45	MET	-	linker	UNP O66529
HC	46	GLU	-	linker	UNP O66529
HC	81	SER	CYS	engineered mutation	UNP O66529
HC	129	CYS	ALA	engineered mutation	UNP O66529
IC	1	MET	-	initiating methionine	UNP O66529
IC	37	GLY	-	linker	UNP O66529
IC	38	THR	-	linker	UNP O66529
IC	39	GLY	-	linker	UNP O66529
IC	40	GLY	-	linker	UNP O66529
IC	41	SER	-	linker	UNP O66529
IC	42	GLY	-	linker	UNP O66529
IC	43	SER	-	linker	UNP O66529
IC	44	SER	-	linker	UNP O66529
IC	45	MET	-	linker	UNP O66529
IC	46	GLU	-	linker	UNP O66529
IC	81	SER	CYS	engineered mutation	UNP O66529
IC	129	CYS	ALA	engineered mutation	UNP O66529
JC	1	MET	-	initiating methionine	UNP O66529
JC	37	GLY	-	linker	UNP O66529
JC	38	THR	-	linker	UNP O66529
JC	39	GLY	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JC	40	GLY	-	linker	UNP O66529
JC	41	SER	-	linker	UNP O66529
JC	42	GLY	-	linker	UNP O66529
JC	43	SER	-	linker	UNP O66529
JC	44	SER	-	linker	UNP O66529
JC	45	MET	-	linker	UNP O66529
JC	46	GLU	-	linker	UNP O66529
JC	81	SER	CYS	engineered mutation	UNP O66529
JC	129	CYS	ALA	engineered mutation	UNP O66529
KC	1	MET	-	initiating methionine	UNP O66529
KC	37	GLY	-	linker	UNP O66529
KC	38	THR	-	linker	UNP O66529
KC	39	GLY	-	linker	UNP O66529
KC	40	GLY	-	linker	UNP O66529
KC	41	SER	-	linker	UNP O66529
KC	42	GLY	-	linker	UNP O66529
KC	43	SER	-	linker	UNP O66529
KC	44	SER	-	linker	UNP O66529
KC	45	MET	-	linker	UNP O66529
KC	46	GLU	-	linker	UNP O66529
KC	81	SER	CYS	engineered mutation	UNP O66529
KC	129	CYS	ALA	engineered mutation	UNP O66529
LC	1	MET	-	initiating methionine	UNP O66529
LC	37	GLY	-	linker	UNP O66529
LC	38	THR	-	linker	UNP O66529
LC	39	GLY	-	linker	UNP O66529
LC	40	GLY	-	linker	UNP O66529
LC	41	SER	-	linker	UNP O66529
LC	42	GLY	-	linker	UNP O66529
LC	43	SER	-	linker	UNP O66529
LC	44	SER	-	linker	UNP O66529
LC	45	MET	-	linker	UNP O66529
LC	46	GLU	-	linker	UNP O66529
LC	81	SER	CYS	engineered mutation	UNP O66529
LC	129	CYS	ALA	engineered mutation	UNP O66529
MC	1	MET	-	initiating methionine	UNP O66529
MC	37	GLY	-	linker	UNP O66529
MC	38	THR	-	linker	UNP O66529
MC	39	GLY	-	linker	UNP O66529
MC	40	GLY	-	linker	UNP O66529
MC	41	SER	-	linker	UNP O66529
MC	42	GLY	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
MC	43	SER	-	linker	UNP O66529
MC	44	SER	-	linker	UNP O66529
MC	45	MET	-	linker	UNP O66529
MC	46	GLU	-	linker	UNP O66529
MC	81	SER	CYS	engineered mutation	UNP O66529
MC	129	CYS	ALA	engineered mutation	UNP O66529
NC	1	MET	-	initiating methionine	UNP O66529
NC	37	GLY	-	linker	UNP O66529
NC	38	THR	-	linker	UNP O66529
NC	39	GLY	-	linker	UNP O66529
NC	40	GLY	-	linker	UNP O66529
NC	41	SER	-	linker	UNP O66529
NC	42	GLY	-	linker	UNP O66529
NC	43	SER	-	linker	UNP O66529
NC	44	SER	-	linker	UNP O66529
NC	45	MET	-	linker	UNP O66529
NC	46	GLU	-	linker	UNP O66529
NC	81	SER	CYS	engineered mutation	UNP O66529
NC	129	CYS	ALA	engineered mutation	UNP O66529
OC	1	MET	-	initiating methionine	UNP O66529
OC	37	GLY	-	linker	UNP O66529
OC	38	THR	-	linker	UNP O66529
OC	39	GLY	-	linker	UNP O66529
OC	40	GLY	-	linker	UNP O66529
OC	41	SER	-	linker	UNP O66529
OC	42	GLY	-	linker	UNP O66529
OC	43	SER	-	linker	UNP O66529
OC	44	SER	-	linker	UNP O66529
OC	45	MET	-	linker	UNP O66529
OC	46	GLU	-	linker	UNP O66529
OC	81	SER	CYS	engineered mutation	UNP O66529
OC	129	CYS	ALA	engineered mutation	UNP O66529
PC	1	MET	-	initiating methionine	UNP O66529
PC	37	GLY	-	linker	UNP O66529
PC	38	THR	-	linker	UNP O66529
PC	39	GLY	-	linker	UNP O66529
PC	40	GLY	-	linker	UNP O66529
PC	41	SER	-	linker	UNP O66529
PC	42	GLY	-	linker	UNP O66529
PC	43	SER	-	linker	UNP O66529
PC	44	SER	-	linker	UNP O66529
PC	45	MET	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
PC	46	GLU	-	linker	UNP O66529
PC	81	SER	CYS	engineered mutation	UNP O66529
PC	129	CYS	ALA	engineered mutation	UNP O66529
QC	1	MET	-	initiating methionine	UNP O66529
QC	37	GLY	-	linker	UNP O66529
QC	38	THR	-	linker	UNP O66529
QC	39	GLY	-	linker	UNP O66529
QC	40	GLY	-	linker	UNP O66529
QC	41	SER	-	linker	UNP O66529
QC	42	GLY	-	linker	UNP O66529
QC	43	SER	-	linker	UNP O66529
QC	44	SER	-	linker	UNP O66529
QC	45	MET	-	linker	UNP O66529
QC	46	GLU	-	linker	UNP O66529
QC	81	SER	CYS	engineered mutation	UNP O66529
QC	129	CYS	ALA	engineered mutation	UNP O66529
RC	1	MET	-	initiating methionine	UNP O66529
RC	37	GLY	-	linker	UNP O66529
RC	38	THR	-	linker	UNP O66529
RC	39	GLY	-	linker	UNP O66529
RC	40	GLY	-	linker	UNP O66529
RC	41	SER	-	linker	UNP O66529
RC	42	GLY	-	linker	UNP O66529
RC	43	SER	-	linker	UNP O66529
RC	44	SER	-	linker	UNP O66529
RC	45	MET	-	linker	UNP O66529
RC	46	GLU	-	linker	UNP O66529
RC	81	SER	CYS	engineered mutation	UNP O66529
RC	129	CYS	ALA	engineered mutation	UNP O66529
SC	1	MET	-	initiating methionine	UNP O66529
SC	37	GLY	-	linker	UNP O66529
SC	38	THR	-	linker	UNP O66529
SC	39	GLY	-	linker	UNP O66529
SC	40	GLY	-	linker	UNP O66529
SC	41	SER	-	linker	UNP O66529
SC	42	GLY	-	linker	UNP O66529
SC	43	SER	-	linker	UNP O66529
SC	44	SER	-	linker	UNP O66529
SC	45	MET	-	linker	UNP O66529
SC	46	GLU	-	linker	UNP O66529
SC	81	SER	CYS	engineered mutation	UNP O66529
SC	129	CYS	ALA	engineered mutation	UNP O66529

Continued on next page...

Continued from previous page...

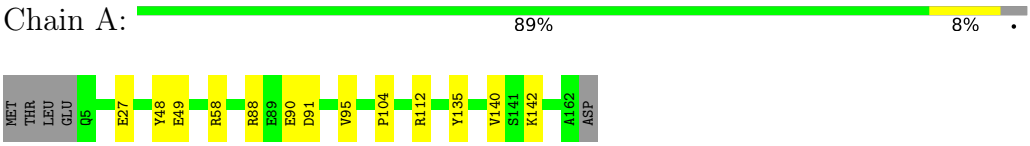
Chain	Residue	Modelled	Actual	Comment	Reference
TC	1	MET	-	initiating methionine	UNP O66529
TC	37	GLY	-	linker	UNP O66529
TC	38	THR	-	linker	UNP O66529
TC	39	GLY	-	linker	UNP O66529
TC	40	GLY	-	linker	UNP O66529
TC	41	SER	-	linker	UNP O66529
TC	42	GLY	-	linker	UNP O66529
TC	43	SER	-	linker	UNP O66529
TC	44	SER	-	linker	UNP O66529
TC	45	MET	-	linker	UNP O66529
TC	46	GLU	-	linker	UNP O66529
TC	81	SER	CYS	engineered mutation	UNP O66529
TC	129	CYS	ALA	engineered mutation	UNP O66529
UC	1	MET	-	initiating methionine	UNP O66529
UC	37	GLY	-	linker	UNP O66529
UC	38	THR	-	linker	UNP O66529
UC	39	GLY	-	linker	UNP O66529
UC	40	GLY	-	linker	UNP O66529
UC	41	SER	-	linker	UNP O66529
UC	42	GLY	-	linker	UNP O66529
UC	43	SER	-	linker	UNP O66529
UC	44	SER	-	linker	UNP O66529
UC	45	MET	-	linker	UNP O66529
UC	46	GLU	-	linker	UNP O66529
UC	81	SER	CYS	engineered mutation	UNP O66529
UC	129	CYS	ALA	engineered mutation	UNP O66529
VC	1	MET	-	initiating methionine	UNP O66529
VC	37	GLY	-	linker	UNP O66529
VC	38	THR	-	linker	UNP O66529
VC	39	GLY	-	linker	UNP O66529
VC	40	GLY	-	linker	UNP O66529
VC	41	SER	-	linker	UNP O66529
VC	42	GLY	-	linker	UNP O66529
VC	43	SER	-	linker	UNP O66529
VC	44	SER	-	linker	UNP O66529
VC	45	MET	-	linker	UNP O66529
VC	46	GLU	-	linker	UNP O66529
VC	81	SER	CYS	engineered mutation	UNP O66529
VC	129	CYS	ALA	engineered mutation	UNP O66529

3 Residue-property plots (i)

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

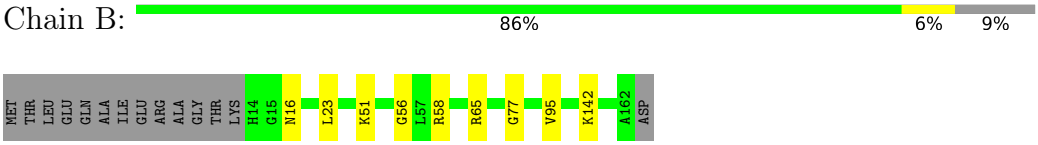
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain A:



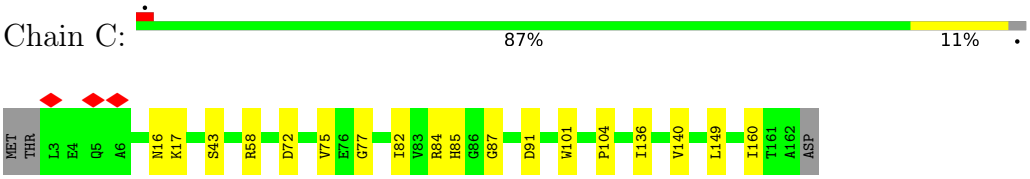
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B:



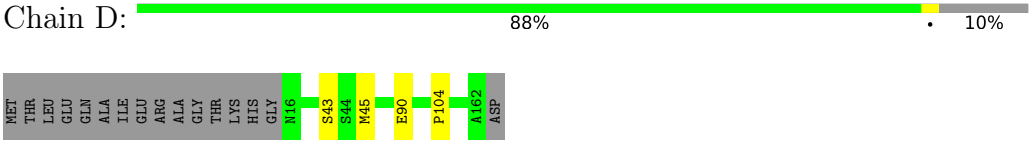
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain C:



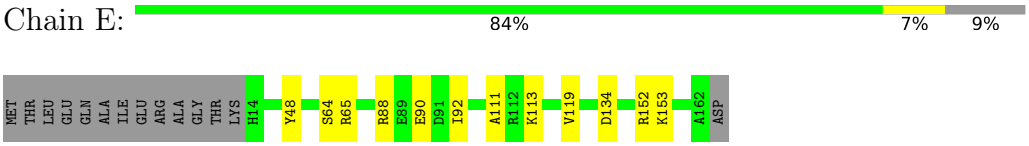
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain D:



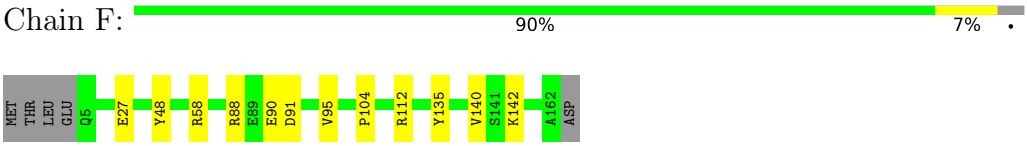
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain E:



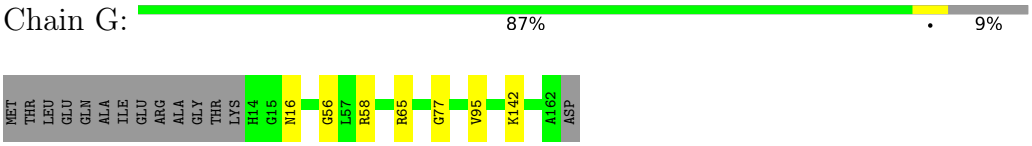
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain F:



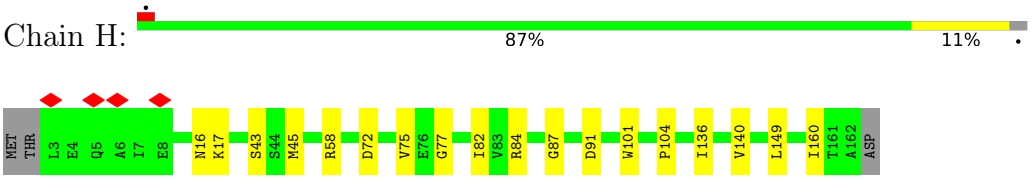
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain G:



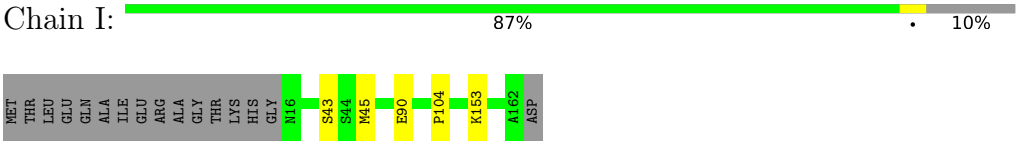
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain H:



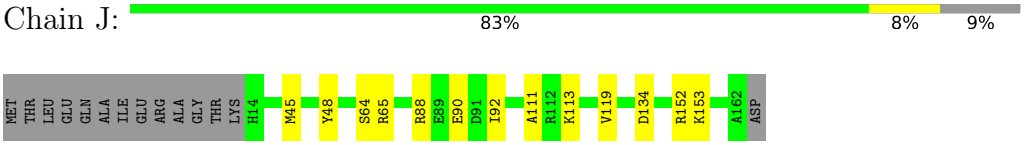
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain I:



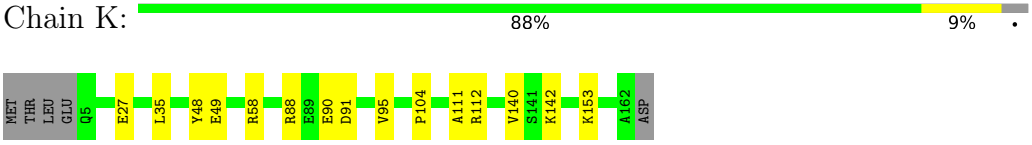
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain J:



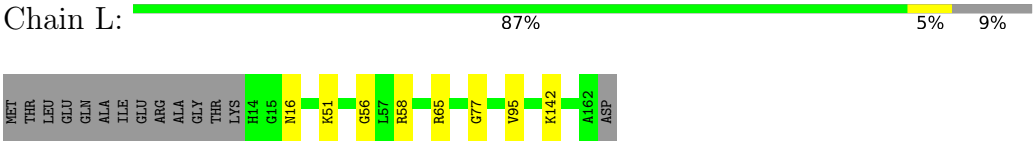
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain K:



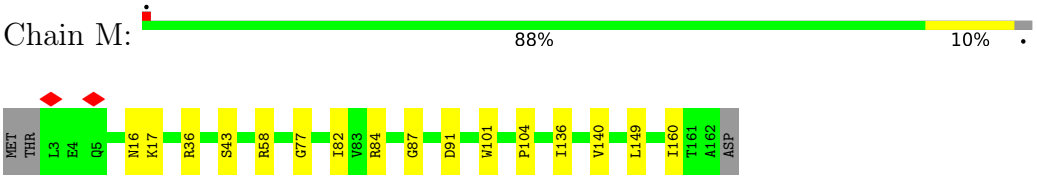
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain L:



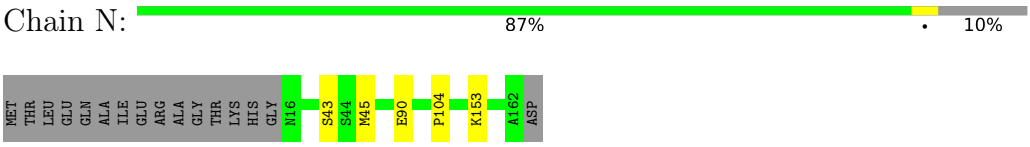
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain M:



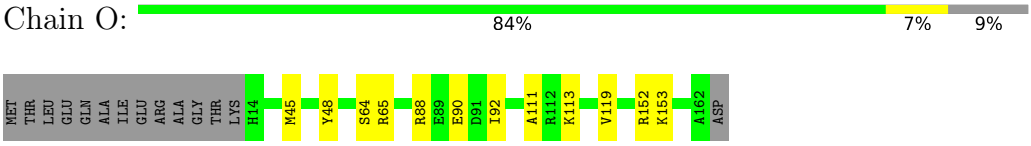
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain N:



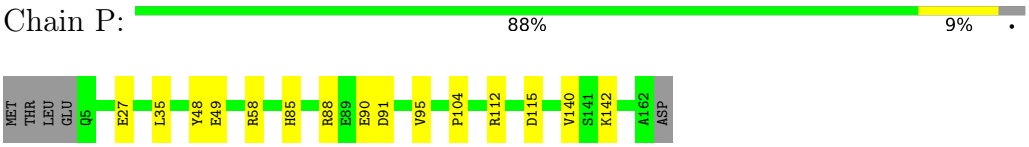
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain O:



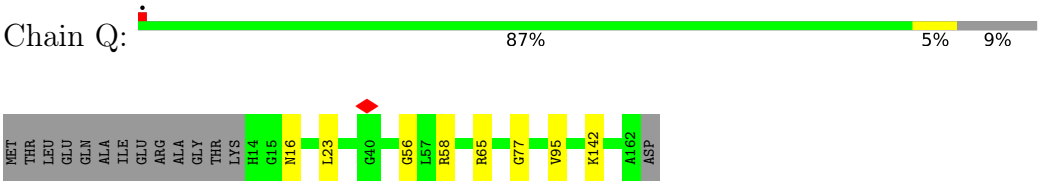
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain P:



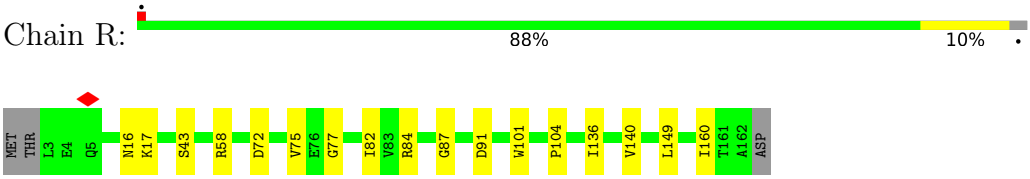
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain Q:



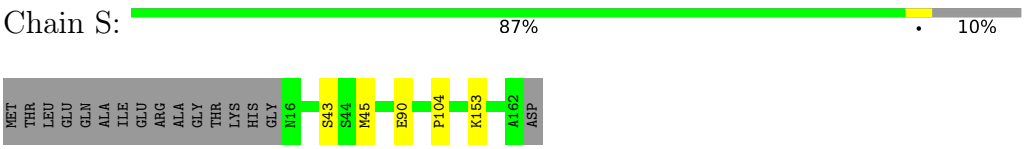
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain R:



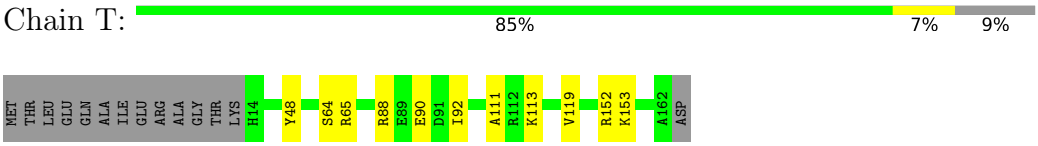
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain S:



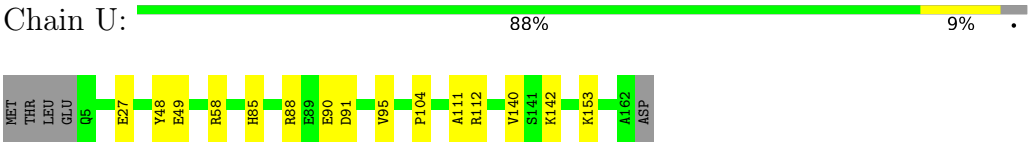
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain T:



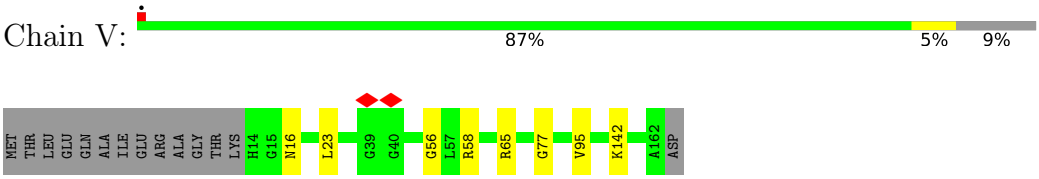
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain U:



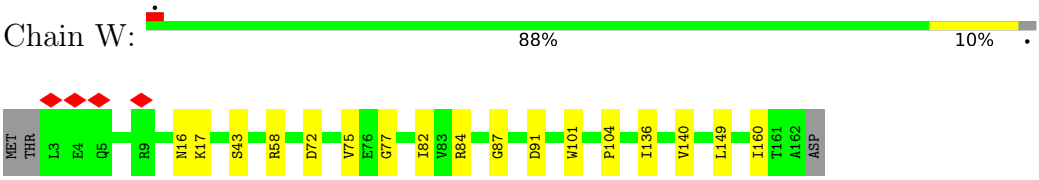
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain V:



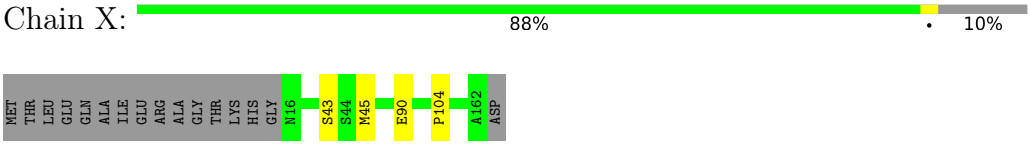
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain W:



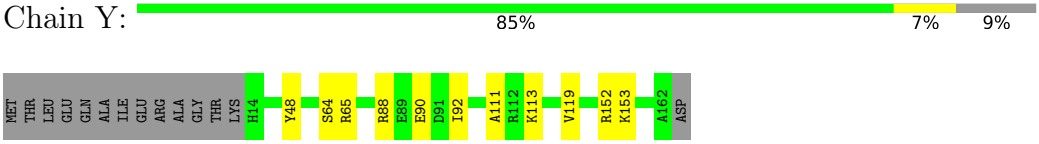
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain X:



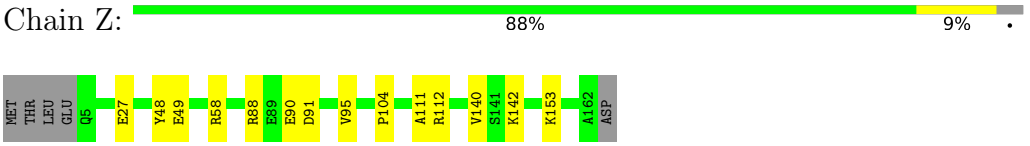
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain Y:



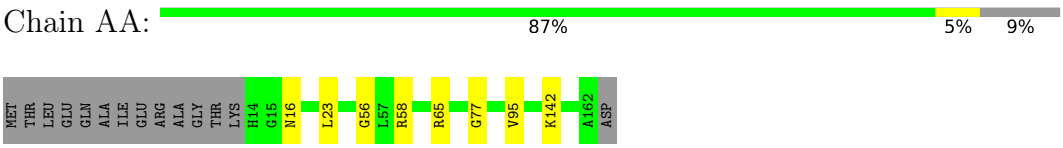
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain Z:



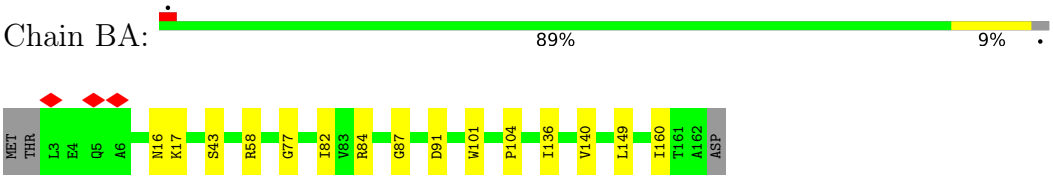
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AA:



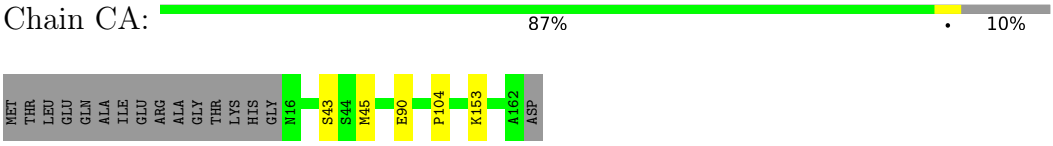
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BA:



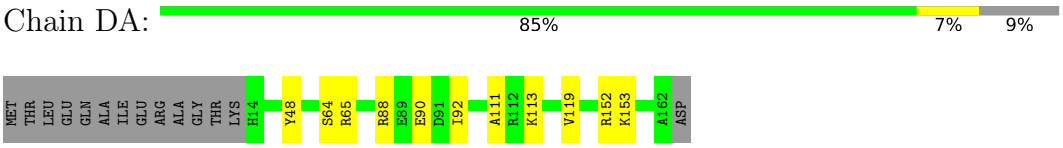
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CA:



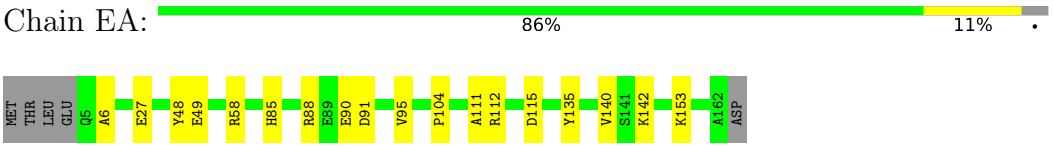
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DA:



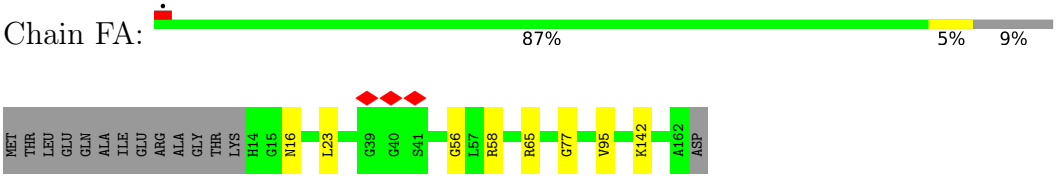
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EA:



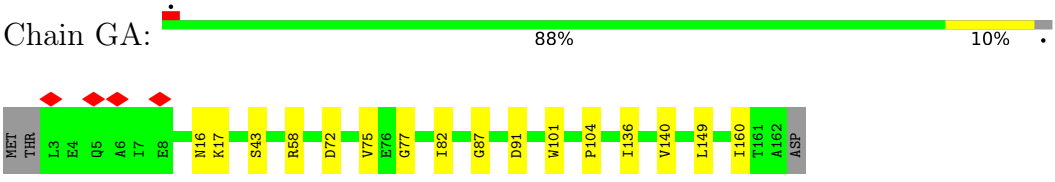
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FA:



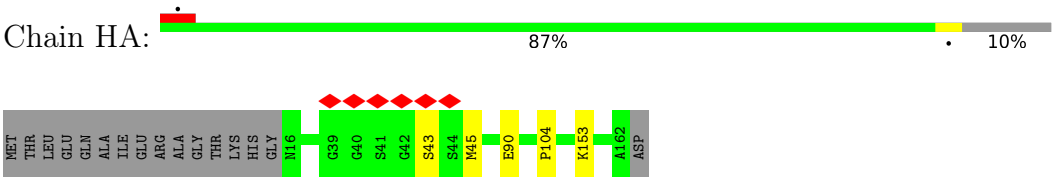
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GA:



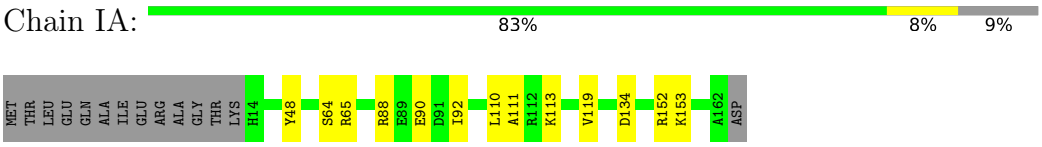
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HA:



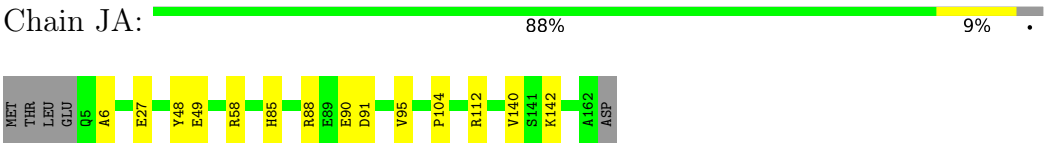
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IA:



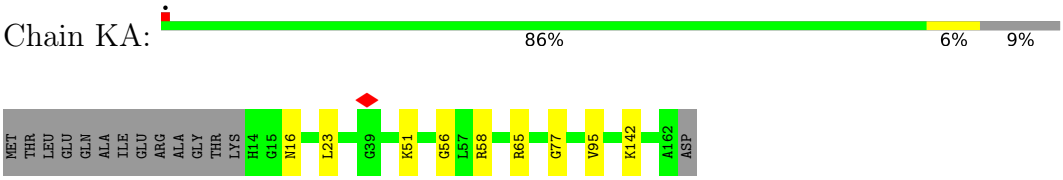
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JA:



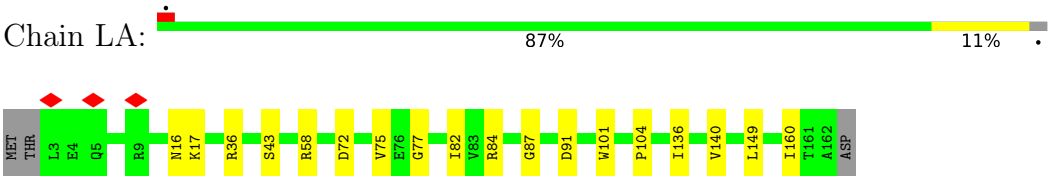
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KA:



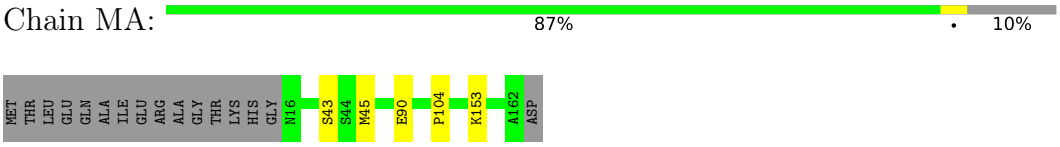
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LA:



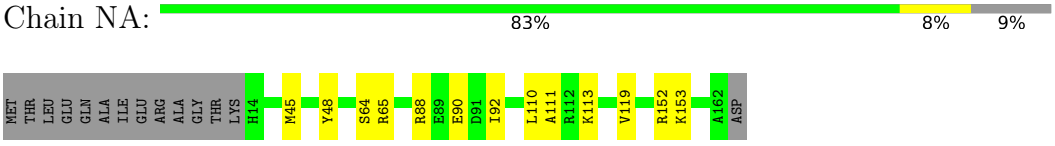
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MA:



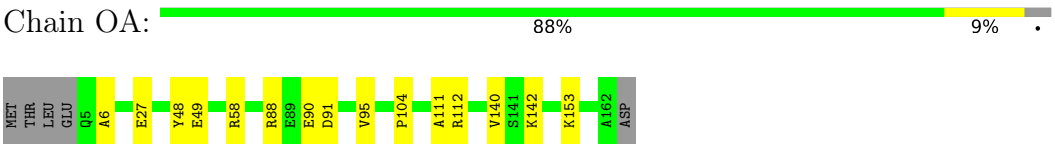
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NA:



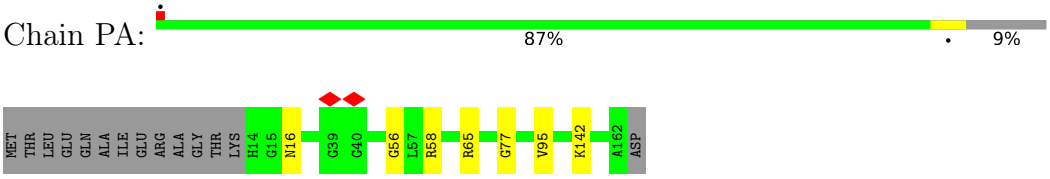
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OA:



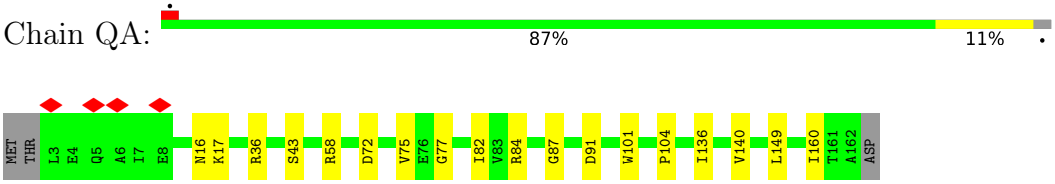
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain PA:



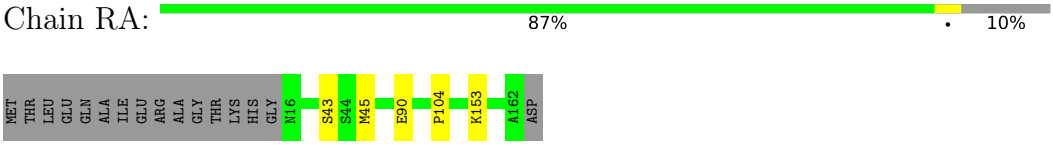
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain QA:



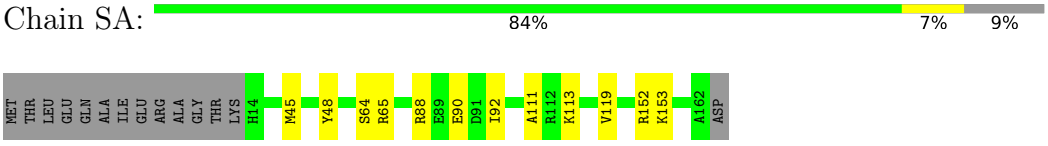
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain RA:



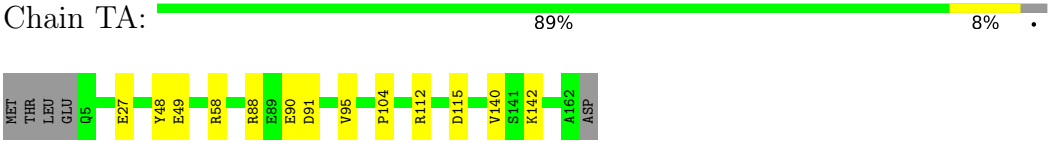
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain SA:



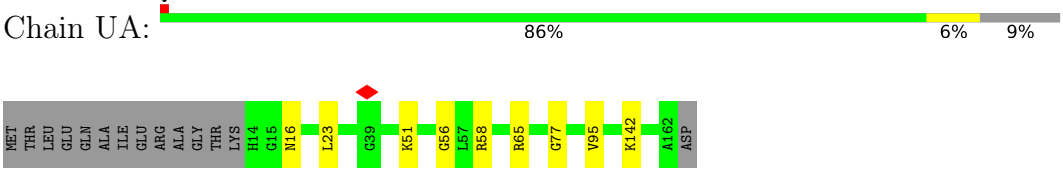
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TA:



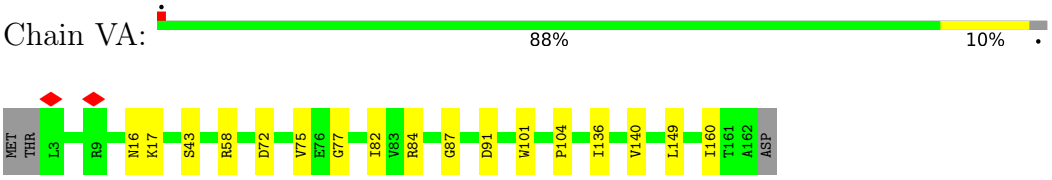
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UA:



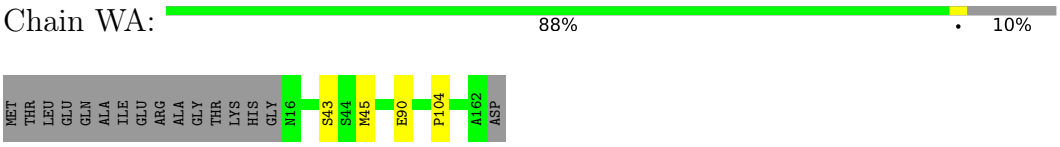
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain VA:



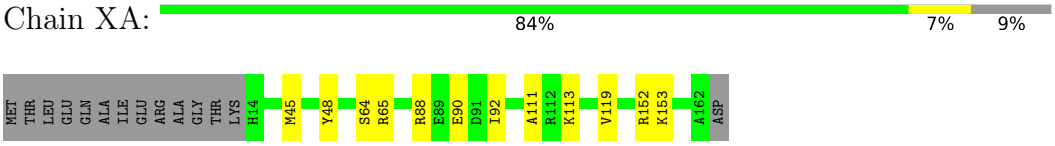
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WA:



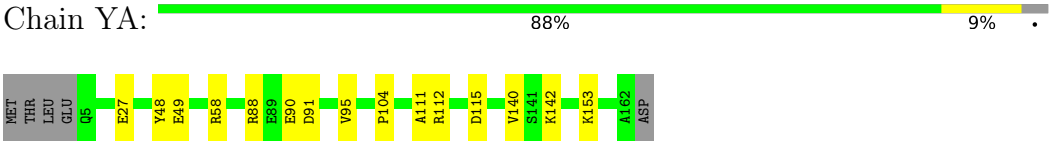
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XA:



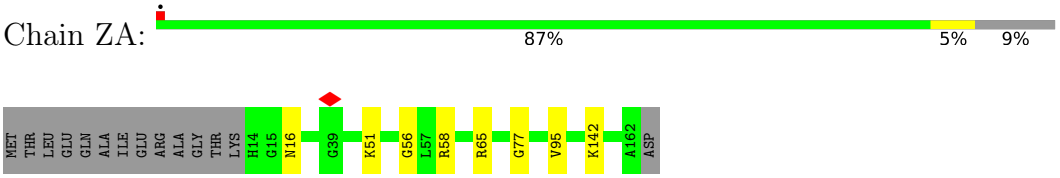
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YA:



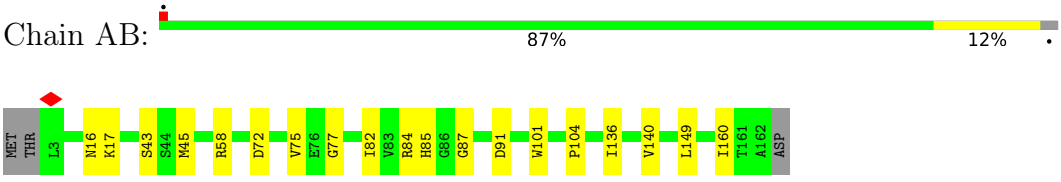
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZA:



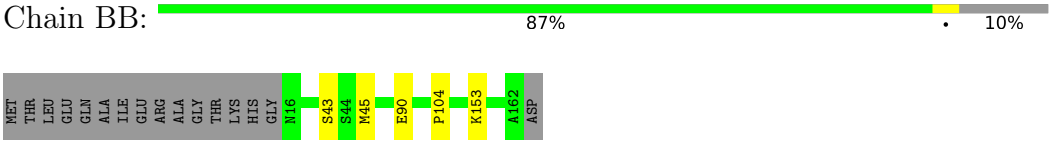
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AB:



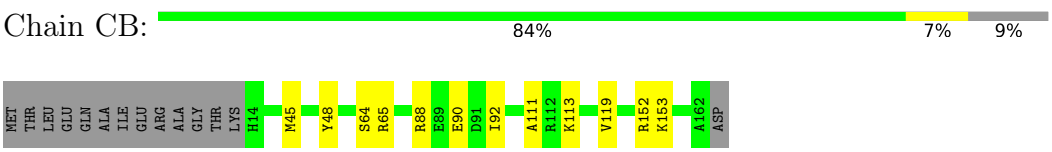
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BB:



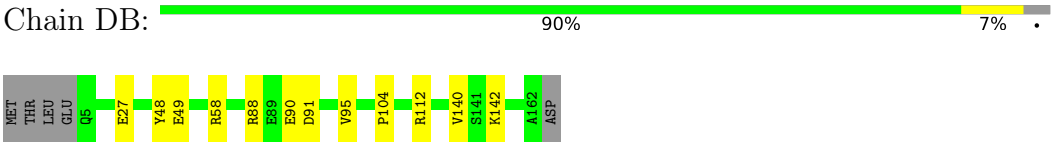
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CB:



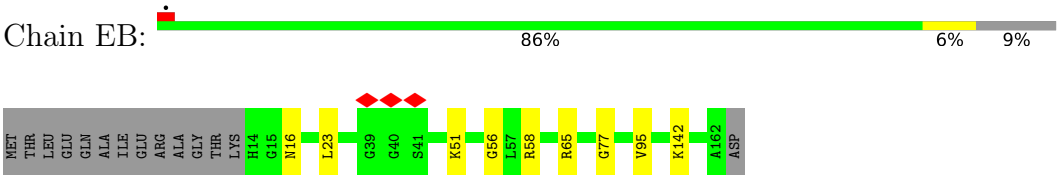
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DB:



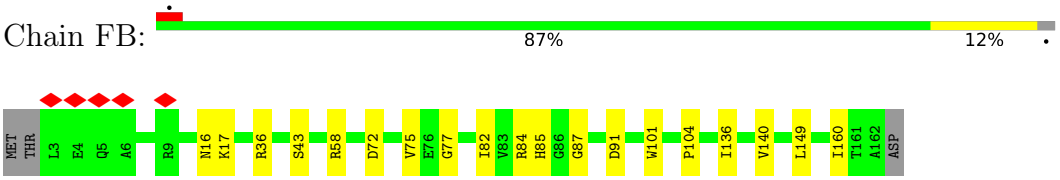
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EB:



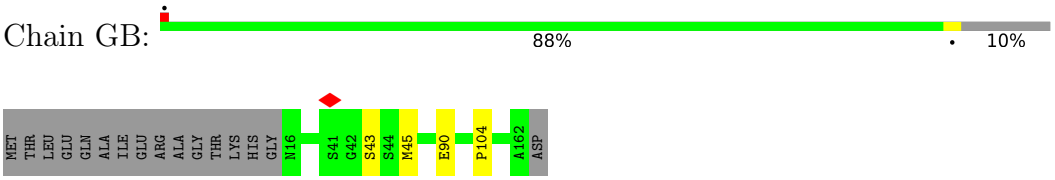
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FB:



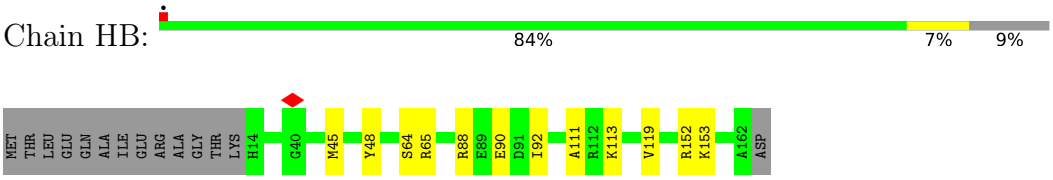
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GB:



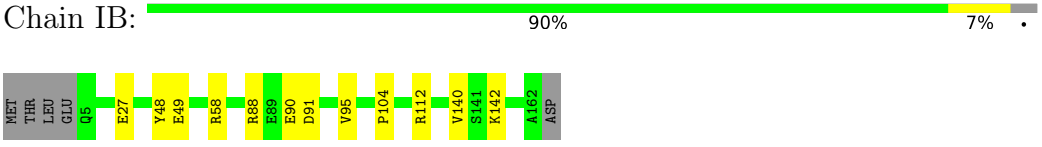
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HB:



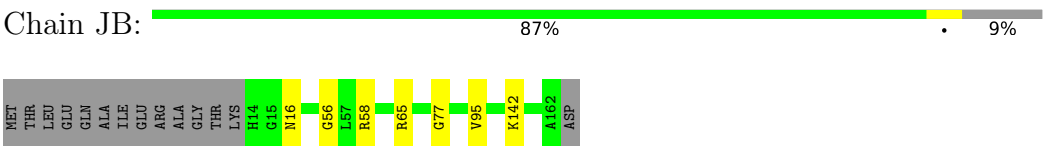
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IB:



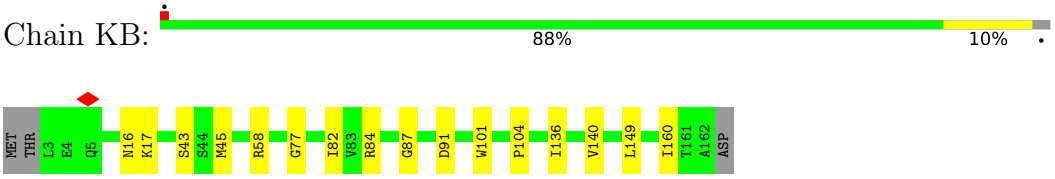
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JB:



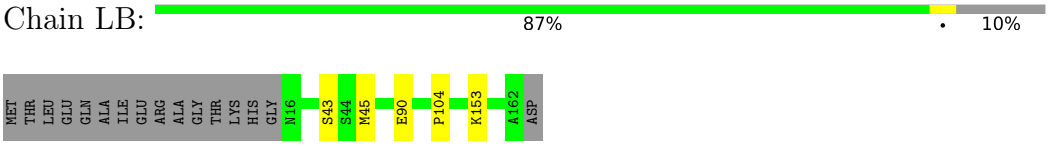
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KB:



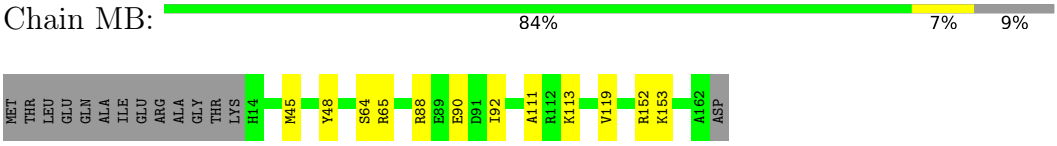
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LB:



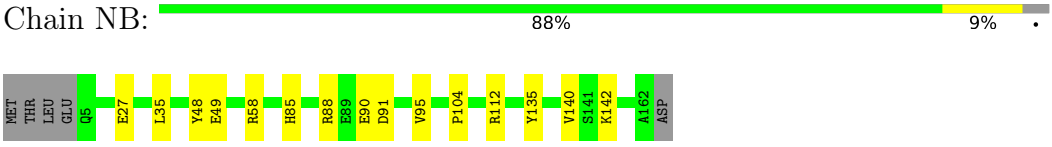
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MB:



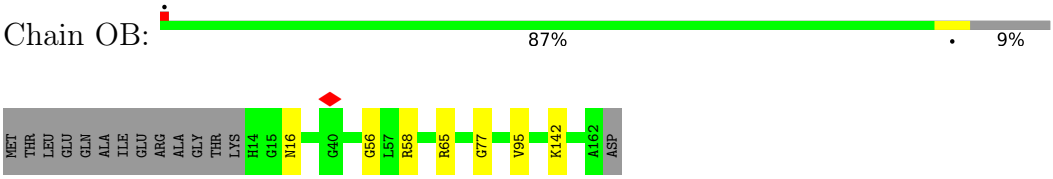
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NB:



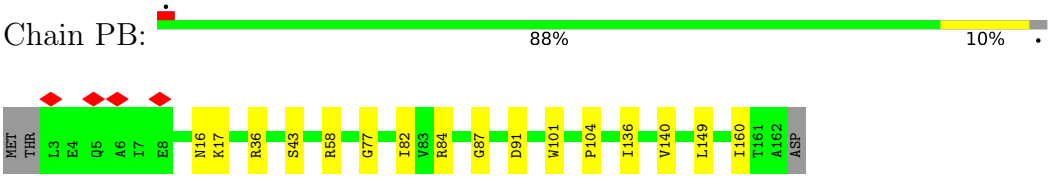
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OB:



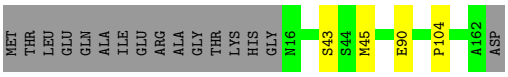
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain PB:



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

Chain QB:



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

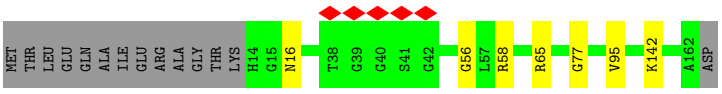
Chain RB:

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

Chain SB:

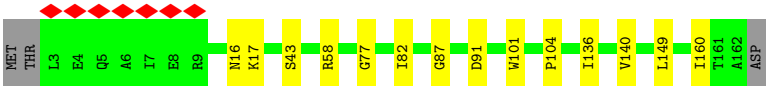
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TB:



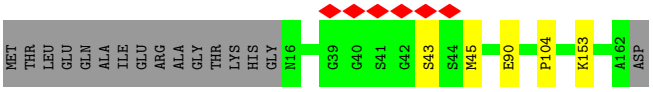
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UB:



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

Chain VB:

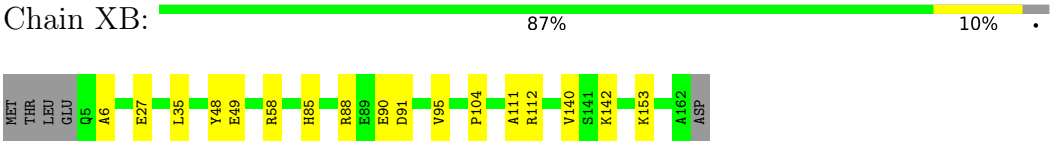


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WB:

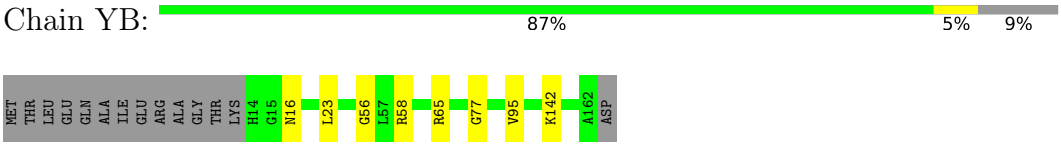
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XB:



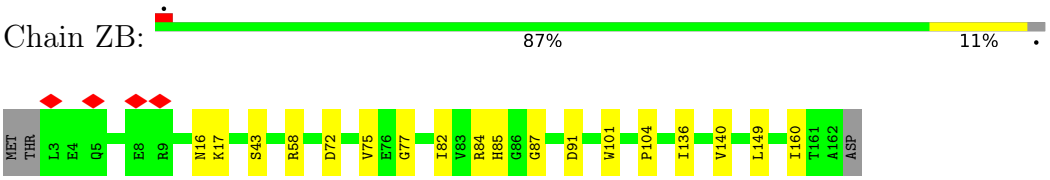
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YB:



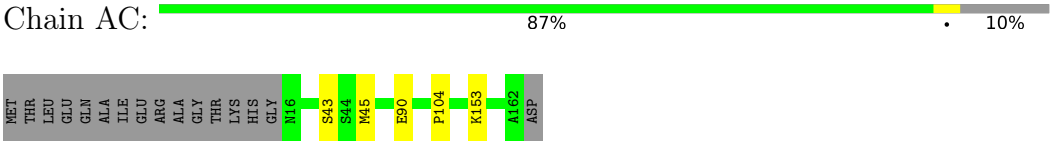
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZB:



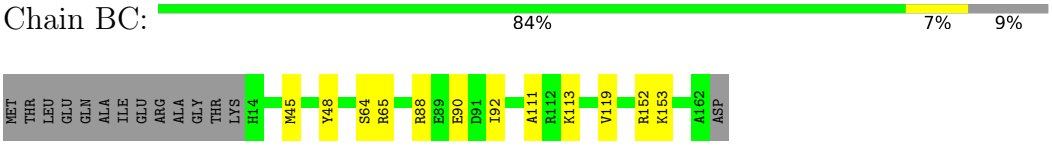
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AC:



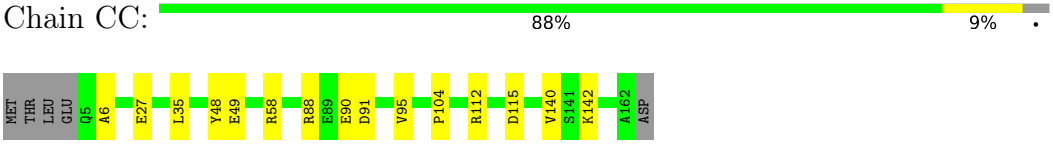
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BC:



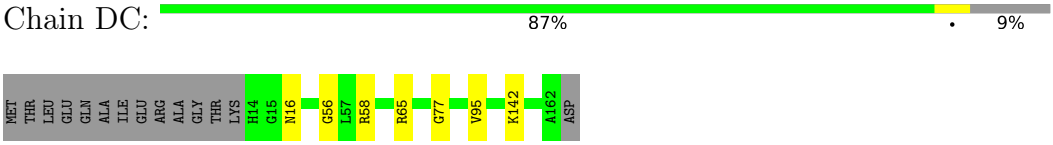
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CC:



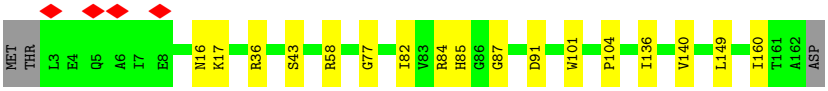
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DC:



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

Chain EC:

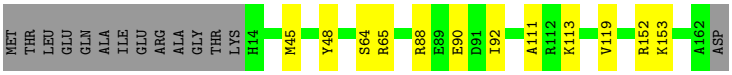


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FC:

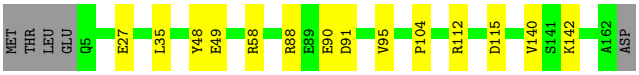
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GC:



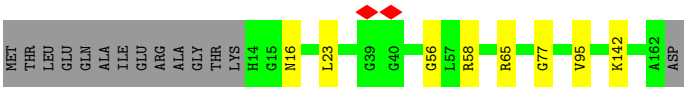
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HC:



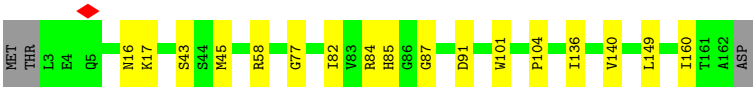
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IC:



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

Chain JC:

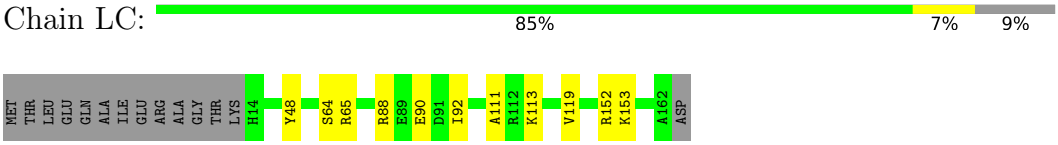


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KC:

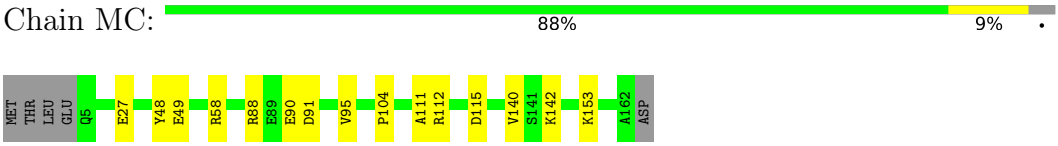
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LC:



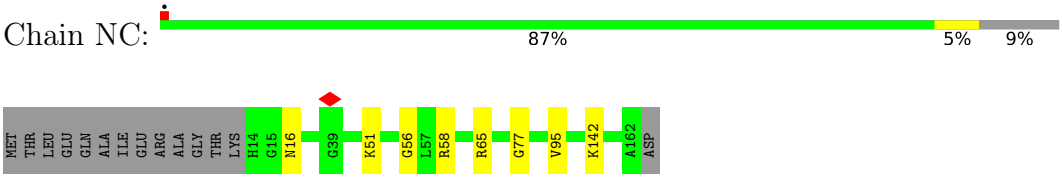
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MC:



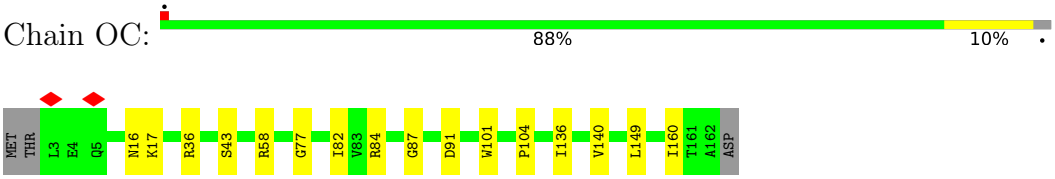
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NC:



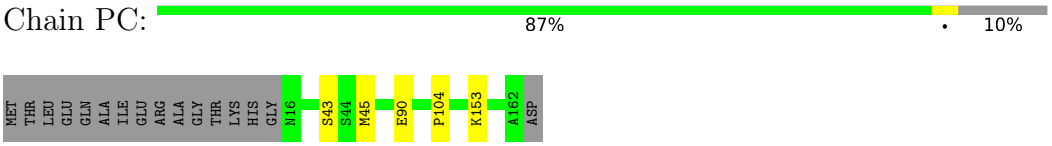
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OC:



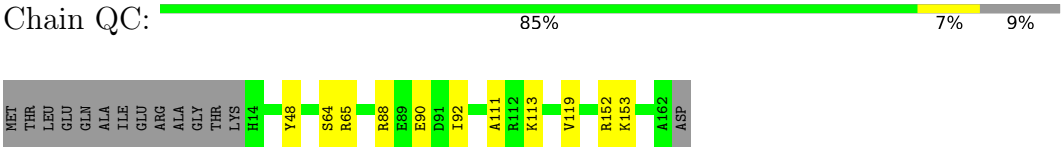
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain PC:



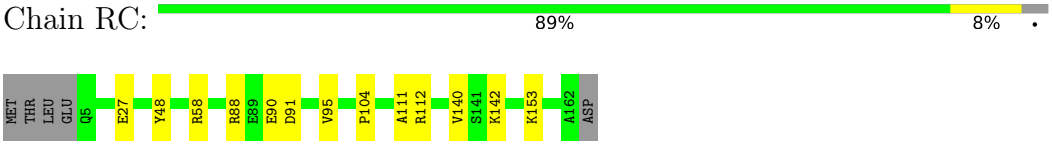
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain QC:



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

Chain RC:

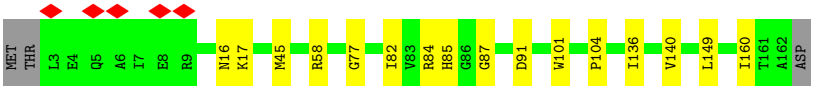


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain SC:

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

Chain TC:

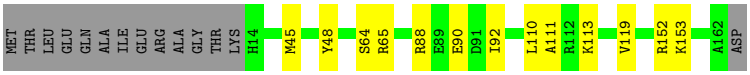


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UC:

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

Chain VC:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=57.0°, rise=24.5 Å, axial sym=C1	Depositor
Number of segments used	192310	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42.44	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.146	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	372.24002, 372.24002, 372.24002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8460001, 0.8460001, 0.8460001	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	A	0.09	0/1204	0.22	0/1624
1	AA	0.08	0/1137	0.26	0/1535
1	AB	0.09	0/1221	0.23	0/1647
1	AC	0.11	0/1122	0.26	0/1515
1	B	0.08	0/1137	0.26	0/1535
1	BA	0.09	0/1221	0.24	0/1647
1	BB	0.11	0/1122	0.26	0/1515
1	BC	0.09	0/1137	0.24	0/1535
1	C	0.09	0/1221	0.23	0/1647
1	CA	0.11	0/1122	0.26	0/1515
1	CB	0.09	0/1137	0.24	0/1535
1	CC	0.09	0/1204	0.22	0/1624
1	D	0.10	0/1122	0.26	0/1515
1	DA	0.09	0/1137	0.24	0/1535
1	DB	0.09	0/1204	0.22	0/1624
1	DC	0.08	0/1137	0.26	0/1535
1	E	0.09	0/1137	0.24	0/1535
1	EA	0.09	0/1204	0.22	0/1624
1	EB	0.09	0/1137	0.26	0/1535
1	EC	0.09	0/1221	0.23	0/1647
1	F	0.09	0/1204	0.22	0/1624
1	FA	0.08	0/1137	0.26	0/1535
1	FB	0.09	0/1221	0.23	0/1647
1	FC	0.11	0/1122	0.26	0/1515
1	G	0.08	0/1137	0.26	0/1535
1	GA	0.09	0/1221	0.23	0/1647
1	GB	0.11	0/1122	0.26	0/1515
1	GC	0.09	0/1137	0.24	0/1535
1	H	0.09	0/1221	0.23	0/1647
1	HA	0.11	0/1122	0.26	0/1515
1	HB	0.09	0/1137	0.24	0/1535
1	HC	0.10	0/1204	0.22	0/1624
1	I	0.11	0/1122	0.26	0/1515
1	IA	0.09	0/1137	0.24	0/1535

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	IB	0.10	0/1204	0.22	0/1624
1	IC	0.08	0/1137	0.26	0/1535
1	J	0.09	0/1137	0.24	0/1535
1	JA	0.09	0/1204	0.22	0/1624
1	JB	0.08	0/1137	0.26	0/1535
1	JC	0.09	0/1221	0.23	0/1647
1	K	0.09	0/1204	0.22	0/1624
1	KA	0.08	0/1137	0.26	0/1535
1	KB	0.09	0/1221	0.23	0/1647
1	KC	0.11	0/1122	0.26	0/1515
1	L	0.08	0/1137	0.26	0/1535
1	LA	0.09	0/1221	0.24	0/1647
1	LB	0.11	0/1122	0.26	0/1515
1	LC	0.09	0/1137	0.24	0/1535
1	M	0.09	0/1221	0.23	0/1647
1	MA	0.11	0/1122	0.26	0/1515
1	MB	0.09	0/1137	0.24	0/1535
1	MC	0.09	0/1204	0.22	0/1624
1	N	0.11	0/1122	0.26	0/1515
1	NA	0.09	0/1137	0.24	0/1535
1	NB	0.09	0/1204	0.22	0/1624
1	NC	0.08	0/1137	0.26	0/1535
1	O	0.09	0/1137	0.24	0/1535
1	OA	0.10	0/1204	0.22	0/1624
1	OB	0.08	0/1137	0.26	0/1535
1	OC	0.09	0/1221	0.23	0/1647
1	P	0.09	0/1204	0.22	0/1624
1	PA	0.08	0/1137	0.26	0/1535
1	PB	0.09	0/1221	0.24	0/1647
1	PC	0.11	0/1122	0.26	0/1515
1	Q	0.08	0/1137	0.26	0/1535
1	QA	0.09	0/1221	0.23	0/1647
1	QB	0.11	0/1122	0.26	0/1515
1	QC	0.09	0/1137	0.24	0/1535
1	R	0.09	0/1221	0.23	0/1647
1	RA	0.11	0/1122	0.26	0/1515
1	RB	0.10	0/1137	0.24	0/1535
1	RC	0.09	0/1204	0.22	0/1624
1	S	0.11	0/1122	0.26	0/1515
1	SA	0.09	0/1137	0.24	0/1535
1	SB	0.09	0/1204	0.22	0/1624
1	SC	0.08	0/1137	0.26	0/1535
1	T	0.09	0/1137	0.24	0/1535

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	TA	0.09	0/1204	0.22	0/1624
1	TB	0.08	0/1137	0.26	0/1535
1	TC	0.09	0/1221	0.23	0/1647
1	U	0.09	0/1204	0.22	0/1624
1	UA	0.08	0/1137	0.26	0/1535
1	UB	0.09	0/1221	0.23	0/1647
1	UC	0.11	0/1122	0.26	0/1515
1	V	0.08	0/1137	0.26	0/1535
1	VA	0.09	0/1221	0.23	0/1647
1	VB	0.11	0/1122	0.26	0/1515
1	VC	0.09	0/1137	0.24	0/1535
1	W	0.09	0/1221	0.23	0/1647
1	WA	0.11	0/1122	0.26	0/1515
1	WB	0.10	0/1137	0.24	0/1535
1	X	0.11	0/1122	0.26	0/1515
1	XA	0.09	0/1137	0.24	0/1535
1	XB	0.09	0/1204	0.22	0/1624
1	Y	0.09	0/1137	0.24	0/1535
1	YA	0.09	0/1204	0.22	0/1624
1	YB	0.08	0/1137	0.26	0/1535
1	Z	0.09	0/1204	0.22	0/1624
1	ZA	0.08	0/1137	0.26	0/1535
1	ZB	0.09	0/1221	0.24	0/1647
All	All	0.09	0/116420	0.24	0/157120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1186	0	1203	10	0
1	AA	1119	0	1133	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1203	0	1221	12	0
1	AC	1105	0	1123	5	0
1	B	1119	0	1133	7	0
1	BA	1203	0	1221	9	0
1	BB	1105	0	1123	5	0
1	BC	1119	0	1133	9	0
1	C	1203	0	1221	11	0
1	CA	1105	0	1123	5	0
1	CB	1119	0	1133	9	0
1	CC	1186	0	1203	12	0
1	D	1105	0	1123	4	0
1	DA	1119	0	1133	8	0
1	DB	1186	0	1204	9	0
1	DC	1119	0	1133	5	0
1	E	1119	0	1133	9	0
1	EA	1186	0	1204	14	0
1	EB	1119	0	1133	7	0
1	EC	1203	0	1221	11	0
1	F	1186	0	1203	9	0
1	FA	1119	0	1133	6	0
1	FB	1203	0	1221	12	0
1	FC	1105	0	1123	5	0
1	G	1119	0	1133	5	0
1	GA	1203	0	1221	9	0
1	GB	1105	0	1123	4	0
1	GC	1119	0	1133	9	0
1	H	1203	0	1221	11	0
1	HA	1105	0	1123	5	0
1	HB	1119	0	1133	9	0
1	HC	1186	0	1204	11	0
1	I	1105	0	1123	5	0
1	IA	1119	0	1133	10	0
1	IB	1186	0	1203	9	0
1	IC	1119	0	1133	6	0
1	J	1119	0	1133	10	0
1	JA	1186	0	1203	11	0
1	JB	1119	0	1133	5	0
1	JC	1203	0	1221	11	0
1	K	1186	0	1203	11	0
1	KA	1119	0	1133	7	0
1	KB	1203	0	1221	10	0
1	KC	1105	0	1123	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1119	0	1133	6	0
1	LA	1203	0	1221	11	0
1	LB	1105	0	1123	5	0
1	LC	1119	0	1133	8	0
1	M	1203	0	1221	10	0
1	MA	1105	0	1123	5	0
1	MB	1119	0	1133	9	0
1	MC	1186	0	1203	11	0
1	N	1105	0	1123	5	0
1	NA	1119	0	1133	10	0
1	NB	1186	0	1203	12	0
1	NC	1119	0	1133	6	0
1	O	1119	0	1133	9	0
1	OA	1186	0	1203	11	0
1	OB	1119	0	1133	5	0
1	OC	1203	0	1221	10	0
1	P	1186	0	1203	12	0
1	PA	1119	0	1133	5	0
1	PB	1203	0	1221	10	0
1	PC	1105	0	1123	5	0
1	Q	1119	0	1133	6	0
1	QA	1203	0	1221	11	0
1	QB	1105	0	1123	4	0
1	QC	1119	0	1133	8	0
1	R	1203	0	1221	10	0
1	RA	1105	0	1123	5	0
1	RB	1119	0	1133	9	0
1	RC	1186	0	1203	9	0
1	S	1105	0	1123	5	0
1	SA	1119	0	1133	9	0
1	SB	1186	0	1204	12	0
1	SC	1119	0	1133	7	0
1	T	1119	0	1133	8	0
1	TA	1186	0	1203	10	0
1	TB	1119	0	1133	5	0
1	TC	1203	0	1221	10	0
1	U	1186	0	1203	11	0
1	UA	1119	0	1133	7	0
1	UB	1203	0	1221	8	0
1	UC	1105	0	1123	4	0
1	V	1119	0	1133	6	0
1	VA	1203	0	1221	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	VB	1105	0	1123	5	0
1	VC	1119	0	1133	10	0
1	W	1203	0	1221	10	0
1	WA	1105	0	1123	4	0
1	WB	1119	0	1133	9	0
1	X	1105	0	1123	4	0
1	XA	1119	0	1133	9	0
1	XB	1186	0	1203	13	0
1	Y	1119	0	1133	8	0
1	YA	1186	0	1203	11	0
1	YB	1119	0	1133	6	0
1	Z	1186	0	1203	10	0
1	ZA	1119	0	1133	6	0
1	ZB	1203	0	1221	11	0
All	All	114640	0	116264	603	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 3.

All (603) 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:VA:84:ARG:NH1	1:MC:49:GLU:OE2	2.26	0.69
1:QA:84:ARG:NH1	1:HC:49:GLU:OE2	2.31	0.64
1:R:84:ARG:NH1	1:Z:49:GLU:OE2	2.31	0.64
1:U:49:GLU:OE2	1:ZB:84:ARG:NH1	2.32	0.62
1:K:49:GLU:OE2	1:LA:84:ARG:NH1	2.31	0.62
1:U:95:VAL:HG12	1:Y:48:TYR:HB2	1.82	0.62
1:K:95:VAL:HG12	1:O:48:TYR:HB2	1.82	0.62
1:W:84:ARG:NH1	1:DB:49:GLU:OE2	2.33	0.62
1:YA:49:GLU:OE2	1:OC:84:ARG:NH1	2.33	0.62
1:A:95:VAL:HG12	1:E:48:TYR:HB2	1.82	0.62
1:RC:95:VAL:HG12	1:VC:48:TYR:HB2	1.82	0.62
1:Z:95:VAL:HG12	1:DA:48:TYR:HB2	1.82	0.62
1:SB:95:VAL:HG12	1:WB:48:TYR:HB2	1.82	0.62
1:EA:95:VAL:HG12	1:IA:48:TYR:HB2	1.82	0.61
1:FB:84:ARG:NH1	1:SB:49:GLU:OE2	2.33	0.61
1:NB:95:VAL:HG12	1:RB:48:TYR:HB2	1.82	0.61
1:HC:95:VAL:HG12	1:LC:48:TYR:HB2	1.82	0.61
1:P:95:VAL:HG12	1:T:48:TYR:HB2	1.82	0.61
1:IB:95:VAL:HG12	1:MB:48:TYR:HB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:95:VAL:HG12	1:NA:48:TYR:HB2	1.82	0.61
1:DB:95:VAL:HG12	1:HB:48:TYR:HB2	1.82	0.61
1:XB:95:VAL:HG12	1:BC:48:TYR:HB2	1.82	0.61
1:YA:95:VAL:HG12	1:CB:48:TYR:HB2	1.82	0.60
1:MC:95:VAL:HG12	1:QC:48:TYR:HB2	1.82	0.60
1:CC:95:VAL:HG12	1:GC:48:TYR:HB2	1.82	0.60
1:M:84:ARG:NH1	1:TA:49:GLU:OE2	2.34	0.60
1:TA:95:VAL:HG12	1:XA:48:TYR:HB2	1.82	0.60
1:F:95:VAL:HG12	1:J:48:TYR:HB2	1.82	0.60
1:OA:95:VAL:HG12	1:SA:48:TYR:HB2	1.82	0.60
1:KB:16:ASN:HD21	1:KB:77:GLY:HA3	1.67	0.60
1:M:16:ASN:HD21	1:M:77:GLY:HA3	1.67	0.60
1:H:16:ASN:HD21	1:H:77:GLY:HA3	1.67	0.59
1:OC:16:ASN:HD21	1:OC:77:GLY:HA3	1.67	0.59
1:FB:16:ASN:HD21	1:FB:77:GLY:HA3	1.67	0.59
1:AB:16:ASN:HD21	1:AB:77:GLY:HA3	1.67	0.59
1:EC:16:ASN:HD21	1:EC:77:GLY:HA3	1.67	0.59
1:A:49:GLU:OE2	1:BA:84:ARG:NH1	2.35	0.59
1:QA:16:ASN:HD21	1:QA:77:GLY:HA3	1.67	0.59
1:ZB:16:ASN:HD21	1:ZB:77:GLY:HA3	1.67	0.59
1:C:16:ASN:HD21	1:C:77:GLY:HA3	1.67	0.59
1:TC:16:ASN:HD21	1:TC:77:GLY:HA3	1.67	0.59
1:R:16:ASN:HD21	1:R:77:GLY:HA3	1.67	0.58
1:IB:49:GLU:OE2	1:PB:84:ARG:NH1	2.36	0.58
1:PB:16:ASN:HD21	1:PB:77:GLY:HA3	1.67	0.58
1:JC:16:ASN:HD21	1:JC:77:GLY:HA3	1.67	0.58
1:GA:16:ASN:HD21	1:GA:77:GLY:HA3	1.67	0.58
1:UB:16:ASN:HD21	1:UB:77:GLY:HA3	1.67	0.58
1:BA:16:ASN:HD21	1:BA:77:GLY:HA3	1.67	0.58
1:VA:16:ASN:HD21	1:VA:77:GLY:HA3	1.67	0.58
1:W:16:ASN:HD21	1:W:77:GLY:HA3	1.67	0.57
1:LA:16:ASN:HD21	1:LA:77:GLY:HA3	1.67	0.57
1:OA:48:TYR:HB2	1:PA:95:VAL:HG22	1.87	0.57
1:XB:48:TYR:HB2	1:YB:95:VAL:HG22	1.87	0.57
1:RC:48:TYR:HB2	1:SC:95:VAL:HG22	1.87	0.57
1:P:48:TYR:HB2	1:Q:95:VAL:HG22	1.87	0.57
1:TA:48:TYR:HB2	1:UA:95:VAL:HG22	1.87	0.57
1:SB:48:TYR:HB2	1:TB:95:VAL:HG22	1.87	0.57
1:NB:48:TYR:HB2	1:OB:95:VAL:HG22	1.87	0.57
1:CC:48:TYR:HB2	1:DC:95:VAL:HG22	1.87	0.57
1:EA:48:TYR:HB2	1:FA:95:VAL:HG22	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:84:ARG:NH1	1:XB:49:GLU:OE2	2.37	0.57
1:YA:48:TYR:HB2	1:ZA:95:VAL:HG22	1.87	0.57
1:HC:48:TYR:HB2	1:IC:95:VAL:HG22	1.87	0.57
1:MC:48:TYR:HB2	1:NC:95:VAL:HG22	1.87	0.56
1:F:48:TYR:HB2	1:G:95:VAL:HG22	1.87	0.56
1:P:49:GLU:OE2	1:EC:84:ARG:NH1	2.39	0.56
1:U:48:TYR:HB2	1:V:95:VAL:HG22	1.87	0.56
1:Z:48:TYR:HB2	1:AA:95:VAL:HG22	1.87	0.56
1:K:48:TYR:HB2	1:L:95:VAL:HG22	1.87	0.56
1:A:48:TYR:HB2	1:B:95:VAL:HG22	1.87	0.56
1:DB:48:TYR:HB2	1:EB:95:VAL:HG22	1.87	0.56
1:JA:48:TYR:HB2	1:KA:95:VAL:HG22	1.87	0.56
1:IB:48:TYR:HB2	1:JB:95:VAL:HG22	1.87	0.56
1:F:104:PRO:HD3	1:F:140:VAL:HG23	1.89	0.55
1:M:17:LYS:HG3	1:M:160:ILE:HD13	1.89	0.55
1:IB:104:PRO:HD3	1:IB:140:VAL:HG23	1.89	0.55
1:OA:104:PRO:HD3	1:OA:140:VAL:HG23	1.89	0.55
1:NB:104:PRO:HD3	1:NB:140:VAL:HG23	1.89	0.55
1:MC:104:PRO:HD3	1:MC:140:VAL:HG23	1.89	0.55
1:K:104:PRO:HD3	1:K:140:VAL:HG23	1.89	0.55
1:SB:104:PRO:HD3	1:SB:140:VAL:HG23	1.89	0.55
1:UB:17:LYS:HG3	1:UB:160:ILE:HD13	1.89	0.55
1:CC:104:PRO:HD3	1:CC:140:VAL:HG23	1.89	0.55
1:YA:104:PRO:HD3	1:YA:140:VAL:HG23	1.89	0.55
1:ZB:101:TRP:HB2	1:ZB:136:ILE:HD11	1.89	0.55
1:A:104:PRO:HD3	1:A:140:VAL:HG23	1.89	0.55
1:R:101:TRP:HB2	1:R:136:ILE:HD11	1.89	0.55
1:OA:142:LYS:HE3	1:PA:142:LYS:HE3	1.89	0.55
1:TA:104:PRO:HD3	1:TA:140:VAL:HG23	1.89	0.55
1:JC:101:TRP:HB2	1:JC:136:ILE:HD11	1.89	0.55
1:TC:101:TRP:HB2	1:TC:136:ILE:HD11	1.89	0.55
1:C:84:ARG:NH1	1:NB:49:GLU:OE2	2.39	0.55
1:YA:142:LYS:HE3	1:ZA:142:LYS:HE3	1.89	0.55
1:PB:17:LYS:HG3	1:PB:160:ILE:HD13	1.89	0.55
1:CC:142:LYS:HE3	1:DC:142:LYS:HE3	1.89	0.55
1:Z:142:LYS:HE3	1:AA:142:LYS:HE3	1.89	0.55
1:EA:142:LYS:HE3	1:FA:142:LYS:HE3	1.89	0.55
1:DB:104:PRO:HD3	1:DB:140:VAL:HG23	1.89	0.55
1:C:17:LYS:HG3	1:C:160:ILE:HD13	1.89	0.55
1:C:101:TRP:HB2	1:C:136:ILE:HD11	1.89	0.55
1:U:142:LYS:HE3	1:V:142:LYS:HE3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:104:PRO:HD3	1:JA:140:VAL:HG23	1.89	0.55
1:KB:101:TRP:HB2	1:KB:136:ILE:HD11	1.89	0.55
1:XB:104:PRO:HD3	1:XB:140:VAL:HG23	1.89	0.55
1:U:104:PRO:HD3	1:U:140:VAL:HG23	1.89	0.54
1:W:17:LYS:HG3	1:W:160:ILE:HD13	1.89	0.54
1:KB:17:LYS:HG3	1:KB:160:ILE:HD13	1.89	0.54
1:MC:142:LYS:HE3	1:NC:142:LYS:HE3	1.89	0.54
1:RC:104:PRO:HD3	1:RC:140:VAL:HG23	1.89	0.54
1:F:142:LYS:HE3	1:G:142:LYS:HE3	1.89	0.54
1:H:101:TRP:HB2	1:H:136:ILE:HD11	1.89	0.54
1:JA:142:LYS:HE3	1:KA:142:LYS:HE3	1.89	0.54
1:FB:101:TRP:HB2	1:FB:136:ILE:HD11	1.89	0.54
1:NB:142:LYS:HE3	1:OB:142:LYS:HE3	1.89	0.54
1:SB:142:LYS:HE3	1:TB:142:LYS:HE3	1.89	0.54
1:EC:101:TRP:HB2	1:EC:136:ILE:HD11	1.89	0.54
1:HC:104:PRO:HD3	1:HC:140:VAL:HG23	1.89	0.54
1:OC:17:LYS:HG3	1:OC:160:ILE:HD13	1.89	0.54
1:OC:101:TRP:HB2	1:OC:136:ILE:HD11	1.89	0.54
1:P:104:PRO:HD3	1:P:140:VAL:HG23	1.89	0.54
1:EA:49:GLU:OE2	1:JC:84:ARG:NH1	2.40	0.54
1:EA:104:PRO:HD3	1:EA:140:VAL:HG23	1.89	0.54
1:AB:101:TRP:HB2	1:AB:136:ILE:HD11	1.89	0.54
1:M:101:TRP:HB2	1:M:136:ILE:HD11	1.89	0.54
1:BA:17:LYS:HG3	1:BA:160:ILE:HD13	1.89	0.54
1:IB:142:LYS:HE3	1:JB:142:LYS:HE3	1.89	0.54
1:TA:142:LYS:HE3	1:UA:142:LYS:HE3	1.89	0.54
1:VA:101:TRP:HB2	1:VA:136:ILE:HD11	1.89	0.54
1:FB:17:LYS:HG3	1:FB:160:ILE:HD13	1.89	0.54
1:TC:17:LYS:HG3	1:TC:160:ILE:HD13	1.89	0.54
1:GA:101:TRP:HB2	1:GA:136:ILE:HD11	1.89	0.54
1:Z:104:PRO:HD3	1:Z:140:VAL:HG23	1.89	0.54
1:QA:101:TRP:HB2	1:QA:136:ILE:HD11	1.89	0.54
1:K:142:LYS:HE3	1:L:142:LYS:HE3	1.89	0.54
1:H:17:LYS:HG3	1:H:160:ILE:HD13	1.89	0.54
1:BA:101:TRP:HB2	1:BA:136:ILE:HD11	1.89	0.54
1:EC:17:LYS:HG3	1:EC:160:ILE:HD13	1.89	0.54
1:HC:142:LYS:HE3	1:IC:142:LYS:HE3	1.89	0.54
1:W:101:TRP:HB2	1:W:136:ILE:HD11	1.89	0.53
1:JC:17:LYS:HG3	1:JC:160:ILE:HD13	1.89	0.53
1:RC:142:LYS:HE3	1:SC:142:LYS:HE3	1.89	0.53
1:H:84:ARG:NH1	1:CC:49:GLU:OE2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:101:TRP:HB2	1:LA:136:ILE:HD11	1.89	0.53
1:OA:49:GLU:OE2	1:KB:84:ARG:NH1	2.41	0.53
1:VA:17:LYS:HG3	1:VA:160:ILE:HD13	1.89	0.53
1:XB:142:LYS:HE3	1:YB:142:LYS:HE3	1.89	0.53
1:P:142:LYS:HE3	1:Q:142:LYS:HE3	1.89	0.53
1:LA:17:LYS:HG3	1:LA:160:ILE:HD13	1.89	0.53
1:UB:101:TRP:HB2	1:UB:136:ILE:HD11	1.89	0.53
1:QA:17:LYS:HG3	1:QA:160:ILE:HD13	1.89	0.53
1:AB:17:LYS:HG3	1:AB:160:ILE:HD13	1.89	0.53
1:DB:142:LYS:HE3	1:EB:142:LYS:HE3	1.89	0.53
1:ZB:17:LYS:HG3	1:ZB:160:ILE:HD13	1.89	0.53
1:R:17:LYS:HG3	1:R:160:ILE:HD13	1.89	0.53
1:PB:101:TRP:HB2	1:PB:136:ILE:HD11	1.89	0.53
1:A:142:LYS:HE3	1:B:142:LYS:HE3	1.89	0.53
1:GA:17:LYS:HG3	1:GA:160:ILE:HD13	1.89	0.52
1:RB:88:ARG:HG3	1:RB:90:GLU:H	1.77	0.50
1:WB:88:ARG:HG3	1:WB:90:GLU:H	1.77	0.50
1:XA:88:ARG:HG3	1:XA:90:GLU:H	1.77	0.50
1:VC:88:ARG:HG3	1:VC:90:GLU:H	1.77	0.50
1:BC:88:ARG:HG3	1:BC:90:GLU:H	1.77	0.50
1:T:88:ARG:HG3	1:T:90:GLU:H	1.77	0.50
1:IA:88:ARG:HG3	1:IA:90:GLU:H	1.77	0.50
1:SA:88:ARG:HG3	1:SA:90:GLU:H	1.77	0.50
1:W:104:PRO:HD3	1:W:140:VAL:HG23	1.94	0.50
1:ZB:104:PRO:HD3	1:ZB:140:VAL:HG23	1.94	0.50
1:GA:104:PRO:HD3	1:GA:140:VAL:HG23	1.94	0.50
1:GC:88:ARG:HG3	1:GC:90:GLU:H	1.77	0.50
1:J:88:ARG:HG3	1:J:90:GLU:H	1.77	0.49
1:Y:88:ARG:HG3	1:Y:90:GLU:H	1.77	0.49
1:DA:88:ARG:HG3	1:DA:90:GLU:H	1.77	0.49
1:JC:104:PRO:HD3	1:JC:140:VAL:HG23	1.94	0.49
1:E:88:ARG:HG3	1:E:90:GLU:H	1.77	0.49
1:CB:88:ARG:HG3	1:CB:90:GLU:H	1.77	0.49
1:LC:88:ARG:HG3	1:LC:90:GLU:H	1.77	0.49
1:LA:104:PRO:HD3	1:LA:140:VAL:HG23	1.94	0.49
1:R:104:PRO:HD3	1:R:140:VAL:HG23	1.94	0.49
1:BA:104:PRO:HD3	1:BA:140:VAL:HG23	1.94	0.49
1:NA:88:ARG:HG3	1:NA:90:GLU:H	1.77	0.49
1:AB:104:PRO:HD3	1:AB:140:VAL:HG23	1.94	0.49
1:HB:88:ARG:HG3	1:HB:90:GLU:H	1.77	0.49
1:QB:43:SER:N	1:RB:90:GLU:OE2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QC:88:ARG:HG3	1:QC:90:GLU:H	1.77	0.49
1:TC:104:PRO:HD3	1:TC:140:VAL:HG23	1.94	0.49
1:C:104:PRO:HD3	1:C:140:VAL:HG23	1.94	0.49
1:O:88:ARG:HG3	1:O:90:GLU:H	1.77	0.49
1:HC:58:ARG:HG2	1:HC:91:ASP:HB3	1.95	0.49
1:P:58:ARG:HG2	1:P:91:ASP:HB3	1.95	0.49
1:MB:88:ARG:HG3	1:MB:90:GLU:H	1.77	0.49
1:EC:104:PRO:HD3	1:EC:140:VAL:HG23	1.94	0.49
1:S:43:SER:N	1:T:90:GLU:OE2	2.45	0.49
1:JA:49:GLU:OE2	1:TC:84:ARG:NH1	2.46	0.49
1:YA:58:ARG:HG2	1:YA:91:ASP:HB3	1.95	0.49
1:XB:58:ARG:HG2	1:XB:91:ASP:HB3	1.95	0.49
1:CC:58:ARG:HG2	1:CC:91:ASP:HB3	1.95	0.49
1:FB:104:PRO:HD3	1:FB:140:VAL:HG23	1.94	0.49
1:AC:43:SER:N	1:BC:90:GLU:OE2	2.45	0.49
1:M:104:PRO:HD3	1:M:140:VAL:HG23	1.94	0.49
1:EA:58:ARG:HG2	1:EA:91:ASP:HB3	1.95	0.49
1:OA:58:ARG:HG2	1:OA:91:ASP:HB3	1.95	0.49
1:RC:58:ARG:HG2	1:RC:91:ASP:HB3	1.95	0.49
1:Z:58:ARG:HG2	1:Z:91:ASP:HB3	1.95	0.48
1:QA:104:PRO:HD3	1:QA:140:VAL:HG23	1.94	0.48
1:MC:111:ALA:O	1:MC:153:LYS:NZ	2.35	0.48
1:KC:43:SER:N	1:LC:90:GLU:OE2	2.45	0.48
1:D:43:SER:N	1:E:90:GLU:OE2	2.45	0.48
1:U:58:ARG:HG2	1:U:91:ASP:HB3	1.95	0.48
1:QA:43:SER:N	1:RA:90:GLU:OE2	2.44	0.48
1:NB:58:ARG:HG2	1:NB:91:ASP:HB3	1.95	0.48
1:NC:56:GLY:O	1:NC:58:ARG:NH1	2.47	0.48
1:UC:43:SER:N	1:VC:90:GLU:OE2	2.45	0.48
1:R:43:SER:N	1:S:90:GLU:OE2	2.43	0.48
1:PB:104:PRO:HD3	1:PB:140:VAL:HG23	1.94	0.48
1:PA:56:GLY:O	1:PA:58:ARG:NH1	2.47	0.48
1:YA:111:ALA:O	1:YA:153:LYS:NZ	2.35	0.48
1:DB:58:ARG:HG2	1:DB:91:ASP:HB3	1.95	0.48
1:OC:104:PRO:HD3	1:OC:140:VAL:HG23	1.94	0.48
1:BB:43:SER:N	1:CB:90:GLU:OE2	2.45	0.48
1:FC:43:SER:N	1:GC:90:GLU:OE2	2.45	0.48
1:H:104:PRO:HD3	1:H:140:VAL:HG23	1.94	0.48
1:JA:58:ARG:HG2	1:JA:91:ASP:HB3	1.95	0.48
1:TA:58:ARG:HG2	1:TA:91:ASP:HB3	1.95	0.48
1:TB:56:GLY:O	1:TB:58:ARG:NH1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UB:104:PRO:HD3	1:UB:140:VAL:HG23	1.94	0.48
1:MC:58:ARG:HG2	1:MC:91:ASP:HB3	1.95	0.48
1:F:58:ARG:HG2	1:F:91:ASP:HB3	1.95	0.48
1:CA:43:SER:N	1:DA:90:GLU:OE2	2.45	0.48
1:RA:43:SER:N	1:SA:90:GLU:OE2	2.45	0.48
1:KB:104:PRO:HD3	1:KB:140:VAL:HG23	1.94	0.48
1:X:43:SER:N	1:Y:90:GLU:OE2	2.45	0.48
1:VA:43:SER:N	1:WA:90:GLU:OE2	2.43	0.48
1:K:58:ARG:HG2	1:K:91:ASP:HB3	1.95	0.48
1:MA:43:SER:N	1:NA:90:GLU:OE2	2.45	0.48
1:VA:104:PRO:HD3	1:VA:140:VAL:HG23	1.94	0.48
1:OC:43:SER:N	1:PC:90:GLU:OE2	2.43	0.48
1:Q:56:GLY:O	1:Q:58:ARG:NH1	2.47	0.47
1:BB:45:MET:HE2	1:CB:92:ILE:HD11	1.96	0.47
1:IB:58:ARG:HG2	1:IB:91:ASP:HB3	1.95	0.47
1:HA:43:SER:N	1:IA:90:GLU:OE2	2.45	0.47
1:SB:58:ARG:HG2	1:SB:91:ASP:HB3	1.94	0.47
1:PC:43:SER:N	1:QC:90:GLU:OE2	2.45	0.47
1:A:58:ARG:HG2	1:A:91:ASP:HB3	1.95	0.47
1:G:56:GLY:O	1:G:58:ARG:NH1	2.47	0.47
1:ZA:56:GLY:O	1:ZA:58:ARG:NH1	2.47	0.47
1:AC:45:MET:HE2	1:BC:92:ILE:HD11	1.96	0.47
1:L:56:GLY:O	1:L:58:ARG:NH1	2.47	0.47
1:OB:56:GLY:O	1:OB:58:ARG:NH1	2.47	0.47
1:M:43:SER:N	1:N:90:GLU:OE2	2.43	0.47
1:W:43:SER:N	1:X:90:GLU:OE2	2.43	0.47
1:GA:149:LEU:HD11	1:HA:104:PRO:HB2	1.97	0.47
1:UB:58:ARG:HG3	1:UB:91:ASP:HB3	1.97	0.47
1:PC:45:MET:HE2	1:QC:92:ILE:HD11	1.96	0.47
1:M:58:ARG:HG3	1:M:91:ASP:HB3	1.97	0.47
1:BA:149:LEU:HD11	1:CA:104:PRO:HB2	1.97	0.47
1:WA:43:SER:N	1:XA:90:GLU:OE2	2.45	0.47
1:ZB:58:ARG:HG3	1:ZB:91:ASP:HB3	1.97	0.47
1:EC:58:ARG:HG3	1:EC:91:ASP:HB3	1.97	0.47
1:FC:45:MET:HE2	1:GC:92:ILE:HD11	1.96	0.47
1:JC:58:ARG:HG3	1:JC:91:ASP:HB3	1.97	0.47
1:KC:45:MET:HE2	1:LC:92:ILE:HD11	1.96	0.47
1:B:56:GLY:O	1:B:58:ARG:NH1	2.47	0.47
1:N:45:MET:HE2	1:O:92:ILE:HD11	1.96	0.47
1:V:56:GLY:O	1:V:58:ARG:NH1	2.47	0.47
1:KA:56:GLY:O	1:KA:58:ARG:NH1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:45:MET:HE2	1:SA:92:ILE:HD11	1.96	0.47
1:AB:149:LEU:HD11	1:BB:104:PRO:HB2	1.97	0.47
1:PB:43:SER:N	1:QB:90:GLU:OE2	2.43	0.47
1:JC:149:LEU:HD11	1:KC:104:PRO:HB2	1.97	0.47
1:TC:149:LEU:HD11	1:UC:104:PRO:HB2	1.97	0.47
1:D:45:MET:HE2	1:E:92:ILE:HD11	1.96	0.47
1:KB:58:ARG:HG3	1:KB:91:ASP:HB3	1.97	0.47
1:QB:45:MET:HE2	1:RB:92:ILE:HD11	1.96	0.47
1:OC:58:ARG:HG3	1:OC:91:ASP:HB3	1.97	0.47
1:BA:58:ARG:HG3	1:BA:91:ASP:HB3	1.97	0.47
1:GB:45:MET:HE2	1:HB:92:ILE:HD11	1.96	0.47
1:PB:58:ARG:HG3	1:PB:91:ASP:HB3	1.97	0.47
1:TC:58:ARG:HG3	1:TC:91:ASP:HB3	1.97	0.47
1:S:45:MET:HE2	1:T:92:ILE:HD11	1.96	0.46
1:HA:45:MET:HE2	1:IA:92:ILE:HD11	1.96	0.46
1:IC:56:GLY:O	1:IC:58:ARG:NH1	2.47	0.46
1:I:45:MET:HE2	1:J:92:ILE:HD11	1.96	0.46
1:W:149:LEU:HD11	1:X:104:PRO:HB2	1.97	0.46
1:FA:56:GLY:O	1:FA:58:ARG:NH1	2.47	0.46
1:MA:45:MET:HE2	1:NA:92:ILE:HD11	1.96	0.46
1:QA:58:ARG:HG3	1:QA:91:ASP:HB3	1.97	0.46
1:G:16:ASN:HD21	1:G:77:GLY:HA3	1.81	0.46
1:R:149:LEU:HD11	1:S:104:PRO:HB2	1.97	0.46
1:W:58:ARG:HG3	1:W:91:ASP:HB3	1.97	0.46
1:XB:111:ALA:O	1:XB:153:LYS:NZ	2.35	0.46
1:NC:16:ASN:HD21	1:NC:77:GLY:HA3	1.81	0.46
1:SC:56:GLY:O	1:SC:58:ARG:NH1	2.47	0.46
1:C:149:LEU:HD11	1:D:104:PRO:HB2	1.97	0.46
1:OB:16:ASN:HD21	1:OB:77:GLY:HA3	1.81	0.46
1:VB:45:MET:HE2	1:WB:92:ILE:HD11	1.96	0.46
1:C:58:ARG:HG3	1:C:91:ASP:HB3	1.97	0.46
1:V:16:ASN:HD21	1:V:77:GLY:HA3	1.81	0.46
1:UA:56:GLY:O	1:UA:58:ARG:NH1	2.47	0.46
1:WA:45:MET:HE2	1:XA:92:ILE:HD11	1.96	0.46
1:UB:43:SER:N	1:VB:90:GLU:OE2	2.43	0.46
1:OC:149:LEU:HD11	1:PC:104:PRO:HB2	1.97	0.46
1:I:43:SER:N	1:J:90:GLU:OE2	2.45	0.46
1:X:45:MET:HE2	1:Y:92:ILE:HD11	1.96	0.46
1:KA:16:ASN:HD21	1:KA:77:GLY:HA3	1.81	0.46
1:FB:58:ARG:HG3	1:FB:91:ASP:HB3	1.97	0.46
1:LB:45:MET:HE2	1:MB:92:ILE:HD11	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:16:ASN:HD21	1:AA:77:GLY:HA3	1.81	0.46
1:CA:45:MET:HE2	1:DA:92:ILE:HD11	1.96	0.46
1:FA:16:ASN:HD21	1:FA:77:GLY:HA3	1.81	0.46
1:QA:149:LEU:HD11	1:RA:104:PRO:HB2	1.97	0.46
1:AB:58:ARG:HG3	1:AB:91:ASP:HB3	1.97	0.46
1:TB:16:ASN:HD21	1:TB:77:GLY:HA3	1.81	0.46
1:EC:149:LEU:HD11	1:FC:104:PRO:HB2	1.97	0.46
1:H:58:ARG:HG3	1:H:91:ASP:HB3	1.97	0.46
1:N:43:SER:N	1:O:90:GLU:OE2	2.45	0.46
1:Q:16:ASN:HD21	1:Q:77:GLY:HA3	1.81	0.46
1:Z:111:ALA:O	1:Z:153:LYS:NZ	2.35	0.46
1:PA:16:ASN:HD21	1:PA:77:GLY:HA3	1.81	0.46
1:VA:149:LEU:HD11	1:WA:104:PRO:HB2	1.97	0.46
1:JB:16:ASN:HD21	1:JB:77:GLY:HA3	1.81	0.46
1:PB:149:LEU:HD11	1:QB:104:PRO:HB2	1.97	0.46
1:VB:43:SER:N	1:WB:90:GLU:OE2	2.45	0.46
1:ZB:149:LEU:HD11	1:AC:104:PRO:HB2	1.97	0.46
1:R:58:ARG:HG3	1:R:91:ASP:HB3	1.97	0.46
1:GA:58:ARG:HG3	1:GA:91:ASP:HB3	1.97	0.46
1:LA:58:ARG:HG3	1:LA:91:ASP:HB3	1.97	0.46
1:LA:149:LEU:HD11	1:MA:104:PRO:HB2	1.97	0.46
1:FB:149:LEU:HD11	1:GB:104:PRO:HB2	1.97	0.46
1:UB:149:LEU:HD11	1:VB:104:PRO:HB2	1.97	0.46
1:YB:16:ASN:HD21	1:YB:77:GLY:HA3	1.81	0.46
1:YB:56:GLY:O	1:YB:58:ARG:NH1	2.47	0.46
1:VA:58:ARG:HG3	1:VA:91:ASP:HB3	1.97	0.46
1:SC:16:ASN:HD21	1:SC:77:GLY:HA3	1.81	0.46
1:H:149:LEU:HD11	1:I:104:PRO:HB2	1.97	0.45
1:L:16:ASN:HD21	1:L:77:GLY:HA3	1.81	0.45
1:UA:16:ASN:HD21	1:UA:77:GLY:HA3	1.81	0.45
1:JB:56:GLY:O	1:JB:58:ARG:NH1	2.47	0.45
1:IC:16:ASN:HD21	1:IC:77:GLY:HA3	1.81	0.45
1:UC:45:MET:HE2	1:VC:92:ILE:HD11	1.96	0.45
1:Z:27:GLU:OE1	1:AA:65:ARG:NH2	2.50	0.45
1:EB:56:GLY:O	1:EB:58:ARG:NH1	2.47	0.45
1:GB:43:SER:N	1:HB:90:GLU:OE2	2.45	0.45
1:KB:149:LEU:HD11	1:LB:104:PRO:HB2	1.97	0.45
1:EC:43:SER:N	1:FC:90:GLU:OE2	2.43	0.45
1:AA:56:GLY:O	1:AA:58:ARG:NH1	2.47	0.45
1:KA:51:LYS:HE2	1:KA:51:LYS:HB2	1.84	0.45
1:M:149:LEU:HD11	1:N:104:PRO:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:43:SER:N	1:MB:90:GLU:OE2	2.45	0.45
1:RC:27:GLU:OE1	1:SC:65:ARG:NH2	2.50	0.45
1:ZA:16:ASN:HD21	1:ZA:77:GLY:HA3	1.81	0.45
1:XB:27:GLU:OE1	1:YB:65:ARG:NH2	2.50	0.45
1:DC:16:ASN:HD21	1:DC:77:GLY:HA3	1.81	0.45
1:EB:16:ASN:HD21	1:EB:77:GLY:HA3	1.81	0.45
1:JA:27:GLU:OE1	1:KA:65:ARG:NH2	2.50	0.45
1:B:16:ASN:HD21	1:B:77:GLY:HA3	1.81	0.45
1:GA:43:SER:N	1:HA:90:GLU:OE2	2.43	0.45
1:EB:51:LYS:HE2	1:EB:51:LYS:HB2	1.84	0.45
1:HB:45:MET:HE2	1:HB:45:MET:HB3	1.89	0.45
1:DC:56:GLY:O	1:DC:58:ARG:NH1	2.47	0.45
1:EA:27:GLU:OE1	1:FA:65:ARG:NH2	2.50	0.45
1:A:27:GLU:OE1	1:B:65:ARG:NH2	2.50	0.45
1:C:43:SER:N	1:D:90:GLU:OE2	2.43	0.45
1:KB:43:SER:N	1:LB:90:GLU:OE2	2.43	0.45
1:BC:45:MET:HE2	1:BC:45:MET:HB3	1.89	0.44
1:JA:85:HIS:CE1	1:TC:85:HIS:HE1	2.35	0.44
1:M:36:ARG:HE	1:M:36:ARG:HB3	1.65	0.44
1:EC:36:ARG:HE	1:EC:36:ARG:HB3	1.65	0.44
1:ZB:43:SER:N	1:AC:90:GLU:OE2	2.44	0.44
1:K:111:ALA:O	1:K:153:LYS:NZ	2.35	0.44
1:ZA:51:LYS:HE2	1:ZA:51:LYS:HB2	1.84	0.44
1:EB:23:LEU:HD23	1:EB:23:LEU:HA	1.89	0.44
1:JA:6:ALA:HB1	1:TC:45:MET:HE2	2.00	0.44
1:MB:45:MET:HE2	1:MB:45:MET:HB3	1.89	0.44
1:RC:111:ALA:O	1:RC:153:LYS:NZ	2.35	0.44
1:T:113:LYS:O	1:T:153:LYS:NZ	2.51	0.44
1:OA:27:GLU:OE1	1:PA:65:ARG:NH2	2.50	0.44
1:HB:113:LYS:O	1:HB:153:LYS:NZ	2.51	0.44
1:VC:113:LYS:O	1:VC:153:LYS:NZ	2.51	0.44
1:DA:113:LYS:O	1:DA:153:LYS:NZ	2.51	0.44
1:EA:111:ALA:O	1:EA:153:LYS:NZ	2.35	0.44
1:XA:113:LYS:O	1:XA:153:LYS:NZ	2.51	0.44
1:MB:113:LYS:O	1:MB:153:LYS:NZ	2.51	0.44
1:GC:113:LYS:O	1:GC:153:LYS:NZ	2.51	0.44
1:NC:51:LYS:HE2	1:NC:51:LYS:HB2	1.84	0.44
1:S:153:LYS:HE3	1:S:153:LYS:HB2	1.83	0.43
1:FA:23:LEU:HD23	1:FA:23:LEU:HA	1.89	0.43
1:SC:23:LEU:HD23	1:SC:23:LEU:HA	1.89	0.43
1:SC:51:LYS:HE2	1:SC:51:LYS:HB2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:SER:N	1:I:90:GLU:OE2	2.43	0.43
1:P:27:GLU:OE1	1:Q:65:ARG:NH2	2.50	0.43
1:LA:43:SER:N	1:MA:90:GLU:OE2	2.44	0.43
1:NA:113:LYS:O	1:NA:153:LYS:NZ	2.51	0.43
1:IB:88:ARG:HG2	1:IB:90:GLU:H	1.83	0.43
1:F:135:TYR:OH	1:J:134:ASP:OD1	2.30	0.43
1:U:111:ALA:O	1:U:153:LYS:NZ	2.35	0.43
1:SB:111:ALA:O	1:SB:153:LYS:NZ	2.35	0.43
1:E:113:LYS:O	1:E:153:LYS:NZ	2.51	0.43
1:U:27:GLU:OE1	1:V:65:ARG:NH2	2.50	0.43
1:EA:88:ARG:HG2	1:EA:90:GLU:H	1.83	0.43
1:HA:153:LYS:HE3	1:HA:153:LYS:HB2	1.83	0.43
1:RB:113:LYS:O	1:RB:153:LYS:NZ	2.51	0.43
1:QC:113:LYS:O	1:QC:153:LYS:NZ	2.51	0.43
1:J:113:LYS:O	1:J:153:LYS:NZ	2.51	0.43
1:IA:113:LYS:O	1:IA:153:LYS:NZ	2.51	0.43
1:UA:51:LYS:HE2	1:UA:51:LYS:HB2	1.84	0.43
1:LC:113:LYS:O	1:LC:153:LYS:NZ	2.51	0.43
1:O:113:LYS:O	1:O:153:LYS:NZ	2.51	0.43
1:EA:6:ALA:HB1	1:JC:45:MET:HE2	2.00	0.43
1:GA:82:ILE:HG22	1:GA:87:GLY:HA3	2.01	0.43
1:TA:88:ARG:HG2	1:TA:90:GLU:H	1.83	0.43
1:AB:82:ILE:HG22	1:AB:87:GLY:HA3	2.01	0.43
1:CB:113:LYS:O	1:CB:153:LYS:NZ	2.51	0.43
1:DB:88:ARG:HG2	1:DB:90:GLU:H	1.83	0.43
1:WB:113:LYS:O	1:WB:153:LYS:NZ	2.51	0.43
1:YB:23:LEU:HD23	1:YB:23:LEU:HA	1.89	0.43
1:GC:45:MET:HE2	1:GC:45:MET:HB3	1.89	0.43
1:MC:88:ARG:HG2	1:MC:90:GLU:H	1.83	0.43
1:TC:82:ILE:HG22	1:TC:87:GLY:HA3	2.01	0.43
1:N:153:LYS:HB2	1:N:153:LYS:HE3	1.83	0.43
1:Y:113:LYS:O	1:Y:153:LYS:NZ	2.51	0.43
1:SA:113:LYS:O	1:SA:153:LYS:NZ	2.51	0.43
1:NB:88:ARG:HG2	1:NB:90:GLU:H	1.83	0.43
1:ZB:82:ILE:HG22	1:ZB:87:GLY:HA3	2.01	0.43
1:BC:113:LYS:O	1:BC:153:LYS:NZ	2.51	0.43
1:EC:82:ILE:HG22	1:EC:87:GLY:HA3	2.01	0.43
1:HC:88:ARG:HG2	1:HC:90:GLU:H	1.83	0.43
1:P:88:ARG:HG2	1:P:90:GLU:H	1.84	0.43
1:YA:115:ASP:OD1	1:YA:115:ASP:N	2.50	0.43
1:K:27:GLU:OE1	1:L:65:ARG:NH2	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:82:ILE:HG22	1:R:87:GLY:HA3	2.01	0.43
1:AB:85:HIS:HE1	1:XB:85:HIS:CE1	2.37	0.43
1:PB:36:ARG:HE	1:PB:36:ARG:HB3	1.65	0.43
1:SB:88:ARG:HG2	1:SB:90:GLU:H	1.83	0.43
1:JC:82:ILE:HG22	1:JC:87:GLY:HA3	2.01	0.43
1:PC:153:LYS:HB2	1:PC:153:LYS:HE3	1.83	0.43
1:RC:88:ARG:HG2	1:RC:90:GLU:H	1.83	0.43
1:Z:88:ARG:HG2	1:Z:90:GLU:H	1.83	0.43
1:KA:23:LEU:HD23	1:KA:23:LEU:HA	1.89	0.43
1:NA:45:MET:HE2	1:NA:45:MET:HB3	1.89	0.43
1:TA:27:GLU:OE1	1:UA:65:ARG:NH2	2.50	0.43
1:MC:115:ASP:OD1	1:MC:115:ASP:N	2.50	0.43
1:BA:82:ILE:HG22	1:BA:87:GLY:HA3	2.01	0.42
1:JA:88:ARG:HG2	1:JA:90:GLU:H	1.83	0.42
1:IB:27:GLU:OE1	1:JB:65:ARG:NH2	2.50	0.42
1:VB:153:LYS:HB2	1:VB:153:LYS:HE3	1.83	0.42
1:WB:45:MET:HE2	1:WB:45:MET:HB3	1.89	0.42
1:WB:111:ALA:HB2	1:WB:119:VAL:HG21	2.02	0.42
1:CC:88:ARG:HG2	1:CC:90:GLU:H	1.83	0.42
1:Q:23:LEU:HD23	1:Q:23:LEU:HA	1.89	0.42
1:Y:111:ALA:HB2	1:Y:119:VAL:HG21	2.02	0.42
1:QA:82:ILE:HG22	1:QA:87:GLY:HA3	2.01	0.42
1:HB:111:ALA:HB2	1:HB:119:VAL:HG21	2.02	0.42
1:NB:112:ARG:HG2	1:RB:152:ARG:HH12	1.85	0.42
1:NB:135:TYR:OH	1:RB:134:ASP:OD1	2.30	0.42
1:F:27:GLU:OE1	1:G:65:ARG:NH2	2.50	0.42
1:TA:112:ARG:HG2	1:XA:152:ARG:HH12	1.85	0.42
1:CC:115:ASP:OD1	1:CC:115:ASP:N	2.50	0.42
1:J:111:ALA:HB2	1:J:119:VAL:HG21	2.01	0.42
1:W:82:ILE:HG22	1:W:87:GLY:HA3	2.01	0.42
1:SB:112:ARG:HG2	1:WB:152:ARG:HH12	1.85	0.42
1:OC:82:ILE:HG22	1:OC:87:GLY:HA3	2.01	0.42
1:A:135:TYR:OH	1:E:134:ASP:OD1	2.30	0.42
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.89	0.42
1:DA:64:SER:OG	1:DA:65:ARG:N	2.53	0.42
1:IA:64:SER:OG	1:IA:65:ARG:N	2.53	0.42
1:OA:88:ARG:HG2	1:OA:90:GLU:H	1.83	0.42
1:XA:64:SER:OG	1:XA:65:ARG:N	2.53	0.42
1:YA:112:ARG:HG2	1:CB:152:ARG:HH12	1.85	0.42
1:UB:82:ILE:HG22	1:UB:87:GLY:HA3	2.01	0.42
1:Y:64:SER:OG	1:Y:65:ARG:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:85:HIS:CE1	1:JC:85:HIS:HE1	2.38	0.42
1:JA:112:ARG:HG2	1:NA:152:ARG:HH12	1.85	0.42
1:LA:82:ILE:HG22	1:LA:87:GLY:HA3	2.01	0.42
1:PB:82:ILE:HG22	1:PB:87:GLY:HA3	2.01	0.42
1:BC:111:ALA:HB2	1:BC:119:VAL:HG21	2.02	0.42
1:HC:112:ARG:HG2	1:LC:152:ARG:HH12	1.85	0.42
1:LC:64:SER:OG	1:LC:65:ARG:N	2.53	0.42
1:QC:64:SER:OG	1:QC:65:ARG:N	2.53	0.42
1:H:82:ILE:HG22	1:H:87:GLY:HA3	2.01	0.42
1:L:51:LYS:HE2	1:L:51:LYS:HB2	1.84	0.42
1:AA:23:LEU:HD23	1:AA:23:LEU:HA	1.89	0.42
1:GC:64:SER:OG	1:GC:65:ARG:N	2.53	0.42
1:A:88:ARG:HG2	1:A:90:GLU:H	1.83	0.42
1:E:64:SER:OG	1:E:65:ARG:N	2.53	0.42
1:T:64:SER:OG	1:T:65:ARG:N	2.53	0.42
1:U:88:ARG:HG2	1:U:90:GLU:H	1.83	0.42
1:U:112:ARG:HG2	1:Y:152:ARG:HH12	1.85	0.42
1:V:23:LEU:HD23	1:V:23:LEU:HA	1.89	0.42
1:IA:111:ALA:HB2	1:IA:119:VAL:HG21	2.02	0.42
1:FB:36:ARG:HE	1:FB:36:ARG:HB3	1.65	0.42
1:HB:64:SER:OG	1:HB:65:ARG:N	2.53	0.42
1:NB:27:GLU:OE1	1:OB:65:ARG:NH2	2.50	0.42
1:SB:27:GLU:OE1	1:TB:65:ARG:NH2	2.50	0.42
1:CC:112:ARG:HG2	1:GC:152:ARG:HH12	1.85	0.42
1:LC:111:ALA:HB2	1:LC:119:VAL:HG21	2.01	0.42
1:C:82:ILE:HG22	1:C:87:GLY:HA3	2.01	0.42
1:E:111:ALA:HB2	1:E:119:VAL:HG21	2.02	0.42
1:H:45:MET:HE2	1:CC:6:ALA:HB1	2.00	0.42
1:M:82:ILE:HG22	1:M:87:GLY:HA3	2.01	0.42
1:P:115:ASP:OD1	1:P:115:ASP:N	2.50	0.42
1:OA:112:ARG:HG2	1:SA:152:ARG:HH12	1.85	0.42
1:YA:27:GLU:OE1	1:ZA:65:ARG:NH2	2.50	0.42
1:YA:88:ARG:HG2	1:YA:90:GLU:H	1.83	0.42
1:LB:153:LYS:HB2	1:LB:153:LYS:HE3	1.83	0.42
1:F:88:ARG:HG2	1:F:90:GLU:H	1.84	0.42
1:O:64:SER:OG	1:O:65:ARG:N	2.53	0.42
1:DA:111:ALA:HB2	1:DA:119:VAL:HG21	2.02	0.42
1:KB:82:ILE:HG22	1:KB:87:GLY:HA3	2.01	0.42
1:J:45:MET:HE2	1:J:45:MET:HB3	1.89	0.41
1:K:88:ARG:HG2	1:K:90:GLU:H	1.83	0.41
1:O:111:ALA:HB2	1:O:119:VAL:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:112:ARG:HG2	1:DA:152:ARG:HH12	1.85	0.41
1:SA:111:ALA:HB2	1:SA:119:VAL:HG21	2.02	0.41
1:VA:82:ILE:HG22	1:VA:87:GLY:HA3	2.01	0.41
1:XA:111:ALA:HB2	1:XA:119:VAL:HG21	2.02	0.41
1:AB:43:SER:N	1:BB:90:GLU:OE2	2.43	0.41
1:IC:23:LEU:HD23	1:IC:23:LEU:HA	1.89	0.41
1:P:112:ARG:HG2	1:T:152:ARG:HH12	1.85	0.41
1:NA:64:SER:OG	1:NA:65:ARG:N	2.53	0.41
1:FB:82:ILE:HG22	1:FB:87:GLY:HA3	2.01	0.41
1:BC:64:SER:OG	1:BC:65:ARG:N	2.53	0.41
1:MC:27:GLU:OE1	1:NC:65:ARG:NH2	2.50	0.41
1:O:45:MET:HE2	1:O:45:MET:HB3	1.89	0.41
1:U:85:HIS:CE1	1:ZB:85:HIS:HE1	2.39	0.41
1:MA:153:LYS:HE3	1:MA:153:LYS:HB2	1.83	0.41
1:BB:153:LYS:HE3	1:BB:153:LYS:HB2	1.83	0.41
1:IB:112:ARG:HG2	1:MB:152:ARG:HH12	1.85	0.41
1:MB:111:ALA:HB2	1:MB:119:VAL:HG21	2.01	0.41
1:RB:111:ALA:HB2	1:RB:119:VAL:HG21	2.02	0.41
1:XB:88:ARG:HG2	1:XB:90:GLU:H	1.83	0.41
1:JC:43:SER:N	1:KC:90:GLU:OE2	2.43	0.41
1:VC:45:MET:HE2	1:VC:45:MET:HB3	1.89	0.41
1:K:35:LEU:HD23	1:K:35:LEU:HA	1.93	0.41
1:EA:112:ARG:HG2	1:IA:152:ARG:HH12	1.85	0.41
1:EA:135:TYR:OH	1:IA:134:ASP:OD1	2.30	0.41
1:NA:111:ALA:HB2	1:NA:119:VAL:HG21	2.01	0.41
1:RA:153:LYS:HE3	1:RA:153:LYS:HB2	1.83	0.41
1:AB:45:MET:HE2	1:XB:6:ALA:HB1	2.02	0.41
1:XB:112:ARG:HG2	1:BC:152:ARG:HH12	1.85	0.41
1:MC:112:ARG:HG2	1:QC:152:ARG:HH12	1.85	0.41
1:VC:111:ALA:HB2	1:VC:119:VAL:HG21	2.01	0.41
1:C:85:HIS:HE1	1:NB:85:HIS:CE1	2.38	0.41
1:F:112:ARG:HG2	1:J:152:ARG:HH12	1.85	0.41
1:CB:64:SER:OG	1:CB:65:ARG:N	2.53	0.41
1:CB:111:ALA:HB2	1:CB:119:VAL:HG21	2.02	0.41
1:DB:112:ARG:HG2	1:HB:152:ARG:HH12	1.85	0.41
1:GC:111:ALA:HB2	1:GC:119:VAL:HG21	2.02	0.41
1:HC:115:ASP:OD1	1:HC:115:ASP:N	2.50	0.41
1:J:64:SER:OG	1:J:65:ARG:N	2.53	0.41
1:K:112:ARG:HG2	1:O:152:ARG:HH12	1.85	0.41
1:CB:45:MET:HE2	1:CB:45:MET:HB3	1.89	0.41
1:VC:64:SER:OG	1:VC:65:ARG:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:111:ALA:O	1:OA:153:LYS:NZ	2.35	0.41
1:TA:115:ASP:OD1	1:TA:115:ASP:N	2.51	0.41
1:HC:35:LEU:HD23	1:HC:35:LEU:HA	1.93	0.41
1:A:112:ARG:HG2	1:E:152:ARG:HH12	1.85	0.41
1:LA:36:ARG:HE	1:LA:36:ARG:HB3	1.65	0.41
1:OA:6:ALA:HB1	1:KB:45:MET:HE2	2.02	0.41
1:MB:64:SER:OG	1:MB:65:ARG:N	2.53	0.41
1:NB:35:LEU:HD23	1:NB:35:LEU:HA	1.93	0.41
1:CC:27:GLU:OE1	1:DC:65:ARG:NH2	2.50	0.41
1:P:85:HIS:CE1	1:EC:85:HIS:HE1	2.39	0.41
1:R:72:ASP:HA	1:R:75:VAL:HG12	2.03	0.41
1:BA:43:SER:N	1:CA:90:GLU:OE2	2.43	0.41
1:GA:72:ASP:HA	1:GA:75:VAL:HG12	2.03	0.41
1:IA:110:LEU:HD23	1:IA:110:LEU:HA	1.95	0.41
1:DB:27:GLU:OE1	1:EB:65:ARG:NH2	2.50	0.41
1:FB:85:HIS:HE1	1:SB:85:HIS:CE1	2.38	0.41
1:AC:153:LYS:HB2	1:AC:153:LYS:HE3	1.83	0.41
1:HC:27:GLU:OE1	1:IC:65:ARG:NH2	2.50	0.41
1:RC:112:ARG:HG2	1:VC:152:ARG:HH12	1.85	0.41
1:VC:110:LEU:HD23	1:VC:110:LEU:HA	1.95	0.41
1:LA:72:ASP:HA	1:LA:75:VAL:HG12	2.03	0.41
1:UA:23:LEU:HD23	1:UA:23:LEU:HA	1.89	0.41
1:FB:43:SER:N	1:GB:90:GLU:OE2	2.43	0.41
1:SB:35:LEU:HD23	1:SB:35:LEU:HA	1.93	0.41
1:WB:64:SER:OG	1:WB:65:ARG:N	2.53	0.41
1:I:153:LYS:HE3	1:I:153:LYS:HB2	1.83	0.40
1:NA:110:LEU:HD23	1:NA:110:LEU:HA	1.95	0.40
1:QA:72:ASP:HA	1:QA:75:VAL:HG12	2.03	0.40
1:XA:45:MET:HE2	1:XA:45:MET:HB3	1.89	0.40
1:P:35:LEU:HD23	1:P:35:LEU:HA	1.93	0.40
1:EA:115:ASP:OD1	1:EA:115:ASP:N	2.50	0.40
1:QA:36:ARG:HE	1:QA:36:ARG:HB3	1.65	0.40
1:SA:64:SER:OG	1:SA:65:ARG:N	2.53	0.40
1:RB:64:SER:OG	1:RB:65:ARG:N	2.53	0.40
1:CC:35:LEU:HD23	1:CC:35:LEU:HA	1.93	0.40
1:FC:153:LYS:HB2	1:FC:153:LYS:HE3	1.83	0.40
1:OC:36:ARG:HE	1:OC:36:ARG:HB3	1.65	0.40
1:QC:111:ALA:HB2	1:QC:119:VAL:HG21	2.01	0.40
1:C:72:ASP:HA	1:C:75:VAL:HG12	2.04	0.40
1:ZB:72:ASP:HA	1:ZB:75:VAL:HG12	2.03	0.40
1:B:51:LYS:HE2	1:B:51:LYS:HB2	1.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:ASP:HA	1:H:75:VAL:HG12	2.03	0.40
1:W:72:ASP:HA	1:W:75:VAL:HG12	2.03	0.40
1:VA:72:ASP:HA	1:VA:75:VAL:HG12	2.03	0.40
1:AB:72:ASP:HA	1:AB:75:VAL:HG12	2.03	0.40
1:FB:72:ASP:HA	1:FB:75:VAL:HG12	2.04	0.40
1:XB:35:LEU:HD23	1:XB:35:LEU:HA	1.93	0.40
1:T:111:ALA:HB2	1:T:119:VAL:HG21	2.02	0.40
1:CA:153:LYS:HB2	1:CA:153:LYS:HE3	1.83	0.40
1:SA:45:MET:HE2	1:SA:45:MET:HB3	1.89	0.40
1:UC:153:LYS:HE3	1:UC:153:LYS:HB2	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	AA	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	AB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	AC	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	B	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	BA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	BB	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	BC	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	C	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	CA	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	CB	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	CC	156/163 (96%)	153 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	DA	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	DB	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	DC	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	E	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	EA	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	EB	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	EC	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	F	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	FA	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	FB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	FC	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	G	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	GA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	GB	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	GC	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	H	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	HA	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	HB	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	HC	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	I	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	IA	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	IB	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	IC	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	J	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	JA	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	JB	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	JC	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	K	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	KA	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	KB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	KC	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	L	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	LA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	LB	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	LC	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	M	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	MA	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	MB	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	MC	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	N	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	NA	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	NB	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	NC	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	O	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	OA	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	OB	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	OC	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	P	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	PA	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	PB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	PC	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	Q	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	QA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	QB	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	QC	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	R	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	RA	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	RB	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	RC	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	S	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	SA	147/163 (90%)	143 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SB	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	SC	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	T	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	TA	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	TB	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	TC	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	U	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	UA	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	UB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	UC	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	V	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	VA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	VB	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	VC	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	W	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	WA	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	WB	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	X	145/163 (89%)	139 (96%)	6 (4%)	0	100	100
1	XA	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	XB	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	Y	147/163 (90%)	143 (97%)	4 (3%)	0	100	100
1	YA	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	YB	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	Z	156/163 (96%)	153 (98%)	3 (2%)	0	100	100
1	ZA	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	ZB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
All	All	15060/16300 (92%)	14600 (97%)	460 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	121/126 (96%)	121 (100%)	0	100	100
1	AA	115/126 (91%)	115 (100%)	0	100	100
1	AB	123/126 (98%)	123 (100%)	0	100	100
1	AC	114/126 (90%)	114 (100%)	0	100	100
1	B	115/126 (91%)	115 (100%)	0	100	100
1	BA	123/126 (98%)	123 (100%)	0	100	100
1	BB	114/126 (90%)	114 (100%)	0	100	100
1	BC	115/126 (91%)	115 (100%)	0	100	100
1	C	123/126 (98%)	123 (100%)	0	100	100
1	CA	114/126 (90%)	114 (100%)	0	100	100
1	CB	115/126 (91%)	115 (100%)	0	100	100
1	CC	121/126 (96%)	121 (100%)	0	100	100
1	D	114/126 (90%)	114 (100%)	0	100	100
1	DA	115/126 (91%)	115 (100%)	0	100	100
1	DB	121/126 (96%)	121 (100%)	0	100	100
1	DC	115/126 (91%)	115 (100%)	0	100	100
1	E	115/126 (91%)	115 (100%)	0	100	100
1	EA	121/126 (96%)	121 (100%)	0	100	100
1	EB	115/126 (91%)	115 (100%)	0	100	100
1	EC	123/126 (98%)	123 (100%)	0	100	100
1	F	121/126 (96%)	121 (100%)	0	100	100
1	FA	115/126 (91%)	115 (100%)	0	100	100
1	FB	123/126 (98%)	123 (100%)	0	100	100
1	FC	114/126 (90%)	114 (100%)	0	100	100
1	G	115/126 (91%)	115 (100%)	0	100	100
1	GA	123/126 (98%)	123 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GB	114/126 (90%)	114 (100%)	0	100	100
1	GC	115/126 (91%)	115 (100%)	0	100	100
1	H	123/126 (98%)	123 (100%)	0	100	100
1	HA	114/126 (90%)	114 (100%)	0	100	100
1	HB	115/126 (91%)	115 (100%)	0	100	100
1	HC	121/126 (96%)	121 (100%)	0	100	100
1	I	114/126 (90%)	114 (100%)	0	100	100
1	IA	115/126 (91%)	115 (100%)	0	100	100
1	IB	121/126 (96%)	121 (100%)	0	100	100
1	IC	115/126 (91%)	115 (100%)	0	100	100
1	J	115/126 (91%)	115 (100%)	0	100	100
1	JA	121/126 (96%)	121 (100%)	0	100	100
1	JB	115/126 (91%)	115 (100%)	0	100	100
1	JC	123/126 (98%)	123 (100%)	0	100	100
1	K	121/126 (96%)	121 (100%)	0	100	100
1	KA	115/126 (91%)	115 (100%)	0	100	100
1	KB	123/126 (98%)	123 (100%)	0	100	100
1	KC	114/126 (90%)	114 (100%)	0	100	100
1	L	115/126 (91%)	115 (100%)	0	100	100
1	LA	123/126 (98%)	123 (100%)	0	100	100
1	LB	114/126 (90%)	114 (100%)	0	100	100
1	LC	115/126 (91%)	115 (100%)	0	100	100
1	M	123/126 (98%)	123 (100%)	0	100	100
1	MA	114/126 (90%)	114 (100%)	0	100	100
1	MB	115/126 (91%)	115 (100%)	0	100	100
1	MC	121/126 (96%)	121 (100%)	0	100	100
1	N	114/126 (90%)	114 (100%)	0	100	100
1	NA	115/126 (91%)	115 (100%)	0	100	100
1	NB	121/126 (96%)	121 (100%)	0	100	100
1	NC	115/126 (91%)	115 (100%)	0	100	100
1	O	115/126 (91%)	115 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	OA	121/126 (96%)	121 (100%)	0	100	100
1	OB	115/126 (91%)	115 (100%)	0	100	100
1	OC	123/126 (98%)	123 (100%)	0	100	100
1	P	121/126 (96%)	121 (100%)	0	100	100
1	PA	115/126 (91%)	115 (100%)	0	100	100
1	PB	123/126 (98%)	123 (100%)	0	100	100
1	PC	114/126 (90%)	114 (100%)	0	100	100
1	Q	115/126 (91%)	115 (100%)	0	100	100
1	QA	123/126 (98%)	123 (100%)	0	100	100
1	QB	114/126 (90%)	114 (100%)	0	100	100
1	QC	115/126 (91%)	115 (100%)	0	100	100
1	R	123/126 (98%)	123 (100%)	0	100	100
1	RA	114/126 (90%)	114 (100%)	0	100	100
1	RB	115/126 (91%)	115 (100%)	0	100	100
1	RC	121/126 (96%)	121 (100%)	0	100	100
1	S	114/126 (90%)	114 (100%)	0	100	100
1	SA	115/126 (91%)	115 (100%)	0	100	100
1	SB	121/126 (96%)	121 (100%)	0	100	100
1	SC	115/126 (91%)	115 (100%)	0	100	100
1	T	115/126 (91%)	115 (100%)	0	100	100
1	TA	121/126 (96%)	121 (100%)	0	100	100
1	TB	115/126 (91%)	115 (100%)	0	100	100
1	TC	123/126 (98%)	123 (100%)	0	100	100
1	U	121/126 (96%)	121 (100%)	0	100	100
1	UA	115/126 (91%)	115 (100%)	0	100	100
1	UB	123/126 (98%)	123 (100%)	0	100	100
1	UC	114/126 (90%)	114 (100%)	0	100	100
1	V	115/126 (91%)	115 (100%)	0	100	100
1	VA	123/126 (98%)	123 (100%)	0	100	100
1	VB	114/126 (90%)	114 (100%)	0	100	100
1	VC	115/126 (91%)	115 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	123/126 (98%)	123 (100%)	0	100	100
1	WA	114/126 (90%)	114 (100%)	0	100	100
1	WB	115/126 (91%)	115 (100%)	0	100	100
1	X	114/126 (90%)	114 (100%)	0	100	100
1	XA	115/126 (91%)	115 (100%)	0	100	100
1	XB	121/126 (96%)	121 (100%)	0	100	100
1	Y	115/126 (91%)	115 (100%)	0	100	100
1	YA	121/126 (96%)	121 (100%)	0	100	100
1	YB	115/126 (91%)	115 (100%)	0	100	100
1	Z	121/126 (96%)	121 (100%)	0	100	100
1	ZA	115/126 (91%)	115 (100%)	0	100	100
1	ZB	123/126 (98%)	123 (100%)	0	100	100
All	All	11760/12600 (93%)	11760 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	C	30	ASN
1	C	85	HIS
1	D	67	ASN
1	E	85	HIS
1	E	146	ASN
1	F	85	HIS
1	H	30	ASN
1	H	85	HIS
1	I	67	ASN
1	J	85	HIS
1	J	146	ASN
1	K	85	HIS
1	M	30	ASN
1	M	85	HIS
1	N	67	ASN
1	O	85	HIS
1	O	146	ASN
1	P	85	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	30	ASN
1	R	85	HIS
1	S	30	ASN
1	S	67	ASN
1	T	85	HIS
1	T	146	ASN
1	U	85	HIS
1	W	16	ASN
1	W	30	ASN
1	W	85	HIS
1	X	67	ASN
1	Y	85	HIS
1	Y	146	ASN
1	Z	85	HIS
1	BA	30	ASN
1	BA	85	HIS
1	CA	30	ASN
1	CA	67	ASN
1	DA	85	HIS
1	DA	146	ASN
1	EA	85	HIS
1	GA	30	ASN
1	GA	85	HIS
1	HA	67	ASN
1	IA	85	HIS
1	IA	146	ASN
1	JA	85	HIS
1	LA	16	ASN
1	LA	30	ASN
1	LA	85	HIS
1	MA	30	ASN
1	MA	67	ASN
1	NA	85	HIS
1	NA	146	ASN
1	OA	85	HIS
1	QA	30	ASN
1	QA	85	HIS
1	RA	67	ASN
1	SA	85	HIS
1	SA	146	ASN
1	TA	85	HIS
1	VA	30	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	VA	85	HIS
1	WA	67	ASN
1	XA	85	HIS
1	XA	146	ASN
1	YA	85	HIS
1	AB	30	ASN
1	AB	85	HIS
1	BB	67	ASN
1	CB	85	HIS
1	CB	146	ASN
1	DB	85	HIS
1	FB	30	ASN
1	FB	85	HIS
1	GB	67	ASN
1	HB	85	HIS
1	HB	146	ASN
1	IB	85	HIS
1	KB	30	ASN
1	KB	85	HIS
1	LB	67	ASN
1	MB	85	HIS
1	MB	146	ASN
1	NB	85	HIS
1	PB	30	ASN
1	PB	85	HIS
1	QB	67	ASN
1	RB	85	HIS
1	RB	146	ASN
1	SB	85	HIS
1	UB	30	ASN
1	UB	85	HIS
1	VB	67	ASN
1	WB	85	HIS
1	WB	146	ASN
1	XB	85	HIS
1	ZB	30	ASN
1	ZB	85	HIS
1	AC	67	ASN
1	BC	85	HIS
1	BC	146	ASN
1	CC	85	HIS
1	EC	30	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	EC	85	HIS
1	FC	67	ASN
1	GC	85	HIS
1	GC	146	ASN
1	HC	85	HIS
1	JC	30	ASN
1	JC	85	HIS
1	KC	67	ASN
1	LC	85	HIS
1	LC	146	ASN
1	MC	85	HIS
1	OC	16	ASN
1	OC	30	ASN
1	OC	85	HIS
1	PC	67	ASN
1	QC	85	HIS
1	QC	146	ASN
1	RC	85	HIS
1	TC	30	ASN
1	TC	85	HIS
1	UC	30	ASN
1	UC	67	ASN
1	VC	85	HIS
1	VC	146	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

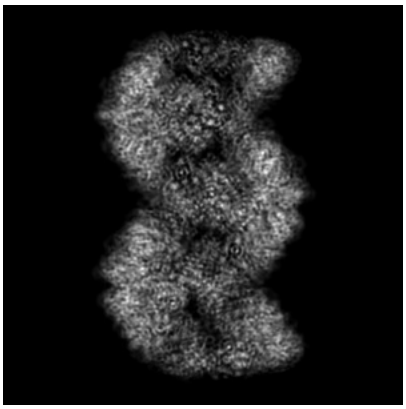
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51001. These allow visual inspection of the internal detail of the map and identification of artifacts.

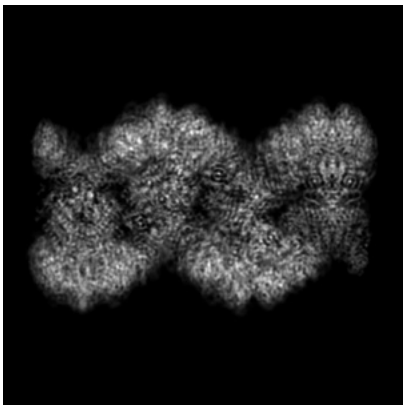
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

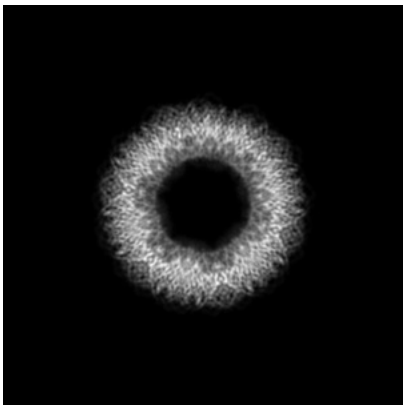
6.1.1 Primary map



X

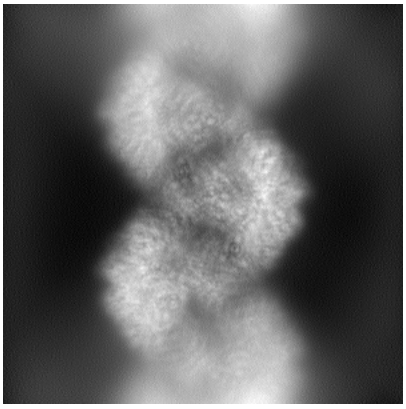


Y

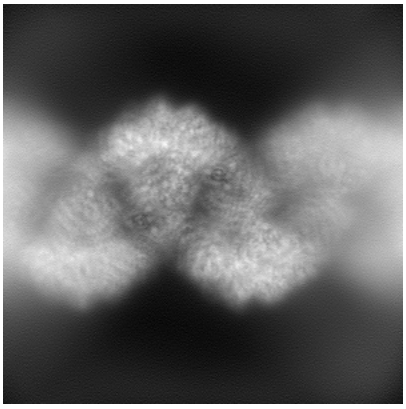


Z

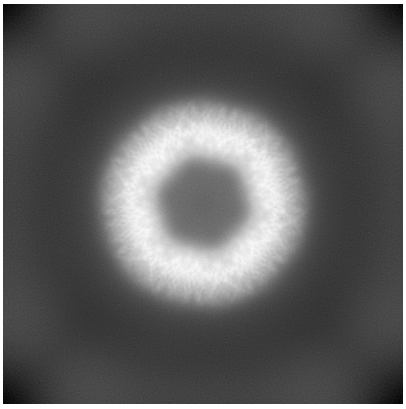
6.1.2 Raw map



X



Y

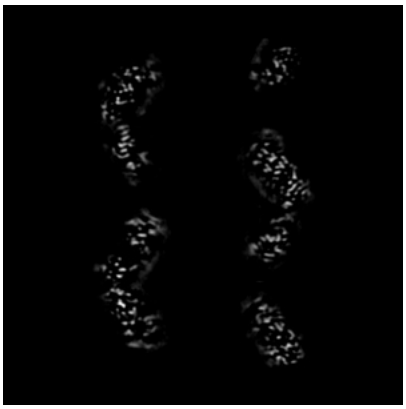


Z

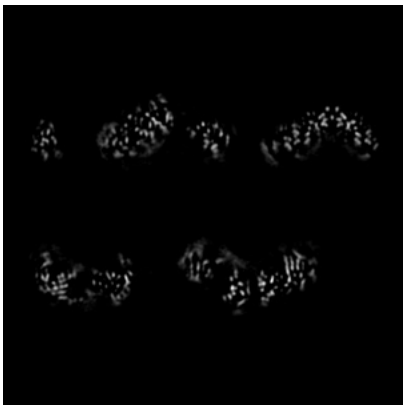
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



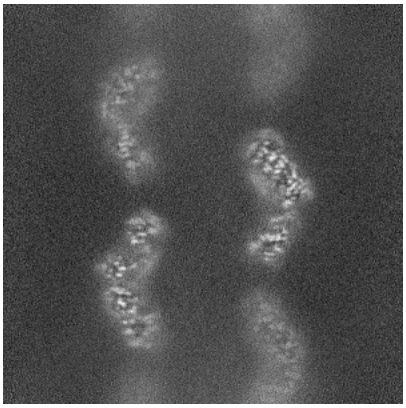
X Index: 220



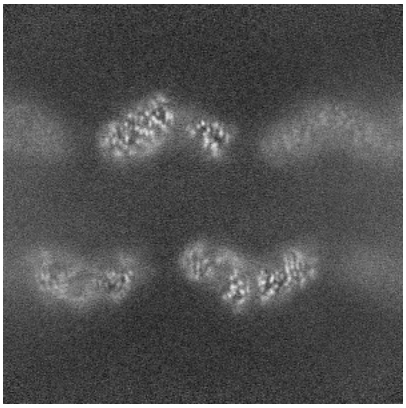
Y Index: 220

Z Index: 220

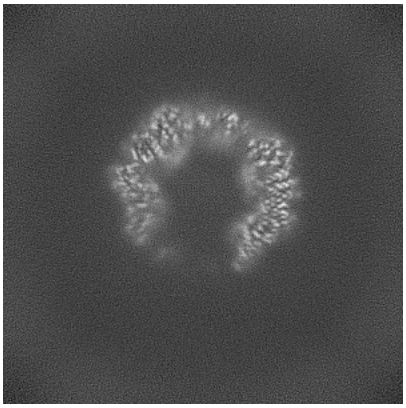
6.2.2 Raw map



X Index: 220



Y Index: 220

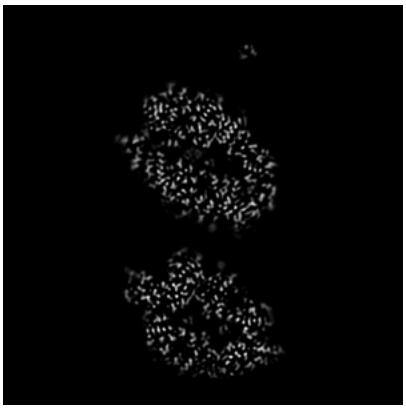


Z Index: 220

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

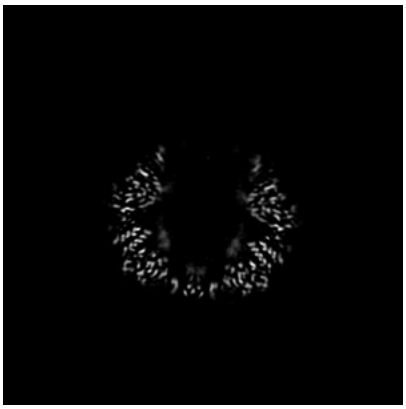
6.3 Largest variance slices (i)

6.3.1 Primary map



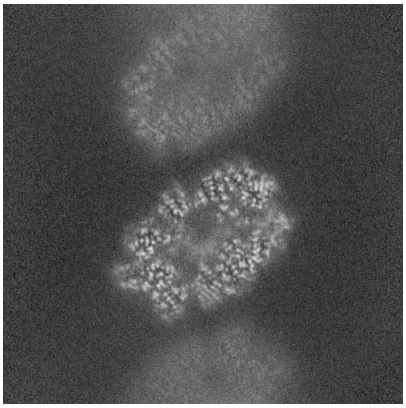
X Index: 144

Y Index: 152

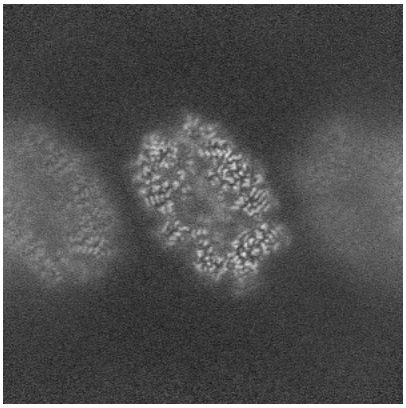


Z Index: 131

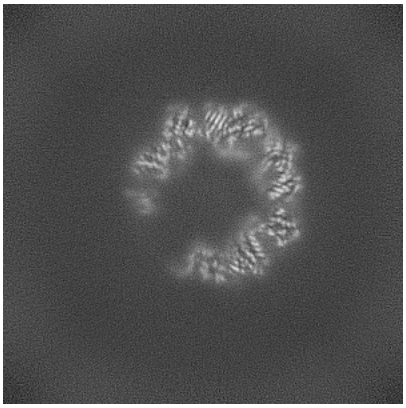
6.3.2 Raw map



X Index: 288



Y Index: 290

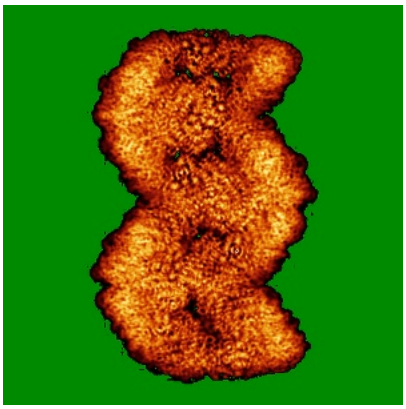


Z Index: 198

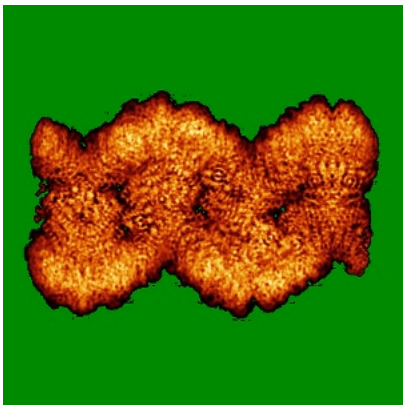
The images above show the largest variance slices of the map in three orthogonal directions.

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

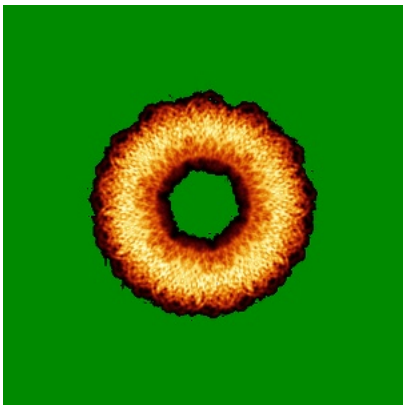
6.4.1 Primary map



X

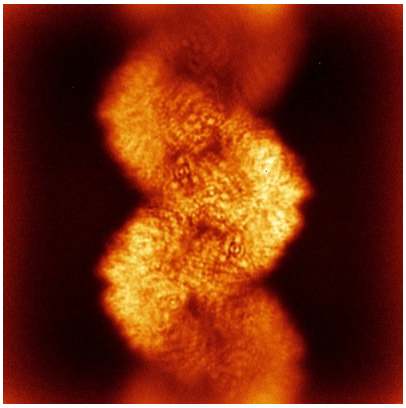


Y

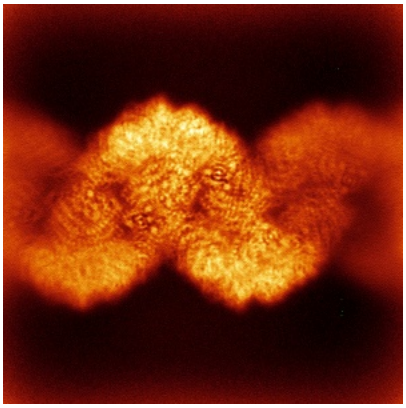


Z

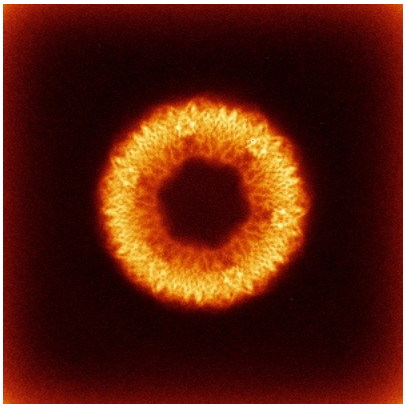
6.4.2 Raw map



X



Y

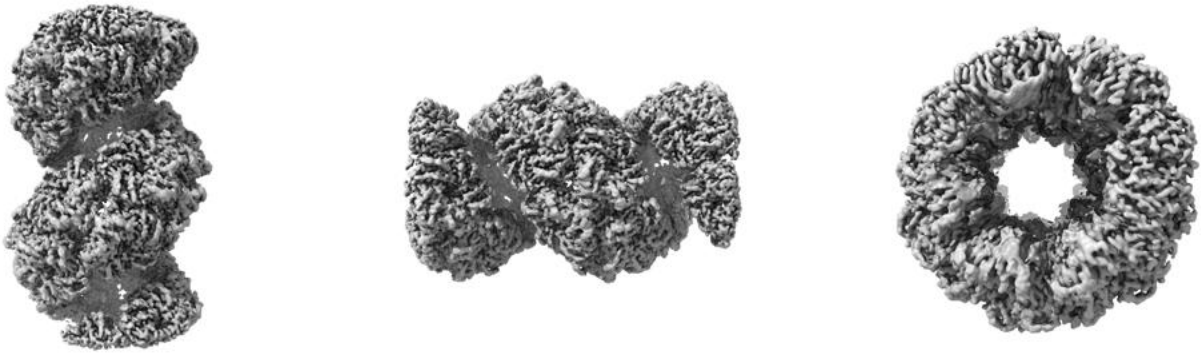


Z

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

6.5 Orthogonal surface views (i)

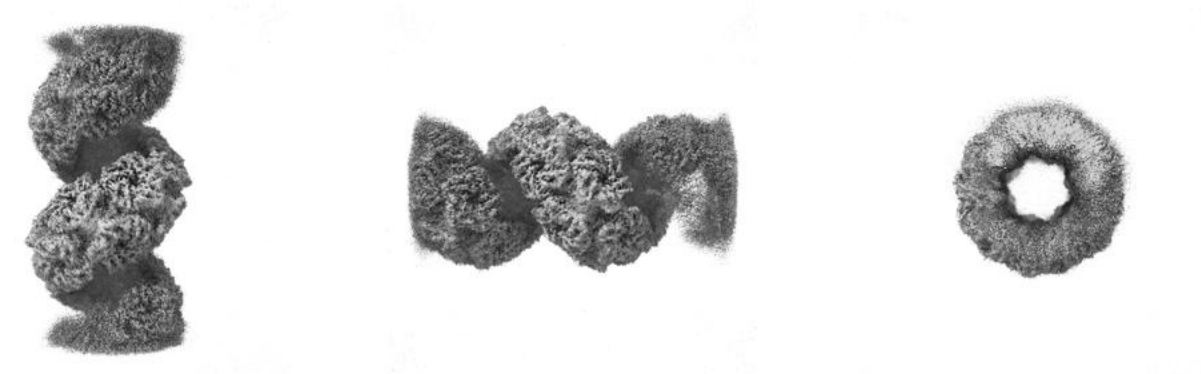
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

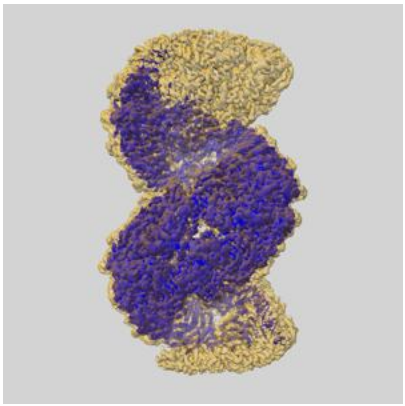
6.6 Mask visualisation

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

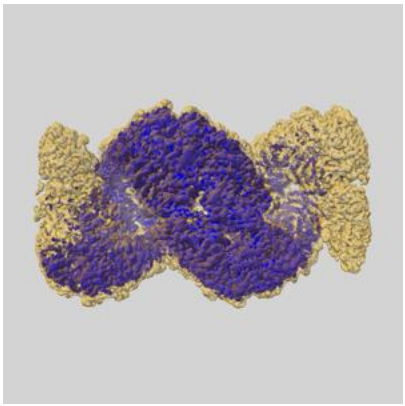
A mask typically either:

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

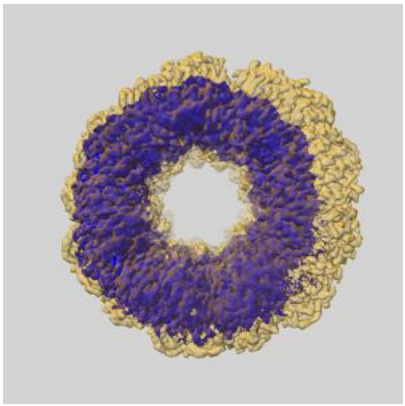
6.6.1 emd_51001_msk_2.map



X

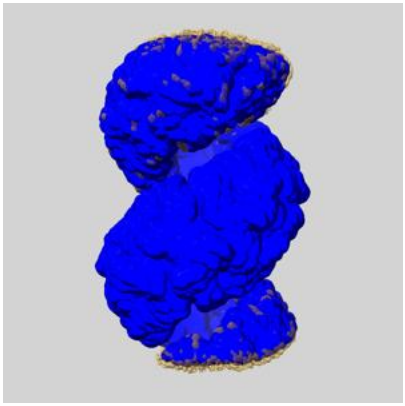


Y

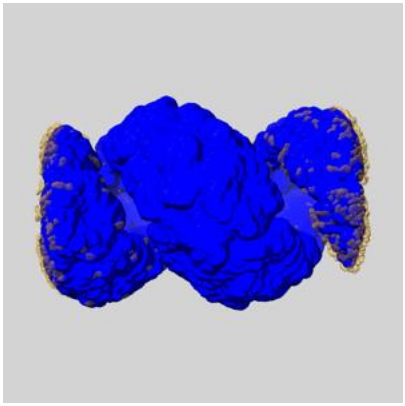


Z

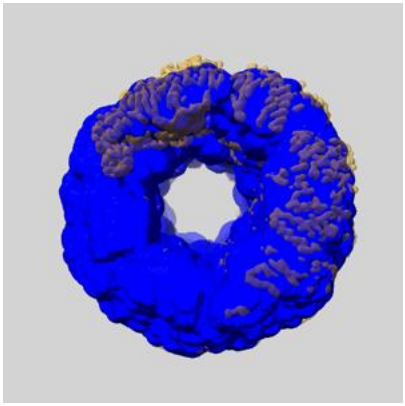
6.6.2 emd_51001_msk_1.map



X



Y

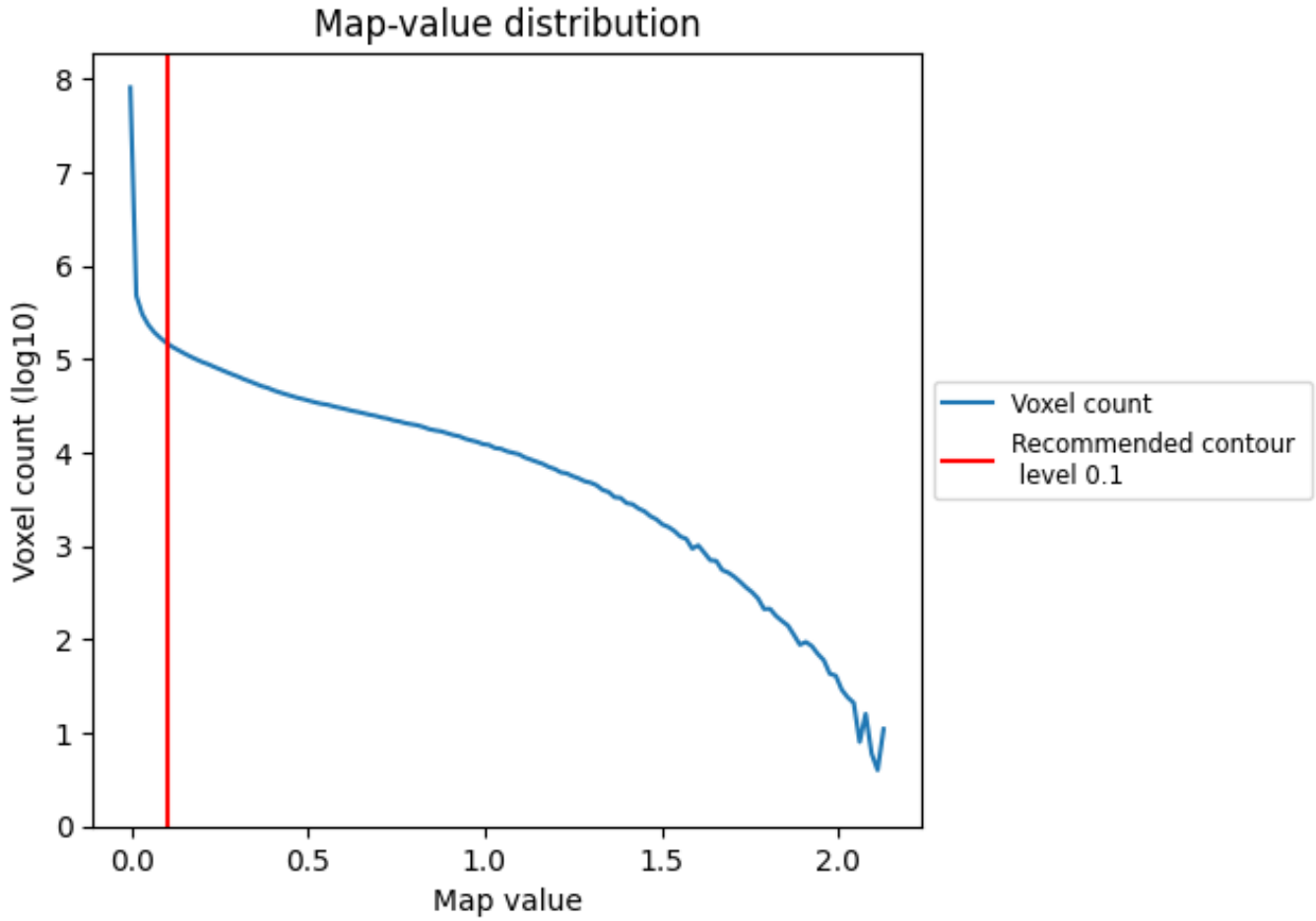


Z

7 Map analysis

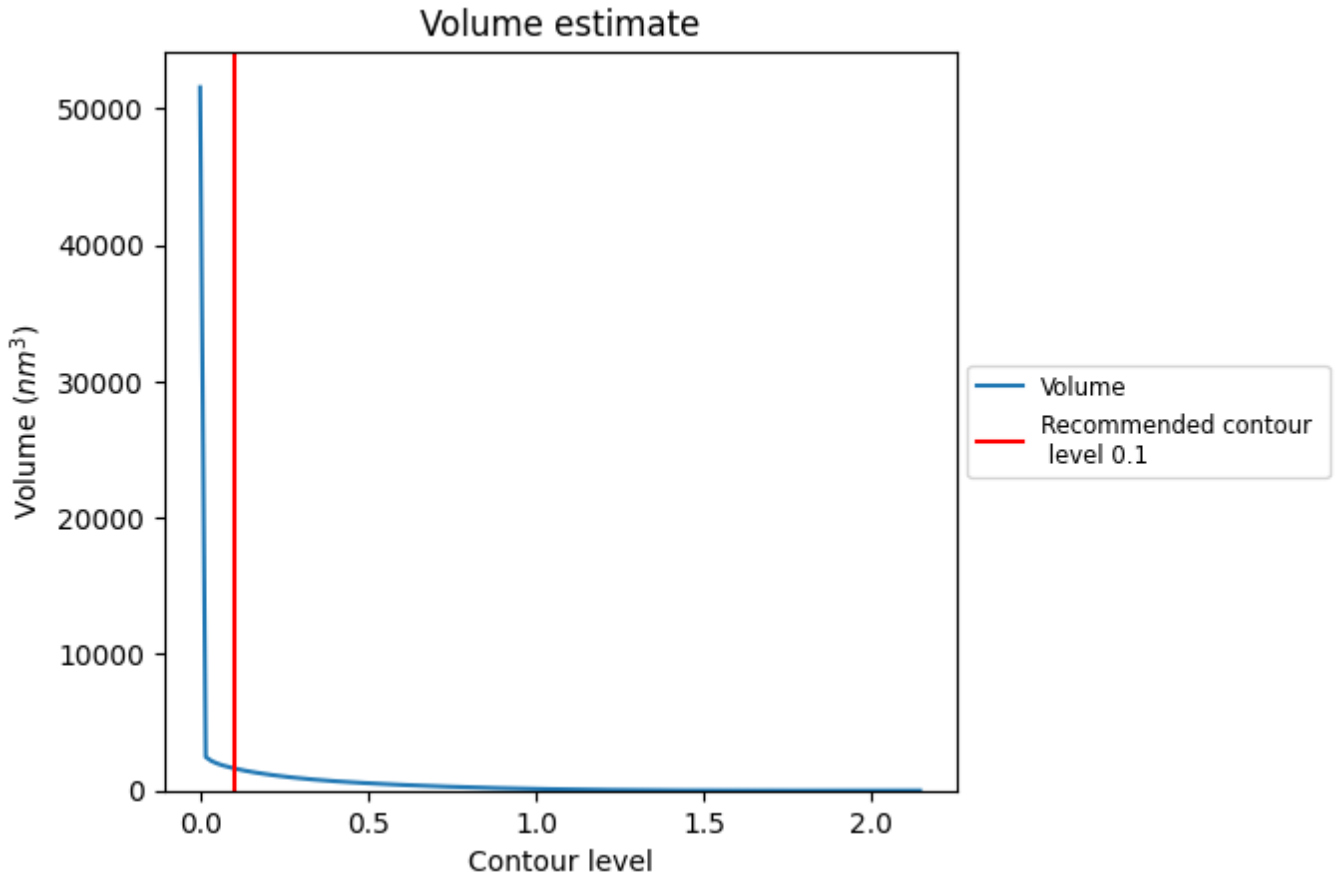
This section contains the results of statistical analysis of the map.

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.

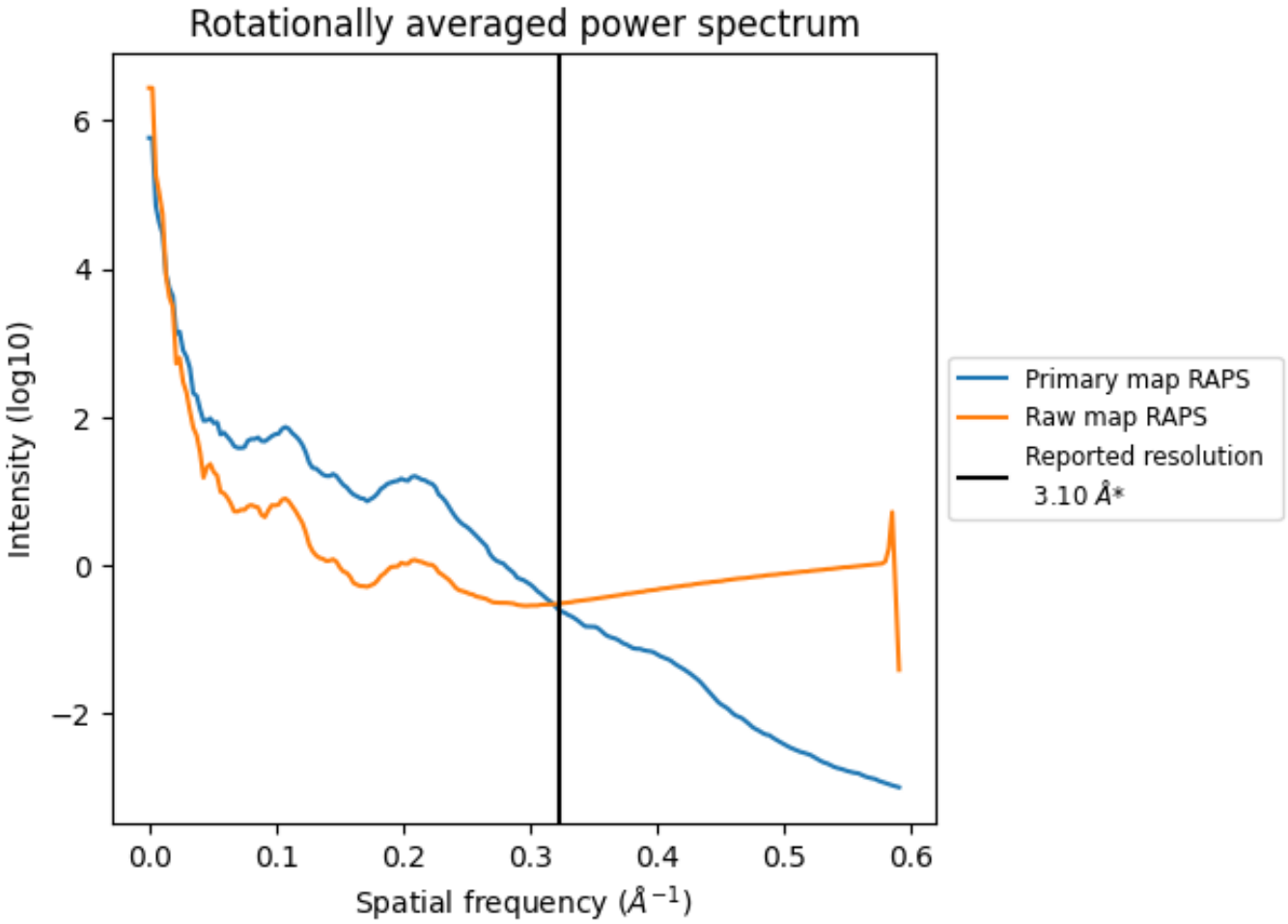
7.2 Volume estimate



The volume at the recommended contour level is 1620 nm^3; this corresponds to an approximate mass of 1463 kDa.

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

7.3 Rotationally averaged power spectrum (i)

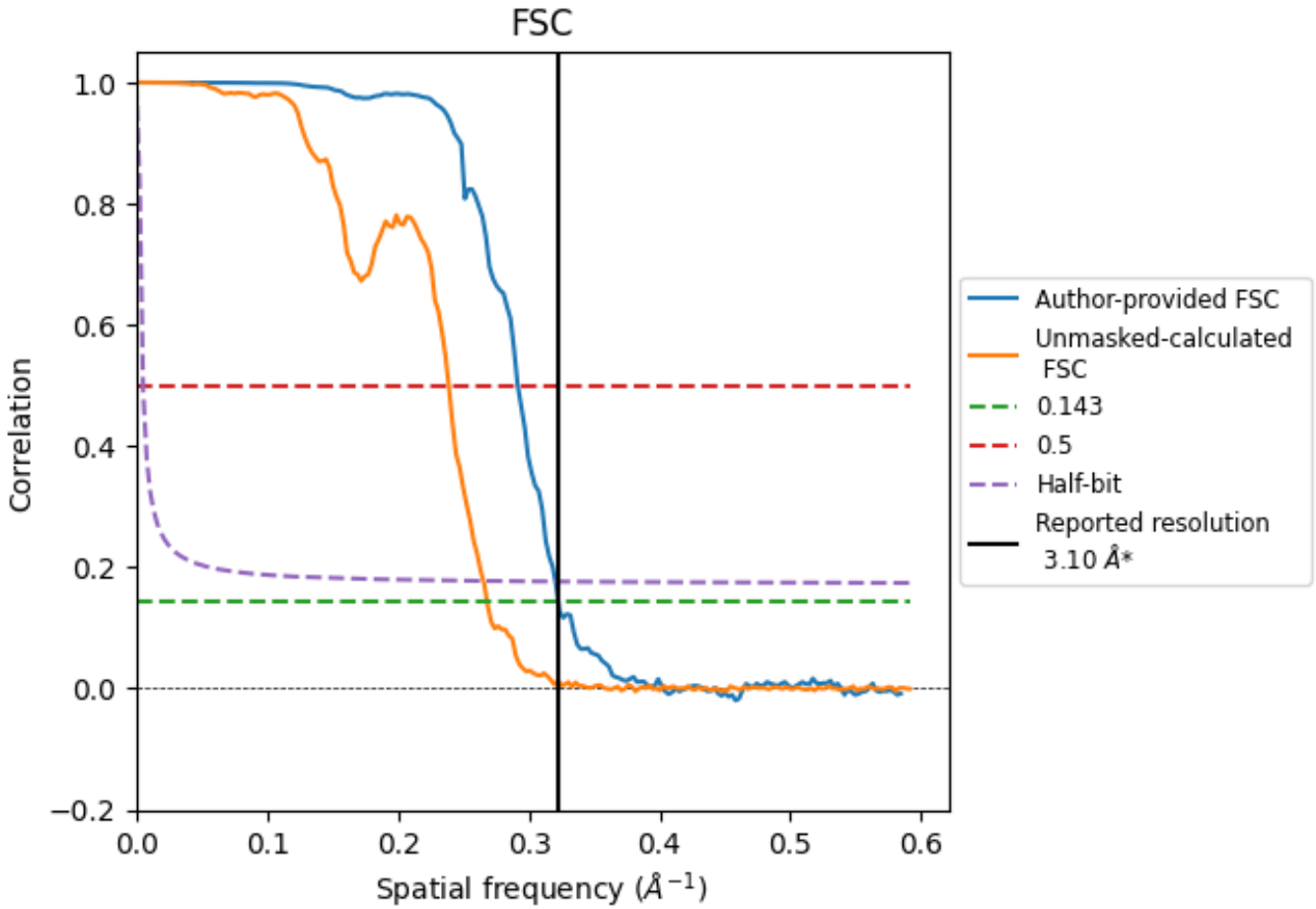


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 $Å^{-1}$

8.2 Resolution estimates (i)

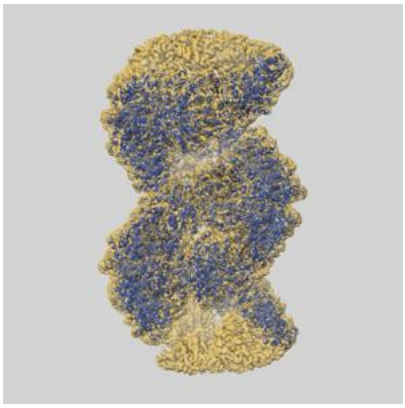
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.43	3.12
Unmasked-calculated*	3.73	4.19	3.77

*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 3.73 differs from the reported value 3.1 by more than 10 %

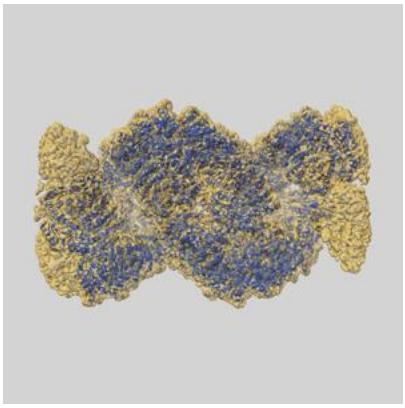
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51001 and PDB model 9G3J. Per-residue inclusion information can be found in section 3 on page 43.

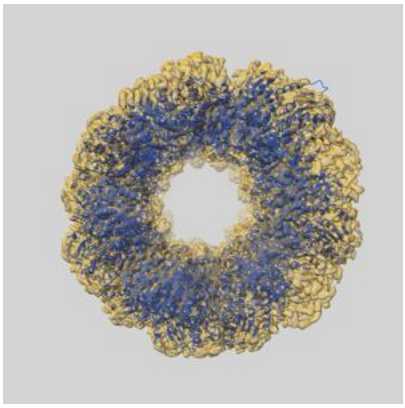
9.1 Map-model overlay



X



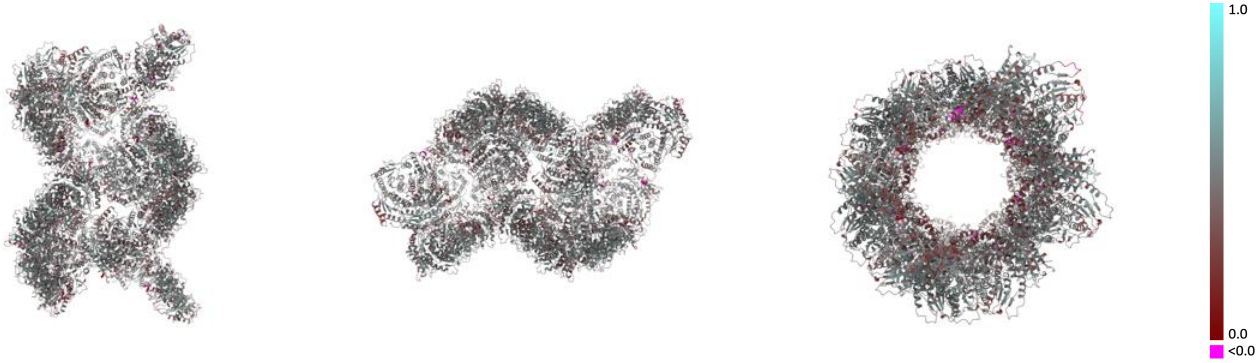
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

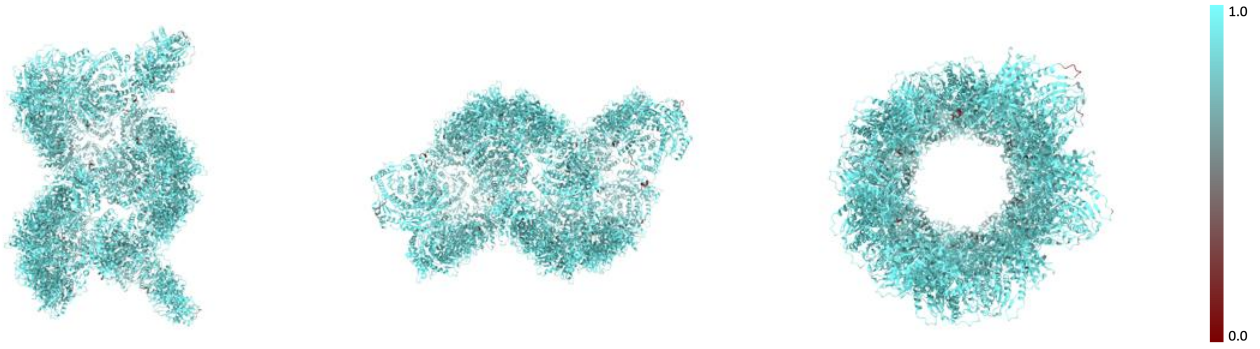
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

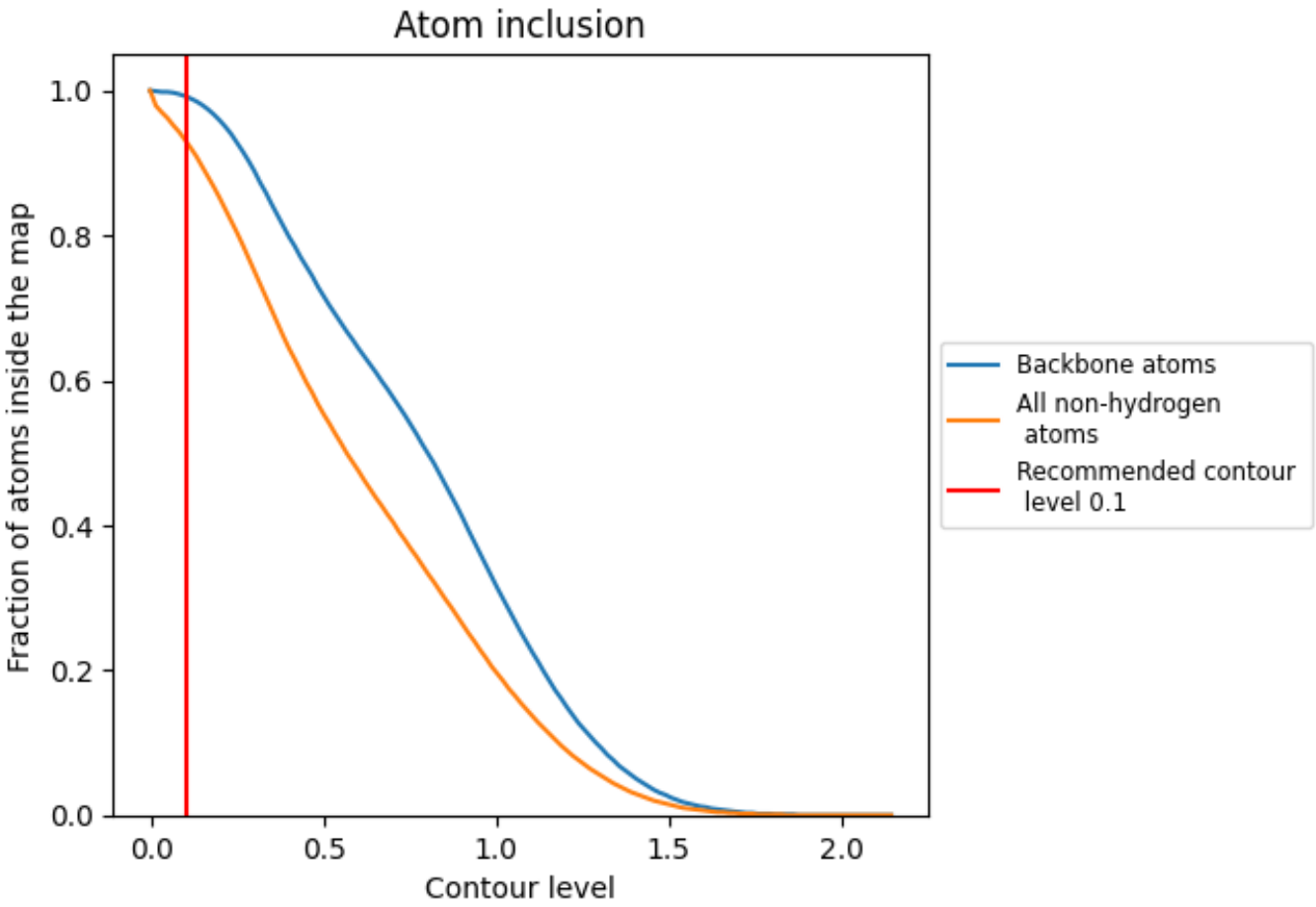
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9310	0.4420
A	0.9590	0.4820
AA	0.9240	0.4180
AB	0.9160	0.4240
AC	0.9340	0.4530
B	0.9370	0.4200
BA	0.9210	0.4450
BB	0.9370	0.4520
BC	0.9280	0.4350
C	0.9250	0.4480
CA	0.9420	0.4630
CB	0.9310	0.4370
CC	0.9600	0.4820
D	0.9390	0.4650
DA	0.9480	0.4510
DB	0.9420	0.4640
DC	0.9270	0.4170
E	0.9470	0.4520
EA	0.9520	0.4800
EB	0.8980	0.3880
EC	0.9210	0.4450
F	0.9570	0.4810
FA	0.9200	0.4130
FB	0.8900	0.4170
FC	0.9430	0.4640
G	0.9230	0.4170
GA	0.9170	0.4440
GB	0.9200	0.4520
GC	0.9510	0.4540
H	0.9170	0.4430
HA	0.8880	0.4460
HB	0.9200	0.4390
HC	0.9590	0.4810
I	0.9410	0.4680
IA	0.9200	0.4420

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
IB	0.9600	0.4810
IC	0.9200	0.4150
J	0.9460	0.4500
JA	0.9520	0.4650
JB	0.9330	0.4190
JC	0.9280	0.4470
K	0.9530	0.4660
KA	0.9190	0.3890
KB	0.9280	0.4430
KC	0.9380	0.4630
L	0.9180	0.3930
LA	0.9150	0.4230
LB	0.9380	0.4640
LC	0.9430	0.4500
M	0.9120	0.4240
MA	0.9400	0.4580
MB	0.9490	0.4510
MC	0.9530	0.4650
N	0.9350	0.4550
NA	0.9330	0.4410
NB	0.9600	0.4800
NC	0.9170	0.3930
O	0.9350	0.4390
OA	0.9610	0.4810
OB	0.9250	0.4190
OC	0.9170	0.4230
P	0.9570	0.4840
PA	0.9240	0.4130
PB	0.9190	0.4450
PC	0.9410	0.4560
Q	0.9270	0.4160
QA	0.9160	0.4430
QB	0.9400	0.4650
QC	0.9360	0.4390
R	0.9230	0.4480
RA	0.9380	0.4630
RB	0.9480	0.4490
RC	0.9530	0.4660
S	0.9440	0.4660
SA	0.9420	0.4500
SB	0.9410	0.4610
SC	0.9220	0.3920

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
T	0.9440	0.4500
TA	0.9490	0.4630
TB	0.8770	0.3830
TC	0.9180	0.4220
U	0.9480	0.4650
UA	0.9200	0.3910
UB	0.8750	0.4160
UC	0.9470	0.4520
V	0.9100	0.3890
VA	0.9110	0.4220
VB	0.8930	0.4380
VC	0.9310	0.4370
W	0.9060	0.4210
WA	0.9370	0.4530
WB	0.8950	0.4300
X	0.9390	0.4540
XA	0.9280	0.4360
XB	0.9490	0.4640
Y	0.9360	0.4380
YA	0.9520	0.4620
YB	0.9180	0.3930
Z	0.9550	0.4820
ZA	0.9110	0.3920
ZB	0.9140	0.4190