



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 11:13 AM UTC

PDB ID : 9G3M / pdb_00009g3m
EMDB ID : EMD-51003
Title : Circularly permuted lumazine synthase triple-stranded straight tube
Authors : Koziej, L.; Azuma, Y.
Deposited on : 2024-07-12
Resolution : 3.09 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

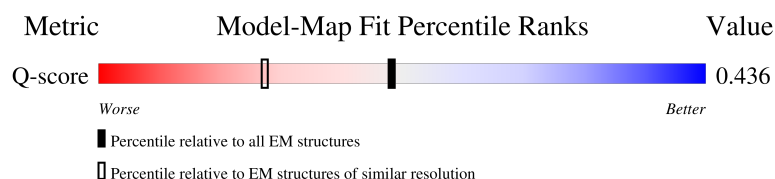
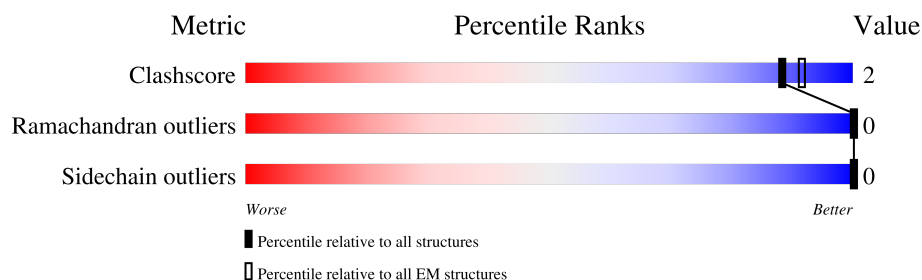
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.09 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	14003 (2.59 - 3.59)

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 $\leq 5\%$. 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	7% 92% 6%
1	AA	163	7% 89% 9%
1	AB	163	10% 93% 5%
1	AC	163	9% 90% 9%

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Mol	Chain	Length	Quality of chain
1	AD	163	9% 86% 6% 9%
1	AE	163	8% 93% 6% .
1	B	163	8% 89% . 9%
1	BA	163	10% 93% 6% .
1	BB	163	10% 88% . 9%
1	BC	163	10% 87% . 9%
1	BD	163	12% 93% 6% .
1	BE	163	9% 89% . 9%
1	C	163	12% 93% 6% .
1	CA	163	9% 88% . 9%
1	CB	163	9% 87% . 9%
1	CC	163	10% 93% 6% .
1	CD	163	11% 90% . 9%
1	CE	163	12% 93% 6% .
1	D	163	10% 88% . 9%
1	DA	163	9% 87% . 9%
1	DB	163	9% 94% . .
1	DC	163	9% 89% . 9%
1	DD	163	12% 94% . .
1	DE	163	9% 88% . 9%
1	E	163	10% 87% . 9%
1	EA	163	10% 93% 6% .
1	EB	163	10% 89% . 9%
1	EC	163	10% 94% . .
1	ED	163	10% 88% . 9%

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Mol	Chain	Length	Quality of chain
1	EE	163	
1	F	163	
1	FA	163	
1	FB	163	
1	FC	163	
1	FD	163	
1	FE	163	
1	G	163	
1	GA	163	
1	GB	163	
1	GC	163	
1	GD	163	
1	GE	163	
1	H	163	
1	HA	163	
1	HB	163	
1	HC	163	
1	HD	163	
1	HE	163	
1	I	163	
1	IA	163	
1	IB	163	
1	IC	163	
1	ID	163	
1	IE	163	

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Mol	Chain	Length	Quality of chain
1	J	163	9% 87% 9%
1	JA	163	10% 94% 9%
1	JB	163	11% 88% 9%
1	JC	163	11% 93% 6%
1	JD	163	14% 90% 9%
1	JE	163	10% 87% 9%
1	K	163	10% 93% 5%
1	KA	163	10% 90% 9%
1	KB	163	11% 94% 9%
1	KC	163	9% 90% 9%
1	KD	163	9% 87% 9%
1	KE	163	12% 94% 9%
1	L	163	10% 89% 9%
1	LA	163	11% 94% 9%
1	LB	163	11% 90% 9%
1	LC	163	11% 86% 6%
1	LD	163	11% 94% 9%
1	LE	163	11% 90% 9%
1	M	163	12% 92% 6%
1	MA	163	10% 90% 9%
1	MB	163	7% 87% 9%
1	MC	163	10% 94% 9%
1	MD	163	12% 90% 9%
1	ME	163	9% 93% 5%
1	N	163	11% 90% 9%

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Mol	Chain	Length	Quality of chain
1	NA	163	
1	NB	163	
1	NC	163	
1	ND	163	
1	NE	163	
1	O	163	
1	OA	163	
1	OB	163	
1	OC	163	
1	OD	163	
1	OE	163	
1	P	163	
1	PA	163	
1	PB	163	
1	PC	163	
1	PD	163	
1	PE	163	
1	Q	163	
1	QA	163	
1	QB	163	
1	QC	163	
1	QD	163	
1	QE	163	
1	R	163	
1	RA	163	

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Mol	Chain	Length	Quality of chain
1	RB	163	
1	RC	163	
1	RD	163	
1	RE	163	
1	S	163	
1	SA	163	
1	SB	163	
1	SC	163	
1	SD	163	
1	SE	163	
1	T	163	
1	TA	163	
1	TB	163	
1	TC	163	
1	TD	163	
1	TE	163	
1	U	163	
1	UA	163	
1	UB	163	
1	UC	163	
1	UD	163	
1	V	163	
1	VA	163	
1	VB	163	
1	VC	163	

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Mol	Chain	Length	Quality of chain
1	VD	163	
1	W	163	
1	WA	163	
1	WB	163	
1	WC	163	
1	WD	163	
1	X	163	
1	XA	163	
1	XB	163	
1	XC	163	
1	XD	163	
1	Y	163	
1	YA	163	
1	YB	163	
1	YC	163	
1	YD	163	
1	Z	163	
1	ZA	163	
1	ZB	163	
1	ZC	163	
1	ZD	163	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 172740 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	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	B	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	C	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	D	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	E	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	F	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	G	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	H	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	I	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	J	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	K	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	L	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	M	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	N	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	O	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	P	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	Q	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	S	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	T	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	U	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	V	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	W	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	X	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	Y	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	Z	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	AA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	BA	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	CA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	DA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	EA	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	FA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	GA	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	HA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	IA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	JA	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	KA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	LA	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	NA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	OA	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	PA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	QA	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	RA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	SA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	TA	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	UA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	VA	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	WA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	XA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	YA	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	ZA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	AB	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	BB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	CB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	DB	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	EB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	FB	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	GB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	IB	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	JB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	KB	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	LB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	MB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	NB	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	OB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	PB	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	QB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	RB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	SB	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	TB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	UB	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	VB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	WB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	XB	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	YB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	ZB	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	AC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	BC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CC	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	DC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	EC	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	FC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	GC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	HC	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	IC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	JC	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	KC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	LC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	MC	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	NC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	OC	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	PC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	QC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	RC	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	SC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	TC	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	UC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	VC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	WC	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	XC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	YC	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	ZC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	AD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	BD	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	CD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	DD	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	ED	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	FD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	GD	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	HD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	ID	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	JD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	KD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	LD	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	MD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	ND	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	OD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	PD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	QD	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	RD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	SD	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	TD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	UD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	VD	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	WD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	XD	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	YD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	ZD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	AE	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	BE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	CE	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	DE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	EE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	FE	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	GE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	HE	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	IE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	JE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	KE	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	LE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	ME	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	NE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	OE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	PE	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	QE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	RE	160	Total	C	N	O	S	0	0
			1202	758	215	226	3		
1	SE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	TE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		

There are 1650 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
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
C	1	MET	-	initiating methionine	UNP O66529
C	37	GLY	-	linker	UNP O66529
C	38	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
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
G	1	MET	-	initiating methionine	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
G	43	SER	-	linker	UNP O66529
G	44	SER	-	linker	UNP O66529
G	45	MET	-	linker	UNP O66529
G	46	GLU	-	linker	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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
J	46	GLU	-	linker	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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
N	44	SER	-	linker	UNP O66529
N	45	MET	-	linker	UNP O66529
N	46	GLU	-	linker	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
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
Q	1	MET	-	initiating methionine	UNP O66529
Q	37	GLY	-	linker	UNP O66529
Q	38	THR	-	linker	UNP O66529
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
W	45	MET	-	linker	UNP O66529
W	46	GLU	-	linker	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
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
Z	1	MET	-	initiating methionine	UNP O66529
Z	37	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
DA	1	MET	-	initiating methionine	UNP O66529
DA	37	GLY	-	linker	UNP O66529
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
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
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
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
GA	41	SER	-	linker	UNP O66529
GA	42	GLY	-	linker	UNP O66529
GA	43	SER	-	linker	UNP O66529
GA	44	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
GA	45	MET	-	linker	UNP O66529
GA	46	GLU	-	linker	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
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
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
JA	44	SER	-	linker	UNP O66529
JA	45	MET	-	linker	UNP O66529
JA	46	GLU	-	linker	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

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Chain	Residue	Modelled	Actual	Comment	Reference
KA	43	SER	-	linker	UNP O66529
KA	44	SER	-	linker	UNP O66529
KA	45	MET	-	linker	UNP O66529
KA	46	GLU	-	linker	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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
QA	1	MET	-	initiating methionine	UNP O66529
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
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
SA	1	MET	-	initiating methionine	UNP O66529
SA	37	GLY	-	linker	UNP O66529
SA	38	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
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
WA	1	MET	-	initiating methionine	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
WA	43	SER	-	linker	UNP O66529
WA	44	SER	-	linker	UNP O66529
WA	45	MET	-	linker	UNP O66529
WA	46	GLU	-	linker	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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
ZA	46	GLU	-	linker	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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
DB	44	SER	-	linker	UNP O66529
DB	45	MET	-	linker	UNP O66529
DB	46	GLU	-	linker	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
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
GB	1	MET	-	initiating methionine	UNP O66529
GB	37	GLY	-	linker	UNP O66529
GB	38	THR	-	linker	UNP O66529
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
MB	45	MET	-	linker	UNP O66529
MB	46	GLU	-	linker	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
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
PB	1	MET	-	initiating methionine	UNP O66529
PB	37	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
TB	1	MET	-	initiating methionine	UNP O66529
TB	37	GLY	-	linker	UNP O66529
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
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
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
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
WB	41	SER	-	linker	UNP O66529
WB	42	GLY	-	linker	UNP O66529
WB	43	SER	-	linker	UNP O66529
WB	44	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
WB	45	MET	-	linker	UNP O66529
WB	46	GLU	-	linker	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
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
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
ZB	44	SER	-	linker	UNP O66529
ZB	45	MET	-	linker	UNP O66529
ZB	46	GLU	-	linker	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

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Chain	Residue	Modelled	Actual	Comment	Reference
AC	43	SER	-	linker	UNP O66529
AC	44	SER	-	linker	UNP O66529
AC	45	MET	-	linker	UNP O66529
AC	46	GLU	-	linker	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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
GC	1	MET	-	initiating methionine	UNP O66529
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
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
IC	1	MET	-	initiating methionine	UNP O66529
IC	37	GLY	-	linker	UNP O66529
IC	38	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
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
MC	1	MET	-	initiating methionine	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
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
MC	43	SER	-	linker	UNP O66529
MC	44	SER	-	linker	UNP O66529
MC	45	MET	-	linker	UNP O66529
MC	46	GLU	-	linker	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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
PC	46	GLU	-	linker	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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
TC	44	SER	-	linker	UNP O66529
TC	45	MET	-	linker	UNP O66529
TC	46	GLU	-	linker	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
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
WC	1	MET	-	initiating methionine	UNP O66529
WC	37	GLY	-	linker	UNP O66529
WC	38	THR	-	linker	UNP O66529
WC	39	GLY	-	linker	UNP O66529
WC	40	GLY	-	linker	UNP O66529
WC	41	SER	-	linker	UNP O66529
WC	42	GLY	-	linker	UNP O66529
WC	43	SER	-	linker	UNP O66529
WC	44	SER	-	linker	UNP O66529
WC	45	MET	-	linker	UNP O66529
WC	46	GLU	-	linker	UNP O66529
XC	1	MET	-	initiating methionine	UNP O66529
XC	37	GLY	-	linker	UNP O66529
XC	38	THR	-	linker	UNP O66529
XC	39	GLY	-	linker	UNP O66529
XC	40	GLY	-	linker	UNP O66529
XC	41	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
XC	42	GLY	-	linker	UNP O66529
XC	43	SER	-	linker	UNP O66529
XC	44	SER	-	linker	UNP O66529
XC	45	MET	-	linker	UNP O66529
XC	46	GLU	-	linker	UNP O66529
YC	1	MET	-	initiating methionine	UNP O66529
YC	37	GLY	-	linker	UNP O66529
YC	38	THR	-	linker	UNP O66529
YC	39	GLY	-	linker	UNP O66529
YC	40	GLY	-	linker	UNP O66529
YC	41	SER	-	linker	UNP O66529
YC	42	GLY	-	linker	UNP O66529
YC	43	SER	-	linker	UNP O66529
YC	44	SER	-	linker	UNP O66529
YC	45	MET	-	linker	UNP O66529
YC	46	GLU	-	linker	UNP O66529
ZC	1	MET	-	initiating methionine	UNP O66529
ZC	37	GLY	-	linker	UNP O66529
ZC	38	THR	-	linker	UNP O66529
ZC	39	GLY	-	linker	UNP O66529
ZC	40	GLY	-	linker	UNP O66529
ZC	41	SER	-	linker	UNP O66529
ZC	42	GLY	-	linker	UNP O66529
ZC	43	SER	-	linker	UNP O66529
ZC	44	SER	-	linker	UNP O66529
ZC	45	MET	-	linker	UNP O66529
ZC	46	GLU	-	linker	UNP O66529
AD	1	MET	-	initiating methionine	UNP O66529
AD	37	GLY	-	linker	UNP O66529
AD	38	THR	-	linker	UNP O66529
AD	39	GLY	-	linker	UNP O66529
AD	40	GLY	-	linker	UNP O66529
AD	41	SER	-	linker	UNP O66529
AD	42	GLY	-	linker	UNP O66529
AD	43	SER	-	linker	UNP O66529
AD	44	SER	-	linker	UNP O66529
AD	45	MET	-	linker	UNP O66529
AD	46	GLU	-	linker	UNP O66529
BD	1	MET	-	initiating methionine	UNP O66529
BD	37	GLY	-	linker	UNP O66529
BD	38	THR	-	linker	UNP O66529
BD	39	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
BD	40	GLY	-	linker	UNP O66529
BD	41	SER	-	linker	UNP O66529
BD	42	GLY	-	linker	UNP O66529
BD	43	SER	-	linker	UNP O66529
BD	44	SER	-	linker	UNP O66529
BD	45	MET	-	linker	UNP O66529
BD	46	GLU	-	linker	UNP O66529
CD	1	MET	-	initiating methionine	UNP O66529
CD	37	GLY	-	linker	UNP O66529
CD	38	THR	-	linker	UNP O66529
CD	39	GLY	-	linker	UNP O66529
CD	40	GLY	-	linker	UNP O66529
CD	41	SER	-	linker	UNP O66529
CD	42	GLY	-	linker	UNP O66529
CD	43	SER	-	linker	UNP O66529
CD	44	SER	-	linker	UNP O66529
CD	45	MET	-	linker	UNP O66529
CD	46	GLU	-	linker	UNP O66529
DD	1	MET	-	initiating methionine	UNP O66529
DD	37	GLY	-	linker	UNP O66529
DD	38	THR	-	linker	UNP O66529
DD	39	GLY	-	linker	UNP O66529
DD	40	GLY	-	linker	UNP O66529
DD	41	SER	-	linker	UNP O66529
DD	42	GLY	-	linker	UNP O66529
DD	43	SER	-	linker	UNP O66529
DD	44	SER	-	linker	UNP O66529
DD	45	MET	-	linker	UNP O66529
DD	46	GLU	-	linker	UNP O66529
ED	1	MET	-	initiating methionine	UNP O66529
ED	37	GLY	-	linker	UNP O66529
ED	38	THR	-	linker	UNP O66529
ED	39	GLY	-	linker	UNP O66529
ED	40	GLY	-	linker	UNP O66529
ED	41	SER	-	linker	UNP O66529
ED	42	GLY	-	linker	UNP O66529
ED	43	SER	-	linker	UNP O66529
ED	44	SER	-	linker	UNP O66529
ED	45	MET	-	linker	UNP O66529
ED	46	GLU	-	linker	UNP O66529
FD	1	MET	-	initiating methionine	UNP O66529
FD	37	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
FD	38	THR	-	linker	UNP O66529
FD	39	GLY	-	linker	UNP O66529
FD	40	GLY	-	linker	UNP O66529
FD	41	SER	-	linker	UNP O66529
FD	42	GLY	-	linker	UNP O66529
FD	43	SER	-	linker	UNP O66529
FD	44	SER	-	linker	UNP O66529
FD	45	MET	-	linker	UNP O66529
FD	46	GLU	-	linker	UNP O66529
GD	1	MET	-	initiating methionine	UNP O66529
GD	37	GLY	-	linker	UNP O66529
GD	38	THR	-	linker	UNP O66529
GD	39	GLY	-	linker	UNP O66529
GD	40	GLY	-	linker	UNP O66529
GD	41	SER	-	linker	UNP O66529
GD	42	GLY	-	linker	UNP O66529
GD	43	SER	-	linker	UNP O66529
GD	44	SER	-	linker	UNP O66529
GD	45	MET	-	linker	UNP O66529
GD	46	GLU	-	linker	UNP O66529
HD	1	MET	-	initiating methionine	UNP O66529
HD	37	GLY	-	linker	UNP O66529
HD	38	THR	-	linker	UNP O66529
HD	39	GLY	-	linker	UNP O66529
HD	40	GLY	-	linker	UNP O66529
HD	41	SER	-	linker	UNP O66529
HD	42	GLY	-	linker	UNP O66529
HD	43	SER	-	linker	UNP O66529
HD	44	SER	-	linker	UNP O66529
HD	45	MET	-	linker	UNP O66529
HD	46	GLU	-	linker	UNP O66529
ID	1	MET	-	initiating methionine	UNP O66529
ID	37	GLY	-	linker	UNP O66529
ID	38	THR	-	linker	UNP O66529
ID	39	GLY	-	linker	UNP O66529
ID	40	GLY	-	linker	UNP O66529
ID	41	SER	-	linker	UNP O66529
ID	42	GLY	-	linker	UNP O66529
ID	43	SER	-	linker	UNP O66529
ID	44	SER	-	linker	UNP O66529
ID	45	MET	-	linker	UNP O66529
ID	46	GLU	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
JD	1	MET	-	initiating methionine	UNP O66529
JD	37	GLY	-	linker	UNP O66529
JD	38	THR	-	linker	UNP O66529
JD	39	GLY	-	linker	UNP O66529
JD	40	GLY	-	linker	UNP O66529
JD	41	SER	-	linker	UNP O66529
JD	42	GLY	-	linker	UNP O66529
JD	43	SER	-	linker	UNP O66529
JD	44	SER	-	linker	UNP O66529
JD	45	MET	-	linker	UNP O66529
JD	46	GLU	-	linker	UNP O66529
KD	1	MET	-	initiating methionine	UNP O66529
KD	37	GLY	-	linker	UNP O66529
KD	38	THR	-	linker	UNP O66529
KD	39	GLY	-	linker	UNP O66529
KD	40	GLY	-	linker	UNP O66529
KD	41	SER	-	linker	UNP O66529
KD	42	GLY	-	linker	UNP O66529
KD	43	SER	-	linker	UNP O66529
KD	44	SER	-	linker	UNP O66529
KD	45	MET	-	linker	UNP O66529
KD	46	GLU	-	linker	UNP O66529
LD	1	MET	-	initiating methionine	UNP O66529
LD	37	GLY	-	linker	UNP O66529
LD	38	THR	-	linker	UNP O66529
LD	39	GLY	-	linker	UNP O66529
LD	40	GLY	-	linker	UNP O66529
LD	41	SER	-	linker	UNP O66529
LD	42	GLY	-	linker	UNP O66529
LD	43	SER	-	linker	UNP O66529
LD	44	SER	-	linker	UNP O66529
LD	45	MET	-	linker	UNP O66529
LD	46	GLU	-	linker	UNP O66529
MD	1	MET	-	initiating methionine	UNP O66529
MD	37	GLY	-	linker	UNP O66529
MD	38	THR	-	linker	UNP O66529
MD	39	GLY	-	linker	UNP O66529
MD	40	GLY	-	linker	UNP O66529
MD	41	SER	-	linker	UNP O66529
MD	42	GLY	-	linker	UNP O66529
MD	43	SER	-	linker	UNP O66529
MD	44	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
MD	45	MET	-	linker	UNP O66529
MD	46	GLU	-	linker	UNP O66529
ND	1	MET	-	initiating methionine	UNP O66529
ND	37	GLY	-	linker	UNP O66529
ND	38	THR	-	linker	UNP O66529
ND	39	GLY	-	linker	UNP O66529
ND	40	GLY	-	linker	UNP O66529
ND	41	SER	-	linker	UNP O66529
ND	42	GLY	-	linker	UNP O66529
ND	43	SER	-	linker	UNP O66529
ND	44	SER	-	linker	UNP O66529
ND	45	MET	-	linker	UNP O66529
ND	46	GLU	-	linker	UNP O66529
OD	1	MET	-	initiating methionine	UNP O66529
OD	37	GLY	-	linker	UNP O66529
OD	38	THR	-	linker	UNP O66529
OD	39	GLY	-	linker	UNP O66529
OD	40	GLY	-	linker	UNP O66529
OD	41	SER	-	linker	UNP O66529
OD	42	GLY	-	linker	UNP O66529
OD	43	SER	-	linker	UNP O66529
OD	44	SER	-	linker	UNP O66529
OD	45	MET	-	linker	UNP O66529
OD	46	GLU	-	linker	UNP O66529
PD	1	MET	-	initiating methionine	UNP O66529
PD	37	GLY	-	linker	UNP O66529
PD	38	THR	-	linker	UNP O66529
PD	39	GLY	-	linker	UNP O66529
PD	40	GLY	-	linker	UNP O66529
PD	41	SER	-	linker	UNP O66529
PD	42	GLY	-	linker	UNP O66529
PD	43	SER	-	linker	UNP O66529
PD	44	SER	-	linker	UNP O66529
PD	45	MET	-	linker	UNP O66529
PD	46	GLU	-	linker	UNP O66529
QD	1	MET	-	initiating methionine	UNP O66529
QD	37	GLY	-	linker	UNP O66529
QD	38	THR	-	linker	UNP O66529
QD	39	GLY	-	linker	UNP O66529
QD	40	GLY	-	linker	UNP O66529
QD	41	SER	-	linker	UNP O66529
QD	42	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
QD	43	SER	-	linker	UNP O66529
QD	44	SER	-	linker	UNP O66529
QD	45	MET	-	linker	UNP O66529
QD	46	GLU	-	linker	UNP O66529
RD	1	MET	-	initiating methionine	UNP O66529
RD	37	GLY	-	linker	UNP O66529
RD	38	THR	-	linker	UNP O66529
RD	39	GLY	-	linker	UNP O66529
RD	40	GLY	-	linker	UNP O66529
RD	41	SER	-	linker	UNP O66529
RD	42	GLY	-	linker	UNP O66529
RD	43	SER	-	linker	UNP O66529
RD	44	SER	-	linker	UNP O66529
RD	45	MET	-	linker	UNP O66529
RD	46	GLU	-	linker	UNP O66529
SD	1	MET	-	initiating methionine	UNP O66529
SD	37	GLY	-	linker	UNP O66529
SD	38	THR	-	linker	UNP O66529
SD	39	GLY	-	linker	UNP O66529
SD	40	GLY	-	linker	UNP O66529
SD	41	SER	-	linker	UNP O66529
SD	42	GLY	-	linker	UNP O66529
SD	43	SER	-	linker	UNP O66529
SD	44	SER	-	linker	UNP O66529
SD	45	MET	-	linker	UNP O66529
SD	46	GLU	-	linker	UNP O66529
TD	1	MET	-	initiating methionine	UNP O66529
TD	37	GLY	-	linker	UNP O66529
TD	38	THR	-	linker	UNP O66529
TD	39	GLY	-	linker	UNP O66529
TD	40	GLY	-	linker	UNP O66529
TD	41	SER	-	linker	UNP O66529
TD	42	GLY	-	linker	UNP O66529
TD	43	SER	-	linker	UNP O66529
TD	44	SER	-	linker	UNP O66529
TD	45	MET	-	linker	UNP O66529
TD	46	GLU	-	linker	UNP O66529
UD	1	MET	-	initiating methionine	UNP O66529
UD	37	GLY	-	linker	UNP O66529
UD	38	THR	-	linker	UNP O66529
UD	39	GLY	-	linker	UNP O66529
UD	40	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
UD	41	SER	-	linker	UNP O66529
UD	42	GLY	-	linker	UNP O66529
UD	43	SER	-	linker	UNP O66529
UD	44	SER	-	linker	UNP O66529
UD	45	MET	-	linker	UNP O66529
UD	46	GLU	-	linker	UNP O66529
VD	1	MET	-	initiating methionine	UNP O66529
VD	37	GLY	-	linker	UNP O66529
VD	38	THR	-	linker	UNP O66529
VD	39	GLY	-	linker	UNP O66529
VD	40	GLY	-	linker	UNP O66529
VD	41	SER	-	linker	UNP O66529
VD	42	GLY	-	linker	UNP O66529
VD	43	SER	-	linker	UNP O66529
VD	44	SER	-	linker	UNP O66529
VD	45	MET	-	linker	UNP O66529
VD	46	GLU	-	linker	UNP O66529
WD	1	MET	-	initiating methionine	UNP O66529
WD	37	GLY	-	linker	UNP O66529
WD	38	THR	-	linker	UNP O66529
WD	39	GLY	-	linker	UNP O66529
WD	40	GLY	-	linker	UNP O66529
WD	41	SER	-	linker	UNP O66529
WD	42	GLY	-	linker	UNP O66529
WD	43	SER	-	linker	UNP O66529
WD	44	SER	-	linker	UNP O66529
WD	45	MET	-	linker	UNP O66529
WD	46	GLU	-	linker	UNP O66529
XD	1	MET	-	initiating methionine	UNP O66529
XD	37	GLY	-	linker	UNP O66529
XD	38	THR	-	linker	UNP O66529
XD	39	GLY	-	linker	UNP O66529
XD	40	GLY	-	linker	UNP O66529
XD	41	SER	-	linker	UNP O66529
XD	42	GLY	-	linker	UNP O66529
XD	43	SER	-	linker	UNP O66529
XD	44	SER	-	linker	UNP O66529
XD	45	MET	-	linker	UNP O66529
XD	46	GLU	-	linker	UNP O66529
YD	1	MET	-	initiating methionine	UNP O66529
YD	37	GLY	-	linker	UNP O66529
YD	38	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
YD	39	GLY	-	linker	UNP O66529
YD	40	GLY	-	linker	UNP O66529
YD	41	SER	-	linker	UNP O66529
YD	42	GLY	-	linker	UNP O66529
YD	43	SER	-	linker	UNP O66529
YD	44	SER	-	linker	UNP O66529
YD	45	MET	-	linker	UNP O66529
YD	46	GLU	-	linker	UNP O66529
ZD	1	MET	-	initiating methionine	UNP O66529
ZD	37	GLY	-	linker	UNP O66529
ZD	38	THR	-	linker	UNP O66529
ZD	39	GLY	-	linker	UNP O66529
ZD	40	GLY	-	linker	UNP O66529
ZD	41	SER	-	linker	UNP O66529
ZD	42	GLY	-	linker	UNP O66529
ZD	43	SER	-	linker	UNP O66529
ZD	44	SER	-	linker	UNP O66529
ZD	45	MET	-	linker	UNP O66529
ZD	46	GLU	-	linker	UNP O66529
AE	1	MET	-	initiating methionine	UNP O66529
AE	37	GLY	-	linker	UNP O66529
AE	38	THR	-	linker	UNP O66529
AE	39	GLY	-	linker	UNP O66529
AE	40	GLY	-	linker	UNP O66529
AE	41	SER	-	linker	UNP O66529
AE	42	GLY	-	linker	UNP O66529
AE	43	SER	-	linker	UNP O66529
AE	44	SER	-	linker	UNP O66529
AE	45	MET	-	linker	UNP O66529
AE	46	GLU	-	linker	UNP O66529
BE	1	MET	-	initiating methionine	UNP O66529
BE	37	GLY	-	linker	UNP O66529
BE	38	THR	-	linker	UNP O66529
BE	39	GLY	-	linker	UNP O66529
BE	40	GLY	-	linker	UNP O66529
BE	41	SER	-	linker	UNP O66529
BE	42	GLY	-	linker	UNP O66529
BE	43	SER	-	linker	UNP O66529
BE	44	SER	-	linker	UNP O66529
BE	45	MET	-	linker	UNP O66529
BE	46	GLU	-	linker	UNP O66529
CE	1	MET	-	initiating methionine	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
CE	37	GLY	-	linker	UNP O66529
CE	38	THR	-	linker	UNP O66529
CE	39	GLY	-	linker	UNP O66529
CE	40	GLY	-	linker	UNP O66529
CE	41	SER	-	linker	UNP O66529
CE	42	GLY	-	linker	UNP O66529
CE	43	SER	-	linker	UNP O66529
CE	44	SER	-	linker	UNP O66529
CE	45	MET	-	linker	UNP O66529
CE	46	GLU	-	linker	UNP O66529
DE	1	MET	-	initiating methionine	UNP O66529
DE	37	GLY	-	linker	UNP O66529
DE	38	THR	-	linker	UNP O66529
DE	39	GLY	-	linker	UNP O66529
DE	40	GLY	-	linker	UNP O66529
DE	41	SER	-	linker	UNP O66529
DE	42	GLY	-	linker	UNP O66529
DE	43	SER	-	linker	UNP O66529
DE	44	SER	-	linker	UNP O66529
DE	45	MET	-	linker	UNP O66529
DE	46	GLU	-	linker	UNP O66529
EE	1	MET	-	initiating methionine	UNP O66529
EE	37	GLY	-	linker	UNP O66529
EE	38	THR	-	linker	UNP O66529
EE	39	GLY	-	linker	UNP O66529
EE	40	GLY	-	linker	UNP O66529
EE	41	SER	-	linker	UNP O66529
EE	42	GLY	-	linker	UNP O66529
EE	43	SER	-	linker	UNP O66529
EE	44	SER	-	linker	UNP O66529
EE	45	MET	-	linker	UNP O66529
EE	46	GLU	-	linker	UNP O66529
FE	1	MET	-	initiating methionine	UNP O66529
FE	37	GLY	-	linker	UNP O66529
FE	38	THR	-	linker	UNP O66529
FE	39	GLY	-	linker	UNP O66529
FE	40	GLY	-	linker	UNP O66529
FE	41	SER	-	linker	UNP O66529
FE	42	GLY	-	linker	UNP O66529
FE	43	SER	-	linker	UNP O66529
FE	44	SER	-	linker	UNP O66529
FE	45	MET	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
FE	46	GLU	-	linker	UNP O66529
GE	1	MET	-	initiating methionine	UNP O66529
GE	37	GLY	-	linker	UNP O66529
GE	38	THR	-	linker	UNP O66529
GE	39	GLY	-	linker	UNP O66529
GE	40	GLY	-	linker	UNP O66529
GE	41	SER	-	linker	UNP O66529
GE	42	GLY	-	linker	UNP O66529
GE	43	SER	-	linker	UNP O66529
GE	44	SER	-	linker	UNP O66529
GE	45	MET	-	linker	UNP O66529
GE	46	GLU	-	linker	UNP O66529
HE	1	MET	-	initiating methionine	UNP O66529
HE	37	GLY	-	linker	UNP O66529
HE	38	THR	-	linker	UNP O66529
HE	39	GLY	-	linker	UNP O66529
HE	40	GLY	-	linker	UNP O66529
HE	41	SER	-	linker	UNP O66529
HE	42	GLY	-	linker	UNP O66529
HE	43	SER	-	linker	UNP O66529
HE	44	SER	-	linker	UNP O66529
HE	45	MET	-	linker	UNP O66529
HE	46	GLU	-	linker	UNP O66529
IE	1	MET	-	initiating methionine	UNP O66529
IE	37	GLY	-	linker	UNP O66529
IE	38	THR	-	linker	UNP O66529
IE	39	GLY	-	linker	UNP O66529
IE	40	GLY	-	linker	UNP O66529
IE	41	SER	-	linker	UNP O66529
IE	42	GLY	-	linker	UNP O66529
IE	43	SER	-	linker	UNP O66529
IE	44	SER	-	linker	UNP O66529
IE	45	MET	-	linker	UNP O66529
IE	46	GLU	-	linker	UNP O66529
JE	1	MET	-	initiating methionine	UNP O66529
JE	37	GLY	-	linker	UNP O66529
JE	38	THR	-	linker	UNP O66529
JE	39	GLY	-	linker	UNP O66529
JE	40	GLY	-	linker	UNP O66529
JE	41	SER	-	linker	UNP O66529
JE	42	GLY	-	linker	UNP O66529
JE	43	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
JE	44	SER	-	linker	UNP O66529
JE	45	MET	-	linker	UNP O66529
JE	46	GLU	-	linker	UNP O66529
KE	1	MET	-	initiating methionine	UNP O66529
KE	37	GLY	-	linker	UNP O66529
KE	38	THR	-	linker	UNP O66529
KE	39	GLY	-	linker	UNP O66529
KE	40	GLY	-	linker	UNP O66529
KE	41	SER	-	linker	UNP O66529
KE	42	GLY	-	linker	UNP O66529
KE	43	SER	-	linker	UNP O66529
KE	44	SER	-	linker	UNP O66529
KE	45	MET	-	linker	UNP O66529
KE	46	GLU	-	linker	UNP O66529
LE	1	MET	-	initiating methionine	UNP O66529
LE	37	GLY	-	linker	UNP O66529
LE	38	THR	-	linker	UNP O66529
LE	39	GLY	-	linker	UNP O66529
LE	40	GLY	-	linker	UNP O66529
LE	41	SER	-	linker	UNP O66529
LE	42	GLY	-	linker	UNP O66529
LE	43	SER	-	linker	UNP O66529
LE	44	SER	-	linker	UNP O66529
LE	45	MET	-	linker	UNP O66529
LE	46	GLU	-	linker	UNP O66529
ME	1	MET	-	initiating methionine	UNP O66529
ME	37	GLY	-	linker	UNP O66529
ME	38	THR	-	linker	UNP O66529
ME	39	GLY	-	linker	UNP O66529
ME	40	GLY	-	linker	UNP O66529
ME	41	SER	-	linker	UNP O66529
ME	42	GLY	-	linker	UNP O66529
ME	43	SER	-	linker	UNP O66529
ME	44	SER	-	linker	UNP O66529
ME	45	MET	-	linker	UNP O66529
ME	46	GLU	-	linker	UNP O66529
NE	1	MET	-	initiating methionine	UNP O66529
NE	37	GLY	-	linker	UNP O66529
NE	38	THR	-	linker	UNP O66529
NE	39	GLY	-	linker	UNP O66529
NE	40	GLY	-	linker	UNP O66529
NE	41	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
NE	42	GLY	-	linker	UNP O66529
NE	43	SER	-	linker	UNP O66529
NE	44	SER	-	linker	UNP O66529
NE	45	MET	-	linker	UNP O66529
NE	46	GLU	-	linker	UNP O66529
OE	1	MET	-	initiating methionine	UNP O66529
OE	37	GLY	-	linker	UNP O66529
OE	38	THR	-	linker	UNP O66529
OE	39	GLY	-	linker	UNP O66529
OE	40	GLY	-	linker	UNP O66529
OE	41	SER	-	linker	UNP O66529
OE	42	GLY	-	linker	UNP O66529
OE	43	SER	-	linker	UNP O66529
OE	44	SER	-	linker	UNP O66529
OE	45	MET	-	linker	UNP O66529
OE	46	GLU	-	linker	UNP O66529
PE	1	MET	-	initiating methionine	UNP O66529
PE	37	GLY	-	linker	UNP O66529
PE	38	THR	-	linker	UNP O66529
PE	39	GLY	-	linker	UNP O66529
PE	40	GLY	-	linker	UNP O66529
PE	41	SER	-	linker	UNP O66529
PE	42	GLY	-	linker	UNP O66529
PE	43	SER	-	linker	UNP O66529
PE	44	SER	-	linker	UNP O66529
PE	45	MET	-	linker	UNP O66529
PE	46	GLU	-	linker	UNP O66529
QE	1	MET	-	initiating methionine	UNP O66529
QE	37	GLY	-	linker	UNP O66529
QE	38	THR	-	linker	UNP O66529
QE	39	GLY	-	linker	UNP O66529
QE	40	GLY	-	linker	UNP O66529
QE	41	SER	-	linker	UNP O66529
QE	42	GLY	-	linker	UNP O66529
QE	43	SER	-	linker	UNP O66529
QE	44	SER	-	linker	UNP O66529
QE	45	MET	-	linker	UNP O66529
QE	46	GLU	-	linker	UNP O66529
RE	1	MET	-	initiating methionine	UNP O66529
RE	37	GLY	-	linker	UNP O66529
RE	38	THR	-	linker	UNP O66529
RE	39	GLY	-	linker	UNP O66529

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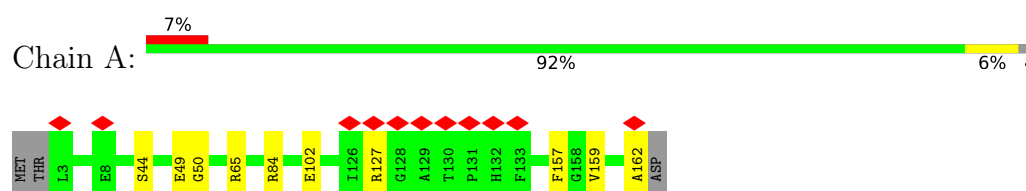
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Chain	Residue	Modelled	Actual	Comment	Reference
RE	40	GLY	-	linker	UNP O66529
RE	41	SER	-	linker	UNP O66529
RE	42	GLY	-	linker	UNP O66529
RE	43	SER	-	linker	UNP O66529
RE	44	SER	-	linker	UNP O66529
RE	45	MET	-	linker	UNP O66529
RE	46	GLU	-	linker	UNP O66529
SE	1	MET	-	initiating methionine	UNP O66529
SE	37	GLY	-	linker	UNP O66529
SE	38	THR	-	linker	UNP O66529
SE	39	GLY	-	linker	UNP O66529
SE	40	GLY	-	linker	UNP O66529
SE	41	SER	-	linker	UNP O66529
SE	42	GLY	-	linker	UNP O66529
SE	43	SER	-	linker	UNP O66529
SE	44	SER	-	linker	UNP O66529
SE	45	MET	-	linker	UNP O66529
SE	46	GLU	-	linker	UNP O66529
TE	1	MET	-	initiating methionine	UNP O66529
TE	37	GLY	-	linker	UNP O66529
TE	38	THR	-	linker	UNP O66529
TE	39	GLY	-	linker	UNP O66529
TE	40	GLY	-	linker	UNP O66529
TE	41	SER	-	linker	UNP O66529
TE	42	GLY	-	linker	UNP O66529
TE	43	SER	-	linker	UNP O66529
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TE	45	MET	-	linker	UNP O66529
TE	46	GLU	-	linker	UNP O66529

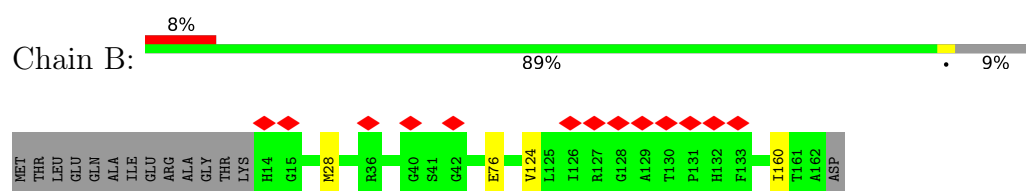
3 Residue-property plots

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

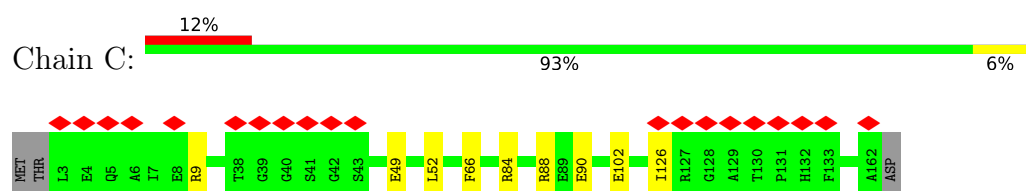
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



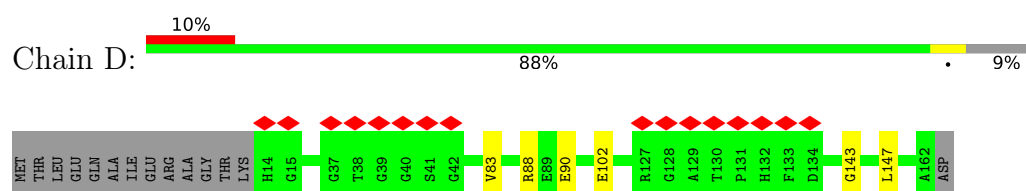
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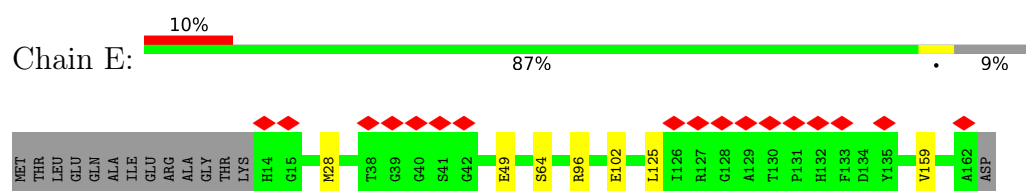
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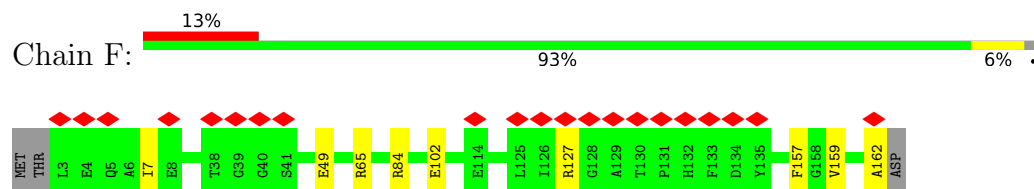
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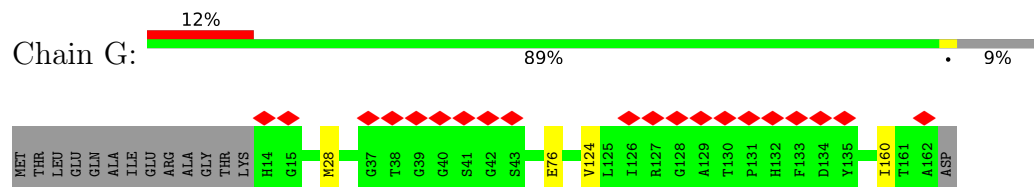
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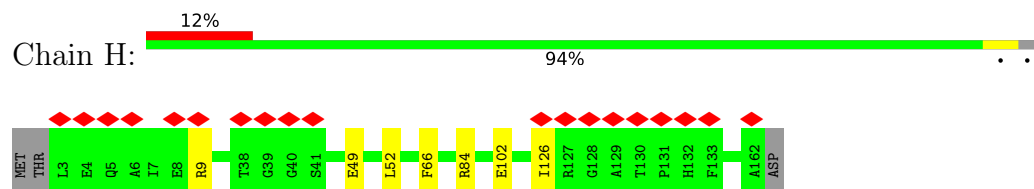
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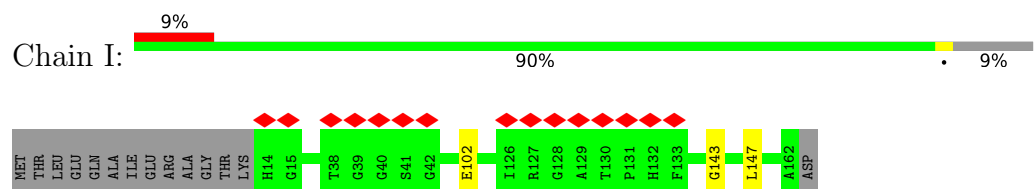
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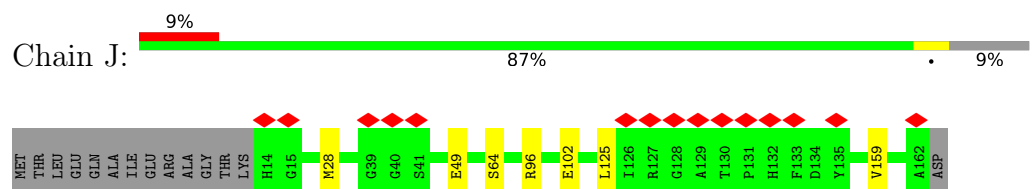
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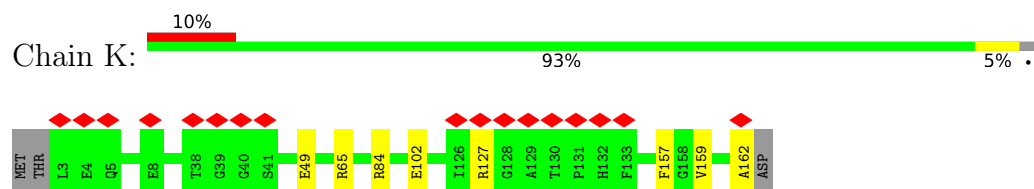
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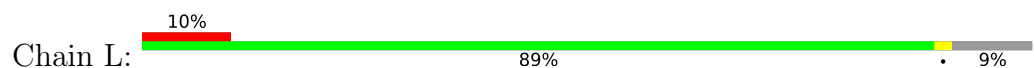
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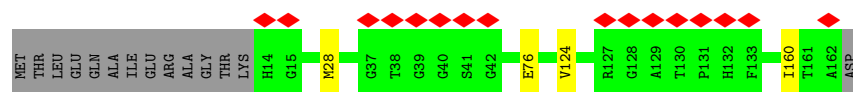


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

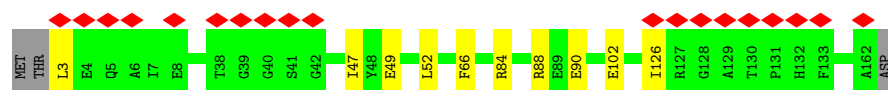


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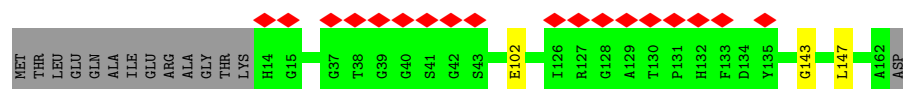




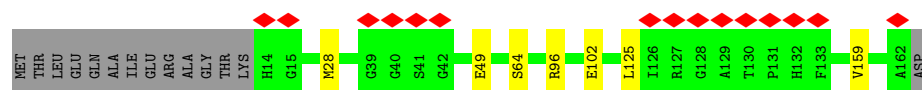
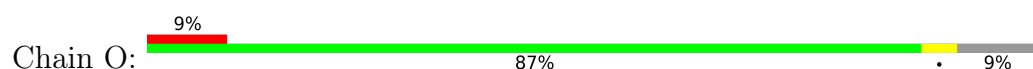
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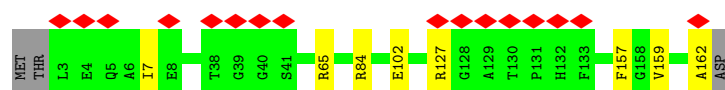
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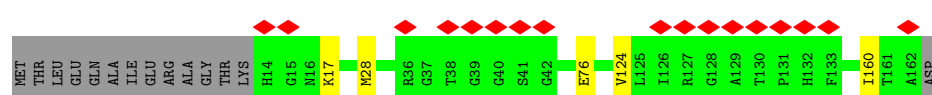
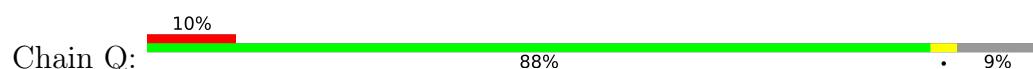
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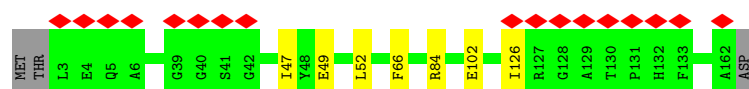
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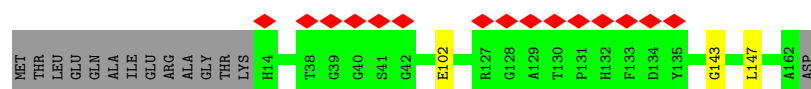
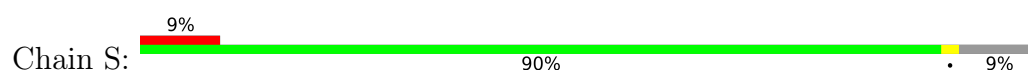
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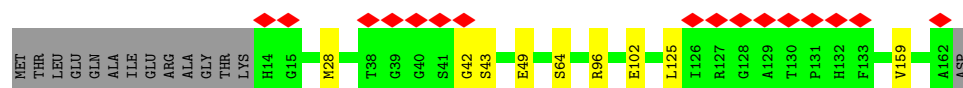
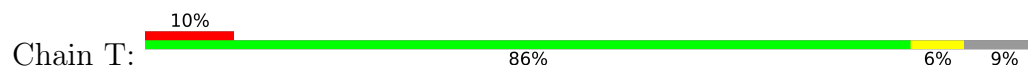
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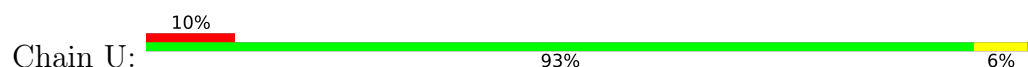
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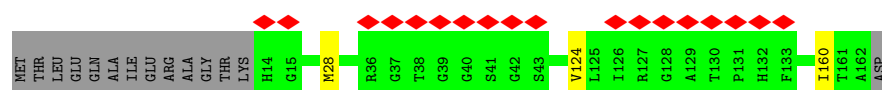
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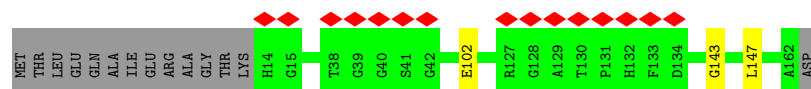
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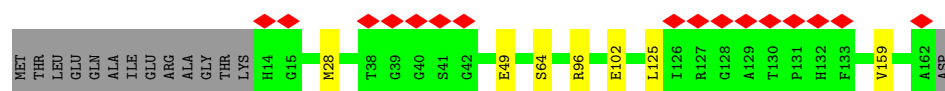
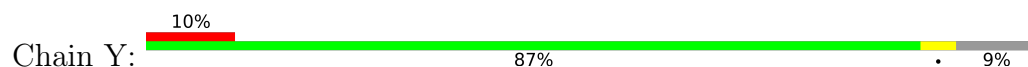
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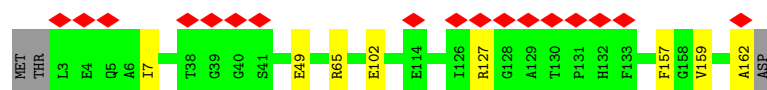
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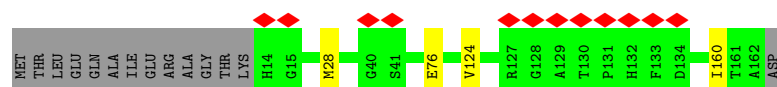
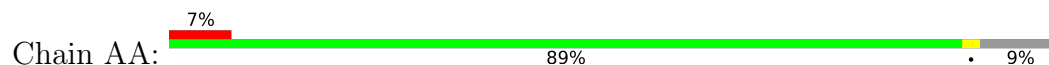
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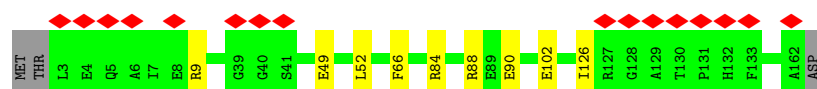
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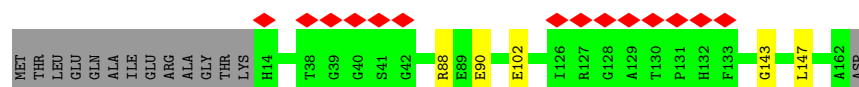
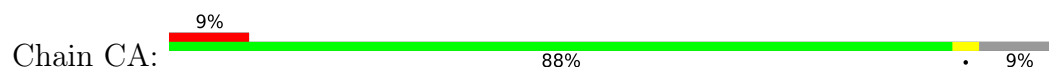
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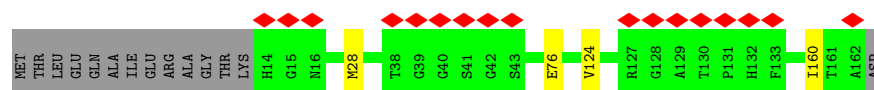


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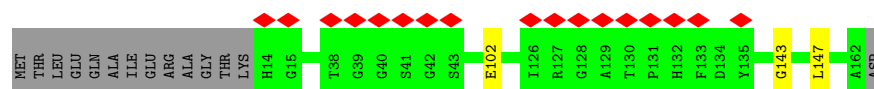




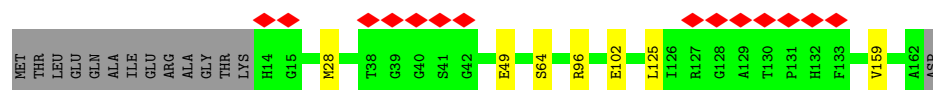
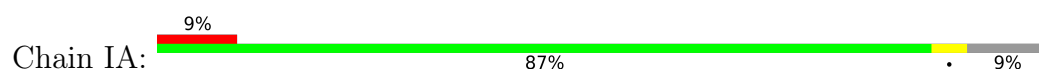
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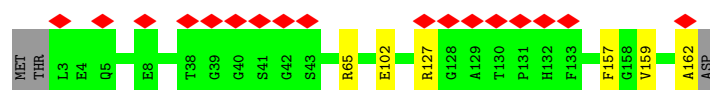
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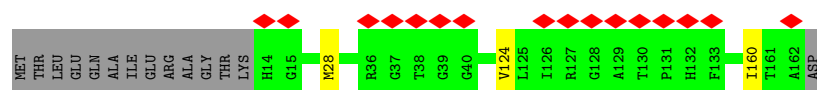
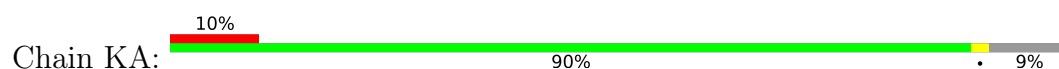
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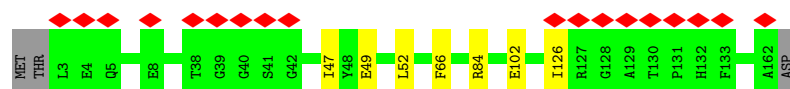
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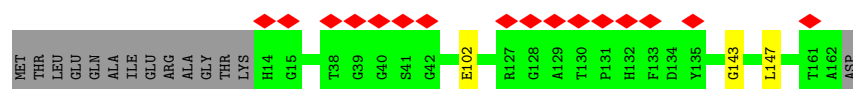
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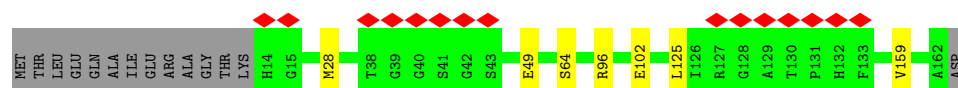
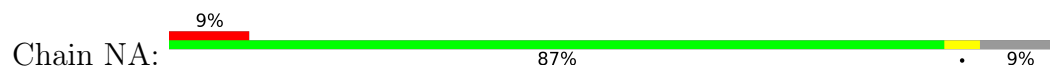
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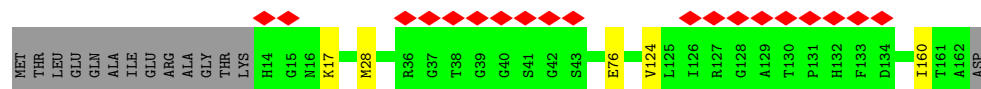
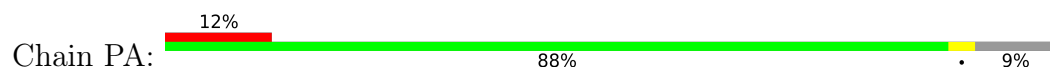
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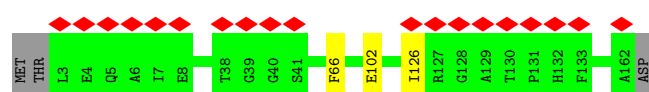
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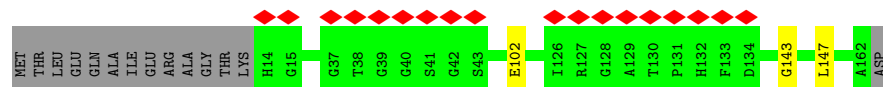
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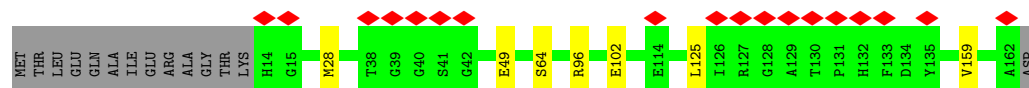
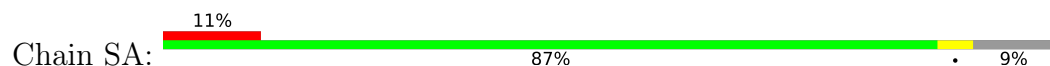
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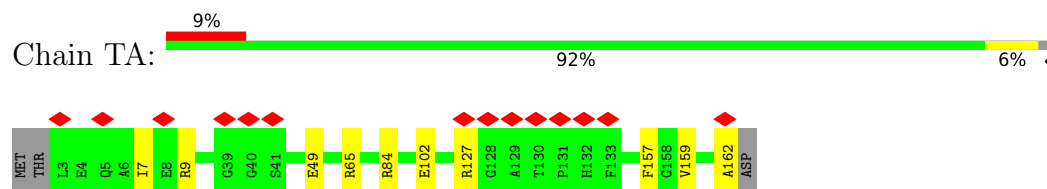
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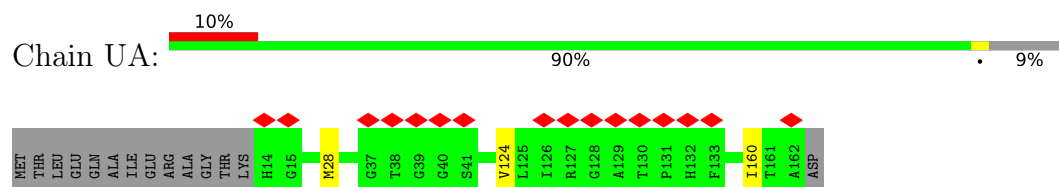
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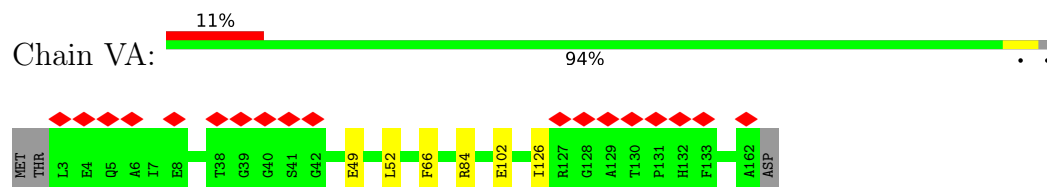
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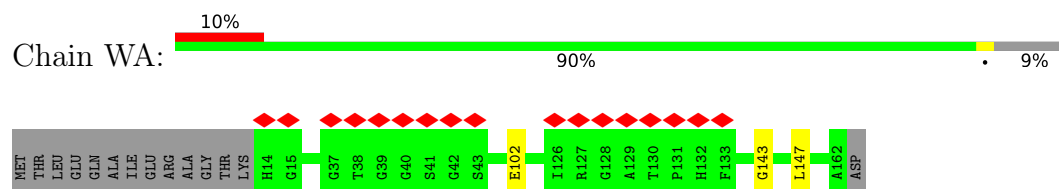
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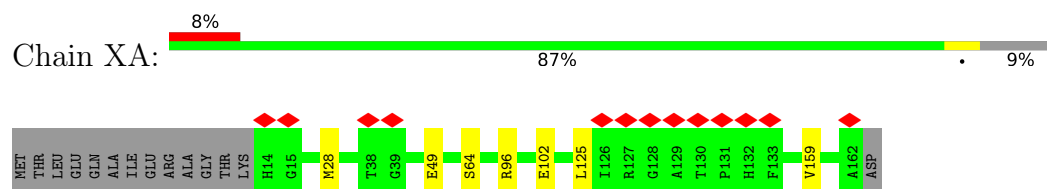
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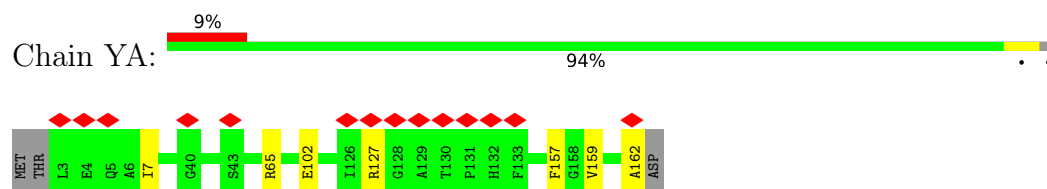
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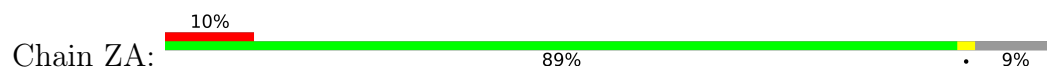
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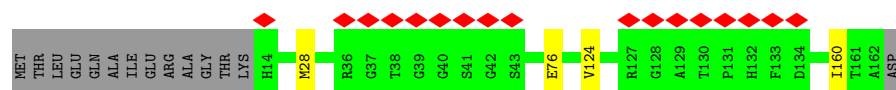


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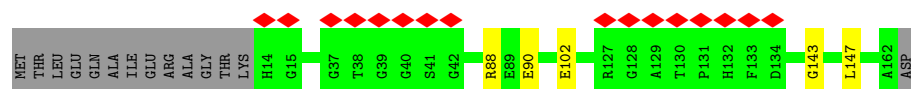




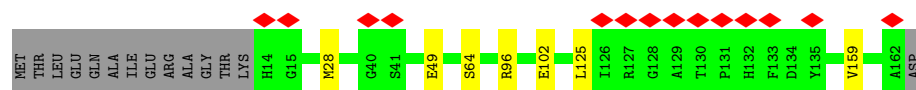
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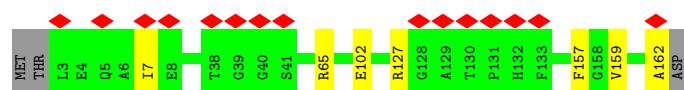
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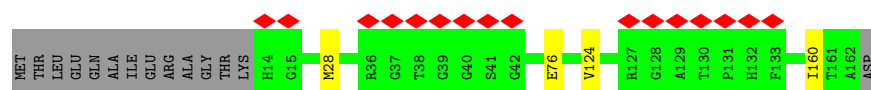
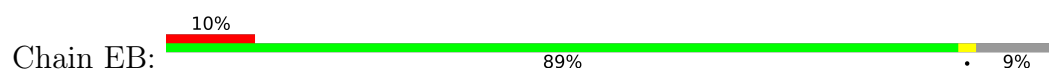
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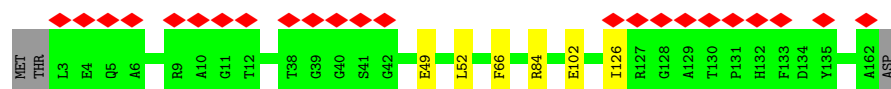
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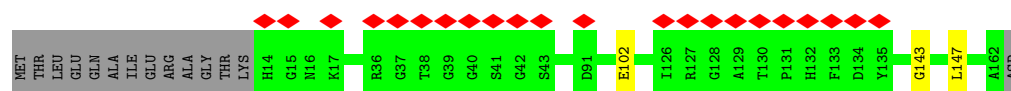
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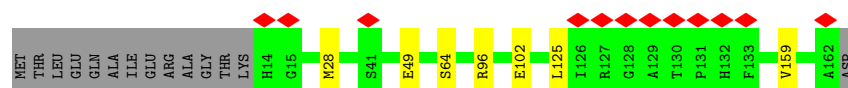
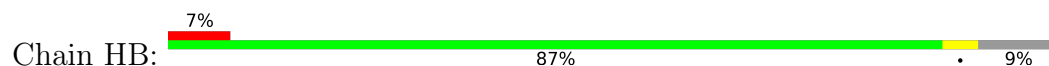
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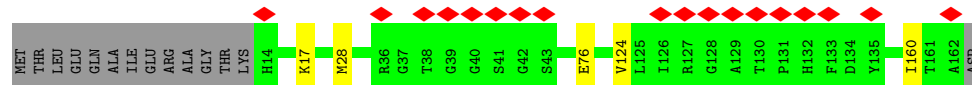
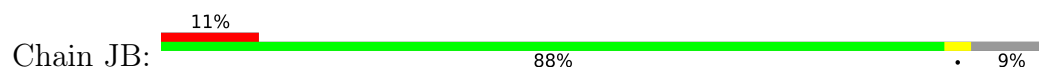
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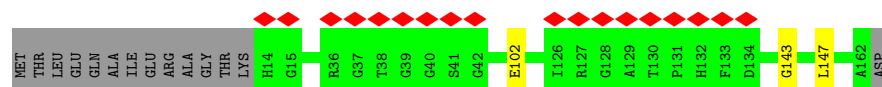
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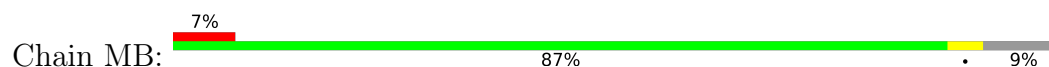
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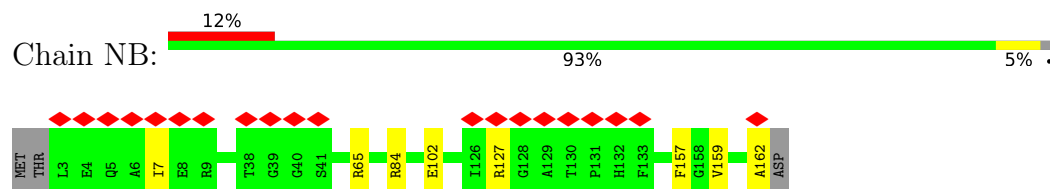
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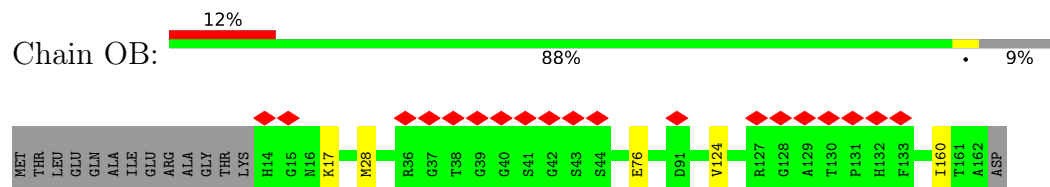
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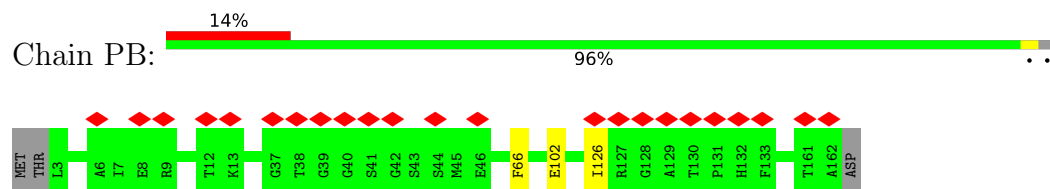
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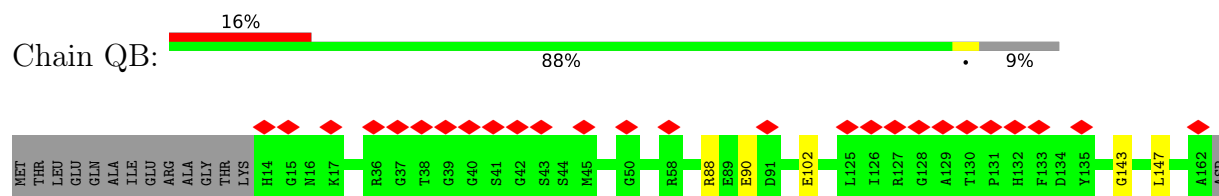
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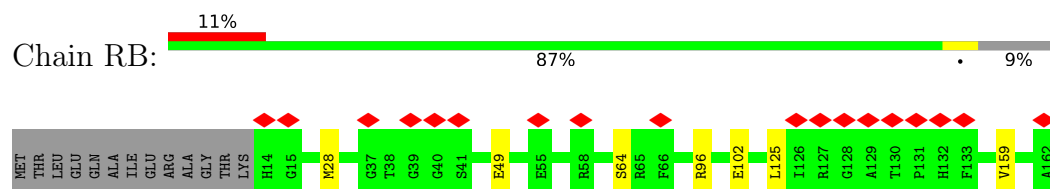
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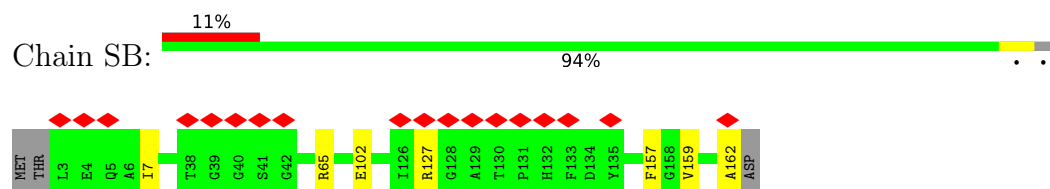
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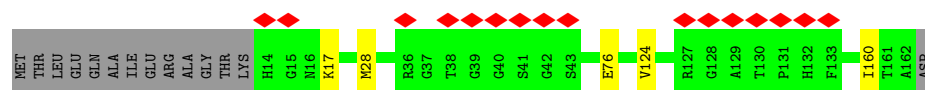


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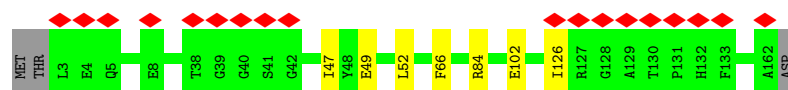


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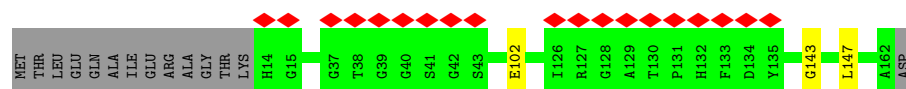




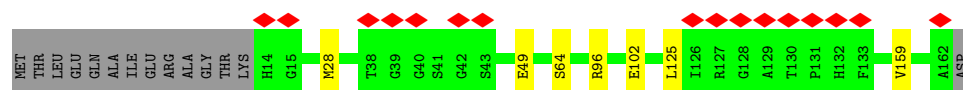
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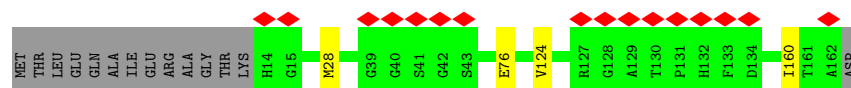
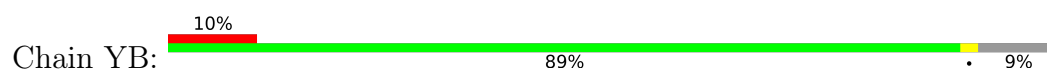
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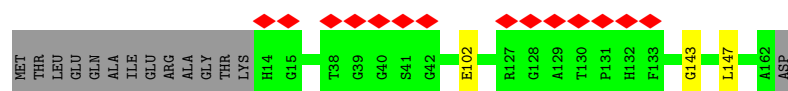
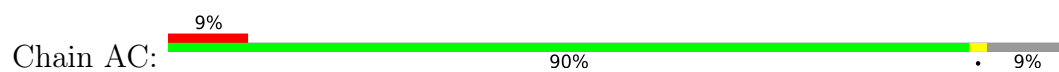
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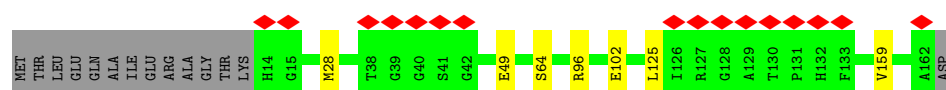
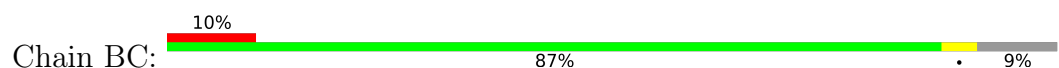
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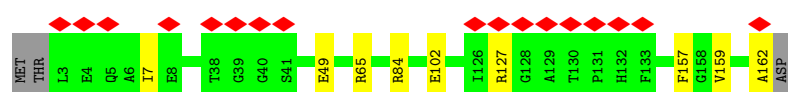
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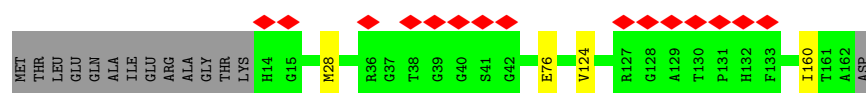
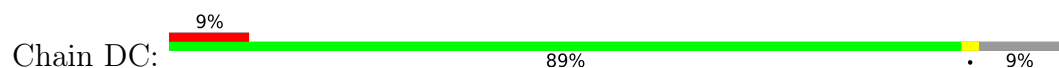
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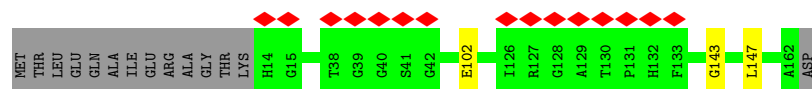
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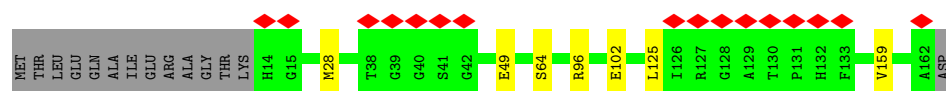
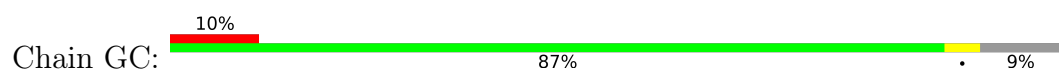
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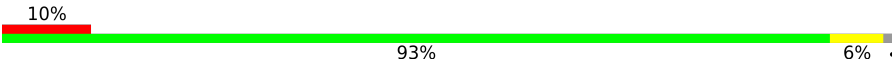
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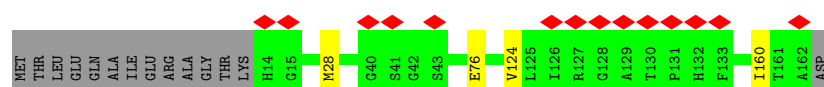
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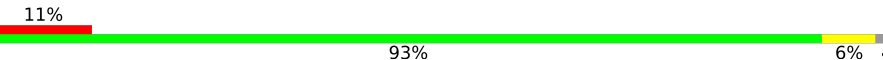


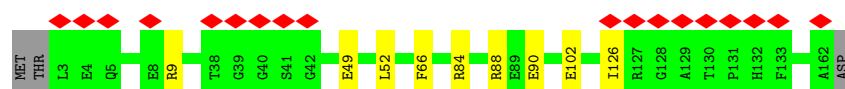
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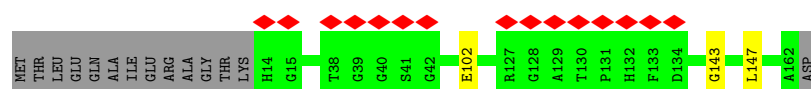
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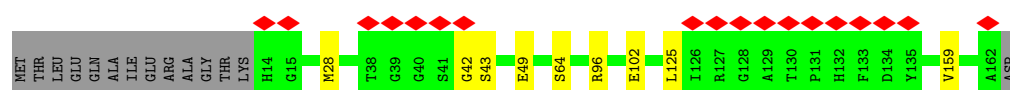
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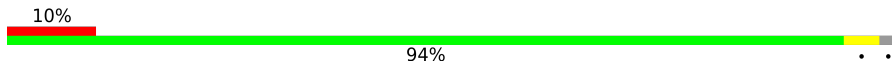


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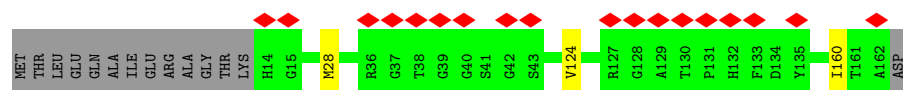
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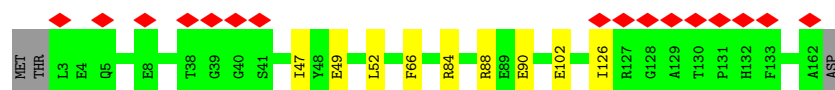


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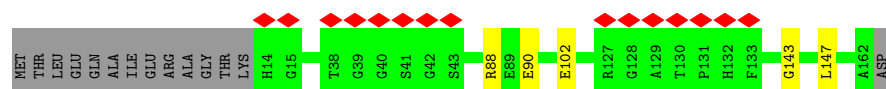
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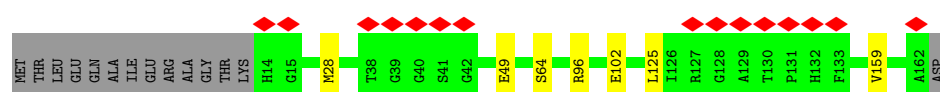
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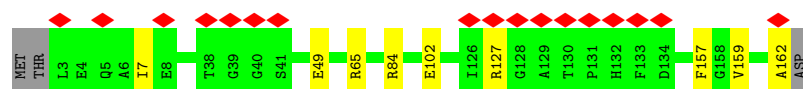
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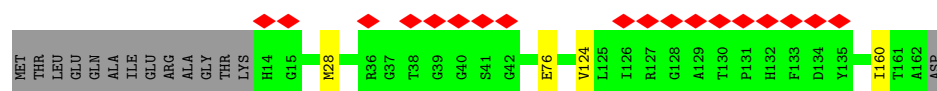
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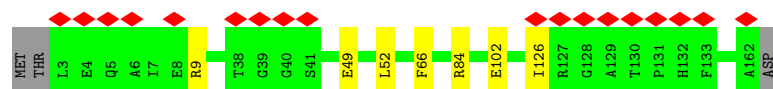
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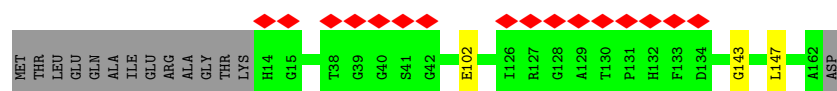
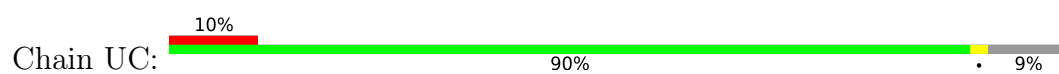
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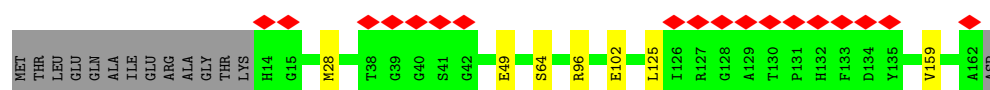
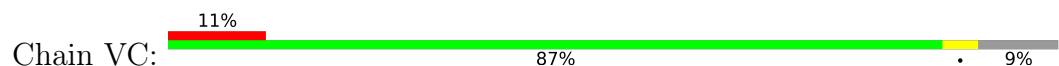
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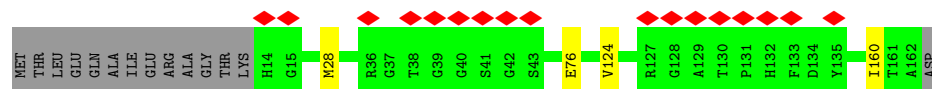
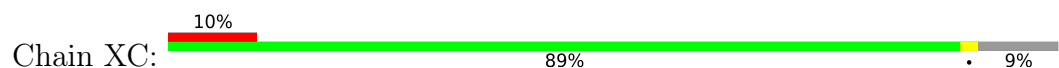
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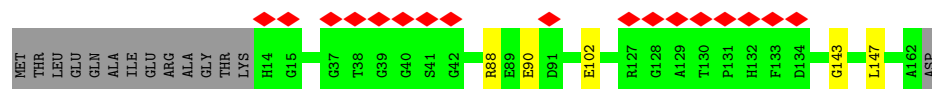
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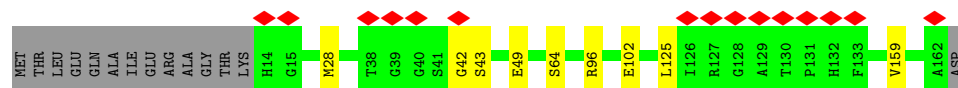
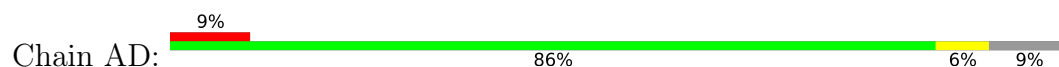
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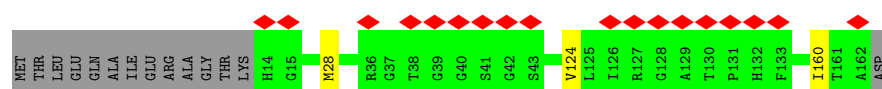
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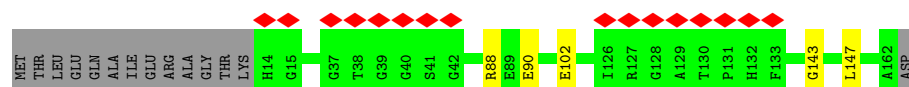
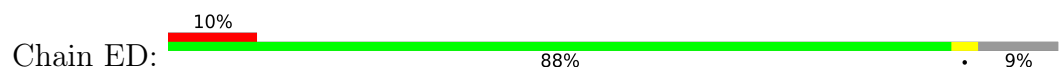
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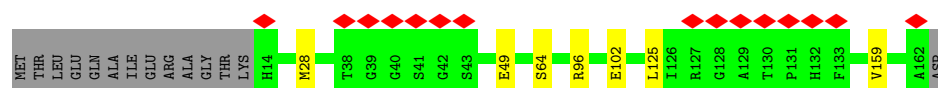
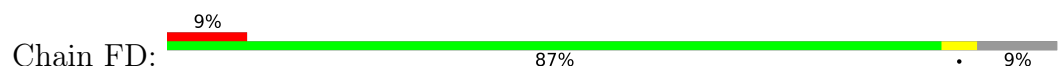
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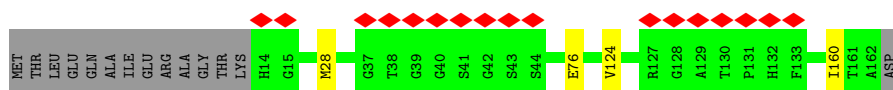


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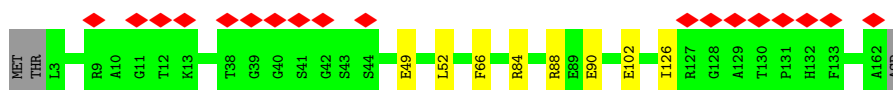


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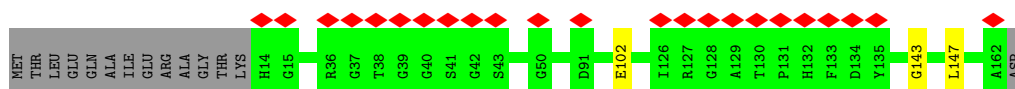




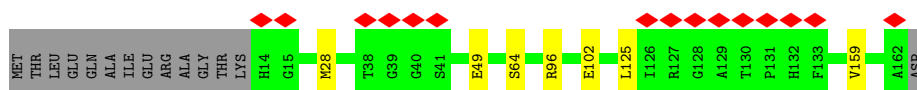
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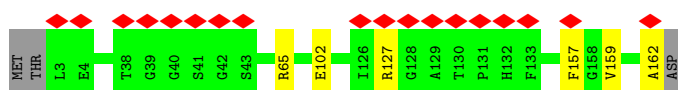
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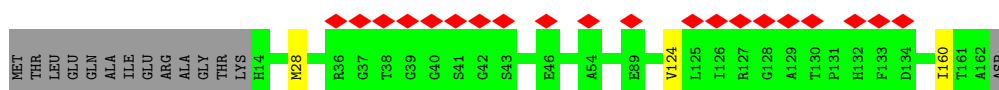
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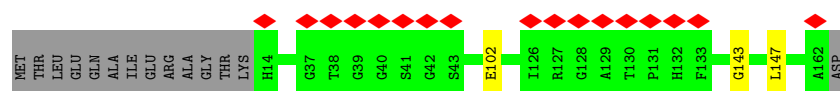
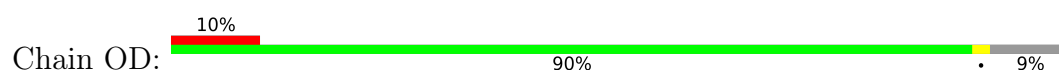
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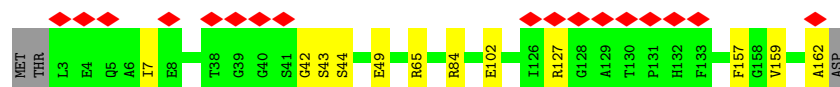
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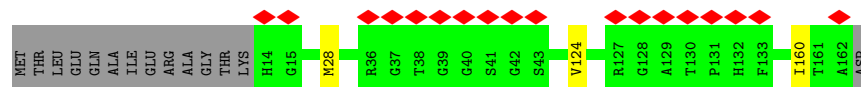
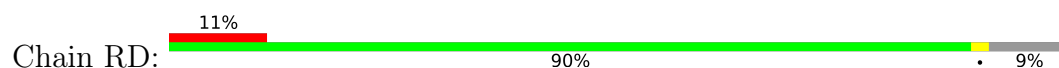
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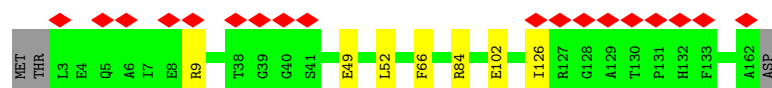
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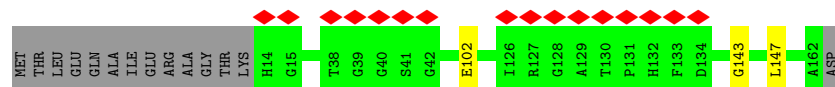
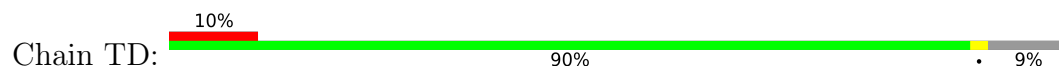
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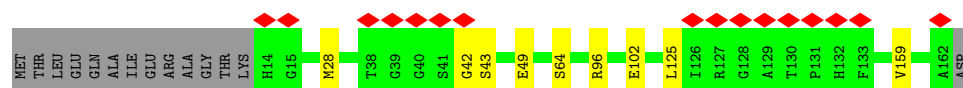
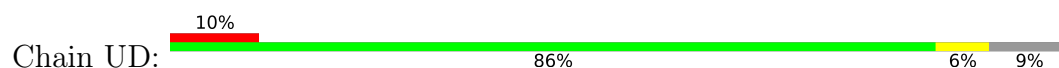
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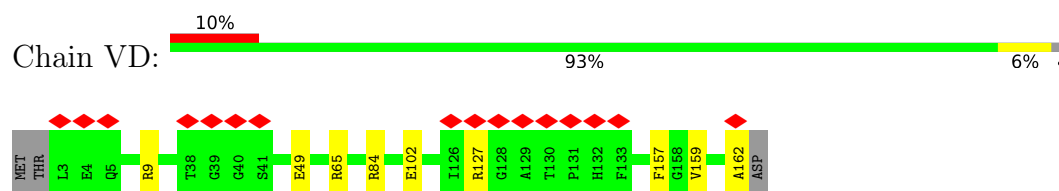
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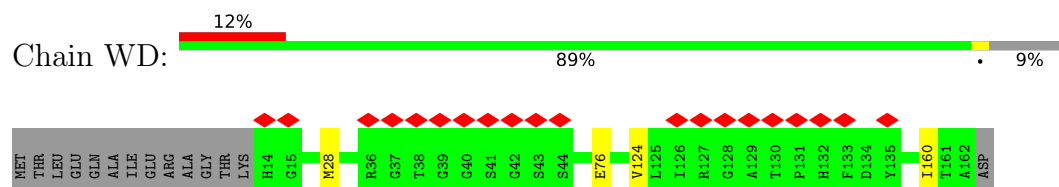
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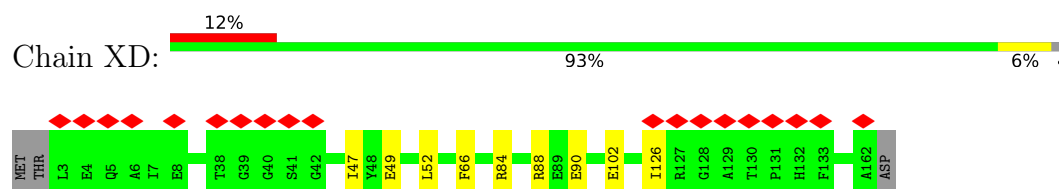
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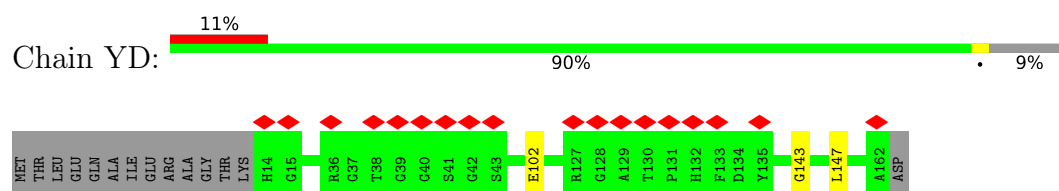
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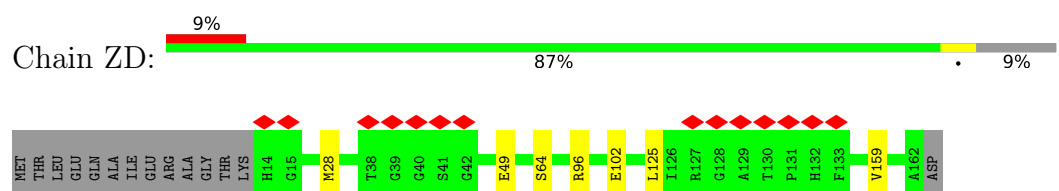
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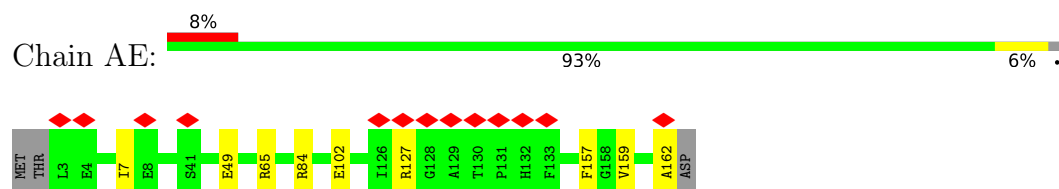
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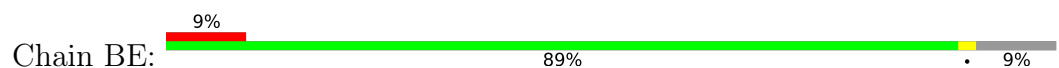
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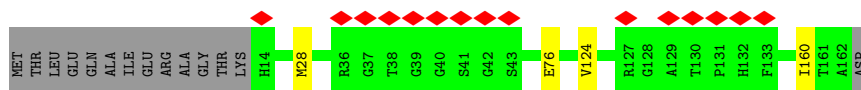


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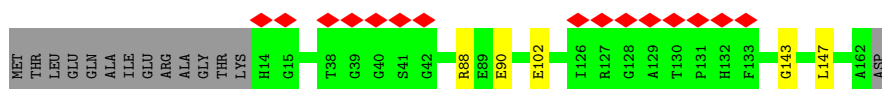




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- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



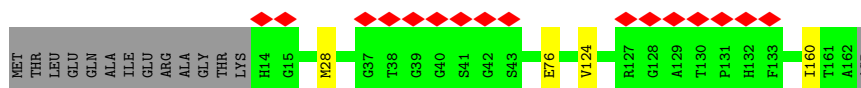
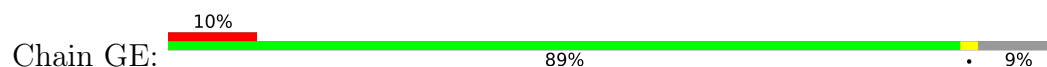
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



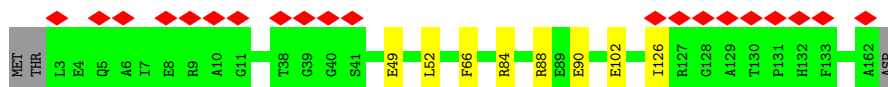
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



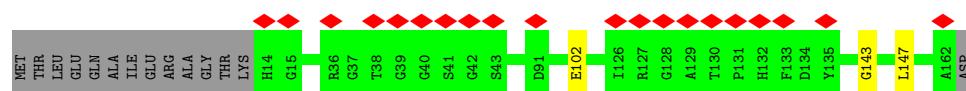
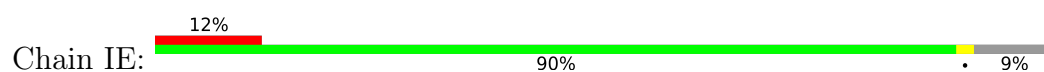
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



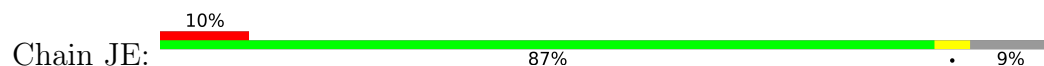
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



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



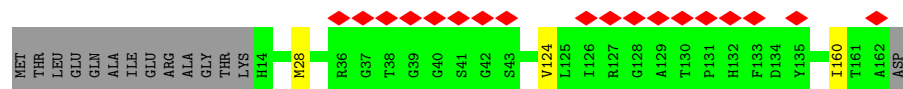
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



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



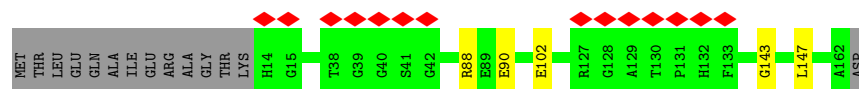
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



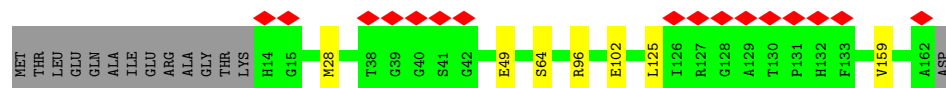
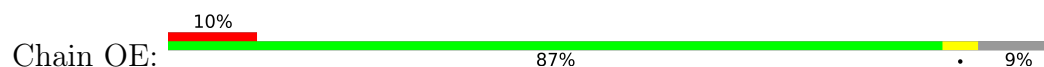
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



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



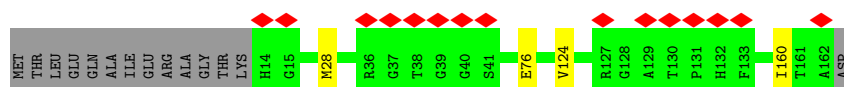
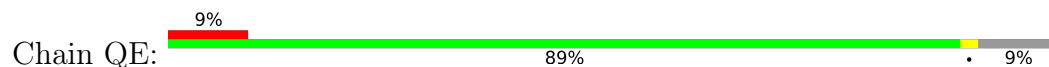
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



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



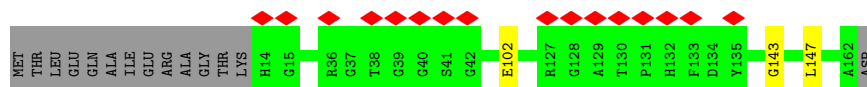
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



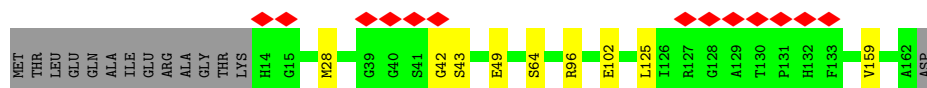
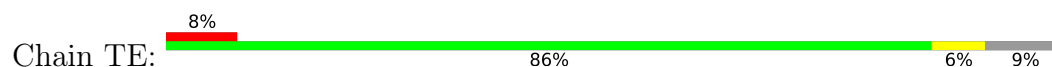
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=81.6°, rise=64.4 Å, axial sym=C1	Depositor
Number of segments used	168323	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 ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	2.273	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	457.6, 457.6, 457.6	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/1220	0.23	0/1646
1	AA	0.13	0/1136	0.23	0/1534
1	AB	0.13	0/1220	0.23	0/1646
1	AC	0.12	0/1136	0.23	0/1534
1	AD	0.14	0/1136	0.25	0/1534
1	AE	0.14	0/1220	0.23	0/1646
1	B	0.12	0/1136	0.23	0/1534
1	BA	0.13	0/1220	0.23	0/1646
1	BB	0.12	0/1136	0.23	0/1534
1	BC	0.14	0/1136	0.25	0/1534
1	BD	0.14	0/1220	0.23	0/1646
1	BE	0.13	0/1136	0.23	0/1534
1	C	0.13	0/1220	0.23	0/1646
1	CA	0.12	0/1136	0.23	0/1534
1	CB	0.14	0/1136	0.25	0/1534
1	CC	0.14	0/1220	0.23	0/1646
1	CD	0.13	0/1136	0.23	0/1534
1	CE	0.13	0/1220	0.23	0/1646
1	D	0.12	0/1136	0.23	0/1534
1	DA	0.14	0/1136	0.25	0/1534
1	DB	0.14	0/1220	0.23	0/1646
1	DC	0.13	0/1136	0.23	0/1534
1	DD	0.13	0/1220	0.23	0/1646
1	DE	0.12	0/1136	0.23	0/1534
1	E	0.13	0/1136	0.25	0/1534
1	EA	0.14	0/1220	0.23	0/1646
1	EB	0.13	0/1136	0.23	0/1534
1	EC	0.13	0/1220	0.23	0/1646
1	ED	0.12	0/1136	0.23	0/1534
1	EE	0.14	0/1136	0.25	0/1534
1	F	0.14	0/1220	0.23	0/1646
1	FA	0.13	0/1136	0.23	0/1534
1	FB	0.13	0/1220	0.23	0/1646
1	FC	0.12	0/1136	0.23	0/1534

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	FD	0.14	0/1136	0.25	0/1534
1	FE	0.14	0/1220	0.23	0/1646
1	G	0.13	0/1136	0.23	0/1534
1	GA	0.13	0/1220	0.23	0/1646
1	GB	0.12	0/1136	0.23	0/1534
1	GC	0.14	0/1136	0.25	0/1534
1	GD	0.14	0/1220	0.23	0/1646
1	GE	0.13	0/1136	0.23	0/1534
1	H	0.13	0/1220	0.23	0/1646
1	HA	0.12	0/1136	0.23	0/1534
1	HB	0.14	0/1136	0.25	0/1534
1	HC	0.14	0/1220	0.23	0/1646
1	HD	0.13	0/1136	0.23	0/1534
1	HE	0.13	0/1220	0.23	0/1646
1	I	0.12	0/1136	0.23	0/1534
1	IA	0.14	0/1136	0.25	0/1534
1	IB	0.14	0/1220	0.23	0/1646
1	IC	0.13	0/1136	0.23	0/1534
1	ID	0.13	0/1220	0.23	0/1646
1	IE	0.12	0/1136	0.23	0/1534
1	J	0.14	0/1136	0.25	0/1534
1	JA	0.14	0/1220	0.23	0/1646
1	JB	0.13	0/1136	0.23	0/1534
1	JC	0.13	0/1220	0.23	0/1646
1	JD	0.12	0/1136	0.23	0/1534
1	JE	0.13	0/1136	0.25	0/1534
1	K	0.14	0/1220	0.23	0/1646
1	KA	0.13	0/1136	0.23	0/1534
1	KB	0.13	0/1220	0.23	0/1646
1	KC	0.12	0/1136	0.23	0/1534
1	KD	0.13	0/1136	0.25	0/1534
1	KE	0.14	0/1220	0.23	0/1646
1	L	0.13	0/1136	0.23	0/1534
1	LA	0.13	0/1220	0.23	0/1646
1	LB	0.12	0/1136	0.23	0/1534
1	LC	0.13	0/1136	0.25	0/1534
1	LD	0.14	0/1220	0.23	0/1646
1	LE	0.13	0/1136	0.23	0/1534
1	M	0.13	0/1220	0.23	0/1646
1	MA	0.12	0/1136	0.23	0/1534
1	MB	0.14	0/1136	0.25	0/1534
1	MC	0.14	0/1220	0.23	0/1646
1	MD	0.13	0/1136	0.23	0/1534

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	ME	0.13	0/1220	0.23	0/1646
1	N	0.12	0/1136	0.23	0/1534
1	NA	0.13	0/1136	0.25	0/1534
1	NB	0.14	0/1220	0.23	0/1646
1	NC	0.13	0/1136	0.23	0/1534
1	ND	0.13	0/1220	0.23	0/1646
1	NE	0.12	0/1136	0.23	0/1534
1	O	0.14	0/1136	0.25	0/1534
1	OA	0.14	0/1220	0.23	0/1646
1	OB	0.13	0/1136	0.23	0/1534
1	OC	0.13	0/1220	0.23	0/1646
1	OD	0.12	0/1136	0.23	0/1534
1	OE	0.14	0/1136	0.25	0/1534
1	P	0.14	0/1220	0.23	0/1646
1	PA	0.13	0/1136	0.23	0/1534
1	PB	0.13	0/1220	0.23	0/1646
1	PC	0.12	0/1136	0.23	0/1534
1	PD	0.14	0/1136	0.25	0/1534
1	PE	0.14	0/1220	0.23	0/1646
1	Q	0.13	0/1136	0.23	0/1534
1	QA	0.13	0/1220	0.23	0/1646
1	QB	0.12	0/1136	0.23	0/1534
1	QC	0.14	0/1136	0.25	0/1534
1	QD	0.14	0/1220	0.23	0/1646
1	QE	0.13	0/1136	0.23	0/1534
1	R	0.13	0/1220	0.23	0/1646
1	RA	0.12	0/1136	0.23	0/1534
1	RB	0.13	0/1136	0.25	0/1534
1	RC	0.14	0/1220	0.23	0/1646
1	RD	0.13	0/1136	0.23	0/1534
1	RE	0.13	0/1220	0.23	0/1646
1	S	0.12	0/1136	0.23	0/1534
1	SA	0.14	0/1136	0.25	0/1534
1	SB	0.14	0/1220	0.23	0/1646
1	SC	0.13	0/1136	0.23	0/1534
1	SD	0.13	0/1220	0.23	0/1646
1	SE	0.12	0/1136	0.23	0/1534
1	T	0.14	0/1136	0.25	0/1534
1	TA	0.14	0/1220	0.23	0/1646
1	TB	0.13	0/1136	0.23	0/1534
1	TC	0.13	0/1220	0.23	0/1646
1	TD	0.12	0/1136	0.23	0/1534
1	TE	0.14	0/1136	0.25	0/1534

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	U	0.14	0/1220	0.23	0/1646
1	UA	0.13	0/1136	0.23	0/1534
1	UB	0.13	0/1220	0.23	0/1646
1	UC	0.12	0/1136	0.23	0/1534
1	UD	0.14	0/1136	0.25	0/1534
1	V	0.13	0/1136	0.23	0/1534
1	VA	0.13	0/1220	0.23	0/1646
1	VB	0.12	0/1136	0.23	0/1534
1	VC	0.14	0/1136	0.25	0/1534
1	VD	0.14	0/1220	0.23	0/1646
1	W	0.13	0/1220	0.23	0/1646
1	WA	0.12	0/1136	0.23	0/1534
1	WB	0.14	0/1136	0.25	0/1534
1	WC	0.14	0/1220	0.23	0/1646
1	WD	0.13	0/1136	0.23	0/1534
1	X	0.12	0/1136	0.23	0/1534
1	XA	0.14	0/1136	0.25	0/1534
1	XB	0.14	0/1220	0.23	0/1646
1	XC	0.13	0/1136	0.23	0/1534
1	XD	0.13	0/1220	0.23	0/1646
1	Y	0.14	0/1136	0.25	0/1534
1	YA	0.14	0/1220	0.23	0/1646
1	YB	0.13	0/1136	0.23	0/1534
1	YC	0.13	0/1220	0.23	0/1646
1	YD	0.12	0/1136	0.23	0/1534
1	Z	0.14	0/1220	0.23	0/1646
1	ZA	0.13	0/1136	0.23	0/1534
1	ZB	0.13	0/1220	0.23	0/1646
1	ZC	0.12	0/1136	0.23	0/1534
1	ZD	0.13	0/1136	0.25	0/1534
All	All	0.13	0/175440	0.23	0/236820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1202	0	1221	10	0
1	AA	1118	0	1133	3	0
1	AB	1202	0	1221	13	0
1	AC	1118	0	1133	2	0
1	AD	1118	0	1133	8	0
1	AE	1202	0	1221	9	0
1	B	1118	0	1133	3	0
1	BA	1202	0	1221	14	0
1	BB	1118	0	1133	3	0
1	BC	1118	0	1133	7	0
1	BD	1202	0	1221	9	0
1	BE	1118	0	1133	3	0
1	C	1202	0	1221	9	0
1	CA	1118	0	1133	3	0
1	CB	1118	0	1133	7	0
1	CC	1202	0	1221	9	0
1	CD	1118	0	1133	2	0
1	CE	1202	0	1221	14	0
1	D	1118	0	1133	4	0
1	DA	1118	0	1133	7	0
1	DB	1202	0	1221	7	0
1	DC	1118	0	1133	3	0
1	DD	1202	0	1221	13	0
1	DE	1118	0	1133	3	0
1	E	1118	0	1133	7	0
1	EA	1202	0	1221	9	0
1	EB	1118	0	1133	3	0
1	EC	1202	0	1221	14	0
1	ED	1118	0	1133	3	0
1	EE	1118	0	1133	7	0
1	F	1202	0	1221	9	0
1	FA	1118	0	1133	3	0
1	FB	1202	0	1221	14	0
1	FC	1118	0	1133	2	0
1	FD	1118	0	1133	7	0
1	FE	1202	0	1221	9	0
1	G	1118	0	1133	3	0
1	GA	1202	0	1221	13	0
1	GB	1118	0	1133	2	0
1	GC	1118	0	1133	7	0
1	GD	1202	0	1221	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GE	1118	0	1133	3	0
1	H	1202	0	1221	14	0
1	HA	1118	0	1133	2	0
1	HB	1118	0	1133	7	0
1	HC	1202	0	1221	9	0
1	HD	1118	0	1133	3	0
1	HE	1202	0	1221	12	0
1	I	1118	0	1133	2	0
1	IA	1118	0	1133	7	0
1	IB	1202	0	1221	8	0
1	IC	1118	0	1133	3	0
1	ID	1202	0	1221	13	0
1	IE	1118	0	1133	2	0
1	J	1118	0	1133	7	0
1	JA	1202	0	1221	6	0
1	JB	1118	0	1133	4	0
1	JC	1202	0	1221	14	0
1	JD	1118	0	1133	2	0
1	JE	1118	0	1133	7	0
1	K	1202	0	1221	8	0
1	KA	1118	0	1133	2	0
1	KB	1202	0	1221	14	0
1	KC	1118	0	1133	2	0
1	KD	1118	0	1133	7	0
1	KE	1202	0	1221	6	0
1	L	1118	0	1133	3	0
1	LA	1202	0	1221	13	0
1	LB	1118	0	1133	2	0
1	LC	1118	0	1133	8	0
1	LD	1202	0	1221	6	0
1	LE	1118	0	1133	2	0
1	M	1202	0	1221	10	0
1	MA	1118	0	1133	2	0
1	MB	1118	0	1133	7	0
1	MC	1202	0	1221	6	0
1	MD	1118	0	1133	2	0
1	ME	1202	0	1221	12	0
1	N	1118	0	1133	2	0
1	NA	1118	0	1133	7	0
1	NB	1202	0	1221	8	0
1	NC	1118	0	1133	2	0
1	ND	1202	0	1221	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	NE	1118	0	1133	3	0
1	O	1118	0	1133	7	0
1	OA	1202	0	1221	9	0
1	OB	1118	0	1133	4	0
1	OC	1202	0	1221	14	0
1	OD	1118	0	1133	2	0
1	OE	1118	0	1133	7	0
1	P	1202	0	1221	8	0
1	PA	1118	0	1133	4	0
1	PB	1202	0	1221	2	0
1	PC	1118	0	1133	3	0
1	PD	1118	0	1133	7	0
1	PE	1202	0	1221	9	0
1	Q	1118	0	1133	4	0
1	QA	1202	0	1221	2	0
1	QB	1118	0	1133	3	0
1	QC	1118	0	1133	7	0
1	QD	1202	0	1221	11	0
1	QE	1118	0	1133	3	0
1	R	1202	0	1221	14	0
1	RA	1118	0	1133	2	0
1	RB	1118	0	1133	7	0
1	RC	1202	0	1221	9	0
1	RD	1118	0	1133	2	0
1	RE	1202	0	1221	13	0
1	S	1118	0	1133	2	0
1	SA	1118	0	1133	7	0
1	SB	1202	0	1221	7	0
1	SC	1118	0	1133	3	0
1	SD	1202	0	1221	13	0
1	SE	1118	0	1133	2	0
1	T	1118	0	1133	8	0
1	TA	1202	0	1221	11	0
1	TB	1118	0	1133	4	0
1	TC	1202	0	1221	14	0
1	TD	1118	0	1133	2	0
1	TE	1118	0	1133	8	0
1	U	1202	0	1221	9	0
1	UA	1118	0	1133	2	0
1	UB	1202	0	1221	14	0
1	UC	1118	0	1133	2	0
1	UD	1118	0	1133	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	1118	0	1133	2	0
1	VA	1202	0	1221	12	0
1	VB	1118	0	1133	2	0
1	VC	1118	0	1133	7	0
1	VD	1202	0	1221	9	0
1	W	1202	0	1221	13	0
1	WA	1118	0	1133	2	0
1	WB	1118	0	1133	7	0
1	WC	1202	0	1221	9	0
1	WD	1118	0	1133	3	0
1	X	1118	0	1133	2	0
1	XA	1118	0	1133	7	0
1	XB	1202	0	1221	7	0
1	XC	1118	0	1133	3	0
1	XD	1202	0	1221	14	0
1	Y	1118	0	1133	7	0
1	YA	1202	0	1221	7	0
1	YB	1118	0	1133	3	0
1	YC	1202	0	1221	13	0
1	YD	1118	0	1133	2	0
1	Z	1202	0	1221	8	0
1	ZA	1118	0	1133	3	0
1	ZB	1202	0	1221	15	0
1	ZC	1118	0	1133	3	0
1	ZD	1118	0	1133	7	0
All	All	172740	0	175230	648	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 2.

All (648) 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:UB:84:ARG:HE	1:TC:52:LEU:CD1	2.06	0.67
1:U:102:GLU:CD	1:Y:28:MET:HE3	2.20	0.67
1:EA:102:GLU:CD	1:IA:28:MET:HE3	2.20	0.66
1:DB:102:GLU:CD	1:HB:28:MET:HE3	2.20	0.66
1:CC:102:GLU:CD	1:GC:28:MET:HE3	2.20	0.66
1:JA:102:GLU:CD	1:NA:28:MET:HE3	2.20	0.66
1:UB:52:LEU:HD11	1:TC:84:ARG:HE	1.59	0.66
1:RC:102:GLU:CD	1:VC:28:MET:HE3	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QD:102:GLU:CD	1:UD:28:MET:HE3	2.20	0.66
1:FB:52:LEU:CD1	1:KB:84:ARG:HE	2.08	0.66
1:PE:102:GLU:CD	1:TE:28:MET:HE3	2.20	0.66
1:H:52:LEU:CD1	1:R:84:ARG:HE	2.08	0.66
1:FB:84:ARG:HE	1:KB:52:LEU:CD1	2.08	0.66
1:LD:102:GLU:CD	1:PD:28:MET:HE3	2.21	0.66
1:F:102:GLU:CD	1:J:28:MET:HE3	2.20	0.66
1:WC:102:GLU:CD	1:AD:28:MET:HE3	2.20	0.66
1:TA:102:GLU:CD	1:XA:28:MET:HE3	2.20	0.66
1:IB:102:GLU:CD	1:MB:28:MET:HE3	2.21	0.66
1:KE:102:GLU:CD	1:OE:28:MET:HE3	2.20	0.66
1:P:102:GLU:CD	1:T:28:MET:HE3	2.20	0.66
1:AE:102:GLU:CD	1:EE:28:MET:HE3	2.20	0.66
1:YA:102:GLU:CD	1:CB:28:MET:HE3	2.21	0.66
1:HC:102:GLU:CD	1:LC:28:MET:HE3	2.21	0.66
1:MC:102:GLU:CD	1:QC:28:MET:HE3	2.20	0.66
1:NB:102:GLU:CD	1:RB:28:MET:HE3	2.21	0.66
1:A:102:GLU:CD	1:E:28:MET:HE3	2.20	0.65
1:K:102:GLU:CD	1:O:28:MET:HE3	2.20	0.65
1:Z:102:GLU:CD	1:DA:28:MET:HE3	2.20	0.65
1:SB:102:GLU:CD	1:WB:28:MET:HE3	2.20	0.65
1:UB:52:LEU:CD1	1:TC:84:ARG:HE	2.09	0.65
1:FE:102:GLU:CD	1:JE:28:MET:HE3	2.21	0.65
1:XB:102:GLU:CD	1:BC:28:MET:HE3	2.21	0.65
1:GD:102:GLU:CD	1:KD:28:MET:HE3	2.20	0.65
1:OA:102:GLU:CD	1:SA:28:MET:HE3	2.20	0.65
1:VD:102:GLU:CD	1:ZD:28:MET:HE3	2.21	0.65
1:H:84:ARG:HE	1:R:52:LEU:HD11	1.61	0.65
1:BD:102:GLU:CD	1:FD:28:MET:HE3	2.21	0.65
1:H:84:ARG:HE	1:R:52:LEU:CD1	2.09	0.65
1:FB:52:LEU:HD11	1:KB:84:ARG:NE	2.13	0.64
1:H:52:LEU:HD11	1:R:84:ARG:NE	2.13	0.63
1:UB:52:LEU:HD11	1:TC:84:ARG:NE	2.13	0.63
1:FB:84:ARG:NE	1:KB:52:LEU:HD11	2.13	0.63
1:H:84:ARG:NE	1:R:52:LEU:HD11	2.13	0.63
1:UB:84:ARG:NE	1:TC:52:LEU:HD11	2.13	0.63
1:JC:52:LEU:CD1	1:OC:84:ARG:HE	2.12	0.63
1:C:84:ARG:NH1	1:M:49:GLU:OE2	2.32	0.63
1:FB:84:ARG:HE	1:KB:52:LEU:HD11	1.64	0.62
1:HE:52:LEU:CD1	1:ME:84:ARG:HE	2.12	0.62
1:HE:84:ARG:HE	1:ME:52:LEU:CD1	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XD:84:ARG:HE	1:CE:52:LEU:CD1	2.11	0.62
1:FB:52:LEU:HD11	1:KB:84:ARG:HE	1.63	0.62
1:W:52:LEU:CD1	1:GA:84:ARG:HE	2.12	0.62
1:ZB:52:LEU:CD1	1:EC:84:ARG:HE	2.12	0.62
1:XD:52:LEU:CD1	1:CE:84:ARG:HE	2.12	0.62
1:ZB:84:ARG:HE	1:EC:52:LEU:CD1	2.13	0.62
1:JC:84:ARG:HE	1:OC:52:LEU:HD11	1.65	0.62
1:YC:84:ARG:HE	1:DD:52:LEU:CD1	2.11	0.62
1:BA:52:LEU:CD1	1:LA:84:ARG:HE	2.13	0.61
1:YC:52:LEU:HD11	1:DD:84:ARG:HE	1.64	0.61
1:JC:84:ARG:HE	1:OC:52:LEU:CD1	2.14	0.61
1:ZB:84:ARG:HE	1:EC:52:LEU:HD11	1.66	0.61
1:BA:84:ARG:HE	1:LA:52:LEU:CD1	2.14	0.60
1:UB:84:ARG:HE	1:TC:52:LEU:HD11	1.67	0.60
1:VA:84:ARG:HE	1:AB:52:LEU:CD1	2.13	0.60
1:XD:52:LEU:HD11	1:CE:84:ARG:HE	1.66	0.60
1:SD:52:LEU:CD1	1:RE:84:ARG:HE	2.13	0.60
1:W:84:ARG:HE	1:GA:52:LEU:CD1	2.13	0.60
1:YC:52:LEU:CD1	1:DD:84:ARG:HE	2.14	0.60
1:K:65:ARG:NH2	1:O:49:GLU:OE1	2.35	0.60
1:VA:52:LEU:CD1	1:AB:84:ARG:HE	2.14	0.60
1:MC:65:ARG:NH2	1:QC:49:GLU:OE1	2.35	0.60
1:JA:65:ARG:NH2	1:NA:49:GLU:OE1	2.35	0.60
1:VD:65:ARG:NH2	1:ZD:49:GLU:OE1	2.35	0.60
1:KE:65:ARG:NH2	1:OE:49:GLU:OE1	2.35	0.60
1:ID:52:LEU:CD1	1:ND:84:ARG:HE	2.15	0.59
1:SB:65:ARG:NH2	1:WB:49:GLU:OE1	2.35	0.59
1:CC:65:ARG:NH2	1:GC:49:GLU:OE1	2.35	0.59
1:BD:65:ARG:NH2	1:FD:49:GLU:OE1	2.35	0.59
1:GD:65:ARG:NH2	1:KD:49:GLU:OE1	2.35	0.59
1:AE:65:ARG:NH2	1:EE:49:GLU:OE1	2.35	0.59
1:A:65:ARG:NH2	1:E:49:GLU:OE1	2.35	0.59
1:H:52:LEU:HD11	1:R:84:ARG:HE	1.66	0.59
1:Z:65:ARG:NH2	1:DA:49:GLU:OE1	2.35	0.59
1:DB:65:ARG:NH2	1:HB:49:GLU:OE1	2.35	0.59
1:EA:65:ARG:NH2	1:IA:49:GLU:OE1	2.35	0.59
1:OA:65:ARG:NH2	1:SA:49:GLU:OE1	2.35	0.59
1:TA:65:ARG:NH2	1:XA:49:GLU:OE1	2.35	0.59
1:NB:65:ARG:NH2	1:RB:49:GLU:OE1	2.35	0.59
1:HC:65:ARG:NH2	1:LC:49:GLU:OE1	2.35	0.59
1:YA:65:ARG:NH2	1:CB:49:GLU:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XB:65:ARG:NH2	1:BC:49:GLU:OE1	2.35	0.59
1:LD:65:ARG:NH2	1:PD:49:GLU:OE1	2.35	0.59
1:QD:65:ARG:NH2	1:UD:49:GLU:OE1	2.35	0.59
1:SD:84:ARG:HE	1:RE:52:LEU:HD11	1.68	0.59
1:PE:65:ARG:NH2	1:TE:49:GLU:OE1	2.35	0.59
1:F:65:ARG:NH2	1:J:49:GLU:OE1	2.35	0.59
1:ID:84:ARG:HE	1:ND:52:LEU:CD1	2.15	0.59
1:P:65:ARG:NH2	1:T:49:GLU:OE1	2.35	0.59
1:WC:65:ARG:NH2	1:AD:49:GLU:OE1	2.35	0.59
1:FE:65:ARG:NH2	1:JE:49:GLU:OE1	2.35	0.59
1:HE:52:LEU:HD11	1:ME:84:ARG:HE	1.67	0.59
1:BA:84:ARG:HE	1:LA:52:LEU:HD11	1.66	0.59
1:IB:65:ARG:NH2	1:MB:49:GLU:OE1	2.35	0.59
1:RC:65:ARG:NH2	1:VC:49:GLU:OE1	2.35	0.59
1:U:65:ARG:NH2	1:Y:49:GLU:OE1	2.35	0.59
1:ZB:52:LEU:HD11	1:EC:84:ARG:NE	2.18	0.58
1:SD:84:ARG:HE	1:RE:52:LEU:CD1	2.15	0.58
1:W:84:ARG:HE	1:GA:52:LEU:HD11	1.66	0.58
1:ZB:84:ARG:NE	1:EC:52:LEU:HD11	2.18	0.58
1:YC:52:LEU:HD11	1:DD:84:ARG:NE	2.19	0.58
1:A:49:GLU:HG2	1:TA:84:ARG:NH2	2.19	0.58
1:HE:52:LEU:HD11	1:ME:84:ARG:NE	2.19	0.58
1:JC:52:LEU:HD11	1:OC:84:ARG:NE	2.19	0.57
1:YC:84:ARG:NE	1:DD:52:LEU:HD11	2.19	0.57
1:JC:84:ARG:NE	1:OC:52:LEU:HD11	2.19	0.57
1:C:49:GLU:OE2	1:M:84:ARG:NH1	2.38	0.57
1:XD:52:LEU:HD11	1:CE:84:ARG:NE	2.19	0.57
1:HE:84:ARG:NE	1:ME:52:LEU:HD11	2.19	0.57
1:W:52:LEU:HD11	1:GA:84:ARG:NE	2.19	0.57
1:BA:52:LEU:HD11	1:LA:84:ARG:NE	2.19	0.57
1:BA:52:LEU:HD11	1:LA:84:ARG:HE	1.70	0.57
1:W:84:ARG:NE	1:GA:52:LEU:HD11	2.20	0.57
1:HE:84:ARG:HE	1:ME:52:LEU:HD11	1.70	0.56
1:BA:84:ARG:NE	1:LA:52:LEU:HD11	2.19	0.56
1:VA:52:LEU:HD11	1:AB:84:ARG:HE	1.68	0.56
1:UB:84:ARG:NE	1:TC:52:LEU:CD1	2.69	0.56
1:XD:84:ARG:NE	1:CE:52:LEU:HD11	2.20	0.56
1:ZB:52:LEU:HD11	1:EC:84:ARG:HE	1.69	0.56
1:SD:52:LEU:HD11	1:RE:84:ARG:NE	2.21	0.56
1:SD:84:ARG:NE	1:RE:52:LEU:HD11	2.21	0.56
1:VA:52:LEU:HD11	1:AB:84:ARG:NE	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ID:52:LEU:HD11	1:ND:84:ARG:HE	1.70	0.56
1:XD:84:ARG:HE	1:CE:52:LEU:HD11	1.71	0.56
1:W:52:LEU:HD11	1:GA:84:ARG:HE	1.70	0.55
1:VA:84:ARG:HE	1:AB:52:LEU:HD11	1.72	0.55
1:VA:84:ARG:NE	1:AB:52:LEU:HD11	2.21	0.55
1:ID:52:LEU:HD11	1:ND:84:ARG:NE	2.21	0.55
1:QD:49:GLU:HG2	1:VD:84:ARG:NH2	2.21	0.55
1:JC:52:LEU:HD11	1:OC:84:ARG:HE	1.72	0.55
1:A:84:ARG:NH2	1:TA:49:GLU:HG2	2.22	0.55
1:H:52:LEU:CD1	1:R:84:ARG:NE	2.70	0.54
1:YC:84:ARG:HE	1:DD:52:LEU:HD11	1.72	0.54
1:ID:84:ARG:HE	1:ND:52:LEU:HD11	1.72	0.54
1:UA:28:MET:HE3	1:VA:102:GLU:HG2	1.90	0.53
1:GE:28:MET:HE3	1:HE:102:GLU:HG2	1.90	0.53
1:V:28:MET:HE3	1:W:102:GLU:HG2	1.90	0.53
1:DC:28:MET:HE3	1:EC:102:GLU:HG2	1.90	0.53
1:IC:28:MET:HE3	1:JC:102:GLU:HG2	1.90	0.53
1:ID:84:ARG:NE	1:ND:52:LEU:HD11	2.23	0.53
1:RD:28:MET:HE3	1:SD:102:GLU:HG2	1.90	0.53
1:KA:28:MET:HE3	1:LA:102:GLU:HG2	1.90	0.53
1:B:28:MET:HE3	1:C:102:GLU:HG2	1.90	0.53
1:EB:28:MET:HE3	1:FB:102:GLU:HG2	1.90	0.53
1:TB:28:MET:HE3	1:UB:102:GLU:HG2	1.90	0.53
1:G:124:VAL:HG23	1:G:160:ILE:HG23	1.91	0.52
1:FA:28:MET:HE3	1:GA:102:GLU:HG2	1.90	0.52
1:FB:84:ARG:NE	1:KB:52:LEU:CD1	2.72	0.52
1:OB:28:MET:HE3	1:PB:102:GLU:HG2	1.90	0.52
1:CD:28:MET:HE3	1:DD:102:GLU:HG2	1.90	0.52
1:QE:28:MET:HE3	1:RE:102:GLU:HG2	1.90	0.52
1:Q:28:MET:HE3	1:R:102:GLU:HG2	1.90	0.52
1:JB:28:MET:HE3	1:KB:102:GLU:HG2	1.90	0.52
1:HD:28:MET:HE3	1:ID:102:GLU:HG2	1.90	0.52
1:MD:28:MET:HE3	1:ND:102:GLU:HG2	1.90	0.52
1:BE:124:VAL:HG23	1:BE:160:ILE:HG23	1.91	0.52
1:AA:28:MET:HE3	1:BA:102:GLU:HG2	1.90	0.52
1:PA:124:VAL:HG23	1:PA:160:ILE:HG23	1.91	0.52
1:WD:28:MET:HE3	1:XD:102:GLU:HG2	1.90	0.52
1:L:28:MET:HE3	1:M:102:GLU:HG2	1.90	0.52
1:SC:28:MET:HE3	1:TC:102:GLU:HG2	1.90	0.52
1:UA:124:VAL:HG23	1:UA:160:ILE:HG23	1.91	0.52
1:SC:124:VAL:HG23	1:SC:160:ILE:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XC:28:MET:HE3	1:YC:102:GLU:HG2	1.90	0.52
1:MD:124:VAL:HG23	1:MD:160:ILE:HG23	1.91	0.52
1:BE:28:MET:HE3	1:CE:102:GLU:HG2	1.90	0.52
1:GE:124:VAL:HG23	1:GE:160:ILE:HG23	1.91	0.52
1:QE:124:VAL:HG23	1:QE:160:ILE:HG23	1.91	0.52
1:B:124:VAL:HG23	1:B:160:ILE:HG23	1.91	0.52
1:L:124:VAL:HG23	1:L:160:ILE:HG23	1.91	0.52
1:FA:124:VAL:HG23	1:FA:160:ILE:HG23	1.91	0.52
1:EB:124:VAL:HG23	1:EB:160:ILE:HG23	1.91	0.52
1:YB:28:MET:HE3	1:ZB:102:GLU:HG2	1.90	0.52
1:XC:124:VAL:HG23	1:XC:160:ILE:HG23	1.91	0.52
1:G:28:MET:HE3	1:H:102:GLU:HG2	1.90	0.52
1:PA:28:MET:HE3	1:QA:102:GLU:HG2	1.90	0.52
1:JB:124:VAL:HG23	1:JB:160:ILE:HG23	1.91	0.52
1:TB:124:VAL:HG23	1:TB:160:ILE:HG23	1.91	0.52
1:DC:124:VAL:HG23	1:DC:160:ILE:HG23	1.91	0.52
1:NC:124:VAL:HG23	1:NC:160:ILE:HG23	1.91	0.52
1:ZA:28:MET:HE3	1:AB:102:GLU:HG2	1.90	0.52
1:LE:28:MET:HE3	1:ME:102:GLU:HG2	1.90	0.52
1:Q:124:VAL:HG23	1:Q:160:ILE:HG23	1.91	0.52
1:IC:124:VAL:HG23	1:IC:160:ILE:HG23	1.91	0.52
1:WD:124:VAL:HG23	1:WD:160:ILE:HG23	1.91	0.52
1:P:102:GLU:CG	1:T:28:MET:HE3	2.41	0.51
1:EA:127:ARG:N	1:EA:162:ALA:O	2.44	0.51
1:SB:127:ARG:N	1:SB:162:ALA:O	2.44	0.51
1:XB:127:ARG:N	1:XB:162:ALA:O	2.44	0.51
1:BD:127:ARG:N	1:BD:162:ALA:O	2.44	0.51
1:JA:102:GLU:CG	1:NA:28:MET:HE3	2.41	0.51
1:IB:102:GLU:CG	1:MB:28:MET:HE3	2.41	0.51
1:NB:102:GLU:CG	1:RB:28:MET:HE3	2.41	0.51
1:NB:127:ARG:N	1:NB:162:ALA:O	2.44	0.51
1:U:102:GLU:CG	1:Y:28:MET:HE3	2.41	0.51
1:KA:124:VAL:HG23	1:KA:160:ILE:HG23	1.91	0.51
1:TA:127:ARG:N	1:TA:162:ALA:O	2.44	0.51
1:SB:102:GLU:CG	1:WB:28:MET:HE3	2.41	0.51
1:NC:28:MET:HE3	1:OC:102:GLU:HG2	1.90	0.51
1:SD:52:LEU:HD11	1:RE:84:ARG:HE	1.72	0.51
1:FE:102:GLU:CG	1:JE:28:MET:HE3	2.41	0.51
1:F:127:ARG:N	1:F:162:ALA:O	2.44	0.51
1:EA:102:GLU:CG	1:IA:28:MET:HE3	2.41	0.51
1:FB:52:LEU:CD1	1:KB:84:ARG:NE	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OB:124:VAL:HG23	1:OB:160:ILE:HG23	1.91	0.51
1:GD:127:ARG:N	1:GD:162:ALA:O	2.44	0.51
1:LD:102:GLU:CG	1:PD:28:MET:HE3	2.41	0.51
1:AE:102:GLU:CG	1:EE:28:MET:HE3	2.41	0.51
1:LE:124:VAL:HG23	1:LE:160:ILE:HG23	1.91	0.51
1:V:124:VAL:HG23	1:V:160:ILE:HG23	1.91	0.51
1:DB:102:GLU:CG	1:HB:28:MET:HE3	2.41	0.51
1:YB:124:VAL:HG23	1:YB:160:ILE:HG23	1.91	0.51
1:HD:124:VAL:HG23	1:HD:160:ILE:HG23	1.91	0.51
1:QD:84:ARG:NH2	1:VD:49:GLU:HG2	2.25	0.51
1:QD:102:GLU:CG	1:UD:28:MET:HE3	2.41	0.51
1:KE:127:ARG:N	1:KE:162:ALA:O	2.44	0.51
1:K:127:ARG:N	1:K:162:ALA:O	2.44	0.51
1:RC:102:GLU:CG	1:VC:28:MET:HE3	2.41	0.51
1:RD:124:VAL:HG23	1:RD:160:ILE:HG23	1.91	0.51
1:AE:127:ARG:N	1:AE:162:ALA:O	2.43	0.51
1:U:127:ARG:N	1:U:162:ALA:O	2.44	0.51
1:AA:124:VAL:HG23	1:AA:160:ILE:HG23	1.91	0.51
1:ZA:124:VAL:HG23	1:ZA:160:ILE:HG23	1.91	0.51
1:PC:102:GLU:OE1	1:PC:102:GLU:N	2.44	0.51
1:WC:102:GLU:CG	1:AD:28:MET:HE3	2.41	0.51
1:D:102:GLU:N	1:D:102:GLU:OE1	2.44	0.51
1:F:102:GLU:CG	1:J:28:MET:HE3	2.41	0.51
1:P:127:ARG:N	1:P:162:ALA:O	2.44	0.51
1:Z:102:GLU:CG	1:DA:28:MET:HE3	2.41	0.51
1:OA:102:GLU:CG	1:SA:28:MET:HE3	2.41	0.51
1:HC:127:ARG:N	1:HC:162:ALA:O	2.44	0.51
1:KC:102:GLU:OE1	1:KC:102:GLU:N	2.44	0.51
1:CD:124:VAL:HG23	1:CD:160:ILE:HG23	1.91	0.51
1:JD:102:GLU:N	1:JD:102:GLU:OE1	2.44	0.51
1:OD:102:GLU:N	1:OD:102:GLU:OE1	2.44	0.51
1:DE:102:GLU:N	1:DE:102:GLU:OE1	2.44	0.51
1:A:102:GLU:CG	1:E:28:MET:HE3	2.41	0.51
1:K:102:GLU:CG	1:O:28:MET:HE3	2.41	0.51
1:N:102:GLU:N	1:N:102:GLU:OE1	2.44	0.51
1:WA:102:GLU:N	1:WA:102:GLU:OE1	2.44	0.51
1:CC:102:GLU:CG	1:GC:28:MET:HE3	2.41	0.51
1:CC:127:ARG:N	1:CC:162:ALA:O	2.44	0.51
1:MC:102:GLU:CG	1:QC:28:MET:HE3	2.41	0.51
1:BD:102:GLU:CG	1:FD:28:MET:HE3	2.41	0.51
1:YD:102:GLU:OE1	1:YD:102:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:102:GLU:N	1:X:102:GLU:OE1	2.44	0.51
1:HA:102:GLU:OE1	1:HA:102:GLU:N	2.44	0.51
1:TA:102:GLU:CG	1:XA:28:MET:HE3	2.41	0.51
1:FC:102:GLU:OE1	1:FC:102:GLU:N	2.44	0.51
1:LD:127:ARG:N	1:LD:162:ALA:O	2.44	0.51
1:MA:102:GLU:N	1:MA:102:GLU:OE1	2.44	0.50
1:XB:102:GLU:CG	1:BC:28:MET:HE3	2.41	0.50
1:TD:102:GLU:N	1:TD:102:GLU:OE1	2.44	0.50
1:GB:102:GLU:OE1	1:GB:102:GLU:N	2.44	0.50
1:WC:127:ARG:N	1:WC:162:ALA:O	2.44	0.50
1:VD:102:GLU:CG	1:ZD:28:MET:HE3	2.41	0.50
1:IE:102:GLU:N	1:IE:102:GLU:OE1	2.44	0.50
1:PE:102:GLU:CG	1:TE:28:MET:HE3	2.41	0.50
1:CA:102:GLU:OE1	1:CA:102:GLU:N	2.44	0.50
1:YA:102:GLU:CG	1:CB:28:MET:HE3	2.41	0.50
1:YA:127:ARG:N	1:YA:162:ALA:O	2.44	0.50
1:LB:102:GLU:OE1	1:LB:102:GLU:N	2.44	0.50
1:VB:102:GLU:OE1	1:VB:102:GLU:N	2.44	0.50
1:MC:127:ARG:N	1:MC:162:ALA:O	2.44	0.50
1:SE:102:GLU:N	1:SE:102:GLU:OE1	2.44	0.50
1:BB:102:GLU:OE1	1:BB:102:GLU:N	2.44	0.50
1:AC:102:GLU:N	1:AC:102:GLU:OE1	2.44	0.50
1:ZC:102:GLU:OE1	1:ZC:102:GLU:N	2.44	0.50
1:ED:102:GLU:N	1:ED:102:GLU:OE1	2.44	0.50
1:GD:102:GLU:CG	1:KD:28:MET:HE3	2.41	0.50
1:NE:102:GLU:N	1:NE:102:GLU:OE1	2.44	0.50
1:HC:102:GLU:CG	1:LC:28:MET:HE3	2.41	0.50
1:UC:102:GLU:OE1	1:UC:102:GLU:N	2.44	0.50
1:A:127:ARG:N	1:A:162:ALA:O	2.44	0.50
1:I:102:GLU:N	1:I:102:GLU:OE1	2.44	0.50
1:S:102:GLU:N	1:S:102:GLU:OE1	2.44	0.50
1:RA:102:GLU:N	1:RA:102:GLU:OE1	2.44	0.50
1:QB:102:GLU:OE1	1:QB:102:GLU:N	2.44	0.50
1:YC:84:ARG:NE	1:DD:52:LEU:CD1	2.75	0.50
1:RC:127:ARG:N	1:RC:162:ALA:O	2.44	0.50
1:VD:127:ARG:N	1:VD:162:ALA:O	2.44	0.50
1:KE:102:GLU:CG	1:OE:28:MET:HE3	2.41	0.50
1:BC:64:SER:O	1:BC:96:ARG:NH1	2.45	0.49
1:QC:64:SER:O	1:QC:96:ARG:NH1	2.45	0.49
1:KD:64:SER:O	1:KD:96:ARG:NH1	2.45	0.49
1:H:84:ARG:NH1	1:R:49:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZB:52:LEU:CD1	1:EC:84:ARG:NE	2.75	0.49
1:LC:64:SER:O	1:LC:96:ARG:NH1	2.45	0.49
1:FE:127:ARG:N	1:FE:162:ALA:O	2.44	0.49
1:IB:7:ILE:HG23	1:OB:76:GLU:HG2	1.94	0.49
1:JC:52:LEU:CD1	1:OC:84:ARG:NE	2.75	0.49
1:PD:64:SER:O	1:PD:96:ARG:NH1	2.45	0.49
1:DB:127:ARG:N	1:DB:162:ALA:O	2.44	0.49
1:CB:64:SER:O	1:CB:96:ARG:NH1	2.45	0.49
1:E:64:SER:O	1:E:96:ARG:NH1	2.45	0.49
1:HB:64:SER:O	1:HB:96:ARG:NH1	2.45	0.49
1:GC:64:SER:O	1:GC:96:ARG:NH1	2.45	0.49
1:FD:64:SER:O	1:FD:96:ARG:NH1	2.45	0.49
1:QD:127:ARG:N	1:QD:162:ALA:O	2.44	0.49
1:A:44:SER:OG	1:TA:9:ARG:NH1	2.45	0.49
1:Z:127:ARG:N	1:Z:162:ALA:O	2.44	0.49
1:AD:64:SER:O	1:AD:96:ARG:NH1	2.45	0.49
1:RB:64:SER:O	1:RB:96:ARG:NH1	2.45	0.48
1:ZD:64:SER:O	1:ZD:96:ARG:NH1	2.45	0.48
1:JA:127:ARG:N	1:JA:162:ALA:O	2.44	0.48
1:Y:64:SER:O	1:Y:96:ARG:NH1	2.45	0.48
1:UB:52:LEU:HD13	1:TC:84:ARG:HB3	1.94	0.48
1:NA:64:SER:O	1:NA:96:ARG:NH1	2.45	0.48
1:UB:52:LEU:CD1	1:TC:84:ARG:NE	2.75	0.48
1:VC:64:SER:O	1:VC:96:ARG:NH1	2.45	0.48
1:HE:84:ARG:NE	1:ME:52:LEU:CD1	2.76	0.48
1:JE:64:SER:O	1:JE:96:ARG:NH1	2.45	0.48
1:J:64:SER:O	1:J:96:ARG:NH1	2.45	0.48
1:MB:64:SER:O	1:MB:96:ARG:NH1	2.45	0.48
1:WB:64:SER:O	1:WB:96:ARG:NH1	2.45	0.48
1:K:84:ARG:NH2	1:U:49:GLU:HG2	2.29	0.48
1:UB:49:GLU:OE2	1:TC:84:ARG:NH1	2.47	0.48
1:ZB:84:ARG:NH1	1:EC:49:GLU:OE2	2.47	0.48
1:JE:102:GLU:OE1	1:JE:102:GLU:N	2.47	0.48
1:H:84:ARG:HB3	1:R:52:LEU:HD13	1.95	0.48
1:AE:7:ILE:HG23	1:GE:76:GLU:HG2	1.94	0.48
1:OE:102:GLU:OE1	1:OE:102:GLU:N	2.47	0.48
1:PE:127:ARG:N	1:PE:162:ALA:O	2.44	0.48
1:TE:64:SER:O	1:TE:96:ARG:NH1	2.45	0.48
1:J:102:GLU:N	1:J:102:GLU:OE1	2.47	0.48
1:T:102:GLU:OE1	1:T:102:GLU:N	2.47	0.48
1:XA:102:GLU:N	1:XA:102:GLU:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:102:GLU:N	1:CB:102:GLU:OE1	2.47	0.48
1:W:52:LEU:CD1	1:GA:84:ARG:NE	2.76	0.48
1:BA:84:ARG:NH1	1:LA:49:GLU:OE2	2.47	0.48
1:SA:102:GLU:N	1:SA:102:GLU:OE1	2.47	0.48
1:WB:102:GLU:N	1:WB:102:GLU:OE1	2.47	0.48
1:JC:84:ARG:NH1	1:OC:49:GLU:OE2	2.47	0.48
1:IA:102:GLU:N	1:IA:102:GLU:OE1	2.47	0.48
1:KD:102:GLU:OE1	1:KD:102:GLU:N	2.47	0.48
1:Y:102:GLU:OE1	1:Y:102:GLU:N	2.47	0.47
1:MB:102:GLU:N	1:MB:102:GLU:OE1	2.47	0.47
1:LC:102:GLU:N	1:LC:102:GLU:OE1	2.47	0.47
1:VC:102:GLU:N	1:VC:102:GLU:OE1	2.47	0.47
1:AD:102:GLU:OE1	1:AD:102:GLU:N	2.47	0.47
1:FD:102:GLU:OE1	1:FD:102:GLU:N	2.47	0.47
1:PD:102:GLU:N	1:PD:102:GLU:OE1	2.47	0.47
1:UD:102:GLU:N	1:UD:102:GLU:OE1	2.47	0.47
1:O:102:GLU:OE1	1:O:102:GLU:N	2.47	0.47
1:XA:64:SER:O	1:XA:96:ARG:NH1	2.45	0.47
1:HB:102:GLU:N	1:HB:102:GLU:OE1	2.47	0.47
1:RB:102:GLU:N	1:RB:102:GLU:OE1	2.47	0.47
1:QC:102:GLU:N	1:QC:102:GLU:OE1	2.47	0.47
1:XD:84:ARG:NE	1:CE:52:LEU:CD1	2.76	0.47
1:GC:102:GLU:N	1:GC:102:GLU:OE1	2.47	0.47
1:OE:64:SER:O	1:OE:96:ARG:NH1	2.45	0.47
1:NA:102:GLU:N	1:NA:102:GLU:OE1	2.47	0.47
1:BC:102:GLU:N	1:BC:102:GLU:OE1	2.47	0.47
1:YC:49:GLU:OE2	1:DD:84:ARG:NH1	2.47	0.47
1:UD:64:SER:O	1:UD:96:ARG:NH1	2.45	0.47
1:ZD:102:GLU:N	1:ZD:102:GLU:OE1	2.47	0.47
1:TE:102:GLU:OE1	1:TE:102:GLU:N	2.47	0.47
1:JC:9:ARG:HH21	1:OC:47:ILE:HD12	1.78	0.47
1:SD:84:ARG:NH1	1:RE:49:GLU:OE2	2.47	0.47
1:E:102:GLU:N	1:E:102:GLU:OE1	2.47	0.47
1:H:84:ARG:NE	1:R:52:LEU:CD1	2.75	0.47
1:DA:64:SER:O	1:DA:96:ARG:NH1	2.45	0.47
1:IA:64:SER:O	1:IA:96:ARG:NH1	2.45	0.47
1:OA:127:ARG:N	1:OA:162:ALA:O	2.44	0.47
1:FB:49:GLU:OE2	1:KB:84:ARG:NH1	2.47	0.47
1:IB:127:ARG:N	1:IB:162:ALA:O	2.44	0.47
1:EE:64:SER:O	1:EE:96:ARG:NH1	2.45	0.47
1:HE:49:GLU:OE2	1:ME:84:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:125:LEU:HD23	1:J:159:VAL:HG13	1.97	0.47
1:K:49:GLU:HG2	1:U:84:ARG:NH2	2.30	0.47
1:DA:102:GLU:N	1:DA:102:GLU:OE1	2.47	0.47
1:SA:125:LEU:HD23	1:SA:159:VAL:HG13	1.97	0.47
1:VA:49:GLU:OE2	1:AB:84:ARG:NH1	2.48	0.47
1:UB:47:ILE:HD12	1:TC:9:ARG:HH21	1.79	0.47
1:BD:102:GLU:HG3	1:FD:28:MET:HE3	1.97	0.47
1:SD:52:LEU:CD1	1:RE:84:ARG:NE	2.77	0.47
1:EE:102:GLU:OE1	1:EE:102:GLU:N	2.47	0.47
1:RB:125:LEU:HD23	1:RB:159:VAL:HG13	1.97	0.47
1:ID:49:GLU:OE2	1:ND:84:ARG:NH1	2.47	0.47
1:P:102:GLU:HG3	1:T:28:MET:HE3	1.97	0.47
1:JE:125:LEU:HD23	1:JE:159:VAL:HG13	1.96	0.47
1:O:64:SER:O	1:O:96:ARG:NH1	2.45	0.47
1:T:125:LEU:HD23	1:T:159:VAL:HG13	1.97	0.47
1:U:102:GLU:HG3	1:Y:28:MET:HE3	1.97	0.47
1:XA:125:LEU:HD23	1:XA:159:VAL:HG13	1.96	0.47
1:DB:102:GLU:HG3	1:HB:28:MET:HE3	1.97	0.47
1:BD:7:ILE:HG23	1:HD:76:GLU:HG2	1.97	0.47
1:SB:102:GLU:HG3	1:WB:28:MET:HE3	1.97	0.46
1:LC:125:LEU:HD23	1:LC:159:VAL:HG13	1.97	0.46
1:VC:125:LEU:HD23	1:VC:159:VAL:HG13	1.97	0.46
1:QD:102:GLU:HG3	1:UD:28:MET:HE3	1.97	0.46
1:F:102:GLU:HG3	1:J:28:MET:HE3	1.97	0.46
1:IA:125:LEU:HD23	1:IA:159:VAL:HG13	1.96	0.46
1:OA:102:GLU:HG3	1:SA:28:MET:HE3	1.97	0.46
1:HB:125:LEU:HD23	1:HB:159:VAL:HG13	1.97	0.46
1:MB:125:LEU:HD23	1:MB:159:VAL:HG13	1.97	0.46
1:QD:44:SER:OG	1:VD:9:ARG:NH1	2.48	0.46
1:TE:125:LEU:HD23	1:TE:159:VAL:HG13	1.97	0.46
1:H:49:GLU:OE2	1:R:84:ARG:NH1	2.49	0.46
1:JA:102:GLU:HG3	1:NA:28:MET:HE3	1.97	0.46
1:WB:125:LEU:HD23	1:WB:159:VAL:HG13	1.97	0.46
1:AD:125:LEU:HD23	1:AD:159:VAL:HG13	1.97	0.46
1:TA:102:GLU:HG3	1:XA:28:MET:HE3	1.97	0.46
1:VA:84:ARG:NE	1:AB:52:LEU:CD1	2.78	0.46
1:IB:102:GLU:HG3	1:MB:28:MET:HE3	1.97	0.46
1:BD:49:GLU:HG2	1:GD:84:ARG:NH2	2.30	0.46
1:OE:125:LEU:HD23	1:OE:159:VAL:HG13	1.97	0.46
1:CC:102:GLU:HG3	1:GC:28:MET:HE3	1.97	0.46
1:SA:64:SER:O	1:SA:96:ARG:NH1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GC:125:LEU:HD23	1:GC:159:VAL:HG13	1.97	0.46
1:FD:125:LEU:HD23	1:FD:159:VAL:HG13	1.97	0.46
1:KD:125:LEU:HD23	1:KD:159:VAL:HG13	1.97	0.46
1:PD:125:LEU:HD23	1:PD:159:VAL:HG13	1.97	0.46
1:UD:125:LEU:HD23	1:UD:159:VAL:HG13	1.97	0.46
1:BA:52:LEU:CD1	1:LA:84:ARG:NE	2.76	0.46
1:DA:125:LEU:HD23	1:DA:159:VAL:HG13	1.97	0.46
1:CB:125:LEU:HD23	1:CB:159:VAL:HG13	1.97	0.46
1:RC:102:GLU:HG3	1:VC:28:MET:HE3	1.97	0.46
1:E:125:LEU:HD23	1:E:159:VAL:HG13	1.97	0.46
1:VD:102:GLU:HG3	1:ZD:28:MET:HE3	1.97	0.46
1:Y:125:LEU:HD23	1:Y:159:VAL:HG13	1.97	0.46
1:QC:125:LEU:HD23	1:QC:159:VAL:HG13	1.97	0.46
1:RC:7:ILE:HG23	1:XC:76:GLU:HG2	1.97	0.46
1:YC:47:ILE:HD12	1:DD:9:ARG:HH21	1.81	0.46
1:K:102:GLU:HG3	1:O:28:MET:HE3	1.97	0.46
1:FB:84:ARG:NH1	1:KB:49:GLU:OE2	2.48	0.46
1:XB:102:GLU:HG3	1:BC:28:MET:HE3	1.97	0.46
1:BC:125:LEU:HD23	1:BC:159:VAL:HG13	1.97	0.46
1:RC:49:GLU:HG2	1:WC:84:ARG:NH2	2.31	0.46
1:ZD:125:LEU:HD23	1:ZD:159:VAL:HG13	1.97	0.46
1:AE:102:GLU:HG3	1:EE:28:MET:HE3	1.97	0.46
1:T:64:SER:O	1:T:96:ARG:NH1	2.45	0.45
1:FE:102:GLU:HG3	1:JE:28:MET:HE3	1.97	0.45
1:Z:102:GLU:HG3	1:DA:28:MET:HE3	1.97	0.45
1:YA:102:GLU:HG3	1:CB:28:MET:HE3	1.97	0.45
1:MC:102:GLU:HG3	1:QC:28:MET:HE3	1.97	0.45
1:GD:102:GLU:HG3	1:KD:28:MET:HE3	1.97	0.45
1:PE:102:GLU:HG3	1:TE:28:MET:HE3	1.97	0.45
1:A:102:GLU:HG3	1:E:28:MET:HE3	1.97	0.45
1:NA:125:LEU:HD23	1:NA:159:VAL:HG13	1.97	0.45
1:EE:125:LEU:HD23	1:EE:159:VAL:HG13	1.97	0.45
1:Q:76:GLU:HG2	1:Z:7:ILE:HG23	1.99	0.45
1:BA:49:GLU:OE2	1:LA:84:ARG:NH1	2.49	0.45
1:EA:102:GLU:HG3	1:IA:28:MET:HE3	1.97	0.45
1:HC:102:GLU:HG3	1:LC:28:MET:HE3	1.97	0.45
1:A:50:GLY:O	1:TA:84:ARG:NH2	2.46	0.45
1:LD:102:GLU:HG3	1:PD:28:MET:HE3	1.97	0.45
1:O:125:LEU:HD23	1:O:159:VAL:HG13	1.97	0.45
1:ZB:49:GLU:OE2	1:EC:84:ARG:NH1	2.49	0.45
1:C:9:ARG:HH21	1:M:47:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:9:ARG:HH21	1:R:47:ILE:HD12	1.81	0.45
1:WC:102:GLU:HG3	1:AD:28:MET:HE3	1.97	0.45
1:JC:84:ARG:HB3	1:OC:52:LEU:HD13	1.99	0.45
1:NB:102:GLU:HG3	1:RB:28:MET:HE3	1.97	0.45
1:CC:84:ARG:NH2	1:HC:49:GLU:HG2	2.32	0.45
1:XD:52:LEU:CD1	1:CE:84:ARG:NE	2.79	0.45
1:KE:102:GLU:HG3	1:OE:28:MET:HE3	1.97	0.45
1:ID:84:ARG:NH1	1:ND:49:GLU:OE2	2.51	0.44
1:XD:49:GLU:OE2	1:CE:84:ARG:NH1	2.50	0.44
1:HE:88:ARG:NH2	1:HE:90:GLU:OE1	2.49	0.44
1:F:49:GLU:HG2	1:PE:84:ARG:NH2	2.32	0.44
1:AB:88:ARG:NH2	1:AB:90:GLU:OE1	2.49	0.44
1:ID:52:LEU:CD1	1:ND:84:ARG:NE	2.80	0.44
1:C:52:LEU:CD1	1:M:84:ARG:HE	2.30	0.44
1:W:84:ARG:NH1	1:GA:49:GLU:OE2	2.50	0.44
1:B:76:GLU:HG2	1:TA:7:ILE:HG23	1.99	0.44
1:FA:76:GLU:HG2	1:OA:7:ILE:HG23	1.98	0.44
1:BD:84:ARG:NH2	1:GD:49:GLU:HG2	2.32	0.44
1:C:88:ARG:NH2	1:C:90:GLU:OE1	2.49	0.44
1:ND:88:ARG:NH2	1:ND:90:GLU:OE1	2.49	0.44
1:SD:49:GLU:OE2	1:RE:84:ARG:NH1	2.50	0.44
1:YA:7:ILE:HG23	1:EB:76:GLU:HG2	2.00	0.44
1:XD:88:ARG:NH2	1:XD:90:GLU:OE1	2.49	0.44
1:DC:76:GLU:HG2	1:HC:7:ILE:HG23	1.99	0.44
1:OC:88:ARG:NH2	1:OC:90:GLU:OE1	2.49	0.44
1:F:7:ILE:HG23	1:QE:76:GLU:HG2	1.98	0.44
1:HE:84:ARG:NH1	1:ME:49:GLU:OE2	2.50	0.44
1:FB:52:LEU:HD13	1:KB:84:ARG:HB3	1.98	0.43
1:ZB:88:ARG:NH2	1:ZB:90:GLU:OE1	2.49	0.43
1:BA:9:ARG:HH21	1:LA:47:ILE:HD12	1.82	0.43
1:ID:88:ARG:NH2	1:ID:90:GLU:OE1	2.49	0.43
1:QD:7:ILE:HG23	1:WD:76:GLU:HG2	2.00	0.43
1:CE:88:ARG:NH2	1:CE:90:GLU:OE1	2.49	0.43
1:WA:143:GLY:O	1:WA:147:LEU:HD23	2.19	0.43
1:FC:143:GLY:O	1:FC:147:LEU:HD23	2.19	0.43
1:IE:143:GLY:O	1:IE:147:LEU:HD23	2.19	0.43
1:MA:143:GLY:O	1:MA:147:LEU:HD23	2.19	0.43
1:JB:76:GLU:HG2	1:NB:7:ILE:HG23	1.99	0.43
1:VA:84:ARG:NH1	1:AB:49:GLU:OE2	2.51	0.43
1:ED:143:GLY:O	1:ED:147:LEU:HD23	2.19	0.43
1:D:143:GLY:O	1:D:147:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:143:GLY:O	1:X:147:LEU:HD23	2.19	0.43
1:Z:157:PHE:CZ	1:Z:159:VAL:HG22	2.54	0.43
1:NB:157:PHE:CZ	1:NB:159:VAL:HG22	2.54	0.43
1:XB:157:PHE:CZ	1:XB:159:VAL:HG22	2.54	0.43
1:CC:49:GLU:HG2	1:HC:84:ARG:NH2	2.33	0.43
1:JC:88:ARG:NH2	1:JC:90:GLU:OE1	2.49	0.43
1:KC:143:GLY:O	1:KC:147:LEU:HD23	2.19	0.43
1:YC:52:LEU:HD13	1:DD:84:ARG:HB3	1.99	0.43
1:DD:66:PHE:HE2	1:DD:126:ILE:HD13	1.84	0.43
1:TD:143:GLY:O	1:TD:147:LEU:HD23	2.19	0.43
1:W:66:PHE:HE2	1:W:126:ILE:HD13	1.84	0.43
1:YA:157:PHE:CZ	1:YA:159:VAL:HG22	2.54	0.43
1:FB:84:ARG:HB3	1:KB:52:LEU:HD13	2.01	0.43
1:JC:66:PHE:HE2	1:JC:126:ILE:HD13	1.84	0.43
1:WC:157:PHE:CZ	1:WC:159:VAL:HG22	2.54	0.43
1:OD:143:GLY:O	1:OD:147:LEU:HD23	2.19	0.43
1:SD:66:PHE:HE2	1:SD:126:ILE:HD13	1.84	0.43
1:DE:143:GLY:O	1:DE:147:LEU:HD23	2.19	0.43
1:HE:66:PHE:HE2	1:HE:126:ILE:HD13	1.84	0.43
1:M:66:PHE:HE2	1:M:126:ILE:HD13	1.84	0.43
1:EA:157:PHE:CZ	1:EA:159:VAL:HG22	2.54	0.43
1:QA:66:PHE:HE2	1:QA:126:ILE:HD13	1.84	0.43
1:UB:66:PHE:HE2	1:UB:126:ILE:HD13	1.84	0.43
1:ZB:84:ARG:HB3	1:EC:52:LEU:HD13	2.01	0.43
1:LA:66:PHE:HE2	1:LA:126:ILE:HD13	1.84	0.43
1:VA:66:PHE:HE2	1:VA:126:ILE:HD13	1.84	0.43
1:IB:157:PHE:CZ	1:IB:159:VAL:HG22	2.54	0.43
1:PE:157:PHE:CZ	1:PE:159:VAL:HG22	2.54	0.43
1:P:157:PHE:CZ	1:P:159:VAL:HG22	2.54	0.43
1:R:66:PHE:HE2	1:R:126:ILE:HD13	1.84	0.43
1:BA:84:ARG:HB3	1:LA:52:LEU:HD13	2.01	0.43
1:CC:157:PHE:CZ	1:CC:159:VAL:HG22	2.54	0.43
1:PC:143:GLY:O	1:PC:147:LEU:HD23	2.19	0.43
1:RC:84:ARG:NH2	1:WC:49:GLU:HG2	2.34	0.43
1:AD:42:GLY:O	1:AD:43:SER:OG	2.31	0.43
1:QD:157:PHE:CZ	1:QD:159:VAL:HG22	2.54	0.43
1:A:157:PHE:CZ	1:A:159:VAL:HG22	2.54	0.42
1:C:84:ARG:HE	1:M:52:LEU:HD11	1.82	0.42
1:M:88:ARG:NH2	1:M:90:GLU:OE1	2.49	0.42
1:U:157:PHE:CZ	1:U:159:VAL:HG22	2.54	0.42
1:AB:66:PHE:HE2	1:AB:126:ILE:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:66:PHE:HE2	1:FB:126:ILE:HD13	1.84	0.42
1:GB:143:GLY:O	1:GB:147:LEU:HD23	2.19	0.42
1:PB:66:PHE:HE2	1:PB:126:ILE:HD13	1.84	0.42
1:EC:66:PHE:HE2	1:EC:126:ILE:HD13	1.84	0.42
1:OC:66:PHE:HE2	1:OC:126:ILE:HD13	1.84	0.42
1:RC:157:PHE:CZ	1:RC:159:VAL:HG22	2.54	0.42
1:BD:157:PHE:CZ	1:BD:159:VAL:HG22	2.54	0.42
1:KE:157:PHE:CZ	1:KE:159:VAL:HG22	2.54	0.42
1:MC:157:PHE:CZ	1:MC:159:VAL:HG22	2.54	0.42
1:ND:66:PHE:HE2	1:ND:126:ILE:HD13	1.84	0.42
1:XD:66:PHE:HE2	1:XD:126:ILE:HD13	1.84	0.42
1:AE:157:PHE:CZ	1:AE:159:VAL:HG22	2.54	0.42
1:C:66:PHE:HE2	1:C:126:ILE:HD13	1.84	0.42
1:H:66:PHE:HE2	1:H:126:ILE:HD13	1.84	0.42
1:K:157:PHE:CZ	1:K:159:VAL:HG22	2.54	0.42
1:N:143:GLY:O	1:N:147:LEU:HD23	2.19	0.42
1:OA:157:PHE:CZ	1:OA:159:VAL:HG22	2.54	0.42
1:TA:157:PHE:CZ	1:TA:159:VAL:HG22	2.54	0.42
1:VA:52:LEU:CD1	1:AB:84:ARG:NE	2.80	0.42
1:SB:157:PHE:CZ	1:SB:159:VAL:HG22	2.54	0.42
1:L:76:GLU:HG2	1:U:7:ILE:HG23	1.99	0.42
1:CA:143:GLY:O	1:CA:147:LEU:HD23	2.19	0.42
1:LB:143:GLY:O	1:LB:147:LEU:HD23	2.19	0.42
1:UB:84:ARG:NH1	1:TC:49:GLU:OE2	2.53	0.42
1:JC:49:GLU:OE2	1:OC:84:ARG:NH1	2.53	0.42
1:ME:66:PHE:HE2	1:ME:126:ILE:HD13	1.84	0.42
1:S:143:GLY:O	1:S:147:LEU:HD23	2.19	0.42
1:EA:84:ARG:NH2	1:OA:49:GLU:HG2	2.34	0.42
1:QB:143:GLY:O	1:QB:147:LEU:HD23	2.19	0.42
1:VB:143:GLY:O	1:VB:147:LEU:HD23	2.19	0.42
1:ME:88:ARG:NH2	1:ME:90:GLU:OE1	2.49	0.42
1:F:84:ARG:NH2	1:PE:49:GLU:HG2	2.35	0.42
1:RA:143:GLY:O	1:RA:147:LEU:HD23	2.19	0.42
1:TB:76:GLU:HG2	1:XB:7:ILE:HG23	2.01	0.42
1:UD:42:GLY:O	1:UD:43:SER:OG	2.31	0.42
1:VD:157:PHE:CZ	1:VD:159:VAL:HG22	2.54	0.42
1:FE:157:PHE:CZ	1:FE:159:VAL:HG22	2.54	0.42
1:G:76:GLU:HG2	1:PE:7:ILE:HG23	2.02	0.42
1:I:143:GLY:O	1:I:147:LEU:HD23	2.19	0.42
1:HC:157:PHE:CZ	1:HC:159:VAL:HG22	2.54	0.42
1:ZC:143:GLY:O	1:ZC:147:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LD:157:PHE:CZ	1:LD:159:VAL:HG22	2.54	0.42
1:NE:143:GLY:O	1:NE:147:LEU:HD23	2.19	0.42
1:F:157:PHE:CZ	1:F:159:VAL:HG22	2.54	0.42
1:GA:66:PHE:HE2	1:GA:126:ILE:HD13	1.84	0.42
1:JA:157:PHE:CZ	1:JA:159:VAL:HG22	2.54	0.42
1:DB:157:PHE:CZ	1:DB:159:VAL:HG22	2.54	0.42
1:ZB:66:PHE:HE2	1:ZB:126:ILE:HD13	1.84	0.42
1:AC:143:GLY:O	1:AC:147:LEU:HD23	2.19	0.42
1:LC:42:GLY:O	1:LC:43:SER:OG	2.31	0.42
1:UC:143:GLY:O	1:UC:147:LEU:HD23	2.19	0.42
1:GD:157:PHE:CZ	1:GD:159:VAL:HG22	2.54	0.42
1:YD:143:GLY:O	1:YD:147:LEU:HD23	2.19	0.42
1:CE:66:PHE:HE2	1:CE:126:ILE:HD13	1.84	0.42
1:P:7:ILE:HG23	1:AA:76:GLU:HG2	2.01	0.42
1:BB:143:GLY:O	1:BB:147:LEU:HD23	2.19	0.42
1:YC:66:PHE:HE2	1:YC:126:ILE:HD13	1.84	0.42
1:HA:143:GLY:O	1:HA:147:LEU:HD23	2.19	0.42
1:KB:66:PHE:HE2	1:KB:126:ILE:HD13	1.84	0.42
1:ZB:9:ARG:HH21	1:EC:47:ILE:HD12	1.85	0.42
1:BE:76:GLU:HG2	1:FE:7:ILE:HG23	2.00	0.42
1:SE:143:GLY:O	1:SE:147:LEU:HD23	2.19	0.42
1:W:49:GLU:OE2	1:GA:84:ARG:NH1	2.52	0.41
1:BA:66:PHE:HE2	1:BA:126:ILE:HD13	1.84	0.41
1:BA:88:ARG:NH2	1:BA:90:GLU:OE1	2.49	0.41
1:JD:143:GLY:O	1:JD:147:LEU:HD23	2.19	0.41
1:W:84:ARG:NE	1:GA:52:LEU:CD1	2.80	0.41
1:EA:7:ILE:HG23	1:PA:76:GLU:HG2	2.02	0.41
1:ID:66:PHE:HE2	1:ID:126:ILE:HD13	1.84	0.41
1:ZB:84:ARG:NE	1:EC:52:LEU:CD1	2.79	0.41
1:RE:66:PHE:HE2	1:RE:126:ILE:HD13	1.84	0.41
1:T:42:GLY:O	1:T:43:SER:OG	2.31	0.41
1:CC:7:ILE:HG23	1:IC:76:GLU:HG2	2.01	0.41
1:SC:76:GLU:HG2	1:WC:7:ILE:HG23	2.02	0.41
1:TC:66:PHE:HE2	1:TC:126:ILE:HD13	1.84	0.41
1:EA:49:GLU:HG2	1:OA:84:ARG:NH2	2.36	0.41
1:C:52:LEU:HD11	1:M:84:ARG:NE	2.36	0.41
1:ZA:76:GLU:HG2	1:DB:7:ILE:HG23	2.02	0.41
1:YC:84:ARG:NH1	1:DD:49:GLU:OE2	2.53	0.41
1:SB:7:ILE:HG23	1:YB:76:GLU:HG2	2.02	0.41
1:ID:84:ARG:NE	1:ND:52:LEU:CD1	2.80	0.41
1:QD:42:GLY:O	1:QD:43:SER:OG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SD:9:ARG:HH21	1:RE:47:ILE:HD12	1.86	0.41
1:XD:84:ARG:NH1	1:CE:49:GLU:OE2	2.54	0.41
1:ZC:88:ARG:NH2	1:ZC:90:GLU:OE1	2.55	0.40
1:AE:49:GLU:HG2	1:FE:84:ARG:NH2	2.36	0.40
1:P:84:ARG:NH2	1:Z:49:GLU:HG2	2.36	0.40
1:OB:17:LYS:CE	1:OB:160:ILE:HD12	2.52	0.40
1:QB:88:ARG:NH2	1:QB:90:GLU:OE1	2.55	0.40
1:XD:47:ILE:HD12	1:CE:9:ARG:HH21	1.86	0.40
1:AE:84:ARG:NH2	1:FE:49:GLU:HG2	2.37	0.40
1:TE:42:GLY:O	1:TE:43:SER:OG	2.31	0.40
1:D:83:VAL:HG21	1:M:3:LEU:HD22	2.02	0.40
1:D:88:ARG:NH2	1:D:90:GLU:OE1	2.55	0.40
1:CA:88:ARG:NH2	1:CA:90:GLU:OE1	2.55	0.40
1:JB:17:LYS:CE	1:JB:160:ILE:HD12	2.52	0.40
1:PC:88:ARG:NH2	1:PC:90:GLU:OE1	2.55	0.40
1:DE:88:ARG:NH2	1:DE:90:GLU:OE1	2.55	0.40
1:Q:17:LYS:CE	1:Q:160:ILE:HD12	2.52	0.40
1:PA:17:LYS:CE	1:PA:160:ILE:HD12	2.52	0.40
1:IB:49:GLU:HG2	1:NB:84:ARG:NH2	2.37	0.40
1:TB:17:LYS:CE	1:TB:160:ILE:HD12	2.52	0.40
1:SD:84:ARG:HB3	1:RE:52:LEU:HD13	2.03	0.40
1:NE:88:ARG:NH2	1:NE:90:GLU:OE1	2.55	0.40
1:W:9:ARG:HH21	1:GA:47:ILE:HD12	1.86	0.40
1:BB:88:ARG:NH2	1:BB:90:GLU:OE1	2.55	0.40
1:ED:88:ARG:NH2	1:ED:90:GLU:OE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/163 (97%)	152 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	AB	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	AC	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	AD	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	AE	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	B	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	BA	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	BB	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	BC	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	BD	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	BE	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	C	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	CA	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	CB	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	CC	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	CD	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	CE	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	D	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	DA	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	DB	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	DC	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	DD	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	DE	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	E	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	EA	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	EB	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	EC	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	ED	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	EE	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	F	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	FA	147/163 (90%)	144 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FB	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	FC	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	FD	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	FE	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	G	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	GA	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	GB	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	GC	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	GD	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	GE	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	H	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	HA	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	HB	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	HC	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	HD	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	HE	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	I	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	IA	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	IB	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	IC	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	ID	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	IE	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	J	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	JA	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	JB	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	JC	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	JD	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	JE	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	K	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	KA	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	KB	158/163 (97%)	156 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	KC	147/163 (90%)	141 (96%)	6 (4%)	0	100	100
1	KD	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	KE	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	L	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	LA	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	LB	147/163 (90%)	141 (96%)	6 (4%)	0	100	100
1	LC	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	LD	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	LE	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	M	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	MA	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	MB	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	MC	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	MD	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	ME	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	N	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	NA	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	NB	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	NC	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	ND	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	NE	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	O	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	OA	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	OB	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	OC	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	OD	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	OE	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	P	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	PA	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	PB	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	PC	147/163 (90%)	140 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	PD	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	PE	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	Q	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	QA	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	QB	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	QC	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	QD	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	QE	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	R	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	RA	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	RB	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	RC	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	RD	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	RE	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	S	147/163 (90%)	141 (96%)	6 (4%)	0	100	100
1	SA	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	SB	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	SC	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	SD	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	SE	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	T	147/163 (90%)	146 (99%)	1 (1%)	0	100	100
1	TA	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	TB	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	TC	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	TD	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	TE	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	U	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	UA	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	UB	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	UC	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	UD	147/163 (90%)	145 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	VA	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	VB	147/163 (90%)	141 (96%)	6 (4%)	0	100	100
1	VC	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	VD	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	W	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	WA	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	WB	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	WC	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	WD	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	X	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	XA	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	XB	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	XC	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	XD	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	Y	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	YA	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	YB	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	YC	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	YD	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
1	Z	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
1	ZA	147/163 (90%)	144 (98%)	3 (2%)	0	100	100
1	ZB	158/163 (97%)	156 (99%)	2 (1%)	0	100	100
1	ZC	147/163 (90%)	141 (96%)	6 (4%)	0	100	100
1	ZD	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
All	All	22710/24450 (93%)	22116 (97%)	594 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	122/125 (98%)	122 (100%)	0	100	100
1	AA	114/125 (91%)	114 (100%)	0	100	100
1	AB	122/125 (98%)	122 (100%)	0	100	100
1	AC	114/125 (91%)	114 (100%)	0	100	100
1	AD	114/125 (91%)	114 (100%)	0	100	100
1	AE	122/125 (98%)	122 (100%)	0	100	100
1	B	114/125 (91%)	114 (100%)	0	100	100
1	BA	122/125 (98%)	122 (100%)	0	100	100
1	BB	114/125 (91%)	114 (100%)	0	100	100
1	BC	114/125 (91%)	114 (100%)	0	100	100
1	BD	122/125 (98%)	122 (100%)	0	100	100
1	BE	114/125 (91%)	114 (100%)	0	100	100
1	C	122/125 (98%)	122 (100%)	0	100	100
1	CA	114/125 (91%)	114 (100%)	0	100	100
1	CB	114/125 (91%)	114 (100%)	0	100	100
1	CC	122/125 (98%)	122 (100%)	0	100	100
1	CD	114/125 (91%)	114 (100%)	0	100	100
1	CE	122/125 (98%)	122 (100%)	0	100	100
1	D	114/125 (91%)	114 (100%)	0	100	100
1	DA	114/125 (91%)	114 (100%)	0	100	100
1	DB	122/125 (98%)	122 (100%)	0	100	100
1	DC	114/125 (91%)	114 (100%)	0	100	100
1	DD	122/125 (98%)	122 (100%)	0	100	100
1	DE	114/125 (91%)	114 (100%)	0	100	100
1	E	114/125 (91%)	114 (100%)	0	100	100
1	EA	122/125 (98%)	122 (100%)	0	100	100
1	EB	114/125 (91%)	114 (100%)	0	100	100
1	EC	122/125 (98%)	122 (100%)	0	100	100
1	ED	114/125 (91%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EE	114/125 (91%)	114 (100%)	0	100	100
1	F	122/125 (98%)	122 (100%)	0	100	100
1	FA	114/125 (91%)	114 (100%)	0	100	100
1	FB	122/125 (98%)	122 (100%)	0	100	100
1	FC	114/125 (91%)	114 (100%)	0	100	100
1	FD	114/125 (91%)	114 (100%)	0	100	100
1	FE	122/125 (98%)	122 (100%)	0	100	100
1	G	114/125 (91%)	114 (100%)	0	100	100
1	GA	122/125 (98%)	122 (100%)	0	100	100
1	GB	114/125 (91%)	114 (100%)	0	100	100
1	GC	114/125 (91%)	114 (100%)	0	100	100
1	GD	122/125 (98%)	122 (100%)	0	100	100
1	GE	114/125 (91%)	114 (100%)	0	100	100
1	H	122/125 (98%)	122 (100%)	0	100	100
1	HA	114/125 (91%)	114 (100%)	0	100	100
1	HB	114/125 (91%)	114 (100%)	0	100	100
1	HC	122/125 (98%)	122 (100%)	0	100	100
1	HD	114/125 (91%)	114 (100%)	0	100	100
1	HE	122/125 (98%)	122 (100%)	0	100	100
1	I	114/125 (91%)	114 (100%)	0	100	100
1	IA	114/125 (91%)	114 (100%)	0	100	100
1	IB	122/125 (98%)	122 (100%)	0	100	100
1	IC	114/125 (91%)	114 (100%)	0	100	100
1	ID	122/125 (98%)	122 (100%)	0	100	100
1	IE	114/125 (91%)	114 (100%)	0	100	100
1	J	114/125 (91%)	114 (100%)	0	100	100
1	JA	122/125 (98%)	122 (100%)	0	100	100
1	JB	114/125 (91%)	114 (100%)	0	100	100
1	JC	122/125 (98%)	122 (100%)	0	100	100
1	JD	114/125 (91%)	114 (100%)	0	100	100
1	JE	114/125 (91%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	122/125 (98%)	122 (100%)	0	100	100
1	KA	114/125 (91%)	114 (100%)	0	100	100
1	KB	122/125 (98%)	122 (100%)	0	100	100
1	KC	114/125 (91%)	114 (100%)	0	100	100
1	KD	114/125 (91%)	114 (100%)	0	100	100
1	KE	122/125 (98%)	122 (100%)	0	100	100
1	L	114/125 (91%)	114 (100%)	0	100	100
1	LA	122/125 (98%)	122 (100%)	0	100	100
1	LB	114/125 (91%)	114 (100%)	0	100	100
1	LC	114/125 (91%)	114 (100%)	0	100	100
1	LD	122/125 (98%)	122 (100%)	0	100	100
1	LE	114/125 (91%)	114 (100%)	0	100	100
1	M	122/125 (98%)	122 (100%)	0	100	100
1	MA	114/125 (91%)	114 (100%)	0	100	100
1	MB	114/125 (91%)	114 (100%)	0	100	100
1	MC	122/125 (98%)	122 (100%)	0	100	100
1	MD	114/125 (91%)	114 (100%)	0	100	100
1	ME	122/125 (98%)	122 (100%)	0	100	100
1	N	114/125 (91%)	114 (100%)	0	100	100
1	NA	114/125 (91%)	114 (100%)	0	100	100
1	NB	122/125 (98%)	122 (100%)	0	100	100
1	NC	114/125 (91%)	114 (100%)	0	100	100
1	ND	122/125 (98%)	122 (100%)	0	100	100
1	NE	114/125 (91%)	114 (100%)	0	100	100
1	O	114/125 (91%)	114 (100%)	0	100	100
1	OA	122/125 (98%)	122 (100%)	0	100	100
1	OB	114/125 (91%)	114 (100%)	0	100	100
1	OC	122/125 (98%)	122 (100%)	0	100	100
1	OD	114/125 (91%)	114 (100%)	0	100	100
1	OE	114/125 (91%)	114 (100%)	0	100	100
1	P	122/125 (98%)	122 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	PA	114/125 (91%)	114 (100%)	0	100	100
1	PB	122/125 (98%)	122 (100%)	0	100	100
1	PC	114/125 (91%)	114 (100%)	0	100	100
1	PD	114/125 (91%)	114 (100%)	0	100	100
1	PE	122/125 (98%)	122 (100%)	0	100	100
1	Q	114/125 (91%)	114 (100%)	0	100	100
1	QA	122/125 (98%)	122 (100%)	0	100	100
1	QB	114/125 (91%)	114 (100%)	0	100	100
1	QC	114/125 (91%)	114 (100%)	0	100	100
1	QD	122/125 (98%)	122 (100%)	0	100	100
1	QE	114/125 (91%)	114 (100%)	0	100	100
1	R	122/125 (98%)	122 (100%)	0	100	100
1	RA	114/125 (91%)	114 (100%)	0	100	100
1	RB	114/125 (91%)	114 (100%)	0	100	100
1	RC	122/125 (98%)	122 (100%)	0	100	100
1	RD	114/125 (91%)	114 (100%)	0	100	100
1	RE	122/125 (98%)	122 (100%)	0	100	100
1	S	114/125 (91%)	114 (100%)	0	100	100
1	SA	114/125 (91%)	114 (100%)	0	100	100
1	SB	122/125 (98%)	122 (100%)	0	100	100
1	SC	114/125 (91%)	114 (100%)	0	100	100
1	SD	122/125 (98%)	122 (100%)	0	100	100
1	SE	114/125 (91%)	114 (100%)	0	100	100
1	T	114/125 (91%)	114 (100%)	0	100	100
1	TA	122/125 (98%)	122 (100%)	0	100	100
1	TB	114/125 (91%)	114 (100%)	0	100	100
1	TC	122/125 (98%)	122 (100%)	0	100	100
1	TD	114/125 (91%)	114 (100%)	0	100	100
1	TE	114/125 (91%)	114 (100%)	0	100	100
1	U	122/125 (98%)	122 (100%)	0	100	100
1	UA	114/125 (91%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UB	122/125 (98%)	122 (100%)	0	100	100
1	UC	114/125 (91%)	114 (100%)	0	100	100
1	UD	114/125 (91%)	114 (100%)	0	100	100
1	V	114/125 (91%)	114 (100%)	0	100	100
1	VA	122/125 (98%)	122 (100%)	0	100	100
1	VB	114/125 (91%)	114 (100%)	0	100	100
1	VC	114/125 (91%)	114 (100%)	0	100	100
1	VD	122/125 (98%)	122 (100%)	0	100	100
1	W	122/125 (98%)	122 (100%)	0	100	100
1	WA	114/125 (91%)	114 (100%)	0	100	100
1	WB	114/125 (91%)	114 (100%)	0	100	100
1	WC	122/125 (98%)	122 (100%)	0	100	100
1	WD	114/125 (91%)	114 (100%)	0	100	100
1	X	114/125 (91%)	114 (100%)	0	100	100
1	XA	114/125 (91%)	114 (100%)	0	100	100
1	XB	122/125 (98%)	122 (100%)	0	100	100
1	XC	114/125 (91%)	114 (100%)	0	100	100
1	XD	122/125 (98%)	122 (100%)	0	100	100
1	Y	114/125 (91%)	114 (100%)	0	100	100
1	YA	122/125 (98%)	122 (100%)	0	100	100
1	YB	114/125 (91%)	114 (100%)	0	100	100
1	YC	122/125 (98%)	122 (100%)	0	100	100
1	YD	114/125 (91%)	114 (100%)	0	100	100
1	Z	122/125 (98%)	122 (100%)	0	100	100
1	ZA	114/125 (91%)	114 (100%)	0	100	100
1	ZB	122/125 (98%)	122 (100%)	0	100	100
1	ZC	114/125 (91%)	114 (100%)	0	100	100
1	ZD	114/125 (91%)	114 (100%)	0	100	100
All	All	17580/18750 (94%)	17580 (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 (26)

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	85	HIS
1	H	85	HIS
1	M	85	HIS
1	W	85	HIS
1	BA	85	HIS
1	GA	85	HIS
1	LA	85	HIS
1	QA	85	HIS
1	VA	85	HIS
1	AB	85	HIS
1	KB	85	HIS
1	PB	85	HIS
1	UB	85	HIS
1	EC	85	HIS
1	JC	85	HIS
1	OC	85	HIS
1	YC	85	HIS
1	DD	85	HIS
1	ID	85	HIS
1	ND	85	HIS
1	SD	85	HIS
1	XD	85	HIS
1	CE	85	HIS
1	HE	85	HIS
1	ME	85	HIS
1	RE	85	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

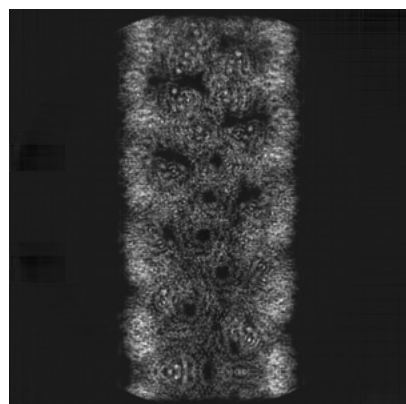
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51003. These allow visual inspection of the internal detail of the map and identification of artifacts.

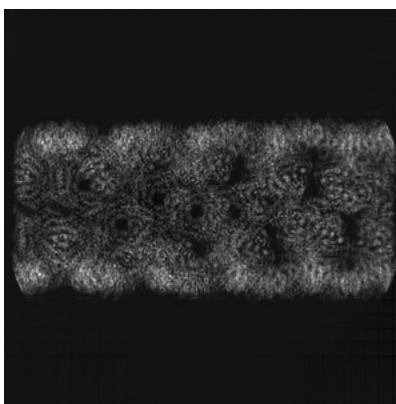
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

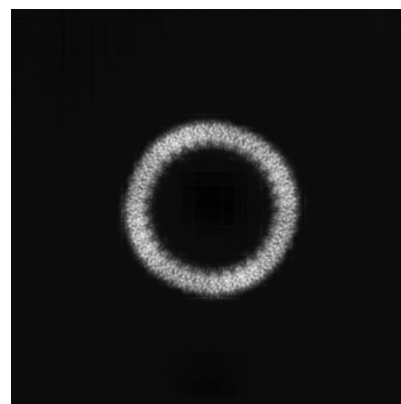
6.1.1 Primary map



X

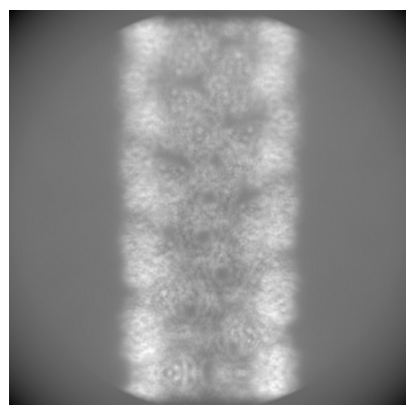


Y

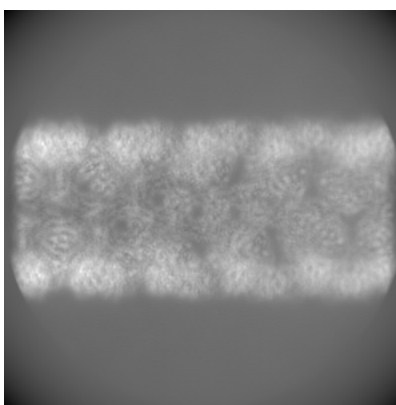


Z

6.1.2 Raw map



X



Y

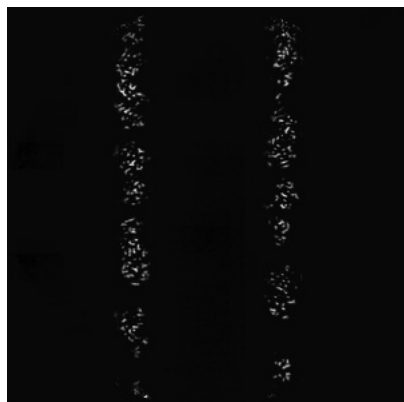


Z

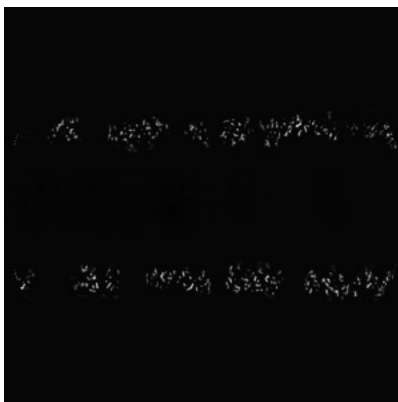
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 208

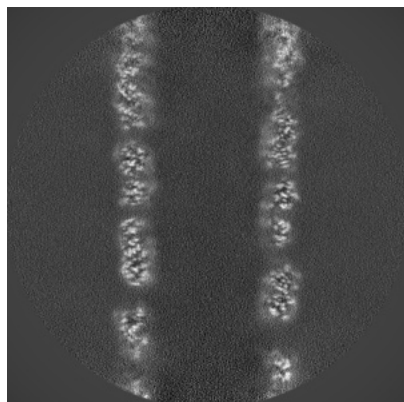


Y Index: 208

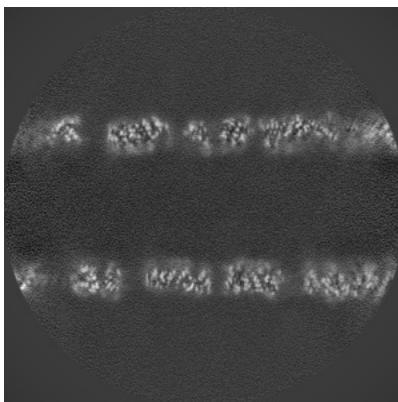


Z Index: 208

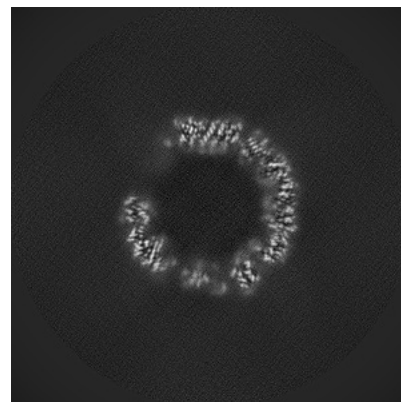
6.2.2 Raw map



X Index: 208



Y Index: 208

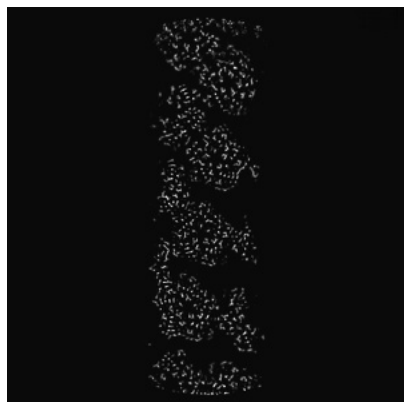


Z Index: 208

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

6.3 Largest variance slices [i](#)

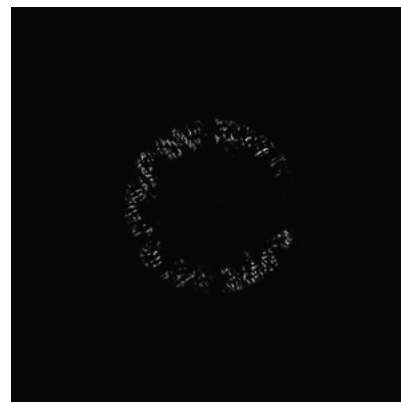
6.3.1 Primary map



X Index: 134

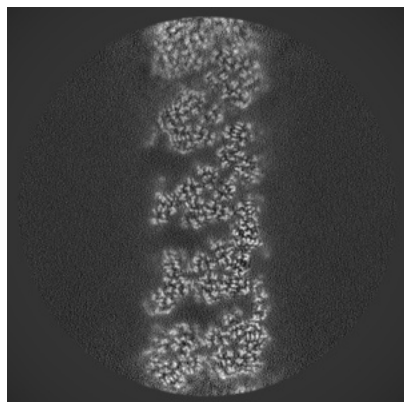


Y Index: 136

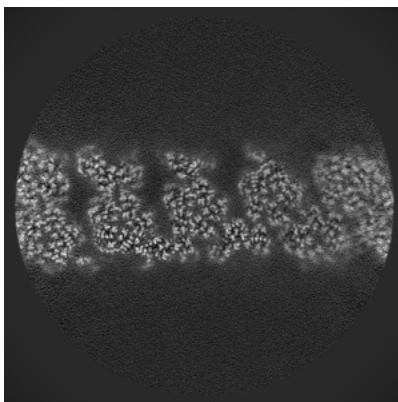


Z Index: 20

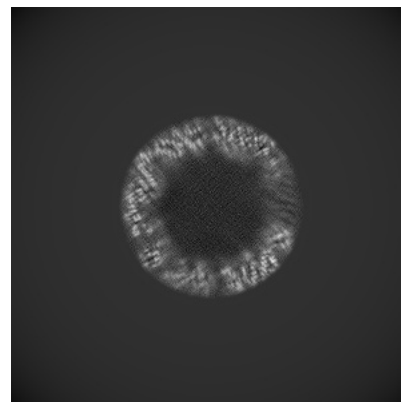
6.3.2 Raw map



X Index: 279



Y Index: 280

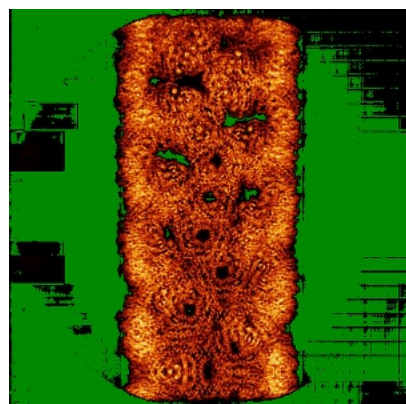


Z Index: 21

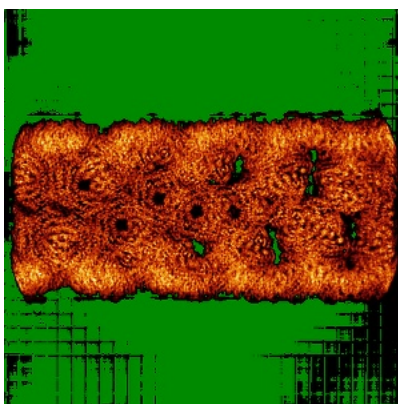
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

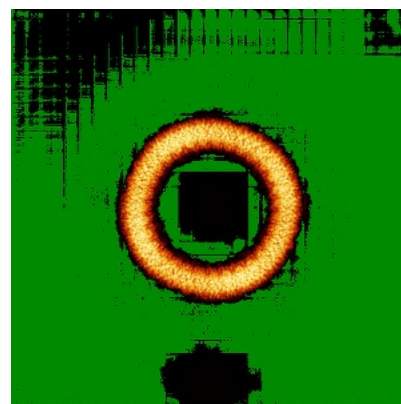
6.4.1 Primary map



X

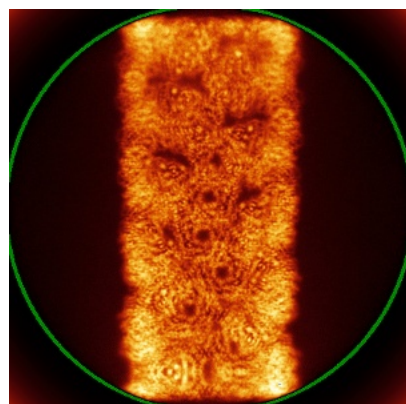


Y

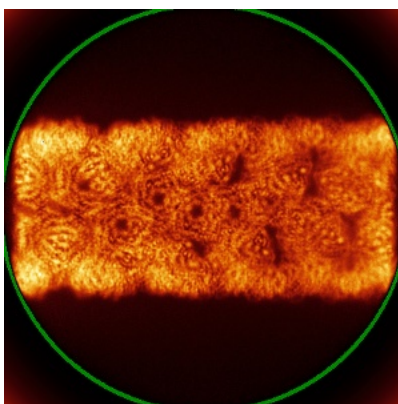


Z

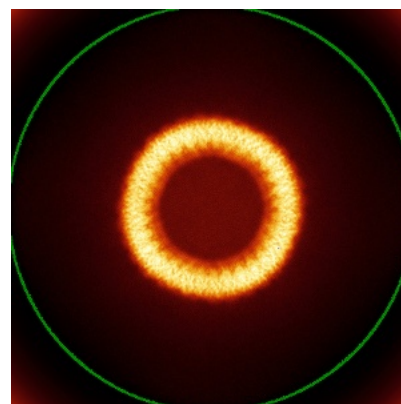
6.4.2 Raw map



X



Y

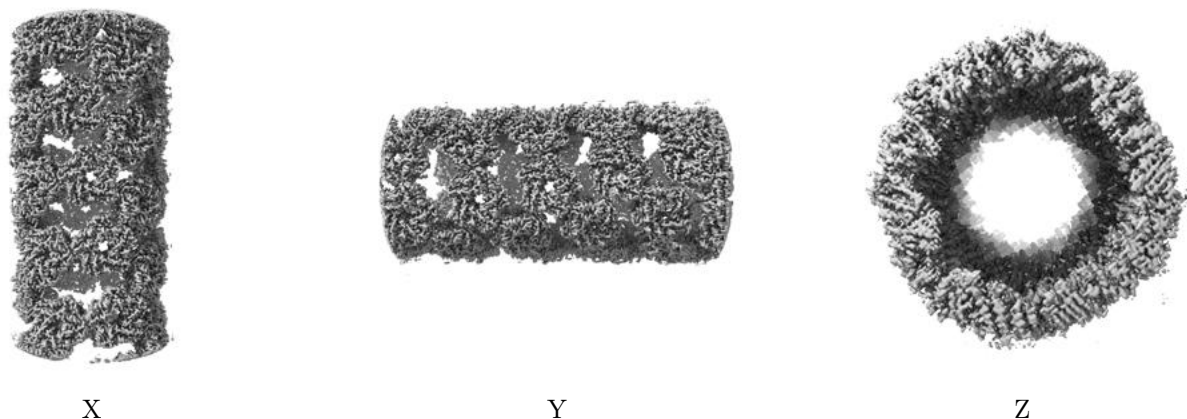


Z

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.

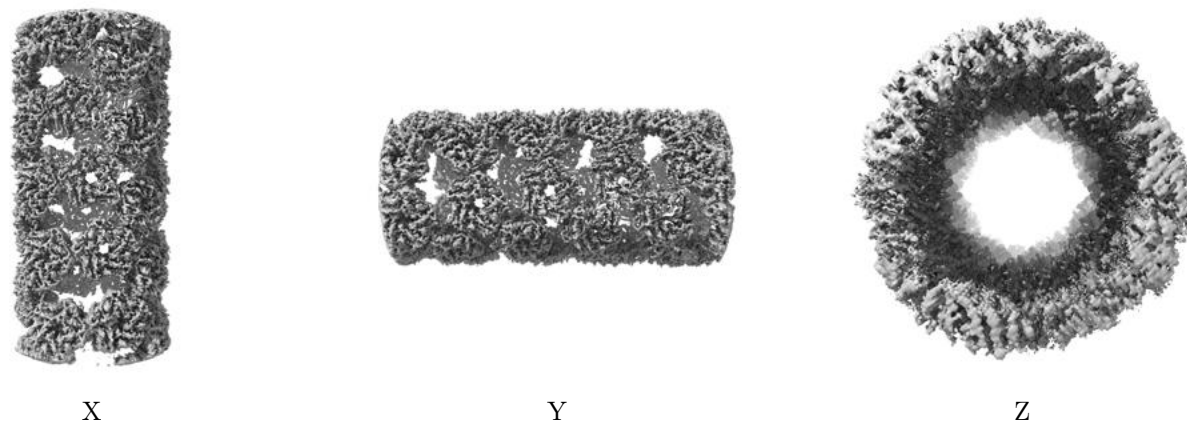
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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

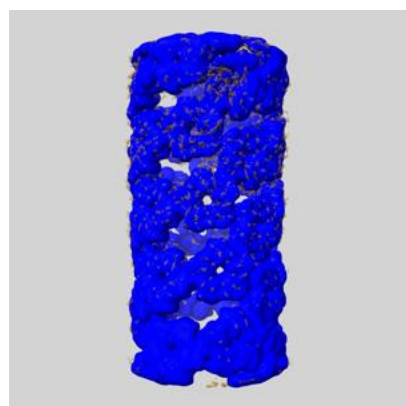
6.6 Mask visualisation [i](#)

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

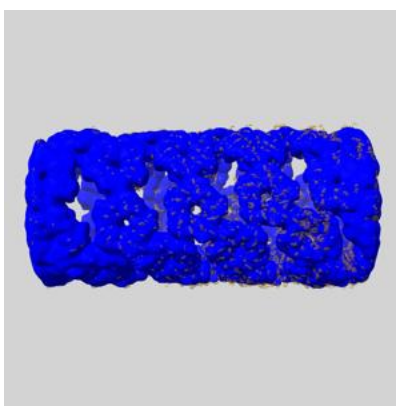
A mask typically either:

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

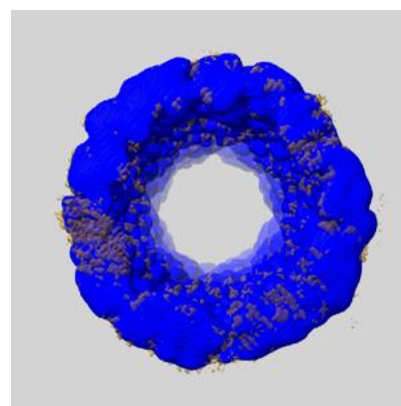
6.6.1 emd_51003_msk_1.map [i](#)



X

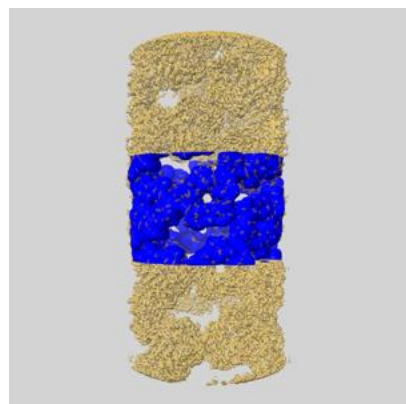


Y

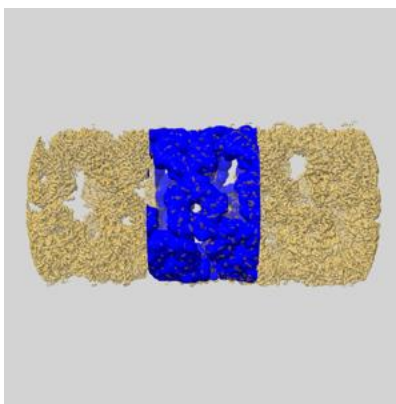


Z

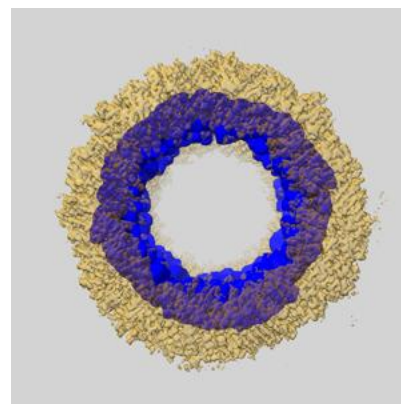
6.6.2 emd_51003_msk_2.map [i](#)



X



Y

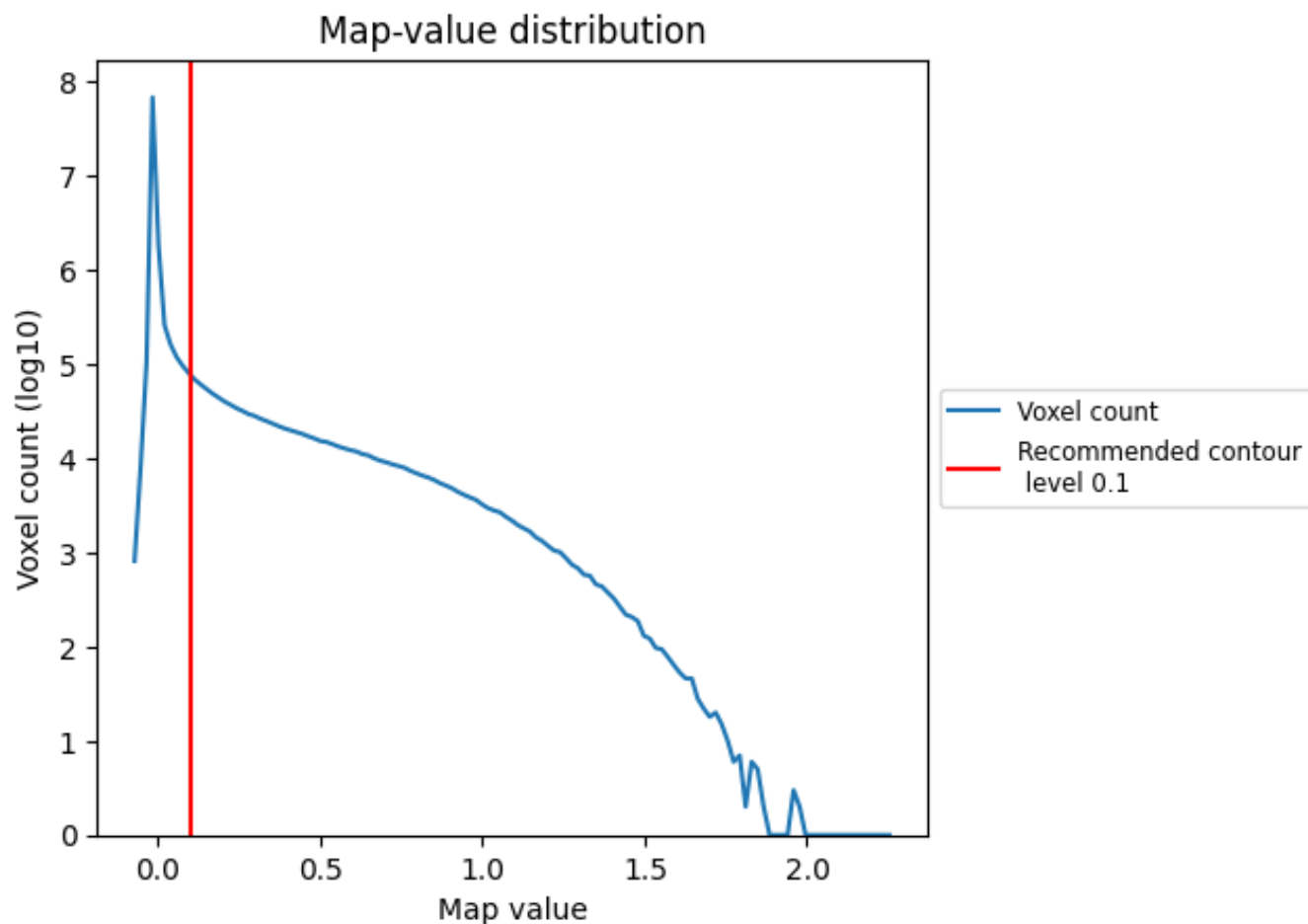


Z

7 Map analysis [i](#)

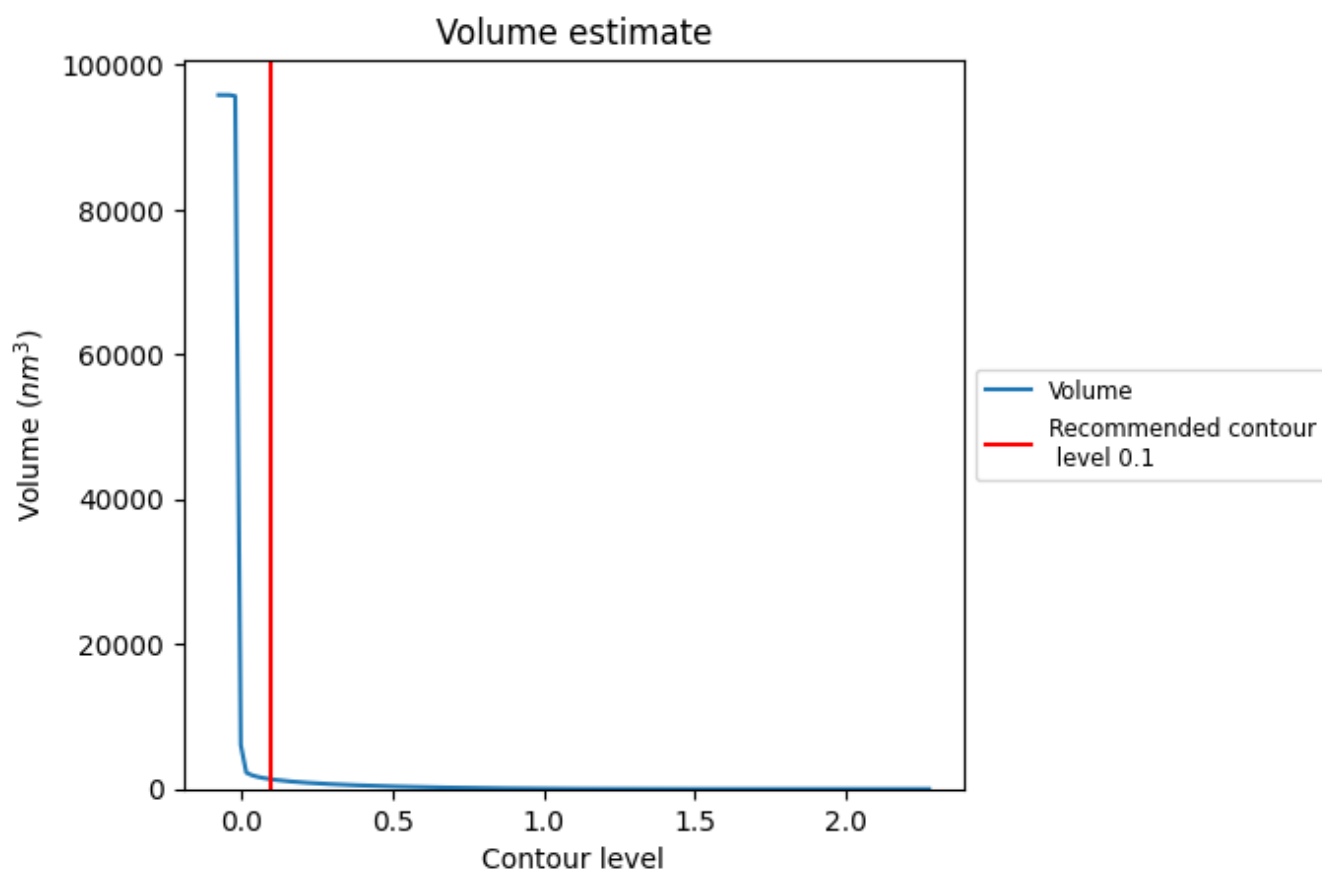
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

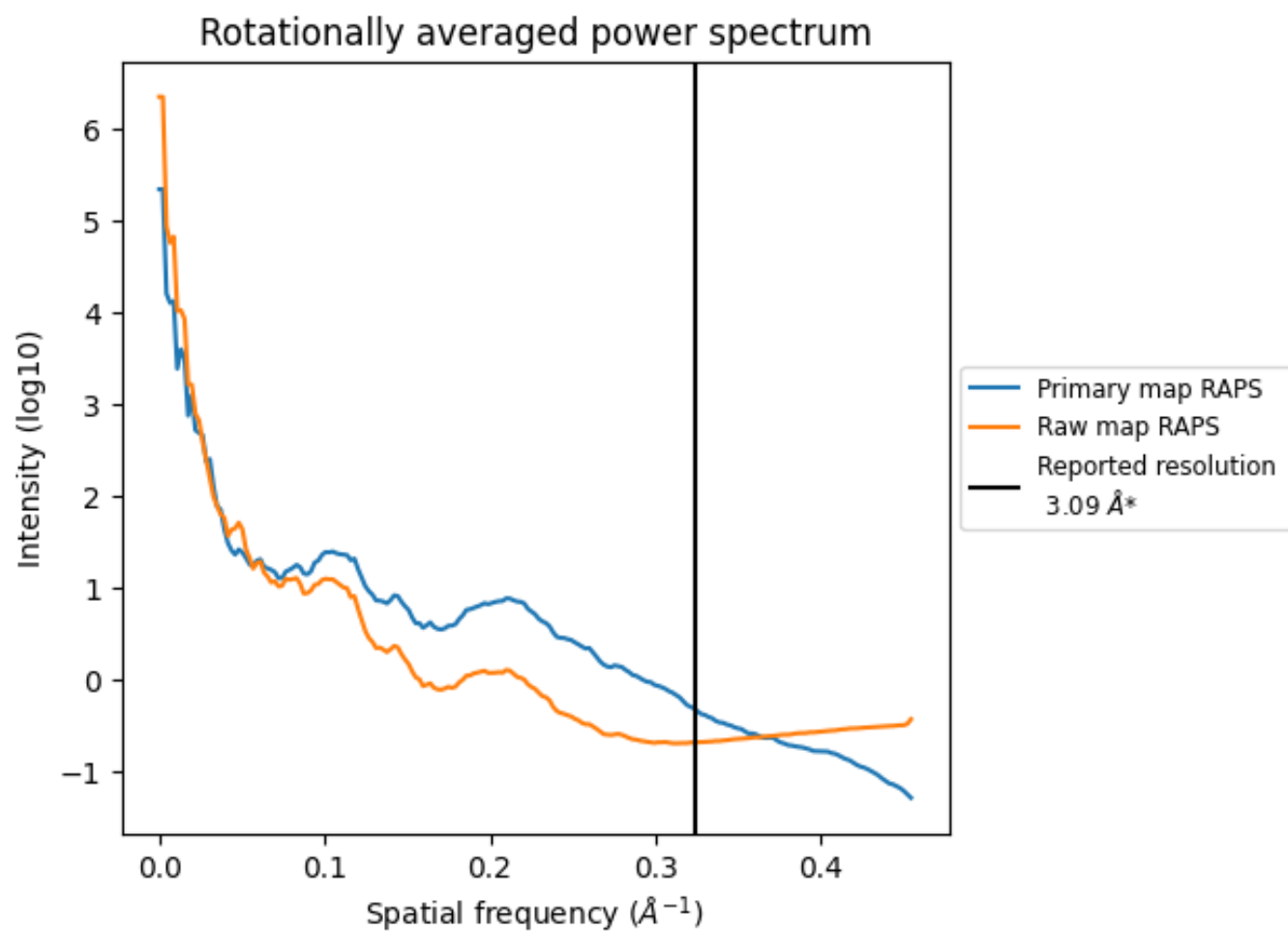
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1344 nm^3 ; this corresponds to an approximate mass of 1214 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

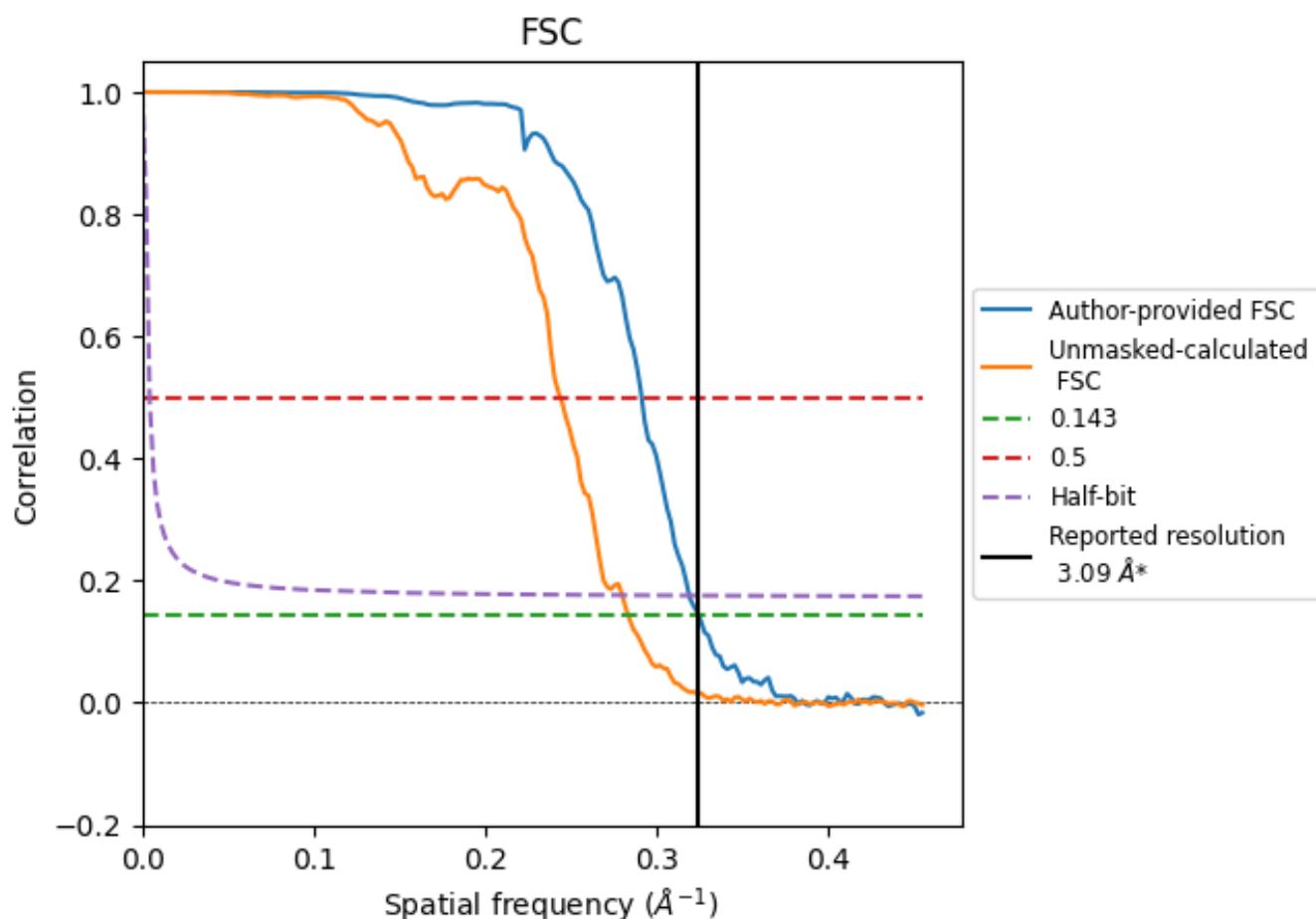


*Reported resolution corresponds to spatial frequency of 0.324 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.324 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

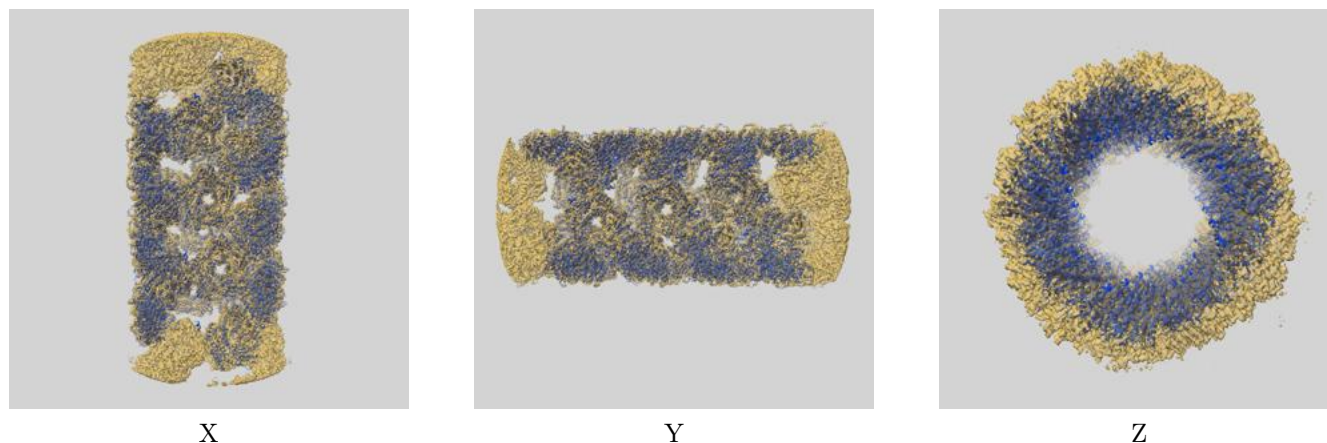
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.08	3.44	3.14
Unmasked-calculated*	3.53	4.11	3.58

*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 3.53 differs from the reported value 3.09 by more than 10 %

9 Map-model fit [i](#)

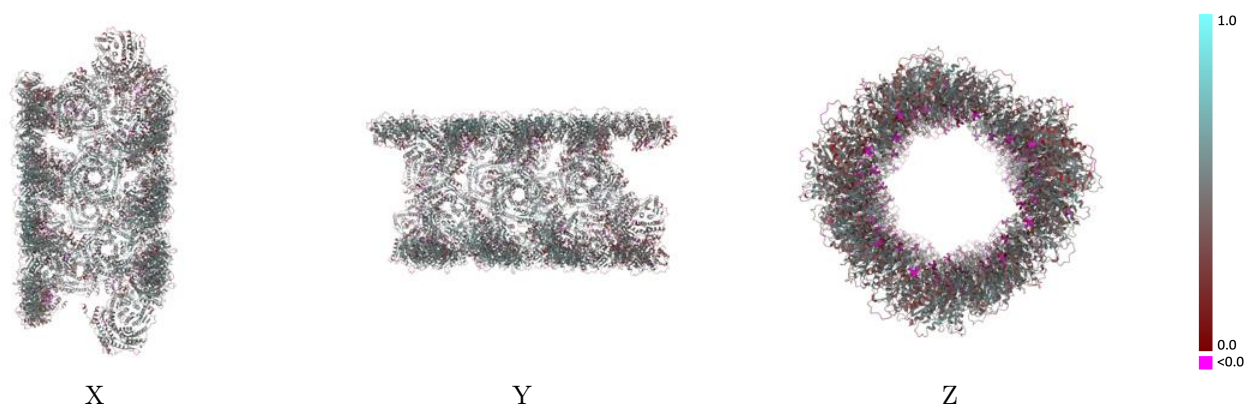
This section contains information regarding the fit between EMDB map EMD-51003 and PDB model 9G3M. Per-residue inclusion information can be found in section [3](#) on page [56](#).

9.1 Map-model overlay [i](#)



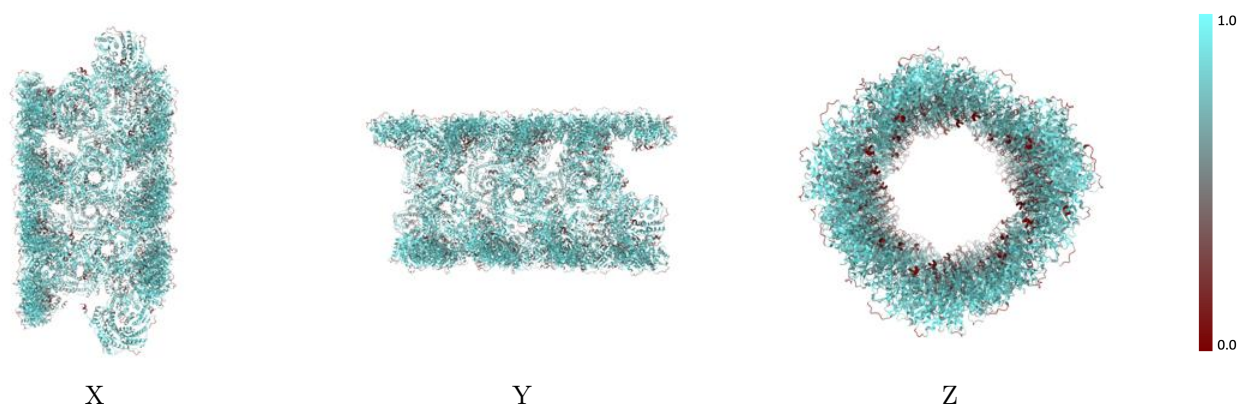
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



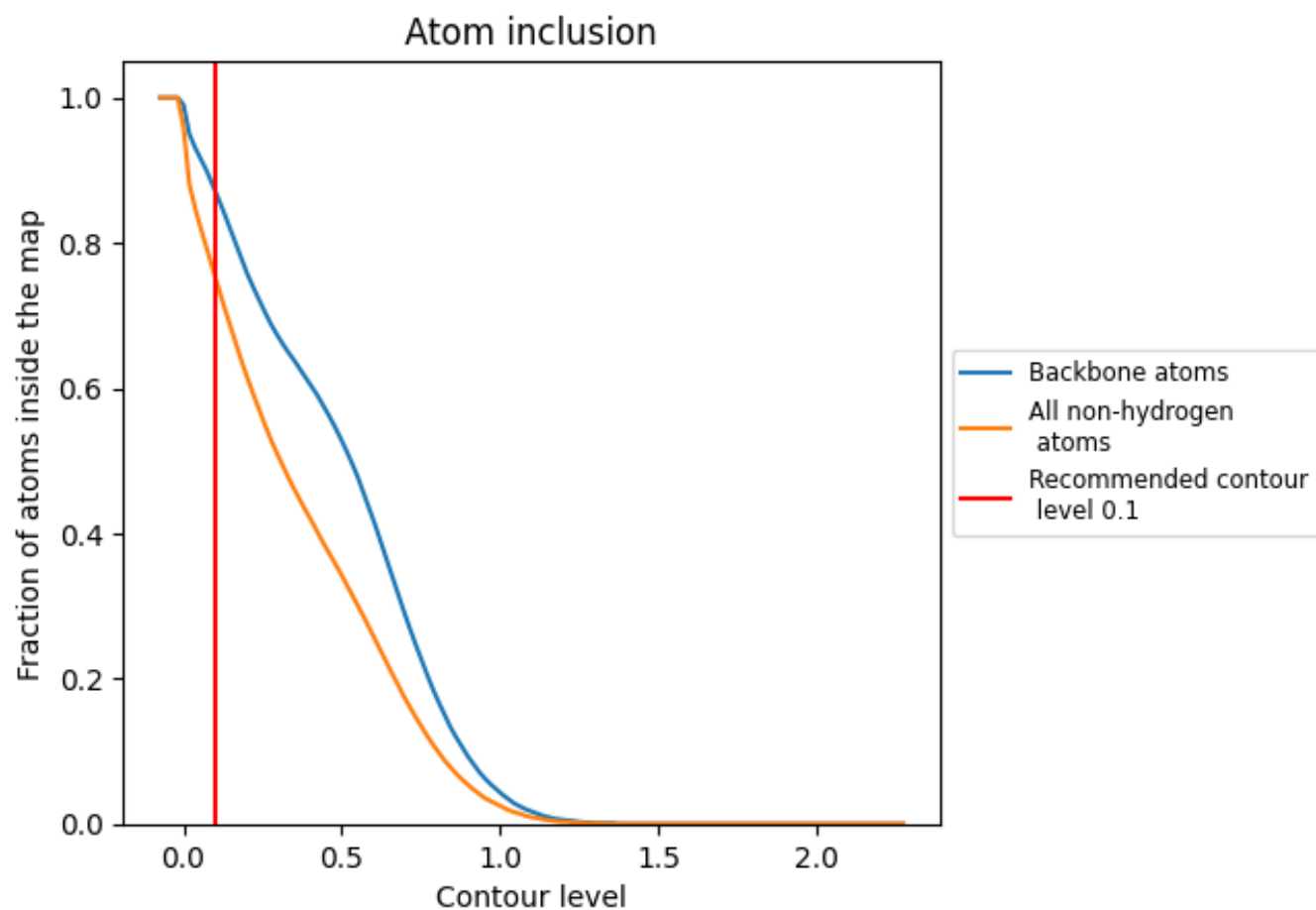
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 75% 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	 0.7540	 0.4360
A	 0.8150	 0.5180
AA	 0.7620	 0.4310
AB	 0.7700	 0.4600
AC	 0.7580	 0.4180
AD	 0.7610	 0.4350
AE	 0.7840	 0.4670
B	 0.7930	 0.4850
BA	 0.7750	 0.4390
BB	 0.7510	 0.4230
BC	 0.7830	 0.4630
BD	 0.7550	 0.4520
BE	 0.7470	 0.4270
C	 0.7770	 0.4860
CA	 0.7560	 0.4040
CB	 0.7830	 0.4700
CC	 0.7950	 0.4830
CD	 0.7470	 0.4190
CE	 0.7540	 0.4430
D	 0.7640	 0.4550
DA	 0.7710	 0.4320
DB	 0.7820	 0.4580
DC	 0.7600	 0.4470
DD	 0.7450	 0.4240
DE	 0.7440	 0.4130
E	 0.7800	 0.4930
EA	 0.7770	 0.4570
EB	 0.7430	 0.4240
EC	 0.7690	 0.4580
ED	 0.7130	 0.3930
EE	 0.7780	 0.4560
F	 0.7650	 0.4790
FA	 0.7470	 0.4190
FB	 0.7270	 0.4180
FC	 0.7290	 0.4200



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Chain	Atom inclusion	Q-score
FD	 0.7640	 0.4400
FE	 0.7700	 0.4580
G	 0.7340	 0.4460
GA	 0.7500	 0.4430
GB	 0.7030	 0.3840
GC	 0.7740	 0.4690
GD	 0.7390	 0.4300
GE	 0.7400	 0.4170
H	 0.7550	 0.4550
HA	 0.7230	 0.4090
HB	 0.7520	 0.4230
HC	 0.7750	 0.4720
HD	 0.7180	 0.3870
HE	 0.7420	 0.4260
I	 0.7450	 0.4290
IA	 0.7600	 0.4490
IB	 0.7470	 0.4380
IC	 0.7700	 0.4500
ID	 0.7300	 0.3930
IE	 0.7120	 0.3830
J	 0.7580	 0.4630
JA	 0.7700	 0.4490
JB	 0.7320	 0.4220
JC	 0.7610	 0.4490
JD	 0.6940	 0.3480
JE	 0.7510	 0.4130
K	 0.7880	 0.4820
KA	 0.7420	 0.4080
KB	 0.7340	 0.4230
KC	 0.7420	 0.4110
KD	 0.7310	 0.3920
KE	 0.7300	 0.4130
L	 0.7630	 0.4400
LA	 0.7480	 0.4280
LB	 0.7300	 0.3950
LC	 0.7560	 0.4560
LD	 0.7240	 0.3780
LE	 0.7250	 0.3930
M	 0.7630	 0.4510
MA	 0.7240	 0.3910
MB	 0.7700	 0.4410
MC	 0.7820	 0.4510

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Chain	Atom inclusion	Q-score
MD	 0.7160	 0.3490
ME	 0.7470	 0.4040
N	 0.7370	 0.4270
NA	 0.7550	 0.4320
NB	 0.7340	 0.4150
NC	 0.7500	 0.4140
ND	 0.7120	 0.3730
NE	 0.7290	 0.3790
O	 0.7790	 0.4620
OA	 0.7640	 0.4730
OB	 0.7160	 0.3870
OC	 0.7580	 0.4320
OD	 0.7100	 0.3650
OE	 0.7520	 0.4150
P	 0.7910	 0.4720
PA	 0.7280	 0.4330
PB	 0.7130	 0.3710
PC	 0.7290	 0.3960
PD	 0.7230	 0.4010
PE	 0.7910	 0.4870
Q	 0.7560	 0.4290
QA	 0.7300	 0.4320
QB	 0.6580	 0.3220
QC	 0.7600	 0.4470
QD	 0.7840	 0.4760
QE	 0.7640	 0.4490
R	 0.7530	 0.4510
RA	 0.7350	 0.4040
RB	 0.6960	 0.3720
RC	 0.7730	 0.4760
RD	 0.7580	 0.4480
RE	 0.7630	 0.4580
S	 0.7260	 0.4100
SA	 0.7270	 0.4310
SB	 0.7980	 0.4800
SC	 0.7470	 0.4510
SD	 0.7630	 0.4510
SE	 0.7370	 0.4230
T	 0.7640	 0.4420
TA	 0.7960	 0.4810
TB	 0.7600	 0.4390
TC	 0.7590	 0.4560

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Chain	Atom inclusion	Q-score
TD	 0.7400	 0.4230
TE	 0.7770	 0.4560
U	 0.7830	 0.4880
UA	 0.7620	 0.4500
UB	 0.7570	 0.4500
UC	 0.7420	 0.4190
UD	 0.7700	 0.4580
V	 0.7620	 0.4520
VA	 0.7550	 0.4490
VB	 0.7240	 0.4050
VC	 0.7630	 0.4660
VD	 0.7830	 0.4710
W	 0.7700	 0.4600
WA	 0.7370	 0.4190
WB	 0.7680	 0.4590
WC	 0.7890	 0.4700
WD	 0.7510	 0.4370
X	 0.7610	 0.4320
XA	 0.7770	 0.4520
XB	 0.8000	 0.4810
XC	 0.7400	 0.4360
XD	 0.7600	 0.4460
Y	 0.7680	 0.4570
YA	 0.8040	 0.4900
YB	 0.7720	 0.4510
YC	 0.7490	 0.4360
YD	 0.7290	 0.3900
Z	 0.7790	 0.4590
ZA	 0.7630	 0.4450
ZB	 0.7830	 0.4580
ZC	 0.7190	 0.3970
ZD	 0.7730	 0.4410