Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 02:06 am GMT

PDB ID	:	9G3N
EMDB ID	:	EMD-51004
Title	:	Circularly permuted lumazine synthase 36-pentamer spherical cage
Authors	:	Koziej, L.; Azuma, Y.
Deposited on	:	2024-07-12
Resolution	:	3.07 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:

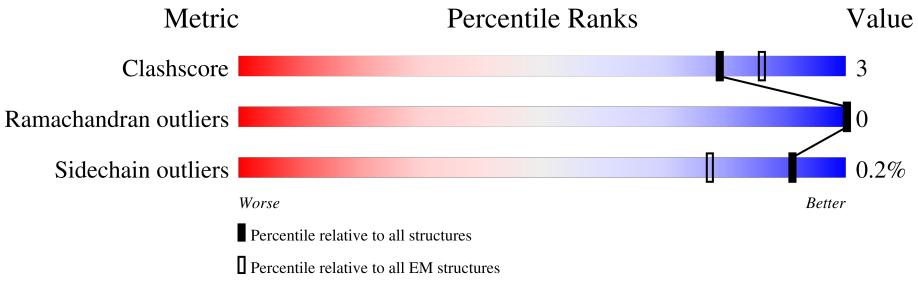
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 3.07 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	163	85% 6% 9%
1	AA	163	85% 6% 9%
1	AB	163	83% 7% 9%
1	AC	163	87% . 9%
1	AD	163	87% 5% 9%
1	AE	163	87% . 9%
1	AF	163	84% 7% 9%
1	B	163	86% 5% 9%
1	BA	163	85% 6% 9%

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Mol	Chain	Length	Quality of chain
1	BB	163	88% · 9%
1	BC	163	85% 6% 9%
1	BD	163	85% 6% 9%
1	BE	163	85% 6% 9%
1	BF	163	83% 7% 9%
1	C	163	82% 9% 9%
1	CA	163	85% 6% 9%
1	CB	163	86% 5% 9%
1	CC	163	83% 8% 9%
1	CD	163	85% 6% 9%
1	CE	163	85% 6% 9%
1	CF	163	87% · 9%
1	D	163	87% · · 9%
1	DA	163	87% 5% 9%
1	DB	163	86% 5% 9%
1	DC	163	84% 7% 9%
1	DD	163	83% 8% 9%
1	DE	163	85% 6% 9%
1	DF	163	87% · 9%
1	E	163	84% 7% 9%
1	EA	163	85% 6% 9%
1	EB	163	85% 6% 9%
1	EC	163	83% 7% 9%
1	ED	163	87% · 9%
1	EE	163	87% 5% 9%

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Mol	Chain	Length	Quality of chain
1	EF	163	86% 5% 9%
1	F	163	83% 8% 9%
1	FA	163	86% 5% 9%
1	FB	163	84% 7% 9%
1	FC	163	87% 9%
1	FD	163	82% 9% 9%
1	FE	163	85% 6% 9%
1	FF	163	85% 6% 9%
1	G	163	84% 7% 9%
1	GA	163	83% 8% 9%
1	GB	163	85% 6% 9%
1	GC	163	85% 6% 9%
1	GD	163	83% 8% 9%
1	GE	163	85% 6% 9%
1	GF	163	84% 7% 9%
1	H	163	83% 7% 9%
1	HA	163	87% 9%
1	HB	163	87% 5% 9%
1	HC	163	86% 5% 9%
1	HD	163	84% 7% 9%
1	HE	163	83% 8% 9%
1	HF	163	85% 6% 9%
1	I	163	88% 9%
1	IA	163	85% 6% 9%
1	IB	163	85% 6% 9%

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Mol	Chain	Length	Quality of chain
1	IC	163	85% 6% 9%
1	ID	163	83% 7% 9%
1	IE	163	87% 9%
1	IF	163	87% 5% 9%
1	J	163	87% 9%
1	JA	163	83% 8% 9%
1	JB	163	86% 5% 9%
1	JC	163	85% 6% 9%
1	JD	163	88% 9%
1	JE	163	84% 7% 9%
1	JF	163	85% 6% 9%
1	K	163	87% 9%
1	KA	163	84% 7% 9%
1	KB	163	82% 9% 9%
1	KC	163	87% 9%
1	KD	163	87% 9%
1	KE	163	83% 8% 9%
1	KF	163	85% 6% 9%
1	L	163	85% 6% 9%
1	LA	163	83% 7% 9%
1	LB	163	87% 9%
1	LC	163	87% 5% 9%
1	LD	163	90% 9%
1	LE	163	84% 7% 9%
1	LF	163	83% 8% 9%

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Mol	Chain	Length	Quality of chain
1	M	163	85% 6% 9%
1	MA	163	88% 9%
1	MB	163	83% 7% 9%
1	MC	163	85% 6% 9%
1	MD	163	85% 6% 9%
1	ME	163	83% 8% 9%
1	MF	163	87% 9%
1	N	163	85% 6% 9%
1	NA	163	86% 5% 9%
1	NB	163	83% 8% 9%
1	NC	163	85% 6% 9%
1	ND	163	85% 6% 9%
1	NE	163	87% 9%
1	NF	163	83% 8% 9%
1	O	163	87% 5% 9%
1	OA	163	87% 9%
1	OB	163	84% 7% 9%
1	OC	163	83% 8% 9%
1	OD	163	85% 6% 9%
1	OE	163	87% 9%
1	OF	163	83% 8% 9%
1	P	163	85% 6% 9%
1	PA	163	85% 6% 9%
1	PB	163	83% 7% 9%
1	PC	163	87% 9%

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Mol	Chain	Length	Quality of chain
1	PD	163	88% · 9%
1	PE	163	86% 5% 9%
1	PF	163	84% 7% 9%
1	Q	163	85% 6% 9%
1	QA	163	85% 6% 9%
1	QB	163	88% · 9%
1	QC	163	82% 9% 9%
1	QD	163	85% 6% 9%
1	QE	163	85% 6% 9%
1	QF	163	83% 7% 9%
1	R	163	82% 9% 9%
1	RA	163	85% 6% 9%
1	RB	163	87% · 9%
1	RC	163	83% 8% 9%
1	RD	163	85% 6% 9%
1	RE	163	84% 7% 9%
1	RF	163	87% · 9%
1	S	163	87% · 9%
1	SA	163	87% 5% 9%
1	SB	163	86% 5% 9%
1	SC	163	84% 7% 9%
1	SD	163	83% 8% 9%
1	SE	163	85% 6% 9%
1	SF	163	85% 6% 9%
1	T	163	84% 7% 9%

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Mol	Chain	Length	Quality of chain
1	TA	163	85% 6% 9%
1	TB	163	85% 6% 9%
1	TC	163	83% 7% 9%
1	TD	163	87% 9%
1	TE	163	87% 5% 9%
1	TF	163	86% 5% 9%
1	U	163	83% 8% 9%
1	UA	163	86% 5% 9%
1	UB	163	85% 6% 9%
1	UC	163	88% 9%
1	UD	163	83% 8% 9%
1	UE	163	85% 6% 9%
1	UF	163	85% 6% 9%
1	V	163	84% 7% 9%
1	VA	163	82% 9% 9%
1	VB	163	85% 6% 9%
1	VC	163	87% 9%
1	VD	163	83% 8% 9%
1	VE	163	86% 5% 9%
1	VF	163	84% 7% 9%
1	W	163	82% 9% 9%
1	WA	163	87% 9%
1	WB	163	87% 5% 9%
1	WC	163	88% 9%
1	WD	163	84% 7% 9%

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Mol	Chain	Length	Quality of chain
1	WE	163	82% 9% 9%
1	WF	163	85% 6% 9%
1	X	163	88% • 9%
1	XA	163	84% 7% 9%
1	XB	163	85% 6% 9%
1	XC	163	85% 6% 9%
1	XD	163	83% 7% 9%
1	XE	163	87% • 9%
1	XF	163	87% 5% 9%
1	Y	163	87% • 9%
1	YA	163	83% 8% 9%
1	YB	163	85% 6% 9%
1	YC	163	84% 7% 9%
1	YD	163	87% • 9%
1	YE	163	83% 7% 9%
1	Z	163	88% • 9%
1	ZA	163	84% 7% 9%
1	ZB	163	82% 9% 9%
1	ZC	163	87% • 9%
1	ZD	163	87% • 9%
1	ZE	163	83% 8% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 199560 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	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	B	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	C	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	D	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	E	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	F	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	G	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	H	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	I	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	J	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	K	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	L	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	M	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	N	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	O	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	P	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	Q	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	S	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	T	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	U	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	V	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	W	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	X	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	Y	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	Z	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	AA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	BA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	CA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	DA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	EA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	FA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	GA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	HA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	IA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	JA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	KA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	LA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	NA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	OA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	PA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	QA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	RA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	SA	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	TA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	UA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	VA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	WA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	XA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	YA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	ZA	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	AB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	BB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	CB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	DB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	EB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	FB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	GB	148	Total	C	N	O	S	0	0
			1108	701	196	208	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	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	JB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	KB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	LB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	MB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	NB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	OB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	PB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	QB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	RB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	SB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	TB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	UB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	VB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	WB	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	XB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	YB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	ZB	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	AC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	BC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	DC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	EC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	FC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	GC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	HC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	IC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	JC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	KC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	LC	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	MC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	NC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	OC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	PC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	QC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	RC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	SC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	TC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	UC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	VC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	WC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	XC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	YC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	ZC	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	AD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	BD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	CD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	DD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	ED	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	FD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	GD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	HD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	ID	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	JD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	KD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	LD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	MD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	ND	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	OD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	PD	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	QD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	RD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	SD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	TD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	UD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	VD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	WD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	XD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	YD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	ZD	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	AE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	BE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	CE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	DE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	EE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	FE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	GE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	HE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	IE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	JE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	KE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	LE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	ME	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	NE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	OE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	PE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	QE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	RE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	SE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	TE	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	UE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	VE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	WE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	XE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	YE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	ZE	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	AF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	BF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	CF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	DF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	EF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	FF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	GF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	HF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IF	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		
1	JF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	KF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	LF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	MF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	NF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	OF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	PF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	QF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	RF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	SF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	TF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	UF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	VF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	WF	148	Total	C	N	O	S	0	0
			1108	701	196	208	3		
1	XF	149	Total	C	N	O	S	0	0
			1118	707	199	209	3		

There are 1980 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
XE	40	GLY	-	linker	UNP O66529
XE	41	SER	-	linker	UNP O66529
XE	42	GLY	-	linker	UNP O66529
XE	43	SER	-	linker	UNP O66529
XE	44	SER	-	linker	UNP O66529
XE	45	MET	-	linker	UNP O66529
XE	46	GLU	-	linker	UNP O66529
YE	1	MET	-	initiating methionine	UNP O66529
YE	37	GLY	-	linker	UNP O66529
YE	38	THR	-	linker	UNP O66529
YE	39	GLY	-	linker	UNP O66529
YE	40	GLY	-	linker	UNP O66529
YE	41	SER	-	linker	UNP O66529
YE	42	GLY	-	linker	UNP O66529
YE	43	SER	-	linker	UNP O66529
YE	44	SER	-	linker	UNP O66529
YE	45	MET	-	linker	UNP O66529
YE	46	GLU	-	linker	UNP O66529
ZE	1	MET	-	initiating methionine	UNP O66529
ZE	37	GLY	-	linker	UNP O66529
ZE	38	THR	-	linker	UNP O66529
ZE	39	GLY	-	linker	UNP O66529
ZE	40	GLY	-	linker	UNP O66529
ZE	41	SER	-	linker	UNP O66529
ZE	42	GLY	-	linker	UNP O66529
ZE	43	SER	-	linker	UNP O66529
ZE	44	SER	-	linker	UNP O66529
ZE	45	MET	-	linker	UNP O66529
ZE	46	GLU	-	linker	UNP O66529
AF	1	MET	-	initiating methionine	UNP O66529
AF	37	GLY	-	linker	UNP O66529
AF	38	THR	-	linker	UNP O66529
AF	39	GLY	-	linker	UNP O66529
AF	40	GLY	-	linker	UNP O66529
AF	41	SER	-	linker	UNP O66529
AF	42	GLY	-	linker	UNP O66529
AF	43	SER	-	linker	UNP O66529
AF	44	SER	-	linker	UNP O66529
AF	45	MET	-	linker	UNP O66529
AF	46	GLU	-	linker	UNP O66529
BF	1	MET	-	initiating methionine	UNP O66529
BF	37	GLY	-	linker	UNP O66529

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
IF	45	MET	-	linker	UNP O66529
IF	46	GLU	-	linker	UNP O66529
JF	1	MET	-	initiating methionine	UNP O66529
JF	37	GLY	-	linker	UNP O66529
JF	38	THR	-	linker	UNP O66529
JF	39	GLY	-	linker	UNP O66529
JF	40	GLY	-	linker	UNP O66529
JF	41	SER	-	linker	UNP O66529
JF	42	GLY	-	linker	UNP O66529
JF	43	SER	-	linker	UNP O66529
JF	44	SER	-	linker	UNP O66529
JF	45	MET	-	linker	UNP O66529
JF	46	GLU	-	linker	UNP O66529
KF	1	MET	-	initiating methionine	UNP O66529
KF	37	GLY	-	linker	UNP O66529
KF	38	THR	-	linker	UNP O66529
KF	39	GLY	-	linker	UNP O66529
KF	40	GLY	-	linker	UNP O66529
KF	41	SER	-	linker	UNP O66529
KF	42	GLY	-	linker	UNP O66529
KF	43	SER	-	linker	UNP O66529
KF	44	SER	-	linker	UNP O66529
KF	45	MET	-	linker	UNP O66529
KF	46	GLU	-	linker	UNP O66529
LF	1	MET	-	initiating methionine	UNP O66529
LF	37	GLY	-	linker	UNP O66529
LF	38	THR	-	linker	UNP O66529
LF	39	GLY	-	linker	UNP O66529
LF	40	GLY	-	linker	UNP O66529
LF	41	SER	-	linker	UNP O66529
LF	42	GLY	-	linker	UNP O66529
LF	43	SER	-	linker	UNP O66529
LF	44	SER	-	linker	UNP O66529
LF	45	MET	-	linker	UNP O66529
LF	46	GLU	-	linker	UNP O66529
MF	1	MET	-	initiating methionine	UNP O66529
MF	37	GLY	-	linker	UNP O66529
MF	38	THR	-	linker	UNP O66529
MF	39	GLY	-	linker	UNP O66529
MF	40	GLY	-	linker	UNP O66529
MF	41	SER	-	linker	UNP O66529
MF	42	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
MF	43	SER	-	linker	UNP O66529
MF	44	SER	-	linker	UNP O66529
MF	45	MET	-	linker	UNP O66529
MF	46	GLU	-	linker	UNP O66529
NF	1	MET	-	initiating methionine	UNP O66529
NF	37	GLY	-	linker	UNP O66529
NF	38	THR	-	linker	UNP O66529
NF	39	GLY	-	linker	UNP O66529
NF	40	GLY	-	linker	UNP O66529
NF	41	SER	-	linker	UNP O66529
NF	42	GLY	-	linker	UNP O66529
NF	43	SER	-	linker	UNP O66529
NF	44	SER	-	linker	UNP O66529
NF	45	MET	-	linker	UNP O66529
NF	46	GLU	-	linker	UNP O66529
OF	1	MET	-	initiating methionine	UNP O66529
OF	37	GLY	-	linker	UNP O66529
OF	38	THR	-	linker	UNP O66529
OF	39	GLY	-	linker	UNP O66529
OF	40	GLY	-	linker	UNP O66529
OF	41	SER	-	linker	UNP O66529
OF	42	GLY	-	linker	UNP O66529
OF	43	SER	-	linker	UNP O66529
OF	44	SER	-	linker	UNP O66529
OF	45	MET	-	linker	UNP O66529
OF	46	GLU	-	linker	UNP O66529
PF	1	MET	-	initiating methionine	UNP O66529
PF	37	GLY	-	linker	UNP O66529
PF	38	THR	-	linker	UNP O66529
PF	39	GLY	-	linker	UNP O66529
PF	40	GLY	-	linker	UNP O66529
PF	41	SER	-	linker	UNP O66529
PF	42	GLY	-	linker	UNP O66529
PF	43	SER	-	linker	UNP O66529
PF	44	SER	-	linker	UNP O66529
PF	45	MET	-	linker	UNP O66529
PF	46	GLU	-	linker	UNP O66529
QF	1	MET	-	initiating methionine	UNP O66529
QF	37	GLY	-	linker	UNP O66529
QF	38	THR	-	linker	UNP O66529
QF	39	GLY	-	linker	UNP O66529
QF	40	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
QF	41	SER	-	linker	UNP O66529
QF	42	GLY	-	linker	UNP O66529
QF	43	SER	-	linker	UNP O66529
QF	44	SER	-	linker	UNP O66529
QF	45	MET	-	linker	UNP O66529
QF	46	GLU	-	linker	UNP O66529
RF	1	MET	-	initiating methionine	UNP O66529
RF	37	GLY	-	linker	UNP O66529
RF	38	THR	-	linker	UNP O66529
RF	39	GLY	-	linker	UNP O66529
RF	40	GLY	-	linker	UNP O66529
RF	41	SER	-	linker	UNP O66529
RF	42	GLY	-	linker	UNP O66529
RF	43	SER	-	linker	UNP O66529
RF	44	SER	-	linker	UNP O66529
RF	45	MET	-	linker	UNP O66529
RF	46	GLU	-	linker	UNP O66529
SF	1	MET	-	initiating methionine	UNP O66529
SF	37	GLY	-	linker	UNP O66529
SF	38	THR	-	linker	UNP O66529
SF	39	GLY	-	linker	UNP O66529
SF	40	GLY	-	linker	UNP O66529
SF	41	SER	-	linker	UNP O66529
SF	42	GLY	-	linker	UNP O66529
SF	43	SER	-	linker	UNP O66529
SF	44	SER	-	linker	UNP O66529
SF	45	MET	-	linker	UNP O66529
SF	46	GLU	-	linker	UNP O66529
TF	1	MET	-	initiating methionine	UNP O66529
TF	37	GLY	-	linker	UNP O66529
TF	38	THR	-	linker	UNP O66529
TF	39	GLY	-	linker	UNP O66529
TF	40	GLY	-	linker	UNP O66529
TF	41	SER	-	linker	UNP O66529
TF	42	GLY	-	linker	UNP O66529
TF	43	SER	-	linker	UNP O66529
TF	44	SER	-	linker	UNP O66529
TF	45	MET	-	linker	UNP O66529
TF	46	GLU	-	linker	UNP O66529
UF	1	MET	-	initiating methionine	UNP O66529
UF	37	GLY	-	linker	UNP O66529
UF	38	THR	-	linker	UNP O66529

Continued on next page...

Continued from previous page...

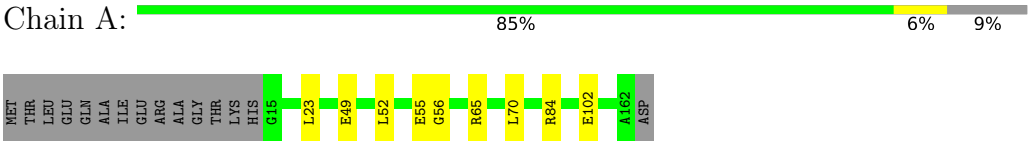
Chain	Residue	Modelled	Actual	Comment	Reference
UF	39	GLY	-	linker	UNP O66529
UF	40	GLY	-	linker	UNP O66529
UF	41	SER	-	linker	UNP O66529
UF	42	GLY	-	linker	UNP O66529
UF	43	SER	-	linker	UNP O66529
UF	44	SER	-	linker	UNP O66529
UF	45	MET	-	linker	UNP O66529
UF	46	GLU	-	linker	UNP O66529
VF	1	MET	-	initiating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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

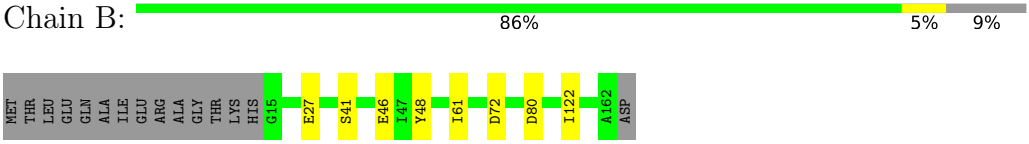
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain A:



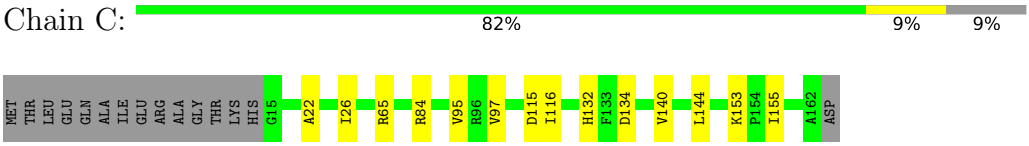
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B:



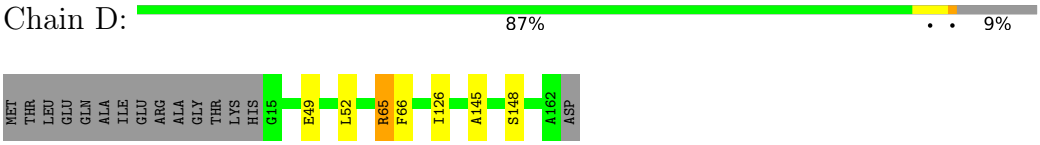
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain C:



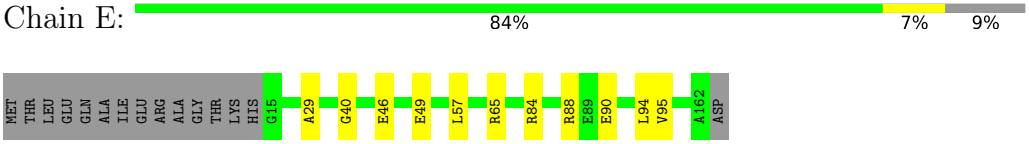
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain D:



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

Chain E:

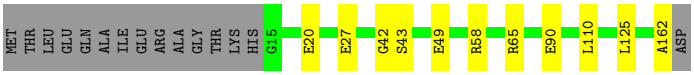


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain F:

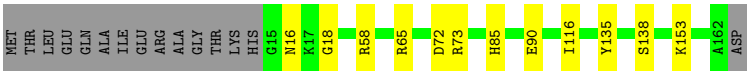
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain G:



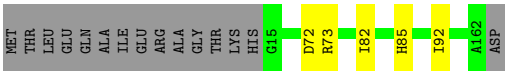
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain H:



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

Chain I:

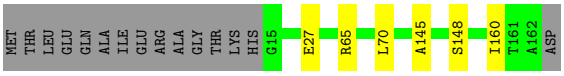


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain J:

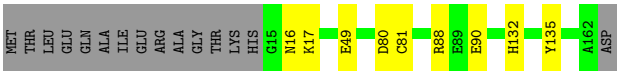
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain K:



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

Chain L:

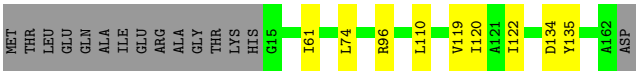


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain M:

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

Chain N:



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

Chain O:

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

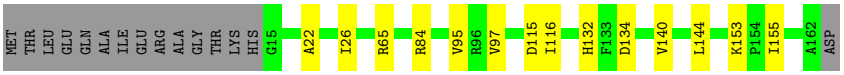
Chain P:

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

Chain Q:

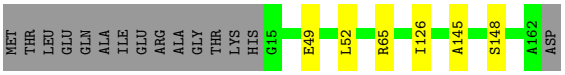
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain R:



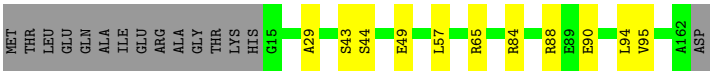
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain S:



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

Chain T:

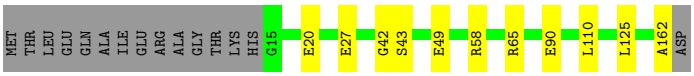


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain U:

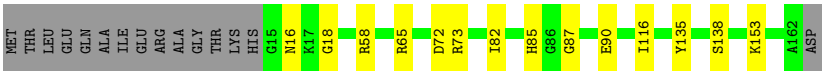
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain V:



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

Chain W:

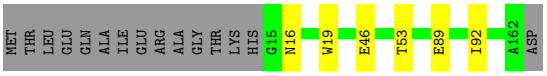


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain X:

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

Chain Y:

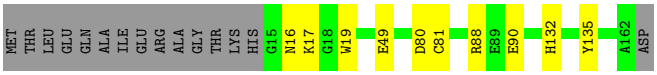


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain Z:

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

Chain AA:

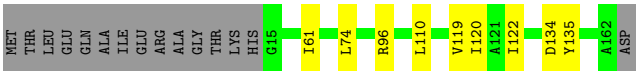


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BA:

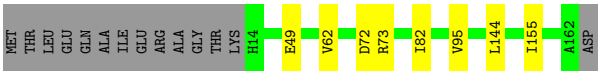
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CA:



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

Chain DA:



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

Chain EA:

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

Chain FA:

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

Chain GA:

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

Chain HA:

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

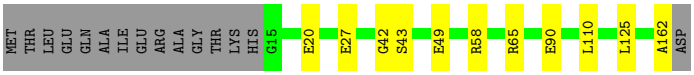
Chain IA:

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

Chain JA:

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

Chain KA:

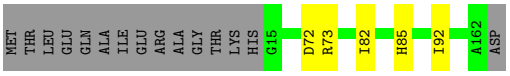


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LA:

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

Chain MA:

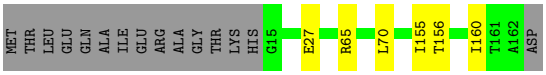


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NA:

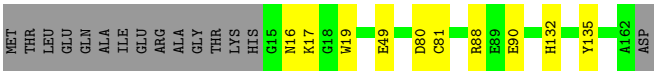
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OA:



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

Chain PA:



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

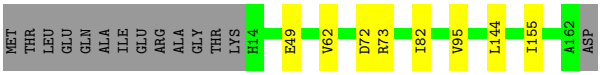
Chain QA:

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

Chain RA:

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

Chain SA:



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

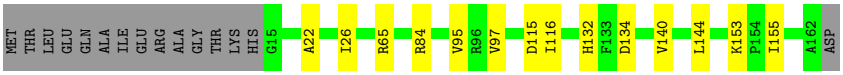
Chain TA:

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

Chain UA:

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

Chain VA:



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

Chain WA:

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

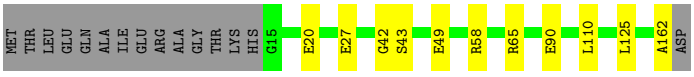
Chain XA:

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

Chain YA:

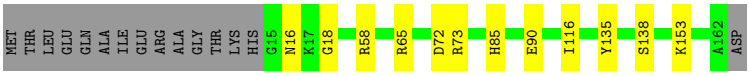
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZA:



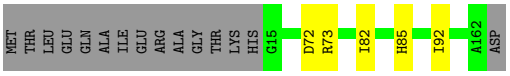
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AB:



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

Chain BB:



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

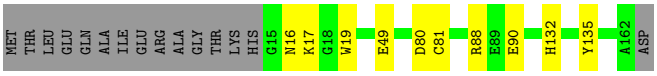
Chain CB:

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

Chain DB:

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

Chain EB:



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

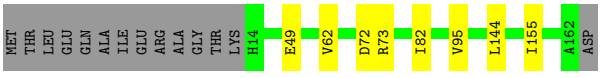
Chain FB:

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

Chain GB:

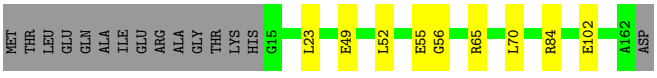
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HB:



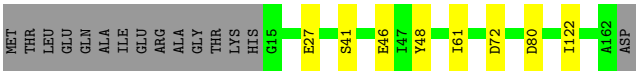
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IB:



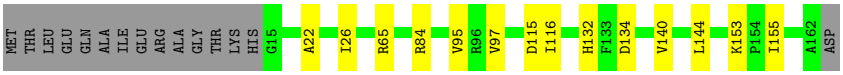
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JB:



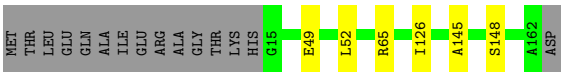
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KB:



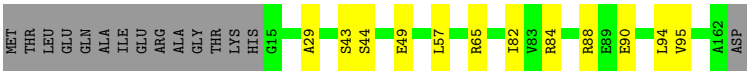
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LB:



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

Chain MB:

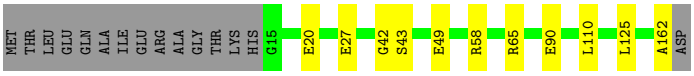


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NB:

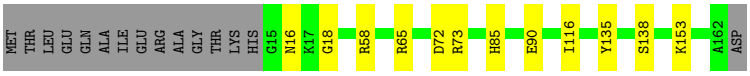
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OB:



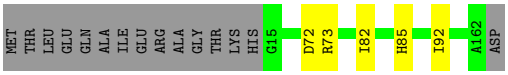
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain PB:



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

Chain QB:



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

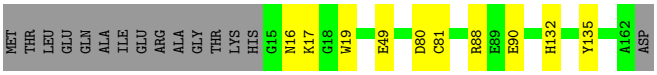
Chain RB:

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

Chain SB:

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

Chain TB:

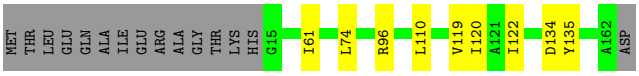


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UB:

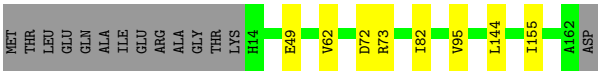
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain VB:



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

Chain WB:

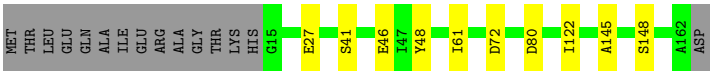


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XB:

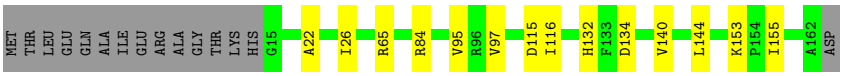
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YB:



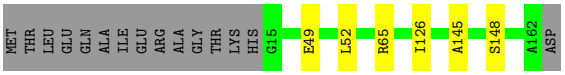
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZB:



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

Chain AC:



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

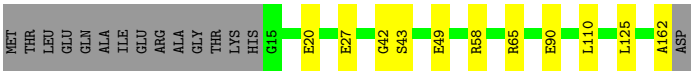
Chain BC:

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

Chain CC:

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

Chain DC:

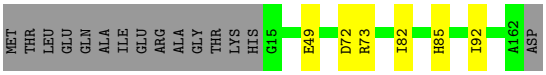


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EC:

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

Chain FC:

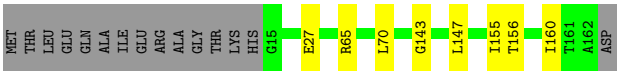


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GC:

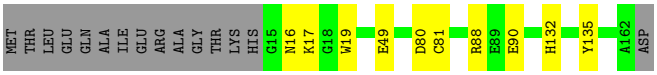
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HC:



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

Chain IC:

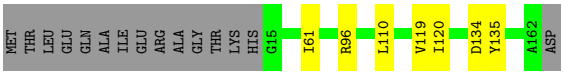


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JC:

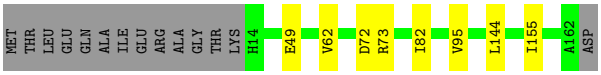
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KC:



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

Chain LC:

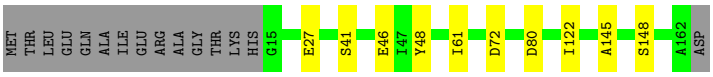


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MC:

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

Chain NC:



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

Chain OC:

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

Chain PC:

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

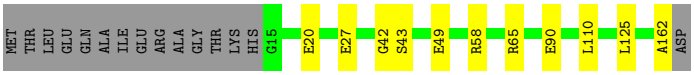
Chain QC:

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

Chain RC:

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

Chain SC:

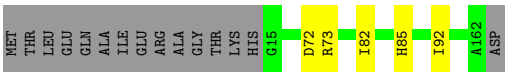


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TC:

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

Chain UC:



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

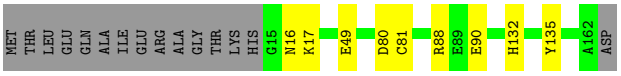
Chain VC:

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

Chain WC:

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

Chain XC:

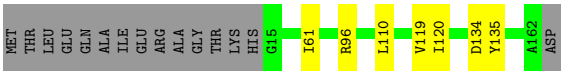


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YC:

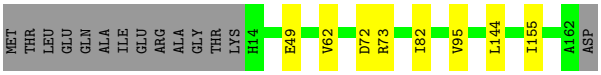
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZC:



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

Chain AD:

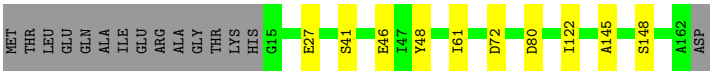


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BD:

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

Chain CD:

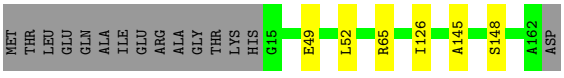


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DD:

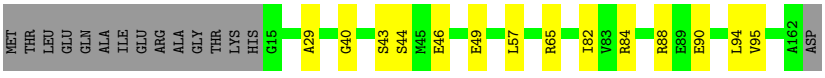
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ED:



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

Chain FD:

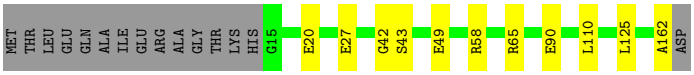


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GD:

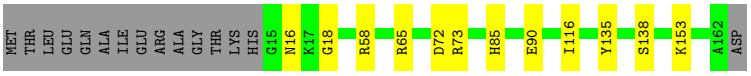
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HD:



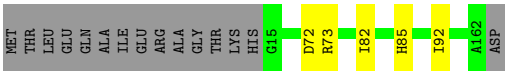
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ID:



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

Chain JD:

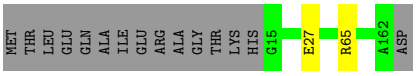


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KD:

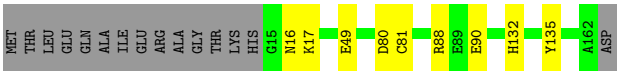
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LD:



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

Chain MD:

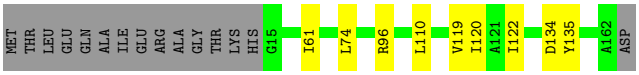


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ND:

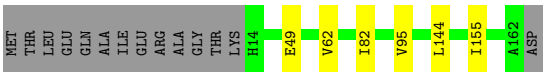
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OD:



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

Chain PD:

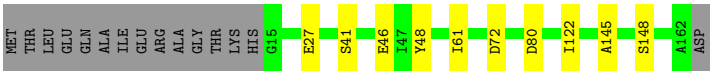


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain QD:

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

Chain RD:

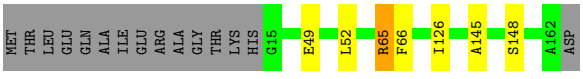


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain SD:

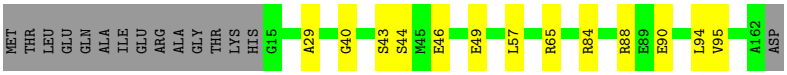
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TD:



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

Chain UD:

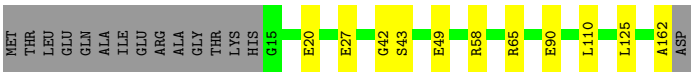


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain VD:

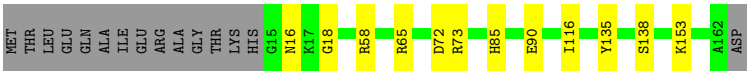
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WD:



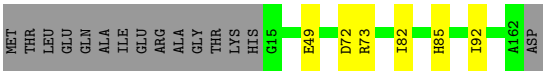
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XD:



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

Chain YD:

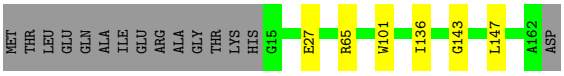


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZD:

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

Chain AE:



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

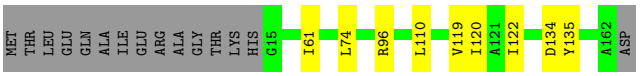
Chain BE:

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

Chain CE:

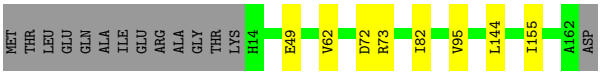
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DE:



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

Chain EE:



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

Chain FE:

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

Chain GE:

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

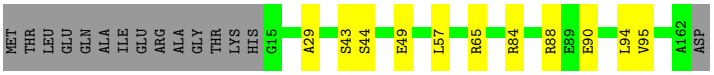
Chain HE:

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

Chain IE:

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

Chain JE:

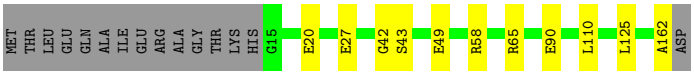


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KE:

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

Chain LE:

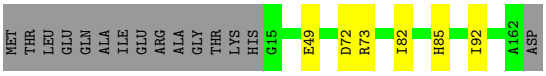


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ME:

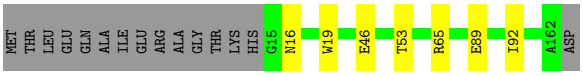
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NE:



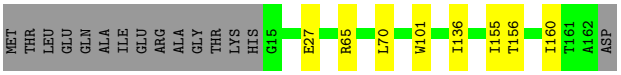
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OE:



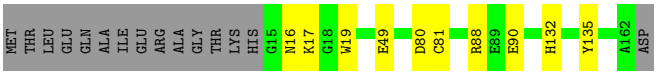
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain PE:



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

Chain QE:

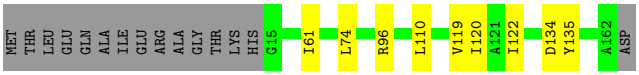


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain RE:

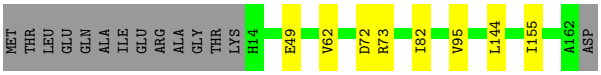
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain SE:



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

Chain TE:

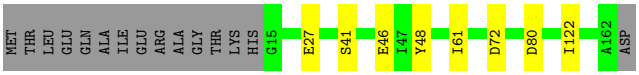


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UE:

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

Chain VE:

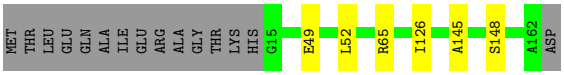


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WE:

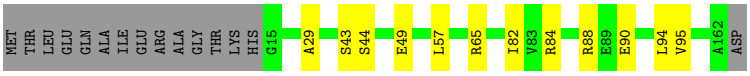
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XE:



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

Chain YE:

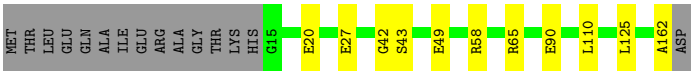


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZE:

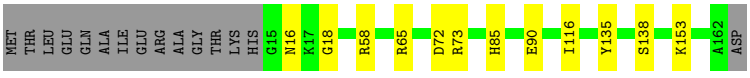
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AF:



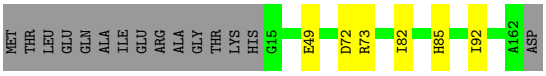
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BF:



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

Chain CF:



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

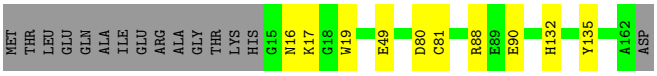
Chain DF:

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

Chain EF:

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

Chain FF:

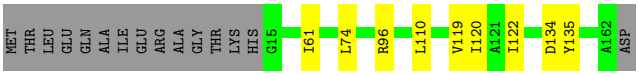


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GF:

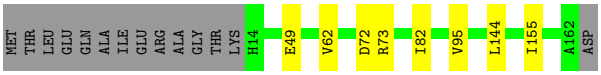
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HF:



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

Chain IF:



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

Chain JF:

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

Chain KF:

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

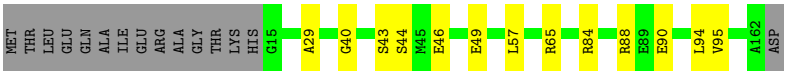
Chain LF:

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

Chain MF:

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

Chain NF:

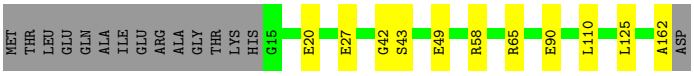


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OF:

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

Chain PF:

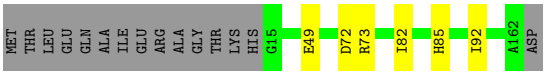


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain QF:

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

Chain RF:

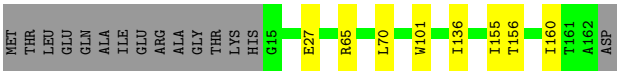


• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain SF:

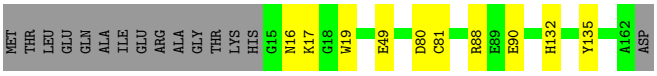
• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TF:



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

Chain UF:



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

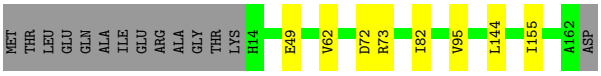
Chain VF:

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

Chain WF:

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

Chain XF:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	22183	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	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	0.24	0/1125	0.53	0/1519
1	AA	0.24	0/1125	0.52	0/1519
1	AB	0.24	0/1125	0.52	0/1519
1	AC	0.25	0/1125	0.53	0/1519
1	AD	0.24	0/1136	0.51	0/1534
1	AE	0.24	0/1125	0.53	0/1519
1	AF	0.25	0/1125	0.53	0/1519
1	B	0.24	0/1125	0.51	0/1519
1	BA	0.24	0/1125	0.52	0/1519
1	BB	0.24	0/1125	0.53	0/1519
1	BC	0.24	0/1125	0.52	0/1519
1	BD	0.24	0/1125	0.53	0/1519
1	BE	0.24	0/1125	0.52	0/1519
1	BF	0.24	0/1125	0.52	0/1519
1	C	0.24	0/1125	0.52	0/1519
1	CA	0.24	0/1125	0.53	0/1519
1	CB	0.24	0/1125	0.54	0/1519
1	CC	0.23	0/1125	0.50	0/1519
1	CD	0.24	0/1125	0.52	0/1519
1	CE	0.24	0/1125	0.52	0/1519
1	CF	0.24	0/1125	0.53	0/1519
1	D	0.25	0/1125	0.53	0/1519
1	DA	0.24	0/1136	0.51	0/1534
1	DB	0.24	0/1125	0.53	0/1519
1	DC	0.25	0/1125	0.53	0/1519
1	DD	0.24	0/1125	0.52	0/1519
1	DE	0.24	0/1125	0.53	0/1519
1	DF	0.24	0/1125	0.54	0/1519
1	E	0.24	0/1125	0.52	0/1519
1	EA	0.24	0/1125	0.53	0/1519
1	EB	0.24	0/1125	0.51	0/1519
1	EC	0.24	0/1125	0.52	0/1519
1	ED	0.25	0/1125	0.53	0/1519
1	EE	0.24	0/1136	0.51	0/1534

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	EF	0.24	0/1125	0.53	0/1519
1	F	0.24	0/1125	0.50	0/1519
1	FA	0.24	0/1125	0.51	0/1519
1	FB	0.24	0/1125	0.52	0/1519
1	FC	0.24	0/1125	0.53	0/1519
1	FD	0.24	0/1125	0.52	0/1519
1	FE	0.24	0/1125	0.53	0/1519
1	FF	0.24	0/1125	0.52	0/1519
1	G	0.25	0/1125	0.53	0/1519
1	GA	0.24	0/1125	0.52	0/1519
1	GB	0.25	0/1125	0.53	0/1519
1	GC	0.24	0/1125	0.54	0/1519
1	GD	0.24	0/1125	0.51	0/1519
1	GE	0.24	0/1125	0.51	0/1519
1	GF	0.24	0/1125	0.52	0/1519
1	H	0.24	0/1125	0.52	0/1519
1	HA	0.25	0/1125	0.53	0/1519
1	HB	0.24	0/1136	0.51	0/1534
1	HC	0.24	0/1125	0.53	0/1519
1	HD	0.25	0/1125	0.53	0/1519
1	HE	0.24	0/1125	0.52	0/1519
1	HF	0.24	0/1125	0.53	0/1519
1	I	0.24	0/1125	0.53	0/1519
1	IA	0.24	0/1125	0.52	0/1519
1	IB	0.24	0/1125	0.53	0/1519
1	IC	0.24	0/1125	0.52	0/1519
1	ID	0.24	0/1125	0.52	0/1519
1	IE	0.25	0/1125	0.53	0/1519
1	IF	0.24	0/1136	0.51	0/1534
1	J	0.24	0/1125	0.54	0/1519
1	JA	0.24	0/1125	0.51	0/1519
1	JB	0.24	0/1125	0.51	0/1519
1	JC	0.24	0/1125	0.52	0/1519
1	JD	0.24	0/1125	0.53	0/1519
1	JE	0.24	0/1125	0.52	0/1519
1	JF	0.24	0/1125	0.53	0/1519
1	K	0.24	0/1125	0.53	0/1519
1	KA	0.25	0/1125	0.53	0/1519
1	KB	0.24	0/1125	0.52	0/1519
1	KC	0.25	0/1125	0.53	0/1519
1	KD	0.24	0/1125	0.54	0/1519
1	KE	0.24	0/1125	0.50	0/1519
1	KF	0.24	0/1125	0.52	0/1519

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	L	0.23	0/1125	0.51	0/1519
1	LA	0.24	0/1125	0.52	0/1519
1	LB	0.25	0/1125	0.53	0/1519
1	LC	0.24	0/1136	0.51	0/1534
1	LD	0.24	0/1125	0.53	0/1519
1	LE	0.25	0/1125	0.53	0/1519
1	LF	0.24	0/1125	0.52	0/1519
1	M	0.24	0/1125	0.52	0/1519
1	MA	0.24	0/1125	0.53	0/1519
1	MB	0.24	0/1125	0.52	0/1519
1	MC	0.24	0/1125	0.53	0/1519
1	MD	0.23	0/1125	0.52	0/1519
1	ME	0.24	0/1125	0.52	0/1519
1	MF	0.25	0/1125	0.53	0/1519
1	N	0.24	0/1125	0.53	0/1519
1	NA	0.24	0/1125	0.54	0/1519
1	NB	0.24	0/1125	0.50	0/1519
1	NC	0.24	0/1125	0.52	0/1519
1	ND	0.24	0/1125	0.52	0/1519
1	NE	0.24	0/1125	0.53	0/1519
1	NF	0.24	0/1125	0.52	0/1519
1	O	0.24	0/1136	0.51	0/1534
1	OA	0.24	0/1125	0.53	0/1519
1	OB	0.25	0/1125	0.53	0/1519
1	OC	0.24	0/1125	0.52	0/1519
1	OD	0.24	0/1125	0.53	0/1519
1	OE	0.24	0/1125	0.54	0/1519
1	OF	0.24	0/1125	0.50	0/1519
1	P	0.24	0/1125	0.53	0/1519
1	PA	0.23	0/1125	0.51	0/1519
1	PB	0.24	0/1125	0.52	0/1519
1	PC	0.25	0/1125	0.53	0/1519
1	PD	0.24	0/1136	0.51	0/1534
1	PE	0.24	0/1125	0.53	0/1519
1	PF	0.25	0/1125	0.53	0/1519
1	Q	0.24	0/1125	0.52	0/1519
1	QA	0.24	0/1125	0.52	0/1519
1	QB	0.24	0/1125	0.53	0/1519
1	QC	0.24	0/1125	0.52	0/1519
1	QD	0.24	0/1125	0.53	0/1519
1	QE	0.23	0/1125	0.51	0/1519
1	QF	0.24	0/1125	0.52	0/1519
1	R	0.24	0/1125	0.52	0/1519

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	RA	0.24	0/1125	0.53	0/1519
1	RB	0.24	0/1125	0.54	0/1519
1	RC	0.23	0/1125	0.50	0/1519
1	RD	0.24	0/1125	0.52	0/1519
1	RE	0.24	0/1125	0.52	0/1519
1	RF	0.24	0/1125	0.53	0/1519
1	S	0.25	0/1125	0.53	0/1519
1	SA	0.24	0/1136	0.51	0/1534
1	SB	0.24	0/1125	0.53	0/1519
1	SC	0.25	0/1125	0.53	0/1519
1	SD	0.24	0/1125	0.52	0/1519
1	SE	0.25	0/1125	0.53	0/1519
1	SF	0.24	0/1125	0.54	0/1519
1	T	0.24	0/1125	0.52	0/1519
1	TA	0.24	0/1125	0.53	0/1519
1	TB	0.24	0/1125	0.51	0/1519
1	TC	0.24	0/1125	0.52	0/1519
1	TD	0.25	0/1125	0.53	0/1519
1	TE	0.24	0/1136	0.51	0/1534
1	TF	0.24	0/1125	0.53	0/1519
1	U	0.23	0/1125	0.50	0/1519
1	UA	0.24	0/1125	0.52	0/1519
1	UB	0.24	0/1125	0.52	0/1519
1	UC	0.24	0/1125	0.53	0/1519
1	UD	0.24	0/1125	0.52	0/1519
1	UE	0.24	0/1125	0.53	0/1519
1	UF	0.24	0/1125	0.51	0/1519
1	V	0.25	0/1125	0.53	0/1519
1	VA	0.24	0/1125	0.52	0/1519
1	VB	0.25	0/1125	0.53	0/1519
1	VC	0.24	0/1125	0.54	0/1519
1	VD	0.24	0/1125	0.50	0/1519
1	VE	0.24	0/1125	0.52	0/1519
1	VF	0.24	0/1125	0.52	0/1519
1	W	0.24	0/1125	0.52	0/1519
1	WA	0.25	0/1125	0.54	0/1519
1	WB	0.24	0/1136	0.51	0/1534
1	WC	0.24	0/1125	0.53	0/1519
1	WD	0.25	0/1125	0.53	0/1519
1	WE	0.24	0/1125	0.52	0/1519
1	WF	0.24	0/1125	0.54	0/1519
1	X	0.24	0/1125	0.53	0/1519
1	XA	0.24	0/1125	0.52	0/1519

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	XB	0.24	0/1125	0.53	0/1519
1	XC	0.23	0/1125	0.52	0/1519
1	XD	0.24	0/1125	0.52	0/1519
1	XE	0.25	0/1125	0.53	0/1519
1	XF	0.24	0/1136	0.51	0/1534
1	Y	0.24	0/1125	0.54	0/1519
1	YA	0.23	0/1125	0.50	0/1519
1	YB	0.24	0/1125	0.52	0/1519
1	YC	0.24	0/1125	0.52	0/1519
1	YD	0.24	0/1125	0.53	0/1519
1	YE	0.24	0/1125	0.52	0/1519
1	Z	0.24	0/1125	0.53	0/1519
1	ZA	0.25	0/1125	0.53	0/1519
1	ZB	0.24	0/1125	0.52	0/1519
1	ZC	0.25	0/1125	0.54	0/1519
1	ZD	0.24	0/1125	0.54	0/1519
1	ZE	0.23	0/1125	0.50	0/1519
All	All	0.24	0/202632	0.52	0/273600

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1108	0	1126	7	0
1	AA	1108	0	1126	6	0
1	AB	1108	0	1126	9	0
1	AC	1108	0	1126	7	0
1	AD	1118	0	1133	5	0
1	AE	1108	0	1126	4	0
1	AF	1108	0	1126	9	0
1	B	1108	0	1126	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	1108	0	1126	7	0
1	BB	1108	0	1126	4	0
1	BC	1108	0	1126	6	0
1	BD	1108	0	1126	7	0
1	BE	1108	0	1126	5	0
1	BF	1108	0	1126	8	0
1	C	1108	0	1126	12	0
1	CA	1108	0	1126	5	0
1	CB	1108	0	1126	5	0
1	CC	1108	0	1126	10	0
1	CD	1108	0	1126	7	0
1	CE	1108	0	1126	7	0
1	CF	1108	0	1126	5	0
1	D	1108	0	1126	5	0
1	DA	1118	0	1133	5	0
1	DB	1108	0	1126	5	0
1	DC	1108	0	1126	9	0
1	DD	1108	0	1126	11	0
1	DE	1108	0	1126	5	0
1	DF	1108	0	1126	4	0
1	E	1108	0	1126	7	0
1	EA	1108	0	1126	7	0
1	EB	1108	0	1126	6	0
1	EC	1108	0	1126	9	0
1	ED	1108	0	1126	8	0
1	EE	1118	0	1133	5	0
1	EF	1108	0	1126	5	0
1	F	1108	0	1126	10	0
1	FA	1108	0	1126	6	0
1	FB	1108	0	1126	8	0
1	FC	1108	0	1126	4	0
1	FD	1108	0	1126	9	0
1	FE	1108	0	1126	7	0
1	FF	1108	0	1126	6	0
1	G	1108	0	1126	9	0
1	GA	1108	0	1126	13	0
1	GB	1108	0	1126	5	0
1	GC	1108	0	1126	6	0
1	GD	1108	0	1126	10	0
1	GE	1108	0	1126	6	0
1	GF	1108	0	1126	8	0
1	H	1108	0	1126	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	HA	1108	0	1126	9	0
1	HB	1118	0	1133	5	0
1	HC	1108	0	1126	5	0
1	HD	1108	0	1126	9	0
1	HE	1108	0	1126	14	0
1	HF	1108	0	1126	5	0
1	I	1108	0	1126	4	0
1	IA	1108	0	1126	6	0
1	IB	1108	0	1126	7	0
1	IC	1108	0	1126	6	0
1	ID	1108	0	1126	8	0
1	IE	1108	0	1126	8	0
1	IF	1118	0	1133	5	0
1	J	1108	0	1126	4	0
1	JA	1108	0	1126	10	0
1	JB	1108	0	1126	6	0
1	JC	1108	0	1126	7	0
1	JD	1108	0	1126	4	0
1	JE	1108	0	1126	7	0
1	JF	1108	0	1126	7	0
1	K	1108	0	1126	4	0
1	KA	1108	0	1126	9	0
1	KB	1108	0	1126	14	0
1	KC	1108	0	1126	4	0
1	KD	1108	0	1126	4	0
1	KE	1108	0	1126	10	0
1	KF	1108	0	1126	7	0
1	L	1108	0	1126	5	0
1	LA	1108	0	1126	8	0
1	LB	1108	0	1126	6	0
1	LC	1118	0	1133	5	0
1	LD	1108	0	1126	2	0
1	LE	1108	0	1126	9	0
1	LF	1108	0	1126	14	0
1	M	1108	0	1126	7	0
1	MA	1108	0	1126	4	0
1	MB	1108	0	1126	8	0
1	MC	1108	0	1126	7	0
1	MD	1108	0	1126	5	0
1	ME	1108	0	1126	9	0
1	MF	1108	0	1126	8	0
1	N	1108	0	1126	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	NA	1108	0	1126	5	0
1	NB	1108	0	1126	10	0
1	NC	1108	0	1126	7	0
1	ND	1108	0	1126	7	0
1	NE	1108	0	1126	5	0
1	NF	1108	0	1126	8	0
1	O	1118	0	1133	5	0
1	OA	1108	0	1126	4	0
1	OB	1108	0	1126	9	0
1	OC	1108	0	1126	15	0
1	OD	1108	0	1126	5	0
1	OE	1108	0	1126	5	0
1	OF	1108	0	1126	10	0
1	P	1108	0	1126	7	0
1	PA	1108	0	1126	6	0
1	PB	1108	0	1126	8	0
1	PC	1108	0	1126	9	0
1	PD	1118	0	1133	4	0
1	PE	1108	0	1126	5	0
1	PF	1108	0	1126	9	0
1	Q	1108	0	1126	7	0
1	QA	1108	0	1126	7	0
1	QB	1108	0	1126	3	0
1	QC	1108	0	1126	9	0
1	QD	1108	0	1126	7	0
1	QE	1108	0	1126	6	0
1	QF	1108	0	1126	9	0
1	R	1108	0	1126	15	0
1	RA	1108	0	1126	5	0
1	RB	1108	0	1126	4	0
1	RC	1108	0	1126	10	0
1	RD	1108	0	1126	7	0
1	RE	1108	0	1126	8	0
1	RF	1108	0	1126	5	0
1	S	1108	0	1126	7	0
1	SA	1118	0	1133	5	0
1	SB	1108	0	1126	5	0
1	SC	1108	0	1126	9	0
1	SD	1108	0	1126	14	0
1	SE	1108	0	1126	5	0
1	SF	1108	0	1126	6	0
1	T	1108	0	1126	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	TA	1108	0	1126	7	0
1	TB	1108	0	1126	6	0
1	TC	1108	0	1126	9	0
1	TD	1108	0	1126	7	0
1	TE	1118	0	1133	5	0
1	TF	1108	0	1126	5	0
1	U	1108	0	1126	10	0
1	UA	1108	0	1126	6	0
1	UB	1108	0	1126	7	0
1	UC	1108	0	1126	3	0
1	UD	1108	0	1126	8	0
1	UE	1108	0	1126	7	0
1	UF	1108	0	1126	6	0
1	V	1108	0	1126	9	0
1	VA	1108	0	1126	12	0
1	VB	1108	0	1126	5	0
1	VC	1108	0	1126	4	0
1	VD	1108	0	1126	10	0
1	VE	1108	0	1126	6	0
1	VF	1108	0	1126	8	0
1	W	1108	0	1126	10	0
1	WA	1108	0	1126	8	0
1	WB	1118	0	1133	5	0
1	WC	1108	0	1126	3	0
1	WD	1108	0	1126	9	0
1	WE	1108	0	1126	15	0
1	WF	1108	0	1126	5	0
1	X	1108	0	1126	3	0
1	XA	1108	0	1126	7	0
1	XB	1108	0	1126	7	0
1	XC	1108	0	1126	5	0
1	XD	1108	0	1126	9	0
1	XE	1108	0	1126	7	0
1	XF	1118	0	1133	5	0
1	Y	1108	0	1126	4	0
1	YA	1108	0	1126	10	0
1	YB	1108	0	1126	7	0
1	YC	1108	0	1126	8	0
1	YD	1108	0	1126	4	0
1	YE	1108	0	1126	8	0
1	Z	1108	0	1126	3	0
1	ZA	1108	0	1126	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	ZB	1108	0	1126	16	0
1	ZC	1108	0	1126	4	0
1	ZD	1108	0	1126	4	0
1	ZE	1108	0	1126	10	0
All	All	199560	0	202764	1028	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (1028) 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:QA:48:TYR:O	1:RA:96:ARG:NH2	2.20	0.75
1:ND:48:TYR:O	1:OD:96:ARG:NH2	2.20	0.75
1:BA:48:TYR:O	1:CA:96:ARG:NH2	2.20	0.75
1:JC:48:TYR:O	1:KC:96:ARG:NH2	2.20	0.75
1:RE:48:TYR:O	1:SE:96:ARG:NH2	2.20	0.75
1:GF:48:TYR:O	1:HF:96:ARG:NH2	2.20	0.74
1:CE:48:TYR:O	1:DE:96:ARG:NH2	2.20	0.74
1:YC:48:TYR:O	1:ZC:96:ARG:NH2	2.20	0.74
1:FB:48:TYR:O	1:GB:96:ARG:NH2	2.20	0.74
1:VF:48:TYR:O	1:WF:96:ARG:NH2	2.20	0.74
1:UB:48:TYR:O	1:VB:96:ARG:NH2	2.20	0.73
1:M:48:TYR:O	1:N:96:ARG:NH2	2.20	0.73
1:QF:116:ILE:O	1:QF:153:LYS:NZ	2.22	0.73
1:TC:116:ILE:O	1:TC:153:LYS:NZ	2.22	0.72
1:ID:116:ILE:O	1:ID:153:LYS:NZ	2.22	0.72
1:BF:116:ILE:O	1:BF:153:LYS:NZ	2.22	0.72
1:ME:116:ILE:O	1:ME:153:LYS:NZ	2.22	0.72
1:PB:116:ILE:O	1:PB:153:LYS:NZ	2.22	0.72
1:W:116:ILE:O	1:W:153:LYS:NZ	2.22	0.72
1:LA:116:ILE:O	1:LA:153:LYS:NZ	2.22	0.72
1:H:116:ILE:O	1:H:153:LYS:NZ	2.22	0.71
1:XD:116:ILE:O	1:XD:153:LYS:NZ	2.22	0.71
1:EC:116:ILE:O	1:EC:153:LYS:NZ	2.22	0.71
1:AB:116:ILE:O	1:AB:153:LYS:NZ	2.22	0.71
1:ZD:16:ASN:OD1	1:ZD:19:TRP:N	2.27	0.68
1:SF:16:ASN:OD1	1:SF:19:TRP:N	2.27	0.68
1:Y:16:ASN:OD1	1:Y:19:TRP:N	2.27	0.68
1:CB:16:ASN:OD1	1:CB:19:TRP:N	2.27	0.68
1:VC:16:ASN:OD1	1:VC:19:TRP:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:ASN:OD1	1:J:19:TRP:N	2.27	0.68
1:OE:16:ASN:OD1	1:OE:19:TRP:N	2.27	0.68
1:RB:16:ASN:OD1	1:RB:19:TRP:N	2.27	0.67
1:FE:55:GLU:OE1	1:FE:56:GLY:N	2.28	0.67
1:DF:16:ASN:OD1	1:DF:19:TRP:N	2.27	0.67
1:UE:55:GLU:OE1	1:UE:56:GLY:N	2.28	0.67
1:P:55:GLU:OE1	1:P:56:GLY:N	2.28	0.67
1:R:115:ASP:OD1	1:R:116:ILE:N	2.28	0.67
1:IB:55:GLU:OE1	1:IB:56:GLY:N	2.28	0.67
1:MC:55:GLU:OE1	1:MC:56:GLY:N	2.28	0.67
1:DD:115:ASP:OD1	1:DD:116:ILE:N	2.28	0.67
1:QD:55:GLU:OE1	1:QD:56:GLY:N	2.28	0.67
1:SD:115:ASP:OD1	1:SD:116:ILE:N	2.28	0.67
1:HE:115:ASP:OD1	1:HE:116:ILE:N	2.28	0.67
1:LF:115:ASP:OD1	1:LF:116:ILE:N	2.28	0.67
1:TA:55:GLU:OE1	1:TA:56:GLY:N	2.28	0.67
1:GC:16:ASN:OD1	1:GC:19:TRP:N	2.27	0.67
1:ZB:115:ASP:OD1	1:ZB:116:ILE:N	2.28	0.67
1:WE:115:ASP:OD1	1:WE:116:ILE:N	2.28	0.67
1:JF:55:GLU:OE1	1:JF:56:GLY:N	2.28	0.67
1:VA:115:ASP:OD1	1:VA:116:ILE:N	2.28	0.67
1:A:49:GLU:OE2	1:F:84:ARG:NH2	2.28	0.67
1:EA:49:GLU:OE2	1:JA:84:ARG:NH2	2.28	0.67
1:EA:55:GLU:OE1	1:EA:56:GLY:N	2.28	0.67
1:NA:16:ASN:OD1	1:NA:19:TRP:N	2.27	0.67
1:KB:115:ASP:OD1	1:KB:116:ILE:N	2.28	0.67
1:BD:55:GLU:OE1	1:BD:56:GLY:N	2.28	0.67
1:QD:49:GLU:OE2	1:VD:84:ARG:NH2	2.28	0.66
1:JF:49:GLU:OE2	1:OF:84:ARG:NH2	2.28	0.66
1:GA:115:ASP:OD1	1:GA:116:ILE:N	2.28	0.66
1:IB:49:GLU:OE2	1:NB:84:ARG:NH2	2.28	0.66
1:XB:49:GLU:OE2	1:CC:84:ARG:NH2	2.28	0.66
1:BD:49:GLU:OE2	1:GD:84:ARG:NH2	2.28	0.66
1:KD:16:ASN:OD1	1:KD:19:TRP:N	2.27	0.66
1:TA:49:GLU:OE2	1:YA:84:ARG:NH2	2.28	0.66
1:OC:115:ASP:OD1	1:OC:116:ILE:N	2.28	0.66
1:C:115:ASP:OD1	1:C:116:ILE:N	2.28	0.66
1:P:49:GLU:OE2	1:U:84:ARG:NH2	2.28	0.65
1:UE:49:GLU:OE2	1:ZE:84:ARG:NH2	2.28	0.65
1:XB:55:GLU:OE1	1:XB:56:GLY:N	2.28	0.65
1:A:55:GLU:OE1	1:A:56:GLY:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MC:49:GLU:OE2	1:RC:84:ARG:NH2	2.28	0.65
1:FE:49:GLU:OE2	1:KE:84:ARG:NH2	2.28	0.65
1:QE:88:ARG:NH2	1:QE:90:GLU:OE1	2.30	0.65
1:UF:88:ARG:NH2	1:UF:90:GLU:OE1	2.30	0.65
1:L:88:ARG:NH2	1:L:90:GLU:OE1	2.30	0.65
1:TB:88:ARG:NH2	1:TB:90:GLU:OE1	2.30	0.65
1:XC:88:ARG:NH2	1:XC:90:GLU:OE1	2.30	0.65
1:BE:88:ARG:NH2	1:BE:90:GLU:OE1	2.30	0.65
1:IC:88:ARG:NH2	1:IC:90:GLU:OE1	2.30	0.64
1:PA:88:ARG:NH2	1:PA:90:GLU:OE1	2.30	0.64
1:MD:88:ARG:NH2	1:MD:90:GLU:OE1	2.30	0.64
1:AA:88:ARG:NH2	1:AA:90:GLU:OE1	2.30	0.64
1:FF:88:ARG:NH2	1:FF:90:GLU:OE1	2.30	0.64
1:H:85:HIS:NE2	1:MA:85:HIS:HE1	1.96	0.64
1:T:88:ARG:NH2	1:T:90:GLU:OE1	2.31	0.64
1:EB:88:ARG:NH2	1:EB:90:GLU:OE1	2.30	0.64
1:FD:88:ARG:NH2	1:FD:90:GLU:OE1	2.31	0.64
1:IA:88:ARG:NH2	1:IA:90:GLU:OE1	2.31	0.64
1:QC:88:ARG:NH2	1:QC:90:GLU:OE1	2.31	0.64
1:MB:88:ARG:NH2	1:MB:90:GLU:OE1	2.31	0.63
1:BC:88:ARG:NH2	1:BC:90:GLU:OE1	2.31	0.63
1:ME:135:TYR:O	1:ME:138:SER:OG	2.15	0.63
1:XA:88:ARG:NH2	1:XA:90:GLU:OE1	2.31	0.63
1:TC:135:TYR:O	1:TC:138:SER:OG	2.15	0.63
1:NF:88:ARG:NH2	1:NF:90:GLU:OE1	2.31	0.63
1:JE:88:ARG:NH2	1:JE:90:GLU:OE1	2.31	0.63
1:YE:88:ARG:NH2	1:YE:90:GLU:OE1	2.31	0.63
1:E:88:ARG:NH2	1:E:90:GLU:OE1	2.31	0.63
1:UD:88:ARG:NH2	1:UD:90:GLU:OE1	2.31	0.62
1:H:135:TYR:O	1:H:138:SER:OG	2.15	0.62
1:BF:135:TYR:O	1:BF:138:SER:OG	2.15	0.62
1:GD:125:LEU:O	1:GD:162:ALA:N	2.33	0.62
1:U:125:LEU:O	1:U:162:ALA:N	2.33	0.61
1:NB:125:LEU:O	1:NB:162:ALA:N	2.33	0.61
1:F:125:LEU:O	1:F:162:ALA:N	2.33	0.61
1:XD:135:TYR:O	1:XD:138:SER:OG	2.15	0.61
1:KE:125:LEU:O	1:KE:162:ALA:N	2.33	0.61
1:YA:125:LEU:O	1:YA:162:ALA:N	2.33	0.61
1:JA:125:LEU:O	1:JA:162:ALA:N	2.33	0.61
1:IB:102:GLU:OE1	1:IB:102:GLU:N	2.34	0.61
1:CC:125:LEU:O	1:CC:162:ALA:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:84:ARG:NH2	1:OA:27:GLU:OE2	2.34	0.61
1:JA:44:SER:N	1:KA:90:GLU:OE1	2.34	0.61
1:QD:102:GLU:N	1:QD:102:GLU:OE1	2.34	0.61
1:A:102:GLU:OE1	1:A:102:GLU:N	2.34	0.61
1:ZB:84:ARG:CG	1:ED:52:LEU:HD13	2.30	0.61
1:BC:84:ARG:NH2	1:HC:27:GLU:OE2	2.34	0.61
1:BD:102:GLU:N	1:BD:102:GLU:OE1	2.34	0.61
1:FE:102:GLU:N	1:FE:102:GLU:OE1	2.34	0.61
1:RC:44:SER:N	1:SC:90:GLU:OE1	2.34	0.61
1:FD:84:ARG:NH2	1:LD:27:GLU:OE2	2.34	0.61
1:KE:44:SER:N	1:LE:90:GLU:OE1	2.34	0.61
1:XD:85:HIS:NE2	1:CF:85:HIS:HE1	1.99	0.61
1:A:84:ARG:NH2	1:F:27:GLU:OE2	2.34	0.61
1:MC:84:ARG:NH2	1:RC:27:GLU:OE2	2.34	0.61
1:UD:84:ARG:NH2	1:AE:27:GLU:OE2	2.34	0.61
1:VD:125:LEU:O	1:VD:162:ALA:N	2.33	0.61
1:B:27:GLU:OE2	1:C:65:ARG:NH2	2.34	0.60
1:EA:102:GLU:OE1	1:EA:102:GLU:N	2.34	0.60
1:FA:27:GLU:OE2	1:GA:65:ARG:NH2	2.34	0.60
1:XB:84:ARG:NH2	1:CC:27:GLU:OE2	2.34	0.60
1:CC:44:SER:N	1:DC:90:GLU:OE1	2.34	0.60
1:ZE:44:SER:N	1:AF:90:GLU:OE1	2.34	0.60
1:JF:84:ARG:NH2	1:OF:27:GLU:OE2	2.34	0.60
1:TA:84:ARG:NH2	1:YA:27:GLU:OE2	2.34	0.60
1:TA:102:GLU:OE1	1:TA:102:GLU:N	2.34	0.60
1:QC:84:ARG:NH2	1:WC:27:GLU:OE2	2.34	0.60
1:RC:125:LEU:O	1:RC:162:ALA:N	2.33	0.60
1:QD:84:ARG:NH2	1:VD:27:GLU:OE2	2.34	0.60
1:VD:44:SER:N	1:WD:90:GLU:OE1	2.34	0.60
1:UE:84:ARG:NH2	1:ZE:27:GLU:OE2	2.34	0.60
1:JF:102:GLU:N	1:JF:102:GLU:OE1	2.34	0.60
1:KF:27:GLU:OE2	1:LF:65:ARG:NH2	2.34	0.60
1:OF:44:SER:N	1:PF:90:GLU:OE1	2.34	0.60
1:OF:125:LEU:O	1:OF:162:ALA:N	2.33	0.60
1:P:102:GLU:N	1:P:102:GLU:OE1	2.34	0.60
1:U:44:SER:N	1:V:90:GLU:OE1	2.34	0.60
1:XA:84:ARG:NH2	1:DB:27:GLU:OE2	2.34	0.60
1:MC:102:GLU:N	1:MC:102:GLU:OE1	2.34	0.60
1:NC:27:GLU:OE2	1:OC:65:ARG:NH2	2.34	0.60
1:JE:84:ARG:NH2	1:PE:27:GLU:OE2	2.34	0.60
1:P:84:ARG:NH2	1:U:27:GLU:OE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XB:102:GLU:OE1	1:XB:102:GLU:N	2.34	0.60
1:TC:85:HIS:NE2	1:RF:85:HIS:HE1	1.99	0.60
1:UE:102:GLU:N	1:UE:102:GLU:OE1	2.34	0.60
1:YE:84:ARG:NH2	1:EF:27:GLU:OE2	2.34	0.60
1:GD:44:SER:N	1:HD:90:GLU:OE1	2.34	0.60
1:ZE:125:LEU:O	1:ZE:162:ALA:N	2.33	0.60
1:YA:44:SER:N	1:ZA:90:GLU:OE1	2.34	0.60
1:ID:135:TYR:O	1:ID:138:SER:OG	2.15	0.60
1:NF:84:ARG:NH2	1:TF:27:GLU:OE2	2.34	0.60
1:F:44:SER:N	1:G:90:GLU:OE1	2.34	0.60
1:V:27:GLU:OE2	1:W:65:ARG:NH2	2.35	0.60
1:MB:84:ARG:NH2	1:SB:27:GLU:OE2	2.34	0.60
1:NB:44:SER:N	1:OB:90:GLU:OE1	2.34	0.60
1:CC:82:ILE:HD12	1:CC:82:ILE:H	1.66	0.60
1:HD:27:GLU:OE2	1:ID:65:ARG:NH2	2.35	0.60
1:F:82:ILE:HD12	1:F:82:ILE:H	1.66	0.60
1:G:27:GLU:OE2	1:H:65:ARG:NH2	2.35	0.60
1:EA:84:ARG:NH2	1:JA:27:GLU:OE2	2.34	0.60
1:ZA:27:GLU:OE2	1:AB:65:ARG:NH2	2.35	0.60
1:E:84:ARG:NH2	1:K:27:GLU:OE2	2.34	0.60
1:BD:84:ARG:NH2	1:GD:27:GLU:OE2	2.34	0.60
1:ZE:82:ILE:HD12	1:ZE:82:ILE:H	1.66	0.60
1:IB:84:ARG:NH2	1:NB:27:GLU:OE2	2.34	0.60
1:OB:27:GLU:OE2	1:PB:65:ARG:NH2	2.35	0.60
1:T:84:ARG:NH2	1:Z:27:GLU:OE2	2.34	0.59
1:U:82:ILE:H	1:U:82:ILE:HD12	1.66	0.59
1:HA:52:LEU:HD13	1:OC:84:ARG:CG	2.32	0.59
1:UA:27:GLU:OE2	1:VA:65:ARG:NH2	2.34	0.59
1:WD:27:GLU:OE2	1:XD:65:ARG:NH2	2.35	0.59
1:LE:27:GLU:OE2	1:ME:65:ARG:NH2	2.35	0.59
1:VE:27:GLU:OE2	1:WE:65:ARG:NH2	2.34	0.59
1:GD:82:ILE:HD12	1:GD:82:ILE:H	1.66	0.59
1:PF:27:GLU:OE2	1:QF:65:ARG:NH2	2.35	0.59
1:SC:27:GLU:OE2	1:TC:65:ARG:NH2	2.35	0.59
1:JA:82:ILE:HD12	1:JA:82:ILE:H	1.66	0.59
1:JB:27:GLU:OE2	1:KB:65:ARG:NH2	2.34	0.59
1:NB:82:ILE:HD12	1:NB:82:ILE:H	1.66	0.59
1:CD:27:GLU:OE2	1:DD:65:ARG:NH2	2.34	0.59
1:FE:84:ARG:NH2	1:KE:27:GLU:OE2	2.34	0.59
1:KE:82:ILE:H	1:KE:82:ILE:HD12	1.66	0.59
1:X:85:HIS:HE1	1:ME:85:HIS:NE2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:85:HIS:NE2	1:NE:85:HIS:HE1	2.00	0.59
1:AF:27:GLU:OE2	1:BF:65:ARG:NH2	2.35	0.59
1:YA:82:ILE:HD12	1:YA:82:ILE:H	1.67	0.59
1:DC:27:GLU:OE2	1:EC:65:ARG:NH2	2.35	0.59
1:YB:27:GLU:OE2	1:ZB:65:ARG:NH2	2.34	0.59
1:RC:82:ILE:HD12	1:RC:82:ILE:H	1.66	0.59
1:OF:82:ILE:H	1:OF:82:ILE:HD12	1.66	0.59
1:R:84:ARG:CG	1:PC:52:LEU:HD13	2.33	0.58
1:QF:135:TYR:O	1:QF:138:SER:OG	2.15	0.58
1:KA:27:GLU:OE2	1:LA:65:ARG:NH2	2.35	0.58
1:Q:27:GLU:OE2	1:R:65:ARG:NH2	2.34	0.58
1:W:135:TYR:O	1:W:138:SER:OG	2.15	0.58
1:RD:27:GLU:OE2	1:SD:65:ARG:NH2	2.34	0.58
1:EC:135:TYR:O	1:EC:138:SER:OG	2.15	0.58
1:JD:85:HIS:HE1	1:QF:85:HIS:NE2	2.01	0.58
1:QB:85:HIS:HE1	1:BF:85:HIS:NE2	2.01	0.58
1:JC:55:GLU:OE1	1:JC:55:GLU:N	2.37	0.58
1:FB:55:GLU:OE1	1:FB:55:GLU:N	2.37	0.58
1:QA:55:GLU:N	1:QA:55:GLU:OE1	2.37	0.58
1:ID:16:ASN:OD1	1:ID:18:GLY:N	2.37	0.58
1:UB:55:GLU:OE1	1:UB:55:GLU:N	2.37	0.58
1:LA:16:ASN:OD1	1:LA:18:GLY:N	2.37	0.58
1:BF:16:ASN:OD1	1:BF:18:GLY:N	2.37	0.58
1:BA:55:GLU:OE1	1:BA:55:GLU:N	2.37	0.58
1:LA:135:TYR:O	1:LA:138:SER:OG	2.15	0.58
1:PB:135:TYR:O	1:PB:138:SER:OG	2.15	0.58
1:EC:16:ASN:OD1	1:EC:18:GLY:N	2.37	0.58
1:YC:55:GLU:OE1	1:YC:55:GLU:N	2.37	0.58
1:CE:55:GLU:N	1:CE:55:GLU:OE1	2.37	0.58
1:PB:16:ASN:OD1	1:PB:18:GLY:N	2.37	0.57
1:PB:85:HIS:NE2	1:YD:85:HIS:HE1	2.01	0.57
1:ND:55:GLU:N	1:ND:55:GLU:OE1	2.37	0.57
1:VD:82:ILE:HD12	1:VD:82:ILE:H	1.66	0.57
1:QF:16:ASN:OD1	1:QF:18:GLY:N	2.37	0.57
1:VF:55:GLU:N	1:VF:55:GLU:OE1	2.37	0.57
1:W:16:ASN:OD1	1:W:18:GLY:N	2.37	0.57
1:VB:134:ASP:OD1	1:VB:135:TYR:N	2.38	0.57
1:XD:16:ASN:OD1	1:XD:18:GLY:N	2.37	0.57
1:RE:55:GLU:N	1:RE:55:GLU:OE1	2.37	0.57
1:SE:134:ASP:OD1	1:SE:135:TYR:N	2.38	0.57
1:H:16:ASN:OD1	1:H:18:GLY:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:134:ASP:OD1	1:RA:135:TYR:N	2.37	0.57
1:W:85:HIS:NE2	1:BB:85:HIS:HE1	2.01	0.57
1:CA:134:ASP:OD1	1:CA:135:TYR:N	2.38	0.57
1:OD:134:ASP:OD1	1:OD:135:TYR:N	2.38	0.57
1:M:55:GLU:N	1:M:55:GLU:OE1	2.37	0.57
1:HF:134:ASP:OD1	1:HF:135:TYR:N	2.38	0.57
1:WF:134:ASP:OD1	1:WF:135:TYR:N	2.38	0.57
1:N:134:ASP:OD1	1:N:135:TYR:N	2.38	0.57
1:GE:27:GLU:OE2	1:HE:65:ARG:NH2	2.34	0.57
1:GF:55:GLU:N	1:GF:55:GLU:OE1	2.37	0.57
1:ZC:134:ASP:OD1	1:ZC:135:TYR:N	2.38	0.57
1:CD:41:SER:OG	1:CD:46:GLU:OE2	2.23	0.57
1:ME:16:ASN:OD1	1:ME:18:GLY:N	2.37	0.57
1:VE:41:SER:OG	1:VE:46:GLU:OE2	2.23	0.57
1:GB:134:ASP:OD1	1:GB:135:TYR:N	2.38	0.57
1:TC:16:ASN:OD1	1:TC:18:GLY:N	2.37	0.57
1:WA:52:LEU:HD13	1:KB:84:ARG:CG	2.35	0.57
1:AB:16:ASN:OD1	1:AB:18:GLY:N	2.37	0.57
1:AC:52:LEU:HD13	1:SD:84:ARG:CG	2.35	0.57
1:FA:48:TYR:HB2	1:GA:95:VAL:HG12	1.87	0.56
1:HD:42:GLY:O	1:HD:43:SER:OG	2.23	0.56
1:VE:48:TYR:HB2	1:WE:95:VAL:HG12	1.87	0.56
1:I:85:HIS:HE1	1:EC:85:HIS:NE2	2.02	0.56
1:JB:48:TYR:HB2	1:KB:95:VAL:HG12	1.87	0.56
1:DC:42:GLY:O	1:DC:43:SER:OG	2.23	0.56
1:KC:134:ASP:OD1	1:KC:135:TYR:N	2.38	0.56
1:GE:48:TYR:HB2	1:HE:95:VAL:HG12	1.87	0.56
1:IE:52:LEU:HD13	1:LF:84:ARG:CG	2.35	0.56
1:B:48:TYR:HB2	1:C:95:VAL:HG12	1.87	0.56
1:NC:48:TYR:HB2	1:OC:95:VAL:HG12	1.87	0.56
1:DE:134:ASP:OD1	1:DE:135:TYR:N	2.38	0.56
1:KF:48:TYR:HB2	1:LF:95:VAL:HG12	1.87	0.56
1:CD:48:TYR:HB2	1:DD:95:VAL:HG12	1.87	0.56
1:YB:48:TYR:HB2	1:ZB:95:VAL:HG12	1.87	0.56
1:KF:41:SER:OG	1:KF:46:GLU:OE2	2.23	0.56
1:RD:48:TYR:HB2	1:SD:95:VAL:HG12	1.87	0.56
1:UA:48:TYR:HB2	1:VA:95:VAL:HG12	1.87	0.55
1:UC:85:HIS:HE1	1:ID:85:HIS:NE2	2.04	0.55
1:WD:42:GLY:O	1:WD:43:SER:OG	2.23	0.55
1:SC:42:GLY:O	1:SC:43:SER:OG	2.23	0.55
1:LB:49:GLU:OE2	1:MB:65:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:115:ASP:OD1	1:CE:116:ILE:N	2.40	0.55
1:WE:84:ARG:CG	1:MF:52:LEU:HD13	2.36	0.55
1:TD:49:GLU:OE2	1:UD:65:ARG:NH2	2.40	0.55
1:GF:115:ASP:OD1	1:GF:116:ILE:N	2.40	0.55
1:VF:115:ASP:OD1	1:VF:116:ILE:N	2.40	0.55
1:FB:115:ASP:OD1	1:FB:116:ILE:N	2.40	0.55
1:JC:115:ASP:OD1	1:JC:116:ILE:N	2.40	0.55
1:LA:85:HIS:NE2	1:FC:85:HIS:HE1	2.04	0.55
1:FA:41:SER:OG	1:FA:46:GLU:OE2	2.23	0.55
1:Q:48:TYR:HB2	1:R:95:VAL:HG12	1.87	0.54
1:QA:115:ASP:OD1	1:QA:116:ILE:N	2.40	0.54
1:MF:49:GLU:OE2	1:NF:65:ARG:NH2	2.40	0.54
1:BA:115:ASP:OD1	1:BA:116:ILE:N	2.40	0.54
1:UA:41:SER:OG	1:UA:46:GLU:OE2	2.23	0.54
1:YC:115:ASP:OD1	1:YC:116:ILE:N	2.40	0.54
1:OB:42:GLY:O	1:OB:43:SER:OG	2.23	0.54
1:NC:41:SER:OG	1:NC:46:GLU:OE2	2.23	0.54
1:GE:41:SER:OG	1:GE:46:GLU:OE2	2.23	0.54
1:WA:49:GLU:OE2	1:XA:65:ARG:NH2	2.40	0.54
1:RE:115:ASP:OD1	1:RE:116:ILE:N	2.40	0.54
1:M:115:ASP:OD1	1:M:116:ILE:N	2.40	0.54
1:S:52:LEU:HD13	1:GA:84:ARG:CG	2.37	0.54
1:TC:72:ASP:OD1	1:TC:73:ARG:N	2.41	0.54
1:XE:49:GLU:OE2	1:YE:65:ARG:NH2	2.40	0.54
1:ZA:42:GLY:O	1:ZA:43:SER:OG	2.23	0.54
1:AB:72:ASP:OD1	1:AB:73:ARG:N	2.41	0.54
1:ND:115:ASP:OD1	1:ND:116:ILE:N	2.40	0.54
1:HE:84:ARG:CG	1:XE:52:LEU:HD13	2.38	0.54
1:PB:72:ASP:OD1	1:PB:73:ARG:N	2.41	0.54
1:ZB:84:ARG:HG2	1:ED:52:LEU:HD13	1.91	0.54
1:H:72:ASP:OD1	1:H:73:ARG:N	2.41	0.53
1:UB:115:ASP:OD1	1:UB:116:ILE:N	2.40	0.53
1:RD:41:SER:OG	1:RD:46:GLU:OE2	2.23	0.53
1:ME:72:ASP:OD1	1:ME:73:ARG:N	2.41	0.53
1:JB:41:SER:OG	1:JB:46:GLU:OE2	2.23	0.53
1:EC:72:ASP:OD1	1:EC:73:ARG:N	2.41	0.53
1:W:72:ASP:OD1	1:W:73:ARG:N	2.41	0.53
1:AB:135:TYR:O	1:AB:138:SER:OG	2.15	0.53
1:Q:41:SER:OG	1:Q:46:GLU:OE2	2.23	0.53
1:HA:49:GLU:OE2	1:IA:65:ARG:NH2	2.40	0.53
1:DD:84:ARG:CG	1:TD:52:LEU:HD13	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XD:72:ASP:OD1	1:XD:73:ARG:N	2.41	0.53
1:XD:90:GLU:N	1:XD:90:GLU:OE1	2.42	0.53
1:TC:90:GLU:OE1	1:TC:90:GLU:N	2.42	0.53
1:ME:90:GLU:N	1:ME:90:GLU:OE1	2.42	0.53
1:BF:72:ASP:OD1	1:BF:73:ARG:N	2.41	0.53
1:QF:72:ASP:OD1	1:QF:73:ARG:N	2.41	0.53
1:QF:90:GLU:N	1:QF:90:GLU:OE1	2.42	0.53
1:LA:72:ASP:OD1	1:LA:73:ARG:N	2.41	0.53
1:LE:42:GLY:O	1:LE:43:SER:OG	2.23	0.53
1:C:84:ARG:CG	1:LB:52:LEU:HD13	2.39	0.53
1:EC:90:GLU:N	1:EC:90:GLU:OE1	2.42	0.53
1:ID:72:ASP:OD1	1:ID:73:ARG:N	2.41	0.53
1:BF:90:GLU:OE1	1:BF:90:GLU:N	2.42	0.53
1:B:41:SER:OG	1:B:46:GLU:OE2	2.23	0.52
1:PC:49:GLU:OE2	1:QC:65:ARG:NH2	2.40	0.52
1:RD:80:ASP:OD1	1:RD:80:ASP:N	2.43	0.52
1:KA:42:GLY:O	1:KA:43:SER:OG	2.23	0.52
1:VE:80:ASP:N	1:VE:80:ASP:OD1	2.43	0.52
1:B:80:ASP:N	1:B:80:ASP:OD1	2.43	0.52
1:UA:80:ASP:OD1	1:UA:80:ASP:N	2.43	0.52
1:S:49:GLU:OE2	1:T:65:ARG:NH2	2.40	0.52
1:LA:90:GLU:OE1	1:LA:90:GLU:N	2.42	0.52
1:EF:65:ARG:NH2	1:IF:49:GLU:OE2	2.39	0.52
1:H:90:GLU:N	1:H:90:GLU:OE1	2.42	0.52
1:FA:80:ASP:OD1	1:FA:80:ASP:N	2.43	0.52
1:W:90:GLU:N	1:W:90:GLU:OE1	2.42	0.52
1:EB:19:TRP:HE1	1:EB:81:CYS:HG	1.57	0.52
1:ZD:46:GLU:N	1:ZD:46:GLU:OE1	2.43	0.52
1:OE:46:GLU:OE1	1:OE:46:GLU:N	2.43	0.52
1:AB:90:GLU:OE1	1:AB:90:GLU:N	2.42	0.52
1:TB:132:HIS:CE1	1:TB:135:TYR:HH	2.28	0.52
1:VC:46:GLU:N	1:VC:46:GLU:OE1	2.43	0.52
1:LD:65:ARG:NH2	1:PD:49:GLU:OE2	2.39	0.52
1:GE:80:ASP:N	1:GE:80:ASP:OD1	2.43	0.52
1:DF:46:GLU:OE1	1:DF:46:GLU:N	2.43	0.52
1:G:42:GLY:O	1:G:43:SER:OG	2.23	0.52
1:KD:46:GLU:N	1:KD:46:GLU:OE1	2.43	0.52
1:MD:132:HIS:CE1	1:MD:135:TYR:HH	2.28	0.52
1:BE:132:HIS:CE1	1:BE:135:TYR:HH	2.28	0.52
1:RB:46:GLU:N	1:RB:46:GLU:OE1	2.43	0.51
1:CB:46:GLU:N	1:CB:46:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XC:132:HIS:CE1	1:XC:135:TYR:HH	2.28	0.51
1:ED:49:GLU:OE2	1:FD:65:ARG:NH2	2.40	0.51
1:ID:90:GLU:N	1:ID:90:GLU:OE1	2.42	0.51
1:IE:49:GLU:OE2	1:JE:65:ARG:NH2	2.40	0.51
1:AF:49:GLU:OE1	1:BF:65:ARG:NH2	2.42	0.51
1:SF:46:GLU:OE1	1:SF:46:GLU:N	2.43	0.51
1:UF:132:HIS:CE1	1:UF:135:TYR:HH	2.28	0.51
1:Y:46:GLU:OE1	1:Y:46:GLU:N	2.43	0.51
1:NC:80:ASP:OD1	1:NC:80:ASP:N	2.43	0.51
1:AF:42:GLY:O	1:AF:43:SER:OG	2.23	0.51
1:PF:42:GLY:O	1:PF:43:SER:OG	2.23	0.51
1:NA:46:GLU:N	1:NA:46:GLU:OE1	2.43	0.51
1:J:46:GLU:OE1	1:J:46:GLU:N	2.43	0.51
1:AA:132:HIS:CE1	1:AA:135:TYR:HH	2.28	0.51
1:HA:52:LEU:HD13	1:OC:84:ARG:HG3	1.92	0.51
1:Q:80:ASP:N	1:Q:80:ASP:OD1	2.43	0.51
1:GC:46:GLU:N	1:GC:46:GLU:OE1	2.43	0.51
1:YB:41:SER:OG	1:YB:46:GLU:OE2	2.23	0.51
1:AC:49:GLU:OE2	1:BC:65:ARG:NH2	2.40	0.51
1:L:132:HIS:CE1	1:L:135:TYR:HH	2.29	0.51
1:PB:90:GLU:OE1	1:PB:90:GLU:N	2.42	0.51
1:Z:65:ARG:NH2	1:DA:49:GLU:OE2	2.39	0.50
1:UC:82:ILE:HG21	1:UC:92:ILE:HD11	1.94	0.50
1:CD:80:ASP:N	1:CD:80:ASP:OD1	2.43	0.50
1:FF:132:HIS:CE1	1:FF:135:TYR:HH	2.29	0.50
1:YB:80:ASP:OD1	1:YB:80:ASP:N	2.43	0.50
1:FC:82:ILE:HG21	1:FC:92:ILE:HD11	1.94	0.50
1:KF:80:ASP:N	1:KF:80:ASP:OD1	2.43	0.50
1:D:49:GLU:OE2	1:E:65:ARG:NH2	2.40	0.50
1:HD:49:GLU:OE1	1:ID:65:ARG:NH2	2.42	0.50
1:K:65:ARG:NH2	1:O:49:GLU:OE2	2.39	0.50
1:X:82:ILE:HG21	1:X:92:ILE:HD11	1.93	0.50
1:BB:82:ILE:HG21	1:BB:92:ILE:HD11	1.94	0.50
1:MD:80:ASP:OD1	1:MD:81:CYS:N	2.45	0.50
1:YD:82:ILE:HG21	1:YD:92:ILE:HD11	1.94	0.50
1:CF:82:ILE:HG21	1:CF:92:ILE:HD11	1.94	0.50
1:TB:80:ASP:OD1	1:TB:81:CYS:N	2.45	0.50
1:JB:80:ASP:OD1	1:JB:80:ASP:N	2.43	0.50
1:IC:132:HIS:CE1	1:IC:135:TYR:HH	2.29	0.50
1:UF:80:ASP:OD1	1:UF:81:CYS:N	2.45	0.49
1:EB:80:ASP:OD1	1:EB:81:CYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QE:80:ASP:OD1	1:QE:81:CYS:N	2.45	0.49
1:QE:132:HIS:CE1	1:QE:135:TYR:HH	2.29	0.49
1:NE:82:ILE:HG21	1:NE:92:ILE:HD11	1.94	0.49
1:FF:80:ASP:OD1	1:FF:81:CYS:N	2.45	0.49
1:L:80:ASP:OD1	1:L:81:CYS:N	2.45	0.49
1:AA:80:ASP:OD1	1:AA:81:CYS:N	2.45	0.49
1:DE:61:ILE:HD12	1:DE:120:ILE:HG23	1.95	0.49
1:MA:82:ILE:HG21	1:MA:92:ILE:HD11	1.94	0.49
1:GB:61:ILE:HD12	1:GB:120:ILE:HG23	1.95	0.49
1:VB:61:ILE:HD12	1:VB:120:ILE:HG23	1.95	0.49
1:ZB:84:ARG:CG	1:ED:52:LEU:CD1	2.90	0.49
1:XC:80:ASP:OD1	1:XC:81:CYS:N	2.45	0.49
1:HF:61:ILE:HD12	1:HF:120:ILE:HG23	1.95	0.49
1:RF:82:ILE:HG21	1:RF:92:ILE:HD11	1.94	0.49
1:N:61:ILE:HD12	1:N:120:ILE:HG23	1.95	0.49
1:CA:61:ILE:HD12	1:CA:120:ILE:HG23	1.95	0.49
1:ZB:84:ARG:HG3	1:ED:52:LEU:HD13	1.94	0.49
1:EB:132:HIS:CE1	1:EB:135:TYR:HH	2.29	0.49
1:IC:80:ASP:OD1	1:IC:81:CYS:N	2.45	0.49
1:AE:65:ARG:NH2	1:EE:49:GLU:OE2	2.39	0.49
1:AF:110:LEU:HD23	1:AF:110:LEU:O	2.13	0.49
1:PA:132:HIS:CE1	1:PA:135:TYR:HH	2.30	0.49
1:OD:61:ILE:HD12	1:OD:120:ILE:HG23	1.95	0.49
1:V:49:GLU:OE1	1:W:65:ARG:NH2	2.42	0.49
1:PA:80:ASP:OD1	1:PA:81:CYS:N	2.45	0.49
1:QB:82:ILE:HG21	1:QB:92:ILE:HD11	1.94	0.49
1:CC:49:GLU:OE1	1:DC:65:ARG:NH1	2.46	0.49
1:QC:43:SER:O	1:QC:44:SER:OG	2.29	0.49
1:LE:110:LEU:HD23	1:LE:110:LEU:O	2.13	0.49
1:I:82:ILE:HG21	1:I:92:ILE:HD11	1.94	0.48
1:G:49:GLU:OE1	1:H:65:ARG:NH2	2.42	0.48
1:PE:65:ARG:NH2	1:TE:49:GLU:OE2	2.39	0.48
1:JD:82:ILE:HG21	1:JD:92:ILE:HD11	1.94	0.48
1:WD:110:LEU:O	1:WD:110:LEU:HD23	2.13	0.48
1:G:110:LEU:HD23	1:G:110:LEU:O	2.13	0.48
1:ZC:61:ILE:HD12	1:ZC:120:ILE:HG23	1.95	0.48
1:DB:65:ARG:NH2	1:HB:49:GLU:OE2	2.39	0.48
1:OB:110:LEU:O	1:OB:110:LEU:HD23	2.13	0.48
1:V:110:LEU:HD23	1:V:110:LEU:O	2.13	0.48
1:KA:110:LEU:HD23	1:KA:110:LEU:O	2.13	0.48
1:DC:49:GLU:OE1	1:EC:65:ARG:NH2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:110:LEU:O	1:DC:110:LEU:HD23	2.13	0.48
1:KC:61:ILE:HD12	1:KC:120:ILE:HG23	1.95	0.48
1:SC:110:LEU:O	1:SC:110:LEU:HD23	2.13	0.48
1:BE:80:ASP:OD1	1:BE:81:CYS:N	2.45	0.48
1:JA:49:GLU:OE1	1:KA:65:ARG:NH1	2.46	0.48
1:RC:49:GLU:OE1	1:SC:65:ARG:NH1	2.46	0.48
1:AD:62:VAL:HG12	1:AD:95:VAL:CG2	2.44	0.48
1:HD:110:LEU:HD23	1:HD:110:LEU:O	2.13	0.48
1:VD:49:GLU:OE1	1:WD:65:ARG:NH1	2.46	0.48
1:SE:61:ILE:HD12	1:SE:120:ILE:HG23	1.95	0.48
1:KA:49:GLU:OE1	1:LA:65:ARG:NH2	2.42	0.48
1:ZA:110:LEU:HD23	1:ZA:110:LEU:O	2.13	0.48
1:OF:49:GLU:OE1	1:PF:65:ARG:NH1	2.46	0.48
1:D:145:ALA:O	1:D:148:SER:OG	2.32	0.47
1:HC:65:ARG:NH2	1:LC:49:GLU:OE2	2.39	0.47
1:PF:49:GLU:OE1	1:QF:65:ARG:NH2	2.42	0.47
1:EE:62:VAL:HG12	1:EE:95:VAL:CG2	2.44	0.47
1:R:84:ARG:HG3	1:PC:52:LEU:HD13	1.95	0.47
1:HB:62:VAL:HG12	1:HB:95:VAL:CG2	2.44	0.47
1:WB:62:VAL:HG12	1:WB:95:VAL:CG2	2.44	0.47
1:IC:19:TRP:HE1	1:IC:81:CYS:HG	1.61	0.47
1:IF:62:VAL:HG12	1:IF:95:VAL:CG2	2.44	0.47
1:WF:61:ILE:HD12	1:WF:120:ILE:HG23	1.95	0.47
1:LC:62:VAL:HG12	1:LC:95:VAL:CG2	2.44	0.47
1:GD:49:GLU:OE1	1:HD:65:ARG:NH1	2.46	0.47
1:G:20:GLU:N	1:G:20:GLU:OE1	2.48	0.47
1:WE:84:ARG:HG3	1:MF:52:LEU:HD13	1.96	0.47
1:AF:20:GLU:N	1:AF:20:GLU:OE1	2.48	0.47
1:R:84:ARG:HG2	1:PC:52:LEU:HD13	1.96	0.47
1:RA:61:ILE:HD12	1:RA:120:ILE:HG23	1.95	0.47
1:OB:20:GLU:OE1	1:OB:20:GLU:N	2.48	0.47
1:DC:20:GLU:N	1:DC:20:GLU:OE1	2.48	0.47
1:RC:80:ASP:N	1:RC:80:ASP:OD1	2.48	0.47
1:SC:20:GLU:OE1	1:SC:20:GLU:N	2.48	0.47
1:ED:145:ALA:O	1:ED:148:SER:OG	2.32	0.47
1:GD:80:ASP:OD1	1:GD:80:ASP:N	2.48	0.47
1:WD:20:GLU:N	1:WD:20:GLU:OE1	2.48	0.47
1:KE:49:GLU:OE1	1:LE:65:ARG:NH1	2.46	0.47
1:LE:20:GLU:N	1:LE:20:GLU:OE1	2.48	0.47
1:S:145:ALA:O	1:S:148:SER:OG	2.32	0.47
1:NB:49:GLU:OE1	1:OB:65:ARG:NH1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LE:49:GLU:OE1	1:ME:65:ARG:NH2	2.42	0.47
1:O:62:VAL:HG12	1:O:95:VAL:CG2	2.44	0.47
1:R:153:LYS:O	1:R:155:ILE:HD12	2.15	0.47
1:U:49:GLU:OE1	1:V:65:ARG:NH1	2.46	0.47
1:V:20:GLU:N	1:V:20:GLU:OE1	2.48	0.47
1:WA:52:LEU:HD13	1:KB:84:ARG:HG3	1.97	0.47
1:PC:145:ALA:O	1:PC:148:SER:OG	2.32	0.47
1:DD:84:ARG:HG3	1:TD:52:LEU:HD13	1.97	0.47
1:PF:110:LEU:HD23	1:PF:110:LEU:O	2.13	0.47
1:XF:62:VAL:HG12	1:XF:95:VAL:CG2	2.44	0.47
1:DA:62:VAL:HG12	1:DA:95:VAL:CG2	2.44	0.47
1:HA:52:LEU:CD1	1:OC:84:ARG:CG	2.93	0.47
1:JA:80:ASP:OD1	1:JA:80:ASP:N	2.48	0.47
1:ZA:20:GLU:N	1:ZA:20:GLU:OE1	2.48	0.47
1:VD:80:ASP:N	1:VD:80:ASP:OD1	2.48	0.47
1:TE:62:VAL:HG12	1:TE:95:VAL:CG2	2.44	0.47
1:OF:80:ASP:OD1	1:OF:80:ASP:N	2.48	0.47
1:C:84:ARG:HG3	1:LB:52:LEU:HD13	1.96	0.46
1:FA:61:ILE:HD11	1:FA:122:ILE:HD11	1.98	0.46
1:SA:62:VAL:HG12	1:SA:95:VAL:CG2	2.44	0.46
1:MB:43:SER:O	1:MB:44:SER:OG	2.29	0.46
1:YB:61:ILE:HD11	1:YB:122:ILE:HD11	1.98	0.46
1:ZB:153:LYS:O	1:ZB:155:ILE:HD12	2.15	0.46
1:WD:49:GLU:OE1	1:XD:65:ARG:NH2	2.42	0.46
1:Q:61:ILE:HD11	1:Q:122:ILE:HD11	1.98	0.46
1:NB:80:ASP:N	1:NB:80:ASP:OD1	2.48	0.46
1:OC:153:LYS:O	1:OC:155:ILE:HD12	2.15	0.46
1:XC:16:ASN:OD1	1:XC:17:LYS:N	2.47	0.46
1:HD:20:GLU:N	1:HD:20:GLU:OE1	2.48	0.46
1:R:84:ARG:CG	1:PC:52:LEU:CD1	2.94	0.46
1:VA:153:LYS:O	1:VA:155:ILE:HD12	2.15	0.46
1:HE:153:LYS:O	1:HE:155:ILE:HD12	2.15	0.46
1:IE:52:LEU:HD13	1:LF:84:ARG:HG2	1.96	0.46
1:ZE:101:TRP:HE3	1:ZE:136:ILE:HD13	1.81	0.46
1:LF:153:LYS:O	1:LF:155:ILE:HD12	2.15	0.46
1:U:101:TRP:HE3	1:U:136:ILE:HD13	1.81	0.46
1:AC:52:LEU:CD1	1:SD:84:ARG:CG	2.94	0.46
1:PD:62:VAL:HG12	1:PD:95:VAL:CG2	2.44	0.46
1:TD:145:ALA:O	1:TD:148:SER:OG	2.32	0.46
1:YA:80:ASP:OD1	1:YA:80:ASP:N	2.48	0.46
1:ZB:132:HIS:O	1:ZB:132:HIS:ND1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RC:101:TRP:HE3	1:RC:136:ILE:HD13	1.81	0.46
1:SC:49:GLU:OE1	1:TC:65:ARG:NH2	2.42	0.46
1:DD:132:HIS:ND1	1:DD:132:HIS:O	2.49	0.46
1:HE:132:HIS:O	1:HE:132:HIS:ND1	2.49	0.46
1:WE:132:HIS:ND1	1:WE:132:HIS:O	2.49	0.46
1:KA:20:GLU:N	1:KA:20:GLU:OE1	2.48	0.46
1:NB:101:TRP:HE3	1:NB:136:ILE:HD13	1.81	0.46
1:CC:101:TRP:HE3	1:CC:136:ILE:HD13	1.81	0.46
1:DD:153:LYS:O	1:DD:155:ILE:HD12	2.15	0.46
1:KE:101:TRP:HE3	1:KE:136:ILE:HD13	1.81	0.46
1:VE:61:ILE:HD11	1:VE:122:ILE:HD11	1.97	0.46
1:LF:132:HIS:O	1:LF:132:HIS:ND1	2.49	0.46
1:B:61:ILE:HD11	1:B:122:ILE:HD11	1.98	0.46
1:C:132:HIS:O	1:C:132:HIS:ND1	2.49	0.46
1:L:16:ASN:OD1	1:L:17:LYS:N	2.47	0.46
1:HA:52:LEU:HD13	1:OC:84:ARG:HG2	1.97	0.46
1:SD:153:LYS:O	1:SD:155:ILE:HD12	2.15	0.46
1:IE:145:ALA:O	1:IE:148:SER:OG	2.32	0.46
1:QA:82:ILE:O	1:QA:87:GLY:N	2.49	0.46
1:JB:61:ILE:HD11	1:JB:122:ILE:HD11	1.98	0.46
1:TB:19:TRP:HE1	1:TB:81:CYS:HG	1.64	0.46
1:PF:20:GLU:N	1:PF:20:GLU:OE1	2.48	0.46
1:VF:82:ILE:O	1:VF:87:GLY:N	2.49	0.46
1:F:49:GLU:OE1	1:G:65:ARG:NH1	2.46	0.46
1:GA:132:HIS:O	1:GA:132:HIS:ND1	2.49	0.46
1:WA:145:ALA:O	1:WA:148:SER:OG	2.32	0.46
1:TB:16:ASN:OD1	1:TB:17:LYS:N	2.47	0.46
1:RD:61:ILE:HD11	1:RD:122:ILE:HD11	1.97	0.46
1:GF:82:ILE:O	1:GF:87:GLY:N	2.49	0.46
1:KF:61:ILE:HD11	1:KF:122:ILE:HD11	1.97	0.46
1:D:52:LEU:HD13	1:VA:84:ARG:CG	2.46	0.46
1:U:80:ASP:OD1	1:U:80:ASP:N	2.48	0.46
1:BA:82:ILE:O	1:BA:87:GLY:N	2.49	0.46
1:JA:101:TRP:HE3	1:JA:136:ILE:HD13	1.81	0.46
1:AC:52:LEU:HD13	1:SD:84:ARG:HG3	1.96	0.46
1:WE:153:LYS:O	1:WE:155:ILE:HD12	2.15	0.46
1:C:153:LYS:O	1:C:155:ILE:HD12	2.15	0.45
1:VA:132:HIS:O	1:VA:132:HIS:ND1	2.49	0.45
1:KB:153:LYS:O	1:KB:155:ILE:HD12	2.15	0.45
1:F:80:ASP:OD1	1:F:80:ASP:N	2.48	0.45
1:OA:65:ARG:NH2	1:SA:49:GLU:OE2	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:82:ILE:O	1:FB:87:GLY:N	2.49	0.45
1:OC:132:HIS:O	1:OC:132:HIS:ND1	2.49	0.45
1:GD:101:TRP:HE3	1:GD:136:ILE:HD13	1.81	0.45
1:R:132:HIS:O	1:R:132:HIS:ND1	2.49	0.45
1:YA:101:TRP:HE3	1:YA:136:ILE:HD13	1.81	0.45
1:NC:61:ILE:HD11	1:NC:122:ILE:HD11	1.98	0.45
1:CD:61:ILE:HD11	1:CD:122:ILE:HD11	1.98	0.45
1:ND:82:ILE:O	1:ND:87:GLY:N	2.49	0.45
1:GA:153:LYS:O	1:GA:155:ILE:HD12	2.15	0.45
1:UA:61:ILE:HD11	1:UA:122:ILE:HD11	1.98	0.45
1:WA:52:LEU:HD13	1:KB:84:ARG:HG2	1.98	0.45
1:VD:101:TRP:HE3	1:VD:136:ILE:HD13	1.81	0.45
1:KE:80:ASP:OD1	1:KE:80:ASP:N	2.48	0.45
1:ZE:80:ASP:OD1	1:ZE:80:ASP:N	2.48	0.45
1:S:52:LEU:HD13	1:GA:84:ARG:HG2	1.98	0.45
1:YA:49:GLU:OE1	1:ZA:65:ARG:NH1	2.46	0.45
1:KB:132:HIS:O	1:KB:132:HIS:ND1	2.49	0.45
1:AC:52:LEU:HD13	1:SD:84:ARG:HG2	1.97	0.45
1:ED:126:ILE:HG23	1:ED:126:ILE:O	2.17	0.45
1:SD:22:ALA:O	1:SD:26:ILE:HD12	2.17	0.45
1:QE:16:ASN:OD1	1:QE:17:LYS:N	2.47	0.45
1:OF:101:TRP:HE3	1:OF:136:ILE:HD13	1.81	0.45
1:UB:82:ILE:O	1:UB:87:GLY:N	2.49	0.45
1:QC:94:LEU:HD23	1:QC:95:VAL:N	2.32	0.45
1:YC:82:ILE:O	1:YC:87:GLY:N	2.49	0.45
1:SD:132:HIS:O	1:SD:132:HIS:ND1	2.49	0.45
1:GE:61:ILE:HD11	1:GE:122:ILE:HD11	1.98	0.45
1:IE:52:LEU:HD13	1:LF:84:ARG:HG3	1.99	0.45
1:ZE:49:GLU:OE1	1:AF:65:ARG:NH1	2.46	0.45
1:R:22:ALA:O	1:R:26:ILE:HD12	2.17	0.45
1:GA:22:ALA:O	1:GA:26:ILE:HD12	2.17	0.45
1:HA:145:ALA:O	1:HA:148:SER:OG	2.32	0.45
1:LB:145:ALA:O	1:LB:148:SER:OG	2.32	0.45
1:CC:80:ASP:N	1:CC:80:ASP:OD1	2.48	0.45
1:JC:82:ILE:O	1:JC:87:GLY:N	2.49	0.45
1:UD:94:LEU:HD23	1:UD:95:VAL:N	2.32	0.45
1:CE:82:ILE:O	1:CE:87:GLY:N	2.49	0.45
1:YE:94:LEU:HD23	1:YE:95:VAL:N	2.32	0.45
1:E:94:LEU:HD23	1:E:95:VAL:N	2.32	0.45
1:M:82:ILE:O	1:M:87:GLY:N	2.49	0.45
1:TA:23:LEU:HD11	1:TA:52:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:49:GLU:OE1	1:AB:65:ARG:NH2	2.42	0.45
1:IB:23:LEU:HD11	1:IB:52:LEU:HD22	1.99	0.45
1:BD:23:LEU:HD11	1:BD:52:LEU:HD22	1.99	0.45
1:RE:82:ILE:O	1:RE:87:GLY:N	2.49	0.45
1:UE:23:LEU:HD11	1:UE:52:LEU:HD22	1.99	0.45
1:AA:16:ASN:OD1	1:AA:17:LYS:N	2.47	0.45
1:XA:94:LEU:HD23	1:XA:95:VAL:N	2.32	0.45
1:BC:94:LEU:HD23	1:BC:95:VAL:N	2.32	0.45
1:YE:43:SER:O	1:YE:44:SER:OG	2.29	0.45
1:F:101:TRP:HE3	1:F:136:ILE:HD13	1.81	0.45
1:P:23:LEU:HD11	1:P:52:LEU:HD22	1.99	0.45
1:XB:23:LEU:HD11	1:XB:52:LEU:HD22	1.99	0.45
1:ZB:22:ALA:O	1:ZB:26:ILE:HD12	2.17	0.45
1:FD:94:LEU:HD23	1:FD:95:VAL:N	2.32	0.45
1:QD:23:LEU:HD11	1:QD:52:LEU:HD22	1.99	0.45
1:HE:22:ALA:O	1:HE:26:ILE:HD12	2.17	0.45
1:ZA:49:GLU:OE2	1:ZA:49:GLU:HA	2.18	0.44
1:OC:22:ALA:O	1:OC:26:ILE:HD12	2.17	0.44
1:FE:23:LEU:HD11	1:FE:52:LEU:HD22	1.99	0.44
1:WE:22:ALA:O	1:WE:26:ILE:HD12	2.17	0.44
1:C:22:ALA:O	1:C:26:ILE:HD12	2.17	0.44
1:G:49:GLU:HA	1:G:49:GLU:OE2	2.18	0.44
1:T:94:LEU:HD23	1:T:95:VAL:N	2.32	0.44
1:IA:94:LEU:HD23	1:IA:95:VAL:N	2.32	0.44
1:LB:126:ILE:HG23	1:LB:126:ILE:O	2.17	0.44
1:OB:49:GLU:OE1	1:PB:65:ARG:NH2	2.42	0.44
1:DC:49:GLU:OE2	1:DC:49:GLU:HA	2.17	0.44
1:IC:16:ASN:OD1	1:IC:17:LYS:N	2.47	0.44
1:WC:65:ARG:NH2	1:AD:49:GLU:OE2	2.39	0.44
1:MF:126:ILE:O	1:MF:126:ILE:HG23	2.17	0.44
1:S:126:ILE:O	1:S:126:ILE:HG23	2.17	0.44
1:BA:161:THR:OG1	1:BA:162:ALA:N	2.51	0.44
1:WA:126:ILE:HG23	1:WA:126:ILE:O	2.17	0.44
1:GC:89:GLU:HA	1:GC:92:ILE:HD12	2.00	0.44
1:VC:89:GLU:HA	1:VC:92:ILE:HD12	2.00	0.44
1:JE:94:LEU:HD23	1:JE:95:VAL:N	2.32	0.44
1:OE:89:GLU:HA	1:OE:92:ILE:HD12	2.00	0.44
1:NF:94:LEU:HD23	1:NF:95:VAL:N	2.32	0.44
1:RF:49:GLU:OE2	1:SF:65:ARG:NH2	2.43	0.44
1:SF:89:GLU:HA	1:SF:92:ILE:HD12	2.00	0.44
1:PA:16:ASN:OD1	1:PA:17:LYS:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MC:23:LEU:HD11	1:MC:52:LEU:HD22	1.99	0.44
1:DD:22:ALA:O	1:DD:26:ILE:HD12	2.17	0.44
1:HD:49:GLU:HA	1:HD:49:GLU:OE2	2.18	0.44
1:IE:126:ILE:HG23	1:IE:126:ILE:O	2.17	0.44
1:PF:49:GLU:HA	1:PF:49:GLU:OE2	2.18	0.44
1:A:23:LEU:HD11	1:A:52:LEU:HD22	1.99	0.44
1:NA:89:GLU:HA	1:NA:92:ILE:HD12	2.00	0.44
1:VA:22:ALA:O	1:VA:26:ILE:HD12	2.17	0.44
1:KB:22:ALA:O	1:KB:26:ILE:HD12	2.17	0.44
1:UB:161:THR:OG1	1:UB:162:ALA:N	2.51	0.44
1:KD:89:GLU:HA	1:KD:92:ILE:HD12	2.00	0.44
1:WD:49:GLU:OE2	1:WD:49:GLU:HA	2.18	0.44
1:QA:161:THR:OG1	1:QA:162:ALA:N	2.51	0.44
1:XE:145:ALA:O	1:XE:148:SER:OG	2.32	0.44
1:FF:16:ASN:OD1	1:FF:17:LYS:N	2.47	0.44
1:LF:22:ALA:O	1:LF:26:ILE:HD12	2.17	0.44
1:EA:65:ARG:NH2	1:IA:49:GLU:OE2	2.51	0.44
1:OB:49:GLU:OE2	1:OB:49:GLU:HA	2.18	0.44
1:XB:65:ARG:NH2	1:BC:49:GLU:OE2	2.51	0.44
1:MC:65:ARG:NH2	1:QC:49:GLU:OE2	2.51	0.44
1:PC:126:ILE:HG23	1:PC:126:ILE:O	2.17	0.44
1:CF:49:GLU:OE2	1:DF:65:ARG:NH2	2.43	0.44
1:D:126:ILE:O	1:D:126:ILE:HG23	2.17	0.44
1:FC:49:GLU:OE2	1:GC:65:ARG:NH2	2.43	0.44
1:SC:49:GLU:OE2	1:SC:49:GLU:HA	2.18	0.44
1:ZD:89:GLU:HA	1:ZD:92:ILE:HD12	2.00	0.44
1:HE:84:ARG:HG3	1:XE:52:LEU:HD13	2.00	0.44
1:T:29:ALA:HB3	1:T:57:LEU:HD23	2.00	0.44
1:AA:19:TRP:HE1	1:AA:81:CYS:HG	1.64	0.44
1:UA:72:ASP:N	1:UA:72:ASP:OD1	2.51	0.44
1:MB:29:ALA:HB3	1:MB:57:LEU:HD23	2.00	0.44
1:MB:94:LEU:HD23	1:MB:95:VAL:N	2.32	0.44
1:YC:161:THR:OG1	1:YC:162:ALA:N	2.51	0.44
1:RD:72:ASP:OD1	1:RD:72:ASP:N	2.51	0.44
1:GF:161:THR:OG1	1:GF:162:ALA:N	2.51	0.44
1:P:70:LEU:O	1:P:70:LEU:HD23	2.18	0.43
1:TD:126:ILE:HG23	1:TD:126:ILE:O	2.17	0.43
1:CE:161:THR:OG1	1:CE:162:ALA:N	2.51	0.43
1:KF:72:ASP:OD1	1:KF:72:ASP:N	2.51	0.43
1:NF:29:ALA:HB3	1:NF:57:LEU:HD23	2.00	0.43
1:TF:65:ARG:NH2	1:XF:49:GLU:OE2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:72:ASP:N	1:Q:72:ASP:OD1	2.51	0.43
1:V:49:GLU:HA	1:V:49:GLU:OE2	2.18	0.43
1:JA:26:ILE:HD12	1:JA:26:ILE:H	1.84	0.43
1:TA:65:ARG:NH2	1:XA:49:GLU:OE2	2.51	0.43
1:VA:134:ASP:N	1:VA:134:ASP:OD1	2.51	0.43
1:YA:26:ILE:HD12	1:YA:26:ILE:H	1.83	0.43
1:YA:144:LEU:HD11	1:YA:155:ILE:HG21	2.00	0.43
1:AC:126:ILE:HG23	1:AC:126:ILE:O	2.17	0.43
1:UD:43:SER:O	1:UD:44:SER:OG	2.29	0.43
1:FE:65:ARG:NH2	1:JE:49:GLU:OE2	2.51	0.43
1:YE:29:ALA:HB3	1:YE:57:LEU:HD23	2.00	0.43
1:DF:89:GLU:HA	1:DF:92:ILE:HD12	2.00	0.43
1:F:26:ILE:H	1:F:26:ILE:HD12	1.84	0.43
1:R:134:ASP:N	1:R:134:ASP:OD1	2.52	0.43
1:V:42:GLY:O	1:V:43:SER:OG	2.23	0.43
1:EA:23:LEU:HD11	1:EA:52:LEU:HD22	1.99	0.43
1:IA:29:ALA:HB3	1:IA:57:LEU:HD23	2.00	0.43
1:IB:65:ARG:NH2	1:MB:49:GLU:OE2	2.51	0.43
1:JB:72:ASP:OD1	1:JB:72:ASP:N	2.51	0.43
1:NC:72:ASP:OD1	1:NC:72:ASP:N	2.51	0.43
1:RC:26:ILE:HD12	1:RC:26:ILE:H	1.84	0.43
1:BD:65:ARG:NH2	1:FD:49:GLU:OE2	2.51	0.43
1:VD:26:ILE:HD12	1:VD:26:ILE:H	1.83	0.43
1:FE:70:LEU:O	1:FE:70:LEU:HD23	2.18	0.43
1:HE:134:ASP:N	1:HE:134:ASP:OD1	2.51	0.43
1:JE:29:ALA:HB3	1:JE:57:LEU:HD23	2.00	0.43
1:XE:126:ILE:HG23	1:XE:126:ILE:O	2.17	0.43
1:ZE:26:ILE:HD12	1:ZE:26:ILE:H	1.84	0.43
1:A:70:LEU:O	1:A:70:LEU:HD23	2.18	0.43
1:T:43:SER:O	1:T:44:SER:OG	2.29	0.43
1:U:26:ILE:HD12	1:U:26:ILE:H	1.83	0.43
1:XB:70:LEU:HD23	1:XB:70:LEU:O	2.18	0.43
1:CC:26:ILE:HD12	1:CC:26:ILE:H	1.84	0.43
1:CC:144:LEU:HD11	1:CC:155:ILE:HG21	2.01	0.43
1:LE:49:GLU:HA	1:LE:49:GLU:OE2	2.18	0.43
1:RE:161:THR:OG1	1:RE:162:ALA:N	2.51	0.43
1:TA:70:LEU:HD23	1:TA:70:LEU:O	2.18	0.43
1:FB:161:THR:OG1	1:FB:162:ALA:N	2.51	0.43
1:KB:134:ASP:OD1	1:KB:134:ASP:N	2.51	0.43
1:FC:72:ASP:OD1	1:FC:73:ARG:N	2.52	0.43
1:MC:70:LEU:HD23	1:MC:70:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QD:65:ARG:NH2	1:UD:49:GLU:OE2	2.51	0.43
1:YD:72:ASP:OD1	1:YD:73:ARG:N	2.52	0.43
1:IE:52:LEU:CD1	1:LF:84:ARG:CG	2.97	0.43
1:AF:49:GLU:OE2	1:AF:49:GLU:HA	2.18	0.43
1:JF:70:LEU:O	1:JF:70:LEU:HD23	2.18	0.43
1:C:134:ASP:N	1:C:134:ASP:OD1	2.51	0.43
1:X:72:ASP:OD1	1:X:73:ARG:N	2.52	0.43
1:HA:126:ILE:HG23	1:HA:126:ILE:O	2.17	0.43
1:KA:49:GLU:OE2	1:KA:49:GLU:HA	2.18	0.43
1:PA:19:TRP:HE1	1:PA:81:CYS:HG	1.66	0.43
1:IB:70:LEU:HD23	1:IB:70:LEU:O	2.18	0.43
1:NB:26:ILE:HD12	1:NB:26:ILE:H	1.84	0.43
1:KE:26:ILE:H	1:KE:26:ILE:HD12	1.84	0.43
1:UE:65:ARG:NH2	1:YE:49:GLU:OE2	2.51	0.43
1:JF:65:ARG:NH2	1:NF:49:GLU:OE2	2.51	0.43
1:J:89:GLU:HA	1:J:92:ILE:HD12	2.00	0.43
1:MA:72:ASP:OD1	1:MA:73:ARG:N	2.52	0.43
1:BB:72:ASP:OD1	1:BB:73:ARG:N	2.52	0.43
1:BC:29:ALA:HB3	1:BC:57:LEU:HD23	2.00	0.43
1:BD:70:LEU:O	1:BD:70:LEU:HD23	2.18	0.43
1:GD:26:ILE:HD12	1:GD:26:ILE:H	1.84	0.43
1:VD:144:LEU:HD11	1:VD:155:ILE:HG21	2.00	0.43
1:CF:72:ASP:OD1	1:CF:73:ARG:N	2.52	0.43
1:VF:161:THR:OG1	1:VF:162:ALA:N	2.51	0.43
1:P:65:ARG:NH2	1:T:49:GLU:OE2	2.51	0.43
1:R:140:VAL:O	1:R:144:LEU:HD23	2.19	0.43
1:UC:72:ASP:OD1	1:UC:73:ARG:N	2.52	0.43
1:BE:16:ASN:OD1	1:BE:17:LYS:N	2.47	0.43
1:KE:144:LEU:HD11	1:KE:155:ILE:HG21	2.01	0.43
1:UE:70:LEU:HD23	1:UE:70:LEU:O	2.18	0.43
1:RF:72:ASP:OD1	1:RF:73:ARG:N	2.52	0.43
1:ZB:140:VAL:O	1:ZB:144:LEU:HD23	2.19	0.43
1:JC:161:THR:OG1	1:JC:162:ALA:N	2.51	0.43
1:UD:29:ALA:HB3	1:UD:57:LEU:HD23	2.00	0.43
1:LE:125:LEU:O	1:LE:162:ALA:N	2.52	0.43
1:JF:23:LEU:HD11	1:JF:52:LEU:HD22	1.99	0.43
1:OF:26:ILE:H	1:OF:26:ILE:HD12	1.84	0.43
1:I:72:ASP:OD1	1:I:73:ARG:N	2.52	0.43
1:M:161:THR:OG1	1:M:162:ALA:N	2.51	0.43
1:EA:70:LEU:HD23	1:EA:70:LEU:O	2.18	0.43
1:FA:72:ASP:OD1	1:FA:72:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KA:125:LEU:O	1:KA:162:ALA:N	2.52	0.43
1:XA:29:ALA:HB3	1:XA:57:LEU:HD23	2.00	0.43
1:ZB:134:ASP:OD1	1:ZB:134:ASP:N	2.51	0.43
1:OC:140:VAL:O	1:OC:144:LEU:HD23	2.19	0.43
1:RD:145:ALA:O	1:RD:148:SER:OG	2.37	0.43
1:SD:134:ASP:N	1:SD:134:ASP:OD1	2.51	0.43
1:JE:43:SER:O	1:JE:44:SER:OG	2.29	0.43
1:LF:134:ASP:N	1:LF:134:ASP:OD1	2.52	0.43
1:MF:145:ALA:O	1:MF:148:SER:OG	2.32	0.43
1:V:125:LEU:O	1:V:162:ALA:N	2.52	0.42
1:GA:134:ASP:N	1:GA:134:ASP:OD1	2.51	0.42
1:WA:52:LEU:CD1	1:KB:84:ARG:CG	2.97	0.42
1:QB:72:ASP:OD1	1:QB:73:ARG:N	2.52	0.42
1:SC:125:LEU:O	1:SC:162:ALA:N	2.52	0.42
1:JD:72:ASP:OD1	1:JD:73:ARG:N	2.52	0.42
1:ND:161:THR:OG1	1:ND:162:ALA:N	2.51	0.42
1:YD:49:GLU:OE2	1:ZD:65:ARG:NH2	2.43	0.42
1:NE:49:GLU:OE2	1:OE:65:ARG:NH2	2.43	0.42
1:AF:125:LEU:O	1:AF:162:ALA:N	2.52	0.42
1:G:125:LEU:O	1:G:162:ALA:N	2.52	0.42
1:VA:140:VAL:O	1:VA:144:LEU:HD23	2.19	0.42
1:AC:145:ALA:O	1:AC:148:SER:OG	2.32	0.42
1:QD:70:LEU:HD23	1:QD:70:LEU:O	2.18	0.42
1:EE:144:LEU:HD12	1:EE:155:ILE:HG21	2.02	0.42
1:ZE:144:LEU:HD11	1:ZE:155:ILE:HG21	2.01	0.42
1:FF:19:TRP:HE1	1:FF:81:CYS:HG	1.66	0.42
1:OF:144:LEU:HD11	1:OF:155:ILE:HG21	2.01	0.42
1:A:65:ARG:NH2	1:E:49:GLU:OE2	2.51	0.42
1:S:52:LEU:HD13	1:GA:84:ARG:HG3	2.01	0.42
1:SA:144:LEU:HD12	1:SA:155:ILE:HG21	2.02	0.42
1:CB:89:GLU:HA	1:CB:92:ILE:HD12	2.00	0.42
1:HB:144:LEU:HD12	1:HB:155:ILE:HG21	2.02	0.42
1:HD:125:LEU:O	1:HD:162:ALA:N	2.52	0.42
1:CE:83:VAL:HG12	1:CE:87:GLY:O	2.19	0.42
1:TE:144:LEU:HD12	1:TE:155:ILE:HG21	2.02	0.42
1:UF:16:ASN:OD1	1:UF:17:LYS:N	2.47	0.42
1:VF:83:VAL:HG12	1:VF:87:GLY:O	2.20	0.42
1:O:82:ILE:HD12	1:O:82:ILE:H	1.85	0.42
1:O:144:LEU:HD12	1:O:155:ILE:HG21	2.02	0.42
1:U:144:LEU:HD11	1:U:155:ILE:HG21	2.01	0.42
1:Y:89:GLU:HA	1:Y:92:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:82:ILE:HD12	1:DA:82:ILE:H	1.85	0.42
1:QA:83:VAL:HG12	1:QA:87:GLY:O	2.19	0.42
1:KB:140:VAL:O	1:KB:144:LEU:HD23	2.19	0.42
1:NB:144:LEU:HD11	1:NB:155:ILE:HG21	2.01	0.42
1:UB:83:VAL:HG12	1:UB:87:GLY:O	2.20	0.42
1:YB:72:ASP:OD1	1:YB:72:ASP:N	2.51	0.42
1:CD:72:ASP:OD1	1:CD:72:ASP:N	2.51	0.42
1:DD:140:VAL:O	1:DD:144:LEU:HD23	2.19	0.42
1:MD:16:ASN:OD1	1:MD:17:LYS:N	2.47	0.42
1:PD:144:LEU:HD12	1:PD:155:ILE:HG21	2.02	0.42
1:GE:145:ALA:O	1:GE:148:SER:OG	2.37	0.42
1:HE:140:VAL:O	1:HE:144:LEU:HD23	2.19	0.42
1:NE:72:ASP:OD1	1:NE:73:ARG:N	2.52	0.42
1:PF:125:LEU:O	1:PF:162:ALA:N	2.52	0.42
1:C:84:ARG:CG	1:LB:52:LEU:CD1	2.98	0.42
1:F:144:LEU:HD11	1:F:155:ILE:HG21	2.01	0.42
1:OB:125:LEU:O	1:OB:162:ALA:N	2.52	0.42
1:DC:125:LEU:O	1:DC:162:ALA:N	2.52	0.42
1:RC:144:LEU:HD11	1:RC:155:ILE:HG21	2.01	0.42
1:DD:134:ASP:OD1	1:DD:134:ASP:N	2.51	0.42
1:SD:140:VAL:O	1:SD:144:LEU:HD23	2.19	0.42
1:WD:125:LEU:O	1:WD:162:ALA:N	2.52	0.42
1:WE:84:ARG:HG2	1:MF:52:LEU:HD13	2.01	0.42
1:WE:140:VAL:O	1:WE:144:LEU:HD23	2.19	0.42
1:LF:140:VAL:O	1:LF:144:LEU:HD23	2.19	0.42
1:KB:65:ARG:N	1:KB:97:VAL:O	2.52	0.42
1:RB:89:GLU:HA	1:RB:92:ILE:HD12	2.00	0.42
1:JC:83:VAL:HG12	1:JC:87:GLY:O	2.20	0.42
1:IF:82:ILE:HD12	1:IF:82:ILE:H	1.85	0.42
1:E:29:ALA:HB3	1:E:57:LEU:HD23	2.00	0.42
1:CD:145:ALA:O	1:CD:148:SER:OG	2.37	0.42
1:RE:83:VAL:HG12	1:RE:87:GLY:O	2.20	0.42
1:S:52:LEU:CD1	1:GA:84:ARG:CG	2.98	0.42
1:SB:65:ARG:NH2	1:WB:49:GLU:OE2	2.39	0.42
1:ZB:84:ARG:HG3	1:ED:52:LEU:CD1	2.50	0.42
1:LC:144:LEU:HD12	1:LC:155:ILE:HG21	2.02	0.42
1:AD:82:ILE:HD12	1:AD:82:ILE:H	1.85	0.42
1:AD:144:LEU:HD12	1:AD:155:ILE:HG21	2.02	0.42
1:IF:144:LEU:HD12	1:IF:155:ILE:HG21	2.02	0.42
1:XF:144:LEU:HD12	1:XF:155:ILE:HG21	2.02	0.42
1:M:83:VAL:HG12	1:M:87:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GA:140:VAL:O	1:GA:144:LEU:HD23	2.19	0.42
1:JA:144:LEU:HD11	1:JA:155:ILE:HG21	2.01	0.42
1:EB:49:GLU:OE2	1:FB:65:ARG:NH2	2.53	0.42
1:QC:29:ALA:HB3	1:QC:57:LEU:HD23	2.00	0.42
1:WE:84:ARG:CG	1:MF:52:LEU:CD1	2.97	0.42
1:FF:49:GLU:OE2	1:GF:65:ARG:NH2	2.53	0.42
1:Q:145:ALA:O	1:Q:148:SER:OG	2.37	0.42
1:SA:82:ILE:HD12	1:SA:82:ILE:H	1.85	0.42
1:LC:82:ILE:H	1:LC:82:ILE:HD12	1.85	0.42
1:HE:84:ARG:HG2	1:XE:52:LEU:HD13	2.00	0.42
1:QE:49:GLU:OE2	1:RE:65:ARG:NH2	2.53	0.42
1:B:72:ASP:N	1:B:72:ASP:OD1	2.51	0.41
1:EB:16:ASN:OD1	1:EB:17:LYS:N	2.47	0.41
1:WB:82:ILE:HD12	1:WB:82:ILE:H	1.85	0.41
1:FD:29:ALA:HB3	1:FD:57:LEU:HD23	2.00	0.41
1:FD:43:SER:O	1:FD:44:SER:OG	2.29	0.41
1:MD:49:GLU:OE2	1:ND:65:ARG:NH2	2.53	0.41
1:ND:83:VAL:HG12	1:ND:87:GLY:O	2.20	0.41
1:BE:49:GLU:OE2	1:CE:65:ARG:NH2	2.53	0.41
1:HF:110:LEU:HD23	1:HF:119:VAL:HG13	2.02	0.41
1:WF:110:LEU:HD23	1:WF:119:VAL:HG13	2.02	0.41
1:H:85:HIS:NE2	1:MA:85:HIS:CE1	2.83	0.41
1:VA:65:ARG:N	1:VA:97:VAL:O	2.52	0.41
1:ZA:125:LEU:O	1:ZA:162:ALA:N	2.52	0.41
1:GB:110:LEU:HD23	1:GB:119:VAL:HG13	2.02	0.41
1:VB:110:LEU:HD23	1:VB:119:VAL:HG13	2.02	0.41
1:YC:83:VAL:HG12	1:YC:87:GLY:O	2.20	0.41
1:DD:84:ARG:CG	1:TD:52:LEU:CD1	2.98	0.41
1:DE:110:LEU:HD23	1:DE:119:VAL:HG13	2.02	0.41
1:KF:145:ALA:O	1:KF:148:SER:OG	2.37	0.41
1:XF:82:ILE:HD12	1:XF:82:ILE:H	1.85	0.41
1:DA:144:LEU:HD12	1:DA:155:ILE:HG21	2.02	0.41
1:XA:43:SER:O	1:XA:44:SER:OG	2.29	0.41
1:TB:49:GLU:OE2	1:UB:65:ARG:NH2	2.53	0.41
1:YB:145:ALA:O	1:YB:148:SER:OG	2.37	0.41
1:KC:110:LEU:HD23	1:KC:119:VAL:HG13	2.02	0.41
1:UD:40:GLY:N	1:UD:46:GLU:OE2	2.53	0.41
1:UF:19:TRP:HE1	1:UF:81:CYS:HG	1.68	0.41
1:N:110:LEU:HD23	1:N:119:VAL:HG13	2.02	0.41
1:BA:83:VAL:HG12	1:BA:87:GLY:O	2.20	0.41
1:CA:110:LEU:HD23	1:CA:119:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QC:40:GLY:N	1:QC:46:GLU:OE2	2.53	0.41
1:HF:74:LEU:HD23	1:HF:122:ILE:CG2	2.51	0.41
1:WF:74:LEU:HD23	1:WF:122:ILE:CG2	2.51	0.41
1:K:70:LEU:HD23	1:K:160:ILE:HD11	2.03	0.41
1:VC:53:THR:O	1:VC:53:THR:HG23	2.21	0.41
1:GD:144:LEU:HD11	1:GD:155:ILE:HG21	2.01	0.41
1:KD:53:THR:HG23	1:KD:53:THR:O	2.21	0.41
1:OD:110:LEU:HD23	1:OD:119:VAL:HG13	2.02	0.41
1:PE:70:LEU:HD23	1:PE:160:ILE:HD11	2.03	0.41
1:GF:83:VAL:HG12	1:GF:87:GLY:O	2.19	0.41
1:C:140:VAL:O	1:C:144:LEU:HD23	2.19	0.41
1:R:65:ARG:N	1:R:97:VAL:O	2.52	0.41
1:HB:72:ASP:OD1	1:HB:73:ARG:N	2.54	0.41
1:SB:70:LEU:HD23	1:SB:160:ILE:HD11	2.03	0.41
1:ZB:65:ARG:N	1:ZB:97:VAL:O	2.52	0.41
1:IC:49:GLU:OE2	1:JC:65:ARG:NH2	2.53	0.41
1:TC:85:HIS:NE2	1:RF:85:HIS:CE1	2.86	0.41
1:XC:49:GLU:OE2	1:YC:65:ARG:NH2	2.53	0.41
1:OD:74:LEU:HD23	1:OD:122:ILE:CG2	2.51	0.41
1:XD:85:HIS:NE2	1:CF:85:HIS:CE1	2.84	0.41
1:SE:110:LEU:HD23	1:SE:119:VAL:HG13	2.02	0.41
1:WE:134:ASP:OD1	1:WE:134:ASP:N	2.52	0.41
1:UF:49:GLU:OE2	1:VF:65:ARG:NH2	2.53	0.41
1:O:72:ASP:OD1	1:O:73:ARG:N	2.54	0.41
1:Y:53:THR:O	1:Y:53:THR:HG23	2.21	0.41
1:OA:70:LEU:HD23	1:OA:160:ILE:HD11	2.03	0.41
1:PA:49:GLU:OE2	1:QA:65:ARG:NH2	2.53	0.41
1:FB:83:VAL:HG12	1:FB:87:GLY:O	2.19	0.41
1:OC:134:ASP:OD1	1:OC:134:ASP:N	2.51	0.41
1:AD:72:ASP:OD1	1:AD:73:ARG:N	2.54	0.41
1:QE:19:TRP:HE1	1:QE:81:CYS:HG	1.68	0.41
1:TE:82:ILE:HD12	1:TE:82:ILE:H	1.85	0.41
1:SF:53:THR:HG23	1:SF:53:THR:O	2.21	0.41
1:N:74:LEU:HD23	1:N:122:ILE:CG2	2.51	0.41
1:FB:82:ILE:HG21	1:FB:92:ILE:HD11	2.03	0.41
1:WB:72:ASP:OD1	1:WB:73:ARG:N	2.54	0.41
1:WB:144:LEU:HD12	1:WB:155:ILE:HG21	2.02	0.41
1:ZC:110:LEU:HD23	1:ZC:119:VAL:HG13	2.02	0.41
1:SD:26:ILE:HD12	1:SD:26:ILE:H	1.86	0.41
1:EE:72:ASP:OD1	1:EE:73:ARG:N	2.54	0.41
1:EF:70:LEU:HD23	1:EF:160:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NF:40:GLY:N	1:NF:46:GLU:OE2	2.53	0.41
1:NF:43:SER:O	1:NF:44:SER:OG	2.29	0.41
1:AA:49:GLU:OE2	1:BA:65:ARG:NH2	2.53	0.41
1:SA:72:ASP:OD1	1:SA:73:ARG:N	2.54	0.41
1:WA:65:ARG:O	1:WA:66:PHE:C	2.60	0.41
1:DB:70:LEU:HD23	1:DB:160:ILE:HD11	2.03	0.41
1:GB:74:LEU:HD23	1:GB:122:ILE:CG2	2.51	0.41
1:HB:82:ILE:H	1:HB:82:ILE:HD12	1.85	0.41
1:NC:145:ALA:O	1:NC:148:SER:OG	2.37	0.41
1:OC:26:ILE:HD12	1:OC:26:ILE:H	1.86	0.41
1:YC:82:ILE:HG21	1:YC:92:ILE:HD11	2.03	0.41
1:FD:40:GLY:N	1:FD:46:GLU:OE2	2.53	0.41
1:EE:82:ILE:HD12	1:EE:82:ILE:H	1.85	0.41
1:TE:72:ASP:OD1	1:TE:73:ARG:N	2.54	0.41
1:VE:72:ASP:OD1	1:VE:72:ASP:N	2.51	0.41
1:E:40:GLY:N	1:E:46:GLU:OE2	2.53	0.41
1:DA:72:ASP:OD1	1:DA:73:ARG:N	2.54	0.41
1:HA:52:LEU:CD1	1:OC:84:ARG:HG3	2.51	0.41
1:ZB:26:ILE:HD12	1:ZB:26:ILE:H	1.86	0.41
1:ZB:144:LEU:HD12	1:ZB:155:ILE:HG21	2.04	0.41
1:PD:82:ILE:H	1:PD:82:ILE:HD12	1.85	0.41
1:HE:84:ARG:CG	1:XE:52:LEU:CD1	2.99	0.41
1:TF:70:LEU:HD23	1:TF:160:ILE:HD11	2.03	0.41
1:C:65:ARG:N	1:C:97:VAL:O	2.52	0.40
1:L:49:GLU:OE2	1:M:65:ARG:NH2	2.53	0.40
1:NA:30:ASN:ND2	1:NA:51:LYS:O	2.55	0.40
1:RA:74:LEU:HD23	1:RA:122:ILE:CG2	2.51	0.40
1:VA:26:ILE:HD12	1:VA:26:ILE:H	1.86	0.40
1:CB:30:ASN:ND2	1:CB:51:LYS:O	2.55	0.40
1:DB:155:ILE:HG22	1:DB:156:THR:N	2.37	0.40
1:HC:70:LEU:HD23	1:HC:160:ILE:HD11	2.03	0.40
1:SD:144:LEU:HD12	1:SD:155:ILE:HG21	2.04	0.40
1:AE:101:TRP:HB2	1:AE:136:ILE:HG23	2.04	0.40
1:EF:101:TRP:HB2	1:EF:136:ILE:HG23	2.04	0.40
1:IF:72:ASP:OD1	1:IF:73:ARG:N	2.54	0.40
1:I:85:HIS:CE1	1:EC:85:HIS:NE2	2.87	0.40
1:HA:65:ARG:O	1:HA:66:PHE:C	2.60	0.40
1:RA:110:LEU:HD23	1:RA:119:VAL:HG13	2.02	0.40
1:CB:53:THR:HG23	1:CB:53:THR:O	2.21	0.40
1:SB:143:GLY:O	1:SB:147:LEU:HD23	2.22	0.40
1:VB:74:LEU:HD23	1:VB:122:ILE:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:143:GLY:O	1:AE:147:LEU:HD23	2.22	0.40
1:HE:144:LEU:HD12	1:HE:155:ILE:HG21	2.04	0.40
1:WE:26:ILE:HD12	1:WE:26:ILE:H	1.86	0.40
1:WE:144:LEU:HD12	1:WE:155:ILE:HG21	2.04	0.40
1:GF:82:ILE:HG21	1:GF:92:ILE:HD11	2.03	0.40
1:SF:30:ASN:ND2	1:SF:51:LYS:O	2.55	0.40
1:TF:155:ILE:HG22	1:TF:156:THR:N	2.37	0.40
1:VF:82:ILE:HG21	1:VF:92:ILE:HD11	2.03	0.40
1:XF:72:ASP:OD1	1:XF:73:ARG:N	2.54	0.40
1:D:65:ARG:O	1:D:66:PHE:C	2.60	0.40
1:K:145:ALA:O	1:K:148:SER:OG	2.37	0.40
1:NA:53:THR:O	1:NA:53:THR:HG23	2.21	0.40
1:OA:155:ILE:HG22	1:OA:156:THR:N	2.37	0.40
1:KB:144:LEU:HD12	1:KB:155:ILE:HG21	2.04	0.40
1:MB:82:ILE:HD12	1:MB:82:ILE:H	1.87	0.40
1:LC:72:ASP:OD1	1:LC:73:ARG:N	2.54	0.40
1:OC:144:LEU:HD12	1:OC:155:ILE:HG21	2.04	0.40
1:QC:82:ILE:H	1:QC:82:ILE:HD12	1.87	0.40
1:WC:70:LEU:HD23	1:WC:160:ILE:HD11	2.03	0.40
1:DE:74:LEU:HD23	1:DE:122:ILE:CG2	2.51	0.40
1:IE:65:ARG:O	1:IE:66:PHE:C	2.60	0.40
1:PE:101:TRP:HB2	1:PE:136:ILE:HG23	2.04	0.40
1:RE:82:ILE:HG21	1:RE:92:ILE:HD11	2.03	0.40
1:SE:74:LEU:HD23	1:SE:122:ILE:CG2	2.51	0.40
1:WE:41:SER:N	1:WE:46:GLU:OE2	2.50	0.40
1:YE:82:ILE:H	1:YE:82:ILE:HD12	1.87	0.40
1:J:30:ASN:ND2	1:J:51:LYS:O	2.55	0.40
1:R:26:ILE:HD12	1:R:26:ILE:H	1.86	0.40
1:W:85:HIS:NE2	1:BB:85:HIS:CE1	2.87	0.40
1:Z:143:GLY:O	1:Z:147:LEU:HD23	2.22	0.40
1:GA:144:LEU:HD12	1:GA:155:ILE:HG21	2.04	0.40
1:VA:144:LEU:HD12	1:VA:155:ILE:HG21	2.04	0.40
1:SB:101:TRP:HB2	1:SB:136:ILE:HG23	2.04	0.40
1:HC:143:GLY:O	1:HC:147:LEU:HD23	2.22	0.40
1:FD:82:ILE:HD12	1:FD:82:ILE:H	1.87	0.40
1:TD:65:ARG:O	1:TD:66:PHE:C	2.60	0.40
1:HE:26:ILE:HD12	1:HE:26:ILE:H	1.86	0.40
1:PE:155:ILE:HG22	1:PE:156:THR:N	2.37	0.40
1:LF:26:ILE:HD12	1:LF:26:ILE:H	1.86	0.40
1:LF:144:LEU:HD12	1:LF:155:ILE:HG21	2.04	0.40
1:R:84:ARG:HG3	1:PC:52:LEU:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:82:ILE:HG22	1:W:87:GLY:HA3	2.04	0.40
1:CA:74:LEU:HD23	1:CA:122:ILE:CG2	2.51	0.40
1:AB:85:HIS:NE2	1:NE:85:HIS:CE1	2.85	0.40
1:DB:101:TRP:HB2	1:DB:136:ILE:HG23	2.03	0.40
1:RB:53:THR:HG23	1:RB:53:THR:O	2.21	0.40
1:GC:30:ASN:ND2	1:GC:51:LYS:O	2.55	0.40
1:GC:64:SER:OG	1:GC:65:ARG:N	2.55	0.40
1:HC:155:ILE:HG22	1:HC:156:THR:N	2.37	0.40
1:PC:65:ARG:O	1:PC:66:PHE:C	2.60	0.40
1:JD:85:HIS:CE1	1:QF:85:HIS:NE2	2.87	0.40
1:ME:134:ASP:OD1	1:ME:135:TYR:N	2.55	0.40
1:OE:53:THR:O	1:OE:53:THR:HG23	2.21	0.40
1:EF:155:ILE:HG22	1:EF:156:THR:N	2.37	0.40
1:MF:65:ARG:O	1:MF:66:PHE:C	2.60	0.40
1:TF:101:TRP:HB2	1:TF:136:ILE:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	AA	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	AB	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	AC	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	AD	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	AE	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	AF	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	B	146/163 (90%)	141 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	BB	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	BC	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	BD	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	BE	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	BF	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	C	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	CA	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	CB	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	CC	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	CD	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	CE	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	CF	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	D	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	DA	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	DB	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	DC	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	DD	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	DE	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	DF	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	E	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	EA	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	EB	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	EC	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	ED	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	EE	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	EF	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	F	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	FA	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	FB	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	FC	146/163 (90%)	140 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FD	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	FE	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	FF	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	G	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	GA	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	GB	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	GC	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	GD	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	GE	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	GF	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	H	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	HA	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	HB	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	HC	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	HD	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	HE	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	HF	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	I	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	IA	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	IB	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	IC	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	ID	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	IE	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	IF	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	J	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	JA	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	JB	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	JC	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	JD	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	JE	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	JF	146/163 (90%)	141 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	KA	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	KB	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	KC	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	KD	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	KE	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	KF	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	L	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	LA	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	LB	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	LC	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	LD	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	LE	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	LF	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	M	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	MA	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	MB	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	MC	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	MD	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	ME	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	MF	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	N	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	NA	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	NB	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	NC	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	ND	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	NE	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	NF	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	O	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	OA	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	OB	146/163 (90%)	140 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OC	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	OD	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	OE	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	OF	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	P	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	PA	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	PB	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	PC	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	PD	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	PE	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	PF	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	Q	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	QA	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	QB	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	QC	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	QD	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	QE	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	QF	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	R	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	RA	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	RB	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	RC	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	RD	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	RE	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	RF	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	S	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	SA	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	SB	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	SC	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	SD	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	SE	146/163 (90%)	143 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SF	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	T	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	TA	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	TB	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	TC	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	TD	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	TE	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	TF	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	U	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	UA	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	UB	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	UC	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	UD	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	UE	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	UF	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	V	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	VA	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	VB	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	VC	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	VD	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	VE	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	VF	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	W	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	WA	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	WB	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	WC	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	WD	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	WE	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	WF	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	X	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	XA	146/163 (90%)	142 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	XB	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	XC	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	XD	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	XE	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	XF	147/163 (90%)	145 (99%)	2 (1%)	0	100	100
1	Y	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	YA	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	YB	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	YC	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	YD	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	YE	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
1	Z	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
1	ZA	146/163 (90%)	140 (96%)	6 (4%)	0	100	100
1	ZB	146/163 (90%)	145 (99%)	1 (1%)	0	100	100
1	ZC	146/163 (90%)	143 (98%)	3 (2%)	0	100	100
1	ZD	146/163 (90%)	141 (97%)	5 (3%)	0	100	100
1	ZE	146/163 (90%)	142 (97%)	4 (3%)	0	100	100
All	All	26292/29340 (90%)	25514 (97%)	778 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/125 (90%)	113 (100%)	0	100	100
1	AA	113/125 (90%)	113 (100%)	0	100	100
1	AB	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	AC	113/125 (90%)	112 (99%)	1 (1%)	75	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AD	114/125 (91%)	114 (100%)	0	100	100
1	AE	113/125 (90%)	113 (100%)	0	100	100
1	AF	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	B	113/125 (90%)	113 (100%)	0	100	100
1	BA	113/125 (90%)	113 (100%)	0	100	100
1	BB	113/125 (90%)	113 (100%)	0	100	100
1	BC	113/125 (90%)	113 (100%)	0	100	100
1	BD	113/125 (90%)	113 (100%)	0	100	100
1	BE	113/125 (90%)	113 (100%)	0	100	100
1	BF	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	C	113/125 (90%)	113 (100%)	0	100	100
1	CA	113/125 (90%)	113 (100%)	0	100	100
1	CB	113/125 (90%)	113 (100%)	0	100	100
1	CC	113/125 (90%)	113 (100%)	0	100	100
1	CD	113/125 (90%)	113 (100%)	0	100	100
1	CE	113/125 (90%)	113 (100%)	0	100	100
1	CF	113/125 (90%)	113 (100%)	0	100	100
1	D	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	DA	114/125 (91%)	114 (100%)	0	100	100
1	DB	113/125 (90%)	113 (100%)	0	100	100
1	DC	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	DD	113/125 (90%)	113 (100%)	0	100	100
1	DE	113/125 (90%)	113 (100%)	0	100	100
1	DF	113/125 (90%)	113 (100%)	0	100	100
1	E	113/125 (90%)	113 (100%)	0	100	100
1	EA	113/125 (90%)	113 (100%)	0	100	100
1	EB	113/125 (90%)	113 (100%)	0	100	100
1	EC	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	ED	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	EE	114/125 (91%)	114 (100%)	0	100	100
1	EF	113/125 (90%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	113/125 (90%)	113 (100%)	0	100	100
1	FA	113/125 (90%)	113 (100%)	0	100	100
1	FB	113/125 (90%)	113 (100%)	0	100	100
1	FC	113/125 (90%)	113 (100%)	0	100	100
1	FD	113/125 (90%)	113 (100%)	0	100	100
1	FE	113/125 (90%)	113 (100%)	0	100	100
1	FF	113/125 (90%)	113 (100%)	0	100	100
1	G	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	GA	113/125 (90%)	113 (100%)	0	100	100
1	GB	113/125 (90%)	113 (100%)	0	100	100
1	GC	113/125 (90%)	113 (100%)	0	100	100
1	GD	113/125 (90%)	113 (100%)	0	100	100
1	GE	113/125 (90%)	113 (100%)	0	100	100
1	GF	113/125 (90%)	113 (100%)	0	100	100
1	H	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	HA	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	HB	114/125 (91%)	114 (100%)	0	100	100
1	HC	113/125 (90%)	113 (100%)	0	100	100
1	HD	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	HE	113/125 (90%)	113 (100%)	0	100	100
1	HF	113/125 (90%)	113 (100%)	0	100	100
1	I	113/125 (90%)	113 (100%)	0	100	100
1	IA	113/125 (90%)	113 (100%)	0	100	100
1	IB	113/125 (90%)	113 (100%)	0	100	100
1	IC	113/125 (90%)	113 (100%)	0	100	100
1	ID	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	IE	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	IF	114/125 (91%)	114 (100%)	0	100	100
1	J	113/125 (90%)	113 (100%)	0	100	100
1	JA	113/125 (90%)	113 (100%)	0	100	100
1	JB	113/125 (90%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JC	113/125 (90%)	113 (100%)	0	100	100
1	JD	113/125 (90%)	113 (100%)	0	100	100
1	JE	113/125 (90%)	113 (100%)	0	100	100
1	JF	113/125 (90%)	113 (100%)	0	100	100
1	K	113/125 (90%)	113 (100%)	0	100	100
1	KA	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	KB	113/125 (90%)	113 (100%)	0	100	100
1	KC	113/125 (90%)	113 (100%)	0	100	100
1	KD	113/125 (90%)	113 (100%)	0	100	100
1	KE	113/125 (90%)	113 (100%)	0	100	100
1	KF	113/125 (90%)	113 (100%)	0	100	100
1	L	113/125 (90%)	113 (100%)	0	100	100
1	LA	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	LB	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	LC	114/125 (91%)	114 (100%)	0	100	100
1	LD	113/125 (90%)	113 (100%)	0	100	100
1	LE	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	LF	113/125 (90%)	113 (100%)	0	100	100
1	M	113/125 (90%)	113 (100%)	0	100	100
1	MA	113/125 (90%)	113 (100%)	0	100	100
1	MB	113/125 (90%)	113 (100%)	0	100	100
1	MC	113/125 (90%)	113 (100%)	0	100	100
1	MD	113/125 (90%)	113 (100%)	0	100	100
1	ME	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	MF	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	N	113/125 (90%)	113 (100%)	0	100	100
1	NA	113/125 (90%)	113 (100%)	0	100	100
1	NB	113/125 (90%)	113 (100%)	0	100	100
1	NC	113/125 (90%)	113 (100%)	0	100	100
1	ND	113/125 (90%)	113 (100%)	0	100	100
1	NE	113/125 (90%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	NF	113/125 (90%)	113 (100%)	0	100	100
1	O	114/125 (91%)	114 (100%)	0	100	100
1	OA	113/125 (90%)	113 (100%)	0	100	100
1	OB	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	OC	113/125 (90%)	113 (100%)	0	100	100
1	OD	113/125 (90%)	113 (100%)	0	100	100
1	OE	113/125 (90%)	113 (100%)	0	100	100
1	OF	113/125 (90%)	113 (100%)	0	100	100
1	P	113/125 (90%)	113 (100%)	0	100	100
1	PA	113/125 (90%)	113 (100%)	0	100	100
1	PB	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	PC	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	PD	114/125 (91%)	114 (100%)	0	100	100
1	PE	113/125 (90%)	113 (100%)	0	100	100
1	PF	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	Q	113/125 (90%)	113 (100%)	0	100	100
1	QA	113/125 (90%)	113 (100%)	0	100	100
1	QB	113/125 (90%)	113 (100%)	0	100	100
1	QC	113/125 (90%)	113 (100%)	0	100	100
1	QD	113/125 (90%)	113 (100%)	0	100	100
1	QE	113/125 (90%)	113 (100%)	0	100	100
1	QF	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	R	113/125 (90%)	113 (100%)	0	100	100
1	RA	113/125 (90%)	113 (100%)	0	100	100
1	RB	113/125 (90%)	113 (100%)	0	100	100
1	RC	113/125 (90%)	113 (100%)	0	100	100
1	RD	113/125 (90%)	113 (100%)	0	100	100
1	RE	113/125 (90%)	113 (100%)	0	100	100
1	RF	113/125 (90%)	113 (100%)	0	100	100
1	S	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	SA	114/125 (91%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	SB	113/125 (90%)	113 (100%)	0	100 100
1	SC	113/125 (90%)	112 (99%)	1 (1%)	75 86
1	SD	113/125 (90%)	113 (100%)	0	100 100
1	SE	113/125 (90%)	113 (100%)	0	100 100
1	SF	113/125 (90%)	113 (100%)	0	100 100
1	T	113/125 (90%)	113 (100%)	0	100 100
1	TA	113/125 (90%)	113 (100%)	0	100 100
1	TB	113/125 (90%)	113 (100%)	0	100 100
1	TC	113/125 (90%)	112 (99%)	1 (1%)	75 86
1	TD	113/125 (90%)	112 (99%)	1 (1%)	75 86
1	TE	114/125 (91%)	114 (100%)	0	100 100
1	TF	113/125 (90%)	113 (100%)	0	100 100
1	U	113/125 (90%)	113 (100%)	0	100 100
1	UA	113/125 (90%)	113 (100%)	0	100 100
1	UB	113/125 (90%)	113 (100%)	0	100 100
1	UC	113/125 (90%)	113 (100%)	0	100 100
1	UD	113/125 (90%)	113 (100%)	0	100 100
1	UE	113/125 (90%)	113 (100%)	0	100 100
1	UF	113/125 (90%)	113 (100%)	0	100 100
1	V	113/125 (90%)	112 (99%)	1 (1%)	75 86
1	VA	113/125 (90%)	113 (100%)	0	100 100
1	VB	113/125 (90%)	113 (100%)	0	100 100
1	VC	113/125 (90%)	113 (100%)	0	100 100
1	VD	113/125 (90%)	113 (100%)	0	100 100
1	VE	113/125 (90%)	113 (100%)	0	100 100
1	VF	113/125 (90%)	113 (100%)	0	100 100
1	W	113/125 (90%)	112 (99%)	1 (1%)	75 86
1	WA	113/125 (90%)	112 (99%)	1 (1%)	75 86
1	WB	114/125 (91%)	114 (100%)	0	100 100
1	WC	113/125 (90%)	113 (100%)	0	100 100
1	WD	113/125 (90%)	112 (99%)	1 (1%)	75 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	WE	113/125 (90%)	113 (100%)	0	100	100
1	WF	113/125 (90%)	113 (100%)	0	100	100
1	X	113/125 (90%)	113 (100%)	0	100	100
1	XA	113/125 (90%)	113 (100%)	0	100	100
1	XB	113/125 (90%)	113 (100%)	0	100	100
1	XC	113/125 (90%)	113 (100%)	0	100	100
1	XD	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	XE	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	XF	114/125 (91%)	114 (100%)	0	100	100
1	Y	113/125 (90%)	113 (100%)	0	100	100
1	YA	113/125 (90%)	113 (100%)	0	100	100
1	YB	113/125 (90%)	113 (100%)	0	100	100
1	YC	113/125 (90%)	113 (100%)	0	100	100
1	YD	113/125 (90%)	113 (100%)	0	100	100
1	YE	113/125 (90%)	113 (100%)	0	100	100
1	Z	113/125 (90%)	113 (100%)	0	100	100
1	ZA	113/125 (90%)	112 (99%)	1 (1%)	75	86
1	ZB	113/125 (90%)	113 (100%)	0	100	100
1	ZC	113/125 (90%)	113 (100%)	0	100	100
1	ZD	113/125 (90%)	113 (100%)	0	100	100
1	ZE	113/125 (90%)	113 (100%)	0	100	100
All	All	20352/22500 (90%)	20316 (100%)	36 (0%)	91	96

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	65	ARG
1	G	58	ARG
1	H	58	ARG
1	S	65	ARG
1	V	58	ARG
1	W	58	ARG
1	HA	65	ARG
1	KA	58	ARG
1	LA	58	ARG

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Mol	Chain	Res	Type
1	WA	65	ARG
1	ZA	58	ARG
1	AB	58	ARG
1	LB	65	ARG
1	OB	58	ARG
1	PB	58	ARG
1	AC	65	ARG
1	DC	58	ARG
1	EC	58	ARG
1	PC	65	ARG
1	SC	58	ARG
1	TC	58	ARG
1	ED	65	ARG
1	HD	58	ARG
1	ID	58	ARG
1	TD	65	ARG
1	WD	58	ARG
1	XD	58	ARG
1	IE	65	ARG
1	LE	58	ARG
1	ME	58	ARG
1	XE	65	ARG
1	AF	58	ARG
1	BF	58	ARG
1	MF	65	ARG
1	PF	58	ARG
1	QF	58	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	85	HIS
1	I	85	HIS
1	S	85	HIS
1	X	85	HIS
1	HA	85	HIS
1	MA	85	HIS
1	WA	85	HIS
1	BB	85	HIS
1	LB	85	HIS
1	QB	85	HIS
1	AC	85	HIS

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Mol	Chain	Res	Type
1	FC	85	HIS
1	PC	85	HIS
1	UC	85	HIS
1	ED	85	HIS
1	HD	146	ASN
1	JD	85	HIS
1	TD	85	HIS
1	YD	85	HIS
1	IE	85	HIS
1	NE	85	HIS
1	XE	85	HIS
1	CF	85	HIS
1	MF	85	HIS
1	RF	85	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.