



## Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 01:03 am GMT

PDB ID : 9G3P  
EMDB ID : EMD-51006  
Title : Circularly permuted lumazine synthase 12-pentamer spherical cage  
Authors : Koziej, L.; Azuma, Y.  
Deposited on : 2024-07-12  
Resolution : 2.08 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](mailto: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>.

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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

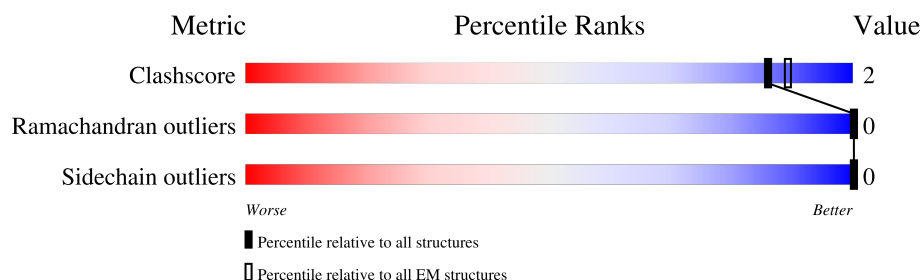
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


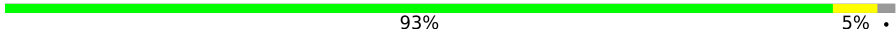
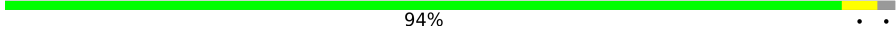
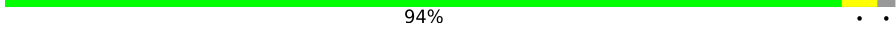
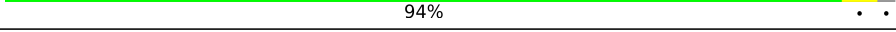
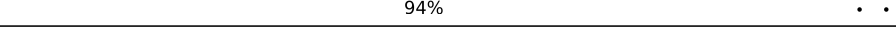
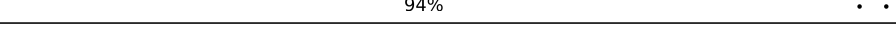
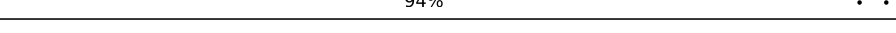
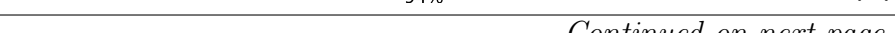
The reported resolution of this entry is 2.08 Å.

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.






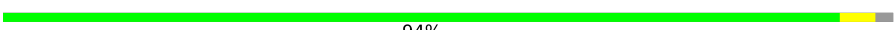






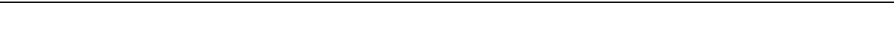

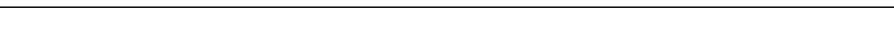
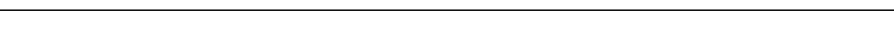
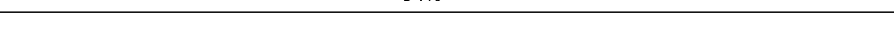
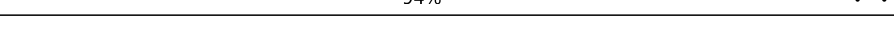
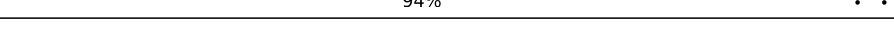
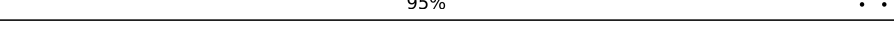
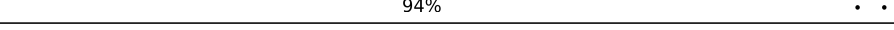
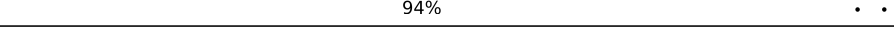
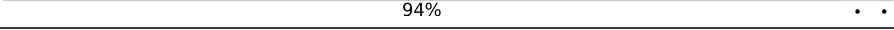
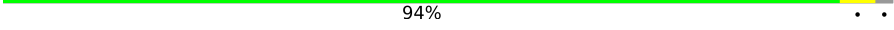
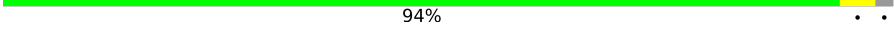

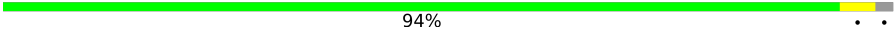
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	163	 94% . .
1	AA	163	 93% 5% .
1	AB	163	 94% . .
1	B	163	 94% . .
1	BA	163	 94% . .
1	BB	163	 94% . .
1	C	163	 94% . .
1	CA	163	 94% . .
1	CB	163	 94% . .














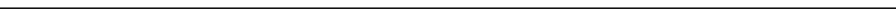

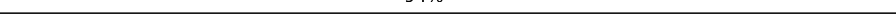
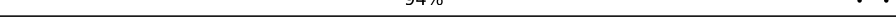
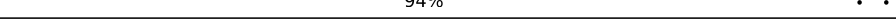
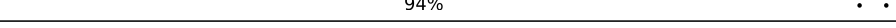
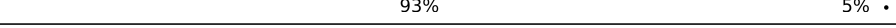
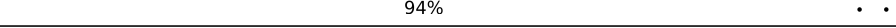
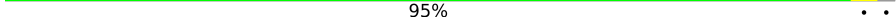
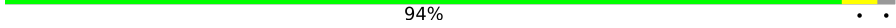
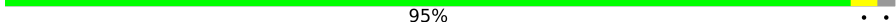
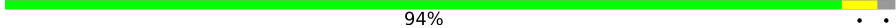
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Mol	Chain	Length	Quality of chain
1	D	163	 94% . .
1	DA	163	 94% . .
1	DB	163	 94% . .
1	E	163	 94% . .
1	EA	163	 94% . .
1	EB	163	 94% . .
1	F	163	 94% . .
1	FA	163	 94% . .
1	FB	163	 94% . .
1	G	163	 94% . .
1	GA	163	 94% . .
1	GB	163	 94% . .
1	H	163	 94% . .
1	HA	163	 94% . .
1	HB	163	 94% . .
1	I	163	 94% . .
1	IA	163	 95% . .
1	J	163	 94% . .
1	JA	163	 94% . .
1	K	163	 94% . .
1	KA	163	 94% . .
1	L	163	 94% . .
1	LA	163	 94% . .
1	M	163	 94% . .
1	MA	163	 94% . .

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Mol	Chain	Length	Quality of chain
1	N	163	 94% . .
1	NA	163	 94% . .
1	O	163	 94% . .
1	OA	163	 94% . .
1	P	163	 93% 5% .
1	PA	163	 94% . .
1	Q	163	 94% . .
1	QA	163	 94% . .
1	R	163	 94% . .
1	RA	163	 94% . .
1	S	163	 94% . .
1	SA	163	 94% . .
1	T	163	 94% . .
1	TA	163	 94% . .
1	U	163	 94% . .
1	UA	163	 94% . .
1	V	163	 94% . .
1	VA	163	 94% . .
1	W	163	 93% 5% .
1	WA	163	 94% . .
1	X	163	 95% . .
1	XA	163	 94% . .
1	Y	163	 95% . .
1	YA	163	 94% . .
1	Z	163	 94% . .

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Mol	Chain	Length	Quality of chain
1	ZA	163	<div><div></div><div>94%</div><div></div></div>

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 72480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	B	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	C	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	D	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	E	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	F	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	G	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	H	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	I	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	J	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	K	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	L	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	M	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	N	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	O	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	P	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	Q	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	S	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	T	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	U	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	V	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	W	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	X	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	Y	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	Z	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	AA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	BA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	CA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	DA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	EA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	FA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	GA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	HA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	IA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	JA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	KA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	LA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	NA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	OA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	PA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	QA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	RA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	SA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	TA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	UA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	VA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	WA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	XA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	YA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	ZA	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	AB	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	BB	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	CB	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	DB	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	EB	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	FB	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		
1	GB	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HB	160	Total	C	N	O	S	0	0
			1208	761	215	229	3		

There are 660 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O66529
A	72	GLY	-	linker	UNP O66529
A	73	THR	-	linker	UNP O66529
A	74	GLY	-	linker	UNP O66529
A	75	GLY	-	linker	UNP O66529
A	76	SER	-	linker	UNP O66529
A	77	GLY	-	linker	UNP O66529
A	78	SER	-	linker	UNP O66529
A	79	SER	-	linker	UNP O66529
A	80	MET	-	linker	UNP O66529
A	81	GLU	-	linker	UNP O66529
B	1	MET	-	initiating methionine	UNP O66529
B	72	GLY	-	linker	UNP O66529
B	73	THR	-	linker	UNP O66529
B	74	GLY	-	linker	UNP O66529
B	75	GLY	-	linker	UNP O66529
B	76	SER	-	linker	UNP O66529
B	77	GLY	-	linker	UNP O66529
B	78	SER	-	linker	UNP O66529
B	79	SER	-	linker	UNP O66529
B	80	MET	-	linker	UNP O66529
B	81	GLU	-	linker	UNP O66529
C	1	MET	-	initiating methionine	UNP O66529
C	72	GLY	-	linker	UNP O66529
C	73	THR	-	linker	UNP O66529
C	74	GLY	-	linker	UNP O66529
C	75	GLY	-	linker	UNP O66529
C	76	SER	-	linker	UNP O66529
C	77	GLY	-	linker	UNP O66529
C	78	SER	-	linker	UNP O66529
C	79	SER	-	linker	UNP O66529
C	80	MET	-	linker	UNP O66529
C	81	GLU	-	linker	UNP O66529
D	1	MET	-	initiating methionine	UNP O66529
D	72	GLY	-	linker	UNP O66529
D	73	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
D	74	GLY	-	linker	UNP O66529
D	75	GLY	-	linker	UNP O66529
D	76	SER	-	linker	UNP O66529
D	77	GLY	-	linker	UNP O66529
D	78	SER	-	linker	UNP O66529
D	79	SER	-	linker	UNP O66529
D	80	MET	-	linker	UNP O66529
D	81	GLU	-	linker	UNP O66529
E	1	MET	-	initiating methionine	UNP O66529
E	72	GLY	-	linker	UNP O66529
E	73	THR	-	linker	UNP O66529
E	74	GLY	-	linker	UNP O66529
E	75	GLY	-	linker	UNP O66529
E	76	SER	-	linker	UNP O66529
E	77	GLY	-	linker	UNP O66529
E	78	SER	-	linker	UNP O66529
E	79	SER	-	linker	UNP O66529
E	80	MET	-	linker	UNP O66529
E	81	GLU	-	linker	UNP O66529
F	1	MET	-	initiating methionine	UNP O66529
F	72	GLY	-	linker	UNP O66529
F	73	THR	-	linker	UNP O66529
F	74	GLY	-	linker	UNP O66529
F	75	GLY	-	linker	UNP O66529
F	76	SER	-	linker	UNP O66529
F	77	GLY	-	linker	UNP O66529
F	78	SER	-	linker	UNP O66529
F	79	SER	-	linker	UNP O66529
F	80	MET	-	linker	UNP O66529
F	81	GLU	-	linker	UNP O66529
G	1	MET	-	initiating methionine	UNP O66529
G	72	GLY	-	linker	UNP O66529
G	73	THR	-	linker	UNP O66529
G	74	GLY	-	linker	UNP O66529
G	75	GLY	-	linker	UNP O66529
G	76	SER	-	linker	UNP O66529
G	77	GLY	-	linker	UNP O66529
G	78	SER	-	linker	UNP O66529
G	79	SER	-	linker	UNP O66529
G	80	MET	-	linker	UNP O66529
G	81	GLU	-	linker	UNP O66529
H	1	MET	-	initiating methionine	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
H	72	GLY	-	linker	UNP O66529
H	73	THR	-	linker	UNP O66529
H	74	GLY	-	linker	UNP O66529
H	75	GLY	-	linker	UNP O66529
H	76	SER	-	linker	UNP O66529
H	77	GLY	-	linker	UNP O66529
H	78	SER	-	linker	UNP O66529
H	79	SER	-	linker	UNP O66529
H	80	MET	-	linker	UNP O66529
H	81	GLU	-	linker	UNP O66529
I	1	MET	-	initiating methionine	UNP O66529
I	72	GLY	-	linker	UNP O66529
I	73	THR	-	linker	UNP O66529
I	74	GLY	-	linker	UNP O66529
I	75	GLY	-	linker	UNP O66529
I	76	SER	-	linker	UNP O66529
I	77	GLY	-	linker	UNP O66529
I	78	SER	-	linker	UNP O66529
I	79	SER	-	linker	UNP O66529
I	80	MET	-	linker	UNP O66529
I	81	GLU	-	linker	UNP O66529
J	1	MET	-	initiating methionine	UNP O66529
J	72	GLY	-	linker	UNP O66529
J	73	THR	-	linker	UNP O66529
J	74	GLY	-	linker	UNP O66529
J	75	GLY	-	linker	UNP O66529
J	76	SER	-	linker	UNP O66529
J	77	GLY	-	linker	UNP O66529
J	78	SER	-	linker	UNP O66529
J	79	SER	-	linker	UNP O66529
J	80	MET	-	linker	UNP O66529
J	81	GLU	-	linker	UNP O66529
K	1	MET	-	initiating methionine	UNP O66529
K	72	GLY	-	linker	UNP O66529
K	73	THR	-	linker	UNP O66529
K	74	GLY	-	linker	UNP O66529
K	75	GLY	-	linker	UNP O66529
K	76	SER	-	linker	UNP O66529
K	77	GLY	-	linker	UNP O66529
K	78	SER	-	linker	UNP O66529
K	79	SER	-	linker	UNP O66529
K	80	MET	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
K	81	GLU	-	linker	UNP O66529
L	1	MET	-	initiating methionine	UNP O66529
L	72	GLY	-	linker	UNP O66529
L	73	THR	-	linker	UNP O66529
L	74	GLY	-	linker	UNP O66529
L	75	GLY	-	linker	UNP O66529
L	76	SER	-	linker	UNP O66529
L	77	GLY	-	linker	UNP O66529
L	78	SER	-	linker	UNP O66529
L	79	SER	-	linker	UNP O66529
L	80	MET	-	linker	UNP O66529
L	81	GLU	-	linker	UNP O66529
M	1	MET	-	initiating methionine	UNP O66529
M	72	GLY	-	linker	UNP O66529
M	73	THR	-	linker	UNP O66529
M	74	GLY	-	linker	UNP O66529
M	75	GLY	-	linker	UNP O66529
M	76	SER	-	linker	UNP O66529
M	77	GLY	-	linker	UNP O66529
M	78	SER	-	linker	UNP O66529
M	79	SER	-	linker	UNP O66529
M	80	MET	-	linker	UNP O66529
M	81	GLU	-	linker	UNP O66529
N	1	MET	-	initiating methionine	UNP O66529
N	72	GLY	-	linker	UNP O66529
N	73	THR	-	linker	UNP O66529
N	74	GLY	-	linker	UNP O66529
N	75	GLY	-	linker	UNP O66529
N	76	SER	-	linker	UNP O66529
N	77	GLY	-	linker	UNP O66529
N	78	SER	-	linker	UNP O66529
N	79	SER	-	linker	UNP O66529
N	80	MET	-	linker	UNP O66529
N	81	GLU	-	linker	UNP O66529
O	1	MET	-	initiating methionine	UNP O66529
O	72	GLY	-	linker	UNP O66529
O	73	THR	-	linker	UNP O66529
O	74	GLY	-	linker	UNP O66529
O	75	GLY	-	linker	UNP O66529
O	76	SER	-	linker	UNP O66529
O	77	GLY	-	linker	UNP O66529
O	78	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
O	79	SER	-	linker	UNP O66529
O	80	MET	-	linker	UNP O66529
O	81	GLU	-	linker	UNP O66529
P	1	MET	-	initiating methionine	UNP O66529
P	72	GLY	-	linker	UNP O66529
P	73	THR	-	linker	UNP O66529
P	74	GLY	-	linker	UNP O66529
P	75	GLY	-	linker	UNP O66529
P	76	SER	-	linker	UNP O66529
P	77	GLY	-	linker	UNP O66529
P	78	SER	-	linker	UNP O66529
P	79	SER	-	linker	UNP O66529
P	80	MET	-	linker	UNP O66529
P	81	GLU	-	linker	UNP O66529
Q	1	MET	-	initiating methionine	UNP O66529
Q	72	GLY	-	linker	UNP O66529
Q	73	THR	-	linker	UNP O66529
Q	74	GLY	-	linker	UNP O66529
Q	75	GLY	-	linker	UNP O66529
Q	76	SER	-	linker	UNP O66529
Q	77	GLY	-	linker	UNP O66529
Q	78	SER	-	linker	UNP O66529
Q	79	SER	-	linker	UNP O66529
Q	80	MET	-	linker	UNP O66529
Q	81	GLU	-	linker	UNP O66529
R	1	MET	-	initiating methionine	UNP O66529
R	72	GLY	-	linker	UNP O66529
R	73	THR	-	linker	UNP O66529
R	74	GLY	-	linker	UNP O66529
R	75	GLY	-	linker	UNP O66529
R	76	SER	-	linker	UNP O66529
R	77	GLY	-	linker	UNP O66529
R	78	SER	-	linker	UNP O66529
R	79	SER	-	linker	UNP O66529
R	80	MET	-	linker	UNP O66529
R	81	GLU	-	linker	UNP O66529
S	1	MET	-	initiating methionine	UNP O66529
S	72	GLY	-	linker	UNP O66529
S	73	THR	-	linker	UNP O66529
S	74	GLY	-	linker	UNP O66529
S	75	GLY	-	linker	UNP O66529
S	76	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
S	77	GLY	-	linker	UNP O66529
S	78	SER	-	linker	UNP O66529
S	79	SER	-	linker	UNP O66529
S	80	MET	-	linker	UNP O66529
S	81	GLU	-	linker	UNP O66529
T	1	MET	-	initiating methionine	UNP O66529
T	72	GLY	-	linker	UNP O66529
T	73	THR	-	linker	UNP O66529
T	74	GLY	-	linker	UNP O66529
T	75	GLY	-	linker	UNP O66529
T	76	SER	-	linker	UNP O66529
T	77	GLY	-	linker	UNP O66529
T	78	SER	-	linker	UNP O66529
T	79	SER	-	linker	UNP O66529
T	80	MET	-	linker	UNP O66529
T	81	GLU	-	linker	UNP O66529
U	1	MET	-	initiating methionine	UNP O66529
U	72	GLY	-	linker	UNP O66529
U	73	THR	-	linker	UNP O66529
U	74	GLY	-	linker	UNP O66529
U	75	GLY	-	linker	UNP O66529
U	76	SER	-	linker	UNP O66529
U	77	GLY	-	linker	UNP O66529
U	78	SER	-	linker	UNP O66529
U	79	SER	-	linker	UNP O66529
U	80	MET	-	linker	UNP O66529
U	81	GLU	-	linker	UNP O66529
V	1	MET	-	initiating methionine	UNP O66529
V	72	GLY	-	linker	UNP O66529
V	73	THR	-	linker	UNP O66529
V	74	GLY	-	linker	UNP O66529
V	75	GLY	-	linker	UNP O66529
V	76	SER	-	linker	UNP O66529
V	77	GLY	-	linker	UNP O66529
V	78	SER	-	linker	UNP O66529
V	79	SER	-	linker	UNP O66529
V	80	MET	-	linker	UNP O66529
V	81	GLU	-	linker	UNP O66529
W	1	MET	-	initiating methionine	UNP O66529
W	72	GLY	-	linker	UNP O66529
W	73	THR	-	linker	UNP O66529
W	74	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
W	75	GLY	-	linker	UNP O66529
W	76	SER	-	linker	UNP O66529
W	77	GLY	-	linker	UNP O66529
W	78	SER	-	linker	UNP O66529
W	79	SER	-	linker	UNP O66529
W	80	MET	-	linker	UNP O66529
W	81	GLU	-	linker	UNP O66529
X	1	MET	-	initiating methionine	UNP O66529
X	72	GLY	-	linker	UNP O66529
X	73	THR	-	linker	UNP O66529
X	74	GLY	-	linker	UNP O66529
X	75	GLY	-	linker	UNP O66529
X	76	SER	-	linker	UNP O66529
X	77	GLY	-	linker	UNP O66529
X	78	SER	-	linker	UNP O66529
X	79	SER	-	linker	UNP O66529
X	80	MET	-	linker	UNP O66529
X	81	GLU	-	linker	UNP O66529
Y	1	MET	-	initiating methionine	UNP O66529
Y	72	GLY	-	linker	UNP O66529
Y	73	THR	-	linker	UNP O66529
Y	74	GLY	-	linker	UNP O66529
Y	75	GLY	-	linker	UNP O66529
Y	76	SER	-	linker	UNP O66529
Y	77	GLY	-	linker	UNP O66529
Y	78	SER	-	linker	UNP O66529
Y	79	SER	-	linker	UNP O66529
Y	80	MET	-	linker	UNP O66529
Y	81	GLU	-	linker	UNP O66529
Z	1	MET	-	initiating methionine	UNP O66529
Z	72	GLY	-	linker	UNP O66529
Z	73	THR	-	linker	UNP O66529
Z	74	GLY	-	linker	UNP O66529
Z	75	GLY	-	linker	UNP O66529
Z	76	SER	-	linker	UNP O66529
Z	77	GLY	-	linker	UNP O66529
Z	78	SER	-	linker	UNP O66529
Z	79	SER	-	linker	UNP O66529
Z	80	MET	-	linker	UNP O66529
Z	81	GLU	-	linker	UNP O66529
AA	1	MET	-	initiating methionine	UNP O66529
AA	72	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
AA	73	THR	-	linker	UNP O66529
AA	74	GLY	-	linker	UNP O66529
AA	75	GLY	-	linker	UNP O66529
AA	76	SER	-	linker	UNP O66529
AA	77	GLY	-	linker	UNP O66529
AA	78	SER	-	linker	UNP O66529
AA	79	SER	-	linker	UNP O66529
AA	80	MET	-	linker	UNP O66529
AA	81	GLU	-	linker	UNP O66529
BA	1	MET	-	initiating methionine	UNP O66529
BA	72	GLY	-	linker	UNP O66529
BA	73	THR	-	linker	UNP O66529
BA	74	GLY	-	linker	UNP O66529
BA	75	GLY	-	linker	UNP O66529
BA	76	SER	-	linker	UNP O66529
BA	77	GLY	-	linker	UNP O66529
BA	78	SER	-	linker	UNP O66529
BA	79	SER	-	linker	UNP O66529
BA	80	MET	-	linker	UNP O66529
BA	81	GLU	-	linker	UNP O66529
CA	1	MET	-	initiating methionine	UNP O66529
CA	72	GLY	-	linker	UNP O66529
CA	73	THR	-	linker	UNP O66529
CA	74	GLY	-	linker	UNP O66529
CA	75	GLY	-	linker	UNP O66529
CA	76	SER	-	linker	UNP O66529
CA	77	GLY	-	linker	UNP O66529
CA	78	SER	-	linker	UNP O66529
CA	79	SER	-	linker	UNP O66529
CA	80	MET	-	linker	UNP O66529
CA	81	GLU	-	linker	UNP O66529
DA	1	MET	-	initiating methionine	UNP O66529
DA	72	GLY	-	linker	UNP O66529
DA	73	THR	-	linker	UNP O66529
DA	74	GLY	-	linker	UNP O66529
DA	75	GLY	-	linker	UNP O66529
DA	76	SER	-	linker	UNP O66529
DA	77	GLY	-	linker	UNP O66529
DA	78	SER	-	linker	UNP O66529
DA	79	SER	-	linker	UNP O66529
DA	80	MET	-	linker	UNP O66529
DA	81	GLU	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
EA	1	MET	-	initiating methionine	UNP O66529
EA	72	GLY	-	linker	UNP O66529
EA	73	THR	-	linker	UNP O66529
EA	74	GLY	-	linker	UNP O66529
EA	75	GLY	-	linker	UNP O66529
EA	76	SER	-	linker	UNP O66529
EA	77	GLY	-	linker	UNP O66529
EA	78	SER	-	linker	UNP O66529
EA	79	SER	-	linker	UNP O66529
EA	80	MET	-	linker	UNP O66529
EA	81	GLU	-	linker	UNP O66529
FA	1	MET	-	initiating methionine	UNP O66529
FA	72	GLY	-	linker	UNP O66529
FA	73	THR	-	linker	UNP O66529
FA	74	GLY	-	linker	UNP O66529
FA	75	GLY	-	linker	UNP O66529
FA	76	SER	-	linker	UNP O66529
FA	77	GLY	-	linker	UNP O66529
FA	78	SER	-	linker	UNP O66529
FA	79	SER	-	linker	UNP O66529
FA	80	MET	-	linker	UNP O66529
FA	81	GLU	-	linker	UNP O66529
GA	1	MET	-	initiating methionine	UNP O66529
GA	72	GLY	-	linker	UNP O66529
GA	73	THR	-	linker	UNP O66529
GA	74	GLY	-	linker	UNP O66529
GA	75	GLY	-	linker	UNP O66529
GA	76	SER	-	linker	UNP O66529
GA	77	GLY	-	linker	UNP O66529
GA	78	SER	-	linker	UNP O66529
GA	79	SER	-	linker	UNP O66529
GA	80	MET	-	linker	UNP O66529
GA	81	GLU	-	linker	UNP O66529
HA	1	MET	-	initiating methionine	UNP O66529
HA	72	GLY	-	linker	UNP O66529
HA	73	THR	-	linker	UNP O66529
HA	74	GLY	-	linker	UNP O66529
HA	75	GLY	-	linker	UNP O66529
HA	76	SER	-	linker	UNP O66529
HA	77	GLY	-	linker	UNP O66529
HA	78	SER	-	linker	UNP O66529
HA	79	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
HA	80	MET	-	linker	UNP O66529
HA	81	GLU	-	linker	UNP O66529
IA	1	MET	-	initiating methionine	UNP O66529
IA	72	GLY	-	linker	UNP O66529
IA	73	THR	-	linker	UNP O66529
IA	74	GLY	-	linker	UNP O66529
IA	75	GLY	-	linker	UNP O66529
IA	76	SER	-	linker	UNP O66529
IA	77	GLY	-	linker	UNP O66529
IA	78	SER	-	linker	UNP O66529
IA	79	SER	-	linker	UNP O66529
IA	80	MET	-	linker	UNP O66529
IA	81	GLU	-	linker	UNP O66529
JA	1	MET	-	initiating methionine	UNP O66529
JA	72	GLY	-	linker	UNP O66529
JA	73	THR	-	linker	UNP O66529
JA	74	GLY	-	linker	UNP O66529
JA	75	GLY	-	linker	UNP O66529
JA	76	SER	-	linker	UNP O66529
JA	77	GLY	-	linker	UNP O66529
JA	78	SER	-	linker	UNP O66529
JA	79	SER	-	linker	UNP O66529
JA	80	MET	-	linker	UNP O66529
JA	81	GLU	-	linker	UNP O66529
KA	1	MET	-	initiating methionine	UNP O66529
KA	72	GLY	-	linker	UNP O66529
KA	73	THR	-	linker	UNP O66529
KA	74	GLY	-	linker	UNP O66529
KA	75	GLY	-	linker	UNP O66529
KA	76	SER	-	linker	UNP O66529
KA	77	GLY	-	linker	UNP O66529
KA	78	SER	-	linker	UNP O66529
KA	79	SER	-	linker	UNP O66529
KA	80	MET	-	linker	UNP O66529
KA	81	GLU	-	linker	UNP O66529
LA	1	MET	-	initiating methionine	UNP O66529
LA	72	GLY	-	linker	UNP O66529
LA	73	THR	-	linker	UNP O66529
LA	74	GLY	-	linker	UNP O66529
LA	75	GLY	-	linker	UNP O66529
LA	76	SER	-	linker	UNP O66529
LA	77	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
LA	78	SER	-	linker	UNP O66529
LA	79	SER	-	linker	UNP O66529
LA	80	MET	-	linker	UNP O66529
LA	81	GLU	-	linker	UNP O66529
MA	1	MET	-	initiating methionine	UNP O66529
MA	72	GLY	-	linker	UNP O66529
MA	73	THR	-	linker	UNP O66529
MA	74	GLY	-	linker	UNP O66529
MA	75	GLY	-	linker	UNP O66529
MA	76	SER	-	linker	UNP O66529
MA	77	GLY	-	linker	UNP O66529
MA	78	SER	-	linker	UNP O66529
MA	79	SER	-	linker	UNP O66529
MA	80	MET	-	linker	UNP O66529
MA	81	GLU	-	linker	UNP O66529
NA	1	MET	-	initiating methionine	UNP O66529
NA	72	GLY	-	linker	UNP O66529
NA	73	THR	-	linker	UNP O66529
NA	74	GLY	-	linker	UNP O66529
NA	75	GLY	-	linker	UNP O66529
NA	76	SER	-	linker	UNP O66529
NA	77	GLY	-	linker	UNP O66529
NA	78	SER	-	linker	UNP O66529
NA	79	SER	-	linker	UNP O66529
NA	80	MET	-	linker	UNP O66529
NA	81	GLU	-	linker	UNP O66529
OA	1	MET	-	initiating methionine	UNP O66529
OA	72	GLY	-	linker	UNP O66529
OA	73	THR	-	linker	UNP O66529
OA	74	GLY	-	linker	UNP O66529
OA	75	GLY	-	linker	UNP O66529
OA	76	SER	-	linker	UNP O66529
OA	77	GLY	-	linker	UNP O66529
OA	78	SER	-	linker	UNP O66529
OA	79	SER	-	linker	UNP O66529
OA	80	MET	-	linker	UNP O66529
OA	81	GLU	-	linker	UNP O66529
PA	1	MET	-	initiating methionine	UNP O66529
PA	72	GLY	-	linker	UNP O66529
PA	73	THR	-	linker	UNP O66529
PA	74	GLY	-	linker	UNP O66529
PA	75	GLY	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
PA	76	SER	-	linker	UNP O66529
PA	77	GLY	-	linker	UNP O66529
PA	78	SER	-	linker	UNP O66529
PA	79	SER	-	linker	UNP O66529
PA	80	MET	-	linker	UNP O66529
PA	81	GLU	-	linker	UNP O66529
QA	1	MET	-	initiating methionine	UNP O66529
QA	72	GLY	-	linker	UNP O66529
QA	73	THR	-	linker	UNP O66529
QA	74	GLY	-	linker	UNP O66529
QA	75	GLY	-	linker	UNP O66529
QA	76	SER	-	linker	UNP O66529
QA	77	GLY	-	linker	UNP O66529
QA	78	SER	-	linker	UNP O66529
QA	79	SER	-	linker	UNP O66529
QA	80	MET	-	linker	UNP O66529
QA	81	GLU	-	linker	UNP O66529
RA	1	MET	-	initiating methionine	UNP O66529
RA	72	GLY	-	linker	UNP O66529
RA	73	THR	-	linker	UNP O66529
RA	74	GLY	-	linker	UNP O66529
RA	75	GLY	-	linker	UNP O66529
RA	76	SER	-	linker	UNP O66529
RA	77	GLY	-	linker	UNP O66529
RA	78	SER	-	linker	UNP O66529
RA	79	SER	-	linker	UNP O66529
RA	80	MET	-	linker	UNP O66529
RA	81	GLU	-	linker	UNP O66529
SA	1	MET	-	initiating methionine	UNP O66529
SA	72	GLY	-	linker	UNP O66529
SA	73	THR	-	linker	UNP O66529
SA	74	GLY	-	linker	UNP O66529
SA	75	GLY	-	linker	UNP O66529
SA	76	SER	-	linker	UNP O66529
SA	77	GLY	-	linker	UNP O66529
SA	78	SER	-	linker	UNP O66529
SA	79	SER	-	linker	UNP O66529
SA	80	MET	-	linker	UNP O66529
SA	81	GLU	-	linker	UNP O66529
TA	1	MET	-	initiating methionine	UNP O66529
TA	72	GLY	-	linker	UNP O66529
TA	73	THR	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
TA	74	GLY	-	linker	UNP O66529
TA	75	GLY	-	linker	UNP O66529
TA	76	SER	-	linker	UNP O66529
TA	77	GLY	-	linker	UNP O66529
TA	78	SER	-	linker	UNP O66529
TA	79	SER	-	linker	UNP O66529
TA	80	MET	-	linker	UNP O66529
TA	81	GLU	-	linker	UNP O66529
UA	1	MET	-	initiating methionine	UNP O66529
UA	72	GLY	-	linker	UNP O66529
UA	73	THR	-	linker	UNP O66529
UA	74	GLY	-	linker	UNP O66529
UA	75	GLY	-	linker	UNP O66529
UA	76	SER	-	linker	UNP O66529
UA	77	GLY	-	linker	UNP O66529
UA	78	SER	-	linker	UNP O66529
UA	79	SER	-	linker	UNP O66529
UA	80	MET	-	linker	UNP O66529
UA	81	GLU	-	linker	UNP O66529
VA	1	MET	-	initiating methionine	UNP O66529
VA	72	GLY	-	linker	UNP O66529
VA	73	THR	-	linker	UNP O66529
VA	74	GLY	-	linker	UNP O66529
VA	75	GLY	-	linker	UNP O66529
VA	76	SER	-	linker	UNP O66529
VA	77	GLY	-	linker	UNP O66529
VA	78	SER	-	linker	UNP O66529
VA	79	SER	-	linker	UNP O66529
VA	80	MET	-	linker	UNP O66529
VA	81	GLU	-	linker	UNP O66529
WA	1	MET	-	initiating methionine	UNP O66529
WA	72	GLY	-	linker	UNP O66529
WA	73	THR	-	linker	UNP O66529
WA	74	GLY	-	linker	UNP O66529
WA	75	GLY	-	linker	UNP O66529
WA	76	SER	-	linker	UNP O66529
WA	77	GLY	-	linker	UNP O66529
WA	78	SER	-	linker	UNP O66529
WA	79	SER	-	linker	UNP O66529
WA	80	MET	-	linker	UNP O66529
WA	81	GLU	-	linker	UNP O66529
XA	1	MET	-	initiating methionine	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
XA	72	GLY	-	linker	UNP O66529
XA	73	THR	-	linker	UNP O66529
XA	74	GLY	-	linker	UNP O66529
XA	75	GLY	-	linker	UNP O66529
XA	76	SER	-	linker	UNP O66529
XA	77	GLY	-	linker	UNP O66529
XA	78	SER	-	linker	UNP O66529
XA	79	SER	-	linker	UNP O66529
XA	80	MET	-	linker	UNP O66529
XA	81	GLU	-	linker	UNP O66529
YA	1	MET	-	initiating methionine	UNP O66529
YA	72	GLY	-	linker	UNP O66529
YA	73	THR	-	linker	UNP O66529
YA	74	GLY	-	linker	UNP O66529
YA	75	GLY	-	linker	UNP O66529
YA	76	SER	-	linker	UNP O66529
YA	77	GLY	-	linker	UNP O66529
YA	78	SER	-	linker	UNP O66529
YA	79	SER	-	linker	UNP O66529
YA	80	MET	-	linker	UNP O66529
YA	81	GLU	-	linker	UNP O66529
ZA	1	MET	-	initiating methionine	UNP O66529
ZA	72	GLY	-	linker	UNP O66529
ZA	73	THR	-	linker	UNP O66529
ZA	74	GLY	-	linker	UNP O66529
ZA	75	GLY	-	linker	UNP O66529
ZA	76	SER	-	linker	UNP O66529
ZA	77	GLY	-	linker	UNP O66529
ZA	78	SER	-	linker	UNP O66529
ZA	79	SER	-	linker	UNP O66529
ZA	80	MET	-	linker	UNP O66529
ZA	81	GLU	-	linker	UNP O66529
AB	1	MET	-	initiating methionine	UNP O66529
AB	72	GLY	-	linker	UNP O66529
AB	73	THR	-	linker	UNP O66529
AB	74	GLY	-	linker	UNP O66529
AB	75	GLY	-	linker	UNP O66529
AB	76	SER	-	linker	UNP O66529
AB	77	GLY	-	linker	UNP O66529
AB	78	SER	-	linker	UNP O66529
AB	79	SER	-	linker	UNP O66529
AB	80	MET	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
AB	81	GLU	-	linker	UNP O66529
BB	1	MET	-	initiating methionine	UNP O66529
BB	72	GLY	-	linker	UNP O66529
BB	73	THR	-	linker	UNP O66529
BB	74	GLY	-	linker	UNP O66529
BB	75	GLY	-	linker	UNP O66529
BB	76	SER	-	linker	UNP O66529
BB	77	GLY	-	linker	UNP O66529
BB	78	SER	-	linker	UNP O66529
BB	79	SER	-	linker	UNP O66529
BB	80	MET	-	linker	UNP O66529
BB	81	GLU	-	linker	UNP O66529
CB	1	MET	-	initiating methionine	UNP O66529
CB	72	GLY	-	linker	UNP O66529
CB	73	THR	-	linker	UNP O66529
CB	74	GLY	-	linker	UNP O66529
CB	75	GLY	-	linker	UNP O66529
CB	76	SER	-	linker	UNP O66529
CB	77	GLY	-	linker	UNP O66529
CB	78	SER	-	linker	UNP O66529
CB	79	SER	-	linker	UNP O66529
CB	80	MET	-	linker	UNP O66529
CB	81	GLU	-	linker	UNP O66529
DB	1	MET	-	initiating methionine	UNP O66529
DB	72	GLY	-	linker	UNP O66529
DB	73	THR	-	linker	UNP O66529
DB	74	GLY	-	linker	UNP O66529
DB	75	GLY	-	linker	UNP O66529
DB	76	SER	-	linker	UNP O66529
DB	77	GLY	-	linker	UNP O66529
DB	78	SER	-	linker	UNP O66529
DB	79	SER	-	linker	UNP O66529
DB	80	MET	-	linker	UNP O66529
DB	81	GLU	-	linker	UNP O66529
EB	1	MET	-	initiating methionine	UNP O66529
EB	72	GLY	-	linker	UNP O66529
EB	73	THR	-	linker	UNP O66529
EB	74	GLY	-	linker	UNP O66529
EB	75	GLY	-	linker	UNP O66529
EB	76	SER	-	linker	UNP O66529
EB	77	GLY	-	linker	UNP O66529
EB	78	SER	-	linker	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
EB	79	SER	-	linker	UNP O66529
EB	80	MET	-	linker	UNP O66529
EB	81	GLU	-	linker	UNP O66529
FB	1	MET	-	initiating methionine	UNP O66529
FB	72	GLY	-	linker	UNP O66529
FB	73	THR	-	linker	UNP O66529
FB	74	GLY	-	linker	UNP O66529
FB	75	GLY	-	linker	UNP O66529
FB	76	SER	-	linker	UNP O66529
FB	77	GLY	-	linker	UNP O66529
FB	78	SER	-	linker	UNP O66529
FB	79	SER	-	linker	UNP O66529
FB	80	MET	-	linker	UNP O66529
FB	81	GLU	-	linker	UNP O66529
GB	1	MET	-	initiating methionine	UNP O66529
GB	72	GLY	-	linker	UNP O66529
GB	73	THR	-	linker	UNP O66529
GB	74	GLY	-	linker	UNP O66529
GB	75	GLY	-	linker	UNP O66529
GB	76	SER	-	linker	UNP O66529
GB	77	GLY	-	linker	UNP O66529
GB	78	SER	-	linker	UNP O66529
GB	79	SER	-	linker	UNP O66529
GB	80	MET	-	linker	UNP O66529
GB	81	GLU	-	linker	UNP O66529
HB	1	MET	-	initiating methionine	UNP O66529
HB	72	GLY	-	linker	UNP O66529
HB	73	THR	-	linker	UNP O66529
HB	74	GLY	-	linker	UNP O66529
HB	75	GLY	-	linker	UNP O66529
HB	76	SER	-	linker	UNP O66529
HB	77	GLY	-	linker	UNP O66529
HB	78	SER	-	linker	UNP O66529
HB	79	SER	-	linker	UNP O66529
HB	80	MET	-	linker	UNP O66529
HB	81	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:  94%



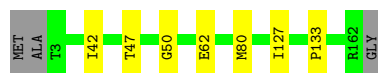
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B:  94%



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

Chain C:  94%



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

Chain D:  94%



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

Chain E:  94%



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

Chain F:  94%



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

Chain G:  94%



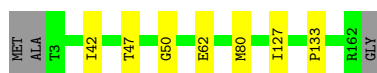
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain H:  94%



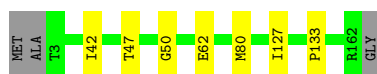
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain I:  94%



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

Chain J:  94%



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

Chain K:  94%



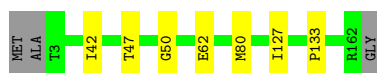
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain L:  94%



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

Chain M:  94%



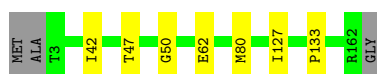
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain N: 94%



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

Chain O: 94%



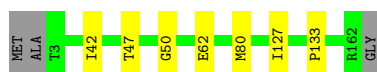
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain P: 93% 5%



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

Chain Q: 94%



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

Chain R: 94%



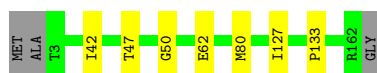
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain S: 94%



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

Chain T: 94%



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

Chain U: 94%



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

Chain V: 94%



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

Chain W: 93%



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

Chain X: 95%



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

Chain Y: 95%



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

Chain Z: 94%



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

Chain AA: 93%



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

Chain BA: 94%



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

Chain CA: 94%



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

Chain DA: 94%



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

Chain EA: 94%



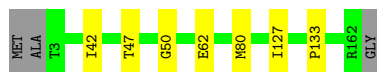
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FA: 94%



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

Chain GA: 94%



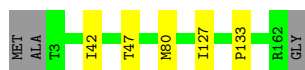
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HA: 94%



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

Chain IA:  95%



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

Chain JA:  94%



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

Chain KA:  94%



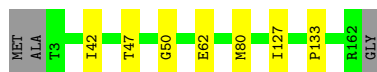
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LA:  94%



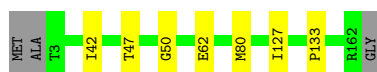
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MA:  94%



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

Chain NA:  94%



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

Chain OA:  94%



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

Chain PA:  94%



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

Chain QA:  94%



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

Chain RA:  94%



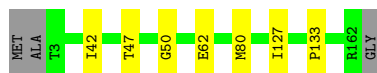
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain SA:  94%



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

Chain TA:  94%



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

Chain UA:  94%



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

Chain VA:  94%



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

Chain WA:  94%



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

Chain XA:  94%



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

Chain YA:  94%



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

Chain ZA:  94%



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

Chain AB:  94%



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

Chain BB:  94%



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

Chain CB:  94%





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

Chain DB:  94%



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

Chain EB:  94%



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

Chain FB:  94%



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

Chain GB:  94%



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

Chain HB:  94%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	98492	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.24	0/1226	0.52	0/1655
1	AA	0.24	0/1226	0.53	0/1655
1	AB	0.24	0/1226	0.52	0/1655
1	B	0.24	0/1226	0.53	0/1655
1	BA	0.24	0/1226	0.52	0/1655
1	BB	0.24	0/1226	0.52	0/1655
1	C	0.24	0/1226	0.52	0/1655
1	CA	0.24	0/1226	0.52	0/1655
1	CB	0.24	0/1226	0.52	0/1655
1	D	0.24	0/1226	0.52	0/1655
1	DA	0.24	0/1226	0.52	0/1655
1	DB	0.24	0/1226	0.52	0/1655
1	E	0.24	0/1226	0.52	0/1655
1	EA	0.24	0/1226	0.52	0/1655
1	EB	0.24	0/1226	0.52	0/1655
1	F	0.24	0/1226	0.52	0/1655
1	FA	0.24	0/1226	0.53	0/1655
1	FB	0.24	0/1226	0.52	0/1655
1	G	0.24	0/1226	0.52	0/1655
1	GA	0.24	0/1226	0.53	0/1655
1	GB	0.24	0/1226	0.53	0/1655
1	H	0.24	0/1226	0.52	0/1655
1	HA	0.24	0/1226	0.52	0/1655
1	HB	0.24	0/1226	0.53	0/1655
1	I	0.24	0/1226	0.52	0/1655
1	IA	0.24	0/1226	0.52	0/1655
1	J	0.24	0/1226	0.53	0/1655
1	JA	0.24	0/1226	0.52	0/1655
1	K	0.24	0/1226	0.52	0/1655
1	KA	0.24	0/1226	0.53	0/1655
1	L	0.24	0/1226	0.53	0/1655
1	LA	0.24	0/1226	0.52	0/1655
1	M	0.24	0/1226	0.53	0/1655
1	MA	0.24	0/1226	0.52	0/1655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	N	0.24	0/1226	0.53	0/1655
1	NA	0.24	0/1226	0.52	0/1655
1	O	0.24	0/1226	0.52	0/1655
1	OA	0.24	0/1226	0.52	0/1655
1	P	0.24	0/1226	0.52	0/1655
1	PA	0.24	0/1226	0.53	0/1655
1	Q	0.24	0/1226	0.53	0/1655
1	QA	0.24	0/1226	0.52	0/1655
1	R	0.24	0/1226	0.52	0/1655
1	RA	0.24	0/1226	0.53	0/1655
1	S	0.24	0/1226	0.53	0/1655
1	SA	0.24	0/1226	0.52	0/1655
1	T	0.24	0/1226	0.53	0/1655
1	TA	0.24	0/1226	0.52	0/1655
1	U	0.24	0/1226	0.52	0/1655
1	UA	0.24	0/1226	0.53	0/1655
1	V	0.24	0/1226	0.53	0/1655
1	VA	0.24	0/1226	0.52	0/1655
1	W	0.24	0/1226	0.52	0/1655
1	WA	0.24	0/1226	0.53	0/1655
1	X	0.24	0/1226	0.52	0/1655
1	XA	0.24	0/1226	0.52	0/1655
1	Y	0.24	0/1226	0.53	0/1655
1	YA	0.24	0/1226	0.53	0/1655
1	Z	0.24	0/1226	0.52	0/1655
1	ZA	0.24	0/1226	0.53	0/1655
All	All	0.24	0/73560	0.52	0/99300

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	1208	0	1224	11	0
1	AA	1208	0	1224	11	0
1	AB	1208	0	1224	8	0
1	B	1208	0	1224	12	0
1	BA	1208	0	1224	7	0
1	BB	1208	0	1224	7	0
1	C	1208	0	1224	9	0
1	CA	1208	0	1224	6	0
1	CB	1208	0	1224	7	0
1	D	1208	0	1224	6	0
1	DA	1208	0	1224	7	0
1	DB	1208	0	1224	9	0
1	E	1208	0	1224	8	0
1	EA	1208	0	1224	9	0
1	EB	1208	0	1224	9	0
1	F	1208	0	1224	9	0
1	FA	1208	0	1224	9	0
1	FB	1208	0	1224	7	0
1	G	1208	0	1224	10	0
1	GA	1208	0	1224	8	0
1	GB	1208	0	1224	7	0
1	H	1208	0	1224	8	0
1	HA	1208	0	1224	6	0
1	HB	1208	0	1224	7	0
1	I	1208	0	1224	7	0
1	IA	1208	0	1224	5	0
1	J	1208	0	1224	7	0
1	JA	1208	0	1224	11	0
1	K	1208	0	1224	9	0
1	KA	1208	0	1224	10	0
1	L	1208	0	1224	9	0
1	LA	1208	0	1224	8	0
1	M	1208	0	1224	9	0
1	MA	1208	0	1224	8	0
1	N	1208	0	1224	7	0
1	NA	1208	0	1224	8	0
1	O	1208	0	1224	7	0
1	OA	1208	0	1224	10	0
1	P	1208	0	1224	12	0
1	PA	1208	0	1224	11	0
1	Q	1208	0	1224	11	0
1	QA	1208	0	1224	8	0
1	R	1208	0	1224	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	1208	0	1224	7	0
1	S	1208	0	1224	6	0
1	SA	1208	0	1224	6	0
1	T	1208	0	1224	8	0
1	TA	1208	0	1224	11	0
1	U	1208	0	1224	10	0
1	UA	1208	0	1224	10	0
1	V	1208	0	1224	9	0
1	VA	1208	0	1224	7	0
1	W	1208	0	1224	9	0
1	WA	1208	0	1224	6	0
1	X	1208	0	1224	5	0
1	XA	1208	0	1224	6	0
1	Y	1208	0	1224	6	0
1	YA	1208	0	1224	9	0
1	Z	1208	0	1224	10	0
1	ZA	1208	0	1224	9	0
All	All	72480	0	73440	292	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (292) 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:S:42:ILE:O	1:S:47:THR:OG1	2.20	0.60
1:K:127:ILE:HG22	1:L:80:MET:HE2	1.83	0.60
1:DB:127:ILE:HG22	1:EB:80:MET:HE2	1.84	0.59
1:XA:42:ILE:O	1:XA:47:THR:OG1	2.20	0.59
1:ZA:42:ILE:O	1:ZA:47:THR:OG1	2.20	0.59
1:CB:42:ILE:O	1:CB:47:THR:OG1	2.20	0.59
1:QA:42:ILE:O	1:QA:47:THR:OG1	2.20	0.59
1:BB:42:ILE:O	1:BB:47:THR:OG1	2.20	0.59
1:VA:42:ILE:O	1:VA:47:THR:OG1	2.20	0.59
1:F:127:ILE:HG22	1:G:80:MET:HE2	1.84	0.59
1:T:42:ILE:O	1:T:47:THR:OG1	2.20	0.59
1:V:42:ILE:O	1:V:47:THR:OG1	2.20	0.58
1:BA:42:ILE:O	1:BA:47:THR:OG1	2.20	0.58
1:X:42:ILE:O	1:X:47:THR:OG1	2.20	0.58
1:Z:42:ILE:O	1:Z:47:THR:OG1	2.20	0.58
1:JA:42:ILE:O	1:JA:47:THR:OG1	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:127:ILE:HG22	1:ZA:80:MET:HE2	1.85	0.58
1:P:127:ILE:HG22	1:Q:80:MET:HE2	1.85	0.58
1:J:42:ILE:O	1:J:47:THR:OG1	2.20	0.57
1:RA:42:ILE:O	1:RA:47:THR:OG1	2.20	0.57
1:TA:127:ILE:HG22	1:UA:80:MET:HE2	1.87	0.57
1:U:42:ILE:O	1:U:47:THR:OG1	2.20	0.57
1:P:42:ILE:O	1:P:47:THR:OG1	2.20	0.57
1:GB:42:ILE:O	1:GB:47:THR:OG1	2.20	0.57
1:DA:42:ILE:O	1:DA:47:THR:OG1	2.20	0.57
1:L:42:ILE:O	1:L:47:THR:OG1	2.20	0.57
1:I:42:ILE:O	1:I:47:THR:OG1	2.20	0.57
1:FB:42:ILE:O	1:FB:47:THR:OG1	2.20	0.57
1:MA:42:ILE:O	1:MA:47:THR:OG1	2.20	0.57
1:UA:42:ILE:O	1:UA:47:THR:OG1	2.20	0.57
1:YA:42:ILE:O	1:YA:47:THR:OG1	2.20	0.57
1:H:42:ILE:O	1:H:47:THR:OG1	2.20	0.56
1:C:42:ILE:O	1:C:47:THR:OG1	2.20	0.56
1:EB:42:ILE:O	1:EB:47:THR:OG1	2.20	0.56
1:HA:42:ILE:O	1:HA:47:THR:OG1	2.20	0.56
1:D:42:ILE:O	1:D:47:THR:OG1	2.20	0.56
1:OA:127:ILE:HG22	1:PA:80:MET:HE2	1.87	0.56
1:G:42:ILE:O	1:G:47:THR:OG1	2.20	0.56
1:N:42:ILE:O	1:N:47:THR:OG1	2.20	0.56
1:IA:42:ILE:O	1:IA:47:THR:OG1	2.20	0.56
1:JA:127:ILE:HG22	1:KA:80:MET:HE2	1.88	0.56
1:OA:42:ILE:O	1:OA:47:THR:OG1	2.20	0.55
1:DB:42:ILE:O	1:DB:47:THR:OG1	2.20	0.55
1:U:127:ILE:HG22	1:V:80:MET:HE2	1.87	0.55
1:Z:127:ILE:HG22	1:AA:80:MET:HE2	1.88	0.55
1:W:42:ILE:O	1:W:47:THR:OG1	2.20	0.55
1:AA:42:ILE:O	1:AA:47:THR:OG1	2.20	0.55
1:EA:127:ILE:HG22	1:FA:80:MET:HE2	1.88	0.55
1:R:42:ILE:O	1:R:47:THR:OG1	2.20	0.55
1:PA:42:ILE:O	1:PA:47:THR:OG1	2.20	0.55
1:A:127:ILE:HG22	1:B:80:MET:HE2	1.88	0.55
1:M:42:ILE:O	1:M:47:THR:OG1	2.20	0.55
1:O:42:ILE:O	1:O:47:THR:OG1	2.20	0.54
1:NA:42:ILE:O	1:NA:47:THR:OG1	2.20	0.54
1:KA:42:ILE:O	1:KA:47:THR:OG1	2.20	0.54
1:A:42:ILE:O	1:A:47:THR:OG1	2.20	0.54
1:FA:42:ILE:O	1:FA:47:THR:OG1	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:42:ILE:O	1:SA:47:THR:OG1	2.20	0.54
1:WA:42:ILE:O	1:WA:47:THR:OG1	2.20	0.54
1:Q:42:ILE:O	1:Q:47:THR:OG1	2.20	0.54
1:F:42:ILE:O	1:F:47:THR:OG1	2.20	0.54
1:JA:80:MET:HE2	1:NA:127:ILE:HG22	1.89	0.54
1:AB:42:ILE:O	1:AB:47:THR:OG1	2.20	0.54
1:Y:42:ILE:O	1:Y:47:THR:OG1	2.20	0.54
1:HB:42:ILE:O	1:HB:47:THR:OG1	2.20	0.54
1:K:42:ILE:O	1:K:47:THR:OG1	2.20	0.53
1:LA:42:ILE:O	1:LA:47:THR:OG1	2.20	0.53
1:CA:42:ILE:O	1:CA:47:THR:OG1	2.20	0.53
1:TA:42:ILE:O	1:TA:47:THR:OG1	2.20	0.53
1:EA:80:MET:HE2	1:IA:127:ILE:HG22	1.91	0.53
1:BA:127:ILE:HG22	1:CA:80:MET:HE2	1.91	0.53
1:GA:42:ILE:O	1:GA:47:THR:OG1	2.20	0.53
1:B:42:ILE:O	1:B:47:THR:OG1	2.20	0.53
1:U:80:MET:HE2	1:Y:127:ILE:HG22	1.91	0.53
1:E:42:ILE:O	1:E:47:THR:OG1	2.20	0.53
1:EA:42:ILE:O	1:EA:47:THR:OG1	2.20	0.53
1:M:127:ILE:HG22	1:N:80:MET:HE2	1.91	0.52
1:YA:80:MET:HE2	1:CB:127:ILE:HG22	1.91	0.52
1:DB:80:MET:HE2	1:HB:127:ILE:HG22	1.92	0.52
1:F:80:MET:HE2	1:J:127:ILE:HG22	1.92	0.52
1:OA:80:MET:HE2	1:SA:127:ILE:HG22	1.92	0.52
1:TA:80:MET:HE2	1:XA:127:ILE:HG22	1.92	0.52
1:EA:127:ILE:CG2	1:FA:80:MET:CE	2.88	0.52
1:YA:127:ILE:CG2	1:ZA:80:MET:CE	2.88	0.52
1:AB:127:ILE:HG22	1:BB:80:MET:HE2	1.92	0.52
1:G:127:ILE:HG22	1:H:80:MET:HE2	1.92	0.51
1:K:127:ILE:CG2	1:L:80:MET:CE	2.88	0.51
1:DB:127:ILE:CG2	1:EB:80:MET:CE	2.88	0.51
1:F:127:ILE:CG2	1:G:80:MET:CE	2.89	0.51
1:Z:127:ILE:CG2	1:AA:80:MET:CE	2.88	0.51
1:TA:127:ILE:CG2	1:UA:80:MET:CE	2.88	0.51
1:K:80:MET:HE2	1:O:127:ILE:HG22	1.92	0.51
1:U:127:ILE:CG2	1:V:80:MET:CE	2.88	0.51
1:JA:127:ILE:CG2	1:KA:80:MET:CE	2.88	0.51
1:P:127:ILE:CG2	1:Q:80:MET:CE	2.88	0.51
1:LA:127:ILE:HG22	1:MA:80:MET:HE2	1.93	0.51
1:UA:127:ILE:HG22	1:VA:80:MET:HE2	1.92	0.50
1:A:127:ILE:CG2	1:B:80:MET:CE	2.88	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:127:ILE:CG2	1:PA:80:MET:CE	2.88	0.50
1:WA:127:ILE:HG22	1:XA:80:MET:HE2	1.94	0.50
1:K:127:ILE:CG2	1:L:80:MET:HE2	2.42	0.49
1:F:127:ILE:CG2	1:G:80:MET:HE2	2.42	0.49
1:CA:127:ILE:HG22	1:DA:80:MET:HE2	1.95	0.49
1:V:127:ILE:HG22	1:W:80:MET:HE2	1.95	0.49
1:FB:127:ILE:HG22	1:GB:80:MET:HE2	1.95	0.48
1:R:127:ILE:HG22	1:S:80:MET:HE2	1.95	0.48
1:EB:127:ILE:HG22	1:FB:80:MET:HE2	1.94	0.48
1:A:62:GLU:OE1	1:E:133:PRO:HD3	2.14	0.48
1:U:62:GLU:OE1	1:Y:133:PRO:HD3	2.14	0.48
1:ZA:127:ILE:HG22	1:AB:80:MET:HE2	1.96	0.48
1:D:127:ILE:HG22	1:E:80:MET:HE2	1.96	0.48
1:Z:62:GLU:OE1	1:DA:133:PRO:HD3	2.14	0.48
1:OA:62:GLU:OE1	1:SA:133:PRO:HD3	2.14	0.48
1:K:62:GLU:OE1	1:O:133:PRO:HD3	2.14	0.48
1:JA:62:GLU:OE1	1:NA:133:PRO:HD3	2.14	0.48
1:YA:62:GLU:OE1	1:CB:133:PRO:HD3	2.14	0.48
1:YA:127:ILE:CG2	1:ZA:80:MET:HE2	2.44	0.48
1:F:62:GLU:OE1	1:J:133:PRO:HD3	2.14	0.48
1:EA:62:GLU:OE1	1:IA:133:PRO:HD3	2.14	0.48
1:TA:62:GLU:OE1	1:XA:133:PRO:HD3	2.14	0.48
1:DB:127:ILE:CG2	1:EB:80:MET:HE2	2.43	0.48
1:GB:127:ILE:HG22	1:HB:80:MET:HE2	1.95	0.47
1:H:127:ILE:HG22	1:I:80:MET:HE2	1.95	0.47
1:P:80:MET:HE2	1:T:127:ILE:HG22	1.97	0.47
1:AA:127:ILE:HG22	1:BA:80:MET:HE2	1.96	0.47
1:I:127:ILE:HG22	1:J:80:MET:HE2	1.97	0.47
1:Z:80:MET:HE2	1:DA:127:ILE:HG22	1.97	0.47
1:BB:127:ILE:HG22	1:CB:80:MET:HE2	1.96	0.47
1:S:127:ILE:HG22	1:T:80:MET:HE2	1.97	0.47
1:DB:62:GLU:OE1	1:HB:133:PRO:HD3	2.14	0.47
1:P:62:GLU:OE1	1:T:133:PRO:HD3	2.14	0.47
1:FA:127:ILE:HG22	1:GA:80:MET:HE2	1.96	0.46
1:KA:127:ILE:HG22	1:LA:80:MET:HE2	1.96	0.46
1:JA:127:ILE:HG21	1:KA:80:MET:HE3	1.98	0.46
1:RA:127:ILE:HG22	1:SA:80:MET:HE2	1.97	0.46
1:L:127:ILE:HG22	1:M:80:MET:HE2	1.98	0.46
1:PA:127:ILE:HG22	1:QA:80:MET:HE2	1.98	0.46
1:U:127:ILE:HG21	1:V:80:MET:HE3	1.98	0.46
1:OA:127:ILE:HG21	1:PA:80:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:127:ILE:HG21	1:AA:80:MET:HE3	1.97	0.46
1:P:127:ILE:CG2	1:Q:80:MET:HE2	2.45	0.45
1:A:127:ILE:HG21	1:B:80:MET:HE3	1.98	0.45
1:Q:127:ILE:HG22	1:R:80:MET:HE2	1.98	0.45
1:QA:127:ILE:HG22	1:RA:80:MET:HE2	1.98	0.45
1:VA:127:ILE:HG22	1:WA:80:MET:HE2	1.98	0.45
1:C:127:ILE:HG22	1:D:80:MET:HE2	1.98	0.45
1:U:133:PRO:HD3	1:V:62:GLU:OE1	2.17	0.45
1:W:127:ILE:HG22	1:X:80:MET:HE2	1.98	0.45
1:Z:133:PRO:HD3	1:AA:62:GLU:OE1	2.17	0.45
1:EA:127:ILE:HG21	1:FA:80:MET:HE3	1.97	0.45
1:TA:133:PRO:HD3	1:UA:62:GLU:OE1	2.17	0.45
1:YA:133:PRO:HD3	1:ZA:62:GLU:OE1	2.17	0.45
1:DB:133:PRO:HD3	1:EB:62:GLU:OE1	2.17	0.45
1:JA:133:PRO:HD3	1:KA:62:GLU:OE1	2.17	0.45
1:A:80:MET:HE2	1:E:127:ILE:HG22	1.97	0.45
1:BA:127:ILE:CG2	1:CA:80:MET:HE2	2.47	0.45
1:N:127:ILE:HG22	1:O:80:MET:HE2	1.99	0.45
1:OA:133:PRO:HD3	1:PA:62:GLU:OE1	2.17	0.45
1:F:133:PRO:HD3	1:G:62:GLU:OE1	2.17	0.44
1:A:133:PRO:HD3	1:B:62:GLU:OE1	2.17	0.44
1:TA:127:ILE:CG2	1:UA:80:MET:HE2	2.47	0.44
1:P:133:PRO:HD3	1:Q:62:GLU:OE1	2.17	0.44
1:EA:133:PRO:HD3	1:FA:62:GLU:OE1	2.17	0.44
1:TA:127:ILE:HG21	1:UA:80:MET:HE3	1.99	0.44
1:HA:127:ILE:HG22	1:IA:80:MET:HE2	2.00	0.44
1:PA:133:PRO:HD3	1:QA:62:GLU:OE1	2.18	0.44
1:B:127:ILE:HG22	1:C:80:MET:HE2	2.00	0.44
1:KA:133:PRO:HD3	1:LA:62:GLU:OE1	2.18	0.44
1:P:127:ILE:HG21	1:Q:80:MET:HE3	2.00	0.44
1:Q:133:PRO:HD3	1:R:62:GLU:OE1	2.18	0.44
1:Z:127:ILE:CG2	1:AA:80:MET:HE3	2.48	0.44
1:EB:133:PRO:HD3	1:FB:62:GLU:OE1	2.18	0.44
1:L:133:PRO:HD3	1:M:62:GLU:OE1	2.18	0.43
1:V:133:PRO:HD3	1:W:62:GLU:OE1	2.18	0.43
1:EA:127:ILE:CG2	1:FA:80:MET:HE3	2.48	0.43
1:K:133:PRO:HD3	1:L:62:GLU:OE1	2.17	0.43
1:JA:80:MET:HE2	1:NA:127:ILE:CG2	2.48	0.43
1:YA:127:ILE:HG21	1:ZA:80:MET:HE3	2.00	0.43
1:AA:133:PRO:HD3	1:BA:62:GLU:OE1	2.18	0.43
1:ZA:133:PRO:HD3	1:AB:62:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UA:133:PRO:HD3	1:VA:62:GLU:OE1	2.18	0.43
1:H:133:PRO:HD3	1:I:62:GLU:OE1	2.19	0.43
1:DB:127:ILE:HG21	1:EB:80:MET:HE3	2.01	0.43
1:G:133:PRO:HD3	1:H:62:GLU:OE1	2.18	0.43
1:UA:127:ILE:CG2	1:VA:80:MET:CE	2.97	0.43
1:B:127:ILE:CG2	1:C:80:MET:CE	2.97	0.43
1:G:127:ILE:CG2	1:H:80:MET:CE	2.97	0.43
1:M:127:ILE:CG2	1:N:80:MET:HE2	2.48	0.43
1:BA:133:PRO:HD3	1:CA:62:GLU:OE1	2.19	0.43
1:FB:133:PRO:HD3	1:GB:62:GLU:OE1	2.19	0.43
1:R:133:PRO:HD3	1:S:62:GLU:OE1	2.19	0.43
1:EB:127:ILE:CG2	1:FB:80:MET:CE	2.97	0.43
1:L:127:ILE:CG2	1:M:80:MET:CE	2.97	0.43
1:Q:127:ILE:CG2	1:R:80:MET:CE	2.97	0.43
1:JA:127:ILE:CG2	1:KA:80:MET:HE3	2.49	0.43
1:KA:127:ILE:CG2	1:LA:80:MET:CE	2.97	0.43
1:M:133:PRO:HD3	1:N:62:GLU:OE1	2.19	0.42
1:W:133:PRO:HD3	1:X:62:GLU:OE1	2.19	0.42
1:AA:127:ILE:CG2	1:BA:80:MET:CE	2.97	0.42
1:FA:133:PRO:HD3	1:GA:62:GLU:OE1	2.18	0.42
1:ZA:127:ILE:CG2	1:AB:80:MET:CE	2.97	0.42
1:E:47:THR:O	1:E:50:GLY:N	2.46	0.42
1:I:47:THR:O	1:I:50:GLY:N	2.46	0.42
1:K:127:ILE:HG21	1:L:80:MET:HE3	2.01	0.42
1:U:80:MET:CE	1:Y:127:ILE:CG2	2.98	0.42
1:LA:133:PRO:HD3	1:MA:62:GLU:OE1	2.19	0.42
1:AB:133:PRO:HD3	1:BB:62:GLU:OE1	2.19	0.42
1:A:80:MET:CE	1:E:127:ILE:CG2	2.98	0.42
1:F:80:MET:CE	1:J:127:ILE:CG2	2.98	0.42
1:F:127:ILE:HG21	1:G:80:MET:HE3	2.01	0.42
1:MA:127:ILE:HG22	1:NA:80:MET:HE2	2.02	0.42
1:PA:127:ILE:CG2	1:QA:80:MET:CE	2.97	0.42
1:VA:133:PRO:HD3	1:WA:62:GLU:OE1	2.19	0.42
1:YA:80:MET:CE	1:CB:127:ILE:CG2	2.98	0.42
1:K:80:MET:CE	1:O:127:ILE:CG2	2.98	0.42
1:P:80:MET:CE	1:T:127:ILE:CG2	2.98	0.42
1:RA:47:THR:O	1:RA:50:GLY:N	2.46	0.42
1:B:133:PRO:HD3	1:C:62:GLU:OE1	2.18	0.42
1:V:127:ILE:CG2	1:W:80:MET:CE	2.97	0.42
1:JA:127:ILE:CG2	1:KA:80:MET:HE2	2.49	0.42
1:A:127:ILE:CG2	1:B:80:MET:HE2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:47:THR:O	1:M:50:GLY:N	2.46	0.42
1:U:127:ILE:CG2	1:V:80:MET:HE3	2.50	0.42
1:P:47:THR:O	1:P:50:GLY:N	2.46	0.42
1:FA:127:ILE:CG2	1:GA:80:MET:CE	2.97	0.42
1:OA:127:ILE:CG2	1:PA:80:MET:HE3	2.50	0.42
1:QA:133:PRO:HD3	1:RA:62:GLU:OE1	2.19	0.42
1:C:133:PRO:HD3	1:D:62:GLU:OE1	2.19	0.42
1:GA:127:ILE:HG22	1:HA:80:MET:HE2	2.01	0.42
1:SA:47:THR:O	1:SA:50:GLY:N	2.46	0.42
1:P:80:MET:HE3	1:T:127:ILE:HG21	2.02	0.42
1:W:47:THR:O	1:W:50:GLY:N	2.46	0.42
1:GA:133:PRO:HD3	1:HA:62:GLU:OE1	2.19	0.42
1:NA:47:THR:O	1:NA:50:GLY:N	2.46	0.42
1:OA:127:ILE:CG2	1:PA:80:MET:HE2	2.48	0.42
1:B:47:THR:O	1:B:50:GLY:N	2.46	0.41
1:EA:80:MET:CE	1:IA:127:ILE:CG2	2.98	0.41
1:OA:80:MET:CE	1:SA:127:ILE:CG2	2.98	0.41
1:TA:80:MET:CE	1:XA:127:ILE:CG2	2.98	0.41
1:Q:47:THR:O	1:Q:50:GLY:N	2.46	0.41
1:AA:47:THR:O	1:AA:50:GLY:N	2.46	0.41
1:DB:80:MET:CE	1:HB:127:ILE:CG2	2.98	0.41
1:JA:80:MET:CE	1:NA:127:ILE:CG2	2.98	0.41
1:QA:47:THR:O	1:QA:50:GLY:N	2.46	0.41
1:Z:80:MET:HE3	1:DA:127:ILE:HG21	2.02	0.41
1:Z:80:MET:CE	1:DA:127:ILE:CG2	2.98	0.41
1:S:133:PRO:HD3	1:T:62:GLU:OE1	2.21	0.41
1:X:133:PRO:HD3	1:Y:62:GLU:OE1	2.21	0.41
1:GA:47:THR:O	1:GA:50:GLY:N	2.46	0.41
1:AB:127:ILE:CG2	1:BB:80:MET:HE2	2.50	0.41
1:I:133:PRO:HD3	1:J:62:GLU:OE1	2.21	0.41
1:MA:133:PRO:HD3	1:NA:62:GLU:OE1	2.21	0.41
1:QA:127:ILE:CG2	1:RA:80:MET:CE	2.99	0.41
1:AB:127:ILE:CG2	1:BB:80:MET:CE	2.99	0.41
1:A:80:MET:HE3	1:E:127:ILE:HG21	2.02	0.41
1:A:127:ILE:CG2	1:B:80:MET:HE3	2.49	0.41
1:T:47:THR:O	1:T:50:GLY:N	2.46	0.41
1:GA:127:ILE:CG2	1:HA:80:MET:CE	2.99	0.41
1:LA:127:ILE:CG2	1:MA:80:MET:CE	2.99	0.41
1:D:133:PRO:HD3	1:E:62:GLU:OE1	2.21	0.41
1:C:47:THR:O	1:C:50:GLY:N	2.46	0.41
1:H:127:ILE:CG2	1:I:80:MET:CE	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:47:THR:O	1:J:50:GLY:N	2.46	0.41
1:N:133:PRO:HD3	1:O:62:GLU:OE1	2.21	0.41
1:U:80:MET:HE2	1:Y:127:ILE:CG2	2.51	0.41
1:CA:133:PRO:HD3	1:DA:62:GLU:OE1	2.21	0.41
1:MA:47:THR:O	1:MA:50:GLY:N	2.46	0.41
1:TA:47:THR:O	1:TA:50:GLY:N	2.46	0.41
1:WA:133:PRO:HD3	1:XA:62:GLU:OE1	2.21	0.41
1:CB:47:THR:O	1:CB:50:GLY:N	2.46	0.41
1:GB:133:PRO:HD3	1:HB:62:GLU:OE1	2.21	0.41
1:W:127:ILE:CG2	1:X:80:MET:CE	2.99	0.41
1:BB:133:PRO:HD3	1:CB:62:GLU:OE1	2.21	0.41
1:Q:127:ILE:HG21	1:R:80:MET:HE3	2.03	0.40
1:HA:47:THR:O	1:HA:50:GLY:N	2.46	0.40
1:LA:127:ILE:CG2	1:MA:80:MET:HE2	2.51	0.40
1:GB:47:THR:O	1:GB:50:GLY:N	2.46	0.40
1:S:7:ASP:OD1	1:S:7:ASP:N	2.55	0.40
1:PA:7:ASP:OD1	1:PA:7:ASP:N	2.55	0.40
1:TA:127:ILE:CG2	1:UA:80:MET:HE3	2.51	0.40
1:VA:127:ILE:CG2	1:WA:80:MET:CE	2.99	0.40
1:B:127:ILE:CG2	1:C:80:MET:HE3	2.52	0.40
1:RA:7:ASP:OD1	1:RA:7:ASP:N	2.55	0.40
1:G:127:ILE:CG2	1:H:80:MET:HE2	2.51	0.40
1:P:7:ASP:OD1	1:P:7:ASP:N	2.55	0.40
1:W:7:ASP:N	1:W:7:ASP:OD1	2.55	0.40
1:FB:127:ILE:CG2	1:GB:80:MET:CE	2.99	0.40
1:C:127:ILE:CG2	1:D:80:MET:CE	2.99	0.40
1:M:127:ILE:CG2	1:N:80:MET:CE	2.99	0.40
1:O:47:THR:O	1:O:50:GLY:N	2.46	0.40
1:AA:7:ASP:N	1:AA:7:ASP:OD1	2.55	0.40
1:HB:7:ASP:OD1	1:HB:7:ASP:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	AA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	AB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	B	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	BA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	BB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	C	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	CA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	CB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	D	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	DA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	DB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	E	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	EA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	EB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	F	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	FA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	FB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	G	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	GA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	GB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	H	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	HA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	HB	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	I	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	IA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	J	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	JA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	K	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	KA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	LA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	M	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	MA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	N	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	NA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	O	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	OA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	P	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	PA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	Q	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	QA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	R	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	RA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	S	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	SA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	T	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	TA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	U	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	UA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	V	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	VA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	W	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	WA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	X	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	XA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	Y	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	YA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	Z	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
1	ZA	158/163 (97%)	155 (98%)	3 (2%)	0	100	100
All	All	9480/9780 (97%)	9300 (98%)	180 (2%)	0	100	100



There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	124/125 (99%)	124 (100%)	0	100	100
1	AA	124/125 (99%)	124 (100%)	0	100	100
1	AB	124/125 (99%)	124 (100%)	0	100	100
1	B	124/125 (99%)	124 (100%)	0	100	100
1	BA	124/125 (99%)	124 (100%)	0	100	100
1	BB	124/125 (99%)	124 (100%)	0	100	100
1	C	124/125 (99%)	124 (100%)	0	100	100
1	CA	124/125 (99%)	124 (100%)	0	100	100
1	CB	124/125 (99%)	124 (100%)	0	100	100
1	D	124/125 (99%)	124 (100%)	0	100	100
1	DA	124/125 (99%)	124 (100%)	0	100	100
1	DB	124/125 (99%)	124 (100%)	0	100	100
1	E	124/125 (99%)	124 (100%)	0	100	100
1	EA	124/125 (99%)	124 (100%)	0	100	100
1	EB	124/125 (99%)	124 (100%)	0	100	100
1	F	124/125 (99%)	124 (100%)	0	100	100
1	FA	124/125 (99%)	124 (100%)	0	100	100
1	FB	124/125 (99%)	124 (100%)	0	100	100
1	G	124/125 (99%)	124 (100%)	0	100	100
1	GA	124/125 (99%)	124 (100%)	0	100	100
1	GB	124/125 (99%)	124 (100%)	0	100	100
1	H	124/125 (99%)	124 (100%)	0	100	100
1	HA	124/125 (99%)	124 (100%)	0	100	100
1	HB	124/125 (99%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	124/125 (99%)	124 (100%)	0	100	100
1	IA	124/125 (99%)	124 (100%)	0	100	100
1	J	124/125 (99%)	124 (100%)	0	100	100
1	JA	124/125 (99%)	124 (100%)	0	100	100
1	K	124/125 (99%)	124 (100%)	0	100	100
1	KA	124/125 (99%)	124 (100%)	0	100	100
1	L	124/125 (99%)	124 (100%)	0	100	100
1	LA	124/125 (99%)	124 (100%)	0	100	100
1	M	124/125 (99%)	124 (100%)	0	100	100
1	MA	124/125 (99%)	124 (100%)	0	100	100
1	N	124/125 (99%)	124 (100%)	0	100	100
1	NA	124/125 (99%)	124 (100%)	0	100	100
1	O	124/125 (99%)	124 (100%)	0	100	100
1	OA	124/125 (99%)	124 (100%)	0	100	100
1	P	124/125 (99%)	124 (100%)	0	100	100
1	PA	124/125 (99%)	124 (100%)	0	100	100
1	Q	124/125 (99%)	124 (100%)	0	100	100
1	QA	124/125 (99%)	124 (100%)	0	100	100
1	R	124/125 (99%)	124 (100%)	0	100	100
1	RA	124/125 (99%)	124 (100%)	0	100	100
1	S	124/125 (99%)	124 (100%)	0	100	100
1	SA	124/125 (99%)	124 (100%)	0	100	100
1	T	124/125 (99%)	124 (100%)	0	100	100
1	TA	124/125 (99%)	124 (100%)	0	100	100
1	U	124/125 (99%)	124 (100%)	0	100	100
1	UA	124/125 (99%)	124 (100%)	0	100	100
1	V	124/125 (99%)	124 (100%)	0	100	100
1	VA	124/125 (99%)	124 (100%)	0	100	100
1	W	124/125 (99%)	124 (100%)	0	100	100
1	WA	124/125 (99%)	124 (100%)	0	100	100
1	X	124/125 (99%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	XA	124/125 (99%)	124 (100%)	0	100	100
1	Y	124/125 (99%)	124 (100%)	0	100	100
1	YA	124/125 (99%)	124 (100%)	0	100	100
1	Z	124/125 (99%)	124 (100%)	0	100	100
1	ZA	124/125 (99%)	124 (100%)	0	100	100
All	All	7440/7500 (99%)	7440 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	B	103	HIS
1	C	103	HIS
1	D	103	HIS
1	E	103	HIS
1	F	103	HIS
1	G	103	HIS
1	H	103	HIS
1	I	103	HIS
1	J	103	HIS
1	K	103	HIS
1	L	103	HIS
1	M	103	HIS
1	N	103	HIS
1	O	103	HIS
1	P	103	HIS
1	Q	103	HIS
1	R	103	HIS
1	S	103	HIS
1	T	103	HIS
1	U	103	HIS
1	V	103	HIS
1	W	103	HIS
1	X	103	HIS
1	Y	103	HIS
1	Z	103	HIS
1	AA	103	HIS
1	BA	103	HIS

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Mol	Chain	Res	Type
1	CA	103	HIS
1	DA	103	HIS
1	EA	103	HIS
1	FA	103	HIS
1	GA	103	HIS
1	HA	103	HIS
1	IA	103	HIS
1	JA	103	HIS
1	KA	103	HIS
1	LA	103	HIS
1	MA	103	HIS
1	NA	103	HIS
1	OA	103	HIS
1	PA	103	HIS
1	QA	103	HIS
1	RA	103	HIS
1	SA	103	HIS
1	TA	103	HIS
1	VA	103	HIS
1	WA	103	HIS
1	XA	103	HIS
1	YA	103	HIS
1	AB	103	HIS
1	BB	103	HIS
1	CB	103	HIS
1	DB	103	HIS
1	FB	103	HIS
1	GB	103	HIS
1	HB	103	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 [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.