



wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 01:48 am BST

PDB ID : 6HJM
Title : Myxococcus xanthus MglB
Authors : Varela, P.F.; Navaza, J.; Trapani, S.; Cherfils, J.
Deposited on : 2018-09-04
Resolution : 2.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

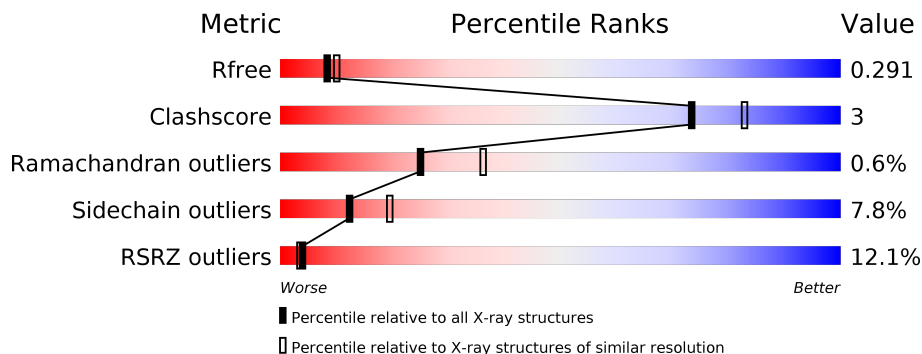
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	192	 3% 59% 7% 33%
1	B	192	 3% 56% 9% 34%
1	C	192	 5% 60% 5% 34%
1	D	192	 12% 55% 7% 38%
1	E	192	 5% 57% 6% 36%
1	F	192	 5% 58% 8% 34%

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Mol	Chain	Length	Quality of chain
1	G	192	
1	H	192	
1	I	192	
1	J	192	
1	K	192	
1	L	192	
1	M	192	
1	N	192	
1	O	192	
1	P	192	
1	Q	192	
1	R	192	
1	S	192	
1	T	192	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19326 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 MglB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	128	976	616	166	190	4	0	0	0
1	B	126	961	606	164	188	3	0	0	0
1	E	123	933	587	161	182	3	0	0	0
1	F	127	969	611	165	189	4	0	0	0
1	C	126	961	605	164	188	4	0	0	0
1	D	120	907	571	158	175	3	0	0	0
1	G	126	961	605	164	188	4	0	0	0
1	H	121	916	576	159	178	3	0	0	0
1	I	127	969	611	165	189	4	0	0	0
1	J	124	948	597	162	185	4	0	0	0
1	M	127	969	611	165	189	4	0	0	0
1	N	123	933	587	161	182	3	0	0	0
1	Q	125	949	597	163	186	3	0	0	0
1	R	125	954	600	163	187	4	0	0	0
1	K	119	901	568	157	173	3	0	0	0
1	L	125	954	601	163	187	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	O	122	925	581	160	181	3	0	0	0
1	P	133	1017	642	173	198	4	0	0	0
1	S	127	969	611	165	189	4	0	0	0
1	T	126	961	605	164	188	4	0	0	0

There are 680 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	initiating methionine	UNP Q50883
A	-31	GLY	-	expression tag	UNP Q50883
A	-30	SER	-	expression tag	UNP Q50883
A	-29	SER	-	expression tag	UNP Q50883
A	-28	HIS	-	expression tag	UNP Q50883
A	-27	HIS	-	expression tag	UNP Q50883
A	-26	HIS	-	expression tag	UNP Q50883
A	-25	HIS	-	expression tag	UNP Q50883
A	-24	HIS	-	expression tag	UNP Q50883
A	-23	HIS	-	expression tag	UNP Q50883
A	-22	SER	-	expression tag	UNP Q50883
A	-21	SER	-	expression tag	UNP Q50883
A	-20	GLY	-	expression tag	UNP Q50883
A	-19	LEU	-	expression tag	UNP Q50883
A	-18	VAL	-	expression tag	UNP Q50883
A	-17	PRO	-	expression tag	UNP Q50883
A	-16	ARG	-	expression tag	UNP Q50883
A	-15	GLY	-	expression tag	UNP Q50883
A	-14	SER	-	expression tag	UNP Q50883
A	-13	HIS	-	expression tag	UNP Q50883
A	-12	MET	-	expression tag	UNP Q50883
A	-11	ALA	-	expression tag	UNP Q50883
A	-10	SER	-	expression tag	UNP Q50883
A	-9	MET	-	expression tag	UNP Q50883
A	-8	THR	-	expression tag	UNP Q50883
A	-7	GLY	-	expression tag	UNP Q50883
A	-6	GLY	-	expression tag	UNP Q50883
A	-5	GLN	-	expression tag	UNP Q50883
A	-4	GLN	-	expression tag	UNP Q50883
A	-3	MET	-	expression tag	UNP Q50883
A	-2	GLY	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP Q50883
A	0	GLY	-	expression tag	UNP Q50883
A	1	SER	-	expression tag	UNP Q50883
B	-32	MET	-	initiating methionine	UNP Q50883
B	-31	GLY	-	expression tag	UNP Q50883
B	-30	SER	-	expression tag	UNP Q50883
B	-29	SER	-	expression tag	UNP Q50883
B	-28	HIS	-	expression tag	UNP Q50883
B	-27	HIS	-	expression tag	UNP Q50883
B	-26	HIS	-	expression tag	UNP Q50883
B	-25	HIS	-	expression tag	UNP Q50883
B	-24	HIS	-	expression tag	UNP Q50883
B	-23	HIS	-	expression tag	UNP Q50883
B	-22	SER	-	expression tag	UNP Q50883
B	-21	SER	-	expression tag	UNP Q50883
B	-20	GLY	-	expression tag	UNP Q50883
B	-19	LEU	-	expression tag	UNP Q50883
B	-18	VAL	-	expression tag	UNP Q50883
B	-17	PRO	-	expression tag	UNP Q50883
B	-16	ARG	-	expression tag	UNP Q50883
B	-15	GLY	-	expression tag	UNP Q50883
B	-14	SER	-	expression tag	UNP Q50883
B	-13	HIS	-	expression tag	UNP Q50883
B	-12	MET	-	expression tag	UNP Q50883
B	-11	ALA	-	expression tag	UNP Q50883
B	-10	SER	-	expression tag	UNP Q50883
B	-9	MET	-	expression tag	UNP Q50883
B	-8	THR	-	expression tag	UNP Q50883
B	-7	GLY	-	expression tag	UNP Q50883
B	-6	GLY	-	expression tag	UNP Q50883
B	-5	GLN	-	expression tag	UNP Q50883
B	-4	GLN	-	expression tag	UNP Q50883
B	-3	MET	-	expression tag	UNP Q50883
B	-2	GLY	-	expression tag	UNP Q50883
B	-1	ARG	-	expression tag	UNP Q50883
B	0	GLY	-	expression tag	UNP Q50883
B	1	SER	-	expression tag	UNP Q50883
E	-32	MET	-	initiating methionine	UNP Q50883
E	-31	GLY	-	expression tag	UNP Q50883
E	-30	SER	-	expression tag	UNP Q50883
E	-29	SER	-	expression tag	UNP Q50883
E	-28	HIS	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-27	HIS	-	expression tag	UNP Q50883
E	-26	HIS	-	expression tag	UNP Q50883
E	-25	HIS	-	expression tag	UNP Q50883
E	-24	HIS	-	expression tag	UNP Q50883
E	-23	HIS	-	expression tag	UNP Q50883
E	-22	SER	-	expression tag	UNP Q50883
E	-21	SER	-	expression tag	UNP Q50883
E	-20	GLY	-	expression tag	UNP Q50883
E	-19	LEU	-	expression tag	UNP Q50883
E	-18	VAL	-	expression tag	UNP Q50883
E	-17	PRO	-	expression tag	UNP Q50883
E	-16	ARG	-	expression tag	UNP Q50883
E	-15	GLY	-	expression tag	UNP Q50883
E	-14	SER	-	expression tag	UNP Q50883
E	-13	HIS	-	expression tag	UNP Q50883
E	-12	MET	-	expression tag	UNP Q50883
E	-11	ALA	-	expression tag	UNP Q50883
E	-10	SER	-	expression tag	UNP Q50883
E	-9	MET	-	expression tag	UNP Q50883
E	-8	THR	-	expression tag	UNP Q50883
E	-7	GLY	-	expression tag	UNP Q50883
E	-6	GLY	-	expression tag	UNP Q50883
E	-5	GLN	-	expression tag	UNP Q50883
E	-4	GLN	-	expression tag	UNP Q50883
E	-3	MET	-	expression tag	UNP Q50883
E	-2	GLY	-	expression tag	UNP Q50883
E	-1	ARG	-	expression tag	UNP Q50883
E	0	GLY	-	expression tag	UNP Q50883
E	1	SER	-	expression tag	UNP Q50883
F	-32	MET	-	initiating methionine	UNP Q50883
F	-31	GLY	-	expression tag	UNP Q50883
F	-30	SER	-	expression tag	UNP Q50883
F	-29	SER	-	expression tag	UNP Q50883
F	-28	HIS	-	expression tag	UNP Q50883
F	-27	HIS	-	expression tag	UNP Q50883
F	-26	HIS	-	expression tag	UNP Q50883
F	-25	HIS	-	expression tag	UNP Q50883
F	-24	HIS	-	expression tag	UNP Q50883
F	-23	HIS	-	expression tag	UNP Q50883
F	-22	SER	-	expression tag	UNP Q50883
F	-21	SER	-	expression tag	UNP Q50883
F	-20	GLY	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	LEU	-	expression tag	UNP Q50883
F	-18	VAL	-	expression tag	UNP Q50883
F	-17	PRO	-	expression tag	UNP Q50883
F	-16	ARG	-	expression tag	UNP Q50883
F	-15	GLY	-	expression tag	UNP Q50883
F	-14	SER	-	expression tag	UNP Q50883
F	-13	HIS	-	expression tag	UNP Q50883
F	-12	MET	-	expression tag	UNP Q50883
F	-11	ALA	-	expression tag	UNP Q50883
F	-10	SER	-	expression tag	UNP Q50883
F	-9	MET	-	expression tag	UNP Q50883
F	-8	THR	-	expression tag	UNP Q50883
F	-7	GLY	-	expression tag	UNP Q50883
F	-6	GLY	-	expression tag	UNP Q50883
F	-5	GLN	-	expression tag	UNP Q50883
F	-4	GLN	-	expression tag	UNP Q50883
F	-3	MET	-	expression tag	UNP Q50883
F	-2	GLY	-	expression tag	UNP Q50883
F	-1	ARG	-	expression tag	UNP Q50883
F	0	GLY	-	expression tag	UNP Q50883
F	1	SER	-	expression tag	UNP Q50883
C	-32	MET	-	initiating methionine	UNP Q50883
C	-31	GLY	-	expression tag	UNP Q50883
C	-30	SER	-	expression tag	UNP Q50883
C	-29	SER	-	expression tag	UNP Q50883
C	-28	HIS	-	expression tag	UNP Q50883
C	-27	HIS	-	expression tag	UNP Q50883
C	-26	HIS	-	expression tag	UNP Q50883
C	-25	HIS	-	expression tag	UNP Q50883
C	-24	HIS	-	expression tag	UNP Q50883
C	-23	HIS	-	expression tag	UNP Q50883
C	-22	SER	-	expression tag	UNP Q50883
C	-21	SER	-	expression tag	UNP Q50883
C	-20	GLY	-	expression tag	UNP Q50883
C	-19	LEU	-	expression tag	UNP Q50883
C	-18	VAL	-	expression tag	UNP Q50883
C	-17	PRO	-	expression tag	UNP Q50883
C	-16	ARG	-	expression tag	UNP Q50883
C	-15	GLY	-	expression tag	UNP Q50883
C	-14	SER	-	expression tag	UNP Q50883
C	-13	HIS	-	expression tag	UNP Q50883
C	-12	MET	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	ALA	-	expression tag	UNP Q50883
C	-10	SER	-	expression tag	UNP Q50883
C	-9	MET	-	expression tag	UNP Q50883
C	-8	THR	-	expression tag	UNP Q50883
C	-7	GLY	-	expression tag	UNP Q50883
C	-6	GLY	-	expression tag	UNP Q50883
C	-5	GLN	-	expression tag	UNP Q50883
C	-4	GLN	-	expression tag	UNP Q50883
C	-3	MET	-	expression tag	UNP Q50883
C	-2	GLY	-	expression tag	UNP Q50883
C	-1	ARG	-	expression tag	UNP Q50883
C	0	GLY	-	expression tag	UNP Q50883
C	1	SER	-	expression tag	UNP Q50883
D	-32	MET	-	initiating methionine	UNP Q50883
D	-31	GLY	-	expression tag	UNP Q50883
D	-30	SER	-	expression tag	UNP Q50883
D	-29	SER	-	expression tag	UNP Q50883
D	-28	HIS	-	expression tag	UNP Q50883
D	-27	HIS	-	expression tag	UNP Q50883
D	-26	HIS	-	expression tag	UNP Q50883
D	-25	HIS	-	expression tag	UNP Q50883
D	-24	HIS	-	expression tag	UNP Q50883
D	-23	HIS	-	expression tag	UNP Q50883
D	-22	SER	-	expression tag	UNP Q50883
D	-21	SER	-	expression tag	UNP Q50883
D	-20	GLY	-	expression tag	UNP Q50883
D	-19	LEU	-	expression tag	UNP Q50883
D	-18	VAL	-	expression tag	UNP Q50883
D	-17	PRO	-	expression tag	UNP Q50883
D	-16	ARG	-	expression tag	UNP Q50883
D	-15	GLY	-	expression tag	UNP Q50883
D	-14	SER	-	expression tag	UNP Q50883
D	-13	HIS	-	expression tag	UNP Q50883
D	-12	MET	-	expression tag	UNP Q50883
D	-11	ALA	-	expression tag	UNP Q50883
D	-10	SER	-	expression tag	UNP Q50883
D	-9	MET	-	expression tag	UNP Q50883
D	-8	THR	-	expression tag	UNP Q50883
D	-7	GLY	-	expression tag	UNP Q50883
D	-6	GLY	-	expression tag	UNP Q50883
D	-5	GLN	-	expression tag	UNP Q50883
D	-4	GLN	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	MET	-	expression tag	UNP Q50883
D	-2	GLY	-	expression tag	UNP Q50883
D	-1	ARG	-	expression tag	UNP Q50883
D	0	GLY	-	expression tag	UNP Q50883
D	1	SER	-	expression tag	UNP Q50883
G	-32	MET	-	initiating methionine	UNP Q50883
G	-31	GLY	-	expression tag	UNP Q50883
G	-30	SER	-	expression tag	UNP Q50883
G	-29	SER	-	expression tag	UNP Q50883
G	-28	HIS	-	expression tag	UNP Q50883
G	-27	HIS	-	expression tag	UNP Q50883
G	-26	HIS	-	expression tag	UNP Q50883
G	-25	HIS	-	expression tag	UNP Q50883
G	-24	HIS	-	expression tag	UNP Q50883
G	-23	HIS	-	expression tag	UNP Q50883
G	-22	SER	-	expression tag	UNP Q50883
G	-21	SER	-	expression tag	UNP Q50883
G	-20	GLY	-	expression tag	UNP Q50883
G	-19	LEU	-	expression tag	UNP Q50883
G	-18	VAL	-	expression tag	UNP Q50883
G	-17	PRO	-	expression tag	UNP Q50883
G	-16	ARG	-	expression tag	UNP Q50883
G	-15	GLY	-	expression tag	UNP Q50883
G	-14	SER	-	expression tag	UNP Q50883
G	-13	HIS	-	expression tag	UNP Q50883
G	-12	MET	-	expression tag	UNP Q50883
G	-11	ALA	-	expression tag	UNP Q50883
G	-10	SER	-	expression tag	UNP Q50883
G	-9	MET	-	expression tag	UNP Q50883
G	-8	THR	-	expression tag	UNP Q50883
G	-7	GLY	-	expression tag	UNP Q50883
G	-6	GLY	-	expression tag	UNP Q50883
G	-5	GLN	-	expression tag	UNP Q50883
G	-4	GLN	-	expression tag	UNP Q50883
G	-3	MET	-	expression tag	UNP Q50883
G	-2	GLY	-	expression tag	UNP Q50883
G	-1	ARG	-	expression tag	UNP Q50883
G	0	GLY	-	expression tag	UNP Q50883
G	1	SER	-	expression tag	UNP Q50883
H	-32	MET	-	initiating methionine	UNP Q50883
H	-31	GLY	-	expression tag	UNP Q50883
H	-30	SER	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-29	SER	-	expression tag	UNP Q50883
H	-28	HIS	-	expression tag	UNP Q50883
H	-27	HIS	-	expression tag	UNP Q50883
H	-26	HIS	-	expression tag	UNP Q50883
H	-25	HIS	-	expression tag	UNP Q50883
H	-24	HIS	-	expression tag	UNP Q50883
H	-23	HIS	-	expression tag	UNP Q50883
H	-22	SER	-	expression tag	UNP Q50883
H	-21	SER	-	expression tag	UNP Q50883
H	-20	GLY	-	expression tag	UNP Q50883
H	-19	LEU	-	expression tag	UNP Q50883
H	-18	VAL	-	expression tag	UNP Q50883
H	-17	PRO	-	expression tag	UNP Q50883
H	-16	ARG	-	expression tag	UNP Q50883
H	-15	GLY	-	expression tag	UNP Q50883
H	-14	SER	-	expression tag	UNP Q50883
H	-13	HIS	-	expression tag	UNP Q50883
H	-12	MET	-	expression tag	UNP Q50883
H	-11	ALA	-	expression tag	UNP Q50883
H	-10	SER	-	expression tag	UNP Q50883
H	-9	MET	-	expression tag	UNP Q50883
H	-8	THR	-	expression tag	UNP Q50883
H	-7	GLY	-	expression tag	UNP Q50883
H	-6	GLY	-	expression tag	UNP Q50883
H	-5	GLN	-	expression tag	UNP Q50883
H	-4	GLN	-	expression tag	UNP Q50883
H	-3	MET	-	expression tag	UNP Q50883
H	-2	GLY	-	expression tag	UNP Q50883
H	-1	ARG	-	expression tag	UNP Q50883
H	0	GLY	-	expression tag	UNP Q50883
H	1	SER	-	expression tag	UNP Q50883
I	-32	MET	-	initiating methionine	UNP Q50883
I	-31	GLY	-	expression tag	UNP Q50883
I	-30	SER	-	expression tag	UNP Q50883
I	-29	SER	-	expression tag	UNP Q50883
I	-28	HIS	-	expression tag	UNP Q50883
I	-27	HIS	-	expression tag	UNP Q50883
I	-26	HIS	-	expression tag	UNP Q50883
I	-25	HIS	-	expression tag	UNP Q50883
I	-24	HIS	-	expression tag	UNP Q50883
I	-23	HIS	-	expression tag	UNP Q50883
I	-22	SER	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-21	SER	-	expression tag	UNP Q50883
I	-20	GLY	-	expression tag	UNP Q50883
I	-19	LEU	-	expression tag	UNP Q50883
I	-18	VAL	-	expression tag	UNP Q50883
I	-17	PRO	-	expression tag	UNP Q50883
I	-16	ARG	-	expression tag	UNP Q50883
I	-15	GLY	-	expression tag	UNP Q50883
I	-14	SER	-	expression tag	UNP Q50883
I	-13	HIS	-	expression tag	UNP Q50883
I	-12	MET	-	expression tag	UNP Q50883
I	-11	ALA	-	expression tag	UNP Q50883
I	-10	SER	-	expression tag	UNP Q50883
I	-9	MET	-	expression tag	UNP Q50883
I	-8	THR	-	expression tag	UNP Q50883
I	-7	GLY	-	expression tag	UNP Q50883
I	-6	GLY	-	expression tag	UNP Q50883
I	-5	GLN	-	expression tag	UNP Q50883
I	-4	GLN	-	expression tag	UNP Q50883
I	-3	MET	-	expression tag	UNP Q50883
I	-2	GLY	-	expression tag	UNP Q50883
I	-1	ARG	-	expression tag	UNP Q50883
I	0	GLY	-	expression tag	UNP Q50883
I	1	SER	-	expression tag	UNP Q50883
J	-32	MET	-	initiating methionine	UNP Q50883
J	-31	GLY	-	expression tag	UNP Q50883
J	-30	SER	-	expression tag	UNP Q50883
J	-29	SER	-	expression tag	UNP Q50883
J	-28	HIS	-	expression tag	UNP Q50883
J	-27	HIS	-	expression tag	UNP Q50883
J	-26	HIS	-	expression tag	UNP Q50883
J	-25	HIS	-	expression tag	UNP Q50883
J	-24	HIS	-	expression tag	UNP Q50883
J	-23	HIS	-	expression tag	UNP Q50883
J	-22	SER	-	expression tag	UNP Q50883
J	-21	SER	-	expression tag	UNP Q50883
J	-20	GLY	-	expression tag	UNP Q50883
J	-19	LEU	-	expression tag	UNP Q50883
J	-18	VAL	-	expression tag	UNP Q50883
J	-17	PRO	-	expression tag	UNP Q50883
J	-16	ARG	-	expression tag	UNP Q50883
J	-15	GLY	-	expression tag	UNP Q50883
J	-14	SER	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-13	HIS	-	expression tag	UNP Q50883
J	-12	MET	-	expression tag	UNP Q50883
J	-11	ALA	-	expression tag	UNP Q50883
J	-10	SER	-	expression tag	UNP Q50883
J	-9	MET	-	expression tag	UNP Q50883
J	-8	THR	-	expression tag	UNP Q50883
J	-7	GLY	-	expression tag	UNP Q50883
J	-6	GLY	-	expression tag	UNP Q50883
J	-5	GLN	-	expression tag	UNP Q50883
J	-4	GLN	-	expression tag	UNP Q50883
J	-3	MET	-	expression tag	UNP Q50883
J	-2	GLY	-	expression tag	UNP Q50883
J	-1	ARG	-	expression tag	UNP Q50883
J	0	GLY	-	expression tag	UNP Q50883
J	1	SER	-	expression tag	UNP Q50883
M	-32	MET	-	initiating methionine	UNP Q50883
M	-31	GLY	-	expression tag	UNP Q50883
M	-30	SER	-	expression tag	UNP Q50883
M	-29	SER	-	expression tag	UNP Q50883
M	-28	HIS	-	expression tag	UNP Q50883
M	-27	HIS	-	expression tag	UNP Q50883
M	-26	HIS	-	expression tag	UNP Q50883
M	-25	HIS	-	expression tag	UNP Q50883
M	-24	HIS	-	expression tag	UNP Q50883
M	-23	HIS	-	expression tag	UNP Q50883
M	-22	SER	-	expression tag	UNP Q50883
M	-21	SER	-	expression tag	UNP Q50883
M	-20	GLY	-	expression tag	UNP Q50883
M	-19	LEU	-	expression tag	UNP Q50883
M	-18	VAL	-	expression tag	UNP Q50883
M	-17	PRO	-	expression tag	UNP Q50883
M	-16	ARG	-	expression tag	UNP Q50883
M	-15	GLY	-	expression tag	UNP Q50883
M	-14	SER	-	expression tag	UNP Q50883
M	-13	HIS	-	expression tag	UNP Q50883
M	-12	MET	-	expression tag	UNP Q50883
M	-11	ALA	-	expression tag	UNP Q50883
M	-10	SER	-	expression tag	UNP Q50883
M	-9	MET	-	expression tag	UNP Q50883
M	-8	THR	-	expression tag	UNP Q50883
M	-7	GLY	-	expression tag	UNP Q50883
M	-6	GLY	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-5	GLN	-	expression tag	UNP Q50883
M	-4	GLN	-	expression tag	UNP Q50883
M	-3	MET	-	expression tag	UNP Q50883
M	-2	GLY	-	expression tag	UNP Q50883
M	-1	ARG	-	expression tag	UNP Q50883
M	0	GLY	-	expression tag	UNP Q50883
M	1	SER	-	expression tag	UNP Q50883
N	-32	MET	-	initiating methionine	UNP Q50883
N	-31	GLY	-	expression tag	UNP Q50883
N	-30	SER	-	expression tag	UNP Q50883
N	-29	SER	-	expression tag	UNP Q50883
N	-28	HIS	-	expression tag	UNP Q50883
N	-27	HIS	-	expression tag	UNP Q50883
N	-26	HIS	-	expression tag	UNP Q50883
N	-25	HIS	-	expression tag	UNP Q50883
N	-24	HIS	-	expression tag	UNP Q50883
N	-23	HIS	-	expression tag	UNP Q50883
N	-22	SER	-	expression tag	UNP Q50883
N	-21	SER	-	expression tag	UNP Q50883
N	-20	GLY	-	expression tag	UNP Q50883
N	-19	LEU	-	expression tag	UNP Q50883
N	-18	VAL	-	expression tag	UNP Q50883
N	-17	PRO	-	expression tag	UNP Q50883
N	-16	ARG	-	expression tag	UNP Q50883
N	-15	GLY	-	expression tag	UNP Q50883
N	-14	SER	-	expression tag	UNP Q50883
N	-13	HIS	-	expression tag	UNP Q50883
N	-12	MET	-	expression tag	UNP Q50883
N	-11	ALA	-	expression tag	UNP Q50883
N	-10	SER	-	expression tag	UNP Q50883
N	-9	MET	-	expression tag	UNP Q50883
N	-8	THR	-	expression tag	UNP Q50883
N	-7	GLY	-	expression tag	UNP Q50883
N	-6	GLY	-	expression tag	UNP Q50883
N	-5	GLN	-	expression tag	UNP Q50883
N	-4	GLN	-	expression tag	UNP Q50883
N	-3	MET	-	expression tag	UNP Q50883
N	-2	GLY	-	expression tag	UNP Q50883
N	-1	ARG	-	expression tag	UNP Q50883
N	0	GLY	-	expression tag	UNP Q50883
N	1	SER	-	expression tag	UNP Q50883
Q	-32	MET	-	initiating methionine	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-31	GLY	-	expression tag	UNP Q50883
Q	-30	SER	-	expression tag	UNP Q50883
Q	-29	SER	-	expression tag	UNP Q50883
Q	-28	HIS	-	expression tag	UNP Q50883
Q	-27	HIS	-	expression tag	UNP Q50883
Q	-26	HIS	-	expression tag	UNP Q50883
Q	-25	HIS	-	expression tag	UNP Q50883
Q	-24	HIS	-	expression tag	UNP Q50883
Q	-23	HIS	-	expression tag	UNP Q50883
Q	-22	SER	-	expression tag	UNP Q50883
Q	-21	SER	-	expression tag	UNP Q50883
Q	-20	GLY	-	expression tag	UNP Q50883
Q	-19	LEU	-	expression tag	UNP Q50883
Q	-18	VAL	-	expression tag	UNP Q50883
Q	-17	PRO	-	expression tag	UNP Q50883
Q	-16	ARG	-	expression tag	UNP Q50883
Q	-15	GLY	-	expression tag	UNP Q50883
Q	-14	SER	-	expression tag	UNP Q50883
Q	-13	HIS	-	expression tag	UNP Q50883
Q	-12	MET	-	expression tag	UNP Q50883
Q	-11	ALA	-	expression tag	UNP Q50883
Q	-10	SER	-	expression tag	UNP Q50883
Q	-9	MET	-	expression tag	UNP Q50883
Q	-8	THR	-	expression tag	UNP Q50883
Q	-7	GLY	-	expression tag	UNP Q50883
Q	-6	GLY	-	expression tag	UNP Q50883
Q	-5	GLN	-	expression tag	UNP Q50883
Q	-4	GLN	-	expression tag	UNP Q50883
Q	-3	MET	-	expression tag	UNP Q50883
Q	-2	GLY	-	expression tag	UNP Q50883
Q	-1	ARG	-	expression tag	UNP Q50883
Q	0	GLY	-	expression tag	UNP Q50883
Q	1	SER	-	expression tag	UNP Q50883
R	-32	MET	-	initiating methionine	UNP Q50883
R	-31	GLY	-	expression tag	UNP Q50883
R	-30	SER	-	expression tag	UNP Q50883
R	-29	SER	-	expression tag	UNP Q50883
R	-28	HIS	-	expression tag	UNP Q50883
R	-27	HIS	-	expression tag	UNP Q50883
R	-26	HIS	-	expression tag	UNP Q50883
R	-25	HIS	-	expression tag	UNP Q50883
R	-24	HIS	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-23	HIS	-	expression tag	UNP Q50883
R	-22	SER	-	expression tag	UNP Q50883
R	-21	SER	-	expression tag	UNP Q50883
R	-20	GLY	-	expression tag	UNP Q50883
R	-19	LEU	-	expression tag	UNP Q50883
R	-18	VAL	-	expression tag	UNP Q50883
R	-17	PRO	-	expression tag	UNP Q50883
R	-16	ARG	-	expression tag	UNP Q50883
R	-15	GLY	-	expression tag	UNP Q50883
R	-14	SER	-	expression tag	UNP Q50883
R	-13	HIS	-	expression tag	UNP Q50883
R	-12	MET	-	expression tag	UNP Q50883
R	-11	ALA	-	expression tag	UNP Q50883
R	-10	SER	-	expression tag	UNP Q50883
R	-9	MET	-	expression tag	UNP Q50883
R	-8	THR	-	expression tag	UNP Q50883
R	-7	GLY	-	expression tag	UNP Q50883
R	-6	GLY	-	expression tag	UNP Q50883
R	-5	GLN	-	expression tag	UNP Q50883
R	-4	GLN	-	expression tag	UNP Q50883
R	-3	MET	-	expression tag	UNP Q50883
R	-2	GLY	-	expression tag	UNP Q50883
R	-1	ARG	-	expression tag	UNP Q50883
R	0	GLY	-	expression tag	UNP Q50883
R	1	SER	-	expression tag	UNP Q50883
K	-32	MET	-	initiating methionine	UNP Q50883
K	-31	GLY	-	expression tag	UNP Q50883
K	-30	SER	-	expression tag	UNP Q50883
K	-29	SER	-	expression tag	UNP Q50883
K	-28	HIS	-	expression tag	UNP Q50883
K	-27	HIS	-	expression tag	UNP Q50883
K	-26	HIS	-	expression tag	UNP Q50883
K	-25	HIS	-	expression tag	UNP Q50883
K	-24	HIS	-	expression tag	UNP Q50883
K	-23	HIS	-	expression tag	UNP Q50883
K	-22	SER	-	expression tag	UNP Q50883
K	-21	SER	-	expression tag	UNP Q50883
K	-20	GLY	-	expression tag	UNP Q50883
K	-19	LEU	-	expression tag	UNP Q50883
K	-18	VAL	-	expression tag	UNP Q50883
K	-17	PRO	-	expression tag	UNP Q50883
K	-16	ARG	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-15	GLY	-	expression tag	UNP Q50883
K	-14	SER	-	expression tag	UNP Q50883
K	-13	HIS	-	expression tag	UNP Q50883
K	-12	MET	-	expression tag	UNP Q50883
K	-11	ALA	-	expression tag	UNP Q50883
K	-10	SER	-	expression tag	UNP Q50883
K	-9	MET	-	expression tag	UNP Q50883
K	-8	THR	-	expression tag	UNP Q50883
K	-7	GLY	-	expression tag	UNP Q50883
K	-6	GLY	-	expression tag	UNP Q50883
K	-5	GLN	-	expression tag	UNP Q50883
K	-4	GLN	-	expression tag	UNP Q50883
K	-3	MET	-	expression tag	UNP Q50883
K	-2	GLY	-	expression tag	UNP Q50883
K	-1	ARG	-	expression tag	UNP Q50883
K	0	GLY	-	expression tag	UNP Q50883
K	1	SER	-	expression tag	UNP Q50883
L	-32	MET	-	initiating methionine	UNP Q50883
L	-31	GLY	-	expression tag	UNP Q50883
L	-30	SER	-	expression tag	UNP Q50883
L	-29	SER	-	expression tag	UNP Q50883
L	-28	HIS	-	expression tag	UNP Q50883
L	-27	HIS	-	expression tag	UNP Q50883
L	-26	HIS	-	expression tag	UNP Q50883
L	-25	HIS	-	expression tag	UNP Q50883
L	-24	HIS	-	expression tag	UNP Q50883
L	-23	HIS	-	expression tag	UNP Q50883
L	-22	SER	-	expression tag	UNP Q50883
L	-21	SER	-	expression tag	UNP Q50883
L	-20	GLY	-	expression tag	UNP Q50883
L	-19	LEU	-	expression tag	UNP Q50883
L	-18	VAL	-	expression tag	UNP Q50883
L	-17	PRO	-	expression tag	UNP Q50883
L	-16	ARG	-	expression tag	UNP Q50883
L	-15	GLY	-	expression tag	UNP Q50883
L	-14	SER	-	expression tag	UNP Q50883
L	-13	HIS	-	expression tag	UNP Q50883
L	-12	MET	-	expression tag	UNP Q50883
L	-11	ALA	-	expression tag	UNP Q50883
L	-10	SER	-	expression tag	UNP Q50883
L	-9	MET	-	expression tag	UNP Q50883
L	-8	THR	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-7	GLY	-	expression tag	UNP Q50883
L	-6	GLY	-	expression tag	UNP Q50883
L	-5	GLN	-	expression tag	UNP Q50883
L	-4	GLN	-	expression tag	UNP Q50883
L	-3	MET	-	expression tag	UNP Q50883
L	-2	GLY	-	expression tag	UNP Q50883
L	-1	ARG	-	expression tag	UNP Q50883
L	0	GLY	-	expression tag	UNP Q50883
L	1	SER	-	expression tag	UNP Q50883
O	-32	MET	-	initiating methionine	UNP Q50883
O	-31	GLY	-	expression tag	UNP Q50883
O	-30	SER	-	expression tag	UNP Q50883
O	-29	SER	-	expression tag	UNP Q50883
O	-28	HIS	-	expression tag	UNP Q50883
O	-27	HIS	-	expression tag	UNP Q50883
O	-26	HIS	-	expression tag	UNP Q50883
O	-25	HIS	-	expression tag	UNP Q50883
O	-24	HIS	-	expression tag	UNP Q50883
O	-23	HIS	-	expression tag	UNP Q50883
O	-22	SER	-	expression tag	UNP Q50883
O	-21	SER	-	expression tag	UNP Q50883
O	-20	GLY	-	expression tag	UNP Q50883
O	-19	LEU	-	expression tag	UNP Q50883
O	-18	VAL	-	expression tag	UNP Q50883
O	-17	PRO	-	expression tag	UNP Q50883
O	-16	ARG	-	expression tag	UNP Q50883
O	-15	GLY	-	expression tag	UNP Q50883
O	-14	SER	-	expression tag	UNP Q50883
O	-13	HIS	-	expression tag	UNP Q50883
O	-12	MET	-	expression tag	UNP Q50883
O	-11	ALA	-	expression tag	UNP Q50883
O	-10	SER	-	expression tag	UNP Q50883
O	-9	MET	-	expression tag	UNP Q50883
O	-8	THR	-	expression tag	UNP Q50883
O	-7	GLY	-	expression tag	UNP Q50883
O	-6	GLY	-	expression tag	UNP Q50883
O	-5	GLN	-	expression tag	UNP Q50883
O	-4	GLN	-	expression tag	UNP Q50883
O	-3	MET	-	expression tag	UNP Q50883
O	-2	GLY	-	expression tag	UNP Q50883
O	-1	ARG	-	expression tag	UNP Q50883
O	0	GLY	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
O	1	SER	-	expression tag	UNP Q50883
P	-32	MET	-	initiating methionine	UNP Q50883
P	-31	GLY	-	expression tag	UNP Q50883
P	-30	SER	-	expression tag	UNP Q50883
P	-29	SER	-	expression tag	UNP Q50883
P	-28	HIS	-	expression tag	UNP Q50883
P	-27	HIS	-	expression tag	UNP Q50883
P	-26	HIS	-	expression tag	UNP Q50883
P	-25	HIS	-	expression tag	UNP Q50883
P	-24	HIS	-	expression tag	UNP Q50883
P	-23	HIS	-	expression tag	UNP Q50883
P	-22	SER	-	expression tag	UNP Q50883
P	-21	SER	-	expression tag	UNP Q50883
P	-20	GLY	-	expression tag	UNP Q50883
P	-19	LEU	-	expression tag	UNP Q50883
P	-18	VAL	-	expression tag	UNP Q50883
P	-17	PRO	-	expression tag	UNP Q50883
P	-16	ARG	-	expression tag	UNP Q50883
P	-15	GLY	-	expression tag	UNP Q50883
P	-14	SER	-	expression tag	UNP Q50883
P	-13	HIS	-	expression tag	UNP Q50883
P	-12	MET	-	expression tag	UNP Q50883
P	-11	ALA	-	expression tag	UNP Q50883
P	-10	SER	-	expression tag	UNP Q50883
P	-9	MET	-	expression tag	UNP Q50883
P	-8	THR	-	expression tag	UNP Q50883
P	-7	GLY	-	expression tag	UNP Q50883
P	-6	GLY	-	expression tag	UNP Q50883
P	-5	GLN	-	expression tag	UNP Q50883
P	-4	GLN	-	expression tag	UNP Q50883
P	-3	MET	-	expression tag	UNP Q50883
P	-2	GLY	-	expression tag	UNP Q50883
P	-1	ARG	-	expression tag	UNP Q50883
P	0	GLY	-	expression tag	UNP Q50883
P	1	SER	-	expression tag	UNP Q50883
S	-32	MET	-	initiating methionine	UNP Q50883
S	-31	GLY	-	expression tag	UNP Q50883
S	-30	SER	-	expression tag	UNP Q50883
S	-29	SER	-	expression tag	UNP Q50883
S	-28	HIS	-	expression tag	UNP Q50883
S	-27	HIS	-	expression tag	UNP Q50883
S	-26	HIS	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-25	HIS	-	expression tag	UNP Q50883
S	-24	HIS	-	expression tag	UNP Q50883
S	-23	HIS	-	expression tag	UNP Q50883
S	-22	SER	-	expression tag	UNP Q50883
S	-21	SER	-	expression tag	UNP Q50883
S	-20	GLY	-	expression tag	UNP Q50883
S	-19	LEU	-	expression tag	UNP Q50883
S	-18	VAL	-	expression tag	UNP Q50883
S	-17	PRO	-	expression tag	UNP Q50883
S	-16	ARG	-	expression tag	UNP Q50883
S	-15	GLY	-	expression tag	UNP Q50883
S	-14	SER	-	expression tag	UNP Q50883
S	-13	HIS	-	expression tag	UNP Q50883
S	-12	MET	-	expression tag	UNP Q50883
S	-11	ALA	-	expression tag	UNP Q50883
S	-10	SER	-	expression tag	UNP Q50883
S	-9	MET	-	expression tag	UNP Q50883
S	-8	THR	-	expression tag	UNP Q50883
S	-7	GLY	-	expression tag	UNP Q50883
S	-6	GLY	-	expression tag	UNP Q50883
S	-5	GLN	-	expression tag	UNP Q50883
S	-4	GLN	-	expression tag	UNP Q50883
S	-3	MET	-	expression tag	UNP Q50883
S	-2	GLY	-	expression tag	UNP Q50883
S	-1	ARG	-	expression tag	UNP Q50883
S	0	GLY	-	expression tag	UNP Q50883
S	1	SER	-	expression tag	UNP Q50883
T	-32	MET	-	initiating methionine	UNP Q50883
T	-31	GLY	-	expression tag	UNP Q50883
T	-30	SER	-	expression tag	UNP Q50883
T	-29	SER	-	expression tag	UNP Q50883
T	-28	HIS	-	expression tag	UNP Q50883
T	-27	HIS	-	expression tag	UNP Q50883
T	-26	HIS	-	expression tag	UNP Q50883
T	-25	HIS	-	expression tag	UNP Q50883
T	-24	HIS	-	expression tag	UNP Q50883
T	-23	HIS	-	expression tag	UNP Q50883
T	-22	SER	-	expression tag	UNP Q50883
T	-21	SER	-	expression tag	UNP Q50883
T	-20	GLY	-	expression tag	UNP Q50883
T	-19	LEU	-	expression tag	UNP Q50883
T	-18	VAL	-	expression tag	UNP Q50883

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-17	PRO	-	expression tag	UNP Q50883
T	-16	ARG	-	expression tag	UNP Q50883
T	-15	GLY	-	expression tag	UNP Q50883
T	-14	SER	-	expression tag	UNP Q50883
T	-13	HIS	-	expression tag	UNP Q50883
T	-12	MET	-	expression tag	UNP Q50883
T	-11	ALA	-	expression tag	UNP Q50883
T	-10	SER	-	expression tag	UNP Q50883
T	-9	MET	-	expression tag	UNP Q50883
T	-8	THR	-	expression tag	UNP Q50883
T	-7	GLY	-	expression tag	UNP Q50883
T	-6	GLY	-	expression tag	UNP Q50883
T	-5	GLN	-	expression tag	UNP Q50883
T	-4	GLN	-	expression tag	UNP Q50883
T	-3	MET	-	expression tag	UNP Q50883
T	-2	GLY	-	expression tag	UNP Q50883
T	-1	ARG	-	expression tag	UNP Q50883
T	0	GLY	-	expression tag	UNP Q50883
T	1	SER	-	expression tag	UNP Q50883

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	32	Total O 32 32	0	0
2	B	27	Total O 27 27	0	0
2	E	12	Total O 12 12	0	0
2	F	23	Total O 23 23	0	0
2	C	13	Total O 13 13	0	0
2	D	7	Total O 7 7	0	0
2	G	9	Total O 9 9	0	0
2	H	12	Total O 12 12	0	0
2	I	18	Total O 18 18	0	0
2	J	12	Total O 12 12	0	0

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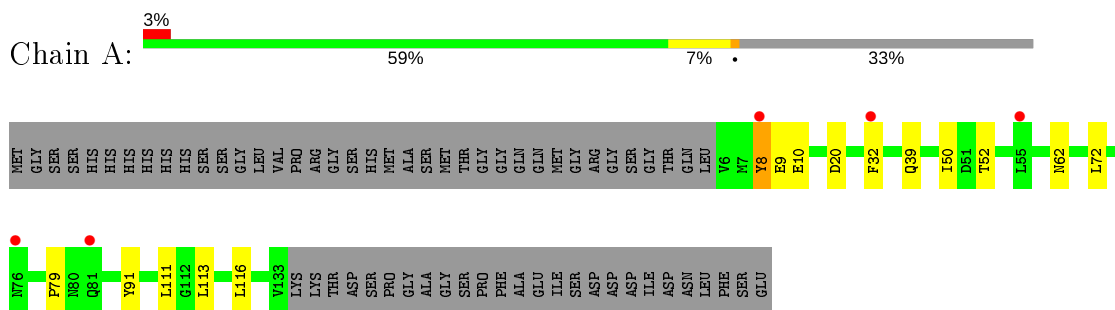
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	M	9	Total O 9 9	0	0
2	N	13	Total O 13 13	0	0
2	Q	19	Total O 19 19	0	0
2	R	18	Total O 18 18	0	0
2	K	7	Total O 7 7	0	0
2	L	13	Total O 13 13	0	0
2	O	6	Total O 6 6	0	0
2	P	17	Total O 17 17	0	0
2	S	12	Total O 12 12	0	0
2	T	14	Total O 14 14	0	0

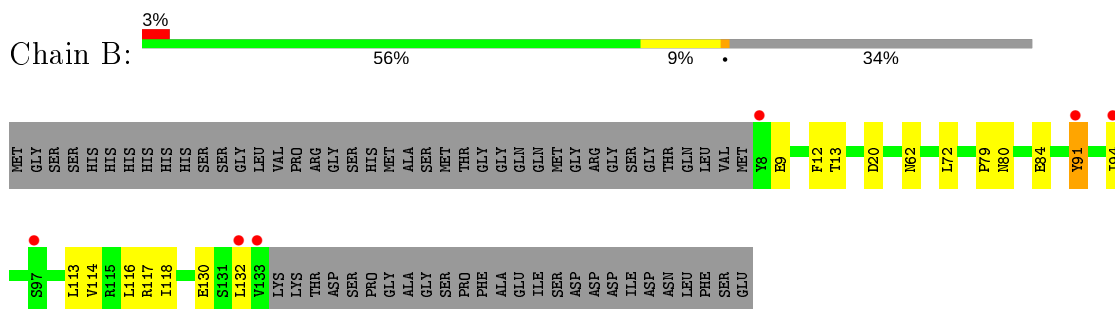
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

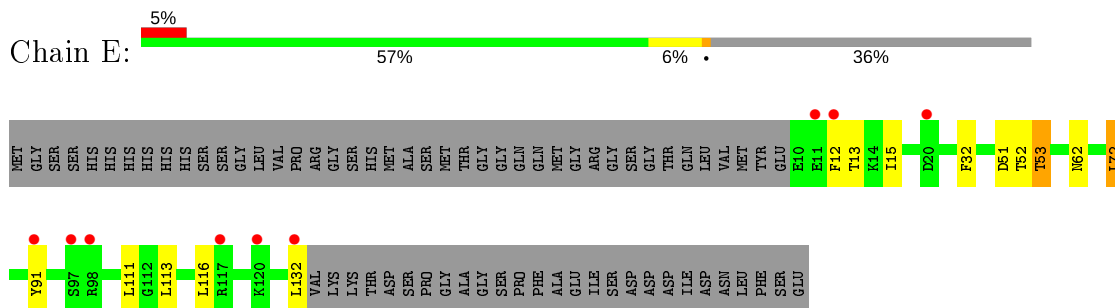
- Molecule 1: MglB



- Molecule 1: MglB

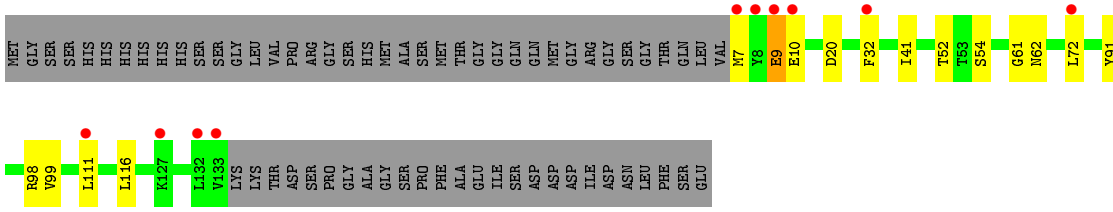


- Molecule 1: MglB

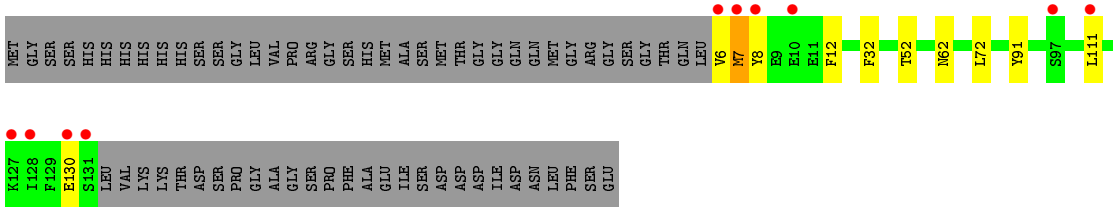


- Molecule 1: MglB

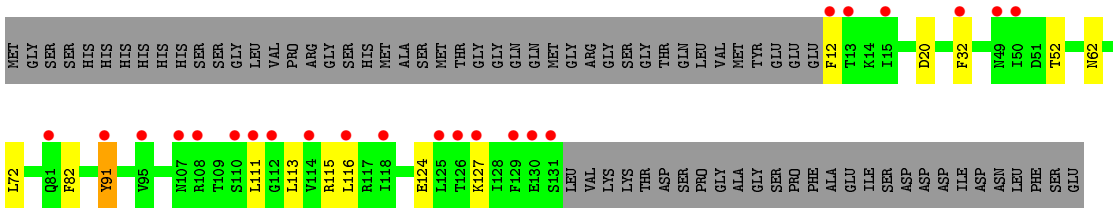




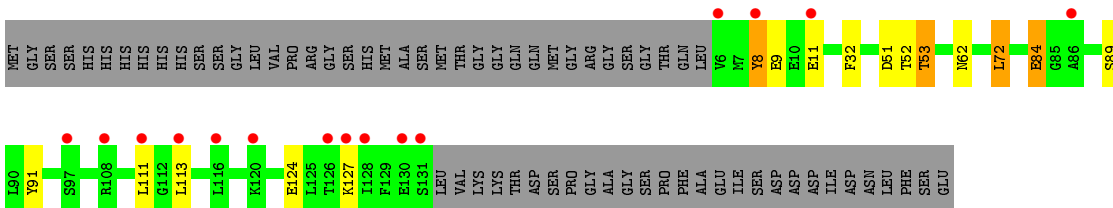
• Molecule 1: MglB



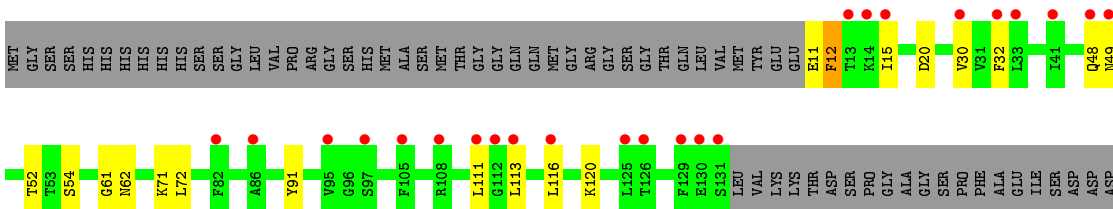
• Molecule 1: MglB

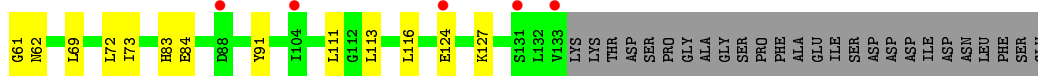
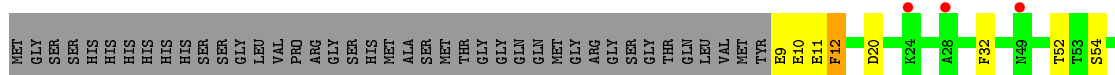


• Molecule 1: MglB

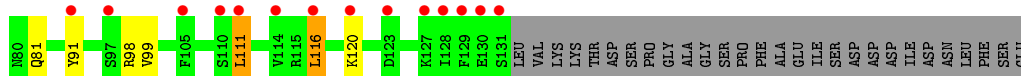
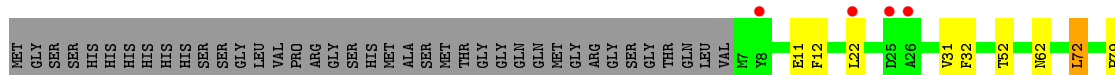


• Molecule 1: MglB

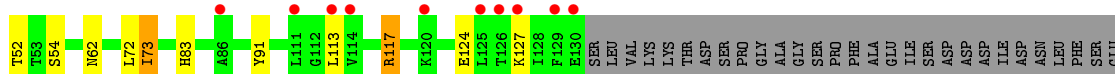
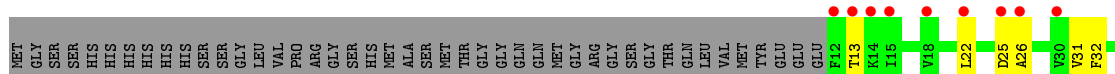




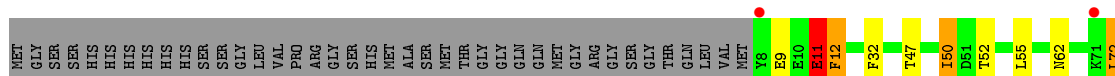
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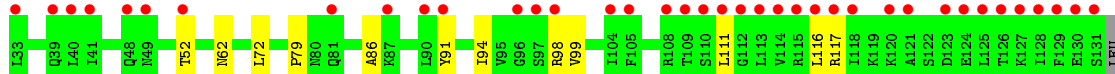
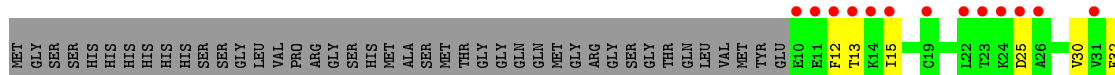
• Molecule 1: MglB



• Molecule 1: MglB



• Molecule 1: MglB



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• Molecule 1: Mg1B



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N62
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I73
G74
P79
Y91
I94

Y95
G96
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L116
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• Molecule 1: Mg1B



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A26
M27
A28
V31
F32
T52
N62

M66
L69
L72
Q81
Y91
F105
D106
T109
S110
L111
V114
R115
L116
R117
I118
K119
K127
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• Molecule 1: Mg1B



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M7
Y8
E9
E10
E11
F12
D20
K24
K28
F32
M49
I50
B51
T52
T53
S54

G61
M62
L72
P79
F82
G85
A86
K87
Y91
I94
R98
V99
I104
R108
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L116
K120
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.78Å 139.60Å 179.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.41 – 2.39 46.91 – 2.39	Depositor EDS
% Data completeness (in resolution range)	72.6 (45.41-2.39) 73.0 (46.91-2.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.39Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.249 , 0.267 0.268 , 0.291	Depositor DCC
R_{free} test set	4276 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19326	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.41	0/985	0.64	1/1328 (0.1%)
1	B	0.40	0/970	0.62	0/1308
1	C	0.38	0/970	0.60	0/1307
1	D	0.39	0/915	0.62	0/1233
1	E	0.41	0/941	0.65	0/1268
1	F	0.41	0/978	0.62	0/1318
1	G	0.38	0/970	0.66	1/1307 (0.1%)
1	H	0.38	0/924	0.61	0/1245
1	I	0.41	0/978	0.62	0/1318
1	J	0.39	0/957	0.62	0/1289
1	K	0.41	0/909	0.64	1/1225 (0.1%)
1	L	0.40	0/963	0.65	1/1298 (0.1%)
1	M	0.41	0/978	0.62	0/1318
1	N	0.40	0/941	0.62	0/1268
1	O	0.38	0/933	0.63	1/1257 (0.1%)
1	P	0.40	0/1026	0.61	0/1382
1	Q	0.42	0/957	0.63	0/1290
1	R	0.41	0/963	0.62	1/1297 (0.1%)
1	S	0.43	0/978	0.69	2/1318 (0.2%)
1	T	0.40	0/970	0.69	3/1307 (0.2%)
All	All	0.40	0/19206	0.63	11/25881 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	85	GLY	N-CA-C	9.18	136.05	113.10
1	S	10	GLU	C-N-CA	7.21	139.72	121.70
1	S	105	PHE	CA-CB-CG	-6.81	97.55	113.90
1	O	86	ALA	N-CA-C	-6.47	93.53	111.00
1	L	11	GLU	C-N-CA	6.15	137.08	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	27	ASN	Mainchain

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	976	0	1004	6	0
1	B	961	0	986	6	0
1	C	961	0	984	3	0
1	D	907	0	939	3	0
1	E	933	0	962	4	0
1	F	969	0	995	7	0
1	G	961	0	984	5	0
1	H	916	0	945	5	0
1	I	969	0	995	5	0
1	J	948	0	970	5	0
1	K	901	0	934	14	0
1	L	954	0	977	10	0
1	M	969	0	995	9	0
1	N	933	0	962	10	0
1	O	925	0	951	7	0
1	P	1017	0	1052	4	0
1	Q	949	0	977	12	0
1	R	954	0	975	11	0
1	S	969	0	995	21	0
1	T	961	0	984	7	0
2	A	32	0	0	0	0
2	B	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	13	0	0	0	0
2	D	7	0	0	0	0
2	E	12	0	0	0	0
2	F	23	0	0	1	0
2	G	9	0	0	0	0
2	H	12	0	0	0	0
2	I	18	0	0	0	0
2	J	12	0	0	0	0
2	K	7	0	0	0	0
2	L	13	0	0	0	0
2	M	9	0	0	0	0
2	N	13	0	0	0	0
2	O	6	0	0	0	0
2	P	17	0	0	0	0
2	Q	19	0	0	0	0
2	R	18	0	0	0	0
2	S	12	0	0	0	0
2	T	14	0	0	0	0
All	All	19326	0	19566	127	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.

The worst 5 of 127 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:10:GLU:HA	1:S:12:PHE:H	1.14	1.10
1:S:10:GLU:HA	1:S:12:PHE:N	1.89	0.87
1:O:12:PHE:O	1:O:15:ILE:HG12	1.75	0.85
1:H:12:PHE:O	1:H:15:ILE:HG12	1.75	0.85
1:F:9:GLU:HA	1:F:10:GLU:HB2	1.60	0.82

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 X-ray entries followed by that with respect to entries of similar resolution.

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	126/192 (66%)	123 (98%)	3 (2%)	0	100	100
1	B	124/192 (65%)	119 (96%)	4 (3%)	1 (1%)	19	29
1	C	124/192 (65%)	122 (98%)	2 (2%)	0	100	100
1	D	118/192 (62%)	117 (99%)	1 (1%)	0	100	100
1	E	121/192 (63%)	120 (99%)	1 (1%)	0	100	100
1	F	125/192 (65%)	121 (97%)	3 (2%)	1 (1%)	19	29
1	G	124/192 (65%)	121 (98%)	2 (2%)	1 (1%)	19	29
1	H	119/192 (62%)	118 (99%)	1 (1%)	0	100	100
1	I	125/192 (65%)	122 (98%)	3 (2%)	0	100	100
1	J	122/192 (64%)	116 (95%)	4 (3%)	2 (2%)	9	13
1	K	117/192 (61%)	114 (97%)	2 (2%)	1 (1%)	17	25
1	L	123/192 (64%)	120 (98%)	2 (2%)	1 (1%)	19	29
1	M	125/192 (65%)	123 (98%)	2 (2%)	0	100	100
1	N	121/192 (63%)	117 (97%)	4 (3%)	0	100	100
1	O	120/192 (62%)	117 (98%)	3 (2%)	0	100	100
1	P	131/192 (68%)	125 (95%)	4 (3%)	2 (2%)	10	14
1	Q	123/192 (64%)	120 (98%)	2 (2%)	1 (1%)	19	29
1	R	123/192 (64%)	120 (98%)	2 (2%)	1 (1%)	19	29
1	S	125/192 (65%)	121 (97%)	2 (2%)	2 (2%)	9	13
1	T	124/192 (65%)	119 (96%)	4 (3%)	1 (1%)	19	29
All	All	2460/3840 (64%)	2395 (97%)	51 (2%)	14 (1%)	25	36

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	84	GLU
1	J	9	GLU
1	R	12	PHE
1	K	13	THR
1	S	9	GLU

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 X-ray entries followed by that with respect to entries of similar resolution.

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	108/159 (68%)	100 (93%)	8 (7%)	13	22
1	B	106/159 (67%)	96 (91%)	10 (9%)	8	13
1	C	106/159 (67%)	99 (93%)	7 (7%)	16	26
1	D	100/159 (63%)	91 (91%)	9 (9%)	9	14
1	E	103/159 (65%)	94 (91%)	9 (9%)	10	15
1	F	107/159 (67%)	100 (94%)	7 (6%)	17	27
1	G	106/159 (67%)	97 (92%)	9 (8%)	10	16
1	H	101/159 (64%)	88 (87%)	13 (13%)	4	5
1	I	107/159 (67%)	98 (92%)	9 (8%)	11	16
1	J	104/159 (65%)	93 (89%)	11 (11%)	6	9
1	K	99/159 (62%)	95 (96%)	4 (4%)	31	49
1	L	105/159 (66%)	96 (91%)	9 (9%)	10	16
1	M	107/159 (67%)	100 (94%)	7 (6%)	17	27
1	N	103/159 (65%)	94 (91%)	9 (9%)	10	15
1	O	102/159 (64%)	95 (93%)	7 (7%)	15	25
1	P	113/159 (71%)	107 (95%)	6 (5%)	22	37
1	Q	105/159 (66%)	98 (93%)	7 (7%)	16	26
1	R	105/159 (66%)	99 (94%)	6 (6%)	20	33
1	S	107/159 (67%)	97 (91%)	10 (9%)	9	13
1	T	106/159 (67%)	100 (94%)	6 (6%)	20	33
All	All	2100/3180 (66%)	1937 (92%)	163 (8%)	12	19

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	13	THR
1	J	116	LEU
1	S	62	ASN

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Mol	Chain	Res	Type
1	I	62	ASN
1	J	9	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	81	GLN
1	Q	83	HIS
1	P	83	HIS
1	N	80	ASN
1	E	83	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	128/192 (66%)	0.51	5 (3%) 39 38	30, 50, 80, 116	0
1	B	126/192 (65%)	0.59	6 (4%) 30 29	32, 48, 90, 130	0
1	C	126/192 (65%)	0.53	10 (7%) 12 11	31, 55, 98, 133	0
1	D	120/192 (62%)	1.30	23 (19%) 1 0	32, 68, 112, 148	0
1	E	123/192 (64%)	0.69	9 (7%) 15 13	38, 60, 98, 128	0
1	F	127/192 (66%)	0.70	10 (7%) 12 11	34, 63, 102, 123	0
1	G	126/192 (65%)	0.83	15 (11%) 4 4	38, 72, 110, 139	0
1	H	121/192 (63%)	1.25	24 (19%) 1 0	40, 82, 118, 148	0
1	I	127/192 (66%)	0.63	12 (9%) 8 7	38, 62, 99, 130	0
1	J	124/192 (64%)	0.77	10 (8%) 12 11	43, 68, 104, 142	0
1	K	119/192 (61%)	1.25	19 (15%) 1 1	44, 78, 126, 153	0
1	L	125/192 (65%)	0.54	6 (4%) 30 29	38, 58, 92, 130	0
1	M	127/192 (66%)	0.66	14 (11%) 5 5	39, 64, 103, 124	0
1	N	123/192 (64%)	0.78	17 (13%) 2 2	42, 76, 112, 137	0
1	O	122/192 (63%)	2.00	51 (41%) 0 0	48, 98, 145, 175	0
1	P	133/192 (69%)	0.71	10 (7%) 14 13	39, 58, 94, 106	0
1	Q	125/192 (65%)	0.67	8 (6%) 19 18	35, 63, 102, 145	0
1	R	125/192 (65%)	0.95	18 (14%) 2 2	34, 58, 95, 138	0
1	S	127/192 (66%)	0.97	19 (14%) 2 1	37, 69, 100, 123	0
1	T	126/192 (65%)	0.76	16 (12%) 3 3	37, 64, 96, 120	0
All	All	2500/3840 (65%)	0.85	302 (12%) 4 3	30, 65, 113, 175	0

The worst 5 of 302 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	7	MET	11.7
1	O	129	PHE	9.2
1	J	8	TYR	9.0
1	D	129	PHE	8.8
1	M	7	MET	8.4

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.