



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 04:26 PM EDT

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 Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

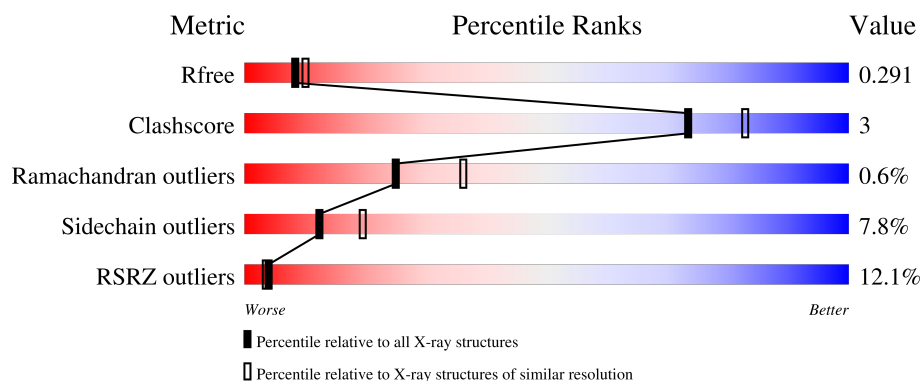
# 1 Overall quality at a glance

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 of the lower 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  $\leq 5\%$ . 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	
1	B	192	
1	C	192	
1	D	192	
1	E	192	

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Mol	Chain	Length	Quality of chain
1	F	192	
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

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

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

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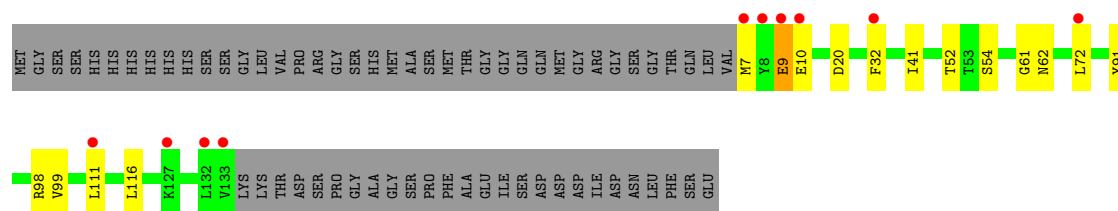
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	M	9	Total 9	O 9	0	0
2	N	13	Total 13	O 13	0	0
2	Q	19	Total 19	O 19	0	0
2	R	18	Total 18	O 18	0	0
2	K	7	Total 7	O 7	0	0
2	L	13	Total 13	O 13	0	0
2	O	6	Total 6	O 6	0	0
2	P	17	Total 17	O 17	0	0
2	S	12	Total 12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

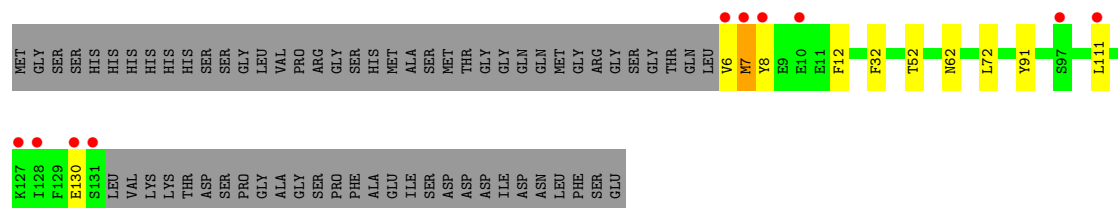


- Molecule 1: MgIB

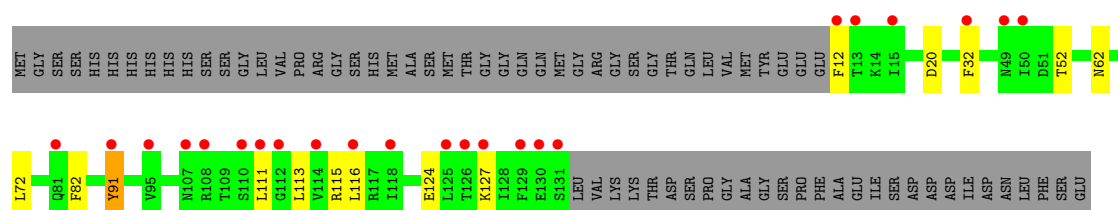




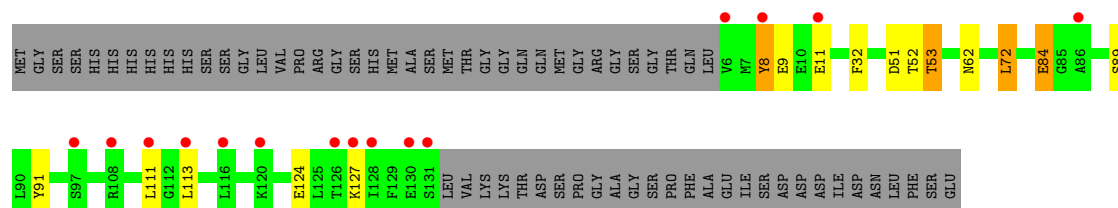
• Molecule 1: MglB



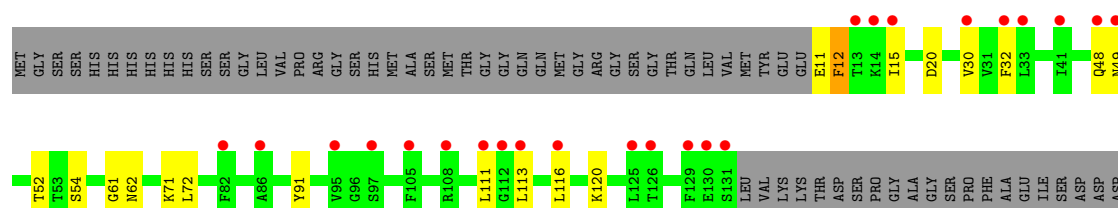
• Molecule 1: MglB



• Molecule 1: MglB



• Molecule 1: MglB





ILE  
ASP  
ASN  
LEU  
PHE  
SER  
GLU

## ● Molecule 1: MglB

Chain I: 

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER SER HIS MET MET ALA SER SER MET MET THR GLY GLY GLN GLN MET GLY ILE ARG GLY SER ASP GLY THR LEU VAL M7 Y8 E9 F12 T13 D20 F32 T82 T53 N62 L72 I73 P79

F82 Y91 R98 V99 L111 L116 R117 E130 S131 V132 V133 LYS THR ASP SER MET MET GLY SER SER MET MET THR GLY SER PRO PHE GLN ALA MET GLY ILE SER ASP GLY SER ASP ASP ASP THR GLN ASP ASN LEU PHE SER GLU

## ● Molecule 1: MglB

Chain J: 

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER SER HIS MET MET ALA SER SER MET MET THR GLY GLY GLN GLN MET GLY ILE ARG GLY SER ASP GLY THR LEU VAL M7 Y8 E9 E10 E11 F12 A17 D20 F32 M49 I50 D51 T52 T53 N62

L72 P79 E84 Y91 I94 S97 L113 L116 L129 E130 SER LEU VAL LYS LYS SER SER ASP SER PRO GLY GLY ALA MET GLY SER PRO PHE GLY ALA GLY ILE SER ASP ASP ASP ASN LEU PHE SER GLU

## ● Molecule 1: MglB

Chain M: 

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER SER HIS MET MET ALA SER SER MET MET THR GLY GLY GLN GLN MET GLY ILE ARG GLY SER ASP GLY THR LEU VAL M7 Y8 E9 E10 E11 F12 D20 F32 Q48 Q49 T52 M62 L69 A70 K71

L72 E75 P79 N80 Q81 F82 Y91 R98 V99 L111 G112 L116 L128 S131 L132 V133 LYS THR ASP GLY ALA GLY SER SER PRO PHE GLY ILE VAL M7 Y8 E9 E10 E11 F12 D20 F32 Q48 Q49 T52 M62 L69 A70 K71

## ● Molecule 1: MglB

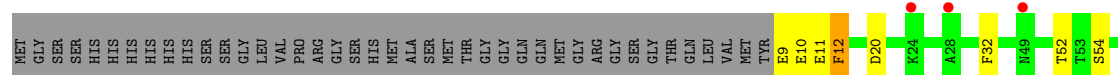
Chain N: 

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER SER HIS MET MET ALA SER SER MET MET THR GLY GLY GLN GLN MET GLY ILE ARG GLY SER ASP GLY THR LEU VAL M7 Y8 E9 E10 E11 F12 D20 F32 Q48 Q49 T52 M62 L69 A70 K71

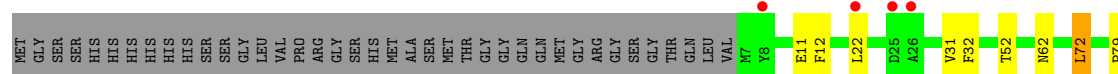
M49 I50 D51 T52 S53 S54 S55 G61 N62 L72 P79 F82 Y91 I94 S97 L111 G112 L113 L116 L117 R128 F129 L132 VAL LYS LYS THR GLY SER SER PRO PHE GLY ILE VAL M7 Y8 E9 E10 E11 F12 D20 F32 Q48 Q49 T52 M62 L69 A70 K71

## ● Molecule 1: MglB

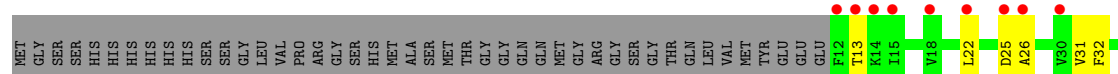
Chain Q: 



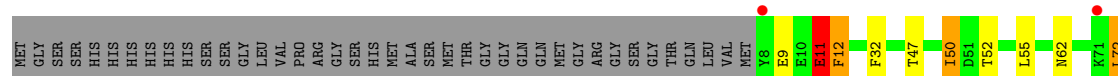
• Molecule 1: MglB



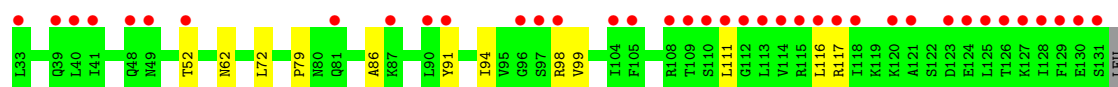
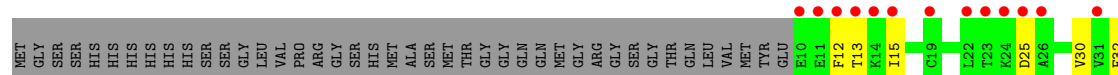
• Molecule 1: MglB



• Molecule 1: MglB



• Molecule 1: MglB



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● Molecule 1: MglB



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● Molecule 1: MglB



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● Molecule 1: MglB



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G85  
A86  
K87  
Y91  
I94  
R98  
V99  
I104  
R108  
L111  
L116  
K120  
E130  
S131  
LEU  
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SER  
ASP  
ASP  
ASP  
ASP  
ASP  
ASN  
PHE  
SER

GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.39Å)	Xtriage
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 <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 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	0.41	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.

All (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
1	G	8	TYR	C-N-CA	5.97	136.63	121.70
1	R	11	GLU	C-N-CA	5.59	135.67	121.70
1	T	86	ALA	C-N-CA	5.50	135.46	121.70
1	K	117	ARG	CB-CG-CD	5.31	125.41	111.60
1	A	8	TYR	C-N-CA	5.25	134.83	121.70
1	T	8	TYR	C-N-CA	5.10	134.44	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:M:9:GLU:HA	1:M:10:GLU:HB2	1.59	0.82
1:K:26:ALA:HA	1:K:117:ARG:HD3	1.66	0.78
1:B:130:GLU:HG2	1:R:116:LEU:HD11	1.65	0.77
1:S:105:PHE:CD1	1:S:106:ASP:N	2.52	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:TYR:HB3	1:C:12:PHE:HB2	1.70	0.73
1:O:25:ASP:HB3	1:O:117:ARG:CZ	2.19	0.72
1:S:105:PHE:CE2	1:S:109:THR:OG1	2.43	0.70
1:M:11:GLU:HG3	1:M:128:ILE:HG23	1.73	0.70
1:N:10:GLU:HB2	1:N:14:LYS:HE2	1.75	0.67
1:S:22:LEU:HD12	1:S:31:VAL:HG21	1.76	0.66
1:S:22:LEU:HD22	1:S:117:ARG:HG3	1.80	0.64
1:S:28:ALA:HA	1:S:105:PHE:CG	2.33	0.62
1:K:113:LEU:HD21	1:K:117:ARG:NH1	2.15	0.61
1:Q:61:GLY:HA2	1:T:61:GLY:HA2	1.83	0.60
1:F:32:PHE:HE2	1:F:52:THR:HG22	1.67	0.60
1:N:61:GLY:HA2	1:P:61:GLY:HA2	1.82	0.59
1:G:84:GLU:O	1:G:89:SER:HA	2.01	0.59
1:Q:9:GLU:N	1:Q:10:GLU:HA	2.17	0.59
1:K:22:LEU:HD12	1:K:31:VAL:HG21	1.85	0.58
1:M:82:PHE:HB2	1:M:91:TYR:CE1	2.38	0.58
1:L:124:GLU:O	1:L:127:LYS:HG2	2.04	0.58
1:S:27:ASN:O	1:S:105:PHE:CZ	2.56	0.58
1:A:39:GLN:HG2	1:F:10:GLU:HG2	1.86	0.58
1:K:124:GLU:O	1:K:127:LYS:HG2	2.04	0.57
1:A:8:TYR:HA	1:A:10:GLU:H	1.69	0.57
1:Q:124:GLU:O	1:Q:127:LYS:HG2	2.05	0.57
1:G:124:GLU:O	1:G:127:LYS:HG2	2.04	0.57
1:D:82:PHE:HB2	1:D:91:TYR:CE1	2.39	0.56
1:K:113:LEU:HD11	1:K:117:ARG:NH1	2.20	0.56
1:S:22:LEU:CD2	1:S:117:ARG:HG3	2.36	0.56
1:I:82:PHE:HB2	1:I:91:TYR:CE1	2.40	0.56
1:D:124:GLU:O	1:D:127:LYS:HG2	2.05	0.56
1:H:32:PHE:HE2	1:H:52:THR:HG22	1.71	0.55
1:Q:69:LEU:O	1:Q:73:ILE:HD12	2.06	0.55
1:L:98:ARG:HG3	1:L:99:VAL:HG23	1.89	0.54
1:N:111:LEU:HD13	1:S:8:TYR:HB3	1.88	0.54
1:O:25:ASP:HB3	1:O:117:ARG:NH1	2.22	0.54
1:T:98:ARG:HG3	1:T:99:VAL:HG23	1.90	0.54
1:Q:83:HIS:HD2	1:R:81:GLN:HG2	1.72	0.54
1:K:73:ILE:HD13	1:K:73:ILE:O	2.07	0.54
1:M:98:ARG:HG3	1:M:99:VAL:HG23	1.91	0.53
1:N:82:PHE:HB2	1:N:91:TYR:CE1	2.43	0.53
1:L:11:GLU:HA	1:L:12:PHE:CB	2.39	0.52
1:I:98:ARG:HG3	1:I:99:VAL:HG23	1.91	0.52
1:L:11:GLU:HA	1:L:12:PHE:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:32:PHE:CZ	1:L:50:ILE:HD12	2.45	0.52
1:O:32:PHE:HE2	1:O:52:THR:HG22	1.73	0.52
1:K:26:ALA:CA	1:K:117:ARG:HD3	2.40	0.51
1:O:79:PRO:HA	1:O:94:ILE:HG13	1.92	0.51
1:Q:54:SER:HB2	1:R:72:LEU:HD11	1.93	0.51
1:M:69:LEU:HD11	1:N:55:LEU:HG	1.93	0.50
1:R:98:ARG:HG3	1:R:99:VAL:HG23	1.91	0.50
1:A:32:PHE:HE1	1:A:52:THR:HG22	1.75	0.50
1:R:22:LEU:HD22	1:R:31:VAL:HG21	1.93	0.50
1:A:8:TYR:HD1	1:A:10:GLU:HB3	1.76	0.50
1:K:73:ILE:HG13	1:L:104:ILE:HG21	1.92	0.50
1:O:98:ARG:HG3	1:O:99:VAL:HG23	1.94	0.50
1:P:79:PRO:HA	1:P:94:ILE:HG13	1.94	0.50
1:C:7:MET:HB2	1:R:111:LEU:HB3	1.94	0.50
1:S:72:LEU:HD11	1:T:54:SER:HB2	1.94	0.50
1:D:32:PHE:HE1	1:D:52:THR:HG22	1.77	0.49
1:F:98:ARG:HG3	1:F:99:VAL:HG23	1.96	0.48
1:T:79:PRO:HA	1:T:94:ILE:HG13	1.95	0.48
1:I:32:PHE:HE1	1:I:52:THR:HG22	1.78	0.48
1:K:25:ASP:O	1:K:117:ARG:NH1	2.46	0.48
1:L:50:ILE:HD11	1:L:55:LEU:HD13	1.95	0.48
2:F:216:HOH:O	1:H:71:LYS:HE2	2.14	0.47
1:J:79:PRO:HA	1:J:94:ILE:HG13	1.96	0.47
1:A:9:GLU:HG2	1:F:41:ILE:HG12	1.97	0.47
1:N:79:PRO:HA	1:N:94:ILE:HG13	1.96	0.47
1:B:80:ASN:HB3	1:B:91:TYR:HE1	1.80	0.47
1:N:21:ARG:HG2	1:N:25:ASP:OD2	2.15	0.47
1:P:32:PHE:HE1	1:P:52:THR:HG22	1.80	0.46
1:M:32:PHE:HE1	1:M:52:THR:HG22	1.81	0.46
1:M:111:LEU:HB3	1:S:7:MET:HB2	1.98	0.46
1:K:83:HIS:HD2	1:L:81:GLN:HG2	1.81	0.46
1:L:32:PHE:HE1	1:L:52:THR:HG22	1.81	0.46
1:T:32:PHE:HE1	1:T:52:THR:HG22	1.81	0.45
1:B:79:PRO:HA	1:B:94:ILE:HG13	1.99	0.45
1:S:66:MET:HE1	1:S:69:LEU:HD22	1.97	0.45
1:E:12:PHE:CB	1:E:15:ILE:HD12	2.47	0.45
1:Q:83:HIS:CD2	1:R:81:GLN:HG2	2.50	0.45
1:R:32:PHE:HE1	1:R:52:THR:HG22	1.81	0.45
1:T:8:TYR:HA	1:T:9:GLU:HB3	1.98	0.45
1:G:51:ASP:OD1	1:G:53:THR:HG23	2.17	0.45
1:M:112:GLY:HA2	1:S:12:PHE:CZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:79:PRO:HA	1:O:94:ILE:CG1	2.47	0.44
1:E:72:LEU:HD11	1:F:54:SER:HB2	1.99	0.44
1:F:61:GLY:HA2	1:H:61:GLY:HA2	1.98	0.44
1:S:32:PHE:HE1	1:S:52:THR:HG22	1.81	0.44
1:J:8:TYR:O	1:J:9:GLU:HB2	2.17	0.44
1:K:32:PHE:HE1	1:K:52:THR:HG22	1.82	0.44
1:G:32:PHE:HE1	1:G:52:THR:HG22	1.83	0.44
1:N:111:LEU:CD1	1:S:8:TYR:HB3	2.48	0.44
1:Q:84:GLU:O	1:R:79:PRO:HD2	2.18	0.44
1:C:32:PHE:HE1	1:C:52:THR:HG22	1.83	0.43
1:G:72:LEU:HD11	1:H:54:SER:HB2	1.99	0.43
1:K:113:LEU:HD21	1:K:117:ARG:HH11	1.82	0.43
1:I:79:PRO:HD2	1:J:84:GLU:O	2.18	0.43
1:T:79:PRO:HA	1:T:94:ILE:CG1	2.48	0.43
1:J:51:ASP:OD1	1:J:53:THR:HG23	2.19	0.43
1:K:54:SER:HB2	1:L:72:LEU:HD11	2.00	0.43
1:Q:83:HIS:HD2	1:R:81:GLN:CG	2.32	0.43
1:S:22:LEU:HD12	1:S:31:VAL:CG2	2.45	0.43
1:S:105:PHE:CG	1:S:106:ASP:N	2.87	0.42
1:R:22:LEU:O	1:R:22:LEU:HD23	2.20	0.42
1:N:32:PHE:HE1	1:N:52:THR:HG22	1.84	0.42
1:Q:32:PHE:HE1	1:Q:52:THR:HG22	1.84	0.42
1:E:32:PHE:HE1	1:E:52:THR:HG22	1.85	0.42
1:K:113:LEU:CG	1:K:117:ARG:NH1	2.82	0.42
1:P:79:PRO:HA	1:P:94:ILE:CG1	2.49	0.42
1:S:105:PHE:HD1	1:S:105:PHE:HA	1.25	0.42
1:I:9:GLU:HB2	1:Q:12:PHE:CZ	2.55	0.41
1:E:51:ASP:OD1	1:E:53:THR:HG23	2.19	0.41
1:M:112:GLY:O	1:S:12:PHE:HZ	2.04	0.41
1:B:80:ASN:HB3	1:B:91:TYR:CE1	2.56	0.41
1:Q:11:GLU:HB3	1:Q:12:PHE:HD2	1.85	0.41
1:B:114:VAL:HG12	1:B:118:ILE:CD1	2.51	0.41
1:J:32:PHE:HE1	1:J:52:THR:HG22	1.85	0.40
1:N:79:PRO:HA	1:N:94:ILE:CG1	2.51	0.40
1:A:79:PRO:HD2	1:B:84:GLU:O	2.22	0.40
1:S:27:ASN:HB3	1:S:105:PHE:HE2	1.86	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 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

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	84	GLU

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Mol	Chain	Res	Type
1	J	9	GLU
1	R	12	PHE
1	K	13	THR
1	S	9	GLU
1	T	87	LYS
1	L	12	PHE
1	P	11	GLU
1	S	11	GLU
1	P	7	MET
1	B	9	GLU
1	F	9	GLU
1	J	8	TYR
1	Q	12	PHE

### 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 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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	50	ILE
1	A	62	ASN
1	A	72	LEU
1	A	91	TYR
1	A	111	LEU
1	A	113	LEU
1	A	116	LEU
1	B	12	PHE
1	B	13	THR
1	B	20	ASP
1	B	62	ASN
1	B	72	LEU
1	B	91	TYR
1	B	113	LEU
1	B	116	LEU
1	B	117	ARG
1	B	132	LEU
1	E	13	THR
1	E	53	THR
1	E	62	ASN
1	E	72	LEU
1	E	91	TYR
1	E	111	LEU
1	E	113	LEU
1	E	116	LEU
1	E	132	LEU
1	F	7	MET
1	F	20	ASP

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Mol	Chain	Res	Type
1	F	62	ASN
1	F	72	LEU
1	F	91	TYR
1	F	111	LEU
1	F	116	LEU
1	C	6	VAL
1	C	7	MET
1	C	62	ASN
1	C	72	LEU
1	C	91	TYR
1	C	111	LEU
1	C	130	GLU
1	D	12	PHE
1	D	20	ASP
1	D	62	ASN
1	D	72	LEU
1	D	91	TYR
1	D	111	LEU
1	D	113	LEU
1	D	115	ARG
1	D	116	LEU
1	G	8	TYR
1	G	9	GLU
1	G	11	GLU
1	G	53	THR
1	G	62	ASN
1	G	72	LEU
1	G	91	TYR
1	G	111	LEU
1	G	113	LEU
1	H	11	GLU
1	H	12	PHE
1	H	20	ASP
1	H	30	VAL
1	H	48	GLN
1	H	49	ASN
1	H	62	ASN
1	H	72	LEU
1	H	91	TYR
1	H	111	LEU
1	H	113	LEU
1	H	116	LEU

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Mol	Chain	Res	Type
1	H	120	LYS
1	I	7	MET
1	I	13	THR
1	I	20	ASP
1	I	62	ASN
1	I	72	LEU
1	I	73	ILE
1	I	91	TYR
1	I	116	LEU
1	I	117	ARG
1	J	8	TYR
1	J	9	GLU
1	J	11	GLU
1	J	12	PHE
1	J	20	ASP
1	J	53	THR
1	J	62	ASN
1	J	72	LEU
1	J	91	TYR
1	J	113	LEU
1	J	116	LEU
1	M	8	TYR
1	M	20	ASP
1	M	62	ASN
1	M	72	LEU
1	M	91	TYR
1	M	111	LEU
1	M	116	LEU
1	N	10	GLU
1	N	11	GLU
1	N	20	ASP
1	N	21	ARG
1	N	62	ASN
1	N	72	LEU
1	N	91	TYR
1	N	116	LEU
1	N	132	LEU
1	Q	20	ASP
1	Q	62	ASN
1	Q	72	LEU
1	Q	91	TYR
1	Q	111	LEU

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Mol	Chain	Res	Type
1	Q	113	LEU
1	Q	116	LEU
1	R	62	ASN
1	R	72	LEU
1	R	91	TYR
1	R	111	LEU
1	R	116	LEU
1	R	120	LYS
1	K	62	ASN
1	K	72	LEU
1	K	73	ILE
1	K	91	TYR
1	L	9	GLU
1	L	11	GLU
1	L	47	THR
1	L	50	ILE
1	L	62	ASN
1	L	72	LEU
1	L	91	TYR
1	L	111	LEU
1	L	116	LEU
1	O	13	THR
1	O	30	VAL
1	O	62	ASN
1	O	72	LEU
1	O	91	TYR
1	O	111	LEU
1	O	116	LEU
1	P	8	TYR
1	P	62	ASN
1	P	72	LEU
1	P	91	TYR
1	P	111	LEU
1	P	116	LEU
1	S	5	LEU
1	S	8	TYR
1	S	9	GLU
1	S	62	ASN
1	S	72	LEU
1	S	91	TYR
1	S	105	PHE
1	S	111	LEU

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Mol	Chain	Res	Type
1	S	116	LEU
1	S	119	LYS
1	T	20	ASP
1	T	62	ASN
1	T	72	LEU
1	T	91	TYR
1	T	111	LEU
1	T	116	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	81	GLN
1	B	62	ASN
1	B	83	HIS
1	E	83	HIS
1	F	80	ASN
1	F	83	HIS
1	D	81	GLN
1	D	83	HIS
1	H	83	HIS
1	J	83	HIS
1	M	16	ASN
1	M	81	GLN
1	N	80	ASN
1	Q	16	ASN
1	Q	83	HIS
1	R	81	GLN
1	R	83	HIS
1	K	83	HIS
1	L	16	ASN
1	L	83	HIS
1	O	62	ASN
1	O	83	HIS
1	P	62	ASN
1	P	83	HIS
1	T	16	ASN
1	T	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 monosaccharides 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	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%)	2.01	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%)	0.66	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

All (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
1	H	129	PHE	7.9
1	O	15	ILE	7.8
1	B	132	LEU	7.8
1	K	15	ILE	7.8
1	O	113	LEU	6.9
1	I	132	LEU	6.6
1	L	132	LEU	6.6
1	K	127	LYS	6.5
1	A	8	TYR	6.4
1	E	11	GLU	6.3
1	R	131	SER	6.3
1	C	8	TYR	6.3
1	O	125	LEU	6.2
1	K	26	ALA	6.1
1	K	113	LEU	6.1
1	O	111	LEU	6.1
1	D	108	ARG	5.9
1	D	15	ILE	5.9
1	R	26	ALA	5.6
1	P	136	THR	5.6
1	H	86	ALA	5.5
1	B	8	TYR	5.4
1	O	131	SER	5.3
1	S	105	PHE	5.3
1	S	7	MET	5.3
1	J	7	MET	5.3
1	O	12	PHE	5.3
1	K	114	VAL	5.2
1	O	114	VAL	5.1
1	K	129	PHE	5.1
1	S	26	ALA	5.0
1	H	97	SER	5.0
1	P	5	LEU	4.9
1	O	10	GLU	4.9
1	I	32	PHE	4.7
1	T	6	VAL	4.7
1	O	108	ARG	4.7
1	A	32	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	127	LYS	4.6
1	O	13	THR	4.6
1	G	111	LEU	4.5
1	R	128	ILE	4.4
1	O	127	LYS	4.4
1	H	49	ASN	4.4
1	T	12	PHE	4.4
1	O	105	PHE	4.3
1	H	113	LEU	4.3
1	I	7	MET	4.3
1	K	111	LEU	4.2
1	K	13	THR	4.2
1	R	114	VAL	4.2
1	D	130	GLU	4.2
1	O	91	TYR	4.2
1	B	97	SER	4.2
1	J	97	SER	4.1
1	N	113	LEU	4.1
1	D	125	LEU	4.0
1	K	25	ASP	4.0
1	O	11	GLU	4.0
1	P	8	TYR	4.0
1	S	116	LEU	3.9
1	B	133	VAL	3.9
1	L	97	SER	3.8
1	N	132	LEU	3.8
1	Q	24	LYS	3.8
1	R	129	PHE	3.8
1	O	22	LEU	3.8
1	O	112	GLY	3.8
1	P	6	VAL	3.8
1	G	8	TYR	3.8
1	O	130	GLU	3.7
1	D	126	THR	3.7
1	C	10	GLU	3.7
1	O	26	ALA	3.7
1	E	98	ARG	3.6
1	O	52	THR	3.6
1	I	8	TYR	3.6
1	M	133	VAL	3.6
1	H	14	LYS	3.6
1	M	98	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	N	49	ASN	3.6
1	C	131	SER	3.6
1	D	110	SER	3.6
1	S	8	TYR	3.6
1	G	130	GLU	3.5
1	N	97	SER	3.5
1	T	8	TYR	3.5
1	H	130	GLU	3.5
1	O	104	ILE	3.5
1	D	112	GLY	3.5
1	H	32	PHE	3.4
1	F	8	TYR	3.4
1	P	74	GLY	3.4
1	O	19	CYS	3.4
1	C	6	VAL	3.4
1	K	14	LYS	3.4
1	H	15	ILE	3.4
1	E	97	SER	3.3
1	R	91	TYR	3.3
1	C	130	GLU	3.3
1	D	111	LEU	3.3
1	K	12	PHE	3.3
1	K	130	GLU	3.3
1	L	116	LEU	3.3
1	O	25	ASP	3.3
1	N	10	GLU	3.3
1	E	120	LYS	3.2
1	O	41	ILE	3.2
1	O	115	ARG	3.2
1	D	116	LEU	3.2
1	G	116	LEU	3.2
1	K	86	ALA	3.2
1	R	105	PHE	3.2
1	O	49	ASN	3.2
1	C	128	ILE	3.2
1	D	12	PHE	3.2
1	O	23	THR	3.2
1	R	120	LYS	3.2
1	L	8	TYR	3.2
1	S	6	VAL	3.1
1	P	97	SER	3.1
1	H	111	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	116	LEU	3.0
1	D	107	ASN	3.0
1	O	116	LEU	3.0
1	M	79	PRO	3.0
1	O	124	GLU	3.0
1	R	127	LYS	3.0
1	S	131	SER	3.0
1	E	12	PHE	3.0
1	S	25	ASP	2.9
1	H	82	PHE	2.9
1	G	126	THR	2.9
1	M	132	LEU	2.9
1	K	22	LEU	2.9
1	G	86	ALA	2.9
1	F	133	VAL	2.9
1	R	22	LEU	2.9
1	P	96	GLY	2.9
1	G	97	SER	2.9
1	K	18	VAL	2.9
1	O	24	LYS	2.9
1	J	51	ASP	2.9
1	N	129	PHE	2.8
1	T	7	MET	2.8
1	K	120	LYS	2.8
1	D	118	ILE	2.8
1	S	81	GLN	2.8
1	B	91	TYR	2.8
1	N	91	TYR	2.8
1	G	127	LYS	2.8
1	K	125	LEU	2.8
1	D	13	THR	2.8
1	H	116	LEU	2.8
1	J	10	GLU	2.8
1	T	116	LEU	2.7
1	N	50	ILE	2.7
1	R	97	SER	2.7
1	S	5	LEU	2.7
1	H	13	THR	2.7
1	O	128	ILE	2.7
1	M	70	ALA	2.7
1	F	10	GLU	2.7
1	O	87	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	111	LEU	2.7
1	I	133	VAL	2.7
1	Q	133	VAL	2.7
1	E	132	LEU	2.7
1	J	12	PHE	2.7
1	M	131	SER	2.7
1	O	121	ALA	2.7
1	T	28	ALA	2.7
1	L	130	GLU	2.7
1	M	48	GLN	2.7
1	Q	131	SER	2.6
1	S	27	ASN	2.6
1	C	127	LYS	2.6
1	N	28	ALA	2.6
1	E	91	TYR	2.6
1	R	25	ASP	2.6
1	I	73	ILE	2.6
1	O	39	GLN	2.6
1	O	117	ARG	2.6
1	G	113	LEU	2.6
1	O	109	THR	2.5
1	H	30	VAL	2.5
1	O	123	ASP	2.5
1	T	82	PHE	2.5
1	O	48	GLN	2.5
1	N	24	LYS	2.5
1	O	33	LEU	2.5
1	H	126	THR	2.5
1	O	98	ARG	2.5
1	J	130	GLU	2.5
1	M	111	LEU	2.5
1	R	111	LEU	2.5
1	R	116	LEU	2.5
1	H	105	PHE	2.5
1	T	32	PHE	2.5
1	Q	28	ALA	2.4
1	J	49	ASN	2.4
1	S	24	LYS	2.4
1	E	20	ASP	2.4
1	D	131	SER	2.4
1	H	108	ARG	2.4
1	I	52	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	S	23	THR	2.4
1	R	123	ASP	2.4
1	D	50	ILE	2.4
1	M	75	GLU	2.4
1	O	120	LYS	2.4
1	D	95	VAL	2.4
1	S	127	LYS	2.4
1	B	94	ILE	2.4
1	I	111	LEU	2.4
1	T	49	ASN	2.4
1	D	32	PHE	2.4
1	M	81	GLN	2.4
1	T	11	GLU	2.4
1	F	72	LEU	2.4
1	H	48	GLN	2.4
1	R	8	TYR	2.3
1	N	55	LEU	2.3
1	D	114	VAL	2.3
1	I	130	GLU	2.3
1	O	14	LYS	2.3
1	S	117	ARG	2.3
1	O	97	SER	2.3
1	R	130	GLU	2.3
1	D	91	TYR	2.3
1	G	11	GLU	2.3
1	J	129	PHE	2.3
1	T	50	ILE	2.3
1	N	21	ARG	2.3
1	D	81	GLN	2.3
1	G	108	ARG	2.3
1	T	108	ARG	2.3
1	N	32	PHE	2.3
1	G	131	SER	2.3
1	O	126	THR	2.2
1	N	53	THR	2.2
1	H	33	LEU	2.2
1	T	24	LYS	2.2
1	K	30	VAL	2.2
1	I	12	PHE	2.2
1	P	137	ASP	2.2
1	M	49	ASN	2.2
1	Q	104	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	52	THR	2.2
1	H	95	VAL	2.2
1	O	118	ILE	2.2
1	S	111	LEU	2.2
1	P	11	GLU	2.2
1	S	130	GLU	2.2
1	Q	49	ASN	2.1
1	M	12	PHE	2.1
1	Q	124	GLU	2.1
1	A	81	GLN	2.1
1	A	76	ASN	2.1
1	C	7	MET	2.1
1	F	9	GLU	2.1
1	T	120	LYS	2.1
1	G	128	ILE	2.1
1	A	55	LEU	2.1
1	C	97	SER	2.1
1	O	40	LEU	2.1
1	L	71	LYS	2.1
1	F	32	PHE	2.1
1	H	131	SER	2.1
1	N	27	ASN	2.1
1	O	110	SER	2.1
1	O	90	LEU	2.1
1	D	49	ASN	2.1
1	T	130	GLU	2.1
1	T	104	ILE	2.1
1	F	127	LYS	2.1
1	N	117	ARG	2.1
1	J	17	ALA	2.1
1	M	8	TYR	2.1
1	F	111	LEU	2.1
1	O	81	GLN	2.1
1	G	120	LYS	2.1
1	O	31	VAL	2.1
1	H	125	LEU	2.0
1	H	112	GLY	2.0
1	O	96	GLY	2.0
1	I	9	GLU	2.0
1	G	6	VAL	2.0
1	S	114	VAL	2.0
1	R	110	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	117	ARG	2.0
1	N	18	VAL	2.0
1	F	132	LEU	2.0
1	H	41	ILE	2.0
1	I	53	THR	2.0
1	Q	88	ASP	2.0
1	K	126	THR	2.0

## 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 monosaccharides 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.