



Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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

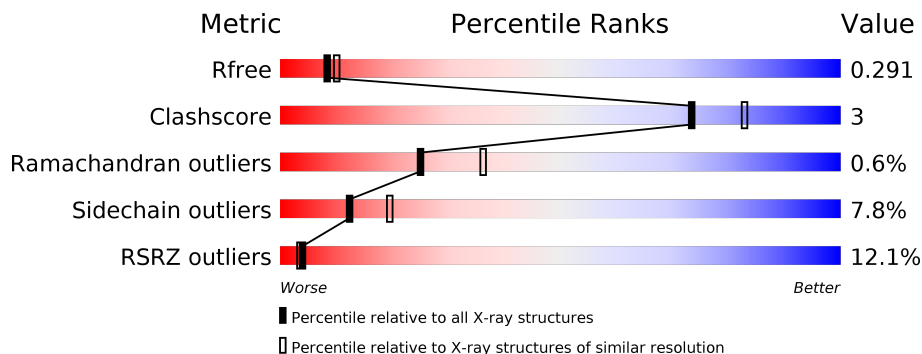
1 Overall quality at a glance

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

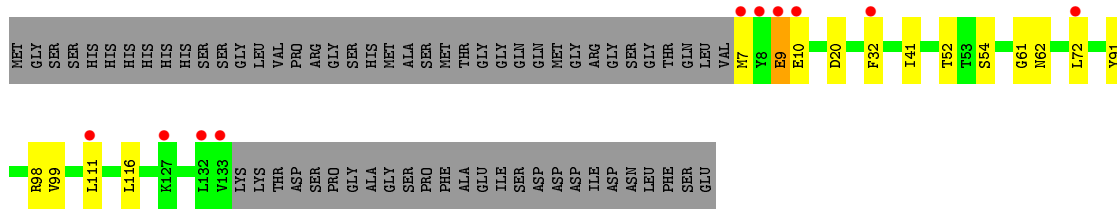
- Molecule 2 is water.

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

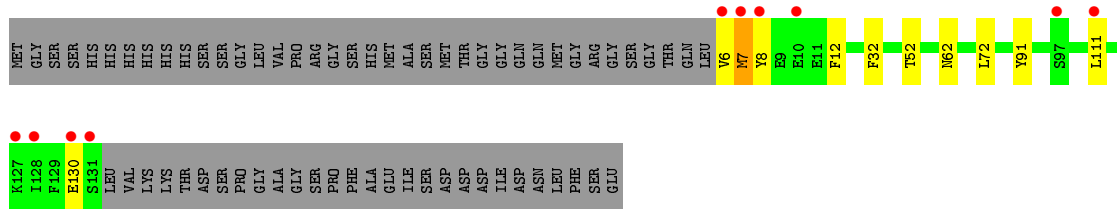
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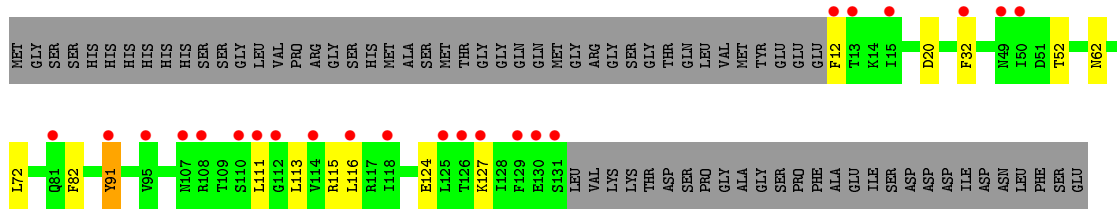
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	M	9	Total O 9 9	0	0
2	N	13	Total O 13 13	0	0
2	Q	19	Total O 19 19	0	0
2	R	18	Total O 18 18	0	0
2	K	7	Total O 7 7	0	0
2	L	13	Total O 13 13	0	0
2	O	6	Total O 6 6	0	0
2	P	17	Total O 17 17	0	0
2	S	12	Total O 12 12	0	0
2	T	14	Total O 14 14	0	0



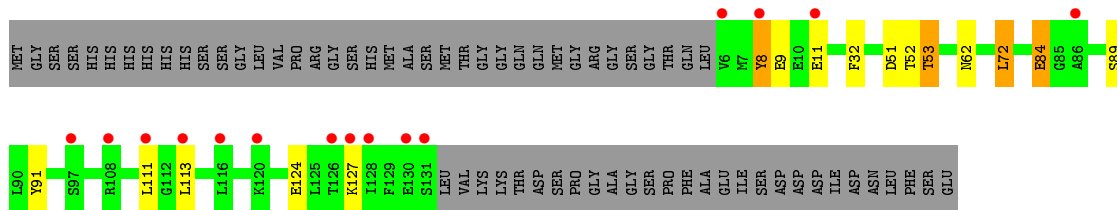
• Molecule 1: Mg1B



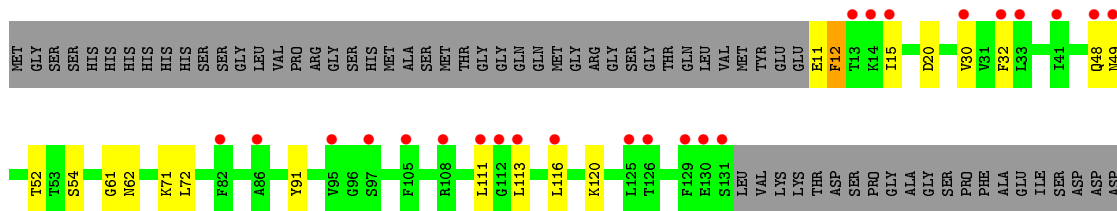
• Molecule 1: Mg1B

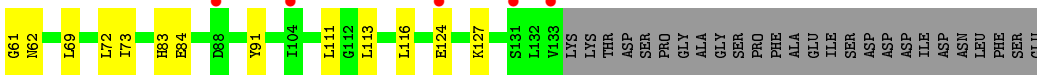
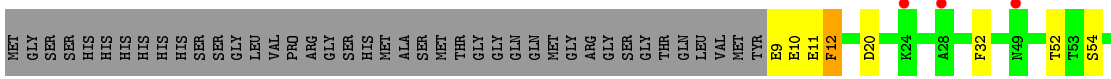


• Molecule 1: Mg1B

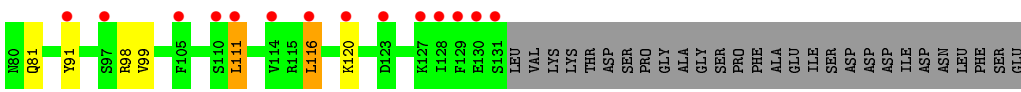
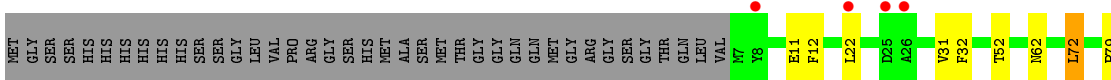


• Molecule 1: Mg1B

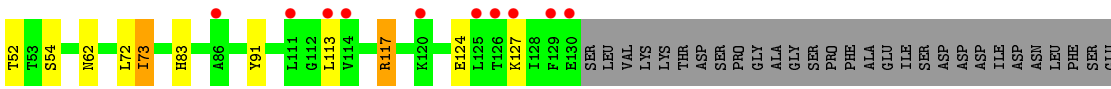
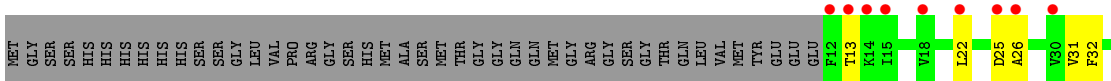




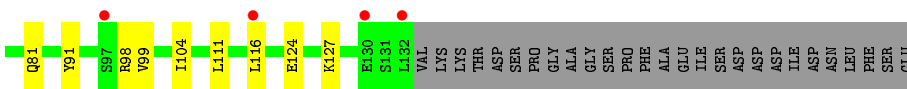
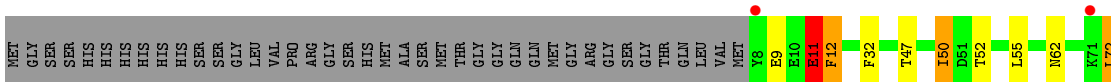
• Molecule 1: MglB



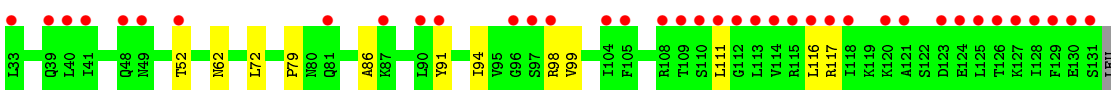
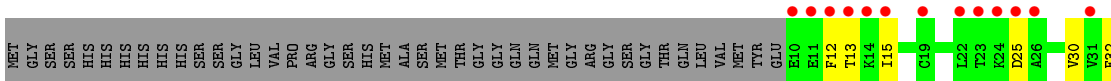
• Molecule 1: MglB



• Molecule 1: MglB



• Molecule 1: MglB



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• Molecule 1: Mg1B



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• Molecule 1: Mg1B



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V31
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N62

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Q81
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F105
D106
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• Molecule 1: Mg1B



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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.

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:L:124:GLU:O	1:L:127:LYS:HG2	2.04	0.58
1:M:82:PHE:HB2	1:M:91:TYR:CE1	2.38	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:O	1:K:73:ILE:HD13	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:K:83:HIS:HD2	1:L:81:GLN:HG2	1.81	0.46
1:M:111:LEU:HB3	1:S:7:MET:HB2	1.98	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:R:32:PHE:HE1	1:R:52:THR:HG22	1.81	0.45
1:Q:83:HIS:CD2	1:R:81:GLN:HG2	2.50	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:O:79:PRO:HA	1:O:94:ILE:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:112:GLY:HA2	1:S:12:PHE:CZ	2.51	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:Q:84:GLU:O	1:R:79:PRO:HD2	2.18	0.44
1:N:111:LEU:CD1	1:S:8:TYR:HB3	2.48	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 [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

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 [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

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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

Some 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 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

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, 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

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	N	49	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	131	SER	3.6
1	D	110	SER	3.6
1	M	98	ARG	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 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.