



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:19 PM GMT

PDB ID : 4HW9
Title : Crystal Structure of Helicobacter pylori MscS (Closed State)
Authors : Lai, J.Y.; Poon, Y.S.; Kaiser, J.; Rees, D.C.
Deposited on : 2012-11-07
Resolution : 4.14 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

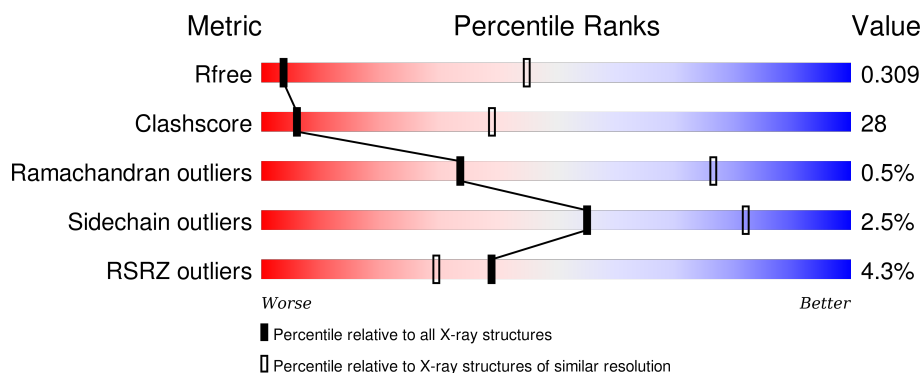
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.14 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}	91344	1023 (4.68-3.60)
Clashscore	102246	1122 (4.68-3.60)
Ramachandran outliers	100387	1068 (4.68-3.60)
Sidechain outliers	100360	1054 (4.68-3.60)
RSRZ outliers	91569	1027 (4.68-3.60)

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. 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	309	<div> <div>6%</div> <div> <div>38%</div> <div>40%</div> <div>18%</div> </div> </div>
1	B	309	<div> <div>2%</div> <div> <div>39%</div> <div>38%</div> <div>18%</div> </div> </div>
1	C	309	<div> <div>3%</div> <div> <div>39%</div> <div>38%</div> <div>18%</div> </div> </div>
1	D	309	<div> <div>3%</div> <div> <div>40%</div> <div>39%</div> <div>18%</div> </div> </div>
1	E	309	<div> <div>4%</div> <div> <div>40%</div> <div>35%</div> <div>5%</div> <div>18%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	309	<p>2% 40% 37% 18%</p>
1	G	309	<p>5% 39% 38% 18%</p>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13797 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 Mechanosensitive channel MscS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	B	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	C	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	D	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	E	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	F	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	G	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0

There are 266 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	EXPRESSION TAG	UNP E8QGV2
A	-22	GLY	-	EXPRESSION TAG	UNP E8QGV2
A	-21	SER	-	EXPRESSION TAG	UNP E8QGV2
A	-20	SER	-	EXPRESSION TAG	UNP E8QGV2
A	-19	HIS	-	EXPRESSION TAG	UNP E8QGV2
A	-18	HIS	-	EXPRESSION TAG	UNP E8QGV2
A	-17	HIS	-	EXPRESSION TAG	UNP E8QGV2
A	-16	HIS	-	EXPRESSION TAG	UNP E8QGV2
A	-15	HIS	-	EXPRESSION TAG	UNP E8QGV2
A	-14	HIS	-	EXPRESSION TAG	UNP E8QGV2
A	-13	SER	-	EXPRESSION TAG	UNP E8QGV2
A	-12	SER	-	EXPRESSION TAG	UNP E8QGV2
A	-11	GLY	-	EXPRESSION TAG	UNP E8QGV2
A	-10	LEU	-	EXPRESSION TAG	UNP E8QGV2
A	-9	VAL	-	EXPRESSION TAG	UNP E8QGV2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	PRO	-	EXPRESSION TAG	UNP E8QGV2
A	-7	ARG	-	EXPRESSION TAG	UNP E8QGV2
A	-6	GLY	-	EXPRESSION TAG	UNP E8QGV2
A	-5	SER	-	EXPRESSION TAG	UNP E8QGV2
A	-4	HIS	-	EXPRESSION TAG	UNP E8QGV2
A	-3	THR	-	EXPRESSION TAG	UNP E8QGV2
A	-2	LEU	-	EXPRESSION TAG	UNP E8QGV2
A	-1	ILE	-	EXPRESSION TAG	UNP E8QGV2
A	0	ASN	-	EXPRESSION TAG	UNP E8QGV2
A	200	THR	ALA	CONFLICT	UNP E8QGV2
A	202	GLU	ASP	CONFLICT	UNP E8QGV2
A	273	PRO	SER	CONFLICT	UNP E8QGV2
A	275	LEU	-	EXPRESSION TAG	UNP E8QGV2
A	276	ILE	-	EXPRESSION TAG	UNP E8QGV2
A	277	ASN	-	EXPRESSION TAG	UNP E8QGV2
A	278	ASP	-	EXPRESSION TAG	UNP E8QGV2
A	279	TYR	-	EXPRESSION TAG	UNP E8QGV2
A	280	LYS	-	EXPRESSION TAG	UNP E8QGV2
A	281	ASP	-	EXPRESSION TAG	UNP E8QGV2
A	282	ASP	-	EXPRESSION TAG	UNP E8QGV2
A	283	ASP	-	EXPRESSION TAG	UNP E8QGV2
A	284	ASP	-	EXPRESSION TAG	UNP E8QGV2
A	285	LYS	-	EXPRESSION TAG	UNP E8QGV2
B	-23	MET	-	EXPRESSION TAG	UNP E8QGV2
B	-22	GLY	-	EXPRESSION TAG	UNP E8QGV2
B	-21	SER	-	EXPRESSION TAG	UNP E8QGV2
B	-20	SER	-	EXPRESSION TAG	UNP E8QGV2
B	-19	HIS	-	EXPRESSION TAG	UNP E8QGV2
B	-18	HIS	-	EXPRESSION TAG	UNP E8QGV2
B	-17	HIS	-	EXPRESSION TAG	UNP E8QGV2
B	-16	HIS	-	EXPRESSION TAG	UNP E8QGV2
B	-15	HIS	-	EXPRESSION TAG	UNP E8QGV2
B	-14	HIS	-	EXPRESSION TAG	UNP E8QGV2
B	-13	SER	-	EXPRESSION TAG	UNP E8QGV2
B	-12	SER	-	EXPRESSION TAG	UNP E8QGV2
B	-11	GLY	-	EXPRESSION TAG	UNP E8QGV2
B	-10	LEU	-	EXPRESSION TAG	UNP E8QGV2
B	-9	VAL	-	EXPRESSION TAG	UNP E8QGV2
B	-8	PRO	-	EXPRESSION TAG	UNP E8QGV2
B	-7	ARG	-	EXPRESSION TAG	UNP E8QGV2
B	-6	GLY	-	EXPRESSION TAG	UNP E8QGV2
B	-5	SER	-	EXPRESSION TAG	UNP E8QGV2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	EXPRESSION TAG	UNP E8QGV2
B	-3	THR	-	EXPRESSION TAG	UNP E8QGV2
B	-2	LEU	-	EXPRESSION TAG	UNP E8QGV2
B	-1	ILE	-	EXPRESSION TAG	UNP E8QGV2
B	0	ASN	-	EXPRESSION TAG	UNP E8QGV2
B	200	THR	ALA	CONFLICT	UNP E8QGV2
B	202	GLU	ASP	CONFLICT	UNP E8QGV2
B	273	PRO	SER	CONFLICT	UNP E8QGV2
B	275	LEU	-	EXPRESSION TAG	UNP E8QGV2
B	276	ILE	-	EXPRESSION TAG	UNP E8QGV2
B	277	ASN	-	EXPRESSION TAG	UNP E8QGV2
B	278	ASP	-	EXPRESSION TAG	UNP E8QGV2
B	279	TYR	-	EXPRESSION TAG	UNP E8QGV2
B	280	LYS	-	EXPRESSION TAG	UNP E8QGV2
B	281	ASP	-	EXPRESSION TAG	UNP E8QGV2
B	282	ASP	-	EXPRESSION TAG	UNP E8QGV2
B	283	ASP	-	EXPRESSION TAG	UNP E8QGV2
B	284	ASP	-	EXPRESSION TAG	UNP E8QGV2
B	285	LYS	-	EXPRESSION TAG	UNP E8QGV2
C	-23	MET	-	EXPRESSION TAG	UNP E8QGV2
C	-22	GLY	-	EXPRESSION TAG	UNP E8QGV2
C	-21	SER	-	EXPRESSION TAG	UNP E8QGV2
C	-20	SER	-	EXPRESSION TAG	UNP E8QGV2
C	-19	HIS	-	EXPRESSION TAG	UNP E8QGV2
C	-18	HIS	-	EXPRESSION TAG	UNP E8QGV2
C	-17	HIS	-	EXPRESSION TAG	UNP E8QGV2
C	-16	HIS	-	EXPRESSION TAG	UNP E8QGV2
C	-15	HIS	-	EXPRESSION TAG	UNP E8QGV2
C	-14	HIS	-	EXPRESSION TAG	UNP E8QGV2
C	-13	SER	-	EXPRESSION TAG	UNP E8QGV2
C	-12	SER	-	EXPRESSION TAG	UNP E8QGV2
C	-11	GLY	-	EXPRESSION TAG	UNP E8QGV2
C	-10	LEU	-	EXPRESSION TAG	UNP E8QGV2
C	-9	VAL	-	EXPRESSION TAG	UNP E8QGV2
C	-8	PRO	-	EXPRESSION TAG	UNP E8QGV2
C	-7	ARG	-	EXPRESSION TAG	UNP E8QGV2
C	-6	GLY	-	EXPRESSION TAG	UNP E8QGV2
C	-5	SER	-	EXPRESSION TAG	UNP E8QGV2
C	-4	HIS	-	EXPRESSION TAG	UNP E8QGV2
C	-3	THR	-	EXPRESSION TAG	UNP E8QGV2
C	-2	LEU	-	EXPRESSION TAG	UNP E8QGV2
C	-1	ILE	-	EXPRESSION TAG	UNP E8QGV2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ASN	-	EXPRESSION TAG	UNP E8QGV2
C	200	THR	ALA	CONFLICT	UNP E8QGV2
C	202	GLU	ASP	CONFLICT	UNP E8QGV2
C	273	PRO	SER	CONFLICT	UNP E8QGV2
C	275	LEU	-	EXPRESSION TAG	UNP E8QGV2
C	276	ILE	-	EXPRESSION TAG	UNP E8QGV2
C	277	ASN	-	EXPRESSION TAG	UNP E8QGV2
C	278	ASP	-	EXPRESSION TAG	UNP E8QGV2
C	279	TYR	-	EXPRESSION TAG	UNP E8QGV2
C	280	LYS	-	EXPRESSION TAG	UNP E8QGV2
C	281	ASP	-	EXPRESSION TAG	UNP E8QGV2
C	282	ASP	-	EXPRESSION TAG	UNP E8QGV2
C	283	ASP	-	EXPRESSION TAG	UNP E8QGV2
C	284	ASP	-	EXPRESSION TAG	UNP E8QGV2
C	285	LYS	-	EXPRESSION TAG	UNP E8QGV2
D	-23	MET	-	EXPRESSION TAG	UNP E8QGV2
D	-22	GLY	-	EXPRESSION TAG	UNP E8QGV2
D	-21	SER	-	EXPRESSION TAG	UNP E8QGV2
D	-20	SER	-	EXPRESSION TAG	UNP E8QGV2
D	-19	HIS	-	EXPRESSION TAG	UNP E8QGV2
D	-18	HIS	-	EXPRESSION TAG	UNP E8QGV2
D	-17	HIS	-	EXPRESSION TAG	UNP E8QGV2
D	-16	HIS	-	EXPRESSION TAG	UNP E8QGV2
D	-15	HIS	-	EXPRESSION TAG	UNP E8QGV2
D	-14	HIS	-	EXPRESSION TAG	UNP E8QGV2
D	-13	SER	-	EXPRESSION TAG	UNP E8QGV2
D	-12	SER	-	EXPRESSION TAG	UNP E8QGV2
D	-11	GLY	-	EXPRESSION TAG	UNP E8QGV2
D	-10	LEU	-	EXPRESSION TAG	UNP E8QGV2
D	-9	VAL	-	EXPRESSION TAG	UNP E8QGV2
D	-8	PRO	-	EXPRESSION TAG	UNP E8QGV2
D	-7	ARG	-	EXPRESSION TAG	UNP E8QGV2
D	-6	GLY	-	EXPRESSION TAG	UNP E8QGV2
D	-5	SER	-	EXPRESSION TAG	UNP E8QGV2
D	-4	HIS	-	EXPRESSION TAG	UNP E8QGV2
D	-3	THR	-	EXPRESSION TAG	UNP E8QGV2
D	-2	LEU	-	EXPRESSION TAG	UNP E8QGV2
D	-1	ILE	-	EXPRESSION TAG	UNP E8QGV2
D	0	ASN	-	EXPRESSION TAG	UNP E8QGV2
D	200	THR	ALA	CONFLICT	UNP E8QGV2
D	202	GLU	ASP	CONFLICT	UNP E8QGV2
D	273	PRO	SER	CONFLICT	UNP E8QGV2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	275	LEU	-	EXPRESSION TAG	UNP E8QGV2
D	276	ILE	-	EXPRESSION TAG	UNP E8QGV2
D	277	ASN	-	EXPRESSION TAG	UNP E8QGV2
D	278	ASP	-	EXPRESSION TAG	UNP E8QGV2
D	279	TYR	-	EXPRESSION TAG	UNP E8QGV2
D	280	LYS	-	EXPRESSION TAG	UNP E8QGV2
D	281	ASP	-	EXPRESSION TAG	UNP E8QGV2
D	282	ASP	-	EXPRESSION TAG	UNP E8QGV2
D	283	ASP	-	EXPRESSION TAG	UNP E8QGV2
D	284	ASP	-	EXPRESSION TAG	UNP E8QGV2
D	285	LYS	-	EXPRESSION TAG	UNP E8QGV2
E	-23	MET	-	EXPRESSION TAG	UNP E8QGV2
E	-22	GLY	-	EXPRESSION TAG	UNP E8QGV2
E	-21	SER	-	EXPRESSION TAG	UNP E8QGV2
E	-20	SER	-	EXPRESSION TAG	UNP E8QGV2
E	-19	HIS	-	EXPRESSION TAG	UNP E8QGV2
E	-18	HIS	-	EXPRESSION TAG	UNP E8QGV2
E	-17	HIS	-	EXPRESSION TAG	UNP E8QGV2
E	-16	HIS	-	EXPRESSION TAG	UNP E8QGV2
E	-15	HIS	-	EXPRESSION TAG	UNP E8QGV2
E	-14	HIS	-	EXPRESSION TAG	UNP E8QGV2
E	-13	SER	-	EXPRESSION TAG	UNP E8QGV2
E	-12	SER	-	EXPRESSION TAG	UNP E8QGV2
E	-11	GLY	-	EXPRESSION TAG	UNP E8QGV2
E	-10	LEU	-	EXPRESSION TAG	UNP E8QGV2
E	-9	VAL	-	EXPRESSION TAG	UNP E8QGV2
E	-8	PRO	-	EXPRESSION TAG	UNP E8QGV2
E	-7	ARG	-	EXPRESSION TAG	UNP E8QGV2
E	-6	GLY	-	EXPRESSION TAG	UNP E8QGV2
E	-5	SER	-	EXPRESSION TAG	UNP E8QGV2
E	-4	HIS	-	EXPRESSION TAG	UNP E8QGV2
E	-3	THR	-	EXPRESSION TAG	UNP E8QGV2
E	-2	LEU	-	EXPRESSION TAG	UNP E8QGV2
E	-1	ILE	-	EXPRESSION TAG	UNP E8QGV2
E	0	ASN	-	EXPRESSION TAG	UNP E8QGV2
E	200	THR	ALA	CONFLICT	UNP E8QGV2
E	202	GLU	ASP	CONFLICT	UNP E8QGV2
E	273	PRO	SER	CONFLICT	UNP E8QGV2
E	275	LEU	-	EXPRESSION TAG	UNP E8QGV2
E	276	ILE	-	EXPRESSION TAG	UNP E8QGV2
E	277	ASN	-	EXPRESSION TAG	UNP E8QGV2
E	278	ASP	-	EXPRESSION TAG	UNP E8QGV2

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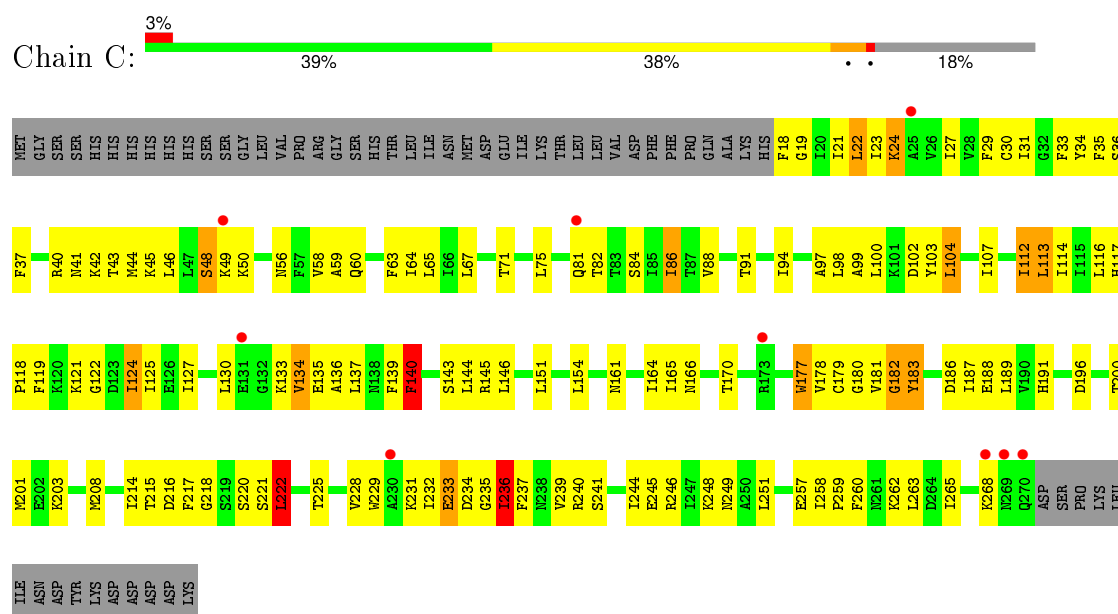
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Chain	Residue	Modelled	Actual	Comment	Reference
E	279	TYR	-	EXPRESSION TAG	UNP E8QGV2
E	280	LYS	-	EXPRESSION TAG	UNP E8QGV2
E	281	ASP	-	EXPRESSION TAG	UNP E8QGV2
E	282	ASP	-	EXPRESSION TAG	UNP E8QGV2
E	283	ASP	-	EXPRESSION TAG	UNP E8QGV2
E	284	ASP	-	EXPRESSION TAG	UNP E8QGV2
E	285	LYS	-	EXPRESSION TAG	UNP E8QGV2
F	-23	MET	-	EXPRESSION TAG	UNP E8QGV2
F	-22	GLY	-	EXPRESSION TAG	UNP E8QGV2
F	-21	SER	-	EXPRESSION TAG	UNP E8QGV2
F	-20	SER	-	EXPRESSION TAG	UNP E8QGV2
F	-19	HIS	-	EXPRESSION TAG	UNP E8QGV2
F	-18	HIS	-	EXPRESSION TAG	UNP E8QGV2
F	-17	HIS	-	EXPRESSION TAG	UNP E8QGV2
F	-16	HIS	-	EXPRESSION TAG	UNP E8QGV2
F	-15	HIS	-	EXPRESSION TAG	UNP E8QGV2
F	-14	HIS	-	EXPRESSION TAG	UNP E8QGV2
F	-13	SER	-	EXPRESSION TAG	UNP E8QGV2
F	-12	SER	-	EXPRESSION TAG	UNP E8QGV2
F	-11	GLY	-	EXPRESSION TAG	UNP E8QGV2
F	-10	LEU	-	EXPRESSION TAG	UNP E8QGV2
F	-9	VAL	-	EXPRESSION TAG	UNP E8QGV2
F	-8	PRO	-	EXPRESSION TAG	UNP E8QGV2
F	-7	ARG	-	EXPRESSION TAG	UNP E8QGV2
F	-6	GLY	-	EXPRESSION TAG	UNP E8QGV2
F	-5	SER	-	EXPRESSION TAG	UNP E8QGV2
F	-4	HIS	-	EXPRESSION TAG	UNP E8QGV2
F	-3	THR	-	EXPRESSION TAG	UNP E8QGV2
F	-2	LEU	-	EXPRESSION TAG	UNP E8QGV2
F	-1	ILE	-	EXPRESSION TAG	UNP E8QGV2
F	0	ASN	-	EXPRESSION TAG	UNP E8QGV2
F	200	THR	ALA	CONFLICT	UNP E8QGV2
F	202	GLU	ASP	CONFLICT	UNP E8QGV2
F	273	PRO	SER	CONFLICT	UNP E8QGV2
F	275	LEU	-	EXPRESSION TAG	UNP E8QGV2
F	276	ILE	-	EXPRESSION TAG	UNP E8QGV2
F	277	ASN	-	EXPRESSION TAG	UNP E8QGV2
F	278	ASP	-	EXPRESSION TAG	UNP E8QGV2
F	279	TYR	-	EXPRESSION TAG	UNP E8QGV2
F	280	LYS	-	EXPRESSION TAG	UNP E8QGV2
F	281	ASP	-	EXPRESSION TAG	UNP E8QGV2
F	282	ASP	-	EXPRESSION TAG	UNP E8QGV2

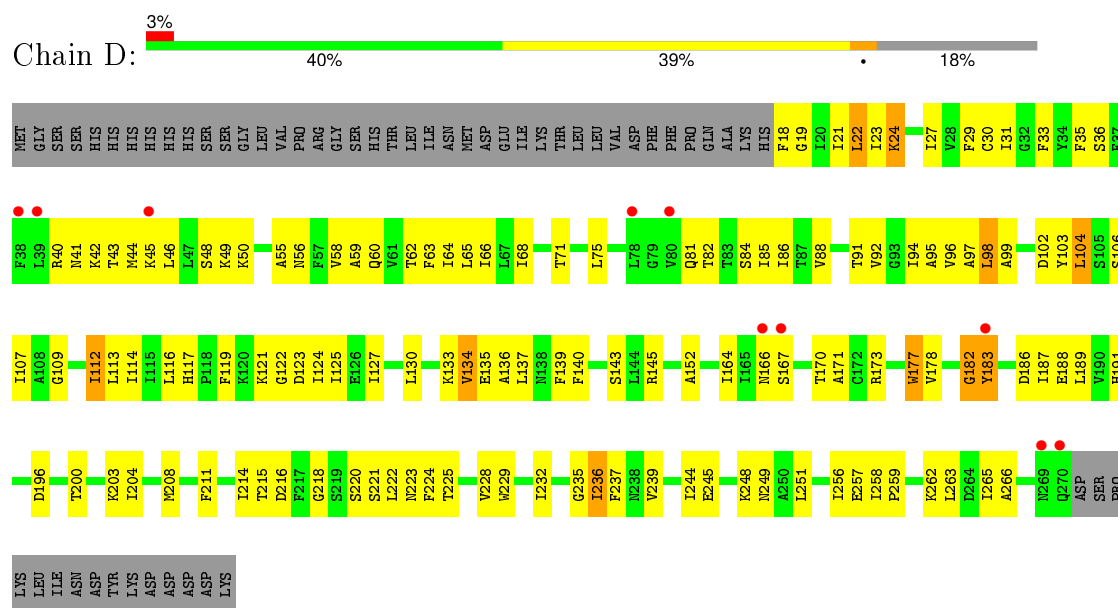
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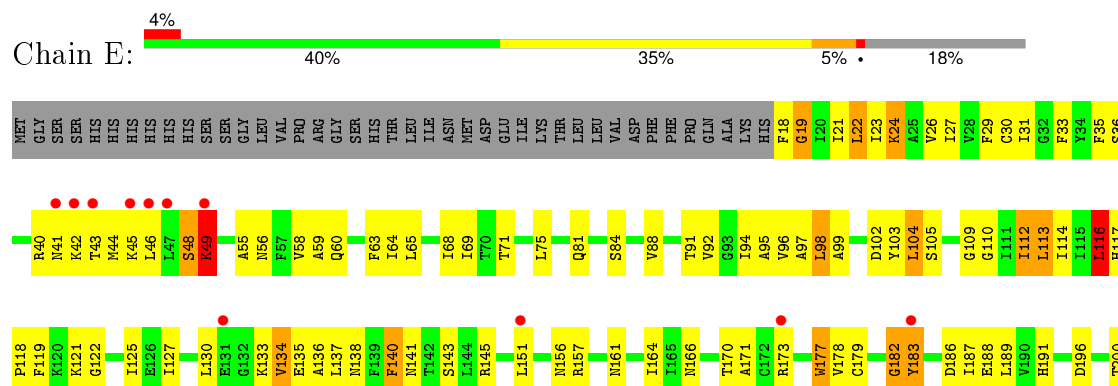
Chain	Residue	Modelled	Actual	Comment	Reference
F	283	ASP	-	EXPRESSION TAG	UNP E8QGV2
F	284	ASP	-	EXPRESSION TAG	UNP E8QGV2
F	285	LYS	-	EXPRESSION TAG	UNP E8QGV2
G	-23	MET	-	EXPRESSION TAG	UNP E8QGV2
G	-22	GLY	-	EXPRESSION TAG	UNP E8QGV2
G	-21	SER	-	EXPRESSION TAG	UNP E8QGV2
G	-20	SER	-	EXPRESSION TAG	UNP E8QGV2
G	-19	HIS	-	EXPRESSION TAG	UNP E8QGV2
G	-18	HIS	-	EXPRESSION TAG	UNP E8QGV2
G	-17	HIS	-	EXPRESSION TAG	UNP E8QGV2
G	-16	HIS	-	EXPRESSION TAG	UNP E8QGV2
G	-15	HIS	-	EXPRESSION TAG	UNP E8QGV2
G	-14	HIS	-	EXPRESSION TAG	UNP E8QGV2
G	-13	SER	-	EXPRESSION TAG	UNP E8QGV2
G	-12	SER	-	EXPRESSION TAG	UNP E8QGV2
G	-11	GLY	-	EXPRESSION TAG	UNP E8QGV2
G	-10	LEU	-	EXPRESSION TAG	UNP E8QGV2
G	-9	VAL	-	EXPRESSION TAG	UNP E8QGV2
G	-8	PRO	-	EXPRESSION TAG	UNP E8QGV2
G	-7	ARG	-	EXPRESSION TAG	UNP E8QGV2
G	-6	GLY	-	EXPRESSION TAG	UNP E8QGV2
G	-5	SER	-	EXPRESSION TAG	UNP E8QGV2
G	-4	HIS	-	EXPRESSION TAG	UNP E8QGV2
G	-3	THR	-	EXPRESSION TAG	UNP E8QGV2
G	-2	LEU	-	EXPRESSION TAG	UNP E8QGV2
G	-1	ILE	-	EXPRESSION TAG	UNP E8QGV2
G	0	ASN	-	EXPRESSION TAG	UNP E8QGV2
G	200	THR	ALA	CONFLICT	UNP E8QGV2
G	202	GLU	ASP	CONFLICT	UNP E8QGV2
G	273	PRO	SER	CONFLICT	UNP E8QGV2
G	275	LEU	-	EXPRESSION TAG	UNP E8QGV2
G	276	ILE	-	EXPRESSION TAG	UNP E8QGV2
G	277	ASN	-	EXPRESSION TAG	UNP E8QGV2
G	278	ASP	-	EXPRESSION TAG	UNP E8QGV2
G	279	TYR	-	EXPRESSION TAG	UNP E8QGV2
G	280	LYS	-	EXPRESSION TAG	UNP E8QGV2
G	281	ASP	-	EXPRESSION TAG	UNP E8QGV2
G	282	ASP	-	EXPRESSION TAG	UNP E8QGV2
G	283	ASP	-	EXPRESSION TAG	UNP E8QGV2
G	284	ASP	-	EXPRESSION TAG	UNP E8QGV2
G	285	LYS	-	EXPRESSION TAG	UNP E8QGV2

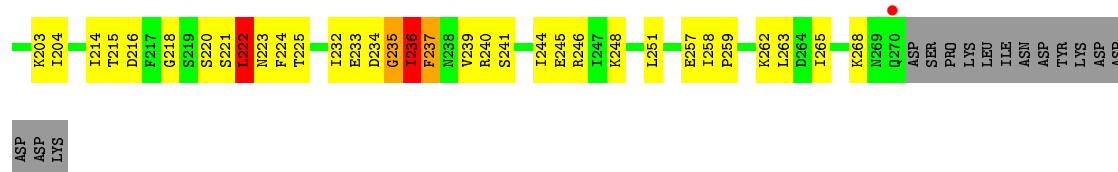


• Molecule 1: Mechanosensitive channel MscS

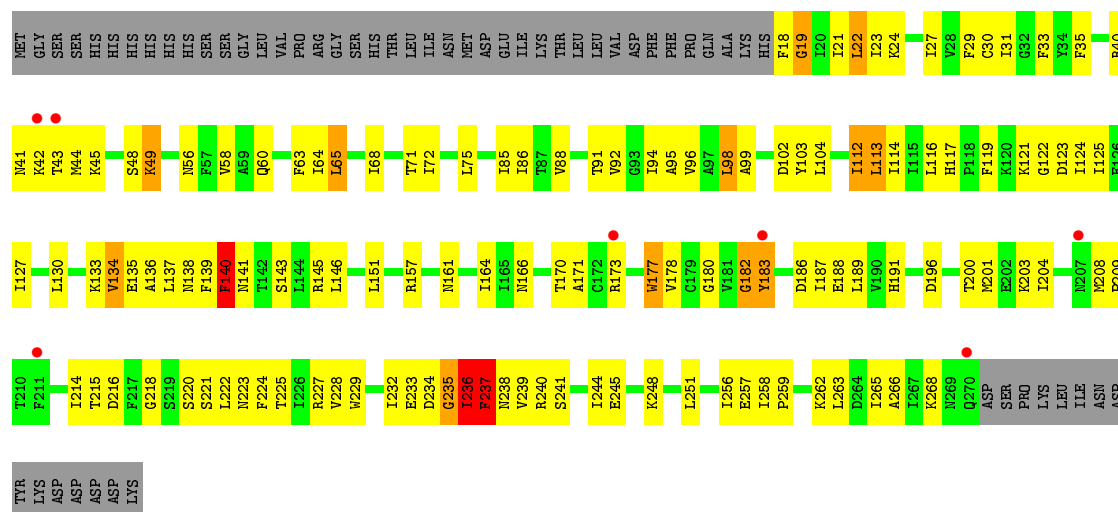


• Molecule 1: Mechanosensitive channel MscS

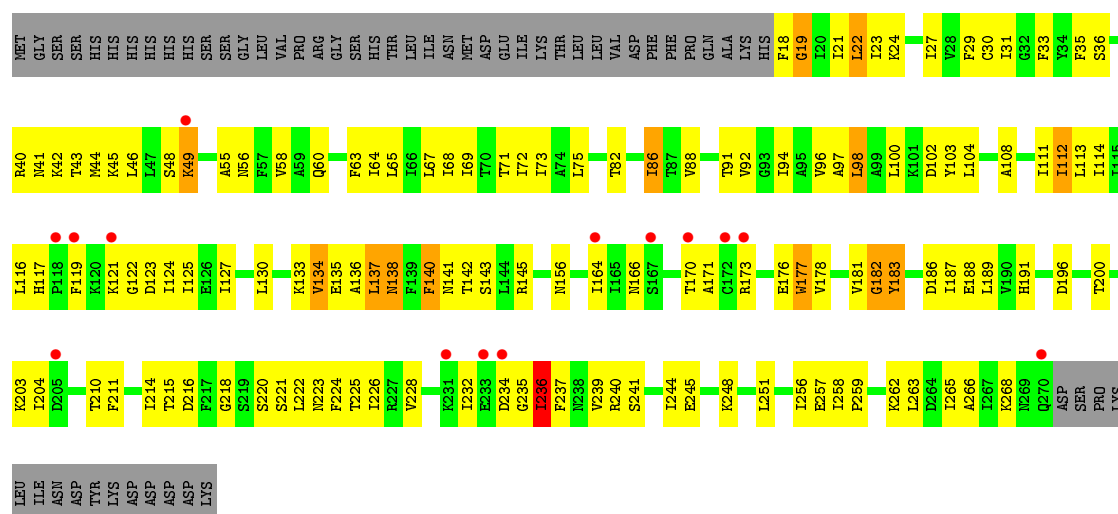
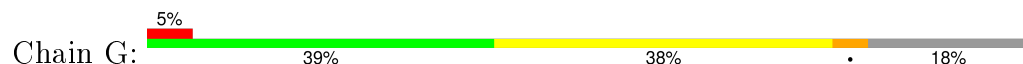




• Molecule 1: Mechanosensitive channel MscS



• Molecule 1: Mechanosensitive channel MscS



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.92Å 143.10Å 178.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.56 – 4.14 46.08 – 4.14	Depositor EDS
% Data completeness (in resolution range)	88.2 (44.56-4.14) 98.6 (46.08-4.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.244 , 0.304 0.250 , 0.309	Depositor DCC
R_{free} test set	1151 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	183.3	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 134.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 22495 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13797	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.97	3/2001 (0.1%)	1.35	20/2707 (0.7%)
1	B	0.97	1/2001 (0.0%)	1.30	18/2707 (0.7%)
1	C	1.05	6/2001 (0.3%)	1.38	34/2707 (1.3%)
1	D	0.99	1/2001 (0.0%)	1.32	16/2707 (0.6%)
1	E	0.98	3/2001 (0.1%)	1.40	29/2707 (1.1%)
1	F	0.94	2/2001 (0.1%)	1.37	26/2707 (1.0%)
1	G	0.97	2/2001 (0.1%)	1.39	21/2707 (0.8%)
All	All	0.98	18/14007 (0.1%)	1.36	164/18949 (0.9%)

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	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	1
All	All	0	7

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	179	CYS	CB-SG	9.23	1.98	1.82
1	C	48	SER	CB-OG	-8.33	1.31	1.42
1	C	177	TRP	CB-CG	-7.89	1.36	1.50
1	D	177	TRP	CB-CG	-7.83	1.36	1.50
1	G	177	TRP	CB-CG	-7.73	1.36	1.50

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	236	ILE	CG1-CB-CG2	-15.14	78.09	111.40
1	A	21	ILE	CG1-CB-CG2	-15.02	78.36	111.40
1	G	86	ILE	CG1-CB-CG2	-12.79	83.25	111.40
1	G	104	LEU	CB-CG-CD2	-10.93	92.42	111.00
1	C	222	LEU	CA-CB-CG	10.36	139.13	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	49	LYS	Mainchain
1	C	236	ILE	Mainchain
1	D	102	ASP	Mainchain
1	E	237	PHE	Mainchain
1	F	234	ASP	Mainchain

5.2 Too-close contacts

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	1971	0	2079	135	0
1	B	1971	0	2079	135	0
1	C	1971	0	2079	134	0
1	D	1971	0	2079	142	0
1	E	1971	0	2079	133	0
1	F	1971	0	2079	135	0
1	G	1971	0	2079	134	0
All	All	13797	0	14553	805	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 28.

The worst 5 of 805 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:C:236:ILE:HG23	1:C:237:PHE:H	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ILE:HG23	1:D:237:PHE:H	1.33	0.91
1:F:220:SER:HB2	1:F:262:LYS:H	1.32	0.91
1:F:91:THR:HA	1:F:94:ILE:HD12	1.52	0.91
1:B:91:THR:HA	1:B:94:ILE:HD12	1.52	0.90

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	251/309 (81%)	235 (94%)	15 (6%)	1 (0%)	39	79
1	B	251/309 (81%)	236 (94%)	14 (6%)	1 (0%)	39	79
1	C	251/309 (81%)	232 (92%)	17 (7%)	2 (1%)	24	69
1	D	251/309 (81%)	234 (93%)	16 (6%)	1 (0%)	39	79
1	E	251/309 (81%)	234 (93%)	16 (6%)	1 (0%)	39	79
1	F	251/309 (81%)	232 (92%)	18 (7%)	1 (0%)	39	79
1	G	251/309 (81%)	232 (92%)	17 (7%)	2 (1%)	24	69
All	All	1757/2163 (81%)	1635 (93%)	113 (6%)	9 (0%)	34	76

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ILE
1	D	236	ILE
1	E	236	ILE
1	F	236	ILE
1	G	236	ILE

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	220/272 (81%)	216 (98%)	4 (2%)	66	87
1	B	220/272 (81%)	214 (97%)	6 (3%)	52	80
1	C	220/272 (81%)	214 (97%)	6 (3%)	52	80
1	D	220/272 (81%)	217 (99%)	3 (1%)	74	89
1	E	220/272 (81%)	211 (96%)	9 (4%)	37	73
1	F	220/272 (81%)	213 (97%)	7 (3%)	46	78
1	G	220/272 (81%)	216 (98%)	4 (2%)	66	87
All	All	1540/1904 (81%)	1501 (98%)	39 (2%)	55	82

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	112	ILE
1	E	49	LYS
1	G	112	ILE
1	D	134	VAL
1	E	35	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	169	ASN
1	E	168	ASN
1	G	169	ASN
1	D	270	GLN
1	E	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	253/309 (81%)	0.37	17 (6%) 21 14	46, 121, 198, 228	0
1	B	253/309 (81%)	0.09	7 (2%) 56 45	52, 120, 196, 222	0
1	C	253/309 (81%)	0.06	9 (3%) 46 36	52, 119, 191, 234	0
1	D	253/309 (81%)	0.00	10 (3%) 42 32	55, 117, 190, 216	0
1	E	253/309 (81%)	0.09	12 (4%) 35 27	55, 117, 191, 221	0
1	F	253/309 (81%)	-0.01	7 (2%) 56 45	54, 117, 189, 235	0
1	G	253/309 (81%)	0.12	14 (5%) 29 21	53, 120, 188, 221	0
All	All	1771/2163 (81%)	0.10	76 (4%) 39 30	46, 119, 194, 235	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	LYS	9.5
1	D	270	GLN	5.0
1	A	270	GLN	5.0
1	C	270	GLN	4.8
1	B	136	ALA	4.4

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.