



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 02:32 am BST

PDB ID : 3PXG
Title : Structure of MecA121 and ClpC1-485 complex
Authors : Wang, F.; Mei, Z.Q.; Wang, J.W.; Shi, Y.G.
Deposited on : 2010-12-09
Resolution : 3.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

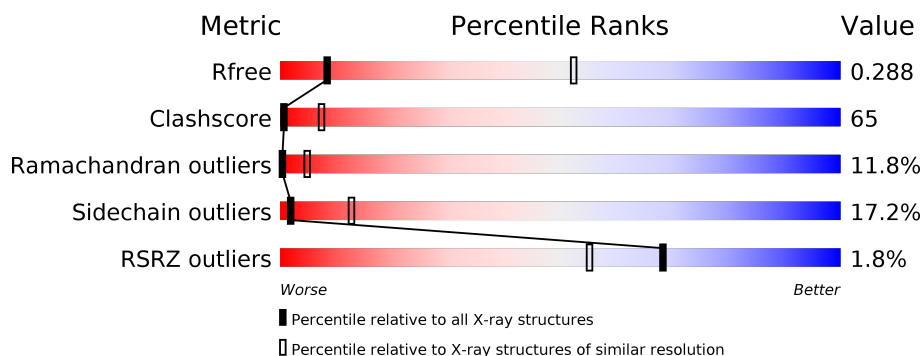
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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	98	<div> <div>0%</div> <div> <div>73%</div> <div>22%</div> <div>•</div> </div> </div>
1	b	98	<div> <div>3%</div> <div> <div>74%</div> <div>21%</div> <div>•</div> </div> </div>
1	c	98	<div> <div>5%</div> <div> <div>76%</div> <div>20%</div> <div>•</div> </div> </div>
1	d	98	<div> <div>73%</div> <div>23%</div> <div>•</div> </div>
1	e	98	<div> <div>73%</div> <div>23%</div> <div>•</div> </div>
1	f	98	<div> <div>2%</div> <div> <div>74%</div> <div>21%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	A	468	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%23%54%16%6%</div></div>
2	B	468	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%21%48%22%7%</div></div>
2	C	468	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%23%53%17%5%</div></div>
2	D	468	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%24%51%16%7%</div></div>
2	E	468	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%22%52%16%7%</div></div>
2	F	468	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%22%53%18%6%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24809 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 Adapter protein mecA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	94	Total	C	N	O	S	0	0	0
			772	496	122	152	2			
1	b	94	Total	C	N	O	S	0	0	0
			772	496	122	152	2			
1	c	94	Total	C	N	O	S	0	0	0
			772	496	122	152	2			
1	d	95	Total	C	N	O	S	0	0	0
			777	499	123	153	2			
1	e	95	Total	C	N	O	S	0	0	0
			777	499	123	153	2			
1	f	94	Total	C	N	O	S	0	0	0
			772	496	122	152	2			

- Molecule 2 is a protein called Negative regulator of genetic competence ClpC/MecB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	442	Total	C	N	O	S	0	0	0
			3380	2092	621	661	6			
2	B	437	Total	C	N	O	S	0	0	0
			3356	2078	616	656	6			
2	C	444	Total	C	N	O	S	0	0	0
			3386	2095	622	663	6			
2	D	434	Total	C	N	O	S	0	0	0
			3342	2070	613	653	6			
2	E	434	Total	C	N	O	S	0	0	0
			3342	2070	613	653	6			
2	F	438	Total	C	N	O	S	0	0	0
			3361	2081	617	657	6			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	DELETION	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	DELETION	UNP P37571
A	?	-	ALA	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	THR	DELETION	UNP P37571
A	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
A	?	-	LEU	DELETION	UNP P37571
A	?	-	HIS	DELETION	UNP P37571
A	?	-	THR	DELETION	UNP P37571
A	?	-	LEU	DELETION	UNP P37571
A	?	-	ILE	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	ALA	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	GLU	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	ALA	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	THR	DELETION	UNP P37571
B	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
B	?	-	LEU	DELETION	UNP P37571
B	?	-	HIS	DELETION	UNP P37571
B	?	-	THR	DELETION	UNP P37571
B	?	-	LEU	DELETION	UNP P37571
B	?	-	ILE	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	ALA	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	GLU	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	ALA	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	THR	DELETION	UNP P37571
C	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
C	?	-	LEU	DELETION	UNP P37571
C	?	-	HIS	DELETION	UNP P37571
C	?	-	THR	DELETION	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	DELETION	UNP P37571
C	?	-	ILE	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	ALA	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	GLU	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
D	?	-	VAL	DELETION	UNP P37571
D	?	-	VAL	DELETION	UNP P37571
D	?	-	ALA	DELETION	UNP P37571
D	?	-	GLY	DELETION	UNP P37571
D	?	-	THR	DELETION	UNP P37571
D	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
D	?	-	LEU	DELETION	UNP P37571
D	?	-	HIS	DELETION	UNP P37571
D	?	-	THR	DELETION	UNP P37571
D	?	-	LEU	DELETION	UNP P37571
D	?	-	ILE	DELETION	UNP P37571
D	?	-	GLY	DELETION	UNP P37571
D	?	-	ALA	DELETION	UNP P37571
D	?	-	GLY	DELETION	UNP P37571
D	?	-	GLY	DELETION	UNP P37571
D	?	-	GLU	DELETION	UNP P37571
D	?	-	GLY	DELETION	UNP P37571
E	?	-	VAL	DELETION	UNP P37571
E	?	-	VAL	DELETION	UNP P37571
E	?	-	ALA	DELETION	UNP P37571
E	?	-	GLY	DELETION	UNP P37571
E	?	-	THR	DELETION	UNP P37571
E	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
E	?	-	LEU	DELETION	UNP P37571
E	?	-	HIS	DELETION	UNP P37571
E	?	-	THR	DELETION	UNP P37571
E	?	-	LEU	DELETION	UNP P37571
E	?	-	ILE	DELETION	UNP P37571
E	?	-	GLY	DELETION	UNP P37571
E	?	-	ALA	DELETION	UNP P37571
E	?	-	GLY	DELETION	UNP P37571
E	?	-	GLY	DELETION	UNP P37571
E	?	-	GLU	DELETION	UNP P37571
E	?	-	GLY	DELETION	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	VAL	DELETION	UNP P37571
F	?	-	VAL	DELETION	UNP P37571
F	?	-	ALA	DELETION	UNP P37571
F	?	-	GLY	DELETION	UNP P37571
F	?	-	THR	DELETION	UNP P37571
F	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
F	?	-	LEU	DELETION	UNP P37571
F	?	-	HIS	DELETION	UNP P37571
F	?	-	THR	DELETION	UNP P37571
F	?	-	LEU	DELETION	UNP P37571
F	?	-	ILE	DELETION	UNP P37571
F	?	-	GLY	DELETION	UNP P37571
F	?	-	ALA	DELETION	UNP P37571
F	?	-	GLY	DELETION	UNP P37571
F	?	-	GLY	DELETION	UNP P37571
F	?	-	GLU	DELETION	UNP P37571
F	?	-	GLY	DELETION	UNP P37571

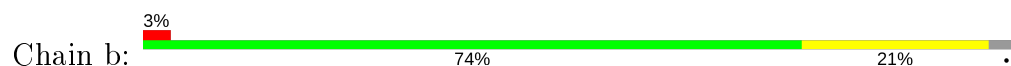
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

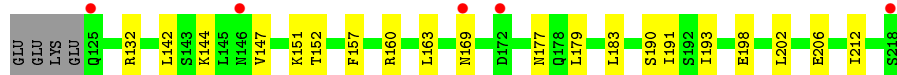
- Molecule 1: Adapter protein mecA 1



- Molecule 1: Adapter protein mecA 1



- Molecule 1: Adapter protein mecA 1



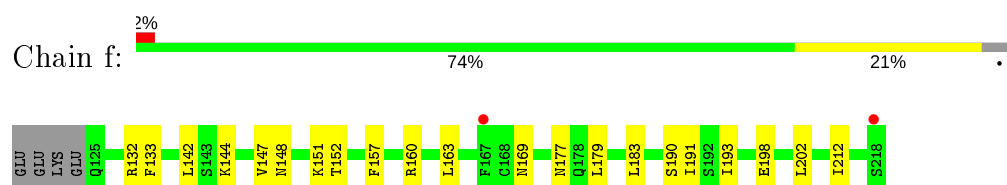
- Molecule 1: Adapter protein mecA 1



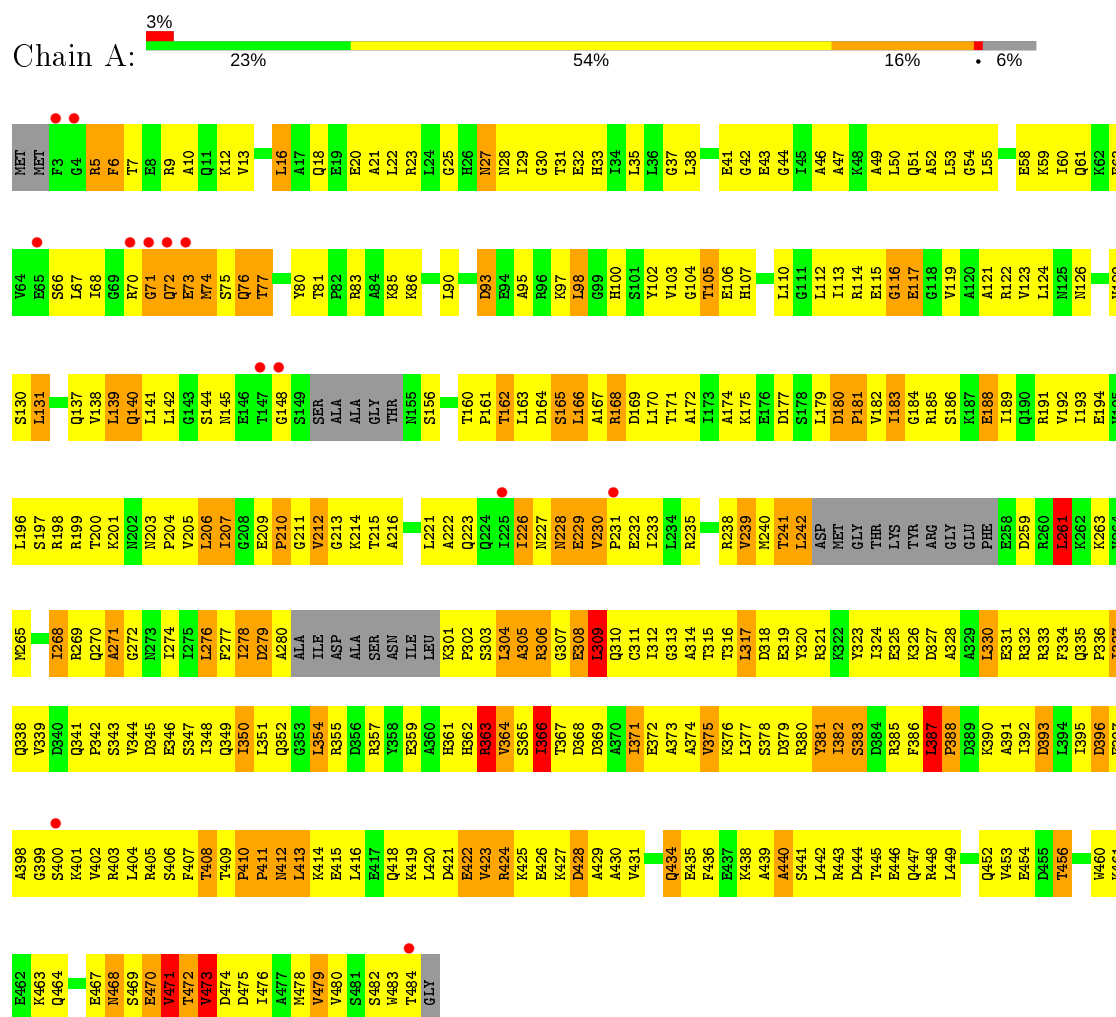
- Molecule 1: Adapter protein mecA 1



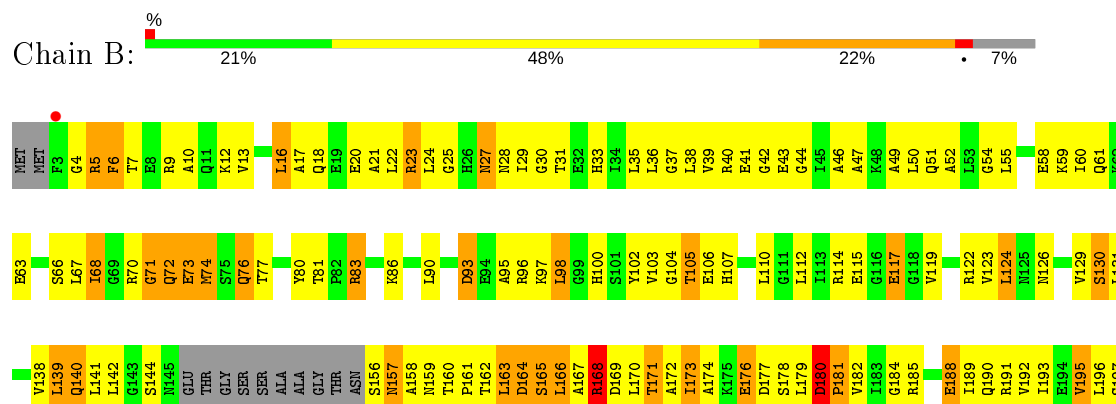
- Molecule 1: Adapter protein mecA 1

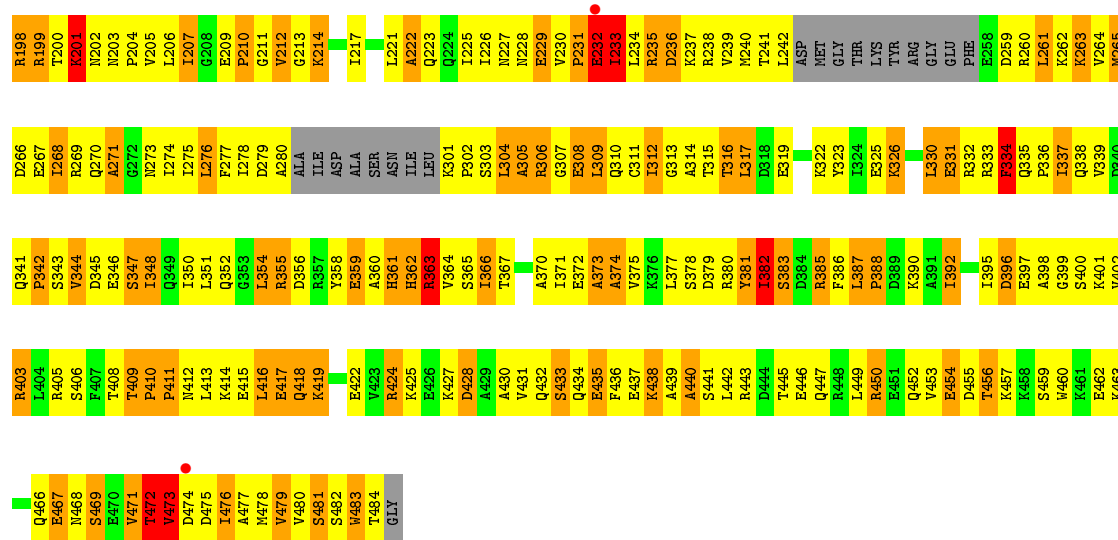


• Molecule 2: Negative regulator of genetic competence ClpC/MecB

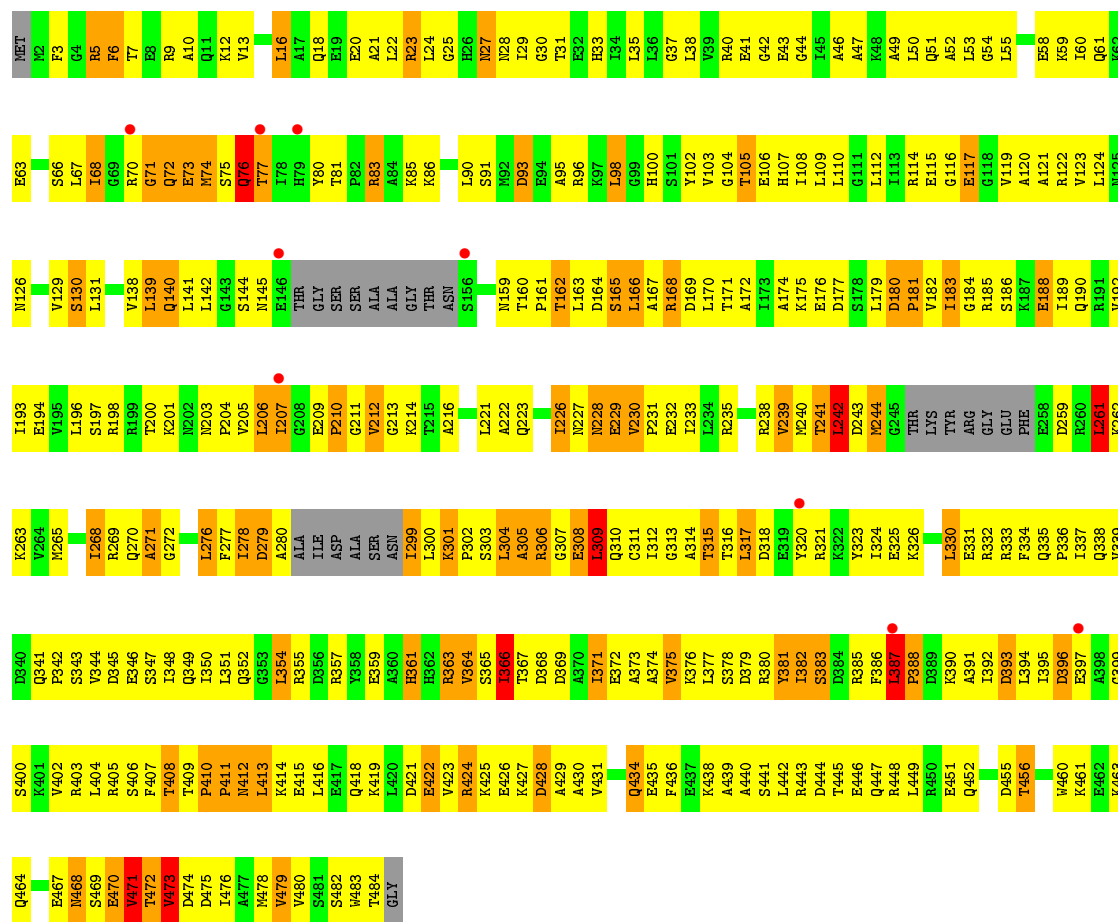


• Molecule 2: Negative regulator of genetic competence ClpC/MecB

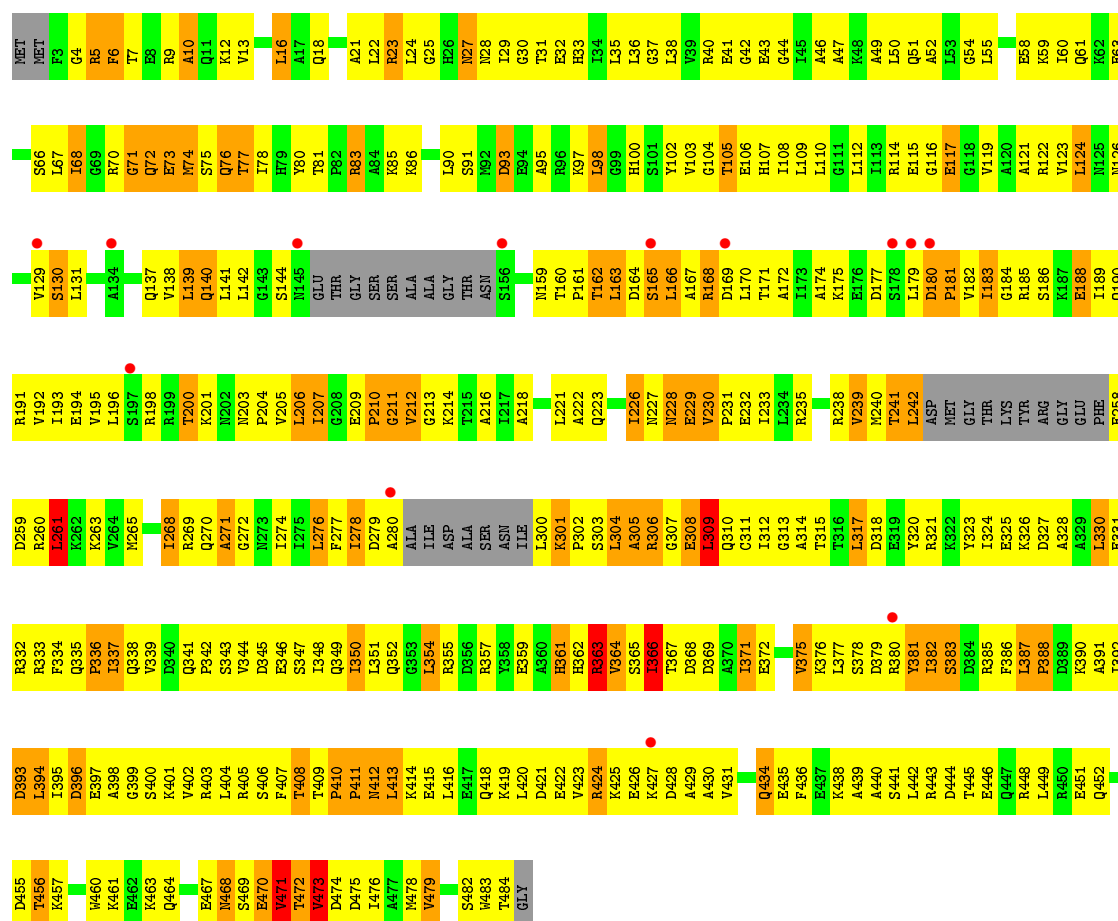




• Molecule 2: Negative regulator of genetic competence ClpC/MecB



• Molecule 2: Negative regulator of genetic competence ClpC/MecB



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.56Å 137.56Å 445.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.52 – 3.65 49.52 – 3.65	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.52-3.65) 96.2 (49.52-3.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, R_{free}	0.257 , 0.303 0.243 , 0.288	Depositor DCC
R_{free} test set	2858 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å ²)	142.2	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 255.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24809	wwPDB-VP
Average B, all atoms (Å ²)	240.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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

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	0.48	0/786	0.66	1/1059 (0.1%)
1	b	0.56	0/786	0.66	0/1059
1	c	0.64	0/786	0.68	0/1059
1	d	0.55	0/791	0.66	0/1066
1	e	0.49	0/791	0.65	0/1066
1	f	0.47	0/786	0.65	0/1059
2	A	0.49	0/3408	0.70	1/4589 (0.0%)
2	B	0.58	1/3384 (0.0%)	0.85	1/4556 (0.0%)
2	C	0.50	0/3415	0.71	1/4602 (0.0%)
2	D	0.48	0/3370	0.69	1/4537 (0.0%)
2	E	0.45	0/3370	0.68	1/4537 (0.0%)
2	F	0.46	0/3389	0.68	1/4563 (0.0%)
All	All	0.50	1/25062 (0.0%)	0.71	7/33752 (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
2	A	0	1
2	C	0	1
2	D	0	1
2	E	0	1
2	F	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	PHE	CA-CB	5.29	1.65	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	161	PRO	N-CA-CB	6.26	110.81	103.30
2	A	161	PRO	N-CA-CB	6.01	110.51	103.30
2	E	161	PRO	N-CA-CB	5.95	110.44	103.30
2	C	161	PRO	N-CA-CB	5.87	110.34	103.30
2	D	161	PRO	N-CA-CB	5.86	110.33	103.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	210	PRO	Peptide
2	C	210	PRO	Peptide
2	D	210	PRO	Peptide
2	E	210	PRO	Peptide
2	F	210	PRO	Peptide

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	772	0	752	0	0
1	b	772	0	752	0	0
1	c	772	0	752	0	0
1	d	777	0	754	0	0
1	e	777	0	754	0	0
1	f	772	0	752	0	0
2	A	3380	0	3390	459	0
2	B	3356	0	3379	549	0
2	C	3386	0	3384	476	0
2	D	3342	0	3372	436	1
2	E	3342	0	3372	476	0
2	F	3361	0	3381	470	1
All	All	24809	0	24794	2773	1

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 65.

The worst 5 of 2773 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)
2:C:363:ARG:CZ	2:C:471:VAL:HA	1.72	1.19
2:E:181:PRO:HB2	2:E:182:VAL:HA	1.25	1.18
2:B:230:VAL:HG12	2:B:231:PRO:CD	1.71	1.18
2:B:304:LEU:HD22	2:B:305:ALA:N	1.58	1.18
2:B:169:ASP:O	2:B:173:ILE:HB	1.44	1.18

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:441:SER:OG	2:F:40:ARG:O[1_565]	1.94	0.26

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	92/98 (94%)	76 (83%)	12 (13%)	4 (4%)	2	24
1	b	92/98 (94%)	76 (83%)	12 (13%)	4 (4%)	2	24
1	c	92/98 (94%)	74 (80%)	14 (15%)	4 (4%)	2	24
1	d	93/98 (95%)	76 (82%)	13 (14%)	4 (4%)	2	24
1	e	93/98 (95%)	76 (82%)	13 (14%)	4 (4%)	2	24
1	f	92/98 (94%)	73 (79%)	15 (16%)	4 (4%)	2	24
2	A	434/468 (93%)	277 (64%)	98 (23%)	59 (14%)	0	3
2	B	429/468 (92%)	272 (63%)	88 (20%)	69 (16%)	0	3
2	C	438/468 (94%)	274 (63%)	103 (24%)	61 (14%)	0	3
2	D	426/468 (91%)	277 (65%)	97 (23%)	52 (12%)	0	5
2	E	426/468 (91%)	276 (65%)	100 (24%)	50 (12%)	0	5
2	F	430/468 (92%)	273 (64%)	103 (24%)	54 (13%)	0	4
All	All	3137/3396 (92%)	2100 (67%)	668 (21%)	369 (12%)	0	5

5 of 369 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	169	ASN
2	A	42	GLY
2	A	98	LEU
2	A	144	SER
2	A	183	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	87/92 (95%)	70 (80%)	17 (20%)	1	9
1	b	87/92 (95%)	70 (80%)	17 (20%)	1	9
1	c	87/92 (95%)	71 (82%)	16 (18%)	1	10
1	d	87/92 (95%)	68 (78%)	19 (22%)	1	6
1	e	87/92 (95%)	68 (78%)	19 (22%)	1	6
1	f	87/92 (95%)	70 (80%)	17 (20%)	1	9
2	A	350/394 (89%)	297 (85%)	53 (15%)	3	17
2	B	350/394 (89%)	280 (80%)	70 (20%)	1	8
2	C	349/394 (89%)	294 (84%)	55 (16%)	2	16
2	D	350/394 (89%)	294 (84%)	56 (16%)	2	15
2	E	350/394 (89%)	294 (84%)	56 (16%)	2	15
2	F	350/394 (89%)	294 (84%)	56 (16%)	2	15
All	All	2621/2916 (90%)	2170 (83%)	451 (17%)	2	13

5 of 451 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	315	THR
2	D	58	GLU
2	F	241	THR
2	C	361	HIS

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Mol	Chain	Res	Type
1	d	132	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	223	GLN
2	D	61	GLN
2	F	100	HIS
2	C	228	ASN
2	C	468	ASN

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	94/98 (95%)	-0.24	1 (1%) 80 70	180, 227, 340, 398	0
1	b	94/98 (95%)	0.11	3 (3%) 47 34	133, 195, 320, 369	0
1	c	94/98 (95%)	0.29	5 (5%) 26 18	127, 194, 315, 374	0
1	d	95/98 (96%)	-0.20	0 100 100	125, 198, 325, 357	0
1	e	95/98 (96%)	-0.21	0 100 100	139, 196, 317, 357	0
1	f	94/98 (95%)	-0.12	2 (2%) 63 50	174, 224, 366, 376	0
2	A	442/468 (94%)	-0.03	13 (2%) 51 37	120, 243, 393, 613	0
2	B	437/468 (93%)	-0.38	3 (0%) 87 80	106, 210, 317, 493	0
2	C	444/468 (94%)	-0.10	9 (2%) 65 52	97, 240, 364, 533	0
2	D	434/468 (92%)	-0.17	7 (1%) 72 59	112, 240, 368, 489	0
2	E	434/468 (92%)	-0.22	3 (0%) 87 80	115, 241, 368, 465	0
2	F	438/468 (93%)	-0.16	13 (2%) 50 36	133, 251, 376, 477	0
All	All	3195/3396 (94%)	-0.16	59 (1%) 68 55	97, 231, 365, 613	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	147	THR	7.2
2	A	3	PHE	6.1
2	F	156	SER	5.8
1	c	218	SER	5.3
2	B	232	GLU	4.9

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.