



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 12:39 AM UTC

PDB ID : 3PXI / pdb_00003pxi
Title : Structure of MecA108:ClpC
Authors : Wang, F.; Mei, Z.Q.; Wang, J.W.; Shi, Y.G.
Deposited on : 2010-12-09
Resolution : 6.93 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

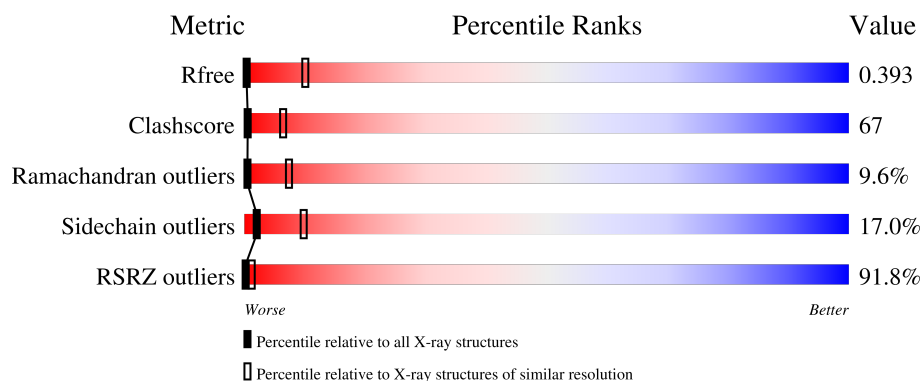
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.93 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}	180053	1166 (9.70-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1053 (9.70-4.00)
Sidechain outliers	187428	1016 (9.70-4.00)
RSRZ outliers	180081	1159 (9.70-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	111	80% 25% 44% 14% • 15%
1	b	111	78% 26% 41% 16% • 15%
1	c	111	79% 23% 46% 15% • 15%
2	A	758	87% 31% 45% 16% • 7%
2	B	758	85% 27% 45% 18% • 7%

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Mol	Chain	Length	Quality of chain
2	C	758	84% 31%46%15%6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18645 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
			755	486	118	149	2			
1	b	94	Total	C	N	O	S	0	0	0
			756	485	120	149	2			
1	c	94	Total	C	N	O	S	0	0	0
			763	491	120	150	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	708	Total	C	N	O	S	0	0	0
			5455	3394	993	1055	13			
2	B	704	Total	C	N	O	S	0	0	0
			5437	3385	985	1054	13			
2	C	711	Total	C	N	O	S	0	0	0
			5479	3410	993	1063	13			

There are 162 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	ALA	deletion	UNP P37571
A	?	-	GLU	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	ARG	deletion	UNP P37571
A	?	-	LEU	deletion	UNP P37571
A	?	-	VAL	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	SER	deletion	UNP P37571
A	?	-	PRO	deletion	UNP P37571
A	?	-	PRO	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	TYR	deletion	UNP P37571
A	?	-	VAL	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	TYR	deletion	UNP P37571
A	?	-	ASP	deletion	UNP P37571
A	?	-	GLU	deletion	UNP P37571
A	618	ALA	GLU	engineered mutation	UNP P37571
A	?	-	LEU	deletion	UNP P37571
A	?	-	LYS	deletion	UNP P37571
A	?	-	ARG	deletion	UNP P37571
A	?	-	ASN	deletion	UNP P37571
A	?	-	LYS	deletion	UNP P37571
A	?	-	TYR	deletion	UNP P37571
A	?	-	VAL	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	PHE	deletion	UNP P37571
A	?	-	ASN	deletion	UNP P37571
A	?	-	VAL	deletion	UNP P37571
A	?	-	GLN	deletion	UNP P37571
A	?	-	ASP	deletion	UNP P37571
A	?	-	GLU	deletion	UNP P37571
A	?	-	THR	deletion	UNP P37571
A	?	-	GLN	deletion	UNP P37571
A	?	-	ASN	deletion	UNP P37571
A	?	-	HIS	deletion	UNP P37571
A	?	-	LYS	deletion	UNP P37571
A	?	-	ASP	deletion	UNP P37571
A	?	-	MET	deletion	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
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	?	-	ALA	deletion	UNP P37571
B	?	-	GLU	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	ARG	deletion	UNP P37571
B	?	-	LEU	deletion	UNP P37571
B	?	-	VAL	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	SER	deletion	UNP P37571
B	?	-	PRO	deletion	UNP P37571
B	?	-	PRO	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	TYR	deletion	UNP P37571
B	?	-	VAL	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	TYR	deletion	UNP P37571
B	?	-	ASP	deletion	UNP P37571
B	?	-	GLU	deletion	UNP P37571
B	618	ALA	GLU	engineered mutation	UNP P37571
B	?	-	LEU	deletion	UNP P37571
B	?	-	LYS	deletion	UNP P37571
B	?	-	ARG	deletion	UNP P37571
B	?	-	ASN	deletion	UNP P37571
B	?	-	LYS	deletion	UNP P37571
B	?	-	TYR	deletion	UNP P37571
B	?	-	VAL	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	PHE	deletion	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP P37571
B	?	-	VAL	deletion	UNP P37571
B	?	-	GLN	deletion	UNP P37571
B	?	-	ASP	deletion	UNP P37571
B	?	-	GLU	deletion	UNP P37571
B	?	-	THR	deletion	UNP P37571
B	?	-	GLN	deletion	UNP P37571
B	?	-	ASN	deletion	UNP P37571
B	?	-	HIS	deletion	UNP P37571
B	?	-	LYS	deletion	UNP P37571
B	?	-	ASP	deletion	UNP P37571
B	?	-	MET	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
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	?	-	ALA	deletion	UNP P37571
C	?	-	GLU	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	ARG	deletion	UNP P37571
C	?	-	LEU	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	SER	deletion	UNP P37571
C	?	-	PRO	deletion	UNP P37571
C	?	-	PRO	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	TYR	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	TYR	deletion	UNP P37571

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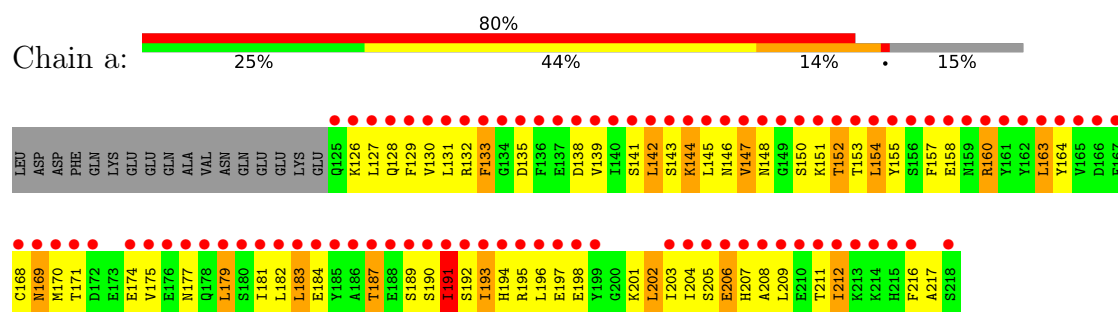
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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	deletion	UNP P37571
C	?	-	GLU	deletion	UNP P37571
C	618	ALA	GLU	engineered mutation	UNP P37571
C	?	-	LEU	deletion	UNP P37571
C	?	-	LYS	deletion	UNP P37571
C	?	-	ARG	deletion	UNP P37571
C	?	-	ASN	deletion	UNP P37571
C	?	-	LYS	deletion	UNP P37571
C	?	-	TYR	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	PHE	deletion	UNP P37571
C	?	-	ASN	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	GLN	deletion	UNP P37571
C	?	-	ASP	deletion	UNP P37571
C	?	-	GLU	deletion	UNP P37571
C	?	-	THR	deletion	UNP P37571
C	?	-	GLN	deletion	UNP P37571
C	?	-	ASN	deletion	UNP P37571
C	?	-	HIS	deletion	UNP P37571
C	?	-	LYS	deletion	UNP P37571
C	?	-	ASP	deletion	UNP P37571
C	?	-	MET	deletion	UNP P37571

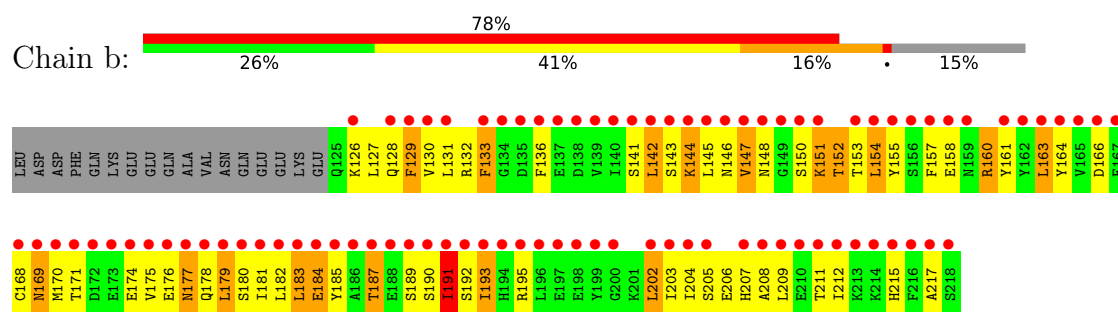
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

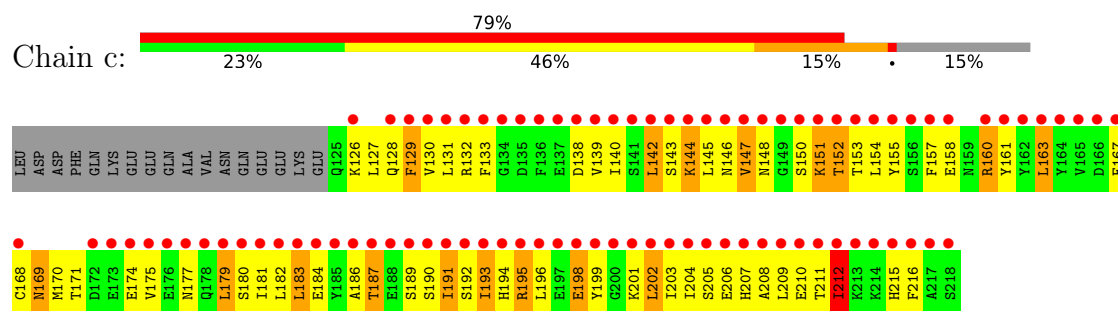
• Molecule 1: Adapter protein mecA 1



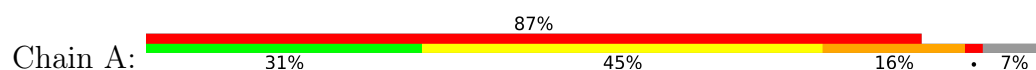
• Molecule 1: Adapter protein mecA 1

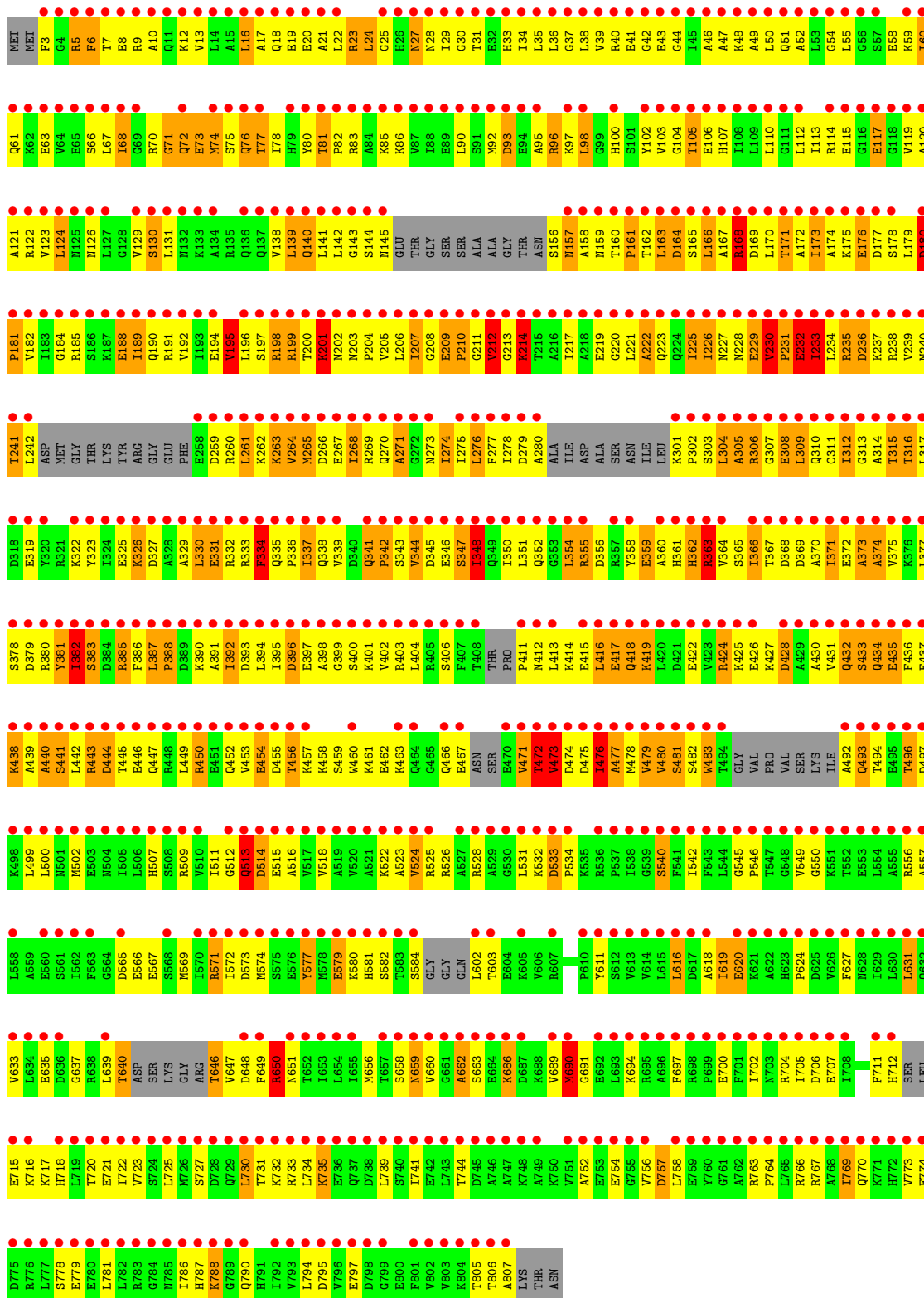


• Molecule 1: Adapter protein mecA 1

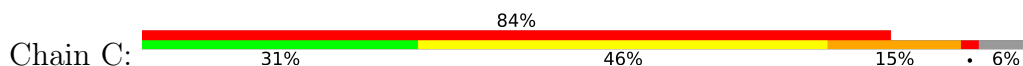


• Molecule 2: Negative regulator of genetic competence ClpC/MecB





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



S778	S779	E779	E780	K716	L781	L782	R783	G784	H785	L786	H787	K788	G789	G790	H791	L792	H793	L794	D795	V796	E797	D798	G799	E800	F801	V802	V803	K804	T805	L743	A807	LYS	THR	ASN																																			
Q632	V633	L634	E635	S636	D636	G637	F663	R638	L639	T640	ASP	SER	SER	L725	GLY	ARG	T646	D648	F649	R650	M650	T652	L653	L654	I655	M656	T657	S658	M659	V660	G661	A662	S663	E664	K686	V687	K688	V689	R689	G785	R690	G691	E692	L693	L694	E695	V696	G699	L765	R766	I702	H703	R704	I705	Q770	K771	H772	V773	E774	D775	R776	L777							
K498	L499	L500	S501	M502	L562	F563	N504	D565	L639	E566	S567	S568	M569	L570	R571	L572	D573	M574	S575	E576	Y577	N651	L652	E579	L654	I655	M656	T657	S658	M659	V660	GLY	GLN	L602	S663	E664	K605	V606	R607	G608	G609	P610	E692	L693	L694	E695	V696	G699	L765	R766	I702	H703	R704	I705	Q770	K771	H772	V773	E774	D775	R776	L777							
K438	A439	A440	S441	L442	R443	D444	T445	E446	Q447	R448	L449	R450	L450	E451	Q452	V453	D454	E455	T456	K457	K458	G459	W460	K461	E462	K463	Q464	G465	GLY	Q466	E467	ASN	SER	E470	V471	V472	V473	D474	D475	L476	A477	M478	V479	V480	S481	S482	W483	T484	GLY	VAL	PRO	VAL	SER	LYS	ILE	A492	Q493	T494	E495	L496	A497								
S378	D379	R380	Y381	I382	S383	D384	R385	F386	L387	P388	D389	K390	E391	D392	L393	L394	I395	D396	E397	K398	G399	S400	K401	V402	R403	L404	R405	S406	F407	T408	THR	PRO	P411	N412	L413	K414	E415	L416	D417	Q418	K419	L420	D421	E422	V423	R424	K425	E426	K427	D428	A429	A430	V431	Q432	S433	Q434	E435	F436	E437										
D318	E319	R320	S321	K322	Y323	L324	E325	K326	D327	L328	A328	L329	A329	E331	R332	R333	F334	K335	P336	L337	Q338	V339	D340	Q341	P342	S343	V344	D345	E346	S347	I348	Q349	I350	L351	Q352	G353	L354	R355	D356	Y357	E358	E359	A360	H361	H362	R363	V364	S365	L366	T367	D368	D369	A370	I371	A372	A373	E374	V375	K376	L377									
S378	D379	R380	Y381	I382	S383	D384	R385	F386	L387	P388	D389	K390	E391	D392	L393	L394	I395	D396	E397	K398	G399	S400	K401	V402	R403	L404	R405	S406	F407	T408	THR	PRO	P411	N412	L413	K414	E415	L416	D417	Q418	K419	L420	D421	E422	V423	R424	K425	E426	K427	D428	A429	A430	V431	Q432	S433	Q434	E435	F436	E437										
K438	A439	A440	S441	L442	R443	D444	T445	E446	Q447	R448	L449	R450	L450	E451	Q452	V453	D454	E455	T456	K457	K458	G459	W460	K461	E462	K463	Q464	G465	GLY	Q466	E467	ASN	SER	E470	V471	V472	V473	D474	D475	L476	A477	M478	V479	V480	S481	S482	W483	T484	GLY	VAL	PRO	VAL	SER	LYS	ILE	A492	Q493	T494	E495	L496	A497								
K498	L499	L500	S501	M502	F503	N504	L505	E506	S507	H508	R509	V510	L511	G512	D513	D514	E515	A516	V517	V518	A519	V520	A521	K522	A523	V524	R525	M526	GLY	Q466	E467	ASN	SER	E470	V471	V472	V473	D474	D475	L476	A477	M478	V479	V480	S481	S482	W483	T484	GLY	VAL	PRO	VAL	SER	LYS	ILE	A492	Q493	T494	E495	L496	A497								
L558	A559	E560	S561	I562	F563	G564	D565	E566	S567	S568	M569	L570	R571	L572	D573	M574	S575	E576	Y577	M578	O579	K580	H581	S582	T583	S584	GLY	GLY	GLN	L602	T603	E604	K605	V606	R607	D608	K609	P610	E692	L693	L694	E695	V696	G699	L765	R766	I702	H703	R704	I705	Q770	K771	H772	V773	E774	D775	R776	L777											
SER	LEU	K716	E781	L782	R783	G784	H785	L786	H787	K788	G789	G790	H791	L792	H793	L794	D795	V796	E797	D798	G799	E800	F801	V802	V803	K804	T805	L743	A807	LYS	THR	ASN																																					
Q61	K62	E63	V64	E65	S66	L67	I68	G69	R70	A10	Q11	K12	E13	V14	L14	A15	Q16	E17	A18	T19	H19	E19	E20	A21	R22	R23	L24	A25	G26	H26	V87	N27	N28	SER	E89	L90	G30	T31	E32	H33	I34	ASN	L35	R36	K97	L98	V99	H100	S101	Y102	V103	L163	G104	T105	E106	H107	K108	L109	L110	L111	L112	R113	E114	E115	G116	E117	G118	V119	E120
A121	R122	V123	L124	E125	N126	L127	G128	S129	Q130	L131	K132	E133	V134	L134	A135	Q136	E137	A138	T139	H139	E139	E140	L141	R142	R143	A144	N145	E146	THR	GLY	SER	SER	ALA	ALA	GLY	THR	ASN	S156	N157	A158	N159	T160	P161	T162	L163	D164	S165	L166	A167	R168	E169	L170	T171	A172	I173	K174	K175	E176	D177	S178	V179	E180							
P181	V182	I183	G184	R185	K186	E187	E188	I189	Q190	R191	V192	I193	E194	L196	S197	K198	R199	T200	K201	N202	N203	P204	V205	L206	L207	G208	E209	P210	L211	V212	G213	K214	T215	A216	T217	A218	E219	L221	A222	Q223	Q224	T225	L226	N227	R228	E229	V230	P231	E232	L233	R234	R235	G236	V237	R238	V239	L240												
T241	L242	D243	M244	G245	THR	LYS	TYS	ARG	GLY	GLU	PHE	E258	D259	R260	L261	K262	K263	V264	M265	D266	E267	L268	R269	Q270	A271	G272	M273	L274	L275	L276	F277	I278	A279	ALA	ILE	ASP	ALA	SER	ASN	L299	L300	K301	P302	S303	L304	S305	R306	G307	E308	L309	Q310	C311	L312	G313	G314	A314	T315	K316	L317										
D318	E319	R320	S321	K322	Y323	L324	E325	K326	D327	L328	A328	L329	A329	E331	R332	R333	F334	K335	P336	L337	Q338	V339	D340	Q341	P342	S343	V344	D345	E346	S347	I348	Q349	I350	L351	Q352	G353	L354	R355	D356	Y357	E358	E359	A360	H361	H362	R363	V364	S365	L366	T367	D368	D369	A370	I371	A372	A373	E374	V375	K376	L377									
S378	D379	R380	Y381	I382	S383	D384	R385	F386	L387	P388	D389	K390	E391	D392	L393	L394	I395	D396	E397	K398	G399	S400	K401	V402	R403	L404	R405	S406	F407	T408	THR	PRO	P411	N412	L413	K414	E415	L416	D417	Q418	K419	L420	D421	E422	V423	R424	K425	E426	K427	D428	A429	A430	V431	Q432	S433	Q434	E435	F436	E437										
K438	A439	A440	S441	L442	R443	D444	T445	E446	Q447	R448	L449	R450	L450	E451	Q452	V453	D454	E455	T456	K457	K458	G459	W460	K461	E462	K463	Q464	G465	GLY	Q466	E467	ASN	SER	E470	V471	V472	V473	D474	D475	L476	A477	M478	V479	V480	S481	S482	W483	T484	GLY	VAL	PRO	VAL	SER	LYS	ILE	A492	Q493	T494	E495	L496	A497								
K498	L499	L500	S501	M502	F503	N504	L505	E506	S507	H508	R509	V510	L511	G512	D513	D514	E515	A516	V517	V518	A519	V520	A521	K522	A523	V524	R525	M526	GLY	Q466	E467	ASN	SER	E470	V471	V472	V473	D474	D475	L476	A477	M478	V479	V480	S481	S482	W483	T484	GLY	VAL	PRO	VAL	SER	LYS	ILE	A492	Q493	T494	E495	L496	A497								
L558	A559	E560	S561	I562	F563	G564	D565	E566	S567	S568	M569	L570	R571	L572	D573	M574	S575	E576	Y577	M578	O579	K580	H581	S582	T583	S584	GLY	GLY	GLN	L602	T603	E604	K605	V606	R607	D608	K609	P610	E692	L693	L694	E695	V696	G699	L765	R766	I702	H703	R704	I705	Q770	K771	H772	V773	E774	D775	R776	L777											
SER	LEU	K716	E781	L782	R783	G784	H785	L786	H787	K788	G789	G790	H791	L792	H793	L794	D795	V796	E797	D798	G799	E800	F801	V802	V803	K804	T805	L743	A807	LYS	THR	ASN																																					

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	141.81Å 141.81Å 656.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.15 – 6.93 49.15 – 6.93	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.15-6.93) 99.2 (49.15-6.93)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.84 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_596)	Depositor
R, R_{free}	0.407 , 0.422 0.373 , 0.393	Depositor DCC
R_{free} test set	333 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	188.0	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 992.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.15	EDS
Total number of atoms	18645	wwPDB-VP
Average B, all atoms (Å ²)	642.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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	0.62	0/768	0.94	2/1035 (0.2%)
1	b	0.73	0/768	0.99	4/1035 (0.4%)
1	c	0.83	1/776 (0.1%)	0.99	2/1046 (0.2%)
2	A	0.67	3/5498 (0.1%)	1.05	27/7386 (0.4%)
2	B	0.76	1/5483 (0.0%)	1.16	36/7369 (0.5%)
2	C	0.71	1/5526 (0.0%)	1.06	24/7431 (0.3%)
All	All	0.72	6/18819 (0.0%)	1.08	95/25302 (0.4%)

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
All	All	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	PHE	CA-CB	7.13	1.65	1.53
2	A	334	PHE	CA-CB	5.46	1.62	1.53
1	c	212	ILE	CA-CB	-5.38	1.47	1.54
2	C	119	VAL	CA-CB	-5.33	1.47	1.54
2	A	366	ILE	CA-C	5.29	1.59	1.52

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	230	VAL	CA-C-N	-10.47	106.75	119.84
2	B	230	VAL	C-N-CA	-10.47	106.75	119.84
2	A	203	ASN	CA-C-N	8.68	128.82	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	203	ASN	C-N-CA	8.68	128.82	120.31
2	B	209	GLU	CA-C-N	8.47	130.43	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	210	PRO	Peptide
2	C	210	PRO	Peptide

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	755	0	728	82	17
1	b	756	0	736	162	0
1	c	763	0	743	141	0
2	A	5455	0	5489	671	34
2	B	5437	0	5491	1053	1
2	C	5479	0	5524	814	24
All	All	18645	0	18711	2510	41

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 67.

The worst 5 of 2510 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:B:694:LYS:HG3	2:C:760:TYR:CE2	1.20	1.59
2:B:694:LYS:CG	2:C:760:TYR:CE2	1.79	1.58
2:B:694:LYS:CD	2:C:760:TYR:HD2	1.05	1.57
2:B:694:LYS:CD	2:C:760:TYR:CD2	1.90	1.55
2:B:694:LYS:HD2	2:C:760:TYR:CD2	1.41	1.53

The worst 5 of 41 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)
1:a:194:HIS:CD2	2:C:48:LYS:NZ[10_445]	1.03	1.17
2:A:500:LEU:CB	2:A:500:LEU:CB[8_555]	1.04	1.16
1:a:128:GLN:NE2	2:A:787:HIS:NE2[8_545]	1.09	1.11
1:a:128:GLN:NE2	2:A:787:HIS:CD2[8_545]	1.25	0.95
1:a:128:GLN:CD	2:A:787:HIS:NE2[8_545]	1.38	0.82

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	92/111 (83%)	76 (83%)	12 (13%)	4 (4%)	2	17
1	b	92/111 (83%)	76 (83%)	12 (13%)	4 (4%)	2	17
1	c	92/111 (83%)	75 (82%)	13 (14%)	4 (4%)	2	17
2	A	686/758 (90%)	493 (72%)	127 (18%)	66 (10%)	0	7
2	B	682/758 (90%)	491 (72%)	115 (17%)	76 (11%)	0	5
2	C	691/758 (91%)	492 (71%)	130 (19%)	69 (10%)	0	7
All	All	2335/2607 (90%)	1703 (73%)	409 (18%)	223 (10%)	0	7

5 of 223 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 [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	83/104 (80%)	67 (81%)	16 (19%)	1	7
1	b	84/104 (81%)	68 (81%)	16 (19%)	1	8
1	c	85/104 (82%)	69 (81%)	16 (19%)	1	8
2	A	571/645 (88%)	481 (84%)	90 (16%)	2	12
2	B	573/645 (89%)	467 (82%)	106 (18%)	1	8
2	C	576/645 (89%)	484 (84%)	92 (16%)	2	11
All	All	1972/2247 (88%)	1636 (83%)	336 (17%)	2	10

5 of 336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	151	LYS
2	C	354	LEU
1	c	190	SER
2	C	131	LEU
2	C	428	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	338	GLN
2	C	349	GLN
2	C	628	ASN
2	B	61	GLN
2	B	51	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	1
2	B	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	664:GLU	C	686:LYS	N	7.77
1	B	664:GLU	C	686:LYS	N	7.77
1	C	664:GLU	C	686:LYS	N	7.77

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	94/111 (84%)	4.28	89 (94%) 0 1	583, 624, 738, 792	0
1	b	94/111 (84%)	4.96	87 (92%) 0 1	543, 603, 730, 756	0
1	c	94/111 (84%)	6.21	88 (93%) 0 1	523, 590, 707, 731	0
2	A	708/758 (93%)	5.14	660 (93%) 0 1	508, 632, 810, 849	0
2	B	704/758 (92%)	5.16	646 (91%) 0 1	523, 661, 747, 823	0
2	C	711/758 (93%)	5.07	637 (89%) 0 1	426, 601, 842, 889	0
All	All	2405/2607 (92%)	5.13	2207 (91%) 0 1	426, 636, 815, 889	0

The worst 5 of 2207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	104	GLY	25.0
2	C	807	ALA	24.3
2	C	276	LEU	21.3
1	c	140	ILE	21.3
2	A	654	LEU	20.3

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 oligosaccharides 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.