wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:46 AM GMT

PDB ID	:	3PXI
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

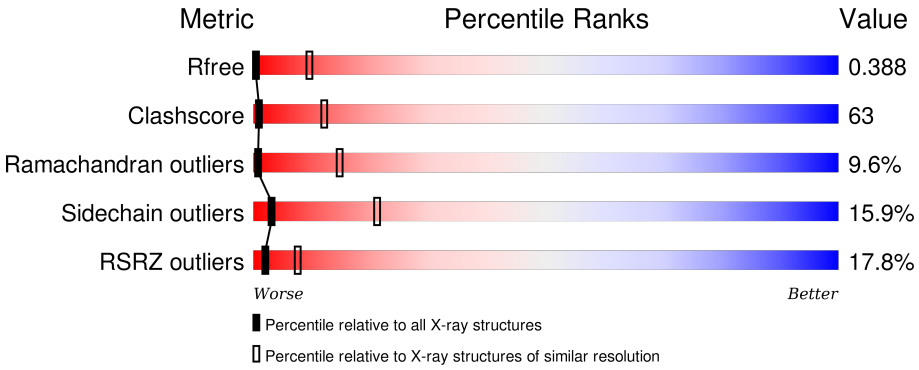
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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 <=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	9% 61% 23% • 15%
1	b	111	35% 67% 18% 15%
1	c	111	22% 67% 18% 15%
2	A	758	15% 35% 44% 13% • 7%
2	B	758	17% 32% 44% 15% • 7%

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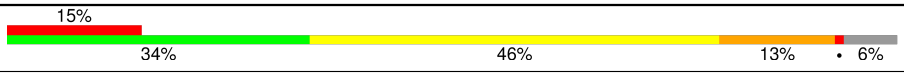
Mol	Chain	Length	Quality of chain
2	C	758	

2 Entry composition (i)

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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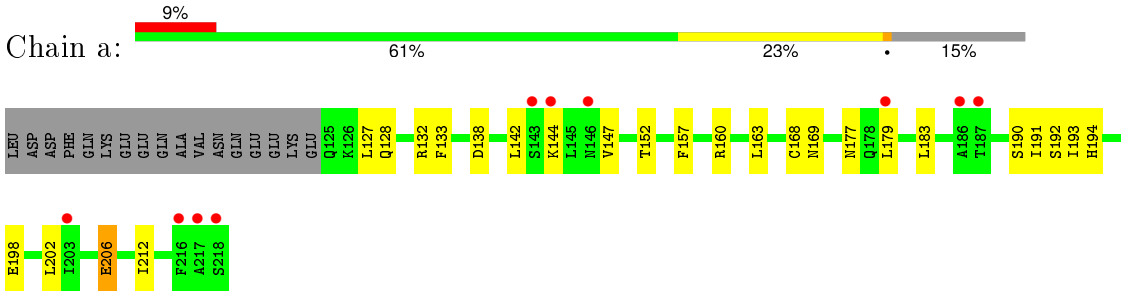
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	DELETION	UNP P37571
C	?	-	GLU	DELETION	UNP P37571
C	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
C	?	-	LEU	DELETION	UNP P37571
C	?	-	LYS	DELETION	UNP P37571
C	?	-	ARG	DELETION	UNP P37571
C	?	-	ASN	DELETION	UNP P37571
C	?	-	LYS	DELETION	UNP P37571
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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

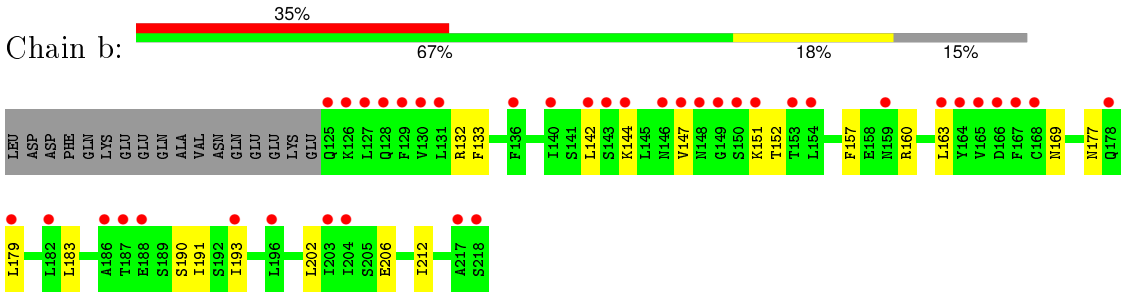
- Molecule 1: Adapter protein mecA 1

Chain a:



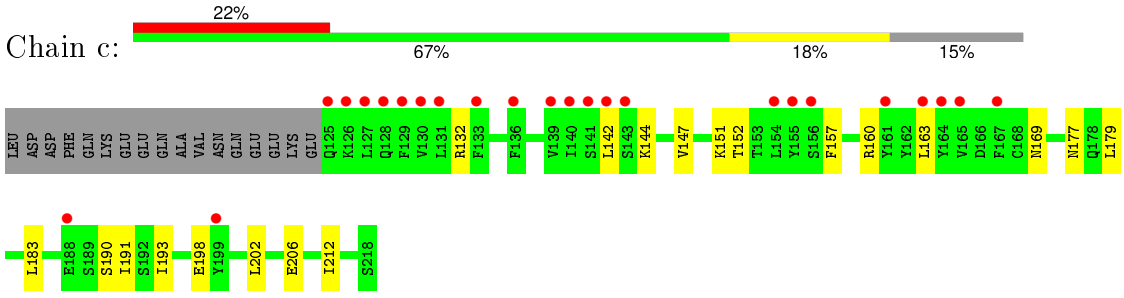
- Molecule 1: Adapter protein mecA 1

Chain b:



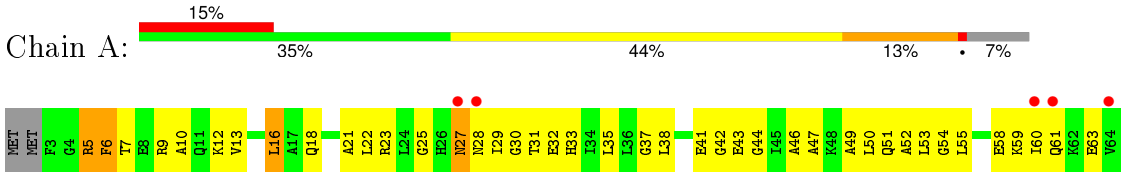
- Molecule 1: Adapter protein mecA 1

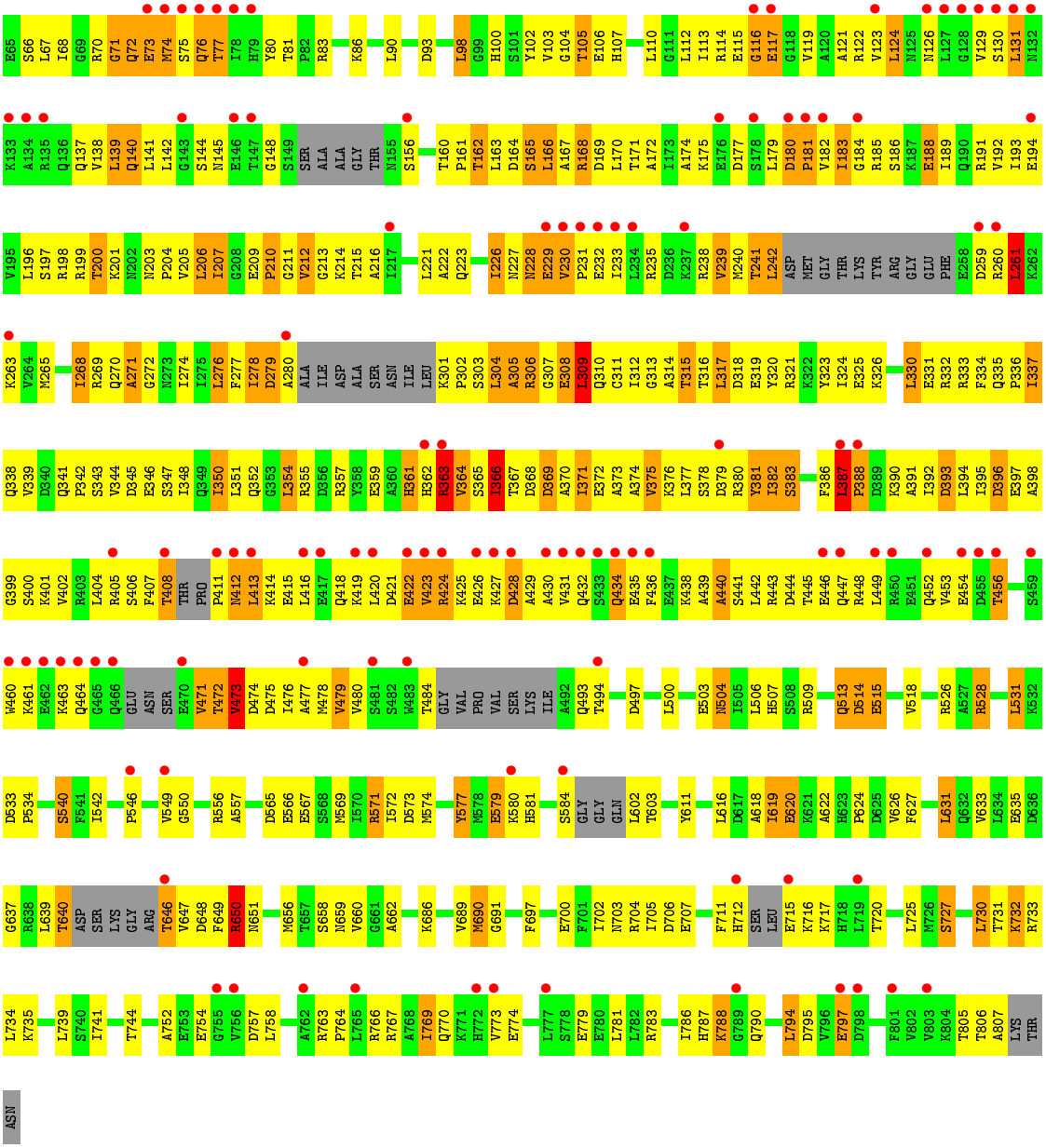
Chain c:



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

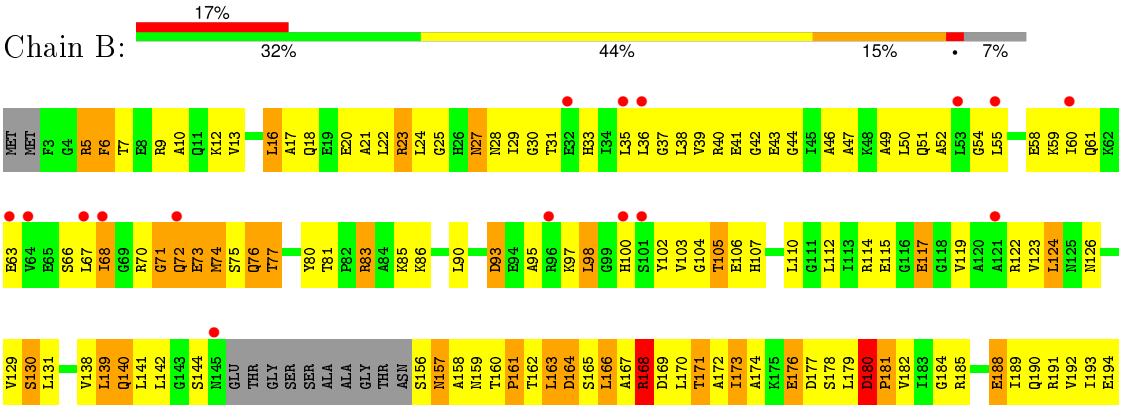
Chain A:

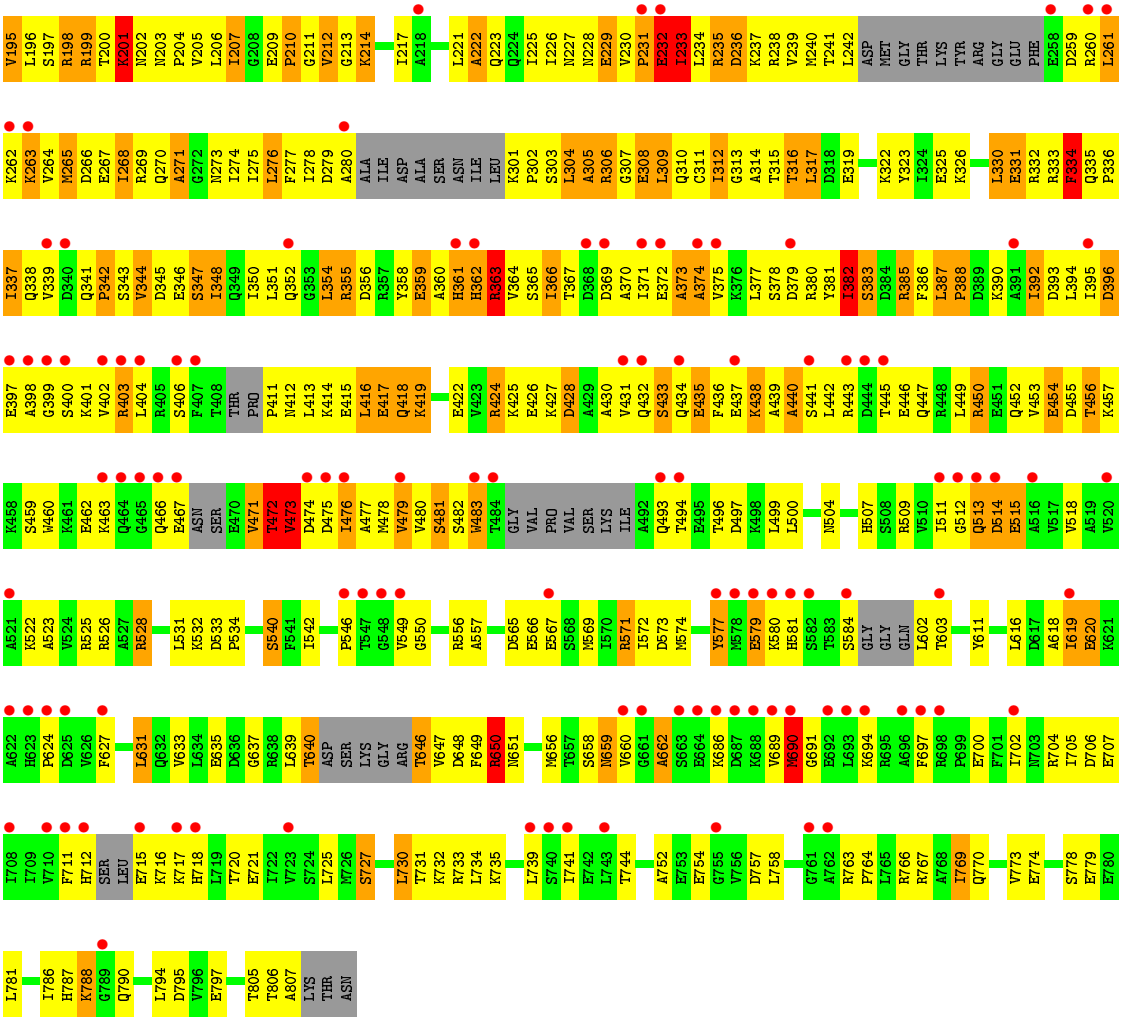




• Molecule 2: Negative regulator of genetic competence ClpC/MecB

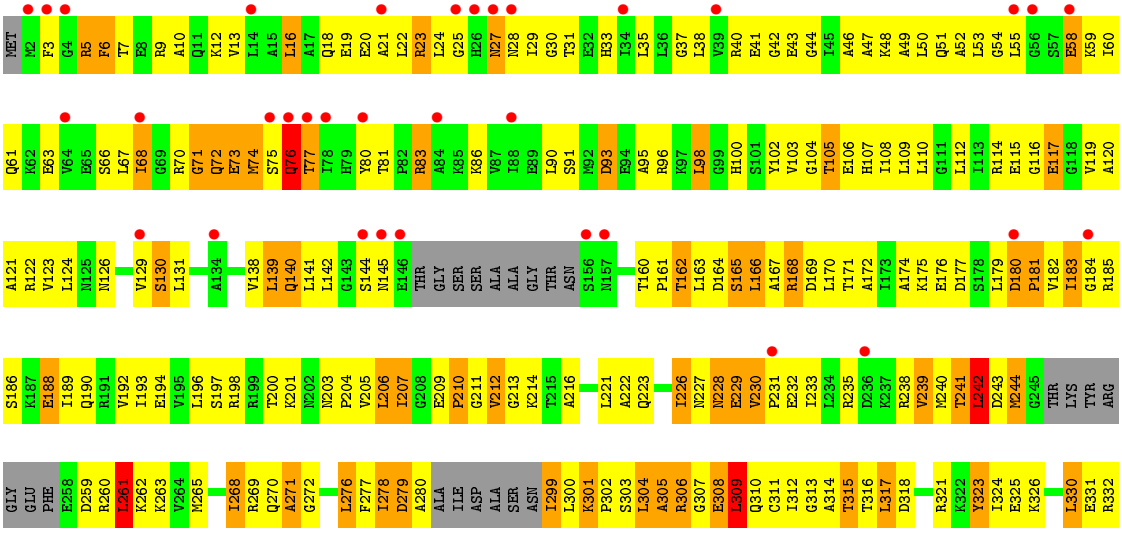
Chain B:

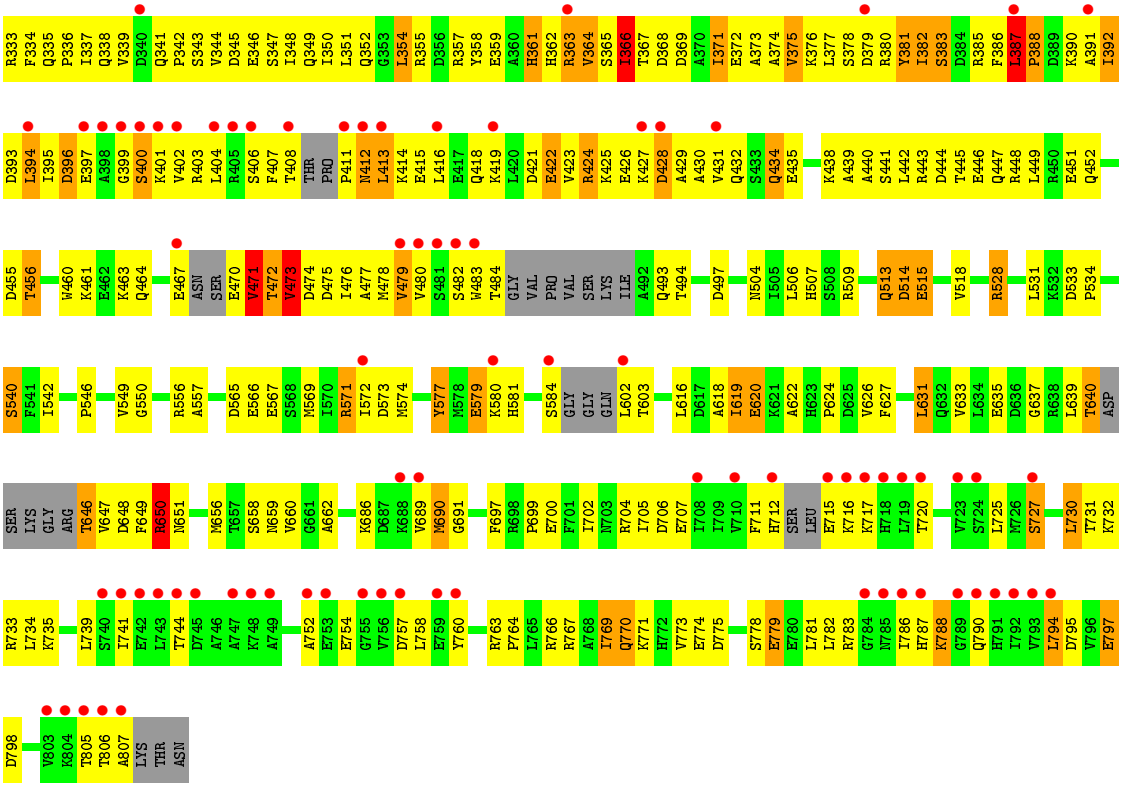




• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain C:




R333 F334 Q335 P336 I337 Q338 V339 D340 Q341 P342 S343 V344 D345 E346 S347 I348 Q349 I350 L351 Q352 G353 L354 R355 D356 R357 Y358 E359 A360 H361 H362 R363 V364 S365 I366 T367 D368 D369 A370 I371 E372 A373 A374 V375 K376 L377 S378 D379 R380 Y381 I382 S383 D384 R385 F386 L387 P388 D389 K390 A391 I392
D393 L394 I395 D396 E397 A398 G399 S400 K401 V402 R403 L404 R405 S406 F407 T408 THR PRO P411 N412 L413 K414 E415 L416 E417 Q418 K419 L420 D421 E422 V423 R424 K425 E426 K427 D428 A429 A430 V431 Q432 S433 Q434 E435 K438 A439 A440 S441 L442 R443 D444 T445 E446 Q447 R448 L449 R450 E451 Q452
D455 T456 W460 K461 E462 K463 Q464 E467 ASN SER E470 V471 T472 V473 D474 D475 I476 A477 M478 V479 V480 S481 S482 W483 T484 GLY VAL PRO VAL SER LYS ILE A492 Q493 T494 D497 N504 I505 L506 H507 S508 R509 Q513 D514 E515 V518 R528 L531 K532 D533 P534
S540 F541 I542 P546 V549 G550 R556 A557 D565 E566 E567 S568 M569 I570 R571 I572 D573 M574 Y577 M578 E579 K580 H581 S584 GLY GLY GLN L602 T603 L616 D617 A618 I619 E620 K621 A622 H623 P624 D625 V626 F627 L631 D632 V633 L634 E635 D636 G637 R638 L639 T640 ASP
SER LYS GLY ARG T646 V647 D648 F649 R650 N651 M656 T657 S658 M659 V660 G661 A662 K686 D687 K688 V689 M690 G691 F697 R698 P699 E700 F701 I702 N703 R704 I705 D706 E707 I708 I709 V710 F711 H712 SER LEU E715 K716 K717 H718 L719 T720 V723 S724 L725 M726 S727 L730 T731 K732
R733 L734 K735 L739 S740 I741 E742 L743 T744 D745 A746 A747 K748 A749 A752 E753 E754 G755 V756 D757 L758 E759 Y760 R763 P764 L765 R766 R767 A768 I769 Q770 K771 H772 V773 E774 D775 S778 E779 E780 L781 L782 R783 G784 N785 I786 H787 K788 G789 Q790 H791 I792 V793 L794 D795 V796 E797
D798 V803 K804 T805 T806 A807 LYS THR ASN

4 Data and refinement statistics (i)

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) 99.6 (49.15-6.93)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.07 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_596)	Depositor
R, R_{free}	0.407 , 0.422 0.363 , 0.388	Depositor DCC
R_{free} test set	332 reflections (4.74%)	DCC
Wilson B-factor (Å^2)	181.7	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 752.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.27$, $< L^2 > = 0.11$	Xtriage
Outliers	0 of 7006 reflections	Xtriage
F_o,F_c correlation	0.67	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 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.48	0/768	0.66	1/1035 (0.1%)
1	b	0.56	0/768	0.67	0/1035
1	c	0.64	0/776	0.68	0/1046
2	A	0.52	1/5498 (0.0%)	0.70	2/7386 (0.0%)
2	B	0.58	2/5483 (0.0%)	0.80	2/7369 (0.0%)
2	C	0.53	1/5526 (0.0%)	0.72	2/7431 (0.0%)
All	All	0.55	4/18819 (0.0%)	0.73	7/25302 (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
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	515	GLU	CG-CD	5.50	1.60	1.51
2	A	515	GLU	CG-CD	5.49	1.60	1.51
2	C	515	GLU	CG-CD	5.42	1.60	1.51
2	B	334	PHE	CA-CB	5.26	1.65	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	161	PRO	N-CA-CB	6.09	110.61	103.30
2	C	161	PRO	N-CA-CB	5.88	110.35	103.30
2	B	161	PRO	N-CA-CB	5.25	109.60	103.30
1	a	138	ASP	CB-CG-OD1	5.23	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	515	GLU	OE1-CD-OE2	-5.15	117.12	123.30

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	0	17
1	b	756	0	736	0	0
1	c	763	0	743	0	0
2	A	5455	0	5489	600	34
2	B	5437	0	5491	871	1
2	C	5479	0	5524	731	24
All	All	18645	0	18711	1994	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 63.

The worst 5 of 1994 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%)	3	34
1	b	92/111 (83%)	76 (83%)	12 (13%)	4 (4%)	3	34
1	c	92/111 (83%)	75 (82%)	13 (14%)	4 (4%)	3	34
2	A	686/758 (90%)	493 (72%)	127 (18%)	66 (10%)	1	15
2	B	682/758 (90%)	491 (72%)	115 (17%)	76 (11%)	0	11
2	C	691/758 (91%)	492 (71%)	130 (19%)	69 (10%)	1	14
All	All	2335/2607 (90%)	1703 (73%)	409 (18%)	223 (10%)	1	15

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%)	2	13
1	b	84/104 (81%)	68 (81%)	16 (19%)	2	13
1	c	85/104 (82%)	69 (81%)	16 (19%)	2	13
2	A	571/645 (88%)	487 (85%)	84 (15%)	4	24
2	B	573/645 (89%)	476 (83%)	97 (17%)	2	18
2	C	576/645 (89%)	492 (85%)	84 (15%)	4	24
All	All	1972/2247 (88%)	1659 (84%)	313 (16%)	3	21

5 of 313 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	235	ARG
2	B	443	ARG
2	C	571	ARG
2	B	276	LEU
2	B	355	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	126	ASN
2	B	310	GLN
2	C	362	HIS
2	B	137	GLN
2	B	203	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.88	10 (10%)	8	13	583, 624, 738, 792	0
1	b	94/111 (84%)	1.74	39 (41%)	0	4	543, 603, 730, 756	0
1	c	94/111 (84%)	1.25	24 (25%)	1	5	523, 590, 707, 731	0
2	A	708/758 (93%)	1.08	116 (16%)	2	8	508, 632, 810, 849	0
2	B	704/758 (92%)	1.03	127 (18%)	2	7	523, 661, 747, 823	0
2	C	711/758 (93%)	0.98	113 (15%)	3	8	426, 601, 842, 889	0
All	All	2405/2607 (92%)	1.06	429 (17%)	2	7	426, 636, 815, 889	0

The worst 5 of 429 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	411	PRO	7.8
2	A	465	GLY	7.5
2	A	231	PRO	7.4
2	A	466	GLN	7.1
2	C	720	THR	6.6

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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.