



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 02:35 PM BST

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

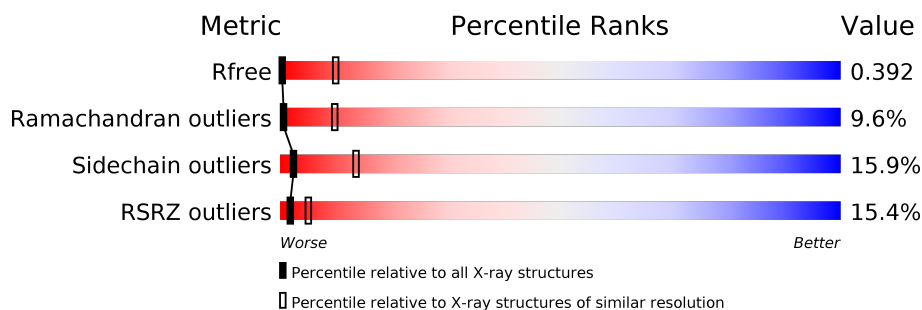
1 Overall quality at a glance

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}	130704	1003 (9.70-3.90)
Ramachandran outliers	138981	1001 (9.70-3.90)
Sidechain outliers	138945	1001 (9.70-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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	111	<div> <div>8%</div> <div>61%</div> <div>23%</div> <div>15%</div> </div>
1	b	111	<div> <div>30%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	c	111	<div> <div>18%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
2	A	758	<div> <div>14%</div> <div>73%</div> <div>19%</div> <div>7%</div> </div>
2	B	758	<div> <div>15%</div> <div>71%</div> <div>20%</div> <div>7%</div> </div>
2	C	758	<div> <div>12%</div> <div>74%</div> <div>19%</div> <div>6%</div> </div>

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

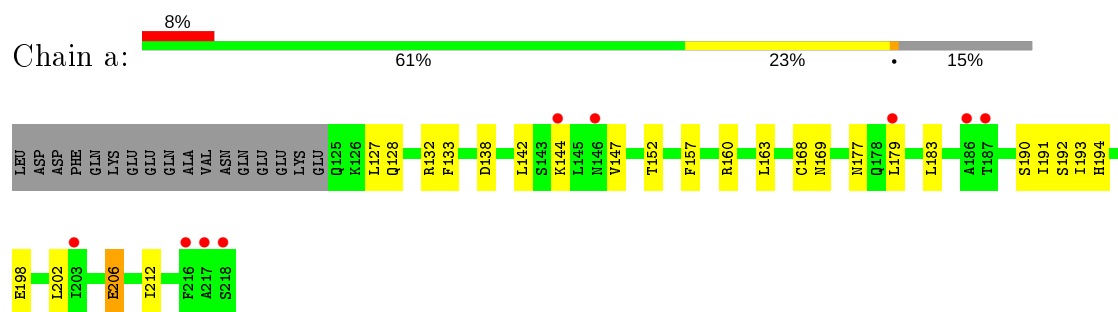
Continued from previous page...

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

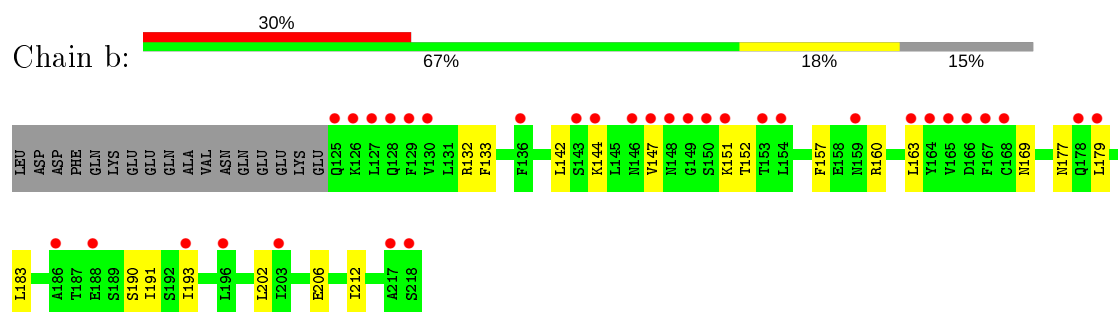
3 Residue-property plots

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.

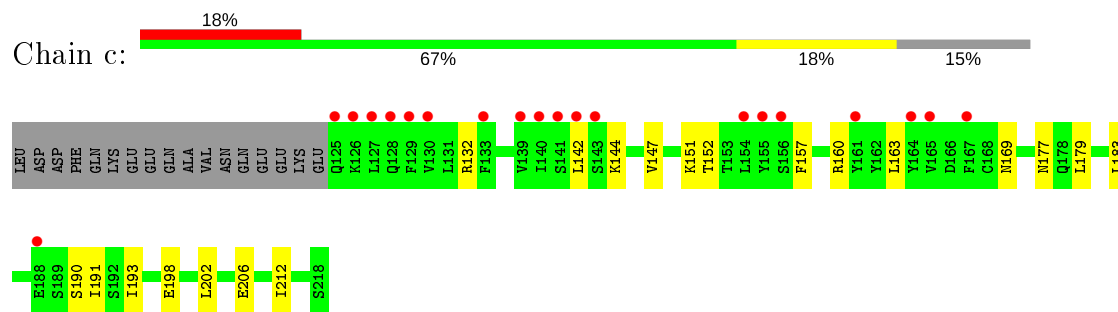
• Molecule 1: Adapter protein mecA 1



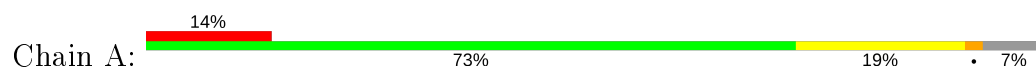
• Molecule 1: Adapter protein mecA 1

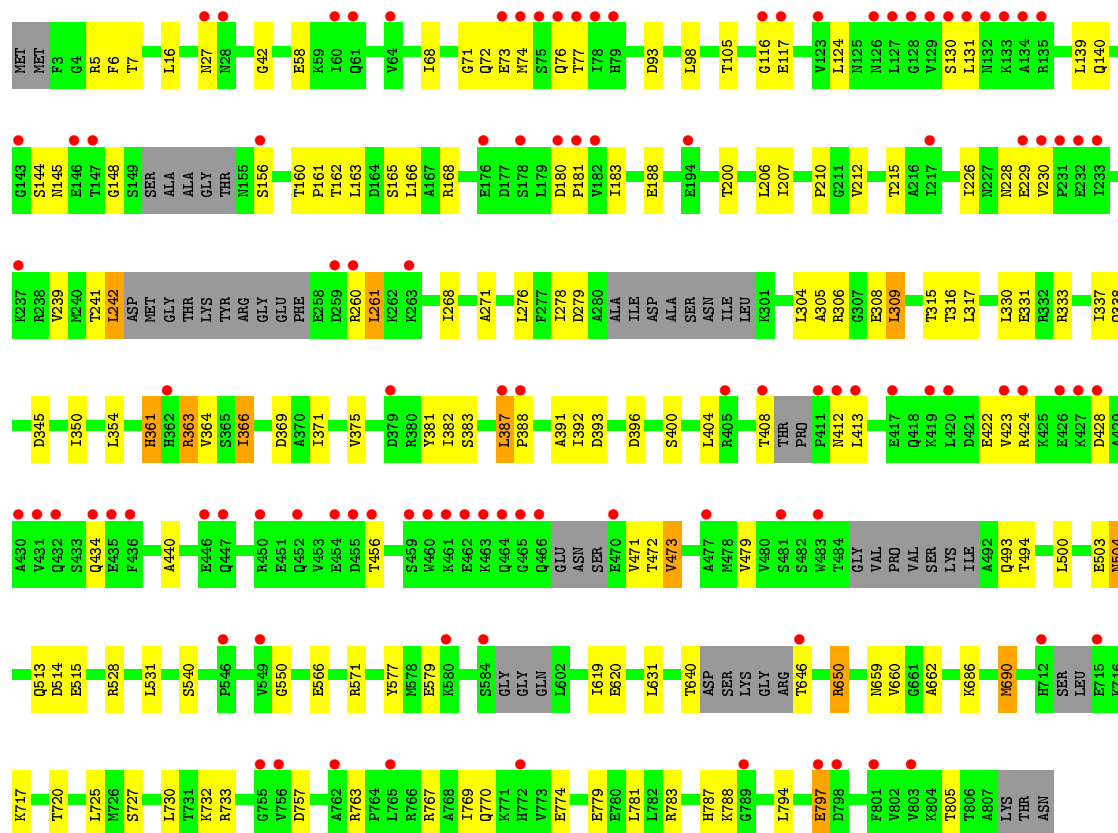


• Molecule 1: Adapter protein mecA 1

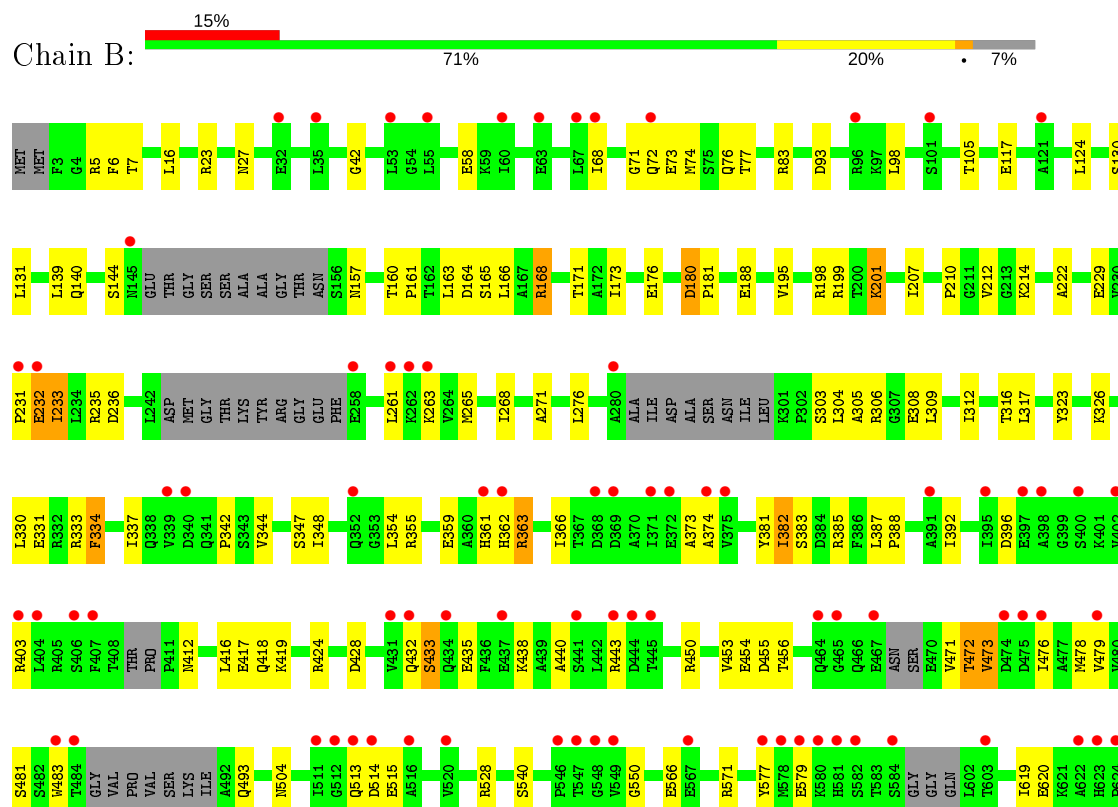


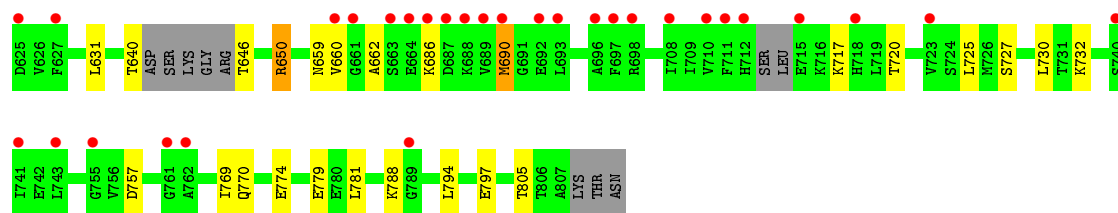
• Molecule 2: Negative regulator of genetic competence ClpC/MecB



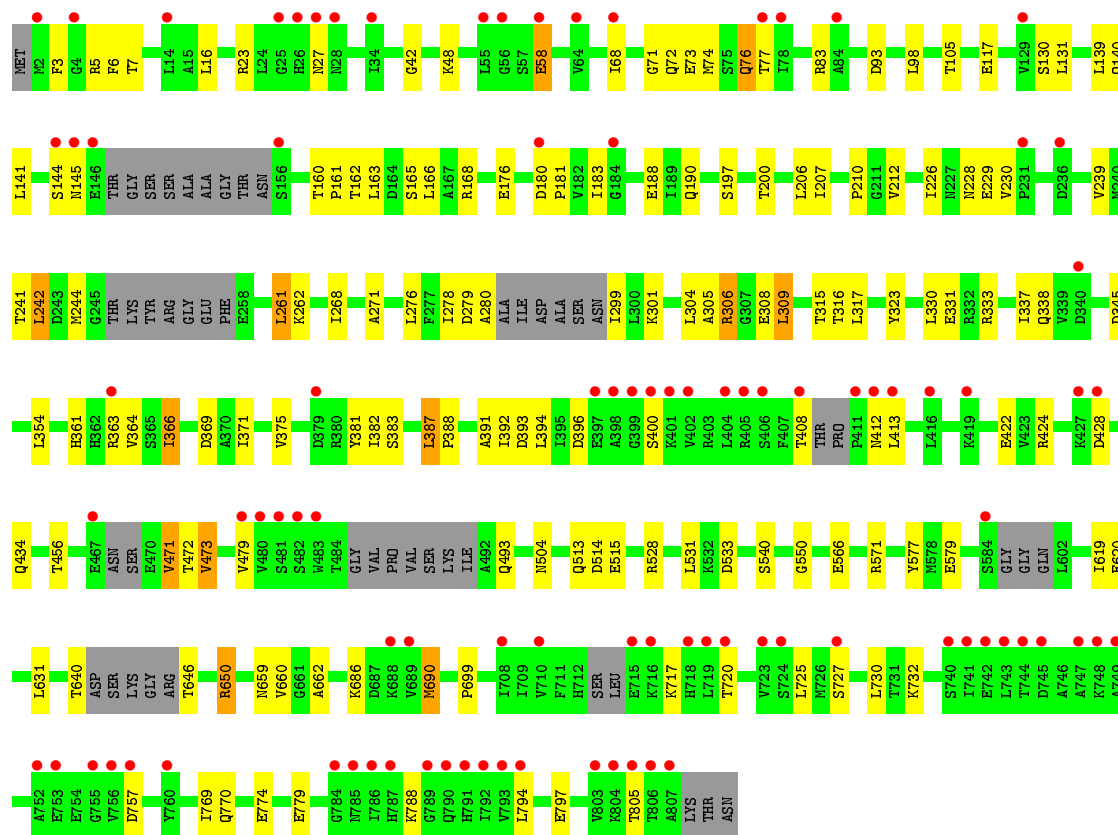


• Molecule 2: Negative regulator of genetic competence ClpC/MecB





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



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) 99.6 (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 0.372 , 0.392	Depositor DCC
R_{free} test set	333 reflections (4.75%)	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)	0.36 , 751.9	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	0.67	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 2.28% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.48	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

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	515	GLU	OE1-CD-OE2	-5.15	117.12	123.30
2	B	515	GLU	OE1-CD-OE2	-5.11	117.17	123.30
2	A	515	GLU	OE1-CD-OE2	-5.09	117.19	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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	22
1	b	92/111 (83%)	76 (83%)	12 (13%)	4 (4%)	2	22
1	c	92/111 (83%)	75 (82%)	13 (14%)	4 (4%)	2	22
2	A	686/758 (90%)	493 (72%)	127 (18%)	66 (10%)	0	10
2	B	682/758 (90%)	491 (72%)	115 (17%)	76 (11%)	0	7
2	C	691/758 (91%)	492 (71%)	130 (19%)	69 (10%)	0	9
All	All	2335/2607 (90%)	1703 (73%)	409 (18%)	223 (10%)	0	10

All (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
2	A	261	LEU
2	A	271	ALA
2	A	306	ARG
2	A	309	LEU
2	A	333	ARG
2	A	363	ARG
2	A	366	ILE
2	A	382	ILE
2	A	471	VAL
2	A	473	VAL
2	A	566	GLU
2	B	42	GLY
2	B	98	LEU
2	B	130	SER
2	B	144	SER
2	B	157	ASN
2	B	164	ASP
2	B	168	ARG
2	B	180	ASP
2	B	181	PRO
2	B	198	ARG
2	B	201	LYS
2	B	210	PRO
2	B	214	LYS
2	B	231	PRO
2	B	232	GLU
2	B	233	ILE
2	B	261	LEU
2	B	271	ALA
2	B	305	ALA
2	B	308	GLU
2	B	333	ARG
2	B	363	ARG
2	B	366	ILE
2	B	373	ALA
2	B	382	ILE
2	B	412	ASN
2	B	438	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	472	THR
2	B	566	GLU
1	c	169	ASN
2	C	42	GLY
2	C	98	LEU
2	C	130	SER
2	C	144	SER
2	C	183	ILE
2	C	242	LEU
2	C	244	MET
2	C	261	LEU
2	C	271	ALA
2	C	299	ILE
2	C	306	ARG
2	C	309	LEU
2	C	333	ARG
2	C	363	ARG
2	C	366	ILE
2	C	382	ILE
2	C	391	ALA
2	C	392	ILE
2	C	471	VAL
2	C	473	VAL
2	C	566	GLU
1	a	144	LYS
1	a	177	ASN
2	A	156	SER
2	A	163	LEU
2	A	165	SER
2	A	166	LEU
2	A	229	GLU
2	A	383	SER
2	A	391	ALA
2	A	493	GLN
2	A	662	ALA
2	A	690	MET
1	b	169	ASN
2	B	166	LEU
2	B	171	THR
2	B	199	ARG
2	B	331	GLU
2	B	362	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	433	SER
2	B	440	ALA
2	B	455	ASP
2	B	493	GLN
2	B	662	ALA
2	B	690	MET
1	c	144	LYS
1	c	206	GLU
2	C	3	PHE
2	C	77	THR
2	C	163	LEU
2	C	165	SER
2	C	166	LEU
2	C	280	ALA
2	C	331	GLU
2	C	383	SER
2	C	493	GLN
2	C	662	ALA
2	C	690	MET
2	A	73	GLU
2	A	77	THR
2	A	130	SER
2	A	162	THR
2	A	168	ARG
2	A	181	PRO
2	A	200	THR
2	A	228	ASN
2	A	305	ALA
2	A	330	LEU
2	A	331	GLU
2	A	375	VAL
2	A	388	PRO
2	A	412	ASN
2	A	413	LEU
2	A	788	LYS
1	b	144	LYS
1	b	206	GLU
2	B	77	THR
2	B	263	LYS
2	B	334	PHE
2	B	388	PRO
2	B	481	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	788	LYS
1	c	177	ASN
2	C	23	ARG
2	C	68	ILE
2	C	73	GLU
2	C	140	GLN
2	C	145	ASN
2	C	162	THR
2	C	168	ARG
2	C	181	PRO
2	C	228	ASN
2	C	229	GLU
2	C	330	LEU
2	C	375	VAL
2	C	388	PRO
2	C	412	ASN
2	C	413	LEU
2	C	788	LYS
2	A	71	GLY
2	A	74	MET
2	A	145	ASN
2	A	148	GLY
2	A	212	VAL
2	A	215	THR
2	A	226	ILE
2	A	316	THR
2	A	400	SER
2	A	422	GLU
2	A	434	GLN
2	A	650	ARG
2	A	757	ASP
2	A	779	GLU
1	b	177	ASN
2	B	68	ILE
2	B	71	GLY
2	B	73	GLU
2	B	74	MET
2	B	140	GLN
2	B	163	LEU
2	B	165	SER
2	B	176	GLU
2	B	212	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	330	LEU
2	B	344	VAL
2	B	359	GLU
2	B	374	ALA
2	B	385	ARG
2	B	450	ARG
2	B	650	ARG
2	B	757	ASP
2	B	779	GLU
2	C	71	GLY
2	C	74	MET
2	C	200	THR
2	C	212	VAL
2	C	226	ILE
2	C	301	LYS
2	C	305	ALA
2	C	316	THR
2	C	422	GLU
2	C	434	GLN
2	C	650	ARG
2	C	757	ASP
2	C	779	GLU
1	a	206	GLU
2	A	68	ILE
2	A	140	GLN
2	A	774	GLU
2	B	23	ARG
2	B	160	THR
2	B	306	ARG
2	B	342	PRO
2	B	774	GLU
2	C	400	SER
2	C	774	GLU
2	A	440	ALA
2	B	222	ALA
2	B	383	SER
2	C	76	GLN
2	C	323	TYR
2	A	116	GLY
2	A	479	VAL
2	B	473	VAL
2	A	160	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	471	VAL
2	B	476	ILE
2	A	392	ILE
2	A	423	VAL
2	C	160	THR
2	C	387	LEU
2	A	387	LEU
2	B	392	ILE
2	A	550	GLY
2	B	550	GLY
2	C	479	VAL
2	C	550	GLY

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	83/104 (80%)	67 (81%)	16 (19%)	1	8
1	b	84/104 (81%)	68 (81%)	16 (19%)	1	8
1	c	85/104 (82%)	69 (81%)	16 (19%)	1	9
2	A	571/645 (88%)	487 (85%)	84 (15%)	3	15
2	B	573/645 (89%)	476 (83%)	97 (17%)	2	12
2	C	576/645 (89%)	492 (85%)	84 (15%)	3	15
All	All	1972/2247 (88%)	1659 (84%)	313 (16%)	2	13

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	132	ARG
1	a	133	PHE
1	a	142	LEU
1	a	147	VAL
1	a	152	THR
1	a	157	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	160	ARG
1	a	163	LEU
1	a	179	LEU
1	a	183	LEU
1	a	190	SER
1	a	191	ILE
1	a	193	ILE
1	a	198	GLU
1	a	202	LEU
1	a	212	ILE
2	A	5	ARG
2	A	6	PHE
2	A	7	THR
2	A	16	LEU
2	A	27	ASN
2	A	58	GLU
2	A	72	GLN
2	A	76	GLN
2	A	93	ASP
2	A	105	THR
2	A	117	GLU
2	A	124	LEU
2	A	131	LEU
2	A	139	LEU
2	A	180	ASP
2	A	188	GLU
2	A	206	LEU
2	A	207	ILE
2	A	230	VAL
2	A	239	VAL
2	A	241	THR
2	A	242	LEU
2	A	261	LEU
2	A	268	ILE
2	A	276	LEU
2	A	278	ILE
2	A	279	ASP
2	A	304	LEU
2	A	308	GLU
2	A	309	LEU
2	A	315	THR
2	A	317	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	337	ILE
2	A	338	GLN
2	A	345	ASP
2	A	350	ILE
2	A	354	LEU
2	A	361	HIS
2	A	363	ARG
2	A	364	VAL
2	A	366	ILE
2	A	369	ASP
2	A	371	ILE
2	A	381	TYR
2	A	387	LEU
2	A	393	ASP
2	A	396	ASP
2	A	408	THR
2	A	424	ARG
2	A	428	ASP
2	A	456	THR
2	A	472	THR
2	A	473	VAL
2	A	504	ASN
2	A	513	GLN
2	A	514	ASP
2	A	528	ARG
2	A	531	LEU
2	A	540	SER
2	A	571	ARG
2	A	577	TYR
2	A	579	GLU
2	A	619	ILE
2	A	620	GLU
2	A	631	LEU
2	A	640	THR
2	A	646	THR
2	A	650	ARG
2	A	659	ASN
2	A	660	VAL
2	A	686	LYS
2	A	690	MET
2	A	717	LYS
2	A	720	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	725	LEU
2	A	727	SER
2	A	730	LEU
2	A	732	LYS
2	A	767	ARG
2	A	769	ILE
2	A	770	GLN
2	A	794	LEU
2	A	797	GLU
2	A	805	THR
1	b	132	ARG
1	b	133	PHE
1	b	142	LEU
1	b	147	VAL
1	b	151	LYS
1	b	152	THR
1	b	157	PHE
1	b	160	ARG
1	b	163	LEU
1	b	179	LEU
1	b	183	LEU
1	b	190	SER
1	b	191	ILE
1	b	193	ILE
1	b	202	LEU
1	b	212	ILE
2	B	5	ARG
2	B	6	PHE
2	B	7	THR
2	B	16	LEU
2	B	27	ASN
2	B	58	GLU
2	B	72	GLN
2	B	76	GLN
2	B	83	ARG
2	B	93	ASP
2	B	105	THR
2	B	117	GLU
2	B	124	LEU
2	B	131	LEU
2	B	139	LEU
2	B	168	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	173	ILE
2	B	180	ASP
2	B	188	GLU
2	B	195	VAL
2	B	201	LYS
2	B	207	ILE
2	B	229	GLU
2	B	232	GLU
2	B	233	ILE
2	B	235	ARG
2	B	236	ASP
2	B	265	MET
2	B	268	ILE
2	B	276	LEU
2	B	303	SER
2	B	304	LEU
2	B	309	LEU
2	B	312	ILE
2	B	316	THR
2	B	317	LEU
2	B	323	TYR
2	B	326	LYS
2	B	337	ILE
2	B	347	SER
2	B	348	ILE
2	B	354	LEU
2	B	355	ARG
2	B	361	HIS
2	B	363	ARG
2	B	381	TYR
2	B	382	ILE
2	B	387	LEU
2	B	396	ASP
2	B	403	ARG
2	B	416	LEU
2	B	417	GLU
2	B	418	GLN
2	B	419	LYS
2	B	424	ARG
2	B	428	ASP
2	B	432	GLN
2	B	433	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	435	GLU
2	B	443	ARG
2	B	453	VAL
2	B	454	GLU
2	B	456	THR
2	B	472	THR
2	B	473	VAL
2	B	478	MET
2	B	479	VAL
2	B	483	TRP
2	B	504	ASN
2	B	513	GLN
2	B	514	ASP
2	B	528	ARG
2	B	540	SER
2	B	571	ARG
2	B	577	TYR
2	B	579	GLU
2	B	619	ILE
2	B	620	GLU
2	B	631	LEU
2	B	640	THR
2	B	646	THR
2	B	650	ARG
2	B	659	ASN
2	B	660	VAL
2	B	686	LYS
2	B	690	MET
2	B	717	LYS
2	B	720	THR
2	B	725	LEU
2	B	727	SER
2	B	730	LEU
2	B	732	LYS
2	B	769	ILE
2	B	770	GLN
2	B	794	LEU
2	B	797	GLU
2	B	805	THR
1	c	132	ARG
1	c	142	LEU
1	c	147	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	c	151	LYS
1	c	152	THR
1	c	157	PHE
1	c	160	ARG
1	c	163	LEU
1	c	179	LEU
1	c	183	LEU
1	c	190	SER
1	c	191	ILE
1	c	193	ILE
1	c	198	GLU
1	c	202	LEU
1	c	212	ILE
2	C	5	ARG
2	C	6	PHE
2	C	7	THR
2	C	16	LEU
2	C	27	ASN
2	C	58	GLU
2	C	72	GLN
2	C	76	GLN
2	C	83	ARG
2	C	93	ASP
2	C	105	THR
2	C	117	GLU
2	C	131	LEU
2	C	139	LEU
2	C	176	GLU
2	C	180	ASP
2	C	188	GLU
2	C	206	LEU
2	C	207	ILE
2	C	230	VAL
2	C	239	VAL
2	C	241	THR
2	C	242	LEU
2	C	261	LEU
2	C	268	ILE
2	C	276	LEU
2	C	278	ILE
2	C	279	ASP
2	C	304	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	308	GLU
2	C	309	LEU
2	C	315	THR
2	C	317	LEU
2	C	337	ILE
2	C	338	GLN
2	C	345	ASP
2	C	354	LEU
2	C	361	HIS
2	C	364	VAL
2	C	366	ILE
2	C	369	ASP
2	C	371	ILE
2	C	381	TYR
2	C	387	LEU
2	C	393	ASP
2	C	394	LEU
2	C	396	ASP
2	C	408	THR
2	C	424	ARG
2	C	428	ASP
2	C	456	THR
2	C	471	VAL
2	C	472	THR
2	C	473	VAL
2	C	504	ASN
2	C	513	GLN
2	C	514	ASP
2	C	528	ARG
2	C	531	LEU
2	C	540	SER
2	C	571	ARG
2	C	577	TYR
2	C	579	GLU
2	C	619	ILE
2	C	620	GLU
2	C	631	LEU
2	C	640	THR
2	C	646	THR
2	C	650	ARG
2	C	659	ASN
2	C	660	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	686	LYS
2	C	690	MET
2	C	717	LYS
2	C	720	THR
2	C	725	LEU
2	C	727	SER
2	C	730	LEU
2	C	732	LYS
2	C	769	ILE
2	C	770	GLN
2	C	794	LEU
2	C	797	GLU
2	C	805	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	159	ASN
1	a	207	HIS
2	A	51	GLN
2	A	61	GLN
2	A	72	GLN
2	A	76	GLN
2	A	100	HIS
2	A	126	ASN
2	A	137	GLN
2	A	223	GLN
2	A	228	ASN
2	A	310	GLN
2	A	338	GLN
2	A	341	GLN
2	A	362	HIS
2	A	432	GLN
2	A	623	HIS
2	A	659	ASN
2	A	770	GLN
2	A	785	ASN
1	b	159	ASN
1	b	207	HIS
2	B	51	GLN
2	B	61	GLN
2	B	72	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	76	GLN
2	B	100	HIS
2	B	126	ASN
2	B	137	GLN
2	B	202	ASN
2	B	203	ASN
2	B	223	GLN
2	B	227	ASN
2	B	228	ASN
2	B	310	GLN
2	B	361	HIS
2	B	362	HIS
2	B	623	HIS
2	B	659	ASN
2	B	770	GLN
2	B	785	ASN
1	c	159	ASN
1	c	194	HIS
1	c	207	HIS
2	C	28	ASN
2	C	51	GLN
2	C	61	GLN
2	C	72	GLN
2	C	76	GLN
2	C	100	HIS
2	C	126	ASN
2	C	137	GLN
2	C	223	GLN
2	C	228	ASN
2	C	338	GLN
2	C	341	GLN
2	C	362	HIS
2	C	432	GLN
2	C	623	HIS
2	C	659	ASN
2	C	785	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 monosaccharides 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	B	1
2	A	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

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	94/111 (84%)	0.76	9 (9%) 8 11	583, 624, 738, 792	0
1	b	94/111 (84%)	1.55	33 (35%) 0 2	543, 603, 730, 756	0
1	c	94/111 (84%)	1.14	20 (21%) 0 3	523, 590, 707, 731	0
2	A	708/758 (93%)	0.97	104 (14%) 2 5	508, 632, 810, 849	0
2	B	704/758 (92%)	0.92	110 (15%) 2 5	523, 661, 747, 823	0
2	C	711/758 (93%)	0.86	94 (13%) 3 7	426, 601, 842, 889	0
All	All	2405/2607 (92%)	0.94	370 (15%) 2 5	426, 636, 815, 889	0

All (370) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	411	PRO	7.9
2	A	231	PRO	7.4
2	A	465	GLY	7.2
2	A	466	GLN	6.9
2	C	720	THR	6.2
2	C	807	ALA	6.0
2	C	806	THR	5.9
2	B	664	GLU	5.8
2	C	741	ILE	5.8
2	A	230	VAL	5.7
2	C	481	SER	5.6
2	B	444	ASP	5.4
2	A	412	ASN	5.2
2	C	748	LYS	5.2
2	A	76	GLN	5.1
2	C	467	GLU	5.0
2	B	688	LYS	4.9
2	C	756	VAL	4.9
2	C	27	ASN	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	689	VAL	4.9
2	B	464	GLN	4.9
2	A	427	LYS	4.8
2	B	687	ASP	4.7
1	b	218	SER	4.7
2	A	27	ASN	4.7
2	C	483	TRP	4.7
2	B	584	SER	4.6
2	A	798	ASP	4.6
2	B	262	LYS	4.6
2	C	719	LEU	4.6
2	A	413	LEU	4.6
2	A	75	SER	4.5
2	B	547	THR	4.5
2	A	130	SER	4.4
2	B	740	SER	4.3
2	C	727	SER	4.3
2	C	716	LYS	4.3
1	b	146	ASN	4.3
2	C	743	LEU	4.2
2	B	374	ALA	4.2
2	B	403	ARG	4.1
2	C	752	ALA	4.1
2	C	28	ASN	4.1
2	C	26	HIS	4.1
2	C	787	HIS	4.1
2	A	28	ASN	4.1
2	C	145	ASN	4.0
2	A	176	GLU	4.0
2	C	723	VAL	4.0
2	A	129	VAL	4.0
2	B	761	GLY	4.0
2	C	405	ARG	3.9
2	B	441	SER	3.9
2	A	431	VAL	3.9
2	B	513	GLN	3.8
2	A	797	GLU	3.8
2	B	512	GLY	3.8
1	b	149	GLY	3.7
1	b	150	SER	3.7
2	A	147	THR	3.7
2	A	77	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	693	LEU	3.7
2	C	755	GLY	3.7
2	A	462	GLU	3.7
2	B	549	VAL	3.6
2	A	78	ILE	3.6
1	b	217	ALA	3.6
2	B	690	MET	3.5
2	B	580	LYS	3.5
2	B	362	HIS	3.5
2	A	463	LYS	3.5
2	A	424	ARG	3.5
1	b	165	VAL	3.5
2	A	464	GLN	3.5
2	A	646	THR	3.5
2	C	77	THR	3.5
2	C	724	SER	3.5
2	B	261	LEU	3.4
2	C	791	HIS	3.4
2	C	715	GLU	3.4
1	b	164	TYR	3.4
2	A	260	ARG	3.4
2	A	455	ASP	3.4
2	A	755	GLY	3.4
2	B	697	PHE	3.4
2	C	401	LYS	3.4
2	C	397	GLU	3.4
2	B	398	ALA	3.4
2	A	74	MET	3.4
2	B	443	ARG	3.4
2	B	361	HIS	3.4
1	b	166	ASP	3.4
2	A	259	ASP	3.3
2	B	352	GLN	3.3
1	b	167	PHE	3.3
2	B	445	THR	3.3
2	C	742	GLU	3.3
2	C	412	ASN	3.3
2	B	511	ILE	3.3
2	C	803	VAL	3.3
2	C	2	MET	3.3
1	c	129	PHE	3.3
2	A	135	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	232	GLU	3.2
2	B	710	VAL	3.2
1	c	188	GLU	3.2
1	c	161	TYR	3.2
2	B	53	LEU	3.2
2	C	402	VAL	3.2
1	c	127	LEU	3.2
2	A	133	LYS	3.2
2	C	792	ILE	3.2
2	A	801	PHE	3.2
2	A	419	LYS	3.1
2	A	432	GLN	3.1
2	C	78	ILE	3.1
2	C	231	PRO	3.1
2	C	398	ALA	3.1
2	B	465	GLY	3.1
2	A	229	GLU	3.1
2	B	369	ASP	3.1
2	C	146	GLU	3.1
2	A	772	HIS	3.1
2	B	431	VAL	3.1
2	B	60	ILE	3.1
2	C	805	THR	3.1
2	A	379	ASP	3.0
2	C	790	GLN	3.0
1	b	188	GLU	3.0
2	B	258	GLU	3.0
2	B	712	HIS	3.0
2	A	481	SER	3.0
2	A	426	GLU	3.0
2	A	446	GLU	3.0
2	C	793	VAL	3.0
1	b	129	PHE	3.0
2	A	182	VAL	3.0
2	C	480	VAL	3.0
2	A	233	ILE	3.0
2	A	61	GLN	2.9
1	c	126	LYS	2.9
2	A	756	VAL	2.9
2	B	68	ILE	2.9
2	A	79	HIS	2.9
1	a	217	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	368	ASP	2.9
2	B	402	VAL	2.9
2	B	434	GLN	2.9
1	c	142	LEU	2.9
2	C	688	LYS	2.8
2	A	237	LYS	2.8
2	B	567	GLU	2.8
2	A	460	TRP	2.8
2	B	582	SER	2.8
2	C	411	PRO	2.8
2	B	546	PRO	2.8
2	B	627	PHE	2.8
2	C	794	LEU	2.8
2	A	178	SER	2.8
2	A	580	LYS	2.7
1	b	203	ILE	2.7
2	B	741	ILE	2.7
2	B	391	ALA	2.7
2	A	156	SER	2.7
2	A	362	HIS	2.7
2	C	745	ASP	2.7
2	C	408	THR	2.7
2	B	603	THR	2.7
2	C	718	HIS	2.7
2	A	146	GLU	2.7
2	B	686	LYS	2.7
2	A	131	LEU	2.7
2	B	516	ALA	2.7
2	B	579	GLU	2.7
2	A	127	LEU	2.7
1	b	130	VAL	2.7
1	b	154	LEU	2.7
2	C	757	ASP	2.7
2	A	430	ALA	2.7
2	B	762	ALA	2.7
2	B	474	ASP	2.6
2	B	755	GLY	2.6
2	B	578	MET	2.6
1	a	218	SER	2.6
2	B	437	GLU	2.6
2	A	132	ASN	2.6
2	C	785	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	a	216	PHE	2.6
2	B	715	GLU	2.6
2	A	549	VAL	2.6
1	b	163	LEU	2.6
1	b	159	ASN	2.6
2	B	121	ALA	2.6
2	B	467	GLU	2.6
2	C	740	SER	2.6
1	b	126	LYS	2.6
2	A	417	GLU	2.6
2	B	432	GLN	2.6
1	c	164	TYR	2.6
2	C	406	SER	2.6
2	C	55	LEU	2.6
1	c	133	PHE	2.6
1	b	148	ASN	2.5
2	A	387	LEU	2.5
1	b	179	LEU	2.5
1	b	178	GLN	2.5
2	B	692	GLU	2.5
2	A	434	GLN	2.5
2	C	789	GLY	2.5
2	A	447	GLN	2.5
1	a	186	ALA	2.5
2	B	718	HIS	2.5
2	A	452	GLN	2.5
2	B	232	GLU	2.5
2	C	749	ALA	2.5
1	c	143	SER	2.5
1	a	179	LEU	2.5
2	A	470	GLU	2.5
2	A	789	GLY	2.5
2	B	663	SER	2.5
2	C	753	GLU	2.5
2	A	456	THR	2.5
1	b	153	THR	2.4
2	C	379	ASP	2.4
2	A	143	GLY	2.4
2	B	625	ASP	2.4
1	c	156	SER	2.4
2	A	459	SER	2.4
2	A	584	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	b	128	GLN	2.4
2	C	710	VAL	2.4
2	C	482	SER	2.4
2	B	548	GLY	2.4
2	C	64	VAL	2.4
2	C	584	SER	2.4
2	B	696	ALA	2.4
2	A	762	ALA	2.4
2	A	116	GLY	2.4
2	B	375	VAL	2.4
2	A	454	GLU	2.4
2	A	180	ASP	2.4
2	C	144	SER	2.4
2	A	450	ARG	2.4
2	C	784	GLY	2.4
2	C	419	LYS	2.4
2	A	181	PRO	2.4
2	A	420	LEU	2.4
2	A	128	GLY	2.4
2	C	184	GLY	2.4
2	A	765	LEU	2.4
2	A	423	VAL	2.4
1	b	151	LYS	2.3
2	C	804	LYS	2.3
2	B	400	SER	2.3
2	B	520	VAL	2.3
2	C	236	ASP	2.3
2	B	698	ARG	2.3
2	B	35	LEU	2.3
2	B	577	TYR	2.3
2	C	363	ARG	2.3
2	B	483	TRP	2.3
2	A	194	GLU	2.3
2	A	712	HIS	2.3
2	A	715	GLU	2.3
2	A	803	VAL	2.3
2	B	406	SER	2.3
2	B	145	ASN	2.3
2	B	263	LYS	2.3
2	B	708	ILE	2.3
2	A	217	ILE	2.3
1	b	147	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	427	LYS	2.3
2	B	63	GLU	2.3
2	B	371	ILE	2.3
2	B	661	GLY	2.3
2	A	388	PRO	2.3
2	A	436	PHE	2.3
1	b	127	LEU	2.3
1	b	144	LYS	2.3
2	B	723	VAL	2.3
1	b	186	ALA	2.3
2	A	134	ALA	2.2
1	a	144	LYS	2.2
1	c	155	TYR	2.2
2	B	484	THR	2.2
1	c	154	LEU	2.2
2	C	340	ASP	2.2
2	C	400	SER	2.2
2	B	395	ILE	2.2
2	B	743	LEU	2.2
2	B	72	GLN	2.2
2	B	624	PRO	2.2
2	B	67	LEU	2.2
2	A	64	VAL	2.2
2	B	280	ALA	2.2
1	b	143	SER	2.2
1	c	167	PHE	2.2
2	C	413	LEU	2.2
2	B	231	PRO	2.2
2	C	156	SER	2.2
2	B	55	LEU	2.2
2	B	407	PHE	2.2
1	b	136	PHE	2.2
2	A	73	GLU	2.2
2	B	475	ASP	2.2
2	C	399	GLY	2.2
2	C	708	ILE	2.2
2	B	479	VAL	2.2
1	b	168	CYS	2.2
2	B	711	PHE	2.2
2	A	60	ILE	2.2
2	C	129	VAL	2.2
2	B	514	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	477	ALA	2.2
2	B	101	SER	2.2
1	b	196	LEU	2.1
2	C	689	VAL	2.1
2	C	180	ASP	2.1
2	A	263	LYS	2.1
1	c	130	VAL	2.1
1	c	140	ILE	2.1
2	B	339	VAL	2.1
2	A	126	ASN	2.1
2	A	546	PRO	2.1
1	c	165	VAL	2.1
2	C	56	GLY	2.1
2	C	416	LEU	2.1
2	A	428	ASP	2.1
2	C	34	ILE	2.1
2	A	123	VAL	2.1
2	C	786	ILE	2.1
2	B	622	ALA	2.1
1	a	187	THR	2.1
2	B	476	ILE	2.1
1	c	128	GLN	2.1
1	b	193	ILE	2.1
2	B	404	LEU	2.1
2	C	68	ILE	2.1
1	c	141	SER	2.1
2	B	623	HIS	2.1
2	B	581	HIS	2.1
1	c	125	GLN	2.1
2	A	483	TRP	2.1
2	C	428	ASP	2.1
1	a	203	ILE	2.1
2	A	435	GLU	2.1
2	C	747	ALA	2.1
2	A	405	ARG	2.1
2	A	461	LYS	2.1
1	b	125	GLN	2.0
2	B	32	GLU	2.0
1	c	139	VAL	2.0
2	A	408	THR	2.0
2	C	479	VAL	2.0
2	C	4	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	25	GLY	2.0
2	C	744	THR	2.0
2	B	96	ARG	2.0
2	C	760	TYR	2.0
2	B	372	GLU	2.0
2	A	117	GLU	2.0
2	B	789	GLY	2.0
2	B	660	VAL	2.0
2	B	340	ASP	2.0
2	B	397	GLU	2.0
2	C	84	ALA	2.0
1	a	146	ASN	2.0
2	C	14	LEU	2.0
2	C	404	LEU	2.0
2	C	58	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.