



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:17 PM GMT

PDB ID : 3WQU  
Title : Staphylococcus aureus FtsA complexed with ATP  
Authors : Fujita, J.; Maeda, Y.; Miyazaki, Y.; Inoue, T.; Matsumura, H.  
Deposited on : 2014-02-01  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

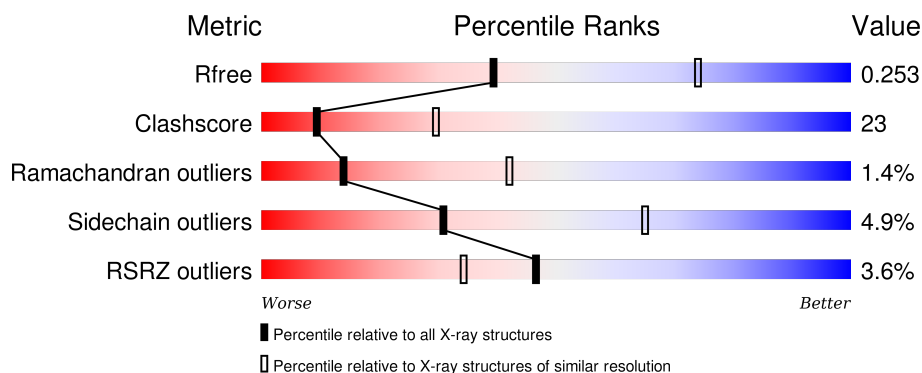
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	484	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>28%</div> <div>•</div> <div>24%</div> </div> </div>
1	B	484	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>28%</div> <div>•</div> <div>23%</div> </div> </div>
1	C	484	<div> <div>%</div> <div> <div></div> <div>50%</div> <div>25%</div> <div>•</div> <div>24%</div> </div> </div>
1	D	484	<div> <div>7%</div> <div> <div></div> <div>35%</div> <div>38%</div> <div>•</div> <div>24%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11659 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 Cell division protein FtsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2871	1811	458	595	7			
1	B	371	Total	C	N	O	S	0	0	0
			2880	1817	460	596	7			
1	C	370	Total	C	N	O	S	0	0	0
			2871	1811	458	595	7			
1	D	369	Total	C	N	O	S	0	0	0
			2861	1805	455	594	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	EXPRESSION TAG	UNP Q6GHQ0
A	-14	ASN	-	EXPRESSION TAG	UNP Q6GHQ0
A	-13	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-12	LYS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-11	VAL	-	EXPRESSION TAG	UNP Q6GHQ0
A	-10	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-9	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-8	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-7	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-6	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-5	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-4	ILE	-	EXPRESSION TAG	UNP Q6GHQ0
A	-3	GLU	-	EXPRESSION TAG	UNP Q6GHQ0
A	-2	GLY	-	EXPRESSION TAG	UNP Q6GHQ0
A	-1	ARG	-	EXPRESSION TAG	UNP Q6GHQ0
A	0	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-15	MET	-	EXPRESSION TAG	UNP Q6GHQ0
B	-14	ASN	-	EXPRESSION TAG	UNP Q6GHQ0
B	-13	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-12	LYS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-11	VAL	-	EXPRESSION TAG	UNP Q6GHQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-9	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-8	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-7	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-6	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-5	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-4	ILE	-	EXPRESSION TAG	UNP Q6GHQ0
B	-3	GLU	-	EXPRESSION TAG	UNP Q6GHQ0
B	-2	GLY	-	EXPRESSION TAG	UNP Q6GHQ0
B	-1	ARG	-	EXPRESSION TAG	UNP Q6GHQ0
B	0	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-15	MET	-	EXPRESSION TAG	UNP Q6GHQ0
C	-14	ASN	-	EXPRESSION TAG	UNP Q6GHQ0
C	-13	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-12	LYS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-11	VAL	-	EXPRESSION TAG	UNP Q6GHQ0
C	-10	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-9	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-8	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-7	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-6	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-5	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-4	ILE	-	EXPRESSION TAG	UNP Q6GHQ0
C	-3	GLU	-	EXPRESSION TAG	UNP Q6GHQ0
C	-2	GLY	-	EXPRESSION TAG	UNP Q6GHQ0
C	-1	ARG	-	EXPRESSION TAG	UNP Q6GHQ0
C	0	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-15	MET	-	EXPRESSION TAG	UNP Q6GHQ0
D	-14	ASN	-	EXPRESSION TAG	UNP Q6GHQ0
D	-13	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-12	LYS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-11	VAL	-	EXPRESSION TAG	UNP Q6GHQ0
D	-10	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-9	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-8	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-7	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-6	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-5	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-4	ILE	-	EXPRESSION TAG	UNP Q6GHQ0
D	-3	GLU	-	EXPRESSION TAG	UNP Q6GHQ0
D	-2	GLY	-	EXPRESSION TAG	UNP Q6GHQ0
D	-1	ARG	-	EXPRESSION TAG	UNP Q6GHQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	EXPRESSION TAG	UNP Q6GHQ0

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- The diagram illustrates the chemical structure of Adenosine Triphosphate (ATP). It consists of an adenine base (a purine ring system with an amino group at C6) linked to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose is connected to a chain of three phosphate groups (labeled alpha, beta, and gamma). The alpha phosphate is directly attached to the 5' carbon of the ribose. The beta and gamma phosphates are linked in series. The structure is color-coded: the adenine base is blue, the ribose sugar is green, and the phosphate groups are pink. Carbon atoms are labeled C1 through C5', and nitrogen atoms are labeled N1 through N7. Oxygen atoms are labeled O1 through O10. Hydrogen atoms are labeled H1 through H10. The phosphate groups are labeled alpha, beta, and gamma. The adenine base is labeled with its constituent atoms: N1, N3, N7, C2, C4, C6, and C8. The ribose sugar is labeled with its constituent atoms: C1', C2', C3', C4', and C5'. The phosphate groups are labeled with their constituent atoms: O1, O2, O3, O4, O5, O6, O7, O8, O9, and O10. The adenine base is connected to the ribose sugar at the N9 position. The ribose sugar is connected to the alpha phosphate at the C5' position. The alpha phosphate is connected to the beta phosphate at the O3 position. The beta phosphate is connected to the gamma phosphate at the O3 position. The gamma phosphate is connected to the O10 position. The adenine base is connected to the N1 position. The N1 position is connected to the C6 position. The C6 position is connected to the N7 position. The N7 position is connected to the C8 position. The C8 position is connected to the C4 position. The C4 position is connected to the N3 position. The N3 position is connected to the C2 position. The C2 position is connected to the N1 position. The ribose sugar is connected to the C1' position. The C1' position is connected to the C2' position. The C2' position is connected to the C3' position. The C3' position is connected to the C4' position. The C4' position is connected to the C5' position. The C5' position is connected to the C1' position. The alpha phosphate is connected to the O1 position. The O1 position is connected to the O2 position. The O2 position is connected to the O3 position. The O3 position is connected to the O4 position. The O4 position is connected to the O5 position. The O5 position is connected to the O6 position. The O6 position is connected to the O7 position. The O7 position is connected to the O8 position. The O8 position is connected to the O9 position. The O9 position is connected to the O10 position. The O10 position is connected to the O1 position. The adenine base is connected to the N1 position. The N1 position is connected to the C6 position. The C6 position is connected to the N7 position. The N7 position is connected to the C8 position. The C8 position is connected to the C4 position. The C4 position is connected to the N3 position. The N3 position is connected to the C2 position. The C2 position is connected to the N1 position. The ribose sugar is connected to the C1' position. The C1' position is connected to the C2' position. The C2' position is connected to the C3' position. The C3' position is connected to the C4' position. The C4' position is connected to the C5' position. The C5' position is connected to the C1' position. The alpha phosphate is connected to the O1 position. The O1 position is connected to the O2 position. The O2 position is connected to the O3 position. The O3 position is connected to the O4 position. The O4 position is connected to the O5 position. The O5 position is connected to the O6 position. The O6 position is connected to the O7 position. The O7 position is connected to the O8 position. The O8 position is connected to the O9 position. The O9 position is connected to the O10 position. The O10 position is connected to the O1 position.

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total 1 Mg 1	0	0
3	A	1	Total 1 Mg 1	0	0
3	D	1	Total 1 Mg 1	0	0
3	C	1	Total 1 Mg 1	0	0

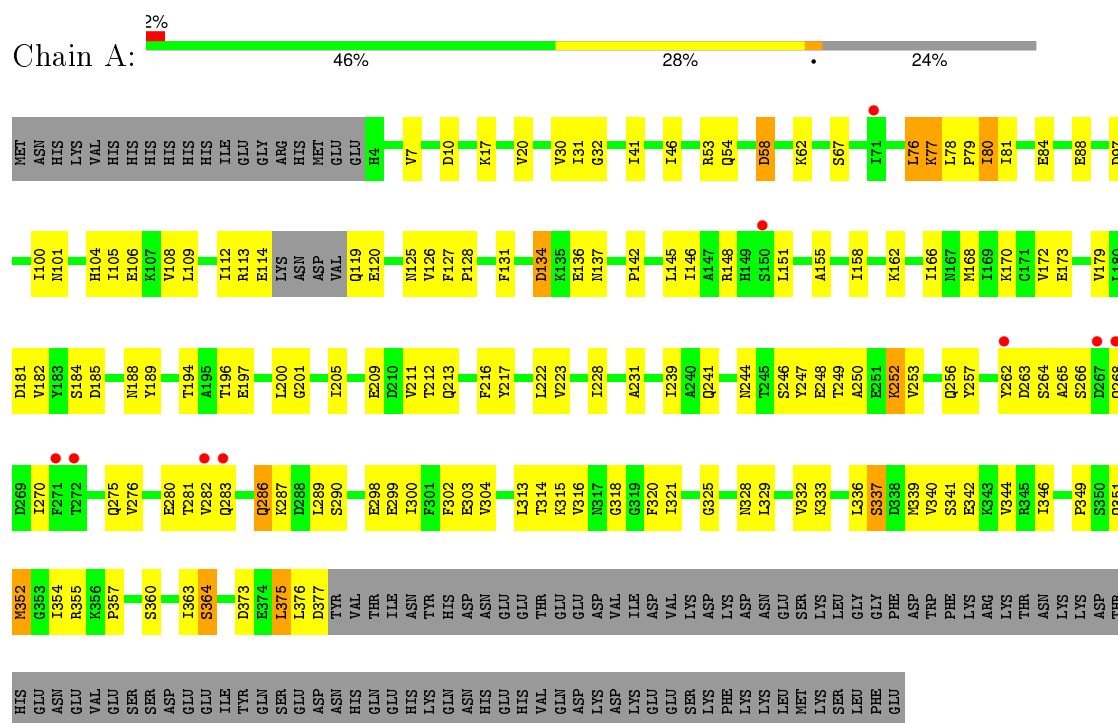
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	10	Total 10	O 10	0	0
4	C	16	Total 16	O 16	0	0
4	D	9	Total 9	O 9	0	0

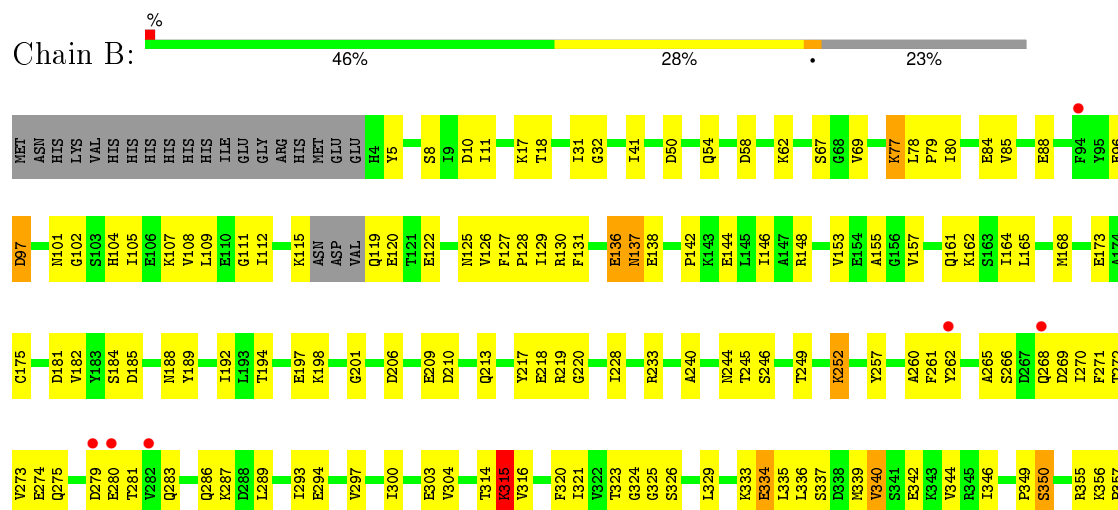
### 3 Residue-property plots [i](#)

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.

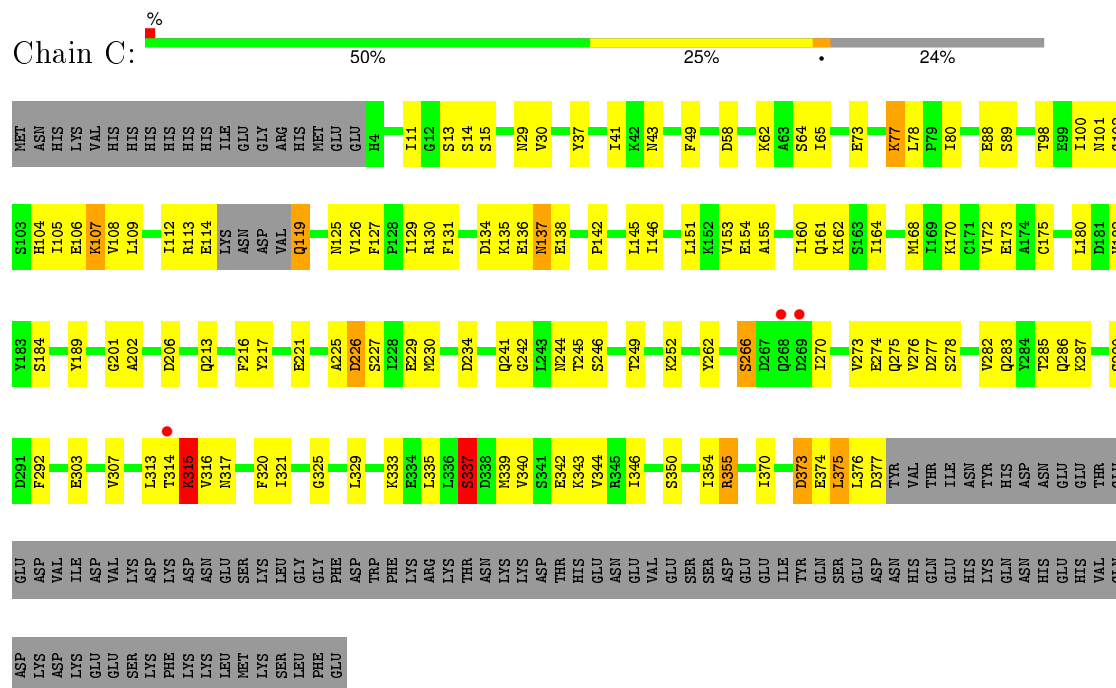
#### • Molecule 1: Cell division protein FtsA



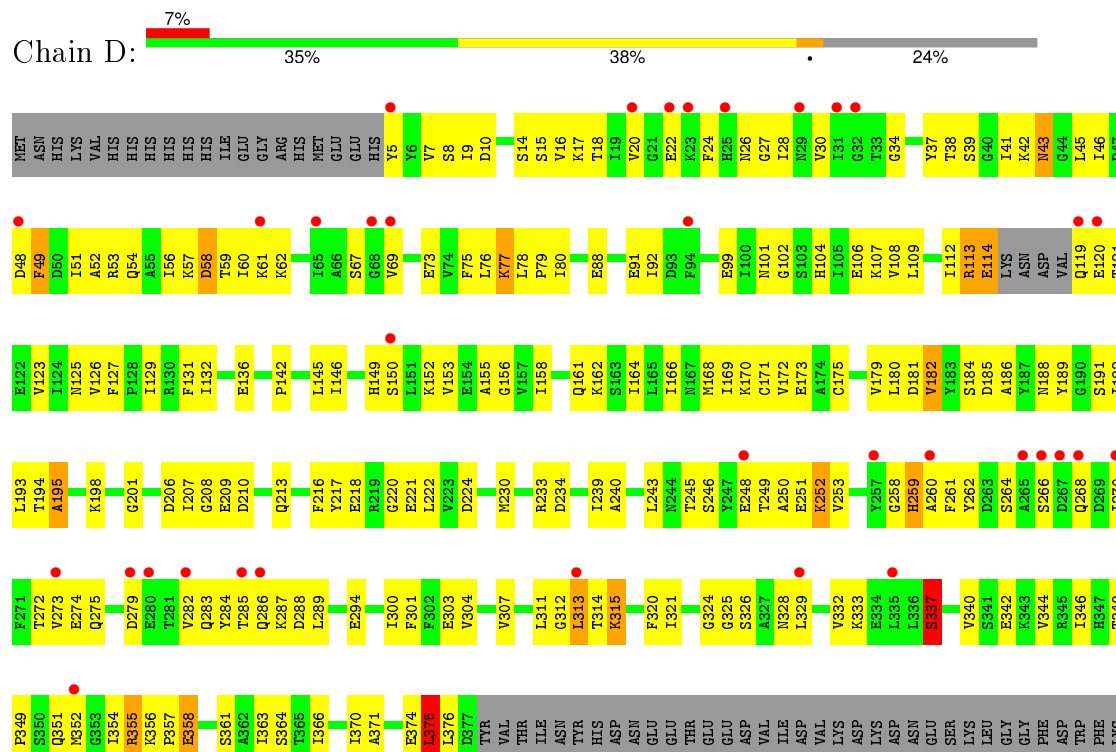
#### • Molecule 1: Cell division protein FtsA



- Molecule 1: Cell division protein FtsA



- Molecule 1: Cell division protein FtsA





ARG	LYS	THR	ASN	LYS	ASP	THR	HIS	GLU	ASN	GLU	VAL	GLU	SER	SER	ASP	GLU	GLU	ILE	TYR	GLN	SER	GLU	ASP	ASN	HIS	GLN	GLU	HIS	LYS	GLN	ASN	HIS	GLU	HIS	VAL	GLN	ASP	LYS	LYS	LYS	GLU	GLU	SER	LYS	PHE	LYS	LYS	LEU	MET	LYS	SER	LEU	PHE	GLU
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.53Å 122.02Å 107.00Å 90.00° 95.66° 90.00°	Depositor
Resolution (Å)	39.65 – 2.80 41.06 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.1 (39.65-2.80) 88.1 (41.06-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.207 , 0.254 0.207 , 0.253	Depositor DCC
$R_{free}$ test set	2289 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.4	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 47816 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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	0.46	2/2910 (0.1%)	0.65	1/3935 (0.0%)
1	B	0.51	4/2919 (0.1%)	0.65	0/3946
1	C	0.52	2/2910 (0.1%)	0.67	2/3935 (0.1%)
1	D	0.42	2/2899 (0.1%)	0.61	0/3920
All	All	0.48	10/11638 (0.1%)	0.65	3/15736 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	LYS	CA-CB	-9.31	1.33	1.53
1	A	252	LYS	C-O	-7.63	1.08	1.23
1	B	252	LYS	C-O	-7.06	1.09	1.23
1	B	337	SER	CA-CB	-6.76	1.42	1.52
1	C	252	LYS	C-O	-6.66	1.10	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	337	SER	N-CA-CB	-8.18	98.24	110.50
1	A	252	LYS	CD-CE-NZ	5.98	125.44	111.70
1	C	337	SER	CB-CA-C	5.74	121.00	110.10

There are no chirality outliers.

There are no planarity outliers.

### 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	2871	0	2813	131	0
1	B	2880	0	2826	115	0
1	C	2871	0	2813	111	0
1	D	2861	0	2806	168	0
2	A	31	0	12	2	0
2	B	31	0	12	2	0
2	C	31	0	12	5	0
2	D	31	0	12	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	13	0	0	0	0
4	B	10	0	0	0	0
4	C	16	0	0	6	0
4	D	9	0	0	3	0
All	All	11659	0	11306	521	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 521 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:GLU:HB3	4:D:604:HOH:O	1.52	1.06
1:B:244:ASN:HD22	1:B:275:GLN:NE2	1.59	1.00
1:D:333:LYS:O	1:D:337:SER:OG	1.84	0.96
1:A:101:ASN:H	1:A:104:HIS:HD2	1.15	0.92
1:C:282:VAL:HG12	1:C:283:GLN:H	1.32	0.91

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/484 (76%)	333 (91%)	29 (8%)	4 (1%)	17	50
1	B	367/484 (76%)	343 (94%)	21 (6%)	3 (1%)	24	58
1	C	366/484 (76%)	338 (92%)	24 (7%)	4 (1%)	17	50
1	D	365/484 (75%)	310 (85%)	45 (12%)	10 (3%)	6	21
All	All	1464/1936 (76%)	1324 (90%)	119 (8%)	21 (1%)	14	42

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASP
1	B	144	GLU
1	B	315	LYS
1	C	135	LYS
1	D	113	ARG

### 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	321/432 (74%)	305 (95%)	16 (5%)	30	64
1	B	322/432 (74%)	305 (95%)	17 (5%)	28	61
1	C	321/432 (74%)	306 (95%)	15 (5%)	32	67
1	D	320/432 (74%)	305 (95%)	15 (5%)	32	67
All	All	1284/1728 (74%)	1221 (95%)	63 (5%)	31	65

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	315	LYS
1	C	107	LYS
1	D	337	SER

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Mol	Chain	Res	Type
1	B	334	GLU
1	B	350	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	317	ASN
1	C	125	ASN
1	D	283	GLN
1	C	26	ASN
1	C	90	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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ATP	A	501	3	24,33,33	1.46	4 (16%)	31,52,52	2.62	6 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ATP	B	501	3	24,33,33	1.47	4 (16%)	31,52,52	2.59	6 (19%)
2	ATP	C	501	3	24,33,33	1.24	4 (16%)	31,52,52	2.75	6 (19%)
2	ATP	D	501	3	24,33,33	1.19	1 (4%)	31,52,52	2.67	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	501	3	-	0/18/38/38	0/3/3/3
2	ATP	B	501	3	-	0/18/38/38	0/3/3/3
2	ATP	C	501	3	-	0/18/38/38	0/3/3/3
2	ATP	D	501	3	-	0/18/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ATP	C8-N7	-2.36	1.30	1.34
2	C	501	ATP	C8-N7	-2.33	1.30	1.34
2	A	501	ATP	C8-N7	-2.23	1.30	1.34
2	A	501	ATP	PB-O1B	-2.13	1.43	1.51
2	C	501	ATP	PB-O2B	-2.10	1.46	1.54

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ATP	N3-C2-N1	-10.90	120.55	128.89
2	A	501	ATP	N3-C2-N1	-10.20	121.09	128.89
2	B	501	ATP	N3-C2-N1	-10.13	121.14	128.89
2	D	501	ATP	N3-C2-N1	-9.47	121.65	128.89
2	D	501	ATP	PA-O3A-PB	-7.92	110.49	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ATP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	ATP	2	0
2	C	501	ATP	5	0
2	D	501	ATP	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	370/484 (76%)	0.22	9 (2%) 62 50	35, 62, 81, 93	0
1	B	371/484 (76%)	0.10	6 (1%) 74 66	25, 53, 75, 94	0
1	C	370/484 (76%)	-0.07	3 (0%) 87 81	30, 46, 70, 85	0
1	D	369/484 (76%)	0.61	35 (9%) 10 5	55, 82, 112, 123	0
All	All	1480/1936 (76%)	0.21	53 (3%) 46 34	25, 60, 100, 123	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	5	TYR	6.7
1	D	25	HIS	6.5
1	D	268	GLN	4.5
1	D	285	THR	3.9
1	D	257	TYR	3.8

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ATP	A	501	31/31	0.99	0.19	-0.03	32,48,55,57	0
3	MG	A	502	1/1	0.88	0.19	-0.07	42,42,42,42	0
2	ATP	B	501	31/31	0.99	0.17	-0.30	30,38,40,41	0
2	ATP	C	501	31/31	0.99	0.17	-0.31	23,31,37,39	0
2	ATP	D	501	31/31	0.97	0.17	-0.69	61,69,78,79	0
3	MG	D	502	1/1	0.85	0.13	-2.41	61,61,61,61	0
3	MG	C	502	1/1	0.98	0.18	-	39,39,39,39	0
3	MG	B	502	1/1	0.97	0.16	-	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.