



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2IUS / pdb\_00002ius  
Title : E. coli FtsK motor domain  
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Deposited on : 2006-06-07  
Resolution : 2.70 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

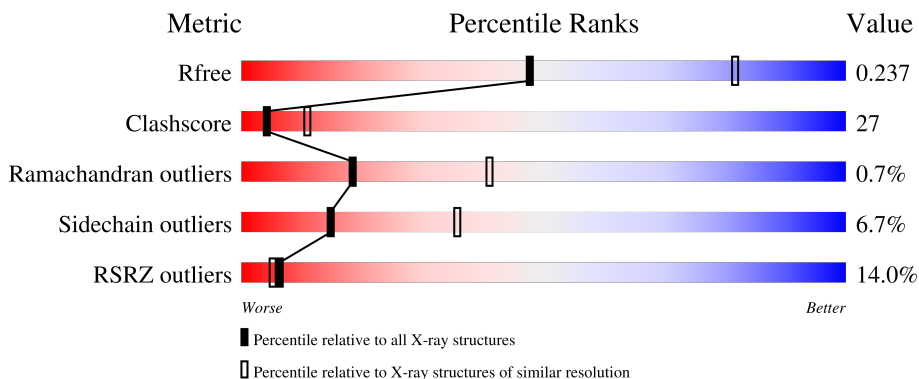
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.



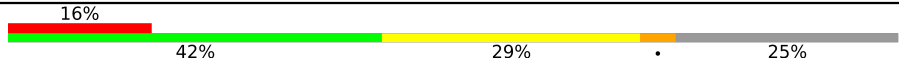
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\geq 3$ , 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	512	 7% 40% 32% 23%
1	B	512	 5% 44% 29% 23%
1	C	512	 15% 41% 33% 23%
1	D	512	 6% 42% 32% 23%
1	E	512	 15% 40% 28% 5% 26%

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Mol	Chain	Length	Quality of chain
1	F	512	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (16%), a green segment (42%), a yellow segment (29%), and a grey segment (14%). The percentages are labeled below the bar. A small black dot is visible on the yellow segment.</p>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18569 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 DNA TRANSLOCASE FTSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	393	3029	1930	532	551	16	0	0	1
1	B	393	3029	1930	532	551	16	0	0	1
1	C	393	3029	1930	532	551	16	0	0	1
1	D	394	3036	1935	533	552	16	0	0	1
1	E	381	2941	1877	512	536	16	0	0	1
1	F	382	2952	1883	516	537	16	0	0	1

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	997	ALA	LYS	engineered mutation	UNP P46889
B	997	ALA	LYS	engineered mutation	UNP P46889
C	997	ALA	LYS	engineered mutation	UNP P46889
D	997	ALA	LYS	engineered mutation	UNP P46889
E	997	ALA	LYS	engineered mutation	UNP P46889
F	997	ALA	LYS	engineered mutation	UNP P46889

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total 91	O 91	0	0
2	B	94	Total 94	O 94	0	0
2	C	80	Total 80	O 80	0	0

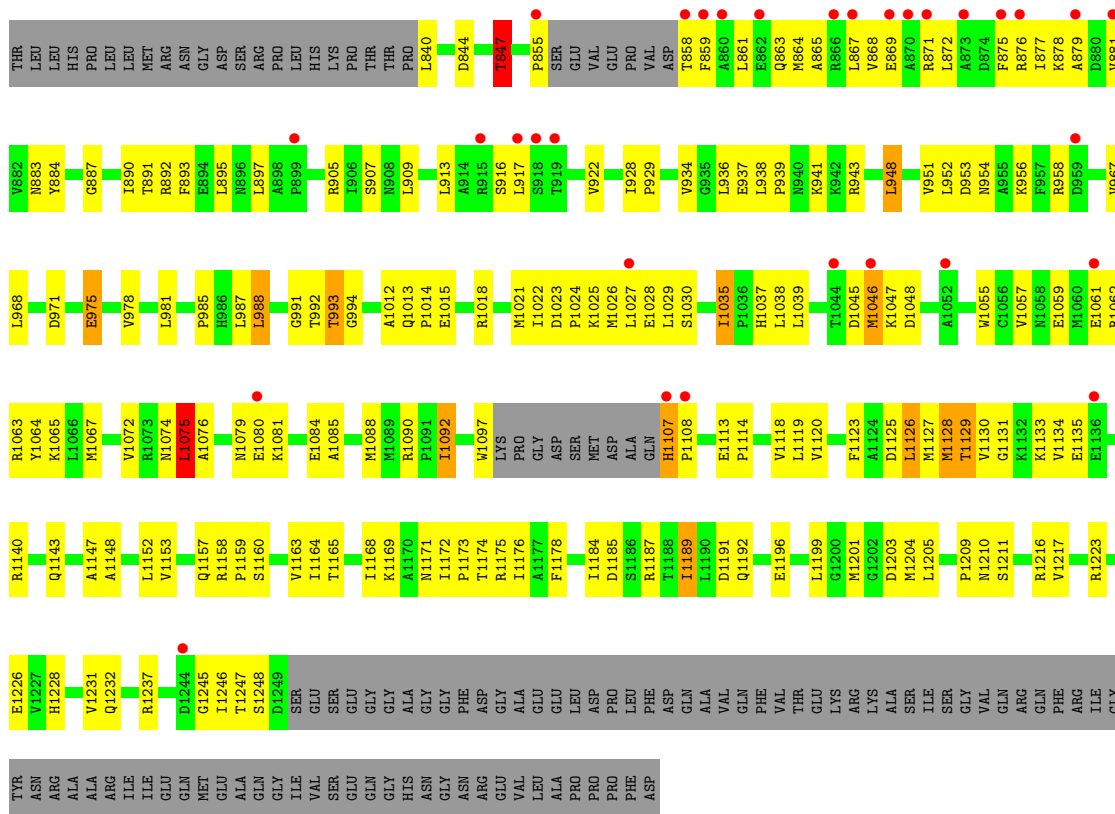
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	D	116	Total 116	O 116	0	0
2	E	99	Total 99	O 99	0	0
2	F	73	Total 73	O 73	0	0









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.60Å 117.20Å 132.80Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	100.00 – 2.70 100.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (100.00-2.70) 99.8 (100.00-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.246 , 0.298 0.243 , 0.237	Depositor DCC
$R_{free}$ test set	4056 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtrriage
Anisotropy	0.266	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 65.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	18569	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8823e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 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	0.47	1/3083 (0.0%)	1.01	10/4186 (0.2%)
1	B	0.53	2/3083 (0.1%)	1.02	17/4186 (0.4%)
1	C	0.45	1/3083 (0.0%)	1.01	12/4186 (0.3%)
1	D	0.49	1/3090 (0.0%)	1.00	12/4194 (0.3%)
1	E	0.51	1/2994 (0.0%)	1.05	17/4066 (0.4%)
1	F	0.45	1/3005 (0.0%)	0.97	6/4080 (0.1%)
All	All	0.48	7/18338 (0.0%)	1.01	74/24898 (0.3%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	918	SER	CA-C	7.14	1.59	1.53
1	D	1248	SER	C-N	-6.04	1.24	1.33
1	B	1248	SER	C-N	-5.76	1.25	1.33
1	E	1248	SER	C-N	-5.49	1.25	1.33
1	F	1248	SER	C-N	-5.37	1.25	1.33

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1107	HIS	CA-C-N	9.42	131.62	119.84
1	E	1107	HIS	C-N-CA	9.42	131.62	119.84
1	B	918	SER	N-CA-C	9.29	122.30	109.11
1	A	1075	LEU	N-CA-C	-9.05	100.83	112.23
1	D	993	THR	N-CA-C	8.26	121.03	111.11

There are no chirality outliers.

There are no planarity outliers.

## 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	3029	0	3146	180	0
1	B	3029	0	3146	165	3
1	C	3029	0	3146	171	0
1	D	3036	0	3153	173	0
1	E	2941	0	3046	173	3
1	F	2952	0	3059	152	0
2	A	91	0	0	19	0
2	B	94	0	0	27	0
2	C	80	0	0	20	0
2	D	116	0	0	26	0
2	E	99	0	0	23	0
2	F	73	0	0	26	0
All	All	18569	0	18696	1003	3

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 27.

The worst 5 of 1003 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:E:1046:MET:HG2	1:E:1129:THR:HG21	1.20	1.10
1:E:1046:MET:HE2	1:E:1126:LEU:HG	1.34	1.08
1:D:1159:PRO:HB3	1:D:1189:ILE:HD11	1.38	1.06
1:E:1159:PRO:HB3	1:E:1189:ILE:HD11	1.34	1.05
1:B:1159:PRO:HB3	1:B:1189:ILE:HD11	1.33	1.05

All (3) 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:B:919:THR:N	1:E:919:THR:N[1_465]	1.90	0.30
1:B:919:THR:O	1:E:919:THR:O[1_465]	2.09	0.11
1:B:917:LEU:O	1:E:919:THR:CG2[1_465]	2.18	0.02

## 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	387/512 (76%)	355 (92%)	29 (8%)	3 (1%)	16	37
1	B	387/512 (76%)	360 (93%)	23 (6%)	4 (1%)	12	32
1	C	387/512 (76%)	354 (92%)	33 (8%)	0	100	100
1	D	387/512 (76%)	355 (92%)	30 (8%)	2 (0%)	24	48
1	E	373/512 (73%)	347 (93%)	22 (6%)	4 (1%)	11	29
1	F	374/512 (73%)	347 (93%)	24 (6%)	3 (1%)	16	37
All	All	2295/3072 (75%)	2118 (92%)	161 (7%)	16 (1%)	18	41

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1131	GLY
1	D	1129	THR
1	E	1026	MET
1	E	1027	LEU
1	E	1108	PRO

### 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	330/429 (77%)	308 (93%)	22 (7%)	15	36
1	B	330/429 (77%)	309 (94%)	21 (6%)	16	38
1	C	330/429 (77%)	310 (94%)	20 (6%)	17	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	331/429 (77%)	311 (94%)	20 (6%)	17	41
1	E	321/429 (75%)	296 (92%)	25 (8%)	11	29
1	F	322/429 (75%)	298 (92%)	24 (8%)	12	31
All	All	1964/2574 (76%)	1832 (93%)	132 (7%)	15	36

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1026	MET
1	F	1054	ARG
1	F	1244	ASP
1	C	981	LEU
1	C	975	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	863	GLN
1	F	883	ASN
1	E	940	ASN
1	E	1157	GLN
1	F	1051	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 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
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	849:PRO	C	855:PRO	N	13.90

## 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	393/512 (76%)	0.67	37 (9%) 14 12	18, 43, 85, 100	0
1	B	393/512 (76%)	0.40	24 (6%) 27 24	14, 37, 77, 94	0
1	C	393/512 (76%)	1.06	75 (19%) 3 3	21, 49, 106, 120	0
1	D	394/512 (76%)	0.48	31 (7%) 18 16	16, 37, 76, 103	0
1	E	381/512 (74%)	0.98	78 (20%) 2 2	20, 45, 106, 128	0
1	F	382/512 (74%)	1.07	82 (21%) 2 2	19, 51, 118, 138	0
All	All	2336/3072 (76%)	0.77	327 (13%) 6 5	14, 43, 96, 138	0

The worst 5 of 327 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	921	ALA	8.6
1	E	918	SER	8.2
1	C	904	ALA	7.7
1	C	1108	PRO	7.4
1	E	915	ARG	6.0

### 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 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.