



Full wwPDB NMR Structure Validation Report ⓘ

Mar 15, 2026 – 11:06 AM UTC

PDB ID : 2J5O / pdb_00002j5o
Title : Pseudomonas aeruginosa FtsK gamma domain
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Deposited on : 2006-09-19

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

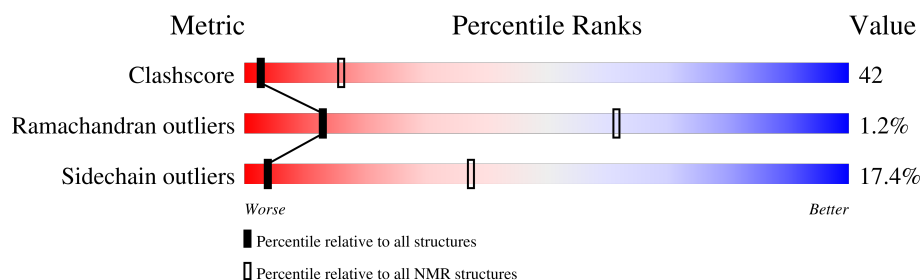
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	72	39% 47% • 10%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:743-A:807 (65)	0.26	15

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 18, 20
2	17, 19

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1096 atoms, of which 547 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA TRANSLOCASE FTSK.

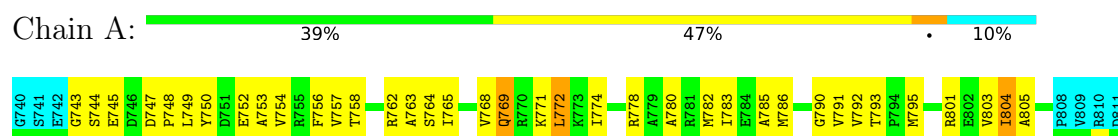
Mol	Chain	Residues	Atoms						Trace
1	A	72	Total	C	H	N	O	S	0
			1096	333	547	102	110	4	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: DNA TRANSLOCASE FTSK

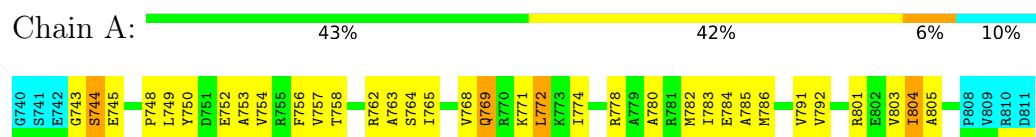


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

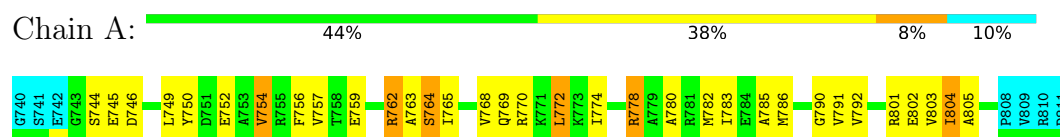
4.2.1 Score per residue for model 1

- Molecule 1: DNA TRANSLOCASE FTSK



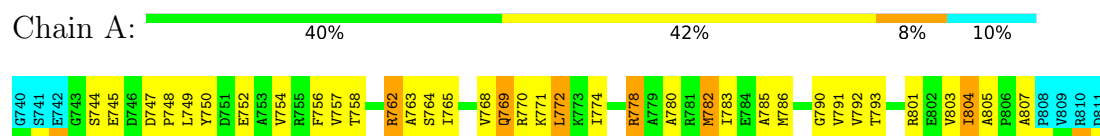
4.2.2 Score per residue for model 2

- Molecule 1: DNA TRANSLOCASE FTSK



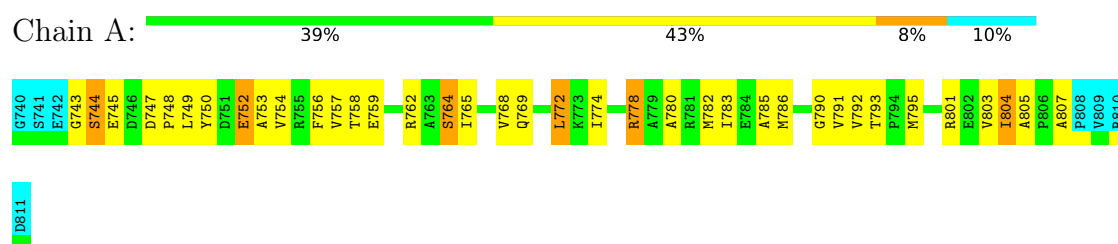
4.2.3 Score per residue for model 3

- Molecule 1: DNA TRANSLOCASE FTSK



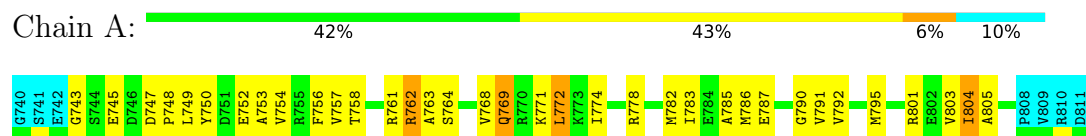
4.2.4 Score per residue for model 4

- Molecule 1: DNA TRANSLOCASE FTSK



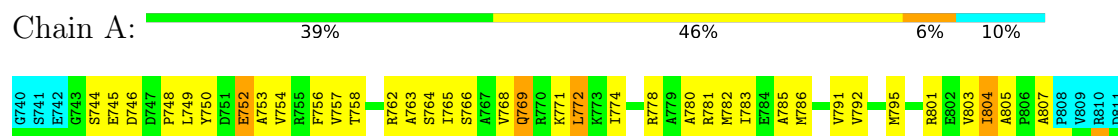
4.2.5 Score per residue for model 5

- Molecule 1: DNA TRANSLOCASE FTSK



4.2.6 Score per residue for model 6

- Molecule 1: DNA TRANSLOCASE FTSK



4.2.7 Score per residue for model 7

- Molecule 1: DNA TRANSLOCASE FTSK





4.2.8 Score per residue for model 8

- Molecule 1: DNA TRANSLOCASE FTSK



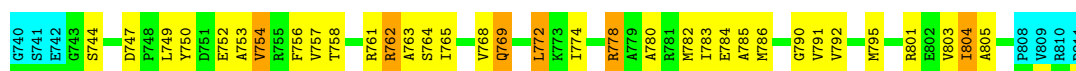
4.2.9 Score per residue for model 9

- Molecule 1: DNA TRANSLOCASE FTSK



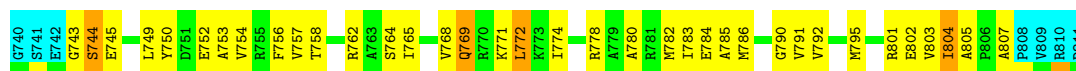
4.2.10 Score per residue for model 10

- Molecule 1: DNA TRANSLOCASE FTSK



4.2.11 Score per residue for model 11

- Molecule 1: DNA TRANSLOCASE FTSK



4.2.12 Score per residue for model 12

- Molecule 1: DNA TRANSLOCASE FTSK

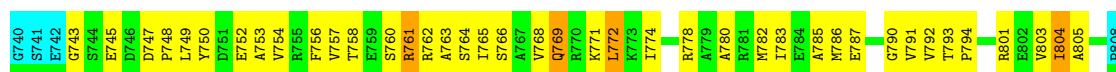




4.2.13 Score per residue for model 13

- Molecule 1: DNA TRANSLOCASE FTSK

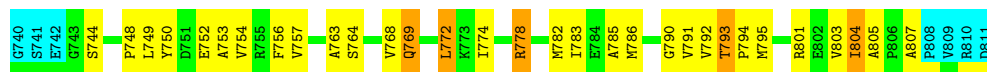
Chain A: 35% 50% 6% 10%



4.2.14 Score per residue for model 14

- Molecule 1: DNA TRANSLOCASE FTSK

Chain A: 47% 36% 7% 10%



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: DNA TRANSLOCASE FTSK

Chain A: 47% 36% 7% 10%



4.2.16 Score per residue for model 16

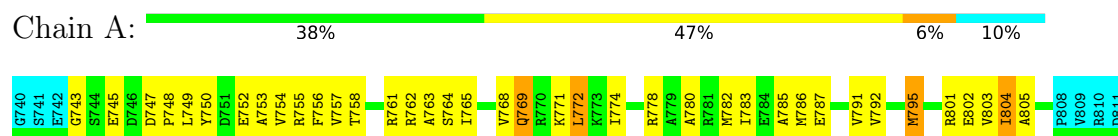
- Molecule 1: DNA TRANSLOCASE FTSK

Chain A: 36% 43% 11% 10%



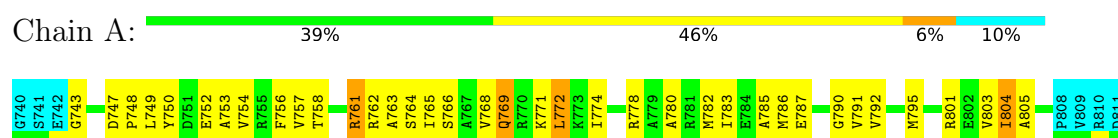
4.2.17 Score per residue for model 17

- Molecule 1: DNA TRANSLOCASE FTSK



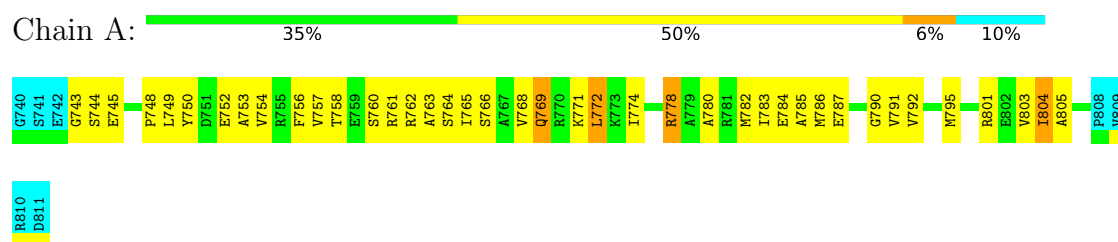
4.2.18 Score per residue for model 18

- Molecule 1: DNA TRANSLOCASE FTSK



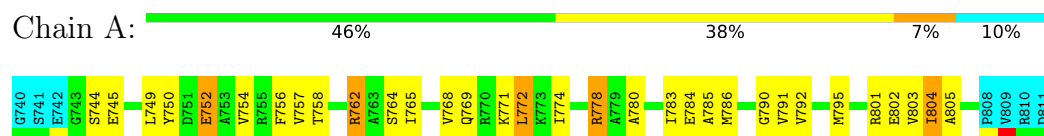
4.2.19 Score per residue for model 19

- Molecule 1: DNA TRANSLOCASE FTSK



4.2.20 Score per residue for model 20

- Molecule 1: DNA TRANSLOCASE FTSK



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CNS*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *NO VIOLATIONS*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	
ANSIG	structure solution	

No chemical shift data was provided.

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	52/58 (90%)	43±2 (83±3%)	9±2 (17±3%)	4	37
All	All	1040/1160 (90%)	859 (83%)	181 (17%)	4	37

All 24 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	772	LEU	20
1	A	804	ILE	20
1	A	745	GLU	15
1	A	769	GLN	15
1	A	771	LYS	15
1	A	795	MET	14
1	A	744	SER	10
1	A	778	ARG	9
1	A	784	GLU	7
1	A	762	ARG	7
1	A	787	GLU	7
1	A	752	GLU	6
1	A	761	ARG	6
1	A	802	GLU	5
1	A	782	MET	5
1	A	754	VAL	4
1	A	793	THR	4
1	A	764	SER	3
1	A	746	ASP	2
1	A	759	GLU	2
1	A	781	ARG	2
1	A	770	ARG	1
1	A	765	ILE	1
1	A	755	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided