



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2026 – 12:22 PM JST

PDB ID : 45LQ / pdb_000045lq
Title : Crystal structure of Escherichia coli YidC in complex with YibN
Authors : Takahashi, Y.S.; Miyazaki, R.; Kohga, H.; Tsukazaki, T.
Deposited on : 2026-09-02
Resolution : 4.09 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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

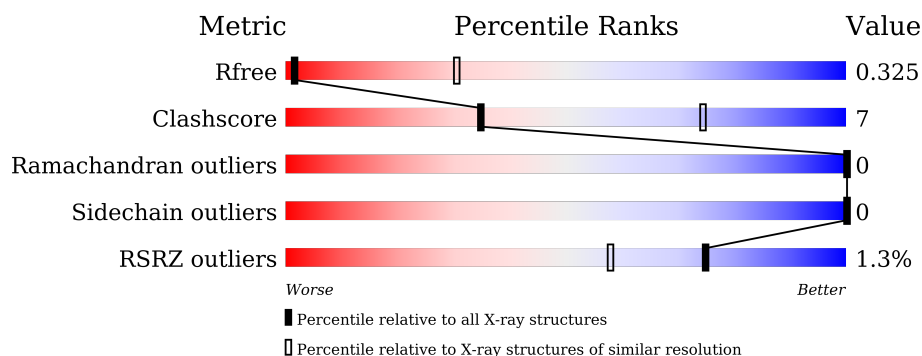
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.09 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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 of 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	548	67% 19% 15%
1	D	548	68% 18% 15%
2	B	27	100%
2	E	27	93% 7%
3	C	167	16% 81%
3	F	167	19% 81%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8392 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 Membrane protein insertase YidC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3719	2424	602	672	21			
1	D	468	Total	C	N	O	S	0	0	0
			3719	2424	602	672	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	THR	SER	conflict	UNP P25714
D	192	THR	SER	conflict	UNP P25714

- Molecule 2 is a protein called Membrane protein insertase YidC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	27	Total	C	N	O	S	0	0	0
			230	151	38	40	1			
2	E	27	Total	C	N	O	S	0	0	0
			230	151	38	40	1			

- Molecule 3 is a protein called YibN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	S	0	0	0
			247	167	40	38	2			
3	F	31	Total	C	N	O	S	0	0	0
			247	167	40	38	2			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	144	LEU	-	expression tag	UNP P0AG27
C	145	GLU	-	expression tag	UNP P0AG27

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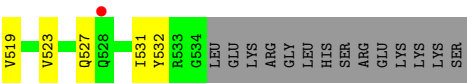
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Chain	Residue	Modelled	Actual	Comment	Reference
C	146	SER	-	expression tag	UNP P0AG27
C	147	SER	-	expression tag	UNP P0AG27
C	148	GLY	-	expression tag	UNP P0AG27
C	149	GLU	-	expression tag	UNP P0AG27
C	150	ASN	-	expression tag	UNP P0AG27
C	151	LEU	-	expression tag	UNP P0AG27
C	152	TYR	-	expression tag	UNP P0AG27
C	153	PHE	-	expression tag	UNP P0AG27
C	154	GLN	-	expression tag	UNP P0AG27
C	155	GLY	-	expression tag	UNP P0AG27
C	156	GLN	-	expression tag	UNP P0AG27
C	157	PHE	-	expression tag	UNP P0AG27
C	158	THR	-	expression tag	UNP P0AG27
C	159	SER	-	expression tag	UNP P0AG27
C	160	HIS	-	expression tag	UNP P0AG27
C	161	HIS	-	expression tag	UNP P0AG27
C	162	HIS	-	expression tag	UNP P0AG27
C	163	HIS	-	expression tag	UNP P0AG27
C	164	HIS	-	expression tag	UNP P0AG27
C	165	HIS	-	expression tag	UNP P0AG27
C	166	HIS	-	expression tag	UNP P0AG27
C	167	HIS	-	expression tag	UNP P0AG27
F	144	LEU	-	expression tag	UNP P0AG27
F	145	GLU	-	expression tag	UNP P0AG27
F	146	SER	-	expression tag	UNP P0AG27
F	147	SER	-	expression tag	UNP P0AG27
F	148	GLY	-	expression tag	UNP P0AG27
F	149	GLU	-	expression tag	UNP P0AG27
F	150	ASN	-	expression tag	UNP P0AG27
F	151	LEU	-	expression tag	UNP P0AG27
F	152	TYR	-	expression tag	UNP P0AG27
F	153	PHE	-	expression tag	UNP P0AG27
F	154	GLN	-	expression tag	UNP P0AG27
F	155	GLY	-	expression tag	UNP P0AG27
F	156	GLN	-	expression tag	UNP P0AG27
F	157	PHE	-	expression tag	UNP P0AG27
F	158	THR	-	expression tag	UNP P0AG27
F	159	SER	-	expression tag	UNP P0AG27
F	160	HIS	-	expression tag	UNP P0AG27
F	161	HIS	-	expression tag	UNP P0AG27
F	162	HIS	-	expression tag	UNP P0AG27
F	163	HIS	-	expression tag	UNP P0AG27

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Chain	Residue	Modelled	Actual	Comment	Reference
F	164	HIS	-	expression tag	UNP P0AG27
F	165	HIS	-	expression tag	UNP P0AG27
F	166	HIS	-	expression tag	UNP P0AG27
F	167	HIS	-	expression tag	UNP P0AG27



• Molecule 2: Membrane protein insertase YidC

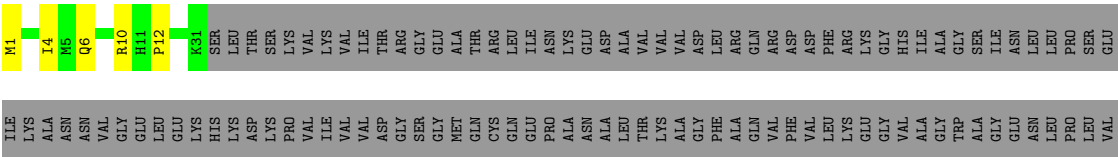


There are no outlier residues recorded for this chain.

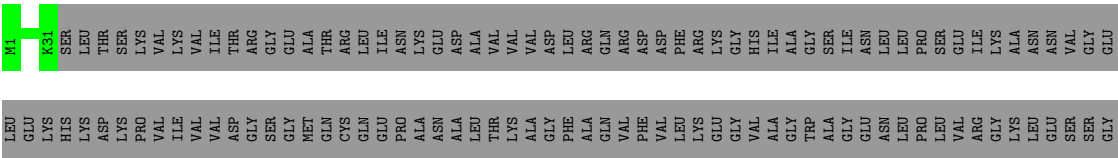
• Molecule 2: Membrane protein insertase YidC



• Molecule 3: YibN



• Molecule 3: YibN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.60Å 182.85Å 100.55Å 90.00° 91.42° 90.00°	Depositor
Resolution (Å)	44.04 – 4.09 44.04 – 4.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.04-4.09) 99.2 (44.04-4.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 4.13Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.266 , 0.325 0.266 , 0.325	Depositor DCC
R_{free} test set	1202 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 18.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	8392	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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	0.13	0/3819	0.32	0/5198
1	D	0.12	0/3819	0.29	0/5198
2	B	0.07	0/235	0.16	0/318
2	E	0.08	0/235	0.18	0/318
3	C	0.08	0/252	0.17	0/342
3	F	0.07	0/252	0.17	0/342
All	All	0.12	0/8612	0.29	0/11716

There are no bond length outliers.

There are no bond angle outliers.

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	3719	0	3722	65	0
1	D	3719	0	3722	59	0
2	B	230	0	226	0	0
2	E	230	0	226	1	0
3	C	247	0	271	3	0
3	F	247	0	271	0	0
All	All	8392	0	8438	126	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 7.

The worst 5 of 126 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:420:LEU:HB3	1:D:424:PHE:HB2	1.62	0.80
1:D:131:TYR:HB3	1:D:151:MET:HB3	1.72	0.71
1:A:372:LEU:HD21	1:A:424:PHE:HE2	1.56	0.71
1:D:377:TYR:CE1	1:D:531:ILE:HD12	2.25	0.70
1:D:120:PRO:HB2	1:D:129:PRO:HG3	1.75	0.69

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	464/548 (85%)	441 (95%)	23 (5%)	0	100	100
1	D	464/548 (85%)	442 (95%)	22 (5%)	0	100	100
2	B	25/27 (93%)	25 (100%)	0	0	100	100
2	E	25/27 (93%)	25 (100%)	0	0	100	100
3	C	29/167 (17%)	29 (100%)	0	0	100	100
3	F	29/167 (17%)	29 (100%)	0	0	100	100
All	All	1036/1484 (70%)	991 (96%)	45 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	402/469 (86%)	402 (100%)	0	100	100
1	D	402/469 (86%)	402 (100%)	0	100	100
2	B	25/25 (100%)	25 (100%)	0	100	100
2	E	25/25 (100%)	25 (100%)	0	100	100
3	C	27/140 (19%)	27 (100%)	0	100	100
3	F	27/140 (19%)	27 (100%)	0	100	100
All	All	908/1268 (72%)	908 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	376	GLN
1	D	387	GLN
3	C	11	HIS
1	D	456	HIS
1	A	338	GLN

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](#)

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, 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	468/548 (85%)	0.31	4 (0%) 81 65	63, 77, 127, 135	0
1	D	468/548 (85%)	0.40	10 (2%) 63 48	66, 82, 134, 144	0
2	B	27/27 (100%)	0.12	0 100 100	88, 92, 102, 103	0
2	E	27/27 (100%)	0.19	0 100 100	100, 103, 110, 110	0
3	C	31/167 (18%)	0.18	0 100 100	89, 91, 99, 100	0
3	F	31/167 (18%)	0.25	0 100 100	95, 101, 108, 110	0
All	All	1052/1484 (70%)	0.33	14 (1%) 75 58	63, 82, 130, 144	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	386	LEU	3.7
1	D	481	MET	3.4
1	D	528	GLN	3.4
1	A	532	TYR	2.8
1	D	111	GLN	2.6

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.