



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:01 am BST

PDB ID : 3WO7
Title : Crystal structure of YidC from Bacillus halodurans (form II)
Authors : Kumazaki, K.; Tsukazaki, T.; Ishitani, R.; Nureki, O.
Deposited on : 2013-12-20
Resolution : 3.20 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	:	2.11
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)	:	2.11

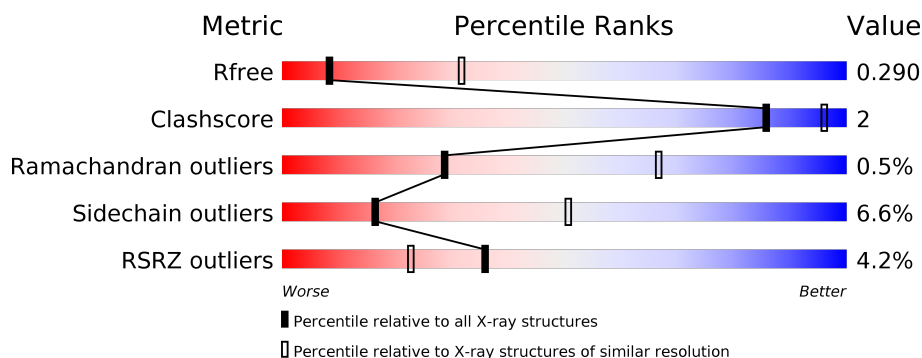
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	254	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>12%</div> </div> </div>
1	B	254	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>11%</div> </div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3590 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1797	1198	279	304	16			
1	B	225	Total	C	N	O	S	0	0	0
			1789	1191	278	303	17			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP Q9KDP2
A	26	GLN	-	expression tag	UNP Q9KDP2
A	107	ALA	GLY	engineered mutation	UNP Q9KDP2
A	268	LEU	-	expression tag	UNP Q9KDP2
A	269	GLU	-	expression tag	UNP Q9KDP2
A	270	SER	-	expression tag	UNP Q9KDP2
A	271	SER	-	expression tag	UNP Q9KDP2
A	272	GLY	-	expression tag	UNP Q9KDP2
A	273	GLU	-	expression tag	UNP Q9KDP2
A	274	ASN	-	expression tag	UNP Q9KDP2
A	275	LEU	-	expression tag	UNP Q9KDP2
A	276	TYR	-	expression tag	UNP Q9KDP2
A	277	PHE	-	expression tag	UNP Q9KDP2
A	278	GLN	-	expression tag	UNP Q9KDP2
B	25	GLY	-	expression tag	UNP Q9KDP2
B	26	GLN	-	expression tag	UNP Q9KDP2
B	107	ALA	GLY	engineered mutation	UNP Q9KDP2
B	268	LEU	-	expression tag	UNP Q9KDP2
B	269	GLU	-	expression tag	UNP Q9KDP2
B	270	SER	-	expression tag	UNP Q9KDP2
B	271	SER	-	expression tag	UNP Q9KDP2
B	272	GLY	-	expression tag	UNP Q9KDP2
B	273	GLU	-	expression tag	UNP Q9KDP2
B	274	ASN	-	expression tag	UNP Q9KDP2
B	275	LEU	-	expression tag	UNP Q9KDP2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	276	TYR	-	expression tag	UNP Q9KDP2
B	277	PHE	-	expression tag	UNP Q9KDP2
B	278	GLN	-	expression tag	UNP Q9KDP2

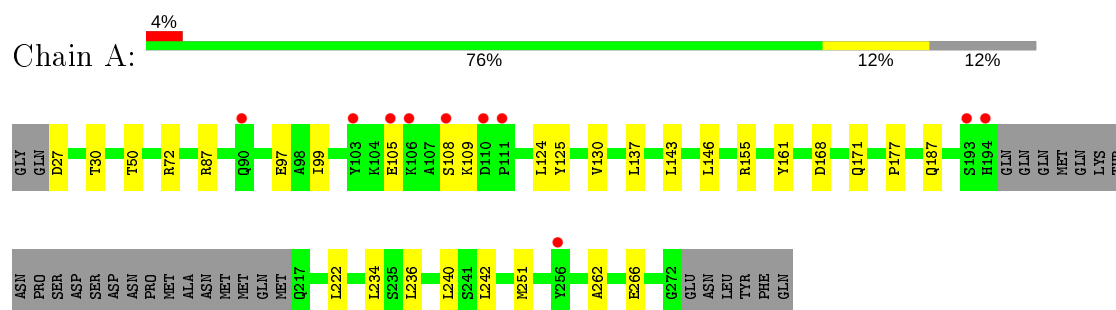
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cu	0	0
			2	2		
2	A	2	Total	Cu	0	0
			2	2		

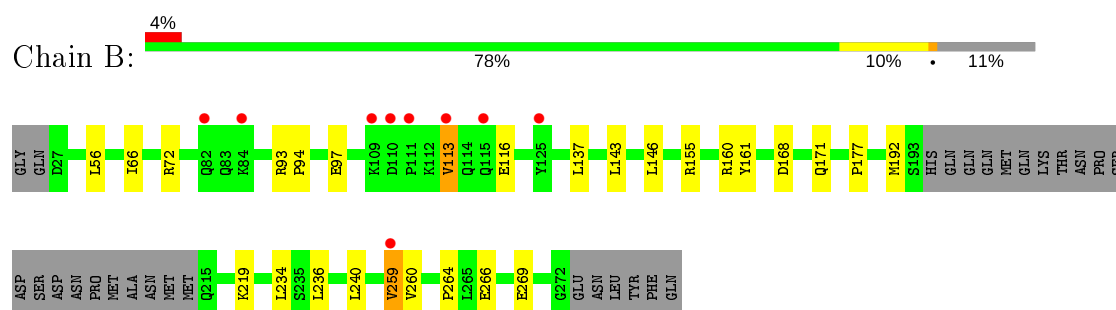
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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: Membrane protein insertase YidC 2



- Molecule 1: Membrane protein insertase YidC 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.03Å 70.06Å 82.91Å 90.00° 92.05° 90.00°	Depositor
Resolution (Å)	45.00 – 3.20 46.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (45.00-3.20) 89.1 (46.00-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, R_{free}	0.260 , 0.291 0.256 , 0.290	Depositor DCC
R_{free} test set	986 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3590	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.15 % 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 8.9692e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

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

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	0.22	0/1843	0.41	0/2499
1	B	0.22	0/1835	0.39	0/2493
All	All	0.22	0/3678	0.40	0/4992

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

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	1797	0	1870	8	0
1	B	1789	0	1839	8	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	3590	0	3709	16	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 2.

All (16) 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:A:27:ASP:N	1:A:30:THR:HG1	1.92	0.67
1:A:187:GLN:HE21	1:A:251:MET:HG2	1.72	0.54
1:B:168:ASP:HB2	1:B:171:GLN:HB2	1.94	0.49
1:B:266:GLU:HA	1:B:269:GLU:HG2	1.95	0.49
1:B:113:VAL:HA	1:B:116:GLU:HB2	1.93	0.48
1:B:177:PRO:HG2	1:B:234:LEU:HD23	1.96	0.48
1:A:177:PRO:HG2	1:A:234:LEU:HD23	1.97	0.47
1:A:168:ASP:HB3	1:A:171:GLN:HB2	1.98	0.46
1:A:108:SER:OG	1:A:109:LYS:N	2.48	0.46
1:A:236:LEU:HD13	1:A:240:LEU:HD22	1.98	0.45
1:B:93:ARG:N	1:B:94:PRO:HD2	2.32	0.44
1:B:264:PRO:HB2	1:B:266:GLU:HG2	2.01	0.43
1:B:56:LEU:HD11	1:B:66:ILE:HD12	2.00	0.42
1:A:87:ARG:HE	1:A:262:ALA:N	2.17	0.42
1:B:236:LEU:HD13	1:B:240:LEU:HD22	2.02	0.42
1:A:125:TYR:HB3	1:A:130:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	220/254 (87%)	212 (96%)	8 (4%)	0	100	100
1	B	221/254 (87%)	207 (94%)	12 (5%)	2 (1%)	17	56
All	All	441/508 (87%)	419 (95%)	20 (4%)	2 (0%)	29	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	VAL
1	B	260	VAL

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	198/229 (86%)	184 (93%)	14 (7%)	14	47
1	B	195/229 (85%)	183 (94%)	12 (6%)	18	53
All	All	393/458 (86%)	367 (93%)	26 (7%)	16	51

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	72	ARG
1	A	97	GLU
1	A	99	ILE
1	A	105	GLU
1	A	124	LEU
1	A	137	LEU
1	A	143	LEU
1	A	146	LEU
1	A	155	ARG
1	A	161	TYR
1	A	222	LEU
1	A	242	LEU
1	A	266	GLU
1	B	72	ARG
1	B	97	GLU
1	B	113	VAL
1	B	137	LEU
1	B	143	LEU
1	B	146	LEU
1	B	155	ARG
1	B	160	ARG
1	B	161	TYR
1	B	192	MET
1	B	219	LYS
1	B	259	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	B	90	GLN
1	B	100	GLN
1	B	114	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	224/254 (88%)	0.48	10 (4%) 33 21	66, 91, 133, 147	0
1	B	225/254 (88%)	0.47	9 (4%) 38 25	68, 95, 132, 166	0
All	All	449/508 (88%)	0.47	19 (4%) 36 23	66, 93, 133, 166	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	SER	6.0
1	A	194	HIS	5.6
1	B	259	VAL	4.1
1	B	113	VAL	4.1
1	A	110	ASP	4.0
1	B	111	PRO	3.9
1	A	105	GLU	3.1
1	A	193	SER	3.0
1	B	82	GLN	3.0
1	A	111	PRO	2.7
1	B	125	TYR	2.7
1	B	109	LYS	2.6
1	A	256	TYR	2.4
1	A	106	LYS	2.3
1	B	84	LYS	2.2
1	B	110	ASP	2.2
1	B	115	GLN	2.2
1	A	90	GLN	2.1
1	A	103	TYR	2.1

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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
2	CU	A	302	1/1	0.90	0.14	131,131,131,131	0
2	CU	B	301	1/1	0.91	0.10	103,103,103,103	1
2	CU	B	302	1/1	0.93	0.14	133,133,133,133	0
2	CU	A	301	1/1	0.97	0.14	115,115,115,115	1

6.5 Other polymers [i](#)

There are no such residues in this entry.