



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:27 PM UTC

PDB ID : 8YSR / pdb_00008ysr
Title : Crystal structure of the Deinococcus wulumuqiensis CD-NTase DwCdnB in complex with hexatungstotellurate(VI) TEW
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Deposited on : 2024-03-23
Resolution : 2.04 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 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

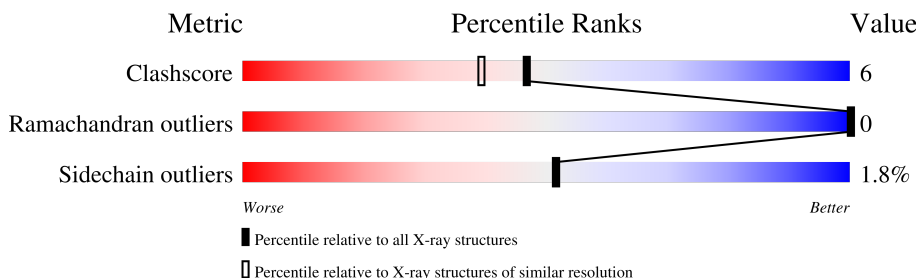
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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))
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	349	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TEW	A	401	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2950 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.

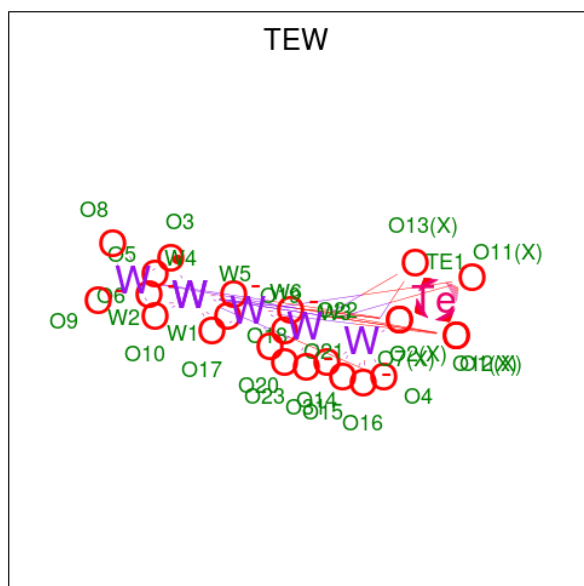
- Molecule 1 is a protein called Nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2654	1672	468	503	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A345ILN6

- Molecule 2 is 6-tungstotellurate(VI) (CCD ID: TEW) (formula: $O_{24}TeW_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	Te	W		
2	A	1	31	24	1	6	0	0

- Molecule 3 is water.

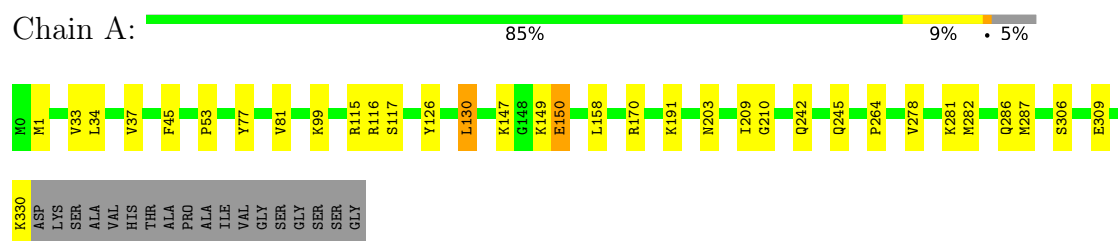
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	265	Total 265	O 265	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Nucleotidyltransferase



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	35.37Å 46.80Å 60.37Å 100.48° 104.89° 100.13°	Depositor
Resolution (Å)	25.58 – 2.04	Depositor
% Data completeness (in resolution range)	95.2 (25.58-2.04)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.08 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.181 , 0.215	Depositor
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.135	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2950	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.65% 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](#)

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

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	0.95	0/2715	0.96	0/3669

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	2654	0	2572	28	0
2	A	31	0	0	11	0
3	A	265	0	0	8	0
All	All	2950	0	2572	30	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 6.

All (30) 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:281:LYS:HG3	2:A:401:TEW:O23	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HE2	2:A:401:TEW:O31	1.63	0.97
1:A:149:LYS:NZ	2:A:401:TEW:O8	2.07	0.88
2:A:401:TEW:TE1	2:A:401:TEW:O7	1.53	0.83
1:A:281:LYS:CE	2:A:401:TEW:O31	2.36	0.71
1:A:245:GLN:OE1	3:A:501:HOH:O	2.13	0.66
1:A:210:GLY:HA2	1:A:278:VAL:HG21	1.78	0.64
1:A:116:ARG:HB3	2:A:401:TEW:O12	1.98	0.62
1:A:281:LYS:CG	2:A:401:TEW:O23	2.44	0.59
1:A:1:MET:HG3	1:A:306:SER:HA	1.87	0.55
1:A:115:ARG:NH2	3:A:506:HOH:O	2.38	0.55
1:A:116:ARG:NE	2:A:401:TEW:O13	2.40	0.54
1:A:242:GLN:HG3	3:A:684:HOH:O	2.08	0.53
1:A:117:SER:OG	1:A:147:LYS:NZ	2.39	0.53
1:A:81:VAL:CG1	1:A:130:LEU:HD23	2.39	0.52
1:A:191:LYS:NZ	3:A:511:HOH:O	2.42	0.51
1:A:309:GLU:HG2	1:A:330:LYS:HD3	1.94	0.50
2:A:401:TEW:O16	3:A:502:HOH:O	2.20	0.49
1:A:34:LEU:O	1:A:37:VAL:HG22	2.12	0.48
1:A:117:SER:HB2	2:A:401:TEW:O18	2.14	0.47
1:A:309:GLU:HG3	3:A:642:HOH:O	2.14	0.47
1:A:170:ARG:NE	3:A:509:HOH:O	2.40	0.46
1:A:33:VAL:O	1:A:37:VAL:HG13	2.16	0.45
1:A:77:TYR:HB2	1:A:126:TYR:HB3	2.01	0.43
1:A:264:PRO:O	1:A:287:MET:HB3	2.19	0.43
1:A:203:ASN:ND2	3:A:519:HOH:O	2.51	0.42
1:A:150:GLU:H	1:A:150:GLU:HG2	1.52	0.42
1:A:116:ARG:CB	2:A:401:TEW:O12	2.65	0.42
1:A:45:PHE:CD2	1:A:53:PRO:HD3	2.55	0.41
1:A:282:MET:HG2	1:A:286:GLN:HB2	2.03	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	329/349 (94%)	325 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	280/293 (96%)	275 (98%)	5 (2%)	51	51

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LYS
1	A	130	LEU
1	A	150	GLU
1	A	158	LEU
1	A	209	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	19	GLN
1	A	60	GLN
1	A	127	HIS
1	A	220	GLN
1	A	245	GLN

5.3.3 RNA ⓘ

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](#)

1 ligand is modelled in this entry.

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	TEW	A	401	1,3	24,42,42	1.54	6 (25%)	12,129,129	11.73	10 (83%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	TEW	W4-O17	-3.67	1.64	1.97
2	A	401	TEW	W2-O8	2.85	1.78	1.72
2	A	401	TEW	W1-O6	2.17	1.76	1.72
2	A	401	TEW	W5-O21	2.13	1.76	1.72
2	A	401	TEW	W4-O18	2.13	1.76	1.72
2	A	401	TEW	W5-O22	-2.05	1.70	2.09

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	TEW	O13-TE1-O12	-20.11	76.55	94.65
2	A	401	TEW	O13-TE1-O11	19.18	107.86	85.21
2	A	401	TEW	O13-TE1-O1	-15.22	80.96	94.65
2	A	401	TEW	O11-TE1-O2	15.00	108.16	94.65
2	A	401	TEW	O7-TE1-O1	-14.18	68.46	85.21
2	A	401	TEW	O7-TE1-O2	8.50	102.31	94.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	TEW	O1-TE1-O12	-8.39	87.10	94.65
2	A	401	TEW	O11-TE1-O7	6.84	100.81	94.65
2	A	401	TEW	O12-TE1-O7	4.27	90.26	85.21
2	A	401	TEW	O1-TE1-O2	-3.21	81.42	85.21

There are no chirality outliers.

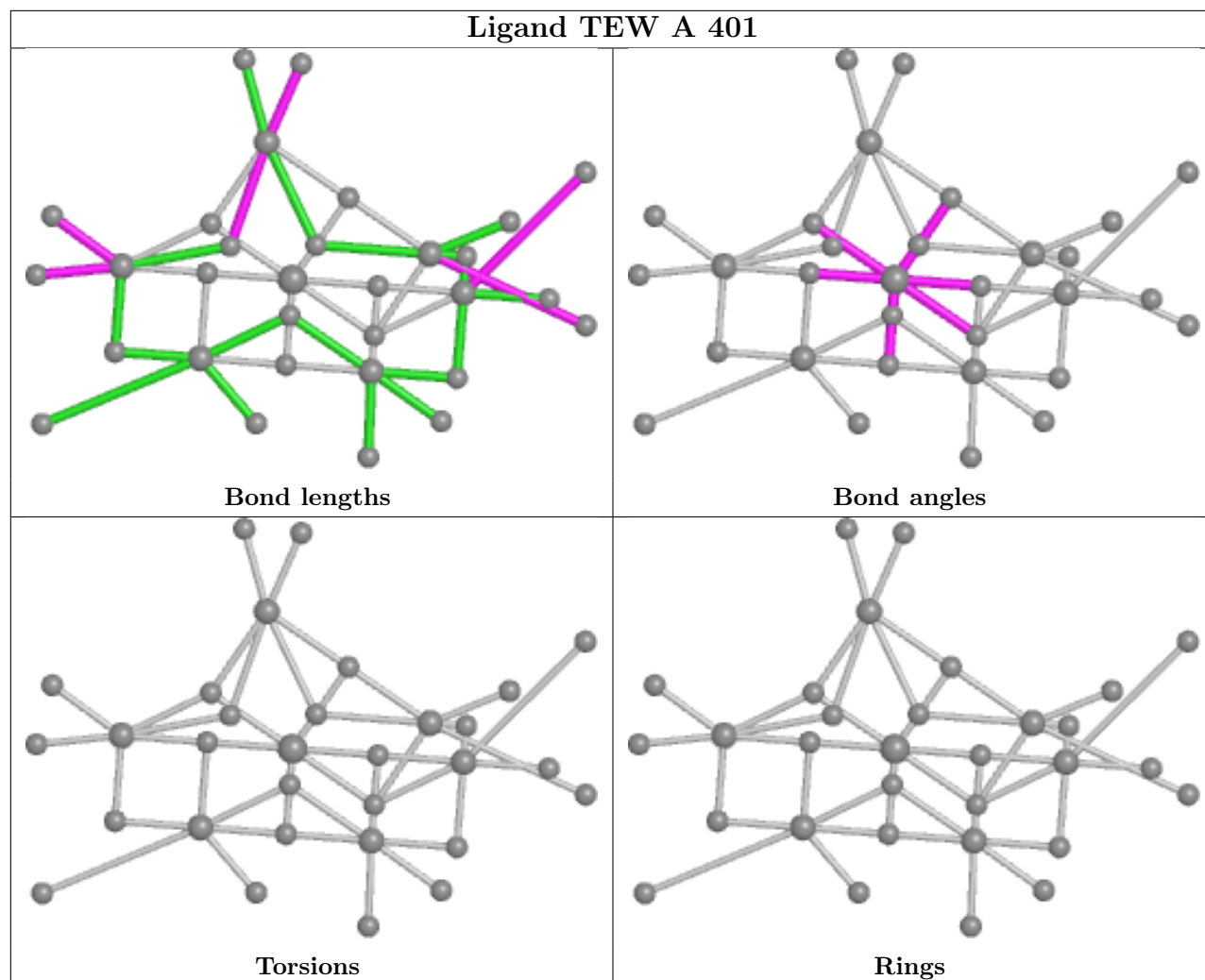
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	TEW	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.