



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:51 pm BST

PDB ID : 1KBZ  
Title : Crystal Structure of apo-dTDP-6-deoxy-L-lyxo-4-hexulose reductase (RmlD) from *Salmonella enterica* serovar Typhimurium  
Authors : Blankenfeldt, W.; Kerr, I.D.; Giraud, M.F.; McMiken, H.J.; Leonard, G.A.; Whitfield, C.; Messner, P.; Graninger, M.; Naismith, J.H.  
Deposited on : 2001-11-07  
Resolution : 2.20 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](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.

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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

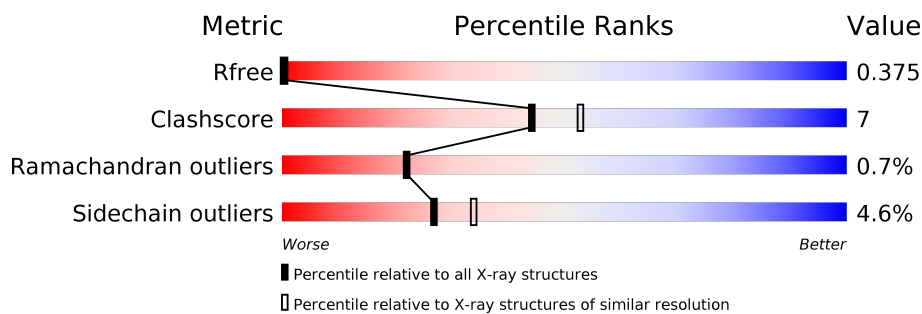
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	299	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2459 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 dTDP-glucose oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2287	1451	396	433	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

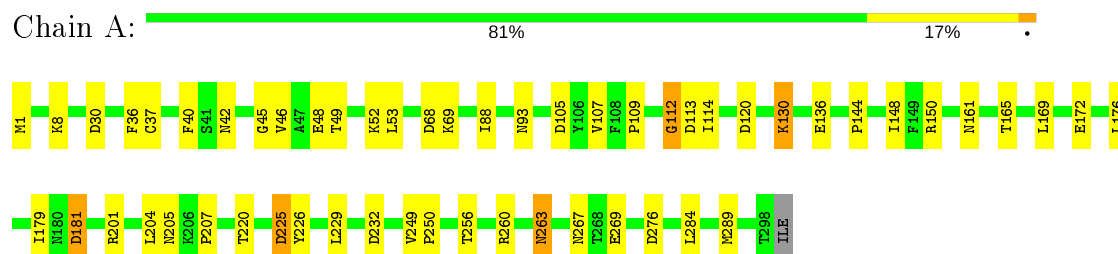
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		

### 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. 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.

- Molecule 1: dTDP-glucose oxidoreductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.53Å 71.90Å 82.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.65 – 2.20 54.11 – 2.21	Depositor EDS
% Data completeness (in resolution range)	96.1 (81.65-2.20) 97.7 (54.11-2.21)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.189 , 0.256 0.320 , 0.375	Depositor DCC
$R_{free}$ test set	730 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	2459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

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

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	0.63	0/2338	0.88	9/3187 (0.3%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH2	-11.67	114.47	120.30
1	A	201	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	276	ASP	CB-CG-OD2	7.18	124.76	118.30
1	A	120	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	225	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	105	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	181	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	232	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	68	ASP	CB-CG-OD2	5.04	122.84	118.30

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	2287	0	2278	30	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	171	0	0	6	1
All	All	2459	0	2278	30	1

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.

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:263:ASN:HD22	1:A:263:ASN:C	1.87	0.76
1:A:267:ASN:OD1	1:A:269:GLU:HG2	1.84	0.76
1:A:249:VAL:CG2	1:A:250:PRO:HD2	2.26	0.65
1:A:37:CYS:SG	3:A:659:HOH:O	2.40	0.63
1:A:93:ASN:ND2	1:A:144:PRO:HD2	2.15	0.62
1:A:52:LYS:HB2	3:A:609:HOH:O	1.99	0.61
1:A:263:ASN:ND2	1:A:263:ASN:C	2.57	0.58
1:A:249:VAL:HG23	1:A:250:PRO:HD2	1.87	0.56
1:A:207:PRO:HG3	3:A:669:HOH:O	2.04	0.56
1:A:136:GLU:OE1	1:A:150:ARG:NH2	2.41	0.51
1:A:169:LEU:HB3	1:A:176:LEU:HD21	1.93	0.51
1:A:179:ILE:HG23	1:A:181:ASP:OD1	2.11	0.50
1:A:69:LYS:HG3	3:A:662:HOH:O	2.11	0.49
1:A:8:LYS:HG2	1:A:30:ASP:HB3	1.95	0.48
1:A:46:VAL:HB	1:A:88:ILE:HD11	1.94	0.48
1:A:205:ASN:HB2	3:A:668:HOH:O	2.16	0.46
1:A:249:VAL:HG22	1:A:250:PRO:HD2	1.96	0.45
1:A:40:PHE:CD1	1:A:46:VAL:HG11	2.51	0.45
1:A:136:GLU:HB2	1:A:148:ILE:HD13	1.98	0.44
1:A:114:ILE:HD12	1:A:114:ILE:O	2.18	0.44
1:A:161:ASN:O	1:A:165:THR:HG23	2.18	0.43
1:A:130:LYS:HB2	1:A:130:LYS:HE3	1.54	0.43
1:A:267:ASN:OD1	1:A:269:GLU:CG	2.60	0.43
1:A:36:PHE:CE2	1:A:53:LEU:HD21	2.53	0.43
1:A:1:MET:CE	1:A:204:LEU:CD1	2.97	0.43
1:A:112:GLY:O	1:A:113:ASP:HB2	2.19	0.42
1:A:48:GLU:CG	3:A:609:HOH:O	2.67	0.42
1:A:42:ASN:O	1:A:45:GLY:N	2.53	0.41
1:A:1:MET:HE1	1:A:204:LEU:CD1	2.51	0.40
1:A:256:THR:OG1	1:A:260:ARG:NH1	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:647:HOH:O	3:A:647:HOH:O[2_555]	2.15	0.05

## 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	296/299 (99%)	282 (95%)	12 (4%)	2 (1%)	22 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	PRO
1	A	112	GLY

### 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	240/241 (100%)	229 (95%)	11 (5%)	27 34

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	107	VAL

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Mol	Chain	Res	Type
1	A	130	LYS
1	A	172	GLU
1	A	220	THR
1	A	225	ASP
1	A	226	TYR
1	A	229	LEU
1	A	263	ASN
1	A	284	LEU
1	A	289	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	60	ASN
1	A	93	ASN
1	A	142	ASN
1	A	263	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.