



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 08:39 PM EST

PDB ID : 1KC1  
Title : Crystal structure of dTDP-6-deoxy-L-lyxo-4-hexulose reductase (RmlD) in complex with NADPH  
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 : 2.60 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.

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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
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) : 2.36

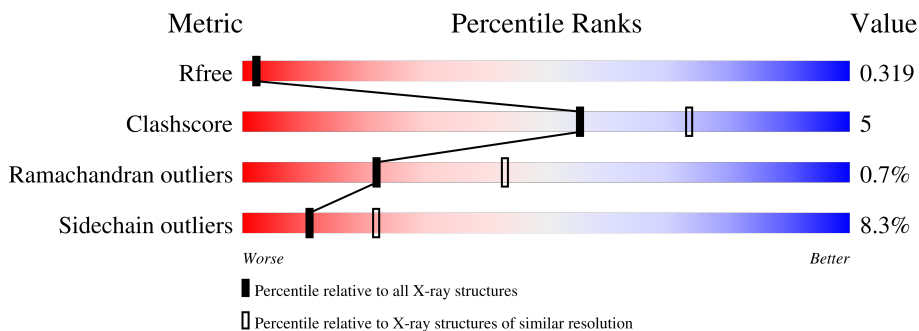
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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  $\geq 3$ , 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	

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
3	SO4	A	601	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2430 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
			Total	C	N	O	S			
1	A	298	2296	1457	398	434	7	0	1	0

- 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		

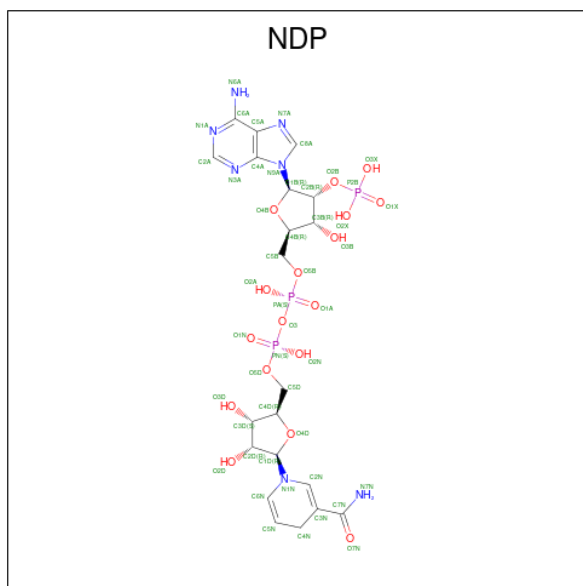
- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
4	A	1	48	21	7	17	3	0	0

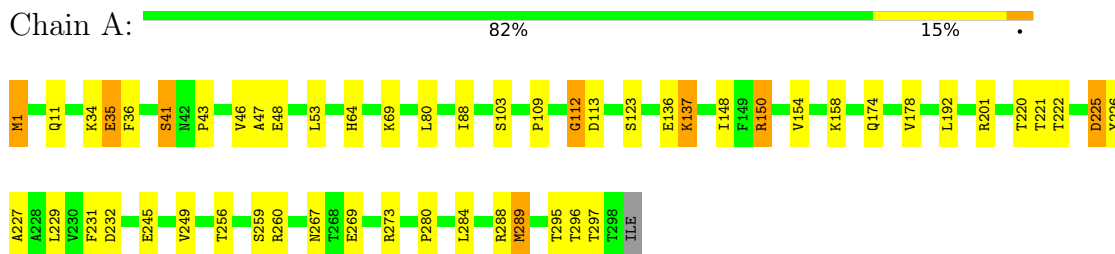
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	80	Total	O	0	0
			80	80		

### 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.

- 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, $\alpha$ , $\beta$ , $\gamma$	47.72Å 72.47Å 82.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.65 – 2.60 39.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (81.65-2.60) 98.9 (39.86-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.169 , 0.251 0.263 , 0.319	Depositor DCC
$R_{free}$ test set	475 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.8	Xtrriage
Anisotropy	0.171	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NDP, 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	1.03	3/2347 (0.1%)	1.07	6/3198 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	ARG	CZ-NH1	-5.62	1.25	1.33
1	A	289	MET	CB-CG	-5.07	1.35	1.51
1	A	289	MET	CG-SD	-5.05	1.68	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ASP	CB-CG-OD2	6.85	124.46	118.30
1	A	201	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	288	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	150	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	201	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	280	PRO	N-CD-CG	-5.04	95.64	103.20

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	2296	0	2290	24	0
2	A	1	0	0	0	0
3	A	5	0	0	3	0
4	A	48	0	26	0	0
5	A	80	0	0	3	0
All	All	2430	0	2316	24	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 5.

All (24) 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:158:LYS:NZ	3:A:601:SO4:O2	2.23	0.71
1:A:136:GLU:OE1	1:A:150:ARG:NH2	2.24	0.71
1:A:11:GLN:OE1	5:A:963:HOH:O	2.13	0.65
1:A:35:GLU:OE1	5:A:955:HOH:O	2.16	0.62
1:A:41:SER:O	1:A:43:PRO:HD3	2.00	0.61
1:A:158:LYS:NZ	3:A:601:SO4:S	2.77	0.56
1:A:1:MET:O	1:A:1:MET:HG3	2.05	0.56
1:A:158:LYS:NZ	3:A:601:SO4:O4	2.28	0.55
1:A:137[B]:LYS:NZ	5:A:962:HOH:O	2.40	0.53
1:A:267:ASN:OD1	1:A:269:GLU:HG2	2.11	0.50
1:A:136:GLU:HB2	1:A:148:ILE:HD13	1.92	0.50
1:A:103:SER:HB3	1:A:150:ARG:HG2	1.94	0.49
1:A:178:VAL:C	1:A:249:VAL:HG12	2.33	0.48
1:A:36:PHE:CZ	1:A:53:LEU:HD21	2.51	0.45
1:A:112:GLY:O	1:A:113:ASP:HB2	2.17	0.45
1:A:221:THR:OG1	1:A:222:THR:N	2.50	0.44
1:A:154:VAL:HG22	1:A:192:LEU:HD11	2.00	0.44
1:A:229:LEU:HD23	1:A:229:LEU:C	2.39	0.43
1:A:295:THR:HG22	1:A:295:THR:O	2.17	0.43
1:A:46:VAL:HG23	1:A:47:ALA:N	2.34	0.43
1:A:64:HIS:HB2	1:A:80:LEU:HD23	2.02	0.42
1:A:88:ILE:HG21	1:A:88:ILE:HD13	1.78	0.41
1:A:256:THR:OG1	1:A:260:ARG:NH1	2.54	0.41
1:A:227:ALA:O	1:A:231:PHE:CD1	2.74	0.41

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	297/299 (99%)	278 (94%)	17 (6%)	2 (1%)	22	43

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	241/241 (100%)	220 (91%)	21 (9%)	10	20

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	34	LYS
1	A	35	GLU
1	A	41	SER
1	A	48	GLU
1	A	69	LYS
1	A	123	SER
1	A	137[A]	LYS
1	A	137[B]	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	174	GLN
1	A	220	THR
1	A	225	ASP
1	A	226	TYR
1	A	232	ASP
1	A	245	GLU
1	A	259	SER
1	A	273	ARG
1	A	284	LEU
1	A	289	MET
1	A	296	THR
1	A	297	THR

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

Mol	Chain	Res	Type
1	A	42	ASN
1	A	60	ASN
1	A	93	ASN
1	A	247	ASN
1	A	272	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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
3	SO4	A	601	-	4,4,4	0.39	0	6,6,6	0.67	0
4	NDP	A	901	-	45,52,52	1.55	8 (17%)	53,80,80	2.06	17 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDP	A	901	-	-	9/30/77/77	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	NDP	C2A-N3A	3.86	1.38	1.32
4	A	901	NDP	O4B-C1B	3.57	1.46	1.41
4	A	901	NDP	P2B-O2B	3.31	1.65	1.59
4	A	901	NDP	C2D-C3D	-2.96	1.45	1.53
4	A	901	NDP	O4D-C1D	-2.60	1.35	1.42
4	A	901	NDP	C2A-N1A	2.34	1.38	1.33
4	A	901	NDP	O2D-C2D	-2.15	1.37	1.43
4	A	901	NDP	C2N-C3N	2.09	1.40	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	NDP	C1D-N1N-C2N	5.77	130.71	121.11
4	A	901	NDP	O4B-C1B-C2B	-4.50	98.77	106.59
4	A	901	NDP	N3A-C2A-N1A	-4.17	122.17	128.68
4	A	901	NDP	C2D-C1D-N1N	-4.14	102.93	113.30
4	A	901	NDP	C2D-C3D-C4D	-3.94	94.98	102.64
4	A	901	NDP	PN-O3-PA	-3.06	122.33	132.83
4	A	901	NDP	O2B-C2B-C1B	2.98	120.83	110.10
4	A	901	NDP	C1B-N9A-C4A	-2.92	121.52	126.64

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	NDP	O3B-C3B-C2B	-2.90	102.93	111.17
4	A	901	NDP	O5D-C5D-C4D	2.87	118.86	108.99
4	A	901	NDP	C3N-C7N-N7N	2.81	122.66	117.67
4	A	901	NDP	O3D-C3D-C2D	-2.74	102.94	111.82
4	A	901	NDP	C3B-C2B-C1B	-2.73	97.75	102.89
4	A	901	NDP	O7N-C7N-N7N	-2.40	117.27	122.88
4	A	901	NDP	C5A-C6A-N6A	2.32	123.87	120.35
4	A	901	NDP	C3N-C2N-N1N	2.27	126.34	123.10
4	A	901	NDP	O4D-C1D-N1N	2.02	112.00	108.06

There are no chirality outliers.

All (9) torsion outliers are listed below:

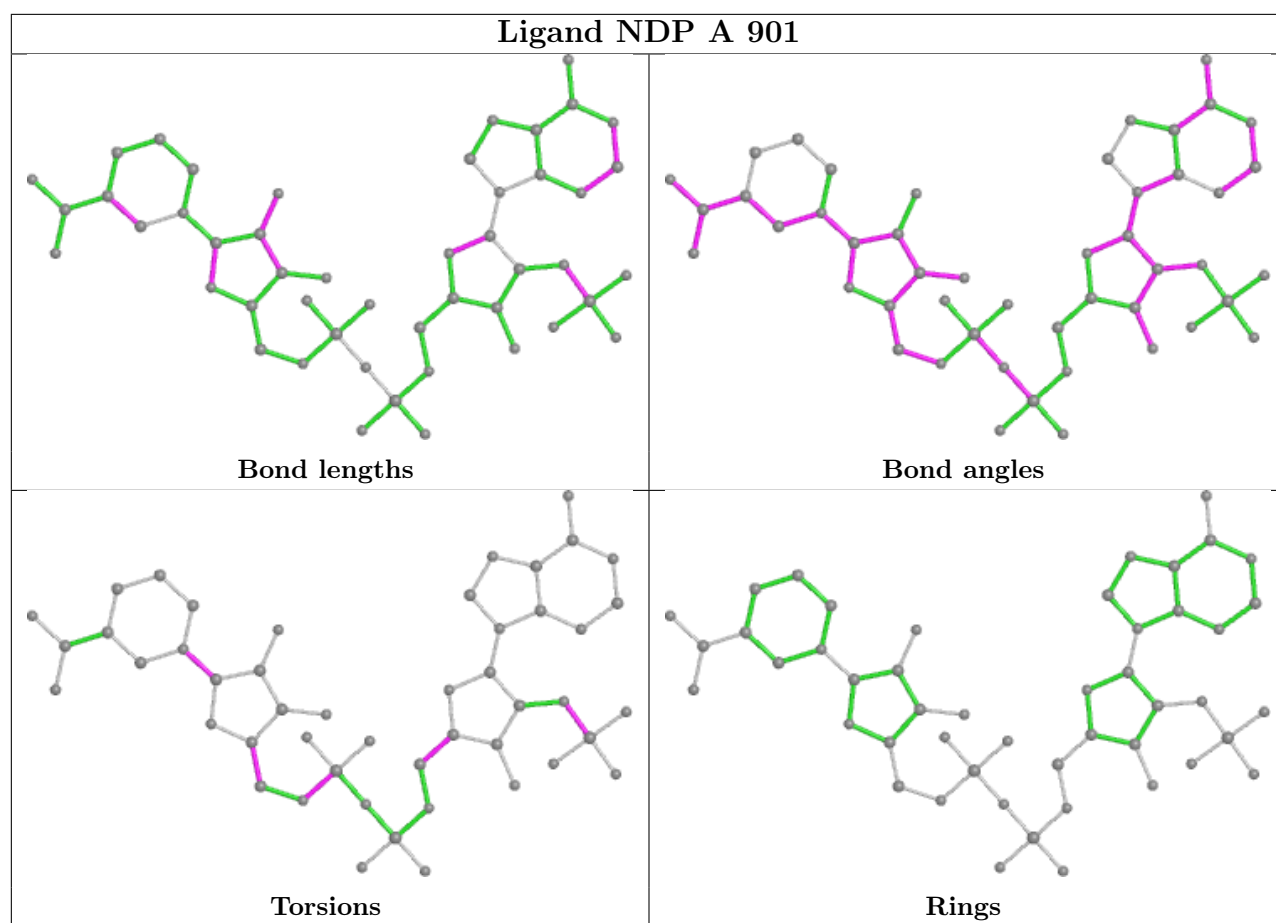
Mol	Chain	Res	Type	Atoms
4	A	901	NDP	C2B-O2B-P2B-O3X
4	A	901	NDP	C5D-O5D-PN-O1N
4	A	901	NDP	O4D-C4D-C5D-O5D
4	A	901	NDP	C3D-C4D-C5D-O5D
4	A	901	NDP	O4D-C1D-N1N-C6N
4	A	901	NDP	O4B-C4B-C5B-O5B
4	A	901	NDP	C2B-O2B-P2B-O1X
4	A	901	NDP	C5D-O5D-PN-O3
4	A	901	NDP	C5D-O5D-PN-O2N

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	SO4	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

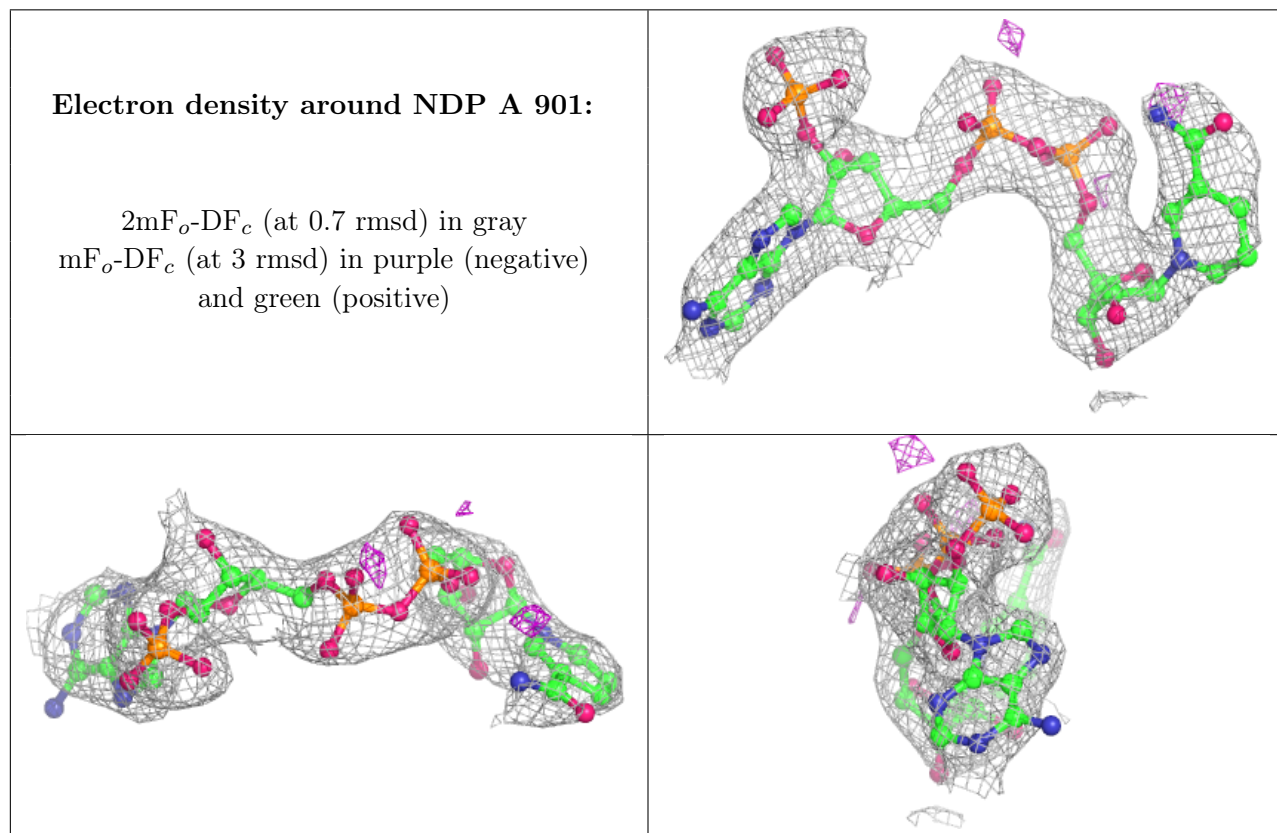
### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

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