

# wwPDB X-ray Structure Validation Summary Report (i)

#### Dec 8, 2022 - 06:16 pm GMT

PDB ID	:	7ZHZ
Title	:	Leishmania donovani Glucose 6-Phosphate Dehydrogenase mutant C138S com-
		plexed with G6P and NADP(H) $(H)$
Authors	:	Fritz-Wolf, K.; Berneburg, I.
Deposited on	:	2022-04-07
Resolution	:	2.50  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 (i) 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 (1)) were used in the production of this report:

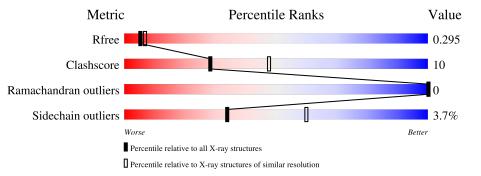
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Mol	Chain	Length	Quality of chain					
1	А	562	72%	22%	• 6%			
1	В	562	67%	26%	• 6%			

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
4	SO4	В	605	-	-	Х	-



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8532 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.

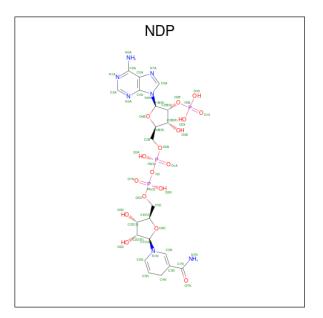
• Molecule 1 is a protein called Glucose-6-phosphate 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	528		С		0	S	0	0	0
			4172	2652	714	790	16			-
1	В	527	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
1	D	021	4172	2654	717	786	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

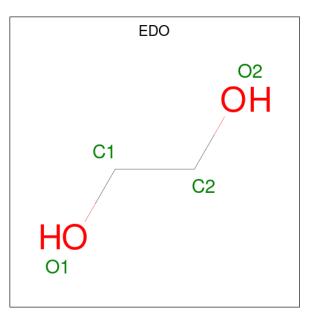
Chain	Residue	Modelled	Actual	Comment	Reference
А	138	SER	CYS	engineered mutation	UNP A2CIL3
В	138	SER	CYS	engineered mutation	UNP A2CIL3

• Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





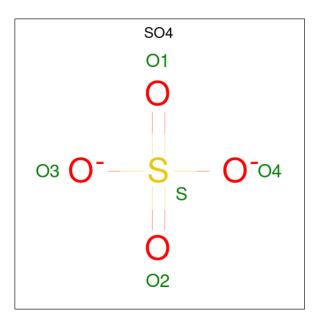
Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
0	Λ	1	Total	С	Ν	Ο	Р	0	0
	A	1	48	21	7	17	3	0	0
0	р	1	Total	С	Ν	Ο	Р	0	0
	D	1	48	21	7	17	3	0	



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

 $\bullet\,$  Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O\_4S).

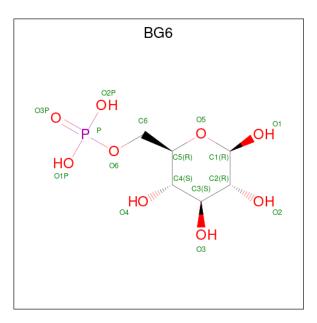




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 5 is 6-O-phosphono-beta-D-glucopyranose (three-letter code: BG6) (formula:  $C_6H_{13}O_9P$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total         C         O         P           16         6         9         1	0	0

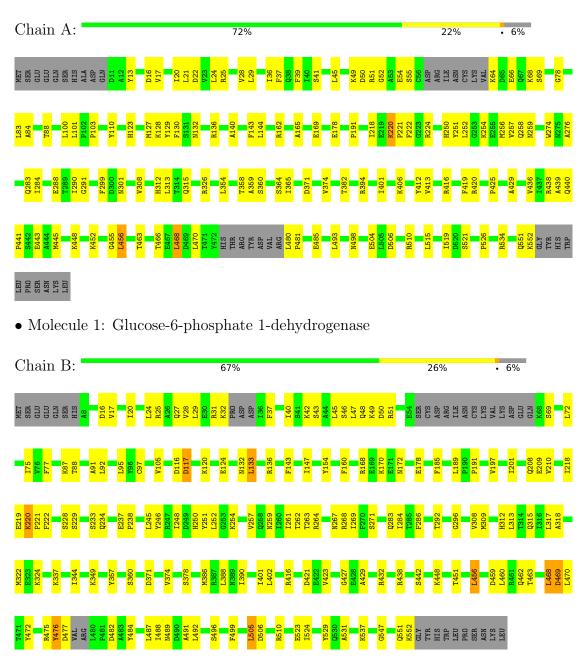
• Molecule 6 is water.

Mo	bl	Chain	Residues	Atoms	ZeroOcc	AltConf
6		А	15	Total O 15 15	0	0
6		В	10	Total         O           10         10	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.



 $\bullet$  Molecule 1: Glucose-6-phosphate 1-dehydrogenase



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	$218.16\text{\AA}$ $66.02\text{\AA}$ $120.02\text{\AA}$	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $120.73^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	48.75 - 2.50	Depositor
Resolution (A)	48.75 - 2.50	EDS
% Data completeness	99.4(48.75-2.50)	Depositor
(in resolution range)	99.7 (48.75 - 2.50)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.22 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
$R, R_{free}$	0.249 , $0.298$	Depositor
II, II, <i>free</i>	0.245 , $0.295$	DCC
$R_{free}$ test set	5105 reflections $(10.00\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	73.9	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8532	wwPDB-VP
Average B, all atoms $(Å^2)$	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: EDO, BG6, SO4, NDP

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		
WIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.25	0/4257	0.51	1/5755~(0.0%)	
1	В	0.27	0/4257	0.52	1/5754~(0.0%)	
All	All	0.26	0/8514	0.52	2/11509~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	468	LEU	CA-CB-CG	7.28	132.04	115.30
1	В	468	LEU	CA-CB-CG	6.09	129.31	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	476	TYR	Peptide

### 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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4172	0	4143	77	0
1	В	4172	0	4143	101	0
2	А	48	0	26	1	0
2	В	48	0	26	1	0
3	А	8	0	12	1	0
3	В	8	0	12	1	0
4	А	15	0	0	2	0
4	В	20	0	0	2	0
5	В	16	0	11	0	0
6	А	15	0	0	1	0
6	В	10	0	0	2	0
All	All	8532	0	8373	166	0

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.

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 10.

The worst 5 of 166 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:B:220:LYS:NZ	6:B:701:HOH:O	2.15	0.79
1:B:69:SER:OG	1:B:178:GLU:OE2	2.00	0.78
1:B:421:ASP:HB2	1:B:432:ARG:HG2	1.67	0.75
1:A:452:LYS:HB2	1:B:262:THR:HG21	1.71	0.73
1:B:250:HIS:ND1	6:B:701:HOH:O	2.22	0.71

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	А	522/562~(93%)	501 (96%)	21 (4%)	0	100 100		
1	В	519/562~(92%)	502 (97%)	17 (3%)	0	100 100		
All	All	1041/1124~(93%)	1003 (96%)	38 (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 side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	450/482~(93%)	436~(97%)	14 (3%)	40 67		
1	В	448/482 (93%)	429 (96%)	19 (4%)	30 54		
All	All	898/964~(93%)	865~(96%)	33~(4%)	34 60		

5 of 33 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	456	LEU
1	В	460	LEU
1	В	505	LEU
1	А	456	LEU
1	А	445	MET

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
1	А	550	HIS
1	В	27	GLN
1	В	312	HIS

### 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)

14 ligands are 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	Turne	Chain	Res	Link	B	ond leng	gths	Bond angles		
	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	А	606	-	$4,\!4,\!4$	0.14	0	6,6,6	0.05	0
4	SO4	В	605	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.04	0
3	EDO	А	602	-	$3,\!3,\!3$	0.46	0	2,2,2	0.33	0
3	EDO	А	603	-	$3,\!3,\!3$	0.46	0	2,2,2	0.34	0
4	SO4	В	607	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	А	604	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	В	606	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	В	603	-	$3,\!3,\!3$	0.45	0	2,2,2	0.34	0
4	SO4	В	608	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	В	601	-	$3,\!3,\!3$	0.46	0	2,2,2	0.33	0
5	BG6	В	604	-	16, 16, 16	1.23	2 (12%)	24,24,24	1.17	3 (12%)
2	NDP	В	602	-	$45,\!52,\!52$	4.02	18 (40%)	53,80,80	2.27	5 (9%)
4	SO4	А	605	-	4,4,4	0.14	0	6,6,6	0.05	0
2	NDP	А	601	-	$45,\!52,\!52$	4.01	18 (40%)	53,80,80	2.30	6 (11%)

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
3	EDO	А	602	-	-	0/1/1/1	-
3	EDO	А	603	-	-	0/1/1/1	-
3	EDO	В	603	-	-	0/1/1/1	-
3	EDO	В	601	-	-	0/1/1/1	-
5	BG6	В	604	-	-	2/6/26/26	0/1/1/1
2	NDP	В	602	-	-	9/30/77/77	0/5/5/5
2	NDP	А	601	_	_	6/30/77/77	0/5/5/5

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	602	NDP	O4B-C1B	13.68	1.60	1.41
2	А	601	NDP	O4B-C1B	13.67	1.60	1.41
2	А	601	NDP	C6N-C5N	12.69	1.56	1.33
2	В	602	NDP	C6N-C5N	12.66	1.55	1.33
2	В	602	NDP	O4D-C1D	7.80	1.60	1.42

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	601	NDP	C5A-C6A-N6A	9.92	135.43	120.35
2	В	602	NDP	C5A-C6A-N6A	9.91	135.42	120.35
2	А	601	NDP	C1B-N9A-C4A	-8.49	111.72	126.64
2	В	602	NDP	C1B-N9A-C4A	-8.43	111.83	126.64
2	А	601	NDP	N6A-C6A-N1A	-6.74	104.59	118.57

There are no chirality outliers.

 $5~{\rm of}~17$  torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	601	NDP	C5D-O5D-PN-O1N
2	А	601	NDP	O4D-C1D-N1N-C6N
2	В	602	NDP	C5D-O5D-PN-O1N
5	В	604	BG6	O5-C5-C6-O6
5	В	604	BG6	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	605	SO4	2	0

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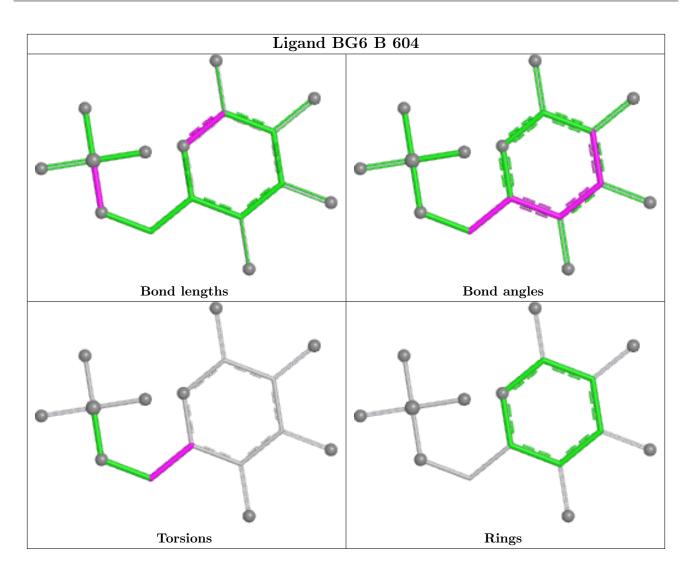
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	602	EDO	1	0
4	А	604	SO4	1	0
3	В	601	EDO	1	0
2	В	602	NDP	1	0
4	А	605	SO4	1	0
2	А	601	NDP	1	0

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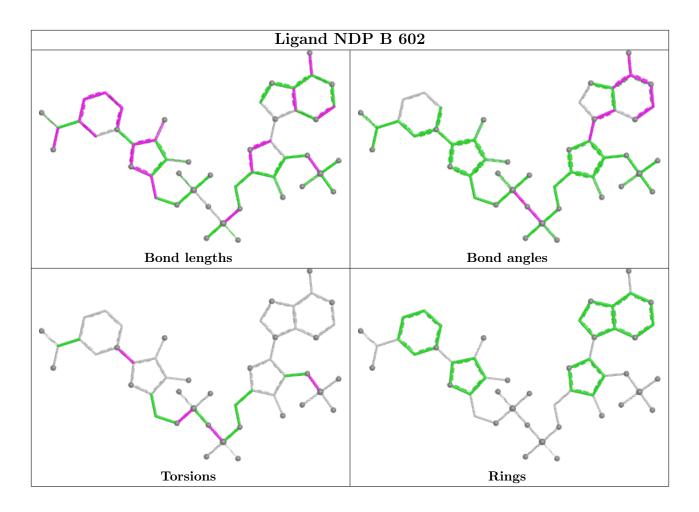
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



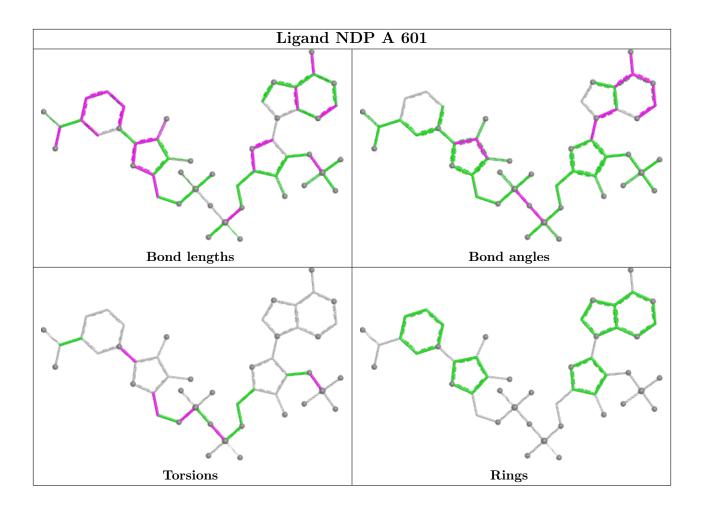












## 5.7 Other polymers (i)

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.

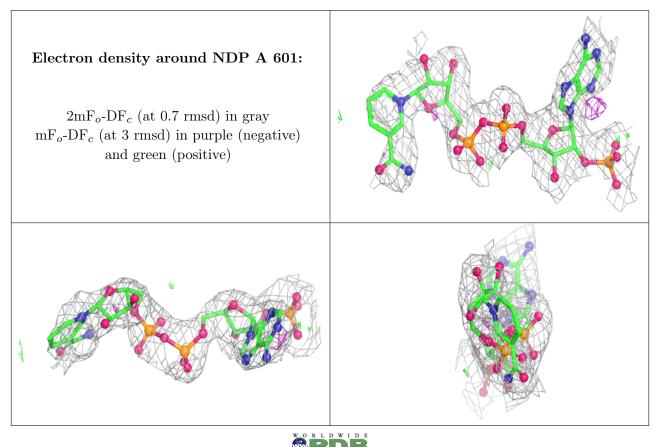
### 6.3 Carbohydrates (i)

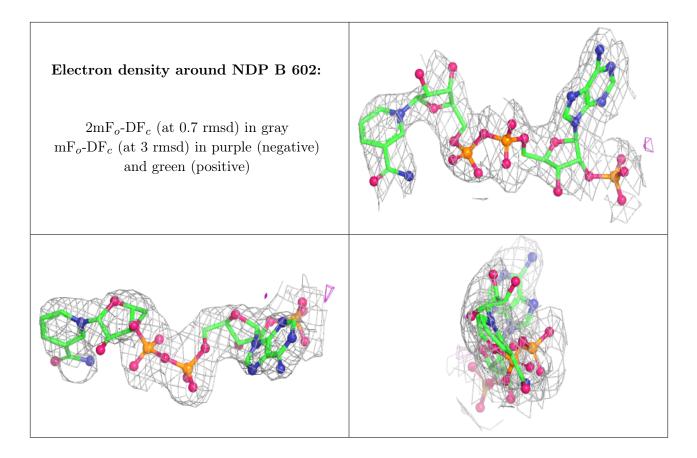
Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

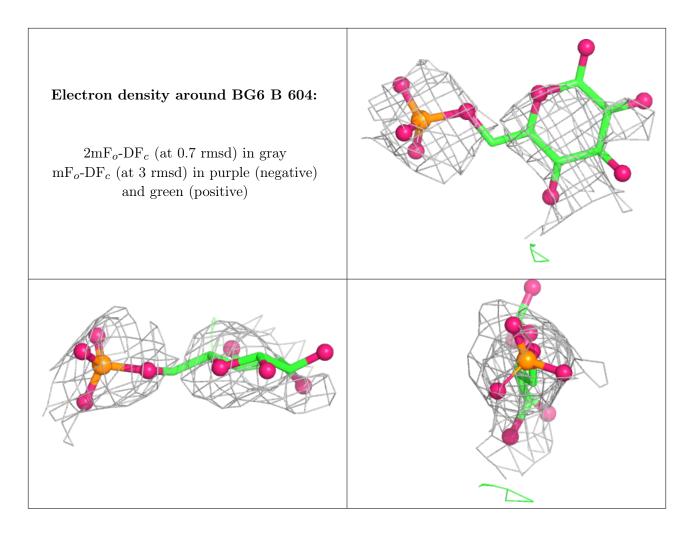
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

