



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 11:49 PM UTC

PDB ID : 7OCP / pdb\_00007ocp  
Title : NADPH bound to the dehydrogenase domain of the bifunctional mannitol-1-phosphate dehydrogenase/phosphatase MtID from *Acinetobacter baumannii*  
Authors : Tam, H.K.; Mueller, V.; Pos, K.M.  
Deposited on : 2021-04-28  
Resolution : 2.75 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](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>.

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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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

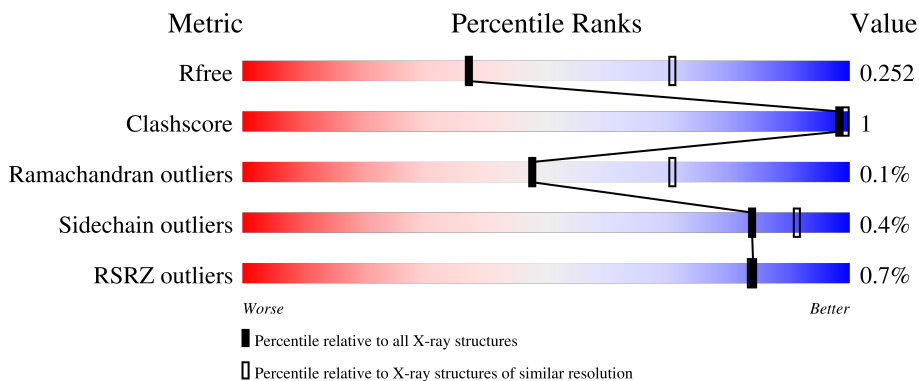
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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  $\leq 5\%$ . 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	727	 93% 5%
1	B	727	 91% 6%

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 11216 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 HAD hydrolase, family IA, variant 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	688	Total	C	N	O	S	0	0	0
			5552	3526	949	1045	32			
1	B	680	Total	C	N	O	S	0	0	0
			5494	3491	940	1031	32			

There are 26 discrepancies between the modelled and reference sequences:

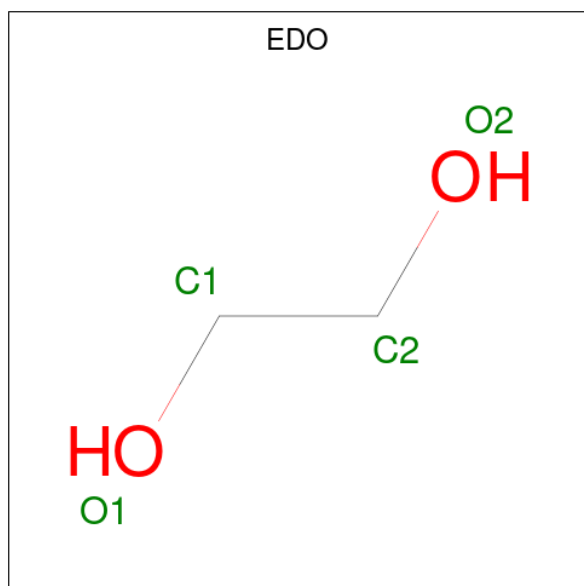
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP D0C7J2
A	2	VAL	-	expression tag	UNP D0C7J2
A	717	ALA	-	expression tag	UNP D0C7J2
A	718	ALA	-	expression tag	UNP D0C7J2
A	719	ALA	-	expression tag	UNP D0C7J2
A	720	LEU	-	expression tag	UNP D0C7J2
A	721	GLU	-	expression tag	UNP D0C7J2
A	722	HIS	-	expression tag	UNP D0C7J2
A	723	HIS	-	expression tag	UNP D0C7J2
A	724	HIS	-	expression tag	UNP D0C7J2
A	725	HIS	-	expression tag	UNP D0C7J2
A	726	HIS	-	expression tag	UNP D0C7J2
A	727	HIS	-	expression tag	UNP D0C7J2
B	1	MET	-	initiating methionine	UNP D0C7J2
B	2	VAL	-	expression tag	UNP D0C7J2
B	717	ALA	-	expression tag	UNP D0C7J2
B	718	ALA	-	expression tag	UNP D0C7J2
B	719	ALA	-	expression tag	UNP D0C7J2
B	720	LEU	-	expression tag	UNP D0C7J2
B	721	GLU	-	expression tag	UNP D0C7J2
B	722	HIS	-	expression tag	UNP D0C7J2
B	723	HIS	-	expression tag	UNP D0C7J2
B	724	HIS	-	expression tag	UNP D0C7J2
B	725	HIS	-	expression tag	UNP D0C7J2
B	726	HIS	-	expression tag	UNP D0C7J2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	727	HIS	-	expression tag	UNP D0C7J2

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

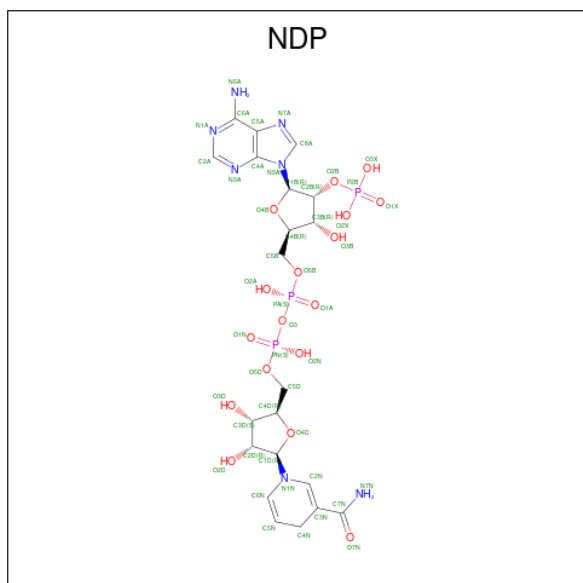
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).

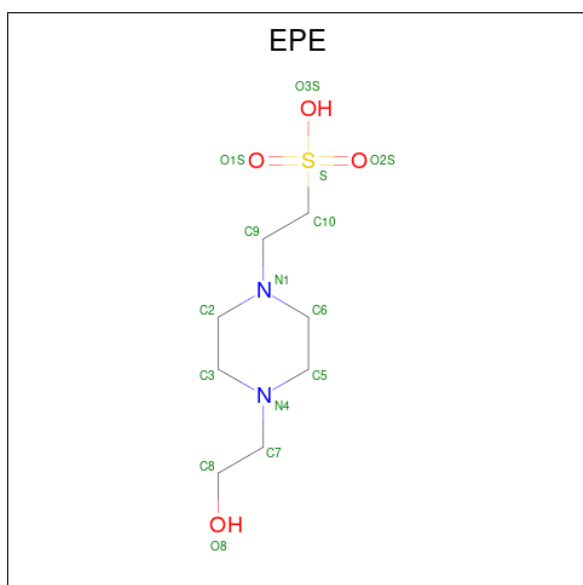


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	26	Total	O	0	0
			26	26		
8	B	10	Total	O	0	0
			10	10		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.66Å 157.69Å 219.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.75 48.59 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.59-2.75) 100.0 (48.59-2.75)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.77Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.220 , 0.255 0.220 , 0.252	Depositor DCC
$R_{free}$ test set	2262 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtrriage
Anisotropy	0.516	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: EDO, EPE, MG, CL, NDP, SO4

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	1.00	0/5656	1.52	0/7636
1	B	1.01	0/5596	1.53	1/7549 (0.0%)
All	All	1.00	0/11252	1.52	1/15185 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	GLY	CA-C-O	-5.60	118.10	122.52

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	5552	0	5527	6	0
1	B	5494	0	5467	9	0
2	A	4	0	6	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	48	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	48	0	26	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	15	0	18	0	0
8	A	26	0	0	0	0
8	B	10	0	0	0	0
All	All	11216	0	11070	14	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 1.

The worst 5 of 14 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:175:GLU:HG2	1:A:180:GLY:C	2.39	0.47
1:A:252:PHE:HB2	1:A:278:ALA:HB1	1.96	0.47
1:A:259:TYR:CE2	1:A:414:VAL:HG13	2.50	0.46
1:B:537:MET:HE1	1:B:638:LEU:HD23	1.97	0.45
1:B:664:LEU:HD11	1:B:685:LEU:HD23	1.99	0.45

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	684/727 (94%)	646 (94%)	36 (5%)	2 (0%)	36	56
1	B	672/727 (92%)	637 (95%)	35 (5%)	0	100	100
All	All	1356/1454 (93%)	1283 (95%)	71 (5%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	A	447	GLU

### 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	607/642 (94%)	605 (100%)	2 (0%)	86	93
1	B	600/642 (94%)	597 (100%)	3 (0%)	81	89
All	All	1207/1284 (94%)	1202 (100%)	5 (0%)	84	91

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

Mol	Chain	Res	Type
1	A	451	GLU
1	A	601	LYS
1	B	359	GLN
1	B	527	LYS
1	B	610	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	402	HIS
1	B	439	GLN
1	B	637	ASN
1	B	476	ASN
1	B	590	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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
4	SO4	A	805	-	4,4,4	0.34	0	6,6,6	0.08	0
2	EDO	A	801	-	3,3,3	0.05	0	2,2,2	0.11	0
5	NDP	B	1002	-	51,52,52	2.56	11 (21%)	71,80,80	1.49	15 (21%)
5	NDP	A	804	-	51,52,52	2.63	10 (19%)	71,80,80	1.43	14 (19%)
4	SO4	B	1003	-	4,4,4	0.34	0	6,6,6	0.06	0
4	SO4	A	803	-	4,4,4	0.34	0	6,6,6	0.08	0
7	EPE	B	1001	-	15,15,15	1.05	2 (13%)	19,20,20	1.96	4 (21%)

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
2	EDO	A	801	-	-	0/1/1/1	-
5	NDP	A	804	-	-	7/34/77/77	0/5/5/5
7	EPE	B	1001	-	-	3/9/19/19	0/1/1/1
5	NDP	B	1002	-	-	7/34/77/77	0/5/5/5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	804	NDP	P2B-O2B	14.19	1.84	1.59
5	B	1002	NDP	P2B-O2B	14.10	1.84	1.59
5	A	804	NDP	PA-O3	6.58	1.66	1.59
5	B	1002	NDP	PA-O3	5.43	1.65	1.59
5	A	804	NDP	PN-O5D	4.59	1.77	1.59

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1001	EPE	O1S-S-C10	6.56	116.64	106.73
5	B	1002	NDP	P2B-O2B-C2B	-3.84	113.19	123.43
5	A	804	NDP	O3-PA-O1A	-3.72	99.52	110.70
5	B	1002	NDP	O2B-P2B-O1X	-3.59	96.55	109.33
5	A	804	NDP	P2B-O2B-C2B	-3.53	114.01	123.43

There are no chirality outliers.

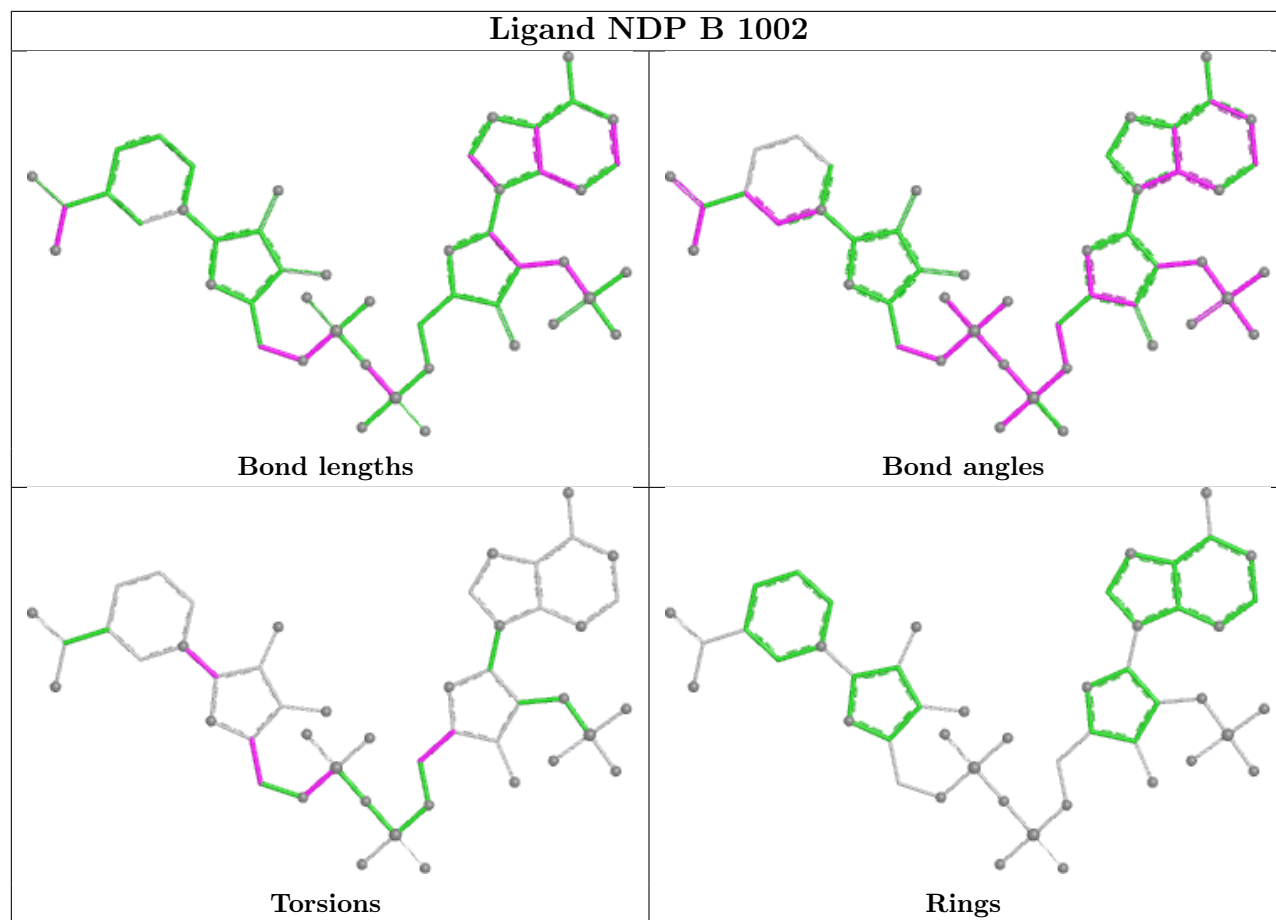
5 of 17 torsion outliers are listed below:

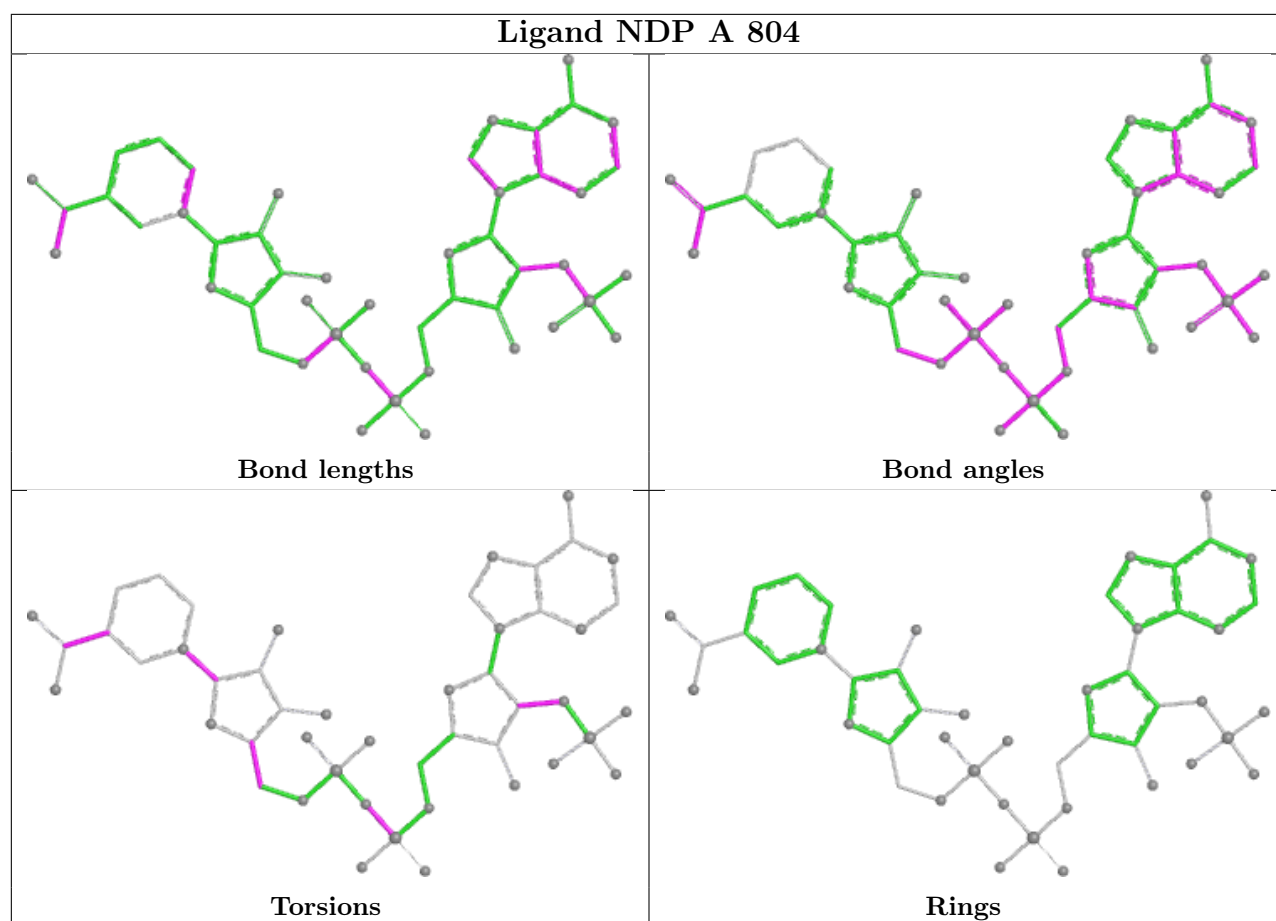
Mol	Chain	Res	Type	Atoms
5	A	804	NDP	C2N-C3N-C7N-N7N
5	B	1002	NDP	C5D-O5D-PN-O3
5	B	1002	NDP	C5D-O5D-PN-O1N
5	B	1002	NDP	C5D-O5D-PN-O2N
5	B	1002	NDP	O4D-C4D-C5D-O5D

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	688/727 (94%)	-0.06	7 (1%) 79 79	50, 87, 147, 165	0
1	B	680/727 (93%)	0.03	2 (0%) 90 91	64, 99, 157, 201	0
All	All	1368/1454 (94%)	-0.02	9 (0%) 84 84	50, 93, 151, 201	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	450	ILE	4.0
1	A	2	VAL	3.1
1	A	603	PRO	2.9
1	A	602	ASP	2.5
1	A	364	ILE	2.4

### 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](#)

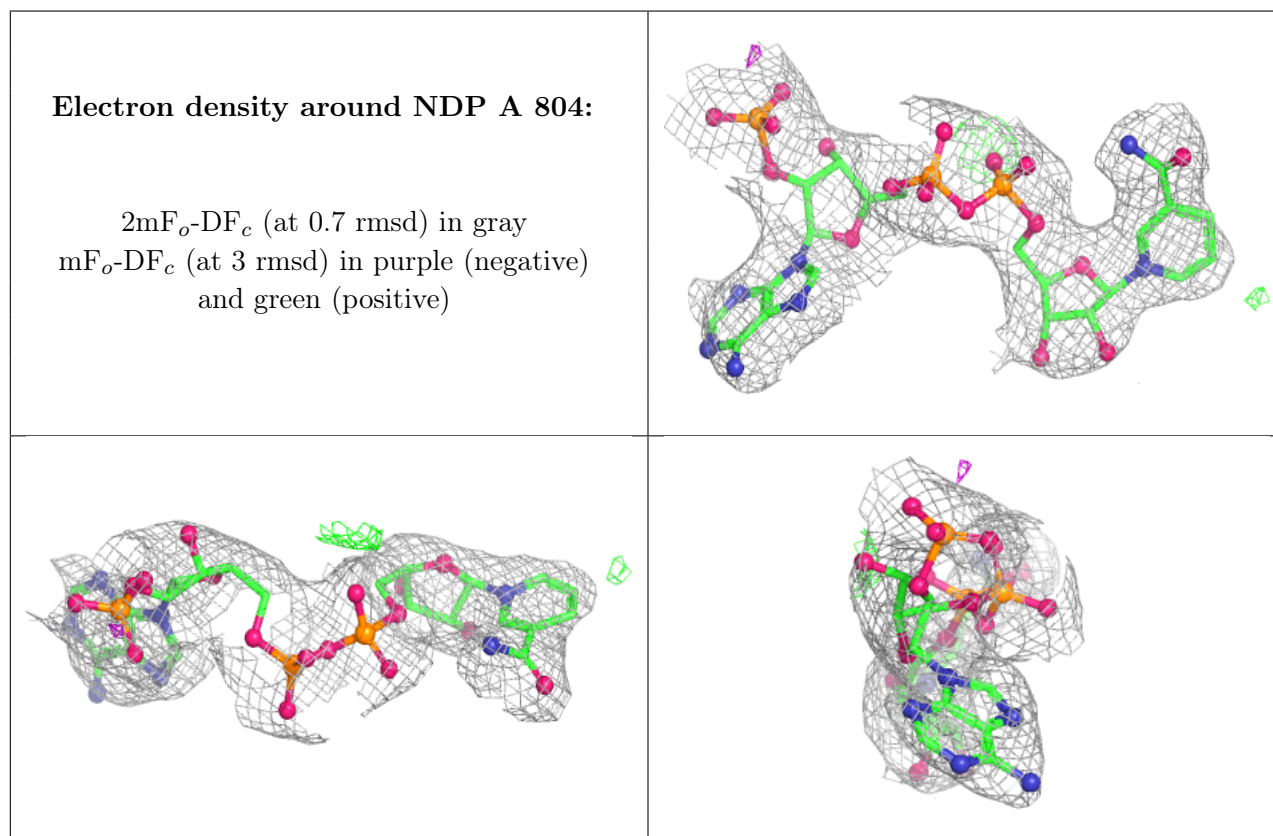
There are no oligosaccharides in this entry.

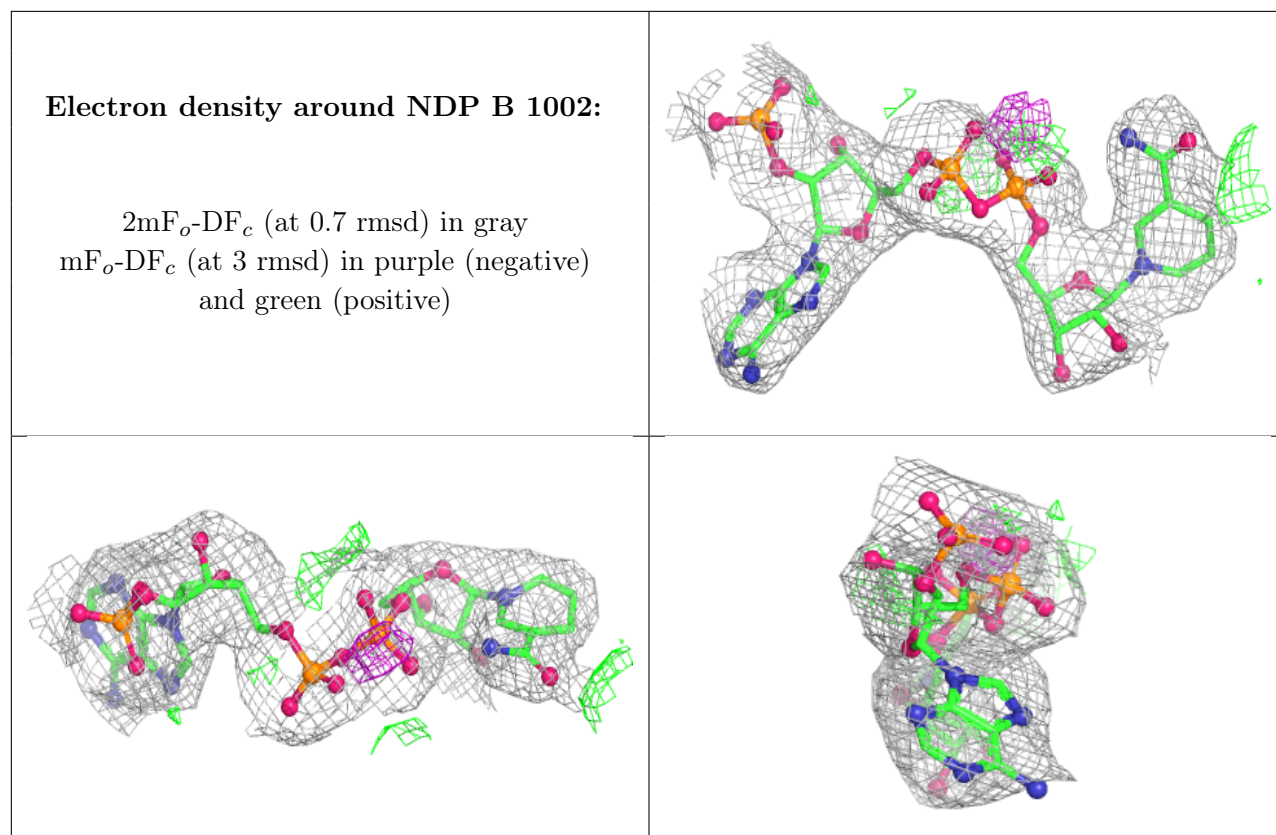
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	EPE	B	1001	15/15	0.78	0.28	91,93,94,95	15
4	SO4	A	805	5/5	0.80	0.08	118,118,118,119	0
6	CL	B	1005	1/1	0.87	0.09	97,97,97,97	0
4	SO4	B	1003	5/5	0.90	0.09	99,99,100,100	0
4	SO4	A	803	5/5	0.90	0.10	96,97,98,98	0
2	EDO	A	801	4/4	0.90	0.15	102,103,103,104	0
3	MG	B	1004	1/1	0.91	0.14	89,89,89,89	0
5	NDP	A	804	48/48	0.92	0.08	97,101,106,111	0
5	NDP	B	1002	48/48	0.92	0.07	75,85,100,102	0
6	CL	A	806	1/1	0.94	0.06	73,73,73,73	0
3	MG	A	802	1/1	0.95	0.14	57,57,57,57	0

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](#)

There are no such residues in this entry.