



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 04:46 pm BST

PDB ID : 1AE4  
Title : ALDEHYDE REDUCTASE COMPLEXED WITH COFACTOR AND INHIBITOR, ALPHA CARBON ATOMS ONLY  
Authors : El-Kabbani, O.  
Deposited on : 1997-03-05  
Resolution : 2.40 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

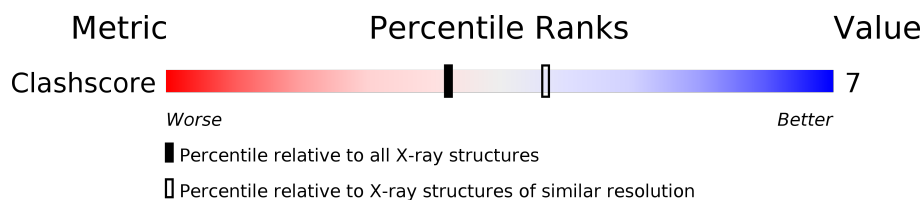
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)

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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	325	 99% .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 396 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 ALDEHYDE REDUCTASE.

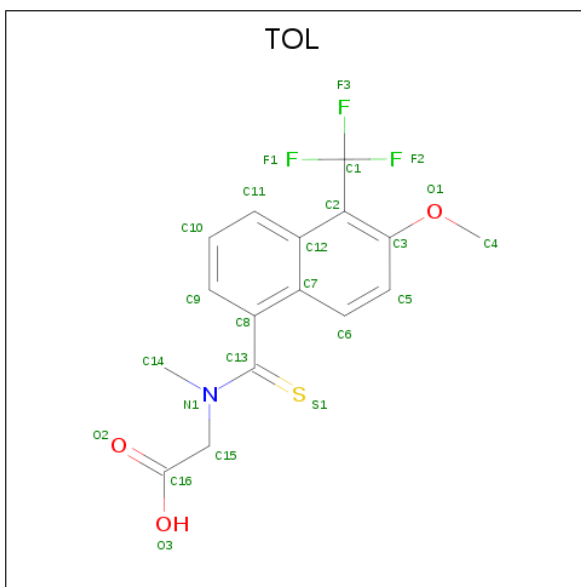
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	324	Total	C	0	0	324
			324	324			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 3 is TOLRESTAT (three-letter code: TOL) (formula: C<sub>16</sub>H<sub>14</sub>F<sub>3</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
3	A	1	24	16	3	1	3	1	0	0

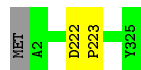
### 3 Residue-property plots

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.

Note EDS was not executed.

- Molecule 1: ALDEHYDE REDUCTASE

Chain A:  99%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.80 Å 67.80 Å 245.28 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.40	Depositor
% Data completeness (in resolution range)	86.0 (8.00-2.40)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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

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	324	0	0	1	0
2	A	48	0	25	1	0
3	A	24	0	13	1	0
All	All	396	0	38	3	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 7.

All (3) 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)
2:A:350:NAP:O1N	2:A:350:NAP:H3D	2.00	0.62
3:A:600:TOL:H11	3:A:600:TOL:F1	2.02	0.50
1:A:222:ASP:CA	1:A:223:PRO:CA	2.99	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	TOL	A	600	-	21,25,25	1.67	5 (23%)	32,37,37	1.50	8 (25%)
2	NAP	A	350	-	45,52,52	1.68	8 (17%)	56,80,80	2.29	18 (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
3	TOL	A	600	-	-	4/18/20/20	0/2/2/2
2	NAP	A	350	-	-	8/31/67/67	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	NAP	C2N-N1N	4.71	1.40	1.35
2	A	350	NAP	O4B-C1B	4.21	1.47	1.41
3	A	600	TOL	C3-C2	4.03	1.42	1.38
2	A	350	NAP	O4D-C1D	3.27	1.45	1.41
2	A	350	NAP	C2D-C1D	-3.07	1.49	1.53
3	A	600	TOL	O1-C3	-2.98	1.32	1.37
3	A	600	TOL	C13-S1	2.83	1.71	1.66
2	A	350	NAP	C6N-N1N	2.55	1.41	1.35
3	A	600	TOL	C8-C13	2.31	1.51	1.49
2	A	350	NAP	C3N-C7N	2.23	1.53	1.50
3	A	600	TOL	C1-C2	2.13	1.54	1.52
2	A	350	NAP	C5A-N7A	-2.09	1.32	1.39
2	A	350	NAP	P2B-O2X	-2.05	1.47	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	NAP	C3B-C2B-C1B	-7.50	88.78	102.89
2	A	350	NAP	PN-O3-PA	5.55	151.88	132.83
2	A	350	NAP	C4A-C5A-N7A	5.36	114.99	109.40
2	A	350	NAP	C1B-N9A-C4A	-4.93	117.98	126.64
2	A	350	NAP	O2B-C2B-C1B	4.25	125.40	110.10
2	A	350	NAP	N6A-C6A-N1A	3.40	125.63	118.57
2	A	350	NAP	O4B-C1B-C2B	3.27	112.27	106.59
2	A	350	NAP	C6N-N1N-C2N	-3.25	119.01	121.97
2	A	350	NAP	O3D-C3D-C2D	-3.20	101.46	111.82
3	A	600	TOL	C3-C2-C12	3.10	119.70	117.53
3	A	600	TOL	C4-O1-C3	-3.02	112.97	117.53
3	A	600	TOL	C5-C3-C2	-2.84	119.34	122.90
2	A	350	NAP	N3A-C2A-N1A	-2.74	124.39	128.68
2	A	350	NAP	O5B-PA-O1A	-2.74	98.35	109.07
2	A	350	NAP	O5B-C5B-C4B	-2.56	100.17	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	TOL	C6-C7-C8	-2.51	119.44	123.31
3	A	600	TOL	S1-C13-N1	-2.45	120.92	124.22
2	A	350	NAP	O2B-C2B-C3B	-2.39	103.00	111.68
2	A	350	NAP	O4D-C4D-C5D	-2.35	101.63	109.37
2	A	350	NAP	C5A-C6A-N1A	-2.29	115.17	120.35
2	A	350	NAP	O4D-C1D-C2D	-2.28	103.60	106.93
2	A	350	NAP	C2A-N1A-C6A	2.23	122.57	118.75
3	A	600	TOL	C9-C8-C13	-2.21	116.86	119.60
3	A	600	TOL	O1-C3-C2	2.19	119.64	116.51
3	A	600	TOL	C1-C2-C3	2.11	123.85	120.21
2	A	350	NAP	C2B-C3B-C4B	2.00	106.34	101.99

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	350	NAP	C1B-C2B-O2B-P2B
2	A	350	NAP	O4B-C4B-C5B-O5B
2	A	350	NAP	PA-O3-PN-O5D
2	A	350	NAP	C2B-O2B-P2B-O1X
3	A	600	TOL	F3-C1-C2-C3
2	A	350	NAP	C4D-C5D-O5D-PN
2	A	350	NAP	C3B-C4B-C5B-O5B
3	A	600	TOL	C16-C15-N1-C14
3	A	600	TOL	F2-C1-C2-C3
3	A	600	TOL	F1-C1-C2-C3
2	A	350	NAP	C2B-O2B-P2B-O3X
2	A	350	NAP	PA-O3-PN-O1N

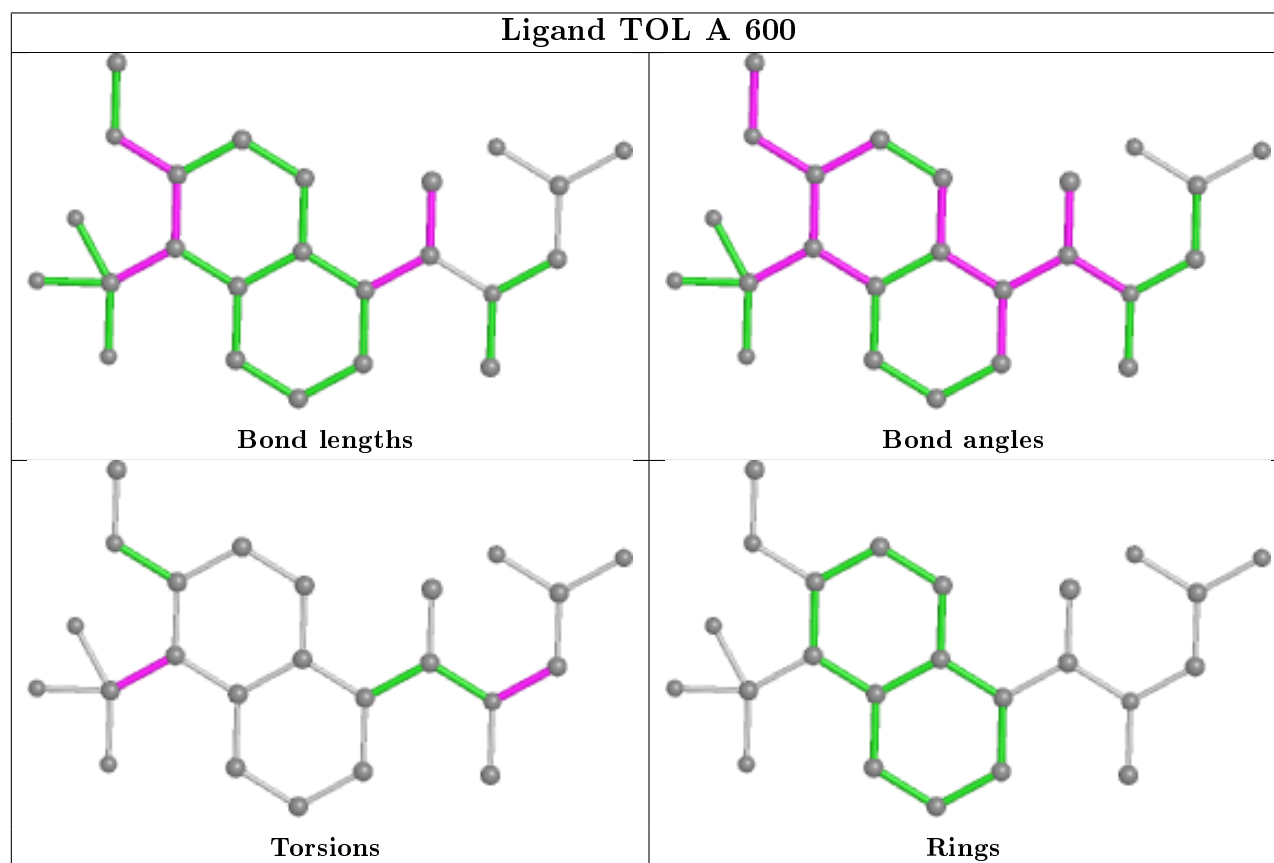
There are no ring outliers.

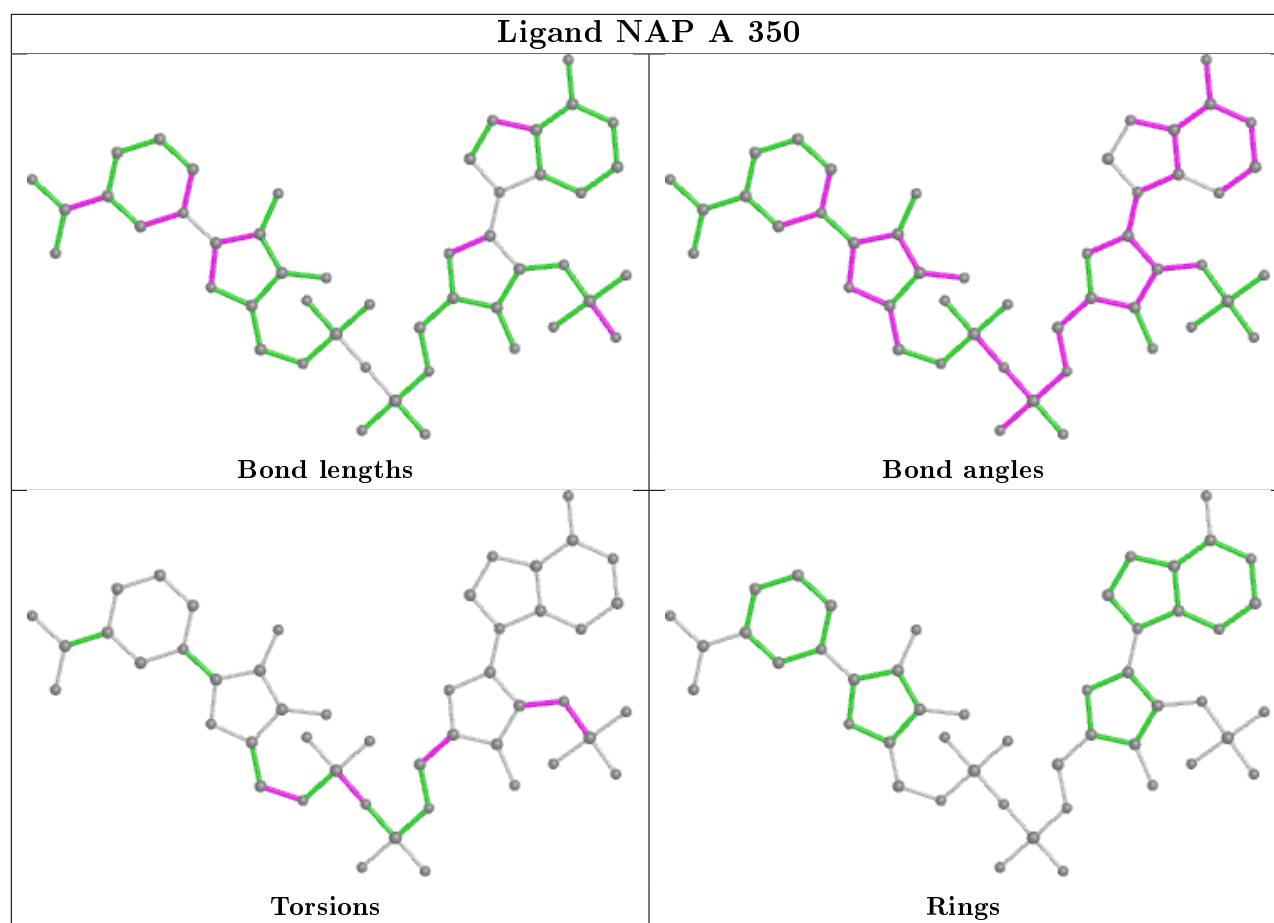
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	TOL	1	0
2	A	350	NAP	1	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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.