



# Full wwPDB X-ray Structure Validation Report i

Apr 21, 2024 – 05:19 am BST

PDB ID : 2WLE  
Title : Crystallographic analysis of the polysialic acid O-acetyltransferase OatWY  
Authors : Lee, H.J.; Rakic, B.; Gilbert, M.; Wakarchuk, W.W.; Withers, S.G.; Strynadka, N.C.J.  
Deposited on : 2009-06-23  
Resolution : 2.19 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 i 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](#) i) were used in the production of this report:

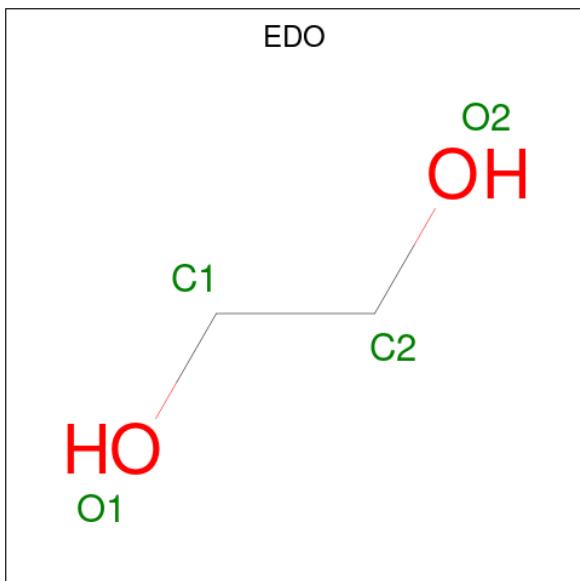
MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2





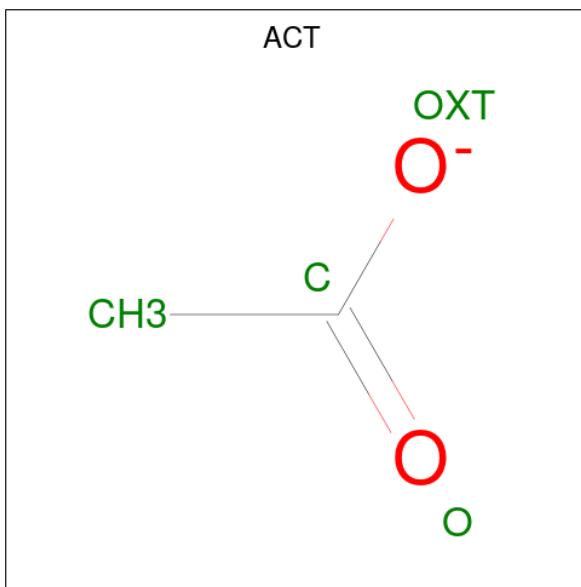
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	48	21	7	16	3	1	0	0
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub><sup>-</sup>).



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

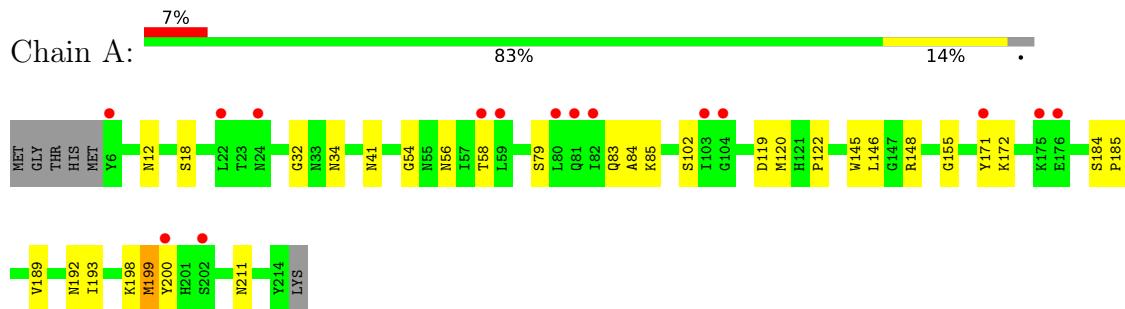
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	105	Total O 105 105	0	0
5	B	39	Total O 39 39	0	0
5	C	71	Total O 71 71	0	0

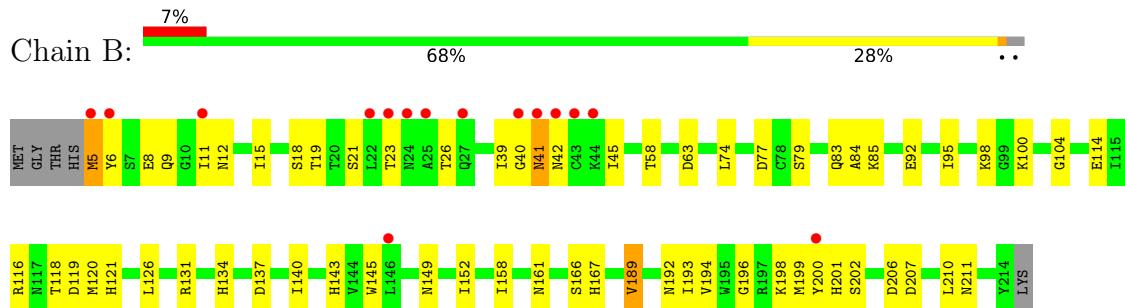
### 3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

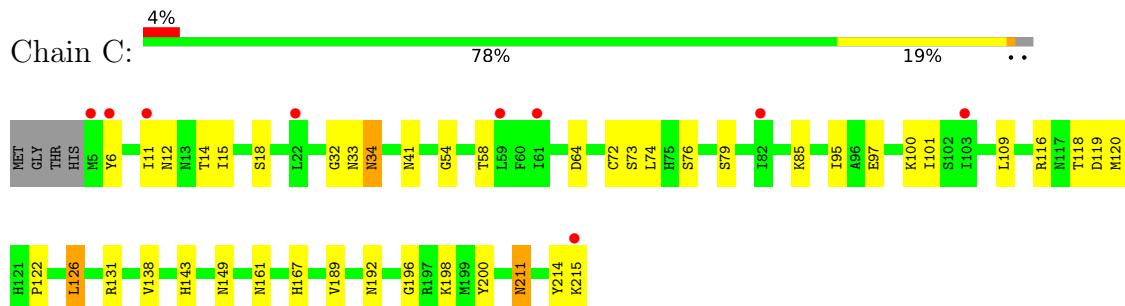
- Molecule 1: POLYSIALIC ACID O-ACETYLTRANSFERASE



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## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.07Å 94.52Å 100.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.19 29.56 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-2.19) 99.3 (29.56-2.19)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	3.68 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
$R$ , $R_{free}$	0.195 , 0.242 0.208 , 0.253	Depositor DCC
$R_{free}$ test set	1966 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.3	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.51$ , $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.











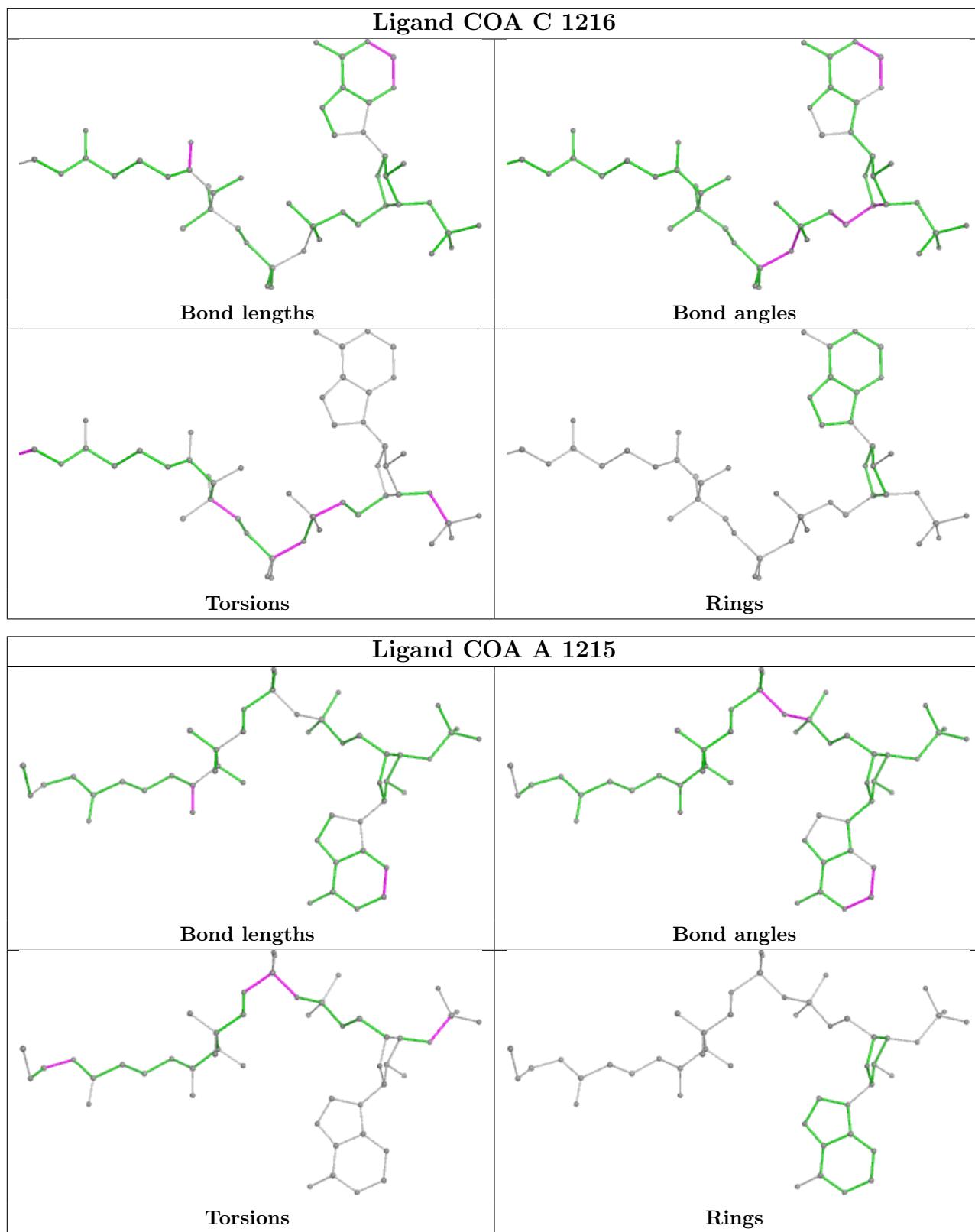












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

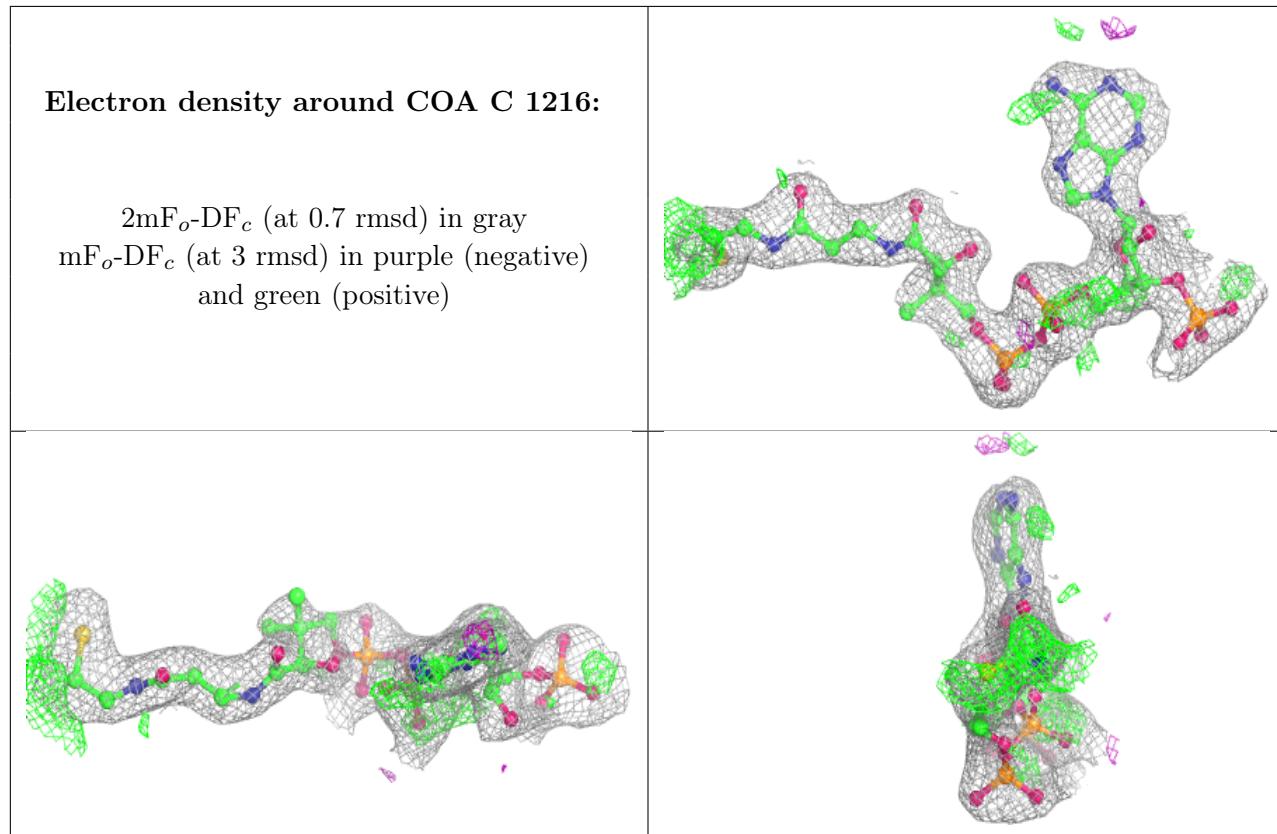
## 5.8 Polymer linkage issues

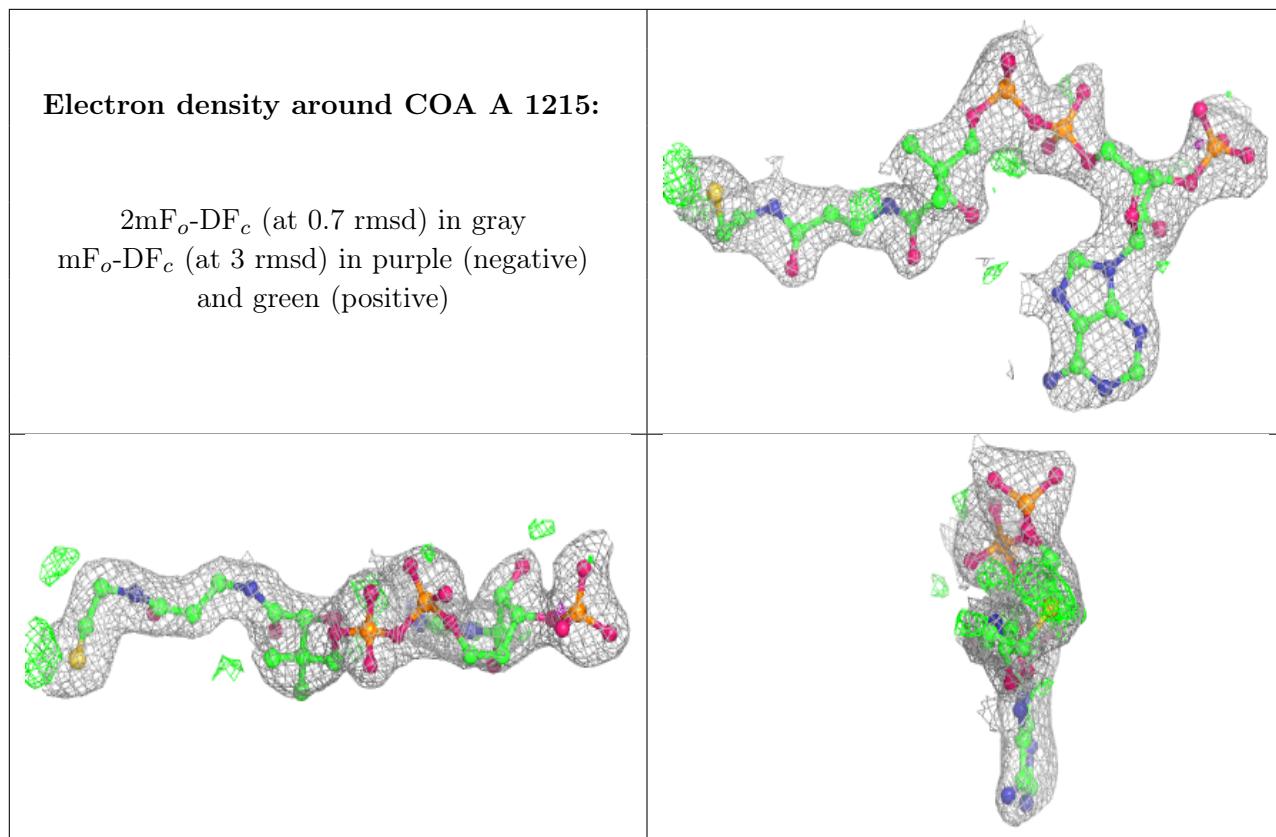
There are no chain breaks in this entry.





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.