Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 05:20 PM EDT

PDB ID	:	6NL2
Title	:	Apo NIS synthetase DesD variant R306Q
Authors	:	Hoffmann, K.M.
Deposited on	:	2019-01-07
Resolution	:	1.92 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*
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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.35.1

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 1.92 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10211 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 desferrioxamine E biosynthesis protein DesD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	3	0
			4704	2993	811	885	15			
1	B	593	Total	C	N	O	S	0	4	0
			4701	2991	811	884	15			

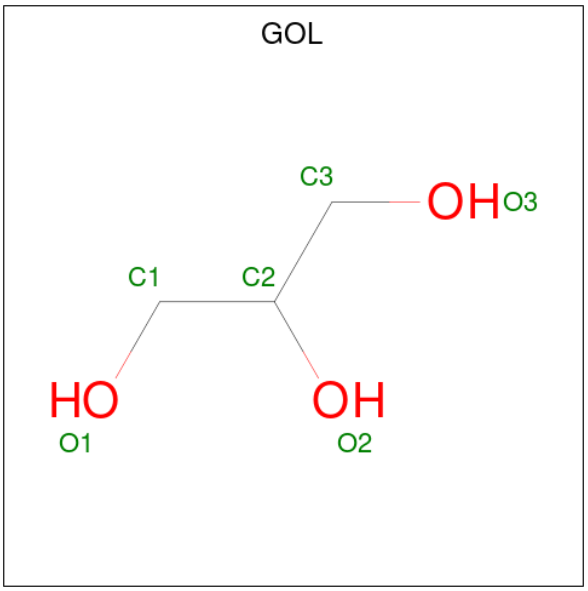
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	GLN	ARG	engineered mutation	UNP Q9L069
A	596	GLY	-	expression tag	UNP Q9L069
B	306	GLN	ARG	engineered mutation	UNP Q9L069
B	596	GLY	-	expression tag	UNP Q9L069

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	2	Total	Cl	0	0
			2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	371	Total O 371 371	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	366	Total 366	O 366	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.32Å 95.70Å 181.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.27 – 1.92	Depositor
% Data completeness (in resolution range)	100.0 (58.27-1.92)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.94 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.160 , 0.186	Depositor
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.061	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10211	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8422e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	GOL	A	602	-	5,5,5	0.46	0	5,5,5	1.76	1 (20%)
3	GOL	A	603	-	5,5,5	0.66	0	5,5,5	1.89	2 (40%)
3	GOL	B	607	-	5,5,5	1.08	0	5,5,5	1.13	0
3	GOL	A	604	-	5,5,5	0.53	0	5,5,5	0.90	0
3	GOL	B	608	-	5,5,5	0.46	0	5,5,5	1.38	1 (20%)
3	GOL	B	609	-	5,5,5	0.70	0	5,5,5	1.50	2 (40%)
3	GOL	B	605	-	5,5,5	0.81	0	5,5,5	1.18	1 (20%)
3	GOL	B	604	-	5,5,5	0.55	0	5,5,5	0.76	0
3	GOL	A	605	-	5,5,5	0.81	0	5,5,5	1.81	1 (20%)
3	GOL	B	606	-	5,5,5	0.63	0	5,5,5	1.34	0
3	GOL	B	603	-	5,5,5	0.60	0	5,5,5	1.97	2 (40%)

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	GOL	A	602	-	-	4/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	B	607	-	-	1/4/4/4	-
3	GOL	A	604	-	-	2/4/4/4	-
3	GOL	B	608	-	-	2/4/4/4	-
3	GOL	B	609	-	-	2/4/4/4	-
3	GOL	B	605	-	-	0/4/4/4	-
3	GOL	B	604	-	-	0/4/4/4	-
3	GOL	A	605	-	-	2/4/4/4	-
3	GOL	B	606	-	-	1/4/4/4	-
3	GOL	B	603	-	-	3/4/4/4	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	GOL	O3-C3-C2	-3.44	93.72	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	605	GOL	O2-C2-C1	3.34	123.85	109.12
3	B	603	GOL	C3-C2-C1	2.81	122.63	111.70
3	A	602	GOL	C3-C2-C1	2.66	122.04	111.70
3	B	609	GOL	O3-C3-C2	2.24	120.95	110.20
3	B	609	GOL	O2-C2-C1	2.14	118.55	109.12
3	B	605	GOL	C3-C2-C1	-2.12	103.45	111.70
3	A	603	GOL	O1-C1-C2	-2.07	100.26	110.20
3	B	608	GOL	O2-C2-C3	-2.06	100.03	109.12
3	B	603	GOL	O3-C3-C2	2.02	119.88	110.20

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	A	603	GOL	C1-C2-C3-O3
3	A	603	GOL	O2-C2-C3-O3
3	A	605	GOL	C1-C2-C3-O3
3	B	603	GOL	O1-C1-C2-C3
3	B	609	GOL	C1-C2-C3-O3
3	A	602	GOL	O2-C2-C3-O3
3	B	603	GOL	O1-C1-C2-O2
3	B	609	GOL	O2-C2-C3-O3
3	A	604	GOL	O1-C1-C2-C3
3	B	607	GOL	C1-C2-C3-O3
3	A	605	GOL	O2-C2-C3-O3
3	B	603	GOL	O2-C2-C3-O3
3	B	606	GOL	O1-C1-C2-C3
3	B	608	GOL	C1-C2-C3-O3
3	B	608	GOL	O2-C2-C3-O3
3	A	602	GOL	O1-C1-C2-O2
3	A	604	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.