Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 – 07:50 am GMT

PDB ID	:	2C81
Title	:	Crystal structures of the PLP- and PMP-bound forms of BtrR, a dual functional aminotransferase involved in butirosin biosynthesis.
Authors	:	Popovic, B.; Tang, X.; Chirgadze, D.Y.; Huang, F.; Blundell, T.L.; Spencer, J.B.
Deposited on	:	2005-11-30
Resolution	:	1.70 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 (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 (i)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.36

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 1.70 Å.

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

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

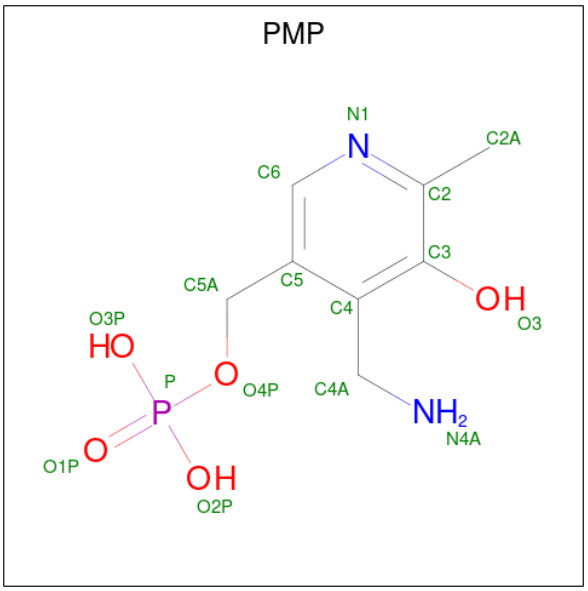
There are 3 unique types of molecules in this entry. The entry contains 3607 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTAMINE-2-DEOXY-SCYLLO-INOSOSE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	409	3196	2036	548	595	17	0	0	1

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	16	8	2	5	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	395	395	395	0	0

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	73.75Å 73.75Å 162.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.37 – 1.70	Depositor
% Data completeness (in resolution range)	91.5 (24.37-1.70)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.189 , 0.209	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3607	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
2	PMP	A	1416	-	16,16,16	5.67	9 (56%)	21,23,23	1.72	4 (19%)

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	PMP	A	1416	-	-	2/8/8/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1416	PMP	P-O1P	11.92	1.89	1.50
2	A	1416	PMP	C5-C4	10.59	1.55	1.40
2	A	1416	PMP	P-O2P	9.13	1.90	1.54
2	A	1416	PMP	O4P-C5A	-9.02	1.11	1.45
2	A	1416	PMP	P-O3P	6.61	1.80	1.54
2	A	1416	PMP	C2-N1	4.98	1.43	1.33
2	A	1416	PMP	C6-N1	2.60	1.39	1.34
2	A	1416	PMP	C3-C4	2.58	1.44	1.40
2	A	1416	PMP	P-O4P	2.03	1.66	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1416	PMP	O4P-P-O1P	5.07	120.69	106.47
2	A	1416	PMP	C5-C6-N1	-3.49	118.01	123.82
2	A	1416	PMP	C6-N1-C2	2.69	124.16	119.17
2	A	1416	PMP	C6-C5-C4	2.05	119.57	118.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1416	PMP	C5-C4-C4A-N4A
2	A	1416	PMP	C3-C4-C4A-N4A

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

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 (i)

5.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

5.4 Ligands (i)

EDS was not executed - this section is therefore empty.

5.5 Other polymers (i)

EDS was not executed - this section is therefore empty.