



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 15, 2026 – 10:36 AM UTC

PDB ID : 1E4O / pdb_00001e4o
Title : Phosphorylase recognition and phosphorolysis of its oligosaccharide substrate:
answers to a long outstanding question
Authors : Watson, K.A.; McCleverty, C.; Geremia, S.; Cottaz, S.; Driguez, H.; Johnson,
L.N.
Deposited on : 2000-07-11
Resolution : 2.90 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

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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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 2.90 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 4 unique types of molecules in this entry. The entry contains 13251 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.

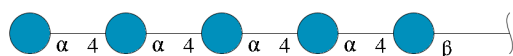
- Molecule 1 is a protein called MALTODEXTRIN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	796	Total	C	N	O	S	0	0	0
			6378	4068	1127	1163	20			
1	B	796	Total	C	N	O	S	0	0	0
			6378	4068	1127	1163	20			

There are 16 discrepancies between the modelled and reference sequences:

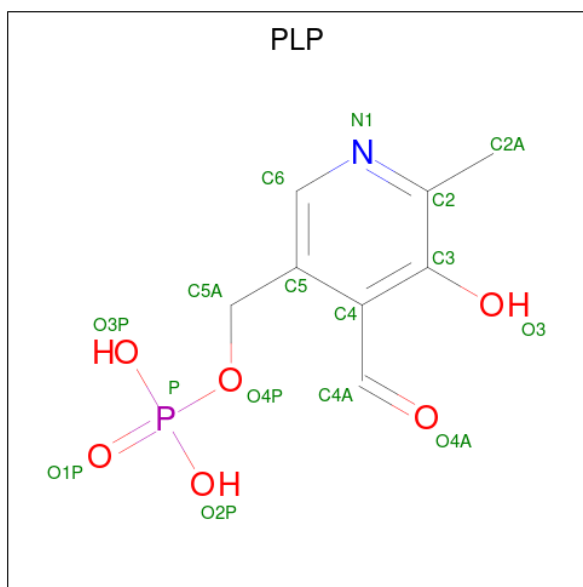
Chain	Residue	Modelled	Actual	Comment	Reference
A	293	LYS	GLU	conflict	UNP P00490
A	487	GLU	VAL	conflict	UNP P00490
A	489	PHE	LEU	conflict	UNP P00490
A	498	GLN	LEU	conflict	UNP P00490
A	501	GLU	VAL	conflict	UNP P00490
A	521	GLU	ASP	conflict	UNP P00490
A	547	HIS	ARG	conflict	UNP P00490
A	681	GLU	LYS	conflict	UNP P00490
B	293	LYS	GLU	conflict	UNP P00490
B	487	GLU	VAL	conflict	UNP P00490
B	489	PHE	LEU	conflict	UNP P00490
B	498	GLN	LEU	conflict	UNP P00490
B	501	GLU	VAL	conflict	UNP P00490
B	521	GLU	ASP	conflict	UNP P00490
B	547	HIS	ARG	conflict	UNP P00490
B	681	GLU	LYS	conflict	UNP P00490

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	5	Total	C	O	0	0	0
			56	30	26			
2	D	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	167	Total	O	0	0
			167	167		
4	B	186	Total	O	0	0
			186	186		

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.45Å 105.69Å 214.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90	Depositor
% Data completeness (in resolution range)	77.2 (50.00-2.90)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.5	Depositor
R, R_{free}	0.245 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13251	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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](#)

10 monosaccharides 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
2	BGC	C	1	2	12,12,12	0.44	0	17,17,17	0.65	0
2	GLC	C	2	2	11,11,12	0.51	0	15,15,17	0.56	0
2	GLC	C	3	2	11,11,12	0.48	0	15,15,17	0.57	0
2	GLC	C	4	2	11,11,12	0.66	0	15,15,17	0.72	0
2	GLC	C	5	2	11,11,12	0.49	0	15,15,17	0.94	2 (13%)
2	BGC	D	1	2	12,12,12	0.44	0	17,17,17	0.65	0
2	GLC	D	2	2	11,11,12	0.50	0	15,15,17	0.56	0
2	GLC	D	3	2	11,11,12	0.49	0	15,15,17	0.56	0
2	GLC	D	4	2	11,11,12	0.66	0	15,15,17	0.71	0
2	GLC	D	5	2	11,11,12	0.48	0	15,15,17	0.94	2 (13%)

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	BGC	C	1	2	-	1/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	D	1	2	-	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	GLC	C1-O5-C5	2.47	115.49	112.19
2	D	5	GLC	C1-O5-C5	2.44	115.46	112.19
2	D	5	GLC	C1-C2-C3	2.28	112.96	109.64
2	C	5	GLC	C1-C2-C3	2.26	112.94	109.64

There are no chirality outliers.

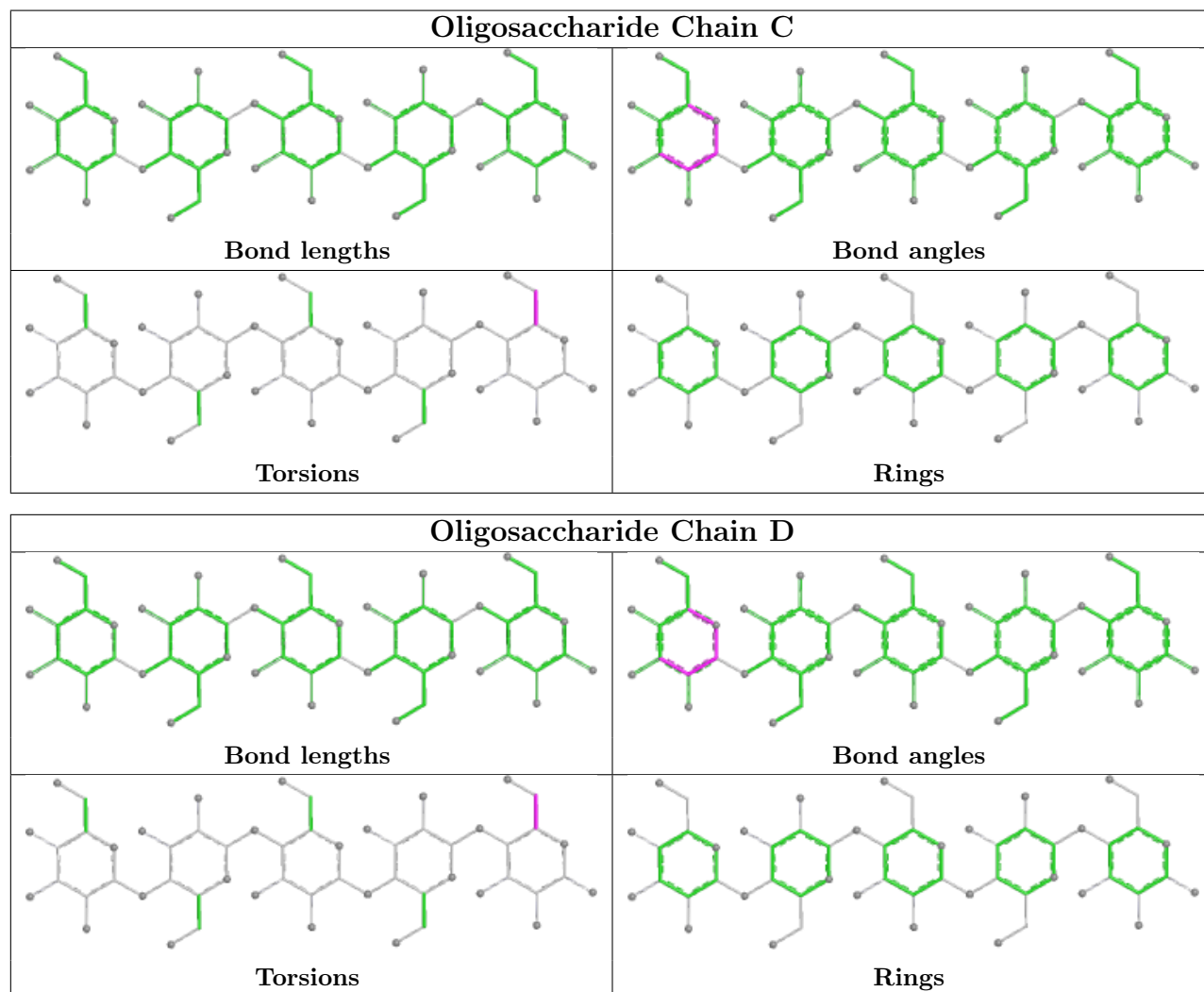
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	BGC	O5-C5-C6-O6
2	D	1	BGC	O5-C5-C6-O6

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 oligosaccharide.



4.6 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	PLP	B	999	1	15,15,16	2.75	6 (40%)	21,22,23	2.02	9 (42%)
3	PLP	A	999	1	15,15,16	2.75	6 (40%)	21,22,23	2.02	9 (42%)

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	PLP	B	999	1	-	1/6/6/8	0/1/1/1
3	PLP	A	999	1	-	1/6/6/8	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	PLP	P-O1P	5.72	1.68	1.50
3	A	999	PLP	P-O1P	5.71	1.68	1.50
3	A	999	PLP	P-O4P	-4.28	1.46	1.60
3	B	999	PLP	P-O4P	-4.27	1.46	1.60
3	B	999	PLP	C2-N1	4.21	1.41	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	PLP	C5-C6-N1	-3.70	117.80	123.83
3	A	999	PLP	C5-C6-N1	-3.69	117.82	123.83
3	A	999	PLP	C4A-C4-C3	-3.44	114.79	120.52
3	B	999	PLP	C4A-C4-C3	-3.44	114.79	120.52
3	A	999	PLP	C5A-C5-C6	-3.26	114.05	119.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	PLP	C4-C5-C5A-O4P
3	B	999	PLP	C4-C5-C5A-O4P

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

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.