



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 03:36 PM UTC

PDB ID : 2C4M / pdb_00002c4m
Title : Starch phosphorylase: structural studies explain oxyanion-dependent kinetic stability and regulatory control.
Authors : Purvis, A.; Nidetzky, B.; Watson, K.
Deposited on : 2005-10-20
Resolution : 1.90 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

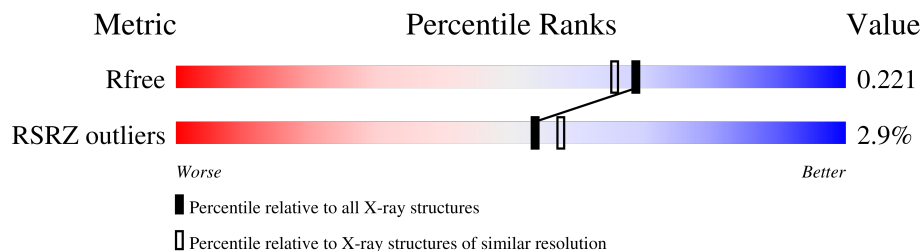
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
R_{free}	180053	7789 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	A	1634	-	X	-	-
2	PLP	C	1634	-	X	-	-
2	PLP	D	1634	-	X	-	-
4	FMT	A	1795	-	X	-	-
4	FMT	A	1796	-	X	-	-
4	FMT	A	1797	-	X	-	-
4	FMT	A	1798	-	X	-	-
4	FMT	A	1799	-	X	-	-
4	FMT	A	1800	-	X	-	-
4	FMT	A	1801	-	X	-	-
4	FMT	A	1802	-	X	-	-
4	FMT	A	1803	-	X	-	-
4	FMT	B	1799	-	X	-	-
4	FMT	B	1800	-	X	-	-
4	FMT	C	1799	-	X	-	-
4	FMT	C	1800	-	X	-	-
4	FMT	C	1801	-	X	-	-
4	FMT	C	1802	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FMT	D	1795	-	X	-	-
4	FMT	D	1796	-	X	-	-
4	FMT	D	1797	-	X	-	-
4	FMT	D	1798	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26654 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.

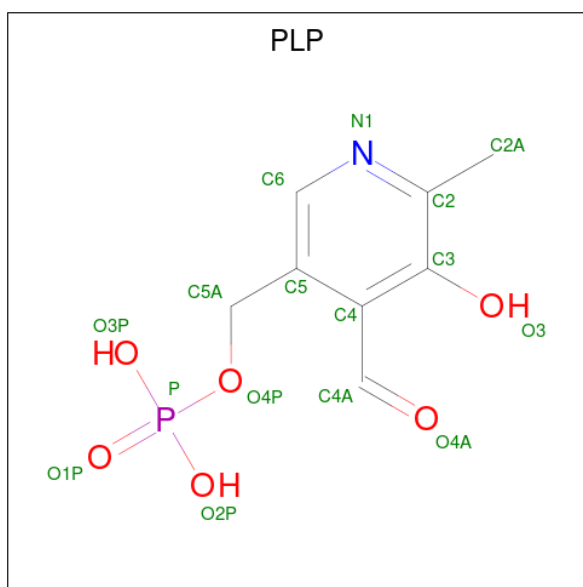
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	789	6328	4014	1088	1204	22	63	0	1
1	B	789	6326	4014	1087	1203	22	56	0	1
1	C	791	6344	4025	1091	1206	22	57	0	1
1	D	789	6328	4014	1088	1204	22	69	0	1

There are 4 discrepancies between the modelled and reference sequences:

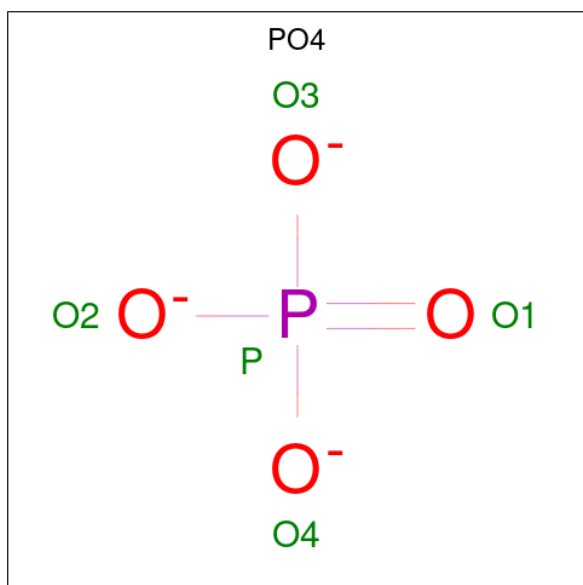
Chain	Residue	Modelled	Actual	Comment	Reference
A	224	ALA	SER	engineered mutation	UNP Q8KQ56
B	224	ALA	SER	engineered mutation	UNP Q8KQ56
C	224	ALA	SER	engineered mutation	UNP Q8KQ56
D	224	ALA	SER	engineered mutation	UNP Q8KQ56

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



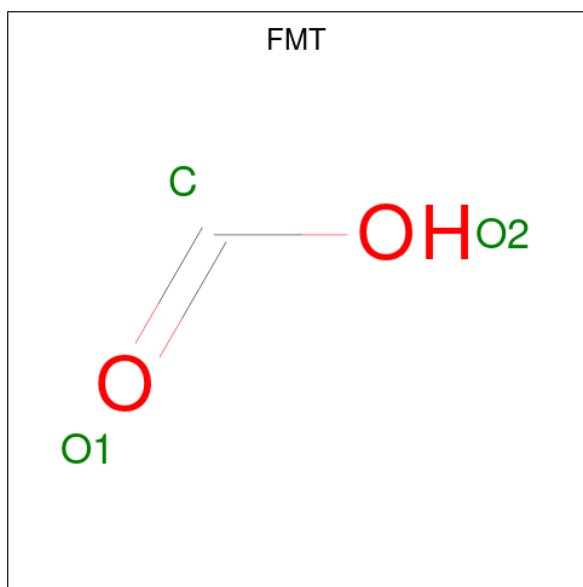
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	303	Total O 303 303	0	0
6	B	306	Total O 306 306	0	0
6	C	340	Total O 340 340	0	0
6	D	205	Total O 205 205	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.27Å 187.62Å 129.31Å 90.00° 112.48° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.3 (30.00-1.90) 89.4 (30.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.91Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.232 0.203 , 0.221	Depositor DCC
R_{free} test set	15209 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtrriage
Anisotropy	0.467	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26654	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.29 % 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 2.7096e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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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 oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

35 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
4	FMT	A	1802	-	2,2,2	5.34	2 (100%)	1,1,1	1.33	0
3	PO4	A	1794	-	4,4,4	1.43	1 (25%)	6,6,6	0.90	0
3	PO4	C	1796	-	4,4,4	1.88	1 (25%)	6,6,6	0.96	0
4	FMT	D	1798	-	2,2,2	5.36	2 (100%)	1,1,1	1.33	0
4	FMT	A	1796	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0
3	PO4	B	1798	-	4,4,4	1.43	1 (25%)	6,6,6	0.90	0
3	PO4	B	1797	-	4,4,4	1.35	1 (25%)	6,6,6	0.86	0
4	FMT	A	1799	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0
4	FMT	D	1795	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0
5	EDO	C	1803	-	3,3,3	0.42	0	2,2,2	0.38	0
3	PO4	D	1794	-	4,4,4	1.75	1 (25%)	6,6,6	0.95	0
2	PLP	D	1634	1	15,15,16	2.12	7 (46%)	21,22,23	2.27	10 (47%)
4	FMT	A	1797	-	2,2,2	5.36	2 (100%)	1,1,1	1.32	0
3	PO4	C	1797	-	4,4,4	1.36	1 (25%)	6,6,6	0.88	0
4	FMT	D	1797	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0
3	PO4	C	1798	-	4,4,4	1.45	1 (25%)	6,6,6	0.90	0
2	PLP	B	1634	1	15,15,16	1.96	5 (33%)	21,22,23	2.12	8 (38%)
4	FMT	A	1803	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0
4	FMT	C	1802	-	2,2,2	5.36	2 (100%)	1,1,1	1.33	0
4	FMT	A	1798	-	2,2,2	5.34	2 (100%)	1,1,1	1.33	0
4	FMT	B	1799	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0
2	PLP	C	1634	1	15,15,16	1.99	7 (46%)	21,22,23	2.09	8 (38%)
3	PO4	B	1795	-	4,4,4	1.65	1 (25%)	6,6,6	0.93	0
3	PO4	B	1796	-	4,4,4	1.35	1 (25%)	6,6,6	0.98	0
4	FMT	A	1795	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0
4	FMT	C	1799	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0
2	PLP	A	1634	1	15,15,16	2.13	7 (46%)	21,22,23	1.88	7 (33%)
4	FMT	C	1801	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0
5	EDO	B	1801	-	3,3,3	0.42	0	2,2,2	0.37	0
5	EDO	B	1802	-	3,3,3	0.42	0	2,2,2	0.38	0
4	FMT	A	1801	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0
4	FMT	B	1800	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMT	C	1800	-	2,2,2	5.36	2 (100%)	1,1,1	1.33	0
4	FMT	A	1800	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0
4	FMT	D	1796	-	2,2,2	5.35	2 (100%)	1,1,1	1.33	0

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
5	EDO	B	1802	-	-	1/1/1/1	-
2	PLP	A	1634	1	-	4/6/6/8	0/1/1/1
5	EDO	B	1801	-	-	1/1/1/1	-
5	EDO	C	1803	-	-	0/1/1/1	-
2	PLP	D	1634	1	-	5/6/6/8	0/1/1/1
2	PLP	C	1634	1	-	3/6/6/8	0/1/1/1
2	PLP	B	1634	1	-	3/6/6/8	0/1/1/1

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1802	FMT	O1-C	5.46	1.52	1.22
4	A	1797	FMT	O1-C	5.44	1.52	1.22
4	A	1795	FMT	O1-C	5.44	1.52	1.22
4	A	1801	FMT	O1-C	5.44	1.52	1.22
4	D	1795	FMT	O1-C	5.44	1.52	1.22

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1634	PLP	O3P-P-O4P	5.42	120.81	106.67
2	C	1634	PLP	C5A-C5-C6	-4.31	112.34	119.36
2	B	1634	PLP	C5-C6-N1	-4.04	117.26	123.83
2	B	1634	PLP	C5A-C5-C6	-3.72	113.29	119.36
2	A	1634	PLP	O2P-P-O4P	3.59	116.03	106.67

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1634	PLP	C5A-O4P-P-O2P
2	A	1634	PLP	C5A-O4P-P-O3P
2	B	1634	PLP	C5A-O4P-P-O3P
2	C	1634	PLP	C5A-O4P-P-O2P
2	C	1634	PLP	C5A-O4P-P-O3P

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](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	789/796 (99%)	0.28	17 (2%) 62 66	10, 28, 46, 75	16 (2%)
1	B	789/796 (99%)	0.29	25 (3%) 50 54	10, 28, 48, 69	14 (1%)
1	C	791/796 (99%)	0.22	17 (2%) 63 67	12, 27, 44, 74	15 (1%)
1	D	789/796 (99%)	0.57	33 (4%) 40 43	13, 34, 52, 71	16 (2%)
All	All	3158/3184 (99%)	0.34	92 (2%) 53 57	10, 29, 48, 75	61 (1%)

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	THR	5.9
1	C	336	VAL	5.7
1	A	337	LEU	5.1
1	C	338	THR	5.0
1	C	337	LEU	4.8

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FMT	A	1802	3/3	0.75	0.20	42,42,42,42	0
4	FMT	C	1802	3/3	0.75	0.16	36,36,38,39	0
4	FMT	A	1801	3/3	0.77	0.15	35,35,36,38	0
4	FMT	A	1800	3/3	0.78	0.17	38,38,40,40	0
4	FMT	B	1800	3/3	0.81	0.14	32,32,36,37	0
4	FMT	A	1803	3/3	0.82	0.13	39,39,39,40	0
4	FMT	A	1797	3/3	0.82	0.14	38,38,38,39	0
4	FMT	A	1796	3/3	0.82	0.15	39,39,39,41	0
3	PO4	C	1798	5/5	0.83	0.15	56,57,58,58	2
4	FMT	A	1795	3/3	0.83	0.16	41,41,43,43	0
4	FMT	A	1799	3/3	0.84	0.13	39,39,40,41	0
4	FMT	D	1796	3/3	0.84	0.13	35,35,37,37	0
4	FMT	C	1801	3/3	0.86	0.12	35,35,37,38	0
3	PO4	A	1794	5/5	0.86	0.14	56,57,57,57	3
4	FMT	C	1799	3/3	0.86	0.13	36,36,38,38	0
4	FMT	D	1797	3/3	0.86	0.11	36,36,37,38	0
3	PO4	B	1798	5/5	0.87	0.16	55,56,57,57	3
4	FMT	D	1798	3/3	0.89	0.10	40,40,40,40	0
5	EDO	B	1802	4/4	0.89	0.11	27,27,31,34	0
4	FMT	D	1795	3/3	0.90	0.13	32,32,33,36	0
5	EDO	C	1803	4/4	0.90	0.12	26,27,30,33	0
4	FMT	B	1799	3/3	0.92	0.10	37,37,40,40	0
4	FMT	C	1800	3/3	0.93	0.10	33,33,35,36	0
2	PLP	B	1634	15/16	0.94	0.08	19,21,42,44	0
2	PLP	C	1634	15/16	0.94	0.08	23,24,42,43	0
5	EDO	B	1801	4/4	0.94	0.13	41,42,43,43	0
2	PLP	D	1634	15/16	0.94	0.08	28,30,48,48	0
3	PO4	D	1794	5/5	0.94	0.11	37,39,41,41	3
3	PO4	C	1796	5/5	0.95	0.10	36,39,41,42	4
4	FMT	A	1798	3/3	0.95	0.08	23,23,26,28	0
3	PO4	C	1797	5/5	0.95	0.10	36,38,40,41	0
2	PLP	A	1634	15/16	0.95	0.07	21,24,42,43	0
3	PO4	B	1795	5/5	0.96	0.11	37,38,39,39	4
3	PO4	B	1796	5/5	0.96	0.09	38,38,40,41	3
3	PO4	B	1797	5/5	0.96	0.08	37,39,41,41	0

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

There are no such residues in this entry.