

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 12, 2023 – 01:22 PM EDT

PDB ID	:	408K
Title	:	Crystal structure of Type III pantothenate kinase from Burkholderia thailan-
		densis, apo structure
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID); Seattle
		Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2013-12-28
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 (1)) were used in the production of this report:

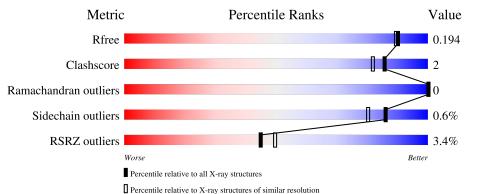
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain						
1	А	280	% <b>8</b> 6%	6%	8%				
1	В	280	83%	•	13%				



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4112 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.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	Δ	257	Total	С	Ν	0	S	Se	0	6	0
1	Л	201	1905	1212	345	341	4	3	0		
1	D	244	Total	С	Ν	0	S	Se	0	2	0
	D	244	1774	1127	320	320	4	3	0	2	0

• Molecule 1 is a protein called Type III pantothenate kinase.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-20	MSE	-	expression tag	UNP Q2T1M2
А	-19	ALA	-	expression tag	UNP Q2T1M2
А	-18	HIS	-	expression tag	UNP Q2T1M2
А	-17	HIS	-	expression tag	UNP Q2T1M2
А	-16	HIS	-	expression tag	UNP Q2T1M2
А	-15	HIS	-	expression tag	UNP Q2T1M2
А	-14	HIS	-	expression tag	UNP Q2T1M2
А	-13	HIS	-	expression tag	UNP Q2T1M2
А	-12	MSE	-	expression tag	UNP Q2T1M2
А	-11	GLY	-	expression tag	UNP Q2T1M2
А	-10	THR	-	expression tag	UNP Q2T1M2
А	-9	LEU	-	expression tag	UNP Q2T1M2
А	-8	GLU	-	expression tag	UNP Q2T1M2
А	-7	ALA	-	expression tag	UNP Q2T1M2
А	-6	GLN	-	expression tag	UNP Q2T1M2
А	-5	THR	-	expression tag	UNP Q2T1M2
А	-4	GLN	-	expression tag	UNP Q2T1M2
А	-3	GLY	-	expression tag	UNP Q2T1M2
А	-2	PRO	-	expression tag	UNP Q2T1M2
А	-1	GLY	-	expression tag	UNP Q2T1M2
А	0	SER	-	expression tag	UNP Q2T1M2
В	-20	MSE	-	expression tag	UNP Q2T1M2
В	-19	ALA	-	expression tag	UNP Q2T1M2
В	-18	HIS	-	expression tag	UNP Q2T1M2
В	-17	HIS	-	expression tag	UNP Q2T1M2

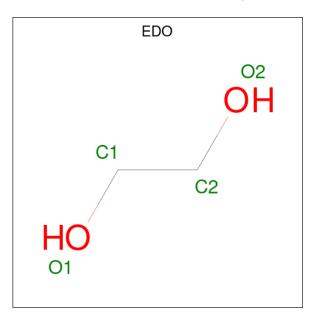
There are 42 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	-16	HIS	-	expression tag	UNP Q2T1M2
В	-15	HIS	-	expression tag	UNP Q2T1M2
В	-14	HIS	-	expression tag	UNP Q2T1M2
В	-13	HIS	-	expression tag	UNP Q2T1M2
В	-12	MSE	-	expression tag	UNP Q2T1M2
В	-11	GLY	-	expression tag	UNP Q2T1M2
В	-10	THR	-	expression tag	UNP Q2T1M2
В	-9	LEU	-	expression tag	UNP Q2T1M2
В	-8	GLU	-	expression tag	UNP Q2T1M2
В	-7	ALA	-	expression tag	UNP Q2T1M2
В	-6	GLN	-	expression tag	UNP Q2T1M2
В	-5	THR	-	expression tag	UNP Q2T1M2
В	-4	GLN	-	expression tag	UNP $Q2T1M2$
В	-3	GLY	-	expression tag	UNP Q2T1M2
В	-2	PRO	-	expression tag	UNP Q2T1M2
В	-1	GLY	-	expression tag	UNP Q2T1M2
В	0	SER	-	expression tag	UNP Q2T1M2

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• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



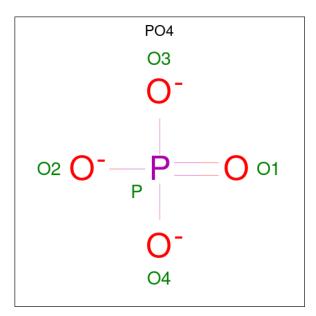
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Cl 1 1	0	0

• Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	В	1	Total 5	0 4	Р 1	0	0

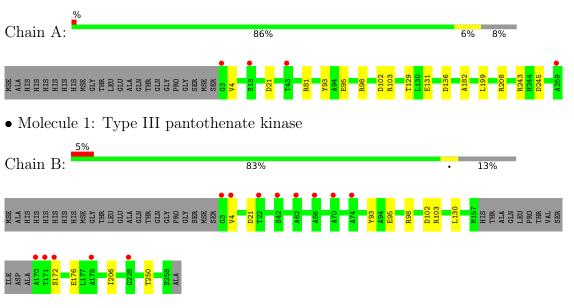
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	240	Total         O           243         243	0	3
5	В	160	Total O 160 160	0	0



# 3 Residue-property plots (i)

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: Type III pantothenate kinase



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	95.94Å 95.94Å 109.20Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	50.00 - 1.70	Depositor
Resolution (A)	47.97 - 1.70	EDS
% Data completeness	99.4 (50.00-1.70)	Depositor
(in resolution range)	$99.4 \ (47.97 - 1.70)$	EDS
$R_{merge}$	0.04	Depositor
R <sub>sym</sub>	0.04	Depositor
$< I/\sigma(I) > 1$	$3.98 (at 1.70 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
$R, R_{free}$	0.162 , $0.186$	Depositor
It, Itfree	0.174 , $0.194$	DCC
$R_{free}$ test set	2797 reflections $(4.97\%)$	wwPDB-VP
Wilson B-factor ( $Å^2$ )	23.1	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34 , $41.7$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4112	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PO4, CL

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| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	Bond lengths		nd angles
		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.71	0/1966	0.82	4/2689~(0.1%)
1	В	0.60	0/1820	0.77	1/2489~(0.0%)
All	All	0.66	0/3786	0.80	5/5178~(0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	81	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	А	102	ASP	CB-CG-OD1	7.79	125.31	118.30
1	В	102	ASP	CB-CG-OD1	7.06	124.65	118.30
1	А	136	ASP	CB-CG-OD1	5.38	123.15	118.30
1	А	208	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1905	0	1905	8	0
1	В	1774	0	1732	8	0
2	А	8	0	12	0	0
2	В	16	0	24	0	1



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	1	0	0	0	0
4	В	5	0	0	0	0
5	А	243	0	0	2	0
5	В	160	0	0	2	0
All	All	4112	0	3673	16	1

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The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129[B]:THR:HG23	5:A:435:HOH:O	1.96	0.64
1:A:129[B]:THR:HG21	5:A:607:HOH:O	1.98	0.61
1:A:95[A]:GLU:OE1	1:A:98:ARG:NE	2.33	0.60
1:B:130:LEU:HD21	1:B:206[A]:ILE:HD12	1.88	0.56
1:B:95[B]:GLU:OE1	1:B:98:ARG:NE	2.40	0.53
1:A:103:ARG:HD3	1:A:131:GLU:OE2	2.10	0.51
1:B:172:SER:O	1:B:176:GLU:HG3	2.10	0.51
1:B:250:THR:HG21	5:B:495:HOH:O	2.11	0.51
1:A:4:VAL:HG12	1:A:21:ASP:HB3	1.95	0.49
1:B:130:LEU:HD21	1:B:206[A]:ILE:CD1	2.45	0.46
1:A:243:ARG:HD2	1:A:245:ASP:OD1	2.16	0.45
1:B:4:VAL:HG12	1:B:21:ASP:HB3	1.99	0.44
1:A:182:ALA:HB1	1:A:199[B]:LEU:HD21	2.02	0.41
1:B:95[B]:GLU:HG2	1:B:98:ARG:HG3	2.03	0.41
1:B:103:ARG:NH1	5:B:433:HOH:O	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:EDO:O1	2:B:305:EDO:O2[8_666]	1.71	0.49



### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percen	tiles
1	А	261/280~(93%)	260 (100%)	1 (0%)	0	100	100
1	В	242/280~(86%)	240 (99%)	2(1%)	0	100	100
All	All	503/560~(90%)	500 (99%)	3~(1%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed Rotameric Outliers		Percentiles			
1	А	183/194~(94%)	182 (100%)	1 (0%)	88 83		
1	В	165/194~(85%)	164 (99%)	1 (1%)	86 80		
All	All	348/388~(90%)	346~(99%)	2(1%)	86 80		

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	93	TYR
1	В	93	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	241	HIS



#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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).

Mal	Mol Type Chain Res		ain Res Link		B	Bond lengths			Bond angles		
intoi Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
2	EDO	А	301	-	$3,\!3,\!3$	0.94	0	$2,\!2,\!2$	0.98	0	
2	EDO	В	303	-	3,3,3	0.49	0	$2,\!2,\!2$	0.24	0	
2	EDO	А	302	-	$3,\!3,\!3$	0.35	0	$2,\!2,\!2$	0.43	0	
2	EDO	В	302	-	3,3,3	0.61	0	$2,\!2,\!2$	0.06	0	
4	PO4	В	301	-	4,4,4	0.89	0	$6,\!6,\!6$	0.33	0	
2	EDO	В	304	-	$3,\!3,\!3$	0.52	0	$2,\!2,\!2$	0.24	0	
2	EDO	В	305	-	3,3,3	0.49	0	$2,\!2,\!2$	0.10	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
2	EDO	А	301	-	-	0/1/1/1	-
2	EDO	В	303	-	-	0/1/1/1	-
2	EDO	А	302	-	-	0/1/1/1	-



Mol	v	Chain	1 0		Chirals	Torsions	Rings
2	EDO	В	302	-	-	0/1/1/1	-
2	EDO	В	304	-	-	0/1/1/1	-
2	EDO	В	305	-	-	0/1/1/1	-

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There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mo	Chain	Res	Type	Clashes	Symm-Clashes
2	В	305	EDO	0	1

### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

### 6.1 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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	254/280~(90%)	-0.30	4 (1%) 72 76	15, 21, 49, 67	0
1	В	241/280~(86%)	-0.00	13 (5%) 25 28	16, 29, 62, 82	0
All	All	495/560~(88%)	-0.16	17 (3%) 45 50	15, 24, 57, 82	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	70	ALA	4.1
1	А	259	ALA	3.9
1	В	3	GLY	3.6
1	В	42	SER	3.5
1	В	170	ALA	3.3
1	В	171	THR	3.2
1	В	22	THR	2.9
1	А	13	SER	2.4
1	В	66	ALA	2.4
1	В	228	GLY	2.3
1	А	43	THR	2.2
1	А	3	GLY	2.2
1	В	74	ALA	2.2
1	В	178	ALA	2.1
1	В	172	SER	2.1
1	В	62	ALA	2.0
1	В	4	VAL	2.0

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

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



### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 6.4 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,  $95^{th}$  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(Å <sup>2</sup> )	Q<0.9
2	EDO	В	304	4/4	0.83	0.17	32,33,34,36	0
2	EDO	В	305	4/4	0.83	0.39	63,78,84,89	0
2	EDO	В	303	4/4	0.86	0.16	27,33,39,40	0
2	EDO	А	301	4/4	0.91	0.11	25,28,28,30	0
3	CL	А	303	1/1	0.93	0.07	59, 59, 59, 59	0
2	EDO	А	302	4/4	0.95	0.11	30,33,33,34	0
2	EDO	В	302	4/4	0.97	0.06	24,25,25,27	0
4	PO4	В	301	5/5	0.97	0.16	53,55,61,63	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

