

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

Dec 3, 2023 - 06.53 am GMT

PDB ID : 2IUC

Title: Structure of alkaline phosphatase from the Antarctic bacterium TAB5

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Deposited on : 2006-06-01

Resolution : 1.95 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.orgA 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 : NOT EXECUTED

Xtriage (Phenix) : 1.13 EDS : 2.36

buster-report : NOT EXECUTED

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)

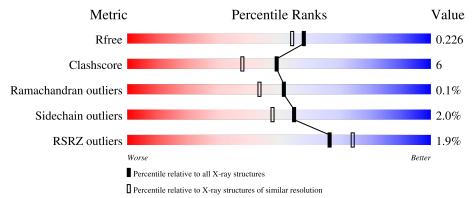
Validation Pipeline (wwPDB-VP) : 2.36

# 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 1.95 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	A	375	79%	11%	•	9%
2	В	375	77%	13%	•	9%

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:



$\mathbf{N}$	/Iol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
	5	PO4	A	1006	_	_	X	_



# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5544 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 ALKALINE PHOSPHATASE.

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	340	Total 2536	C 1601	N 414	O 514	S 7	5	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	SER	LYS	$\operatorname{conflict}$	UNP Q9KWY4
A	225	SER	LYS	$\operatorname{conflict}$	UNP Q9KWY4
A	327	SER	GLU	conflict	UNP Q9KWY4
A	331	SER	THR	conflict	UNP Q9KWY4

• Molecule 2 is a protein called ALKALINE PHOSPHATASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	342	Total 2553	C 1611	N 415	O 520	S 7	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	58	SER	GLU	$\operatorname{conflict}$	UNP Q9KWY4
В	122	SER	ASN	conflict	UNP Q9KWY4
В	176	SER	LYS	$\operatorname{conflict}$	UNP Q9KWY4
В	178	SER	LYS	$\operatorname{conflict}$	UNP Q9KWY4
В	180	SER	LYS	conflict	UNP Q9KWY4
В	290	SER	LYS	$\operatorname{conflict}$	UNP Q9KWY4
В	313	SER	LYS	conflict	UNP Q9KWY4

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

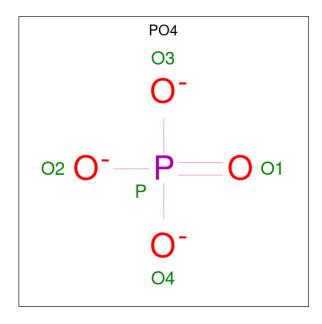


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	В	2	Total Zn 2 2	0	0

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0
4	В	3	Total Mg 3 3	0	0

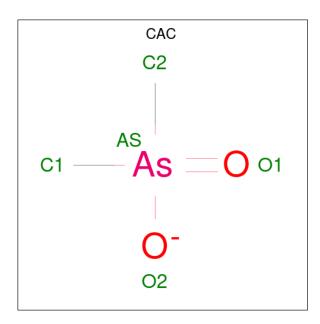
 $\bullet$  Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total P 1 1	0	0
5	В	1	Total P 1 1	0	0

 $\bullet$  Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula:  $\mathrm{C_2H_6AsO_2}).$ 





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	В	1	Total 5	As 1	C 2	O 2	0	0

### • Molecule 7 is water.

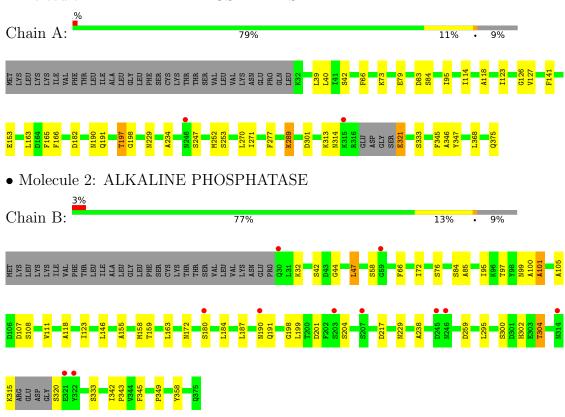
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	252	Total O 252 252	0	0
7	В	186	Total O 186 186	0	0



# 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: ALKALINE PHOSPHATASE





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	70.04Å 173.18Å 55.34Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.74 - 1.95	Depositor
resolution (A)	8.72 - 1.95	EDS
% Data completeness	97.2 (8.74-1.95)	Depositor
(in resolution range)	97.2 (8.72-1.95)	EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.92 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
P. P.	0.162 , $0.225$	Depositor
$R, R_{free}$	0.164 , $0.226$	DCC
$R_{free}$ test set	2433 reflections $(5.07\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.47,62.4	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.22% of the height of the origin peak. No significant pseudotranslation is detected.

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



<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: CAC, ZN, MG, PO4

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			nd lengths	Bond angles	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	1.29	$7/2583 \ (0.3\%)$	0.96	4/3499 (0.1%)
2	В	1.27	2/2600 (0.1%)	0.94	5/3523 (0.1%)
All	All	1.28	9/5183 (0.2%)	0.95	9/7022 (0.1%)

#### All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
1	A	321	GLU	CA-CB	-6.07	1.40	1.53
1	A	346	ALA	CA-CB	5.96	1.65	1.52
1	A	141	PHE	CE1-CZ	5.56	1.48	1.37
1	A	153	GLU	CG-CD	5.24	1.59	1.51
2	В	238	ALA	CA-CB	5.24	1.63	1.52
1	A	73	LYS	CD-CE	5.23	1.64	1.51
2	В	101	ALA	CA-CB	-5.23	1.41	1.52
1	A	79	GLU	CB-CG	5.21	1.62	1.52
1	A	234	ALA	CA-CB	5.07	1.63	1.52

#### All (9) bond angle outliers are listed below:

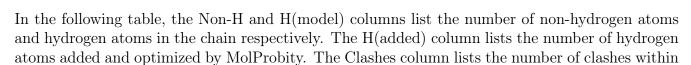
Mol	Chain	Res	Type	Atoms	Z	${\bf Observed}(^o)$	$\operatorname{Ideal}(^{o})$
2	В	47	LEU	CB-CG-CD2	6.69	122.36	111.00
2	В	199	LEU	CB-CG-CD1	-5.79	101.16	111.00
1	A	83	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	301	ASP	CB-CG-OD1	5.66	123.39	118.30
2	В	111	VAL	CG1-CB-CG2	-5.47	102.15	110.90
2	В	295	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	A	321	GLU	N-CA-CB	5.03	119.65	110.60
1	A	289	LYS	CD-CE-NZ	5.02	123.24	111.70
2	В	217	ASP	CB-CG-OD1	5.00	122.80	118.30



There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2536	0	2434	23	0
2	В	2553	0	2453	37	0
3	A	2	0	0	0	0
3	В	2	0	0	0	0
4	A	3	0	0	0	0
4	В	3	0	0	0	0
5	A	1	0	0	2	0
5	В	1	0	0	1	0
6	В	5	0	0	0	0
7	A	252	0	0	6	0
7	В	186	0	0	6	0
All	All	5544	0	4887	59	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 6.

All (59) 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:84:SER:OG	5:A:1006:PO4:P	2.08	1.11
2:B:84:SER:OG	5:B:1757:PO4:P	2.08	1.11
2:B:184:LEU:HB3	7:B:2096:HOH:O	1.59	1.00
1:A:198:GLY:HA3	7:A:2136:HOH:O	1.62	0.97
2:B:198:GLY:HA3	7:B:2102:HOH:O	1.65	0.96
2:B:259:ASP:OD1	2:B:304:THR:HG21	1.80	0.82
2:B:201:ASP:CB	7:B:2105:HOH:O	2.29	0.79
2:B:184:LEU:HD13	7:B:2096:HOH:O	1.82	0.77
2:B:302:HIS:CE1	2:B:304:THR:HG22	2.23	0.73
2:B:198:GLY:CA	7:B:2102:HOH:O	2.28	0.71
1:A:314:ASN:O	1:A:321:GLU:HA	1.89	0.71
2:B:44:GLY:CA	2:B:304:THR:HG23	2.24	0.68

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Continuea from prev		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:271:ILE:HG23	7:A:2190:HOH:O	1.94	0.67
2:B:44:GLY:HA2	2:B:304:THR:HG23	1.76	0.66
1:A:247:SER:HB3	7:A:2170:HOH:O	1.95	0.66
2:B:159:THR:O	2:B:190:ASN:ND2	2.30	0.65
2:B:95:ILE:CD1	2:B:105:ALA:HA	2.28	0.63
1:A:197:THR:CG2	7:A:2135:HOH:O	2.48	0.61
1:A:118:ALA:HB1	1:A:123:ILE:HB	1.84	0.60
1:A:197:THR:HG22	7:A:2135:HOH:O	2.02	0.59
2:B:302:HIS:CE1	2:B:304:THR:CG2	2.86	0.59
2:B:315:LYS:HA	2:B:320:SER:O	2.05	0.56
2:B:302:HIS:ND1	2:B:304:THR:HG22	2.21	0.55
2:B:107:ASP:O	2:B:108:SER:HB2	2.08	0.54
2:B:302:HIS:HE1	2:B:304:THR:CG2	2.20	0.54
2:B:44:GLY:HA2	2:B:304:THR:CG2	2.38	0.53
2:B:158:MET:HG3	2:B:187:LEU:HD21	1.90	0.53
1:A:84:SER:CB	5:A:1006:PO4:P	2.96	0.53
1:A:375:GLN:O	7:A:2252:HOH:O	2.18	0.53
2:B:118:ALA:HB1	2:B:123:ILE:HB	1.93	0.50
1:A:182:ASP:OD1	1:A:182:ASP:C	2.50	0.50
1:A:126:GLY:HA2	1:A:165:PHE:O	2.12	0.50
1:A:40:LEU:HD23	1:A:253:SER:HB2	1.93	0.49
2:B:76:SER:HB2	2:B:97:THR:O	2.11	0.49
1:A:333:SER:HB3	2:B:333:SER:HB3	1.94	0.48
1:A:270:LEU:C	1:A:270:LEU:HD23	2.34	0.47
1:A:289:LYS:HG2	1:A:347:TYR:OH	2.15	0.47
2:B:72:ILE:HA	2:B:358:TYR:O	2.15	0.46
1:A:190:ASN:O	1:A:191:GLN:HB2	2.15	0.46
2:B:66:PHE:CG	2:B:345:PHE:HB3	2.50	0.46
2:B:108:SER:HB3	2:B:146:LEU:HD22	1.99	0.45
2:B:190:ASN:O	2:B:191:GLN:HB2	2.16	0.45
1:A:127:VAL:O	1:A:166:PHE:HA	2.18	0.44
2:B:302:HIS:HD1	2:B:304:THR:HG22	1.83	0.44
2:B:99:ASN:O	2:B:100:ALA:HB3	2.17	0.44
1:A:66:PHE:CG	1:A:345:PHE:HB3	2.53	0.44
1:A:39:LEU:O	1:A:252:MET:HA	2.17	0.43
2:B:342:ILE:HA	2:B:343:PRO:HD3	1.84	0.43
2:B:32:LYS:HB3	2:B:349:PRO:HB3	2.01	0.43
1:A:114:ILE:CD1	1:A:368:LEU:HD21	2.49	0.43
2:B:85:ALA:HB1	2:B:101:ALA:O	2.19	0.42
2:B:42:SER:O	2:B:300:SER:HB3	2.20	0.42
1:A:42:SER:HB3	1:A:277:PHE:CE2	2.55	0.42

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	.,	10	1

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap (Å)
2:B:172:ASN:OD1	7:B:2088:HOH:O	2.22	0.42
1:A:40:LEU:CD2	1:A:253:SER:HB2	2.50	0.42
2:B:44:GLY:HA3	2:B:304:THR:HG23	2.01	0.41
2:B:108:SER:HB3	2:B:146:LEU:CD2	2.51	0.41
2:B:302:HIS:HE1	2:B:304:THR:HG21	1.86	0.40
2:B:155:ALA:O	2:B:158:MET:HB3	2.20	0.40

There are no symmetry-related clashes.

### 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	Perce	$\mathbf{ntiles}$
1	A	336/375~(90%)	322 (96%)	14 (4%)	0	100	100
2	В	338/375~(90%)	326 (96%)	11 (3%)	1 (0%)	41	30
All	All	674/750 (90%)	648 (96%)	25 (4%)	1 (0%)	51	43

#### All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	180	SER

#### 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	A	268/307 (87%)	263 (98%)	5 (2%)	57 50
2	В	272/307 (89%)	266 (98%)	6 (2%)	52 44
All	All	540/614 (88%)	529 (98%)	11 (2%)	55 48

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ILE
1	A	163	LEU
1	A	197	THR
1	A	229	ASN
1	A	313	LYS
2	В	47	LEU
2	В	58	SER
2	В	163	LEU
2	В	204	SER
2	В	229	ASN
2	В	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	240	GLN
1	A	265	ASN
2	В	68	ASN
2	В	229	ASN

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

Mogul was not executed - this section is therefore empty.

# 5.5 Carbohydrates (i)

Mogul was not executed - this section is therefore empty.



## 5.6 Ligand geometry (i)

Mogul was not executed - this section is therefore empty.

## 5.7 Other polymers (i)

Mogul was not executed - this section is therefore empty.

## 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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	A	340/375 (90%)	-0.27	2 (0%) 89 93	9, 15, 28, 51	1 (0%)
2	В	342/375 (91%)	-0.10	11 (3%) 47 57	10, 17, 34, 49	0
All	All	682/750 (90%)	-0.19	13 (1%) 66 74	9, 16, 32, 51	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	59	GLY	4.1
2	В	322	TYR	3.2
2	В	245	ASP	3.0
2	В	246	ASN	3.0
2	В	207	SER	2.7
2	В	314	ASN	2.6
2	В	203	SER	2.6
1	A	246	ASN	2.5
2	В	180	SER	2.4
1	A	315	LYS	2.3
2	В	30	GLN	2.3
2	В	321	GLU	2.2
2	В	190	ASN	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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	PO4	В	1757	1/5	0.95	0.18	28,28,28,28	0
5	PO4	A	1006	1/5	0.96	0.15	24,24,24,24	0
4	MG	В	1010	1/1	0.97	0.09	29,29,29,29	0
6	CAC	В	1756	5/5	0.97	0.12	17,22,25,28	5
4	MG	A	1003	1/1	0.98	0.05	15,15,15,15	0
4	MG	В	1008	1/1	0.98	0.05	19,19,19,19	0
4	MG	A	1004	1/1	0.99	0.03	22,22,22,22	0
4	MG	В	1009	1/1	0.99	0.05	13,13,13,13	0
4	MG	A	1005	1/1	0.99	0.12	23,23,23,23	0
3	ZN	A	1002	1/1	1.00	0.03	18,18,18,18	0
3	ZN	В	1006	1/1	1.00	0.04	25,25,25,25	0
3	ZN	В	1007	1/1	1.00	0.04	18,18,18,18	0
3	ZN	A	1001	1/1	1.00	0.08	28,28,28,28	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

