

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

#### Apr 14, 2025 – 12:16 PM JST

PDB ID	:	$9 \mathrm{JIX} \ / \ \mathrm{pdb} \ 00009 \mathrm{jix}$
Title	:	Crystal structure of de novo designed ATPase, $PL2x4_2$
Authors	:	Kosugi, T.; Tanabe, M.; Koga, N.
Deposited on	:	2024-09-12
Resolution	:	2.29  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:

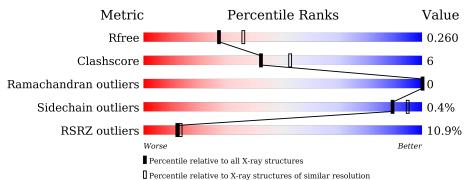
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

# 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 2.29 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	158	84%	13%	•••
1	С	158	80%	14%	6%



#### 9JIX

## 2 Entry composition (i)

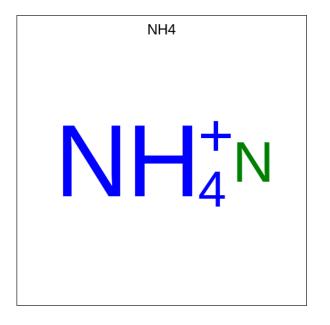
There are 6 unique types of molecules in this entry. The entry contains 2358 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 De Novo Designed ATPase, PL2x4\_2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	А	154	Total         C         N         O         S           1166         734         204         227         1	0	0	0
1	С	149	Total         C         N         O           1142         719         202         221	0	1	0

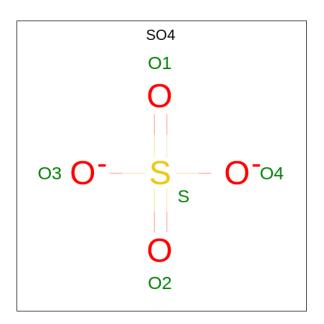
• Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula:  $H_4N$ ).



[	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	2	А	1	Total N 1 1	0	0

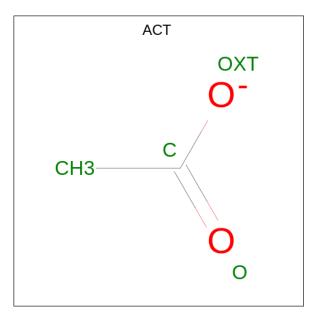
• Molecule 3 is SULFATE ION (CCD ID: SO4) (formula:  $O_4S$ ).





M	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	}	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	8	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



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

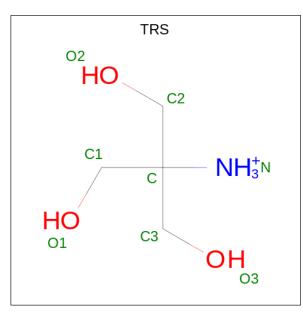
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Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
4	А	1	Total 4	${ m C} 2$	O 2	0	0

• Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{N} \\ 8 & 4 & 1 \end{array}$	O 3	0	0

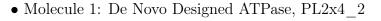
• Molecule 6 is water.

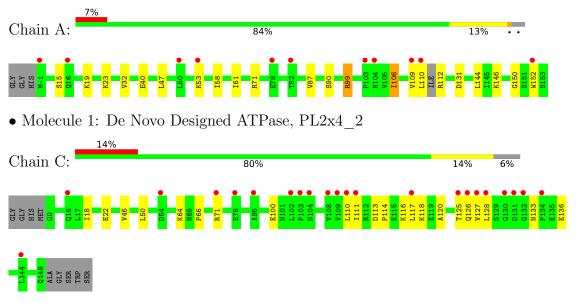
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	18	Total         O           18         18	0	0
6	С	1	Total O 1 1	0	0



## 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.







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	$\begin{array}{cccc} 77.66 \text{\AA} & 77.66 \text{\AA} & 101.53 \text{\AA} \\ 90.00^{\circ} & 90.00^{\circ} & 120.00^{\circ} \end{array}$	Depositor
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness (in resolution range)	$100.0 (40.52-2.29) \\ 100.0 (40.52-2.29)$	Depositor EDS
R <sub>merge</sub>	0.06	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.19 (at 2.29 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
$R, R_{free}$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor DCC
$R_{free}$ test set	846 reflections $(5.15\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	58.2	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.31, $46.9$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2358	wwPDB-VP
Average B, all atoms $(Å^2)$	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.70% 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: SO4, NH4, TRS, ACT

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	Bo	nd lengths	Bond angles	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.47	0/1176	0.74	1/1591~(0.1%)
1	С	0.45	2/1151~(0.2%)	0.71	0/1558
All	All	0.46	2/2327~(0.1%)	0.72	1/3149~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	С	126	GLN	C-N	6.64	1.49	1.34
1	С	125	THR	C-N	6.38	1.48	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	А	99	ARG	NE-CZ-NH2	-5.59	117.50	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	152	TRP	Peptide



#### 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	1166	0	1246	16	4
1	С	1142	0	1233	13	0
2	А	1	0	0	0	0
3	А	5	0	0	0	0
3	С	5	0	0	0	0
4	А	12	0	9	1	0
5	С	8	0	12	0	0
6	А	18	0	0	3	0
6	С	1	0	0	0	0
All	All	2358	0	2500	30	4

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 (30) 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:40:GLU:HG3	1:A:71:ARG:HB3	1.77	0.65
1:C:114:PRO:O	1:C:118:LYS:HG2	1.98	0.64
1:C:111:ILE:HD12	1:C:113:ASP:HB2	1.83	0.58
1:C:110:LEU:HD12	1:C:127:VAL:HG21	1.88	0.56
1:A:109:VAL:HG22	6:A:1306:HOH:O	2.05	0.56
1:A:146:LYS:HA	1:A:150:GLY:O	2.06	0.56
1:A:32:VAL:HG22	1:A:58:ILE:HB	1.91	0.53
1:A:110:LEU:O	1:A:112:ARG:N	2.43	0.52
1:C:114:PRO:HA	1:C:117:LEU:HB3	1.91	0.51
1:A:87:VAL:HB	1:A:106:ILE:HD13	1.92	0.51
1:A:144:LEU:C	1:A:144:LEU:HD23	2.33	0.48
1:A:15:SER:O	1:A:19:LYS:HG2	2.13	0.48
1:A:53:LYS:O	1:A:53:LYS:HG2	2.13	0.47
1:C:71[A]:ARG:HD2	1:C:71[A]:ARG:HA	1.62	0.47
1:A:99:ARG:HD2	1:A:106:ILE:HG13	1.97	0.47
1:C:110:LEU:HB3	1:C:111:ILE:H	1.56	0.47
1:C:133:ASN:HD22	1:C:136:GLU:H	1.64	0.45
1:A:112:ARG:NE	6:A:1301:HOH:O	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LYS:O	1:C:120:ALA:N	2.47	0.44
1:A:99:ARG:HD2	1:A:99:ARG:HA	1.79	0.44
1:A:23:LYS:HB2	1:A:23:LYS:HE3	1.76	0.43
1:A:19:LYS:HD3	1:A:19:LYS:HA	1.93	0.43
1:C:18:ILE:HG22	1:C:22:GLU:OE2	2.19	0.42
4:A:1204:ACT:H2	6:A:1306:HOH:O	2.18	0.42
1:A:90:SER:O	1:A:110:LEU:HD12	2.20	0.42
1:C:64:LYS:O	1:C:66:PRO:HD3	2.21	0.41
1:C:100:GLU:OE1	1:C:100:GLU:HA	2.20	0.41
1:A:47:LEU:HD21	1:A:61:ILE:HD11	2.02	0.41
1:C:46:VAL:O	1:C:50:LEU:HB2	2.21	0.40
1:C:127:VAL:O	1:C:128:LEU:C	2.60	0.40

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All (4) 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)
1:A:110:LEU:CD2	$1:A:131:ASP:OD2[4_555]$	1.49	0.71
1:A:109:VAL:O	$1:A:112:ARG:CD[4_555]$	1.60	0.60
1:A:110:LEU:CD2	1:A:131:ASP:CG[4_555]	2.10	0.10
1:A:131:ASP:OD2	$1:A:131:ASP:OD2[4_555]$	2.11	0.09

### 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	Percer	ntiles
1	А	150/158~(95%)	146~(97%)	4(3%)	0	100	100
1	С	148/158~(94%)	140 (95%)	8 (5%)	0	100	100
All	All	298/316~(94%)	286 (96%)	12~(4%)	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	131/133~(98%)	130~(99%)	1 (1%)	79 89
1	С	129/133~(97%)	129 (100%)	0	100 100
All	All	260/266~(98%)	259 (100%)	1 (0%)	89 95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	106	ILE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	А	28	GLN
1	А	126	GLN
1	А	148	GLN
1	С	133	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)

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

### 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is modelled with single atom - leaving 6 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).

Mol	Trune	Chain	Dec	Link	В	ond leng	gths	В	ond ang	gles
	Type	Chain	Res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	ACT	А	1204	-	$3,\!3,\!3$	0.94	0	$3,\!3,\!3$	0.79	0
4	ACT	А	1203	-	3,3,3	0.93	0	$3,\!3,\!3$	0.82	0
5	TRS	С	401	-	7,7,7	0.11	0	$9,\!9,\!9$	0.23	0
3	SO4	С	402	-	4,4,4	0.45	0	$6,\!6,\!6$	0.06	0
4	ACT	А	1205	-	3,3,3	0.95	0	$3,\!3,\!3$	0.79	0
3	SO4	А	1202	-	4,4,4	0.52	0	$6,\!6,\!6$	0.05	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	TRS	С	401	-	-	0/9/9/9	-

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:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	1204	ACT	1	0

### 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	154/158~(97%)	0.44	11 (7%) 23 25	38, 58, 88, 115	0
1	С	149/158~(94%)	1.04	22 (14%) 7 8	38, 89, 167, 185	1 (0%)
All	All	303/316~(95%)	0.74	33 (10%) 12 13	38, 71, 149, 185	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	110	LEU	5.3
1	А	103	PRO	4.6
1	С	127	VAL	4.5
1	С	110	LEU	4.1
1	А	104	ASN	4.1
1	С	109	VAL	3.9
1	А	152	TRP	3.9
1	С	103	PRO	3.9
1	С	125	THR	3.8
1	С	117	LEU	3.3
1	А	-1	MET	3.3
1	С	111	ILE	3.1
1	С	131	ASP	3.0
1	А	50	LEU	2.7
1	С	144	LEU	2.7
1	С	134	PRO	2.6
1	А	78	GLU	2.6
1	С	78	GLU	2.5
1	С	130	GLY	2.5
1	А	82	THR	2.5
1	С	95	ALA	2.5
1	С	16	GLN	2.3
1	А	109	VAL	2.3
1	С	128	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	А	53	LYS	2.3
1	С	132	GLY	2.3
1	С	71[A]	ARG	2.2
1	А	16	GLN	2.2
1	С	102	LEU	2.2
1	С	108	VAL	2.2
1	С	54	ASP	2.1
1	С	104	ASN	2.1
1	С	126	GLN	2.1

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#### 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
5	TRS	С	401	8/8	0.59	0.14	108,115,122,126	0
4	ACT	А	1205	4/4	0.60	0.16	95,98,98,101	0
4	ACT	А	1203	4/4	0.75	0.15	83,91,94,94	0
4	ACT	А	1204	4/4	0.78	0.23	62,67,70,74	0
3	SO4	С	402	5/5	0.89	0.08	92,94,101,107	0
3	SO4	А	1202	5/5	0.96	0.10	56,57,59,61	0
2	NH4	А	1201	1/1	0.99	0.24	35,35,35,35	1

#### 6.5 Other polymers (i)

There are no such residues in this entry.

