



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:12 AM GMT

PDB ID : 1YJ5  
Title : Molecular architecture of mammalian polynucleotide kinase, a DNA repair enzyme  
Authors : Bernstein, N.K.; Williams, R.S.; Rakovszky, M.L.; Cui, D.; Green, R.; Karimi-Busheri, F.; Mani, R.S.; Galicia, S.; Koch, C.A.; Cass, C.E.; Durocher, D.; Weinfeld, M.; Glover, J.N.M.  
Deposited on : 2005-01-13  
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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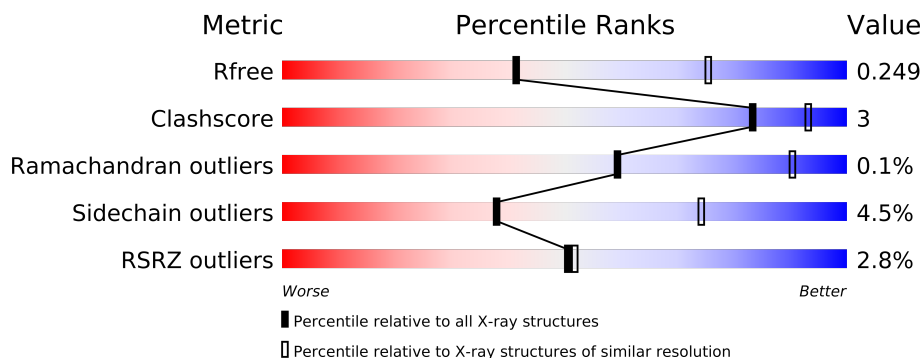
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	383	
1	B	383	
2	C	143	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	105	-	X
3	SO4	A	107	-	X
3	SO4	A	108	-	X
3	SO4	A	110	-	X
3	SO4	B	106	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	B	109	-	X
3	SO4	B	111	-	X
3	SO4	B	112	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6844 atoms, of which 0 are hydrogen and 0 are deuterium.

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 5' polynucleotide kinase-3' phosphatase catalytic domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	Se	0	0	0
			2955	1891	517	535	7	5			
1	B	383	Total	C	N	O	S	Se	0	0	0
			2979	1905	521	541	7	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MSE	MET	MODIFIED RESIDUE	UNP Q9JLV6
A	264	MSE	MET	MODIFIED RESIDUE	UNP Q9JLV6
A	465	MSE	MET	MODIFIED RESIDUE	UNP Q9JLV6
A	476	MSE	MET	MODIFIED RESIDUE	UNP Q9JLV6
A	478	MSE	MET	MODIFIED RESIDUE	UNP Q9JLV6
B	219	MSE	MET	MODIFIED RESIDUE	UNP Q9JLV6
B	264	MSE	MET	MODIFIED RESIDUE	UNP Q9JLV6
B	465	MSE	MET	MODIFIED RESIDUE	UNP Q9JLV6
B	476	MSE	MET	MODIFIED RESIDUE	UNP Q9JLV6
B	478	MSE	MET	MODIFIED RESIDUE	UNP Q9JLV6

- Molecule 2 is a protein called 5' polynucleotide kinase-3' phosphatase FHA domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	105	Total	C	N	O	S	0	0	0
			772	491	137	143	1			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total 50	O 50	0	0
4	B	26	Total 26	O 26	0	0
4	C	2	Total 2	O 2	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.47Å 169.87Å 77.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 2.80 29.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.75-2.80) 99.5 (29.80-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.219 , 0.253 0.218 , 0.249	Depositor DCC
$R_{free}$ test set	1562 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 13.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 31575 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6844	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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 lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/3027	0.46	0/4099
1	B	0.31	0/3052	0.47	0/4132
2	C	0.28	0/789	0.48	0/1081
All	All	0.30	0/6868	0.47	0/9312

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2955	0	2947	19	0
1	B	2979	0	2958	18	0
2	C	772	0	772	4	0
3	A	35	0	0	0	0
3	B	25	0	0	0	0
4	A	50	0	0	0	0
4	B	26	0	0	0	0
4	C	2	0	0	0	0
All	All	6844	0	6677	40	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (40) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:461:ARG:HH11	1:A:520:SER:HB2	1.41	0.85
1:A:403:ARG:NH2	1:B:338:PRO:O	2.26	0.69
1:A:269:GLN:HE22	1:A:278:ILE:H	1.41	0.67
1:B:400:SER:HB2	1:B:402:GLN:HE21	1.61	0.65
1:A:430:ARG:NH2	1:A:486:GLU:O	2.32	0.61
1:B:150:LYS:H	1:B:150:LYS:HD3	1.69	0.58
1:A:400:SER:HB2	1:A:402:GLN:HE21	1.68	0.57
1:A:290:ALA:HB3	1:A:292:ARG:HD2	1.87	0.57
1:A:457:ARG:HG3	1:A:478:MSE:HE2	1.92	0.51
1:A:377:LYS:O	1:A:381:ILE:HG12	2.12	0.50
1:A:178:THR:HG22	1:A:181:GLY:H	1.78	0.49
1:B:206:ALA:HB2	1:B:212:LEU:HD11	1.96	0.48
1:A:171:LEU:HD22	1:A:176:ILE:HG12	1.95	0.48
1:A:153:LEU:HB2	1:A:250:VAL:HB	1.95	0.48
2:C:54:ILE:HG23	2:C:63:ALA:HB3	1.96	0.47
1:B:153:LEU:HB2	1:B:250:VAL:HB	1.97	0.47
1:B:166:VAL:HG22	1:B:211:LYS:HB3	1.96	0.47
1:B:461:ARG:NH1	1:B:520:SER:OG	2.48	0.47
2:C:35:ARG:HA	2:C:41:VAL:HB	1.99	0.45
1:A:487:PRO:HA	1:A:488:PRO:HD3	1.87	0.45
1:A:268:LEU:HA	1:A:272:ALA:HB3	2.00	0.43
1:B:290:ALA:O	1:B:310:ARG:NH1	2.48	0.43
2:C:19:PRO:HA	2:C:20:PRO:HD3	1.90	0.43
1:A:276:ILE:HA	1:A:277:PRO:HD3	1.84	0.43
1:A:364:PRO:HA	1:A:417:ARG:HG2	2.00	0.43
1:B:177:THR:HB	1:B:194:LEU:HD13	2.01	0.42
1:B:292:ARG:HE	1:B:322:THR:HG21	1.83	0.42
1:A:467:ASP:HA	1:A:468:PRO:HD3	1.84	0.42
1:A:174:THR:HG23	1:A:323:PRO:HG3	2.00	0.42
1:B:174:THR:HG23	1:B:323:PRO:HG3	2.02	0.42
1:B:457:ARG:HG3	1:B:478:MSE:HE2	2.00	0.42
1:B:268:LEU:HA	1:B:272:ALA:HB3	2.00	0.42
1:B:471:ALA:HA	1:B:472:PRO:HD3	1.88	0.42
1:B:292:ARG:HD3	1:B:333:ALA:HB3	2.02	0.41
1:B:150:LYS:O	1:B:150:LYS:HG2	2.20	0.41
1:B:292:ARG:HH21	1:B:322:THR:HB	1.84	0.41
1:B:368:VAL:HG11	1:B:430:ARG:HB2	2.03	0.41
1:A:273:ASN:O	1:A:275:GLY:N	2.48	0.41
1:A:459:ASN:HD22	1:A:459:ASN:HA	1.65	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:96:VAL:HB	2:C:97:ASN:H	1.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	Percentiles	
1	A	377/383 (98%)	365 (97%)	12 (3%)	0	100	100
1	B	381/383 (100%)	371 (97%)	10 (3%)	0	100	100
2	C	103/143 (72%)	97 (94%)	5 (5%)	1 (1%)	22	60
All	All	861/909 (95%)	833 (97%)	27 (3%)	1 (0%)	59	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	96	VAL

### 5.3.2 Protein sidechains ⓘ

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	316/316 (100%)	303 (96%)	13 (4%)	41	77
1	B	318/316 (101%)	303 (95%)	15 (5%)	36	73
2	C	83/123 (68%)	79 (95%)	4 (5%)	35	72
All	All	717/755 (95%)	685 (96%)	32 (4%)	38	74

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	LYS
1	A	171	LEU
1	A	200	LYS
1	A	240	GLU
1	A	284	VAL
1	A	292	ARG
1	A	303	LYS
1	A	395	ARG
1	A	402	GLN
1	A	418	VAL
1	A	419	VAL
1	A	457	ARG
1	A	459	ASN
1	B	150	LYS
1	B	171	LEU
1	B	186	THR
1	B	200	LYS
1	B	208	GLU
1	B	244	VAL
1	B	258	ARG
1	B	337	LEU
1	B	378	SER
1	B	383	GLU
1	B	402	GLN
1	B	417	ARG
1	B	419	VAL
1	B	506	GLU
1	B	509	ASP
2	C	9	ARG
2	C	42	THR
2	C	54	ILE
2	C	96	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	HIS
1	A	269	GLN
1	A	402	GLN
1	A	459	ASN
1	B	163	GLN
1	B	217	ASN
1	B	295	ASN

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Mol	Chain	Res	Type
1	B	402	GLN
1	B	409	GLN
1	B	460	ASN
1	B	505	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 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	SO4	A	101	-	4,4,4	0.21	0	6,6,6	0.08	0
3	SO4	A	102	-	4,4,4	0.20	0	6,6,6	0.07	0
3	SO4	A	103	-	4,4,4	0.26	0	6,6,6	0.19	0
3	SO4	A	105	-	4,4,4	0.09	0	6,6,6	0.07	0
3	SO4	A	107	-	4,4,4	0.19	0	6,6,6	0.10	0
3	SO4	A	108	-	4,4,4	0.21	0	6,6,6	0.11	0
3	SO4	A	110	-	4,4,4	0.19	0	6,6,6	0.12	0
3	SO4	B	104	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	B	106	-	4,4,4	0.20	0	6,6,6	0.09	0
3	SO4	B	109	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	B	111	-	4,4,4	0.20	0	6,6,6	0.14	0
3	SO4	B	112	-	4,4,4	0.22	0	6,6,6	0.07	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
3	SO4	A	101	-	-	0/0/0/0	0/0/0/0
3	SO4	A	102	-	-	0/0/0/0	0/0/0/0
3	SO4	A	103	-	-	0/0/0/0	0/0/0/0
3	SO4	A	105	-	-	0/0/0/0	0/0/0/0
3	SO4	A	107	-	-	0/0/0/0	0/0/0/0
3	SO4	A	108	-	-	0/0/0/0	0/0/0/0
3	SO4	A	110	-	-	0/0/0/0	0/0/0/0
3	SO4	B	104	-	-	0/0/0/0	0/0/0/0
3	SO4	B	106	-	-	0/0/0/0	0/0/0/0
3	SO4	B	109	-	-	0/0/0/0	0/0/0/0
3	SO4	B	111	-	-	0/0/0/0	0/0/0/0
3	SO4	B	112	-	-	0/0/0/0	0/0/0/0

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	379/383 (98%)	-0.28	1 (0%) 91 93	15, 22, 35, 44	0
1	B	383/383 (100%)	-0.13	9 (2%) 57 58	13, 25, 35, 47	0
2	C	105/143 (73%)	0.92	15 (14%) 3 3	38, 39, 42, 42	0
All	All	867/909 (95%)	-0.07	25 (2%) 50 50	13, 24, 39, 47	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	SER	6.3
2	C	108	GLU	5.3
1	B	141	LYS	4.8
1	B	507	HIS	4.2
1	B	140	ARG	4.1
2	C	42	THR	3.2
2	C	16	THR	3.2
2	C	44	ARG	3.1
2	C	45	LYS	3.0
1	B	223	ARG	2.8
2	C	6	SER	2.8
1	B	225	LYS	2.7
2	C	100	TYR	2.7
2	C	18	GLY	2.6
2	C	110	SER	2.5
2	C	46	CYS	2.5
2	C	37	PRO	2.5
1	B	505	GLN	2.5
2	C	70	ASN	2.4
2	C	36	GLY	2.3
1	B	299	GLY	2.2
2	C	69	VAL	2.1
2	C	97	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	143	SER	2.1
1	A	522	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	B	111	5/5	0.34	6.61	33,33,33,34	5
3	SO4	A	107	5/5	0.40	4.48	90,91,91,91	0
3	SO4	A	108	5/5	0.33	4.27	93,93,93,93	0
3	SO4	B	109	5/5	0.35	3.40	119,120,120,120	0
3	SO4	A	110	5/5	0.34	3.29	40,40,40,41	5
3	SO4	B	112	5/5	0.24	3.03	35,35,35,36	5
3	SO4	B	106	5/5	0.33	2.71	111,111,111,111	0
3	SO4	A	105	5/5	0.23	2.26	84,84,85,85	0
3	SO4	A	102	5/5	0.23	0.99	73,73,73,73	0
3	SO4	A	101	5/5	0.13	-0.38	31,32,32,32	0
3	SO4	B	104	5/5	0.12	-1.34	24,25,25,25	0
3	SO4	A	103	5/5	0.15	-1.54	46,46,47,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.