



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:05 PM BST

PDB ID : 6VBH  
Title : Human XPG endonuclease catalytic domain  
Authors : Tsutakawa, S.E.; Arvai, A.S.; Tainer, J.A.  
Deposited on : 2019-12-18  
Resolution : 2.00 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

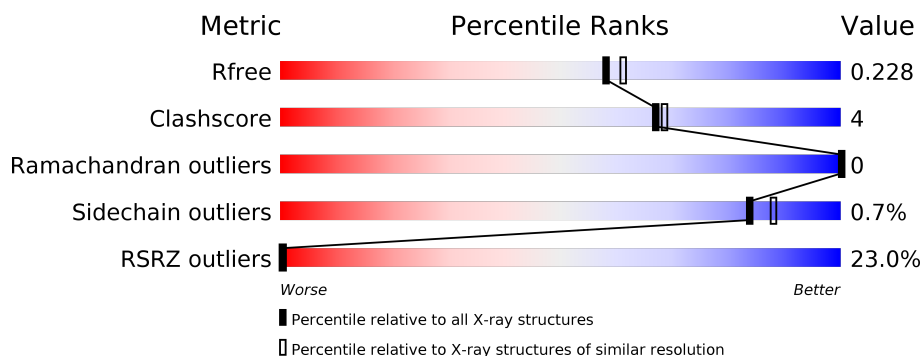
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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  $\leq 5\%$ . 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	346	<div> <div>22%</div> <div>86%</div> <div>8%</div> <div>6%</div> </div>

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	SO4	A	1012	-	-	-	X
2	SO4	A	1013	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1015	-	-	-	X

## 2 Entry composition [i](#)

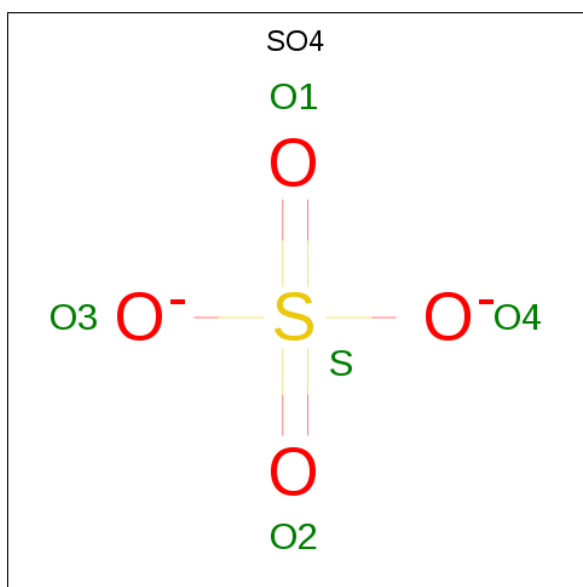
There are 3 unique types of molecules in this entry. The entry contains 5566 atoms, of which 2677 are hydrogens and 0 are deuteriums.

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 DNA repair protein complementing XP-G cells, Flap endonuclease 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	326	Total	C	H	N	O	S	0	4	0
			5372	1733	2677	462	492	8			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

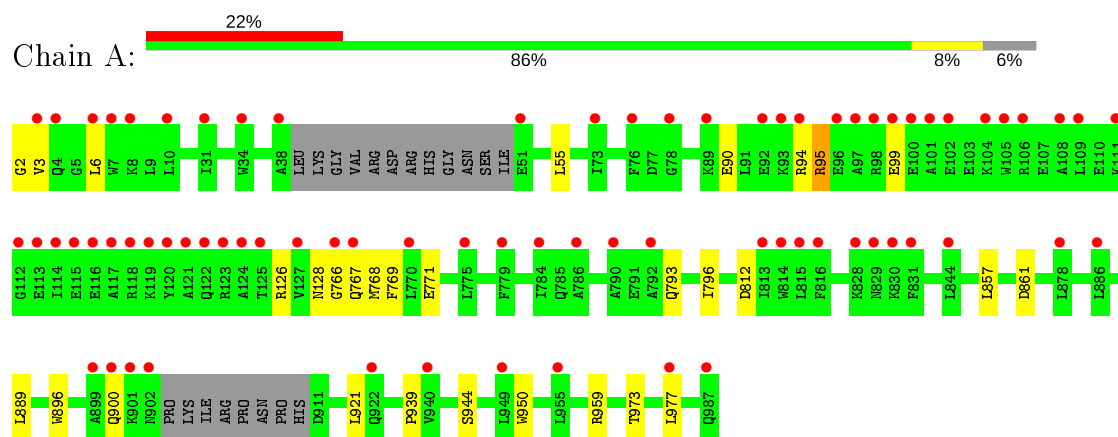
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		

### 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: DNA repair protein complementing XP-G cells, Flap endonuclease 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.44Å 173.40Å 101.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.83 – 2.00 43.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	82.5 (43.83-2.00) 79.2 (43.83-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.00Å)	Xtriage
Refinement program	PHENIX phenix-dev 2722	Depositor
R, $R_{free}$	0.220 , 0.244 0.217 , 0.228	Depositor DCC
$R_{free}$ test set	1731 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.752	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 60.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<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.

## 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

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	0.62	0/2770	0.73	0/3739

There are no bond length outliers.

There are no bond angle outliers.

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	A	2695	2677	2670	21	0
2	A	75	0	0	2	0
3	A	119	0	0	2	0
All	All	2889	2677	2670	21	0

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 4.

All (21) 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:2:GLY:N	1:A:861:ASP:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:ARG:HA	1:A:973:THR:HG21	1.89	0.54
1:A:95:ARG:O	1:A:99:GLU:HG3	2.10	0.52
1:A:95:ARG:HH11	1:A:99:GLU:HG3	1.76	0.50
1:A:128:ASN:OD1	1:A:766:GLY:N	2.45	0.49
1:A:950:TRP:HB3	2:A:1012:SO4:O1	2.13	0.48
1:A:857:LEU:HD11	1:A:889:LEU:HD22	1.96	0.48
1:A:3:VAL:HB	1:A:6:LEU:HB3	1.96	0.47
1:A:857:LEU:HD11	1:A:889:LEU:CD2	2.45	0.47
1:A:900:GLN:HA	1:A:900:GLN:OE1	2.15	0.46
1:A:55:LEU:HD11	1:A:771:GLU:OE1	2.15	0.46
1:A:90:GLU:OE1	1:A:94:ARG:NH2	2.50	0.45
1:A:939:PRO:O	3:A:1101:HOH:O	2.21	0.45
1:A:896:TRP:NE1	1:A:921:LEU:O	2.50	0.44
1:A:793:GLN:O	1:A:796:ILE:HG22	2.18	0.44
1:A:128:ASN:OD1	1:A:767:GLN:N	2.49	0.43
1:A:944:SER:HB3	3:A:1113:HOH:O	2.17	0.43
1:A:3:VAL:CG1	1:A:6:LEU:HB2	2.49	0.42
1:A:973:THR:HG22	1:A:977:LEU:CD1	2.50	0.42
1:A:126:ARG:HD2	2:A:1014:SO4:O2	2.21	0.40
1:A:768:MET:O	1:A:769:PHE:C	2.59	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	Percentiles	
1	A	324/346 (94%)	317 (98%)	7 (2%)	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	A	288/302 (95%)	286 (99%)	2 (1%)	84 88

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

Mol	Chain	Res	Type
1	A	95	ARG
1	A	812	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

15 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	$\# Z  > 2$
2	SO4	A	1005	-	4,4,4	0.20	0	6,6,6	0.29	0
2	SO4	A	1014	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	A	1010	-	4,4,4	0.11	0	6,6,6	0.15	0
2	SO4	A	1001	-	4,4,4	0.16	0	6,6,6	0.41	0
2	SO4	A	1006	-	4,4,4	0.16	0	6,6,6	0.40	0
2	SO4	A	1011	-	4,4,4	0.21	0	6,6,6	0.19	0
2	SO4	A	1002	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	A	1003	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	A	1015	-	4,4,4	0.19	0	6,6,6	0.35	0
2	SO4	A	1008	-	4,4,4	0.17	0	6,6,6	0.25	0
2	SO4	A	1004	-	4,4,4	0.18	0	6,6,6	0.22	0
2	SO4	A	1013	-	4,4,4	0.11	0	6,6,6	0.16	0
2	SO4	A	1007	-	4,4,4	0.16	0	6,6,6	0.34	0
2	SO4	A	1009	-	4,4,4	0.22	0	6,6,6	0.31	0
2	SO4	A	1012	-	4,4,4	0.11	0	6,6,6	0.41	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1014	SO4	1	0
2	A	1012	SO4	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 ⓘ

### 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	326/346 (94%)	1.58	75 (23%) 0 0	41, 62, 133, 163	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	ILE	15.3
1	A	101	ALA	11.0
1	A	120	TYR	10.2
1	A	113	GLU	10.2
1	A	112	GLY	8.7
1	A	111	LYS	7.9
1	A	38	ALA	7.8
1	A	117	ALA	7.4
1	A	100	GLU	7.4
1	A	828	LYS	6.9
1	A	109	LEU	6.9
1	A	830	LYS	6.7
1	A	97	ALA	6.0
1	A	96	GLU	6.0
1	A	902	ASN	5.6
1	A	831	PHE	5.5
1	A	987	GLN	5.5
1	A	108	ALA	5.5
1	A	104	LYS	5.1
1	A	105	TRP	5.1
1	A	116	GLU	4.9
1	A	106[A]	ARG	4.8
1	A	115	GLU	4.7
1	A	127	VAL	4.7
1	A	901	LYS	4.6
1	A	121	ALA	4.6
1	A	119	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	3	VAL	4.0
1	A	98	ARG	4.0
1	A	118	ARG	3.7
1	A	123	ARG	3.7
1	A	102	GLU	3.6
1	A	51	GLU	3.6
1	A	93	LYS	3.5
1	A	125	THR	3.4
1	A	770	LEU	3.3
1	A	977	LEU	3.3
1	A	124	ALA	3.3
1	A	4	GLN	3.2
1	A	900	GLN	3.2
1	A	940	VAL	3.0
1	A	94	ARG	2.9
1	A	89	LYS	2.9
1	A	792	ALA	2.9
1	A	816	PHE	2.8
1	A	899	ALA	2.7
1	A	92	GLU	2.7
1	A	7	TRP	2.6
1	A	815	LEU	2.5
1	A	767	GLN	2.5
1	A	99	GLU	2.5
1	A	786	ALA	2.5
1	A	813	ILE	2.4
1	A	814	TRP	2.4
1	A	775	LEU	2.4
1	A	829	ASN	2.4
1	A	766	GLY	2.4
1	A	955	LEU	2.4
1	A	790	ALA	2.4
1	A	878	LEU	2.4
1	A	78	GLY	2.3
1	A	6	LEU	2.3
1	A	8	LYS	2.3
1	A	784	ILE	2.2
1	A	76	PHE	2.2
1	A	73	ILE	2.1
1	A	34	TRP	2.1
1	A	922	GLN	2.1
1	A	886	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	779	PHE	2.1
1	A	31	ILE	2.1
1	A	10	LEU	2.0
1	A	844	LEU	2.0
1	A	122	GLN	2.0
1	A	949	LEU	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<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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1006	5/5	0.53	0.36	102,107,124,138	0
2	SO4	A	1012	5/5	0.61	0.52	97,100,138,140	0
2	SO4	A	1013	5/5	0.63	0.70	136,141,158,160	0
2	SO4	A	1010	5/5	0.66	0.32	108,119,157,186	0
2	SO4	A	1015	5/5	0.71	0.59	98,100,149,167	0
2	SO4	A	1011	5/5	0.82	0.15	100,110,152,158	0
2	SO4	A	1009	5/5	0.82	0.20	74,104,117,140	0
2	SO4	A	1005	5/5	0.82	0.16	89,105,126,138	0
2	SO4	A	1014	5/5	0.87	0.11	86,91,109,129	0
2	SO4	A	1008	5/5	0.88	0.10	100,113,137,138	0
2	SO4	A	1007	5/5	0.90	0.09	69,105,111,134	0
2	SO4	A	1003	5/5	0.93	0.15	93,111,130,152	0
2	SO4	A	1002	5/5	0.96	0.10	86,90,101,120	0
2	SO4	A	1001	5/5	0.97	0.17	66,68,87,93	0
2	SO4	A	1004	5/5	0.98	0.22	84,92,114,141	0

## 6.5 Other polymers

There are no such residues in this entry.