



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 02:04 pm GMT

PDB ID : 2PP9  
Title : Nitrate bound wild type oxidized AfNiR  
Authors : Murphy, M.E.P.; Tocheva, E.I.  
Deposited on : 2007-04-28  
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

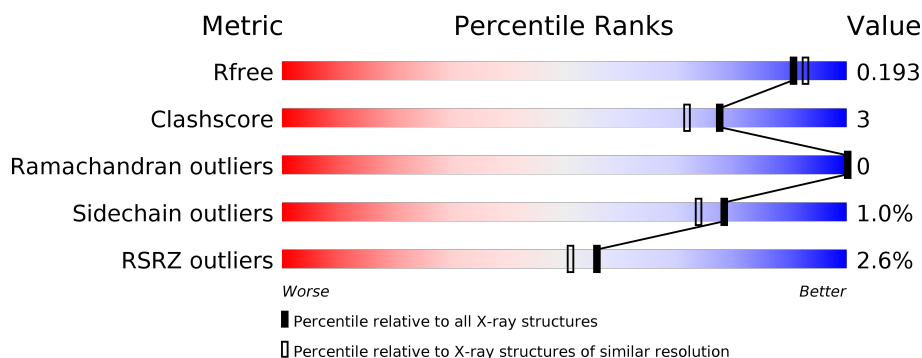
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

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. 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	341	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>7% •</div> </div> </div>
1	B	341	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>6% •</div> </div> </div>
1	C	341	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>6% ••</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8746 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	4	0
			2594	1660	438	485	11			
1	B	337	Total	C	N	O	S	0	1	0
			2573	1646	432	484	11			
1	C	336	Total	C	N	O	S	0	1	0
			2571	1645	434	481	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	ILE	-	EXPRESSION TAG	UNP P38501
A	342	GLU	-	EXPRESSION TAG	UNP P38501
A	343	GLY	-	EXPRESSION TAG	UNP P38501
A	344	ARG	-	EXPRESSION TAG	UNP P38501
B	341	ILE	-	EXPRESSION TAG	UNP P38501
B	342	GLU	-	EXPRESSION TAG	UNP P38501
B	343	GLY	-	EXPRESSION TAG	UNP P38501
B	344	ARG	-	EXPRESSION TAG	UNP P38501
C	341	ILE	-	EXPRESSION TAG	UNP P38501
C	342	GLU	-	EXPRESSION TAG	UNP P38501
C	343	GLY	-	EXPRESSION TAG	UNP P38501
C	344	ARG	-	EXPRESSION TAG	UNP P38501

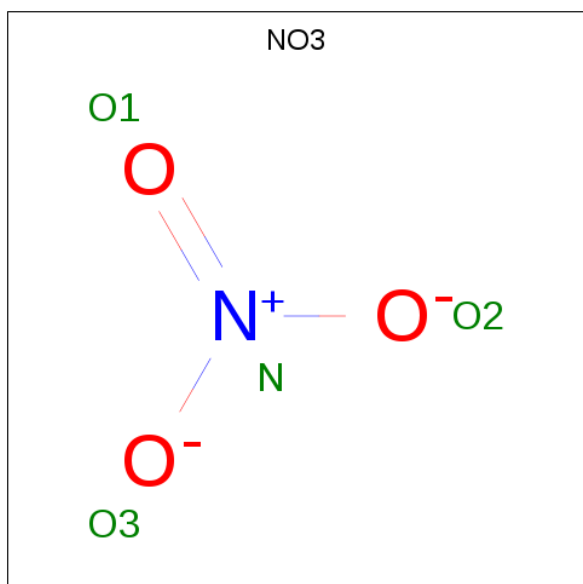
- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cu	0	0
			1	1		
3	A	1	Total	Cu	0	0
			1	1		
3	C	1	Total	Cu	0	0
			1	1		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		
4	C	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	334	Total	O	0	0
			334	334		
7	B	330	Total	O	0	0
			330	330		
7	C	287	Total	O	0	0
			287	287		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.91Å 102.08Å 145.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.67 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (30.00-1.80) 95.1 (29.67-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.66 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.169 , 0.195 0.167 , 0.193	Depositor DCC
$R_{free}$ test set	4046 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8746	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, NO3, CU, CU1, 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	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.59	0/2665	0.64	0/3634
1	B	0.59	1/2644 (0.0%)	0.66	1/3606 (0.0%)
1	C	0.56	0/2642	0.63	0/3602
All	All	0.58	1/7951 (0.0%)	0.64	1/10842 (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	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	325	GLU	CG-CD	5.21	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	HIS	Peptide
1	B	306	HIS	Peptide
1	C	306	HIS	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	A	2594	0	2524	19	0
1	B	2573	0	2496	17	0
1	C	2571	0	2497	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
5	A	4	0	3	0	0
5	B	12	0	9	0	0
5	C	16	0	12	2	0
6	A	7	0	9	1	0
7	A	334	0	0	3	0
7	B	330	0	0	2	0
7	C	287	0	0	1	0
All	All	8746	0	7550	49	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 3.

The worst 5 of 49 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:C:26:HIS:HE1	1:C:74:VAL:H	1.24	0.84
1:A:26:HIS:HE1	1:A:74:VAL:H	1.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:HIS:HE1	1:B:74:VAL:H	1.26	0.81
1:A:300:ILE:HD12	1:A:321:LYS:HG2	1.63	0.79
1:C:22:PRO:HB2	1:C:221:ASN:HD21	1.52	0.74

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	338/341 (99%)	336 (99%)	2 (1%)	0	100	100
1	B	336/341 (98%)	331 (98%)	5 (2%)	0	100	100
1	C	335/341 (98%)	328 (98%)	7 (2%)	0	100	100
All	All	1009/1023 (99%)	995 (99%)	14 (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	A	268/268 (100%)	265 (99%)	3 (1%)	76	71
1	B	266/268 (99%)	263 (99%)	3 (1%)	76	71
1	C	265/268 (99%)	263 (99%)	2 (1%)	83	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	799/804 (99%)	791 (99%)	8 (1%)	78	74

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37	LYS
1	C	332	THR
1	B	253	ARG
1	A	253	ARG
1	B	168	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	115	ASN
1	B	221	ASN
1	C	77	GLN
1	B	77	GLN
1	C	60	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	TRS	A	2001	-	6,6,7	0.35	0	3,6,9	0.89	0
5	ACT	A	2010	-	1,3,3	1.51	0	0,3,3	0.00	-
4	NO3	A	503	3	1,3,3	3.30	1 (100%)	0,3,3	0.00	-
5	ACT	B	2003	-	1,3,3	0.97	0	0,3,3	0.00	-
5	ACT	B	2004	-	1,3,3	1.68	0	0,3,3	0.00	-
5	ACT	B	2005	-	1,3,3	1.48	0	0,3,3	0.00	-
4	NO3	B	503	3	1,3,3	3.31	1 (100%)	0,3,3	0.00	-
5	ACT	C	2006	-	1,3,3	1.11	0	0,3,3	0.00	-
5	ACT	C	2007	-	1,3,3	1.66	0	0,3,3	0.00	-
5	ACT	C	2008	-	1,3,3	1.51	0	0,3,3	0.00	-
5	ACT	C	2009	-	1,3,3	1.47	0	0,3,3	0.00	-
4	NO3	C	503	3	1,3,3	3.34	1 (100%)	0,3,3	0.00	-

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
6	TRS	A	2001	-	-	0/6/6/9	0/0/0/0
5	ACT	A	2010	-	-	0/0/0/0	0/0/0/0
4	NO3	A	503	3	-	0/0/0/0	0/0/0/0
5	ACT	B	2003	-	-	0/0/0/0	0/0/0/0
5	ACT	B	2004	-	-	0/0/0/0	0/0/0/0
5	ACT	B	2005	-	-	0/0/0/0	0/0/0/0
4	NO3	B	503	3	-	0/0/0/0	0/0/0/0
5	ACT	C	2006	-	-	0/0/0/0	0/0/0/0
5	ACT	C	2007	-	-	0/0/0/0	0/0/0/0
5	ACT	C	2008	-	-	0/0/0/0	0/0/0/0
5	ACT	C	2009	-	-	0/0/0/0	0/0/0/0
4	NO3	C	503	3	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	NO3	O1-N	3.30	1.39	1.24
4	B	503	NO3	O1-N	3.31	1.39	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	NO3	O1-N	3.34	1.39	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2001	TRS	1	0
5	C	2006	ACT	1	0
5	C	2009	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<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	336/341 (98%)	-0.15	5 (1%) 73 70	12, 17, 28, 43	0
1	B	337/341 (98%)	-0.08	9 (2%) 54 49	12, 18, 31, 39	0
1	C	336/341 (98%)	0.07	12 (3%) 42 37	13, 21, 32, 41	0
All	All	1009/1023 (98%)	-0.05	26 (2%) 56 51	12, 19, 31, 43	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	34	GLY	4.2
1	A	339	GLY	4.1
1	A	4	ALA	3.8
1	B	33	GLU	3.5
1	B	340	THR	3.4

### 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 carbohydrates 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
5	ACT	B	2004	4/4	0.78	0.31	27,28,28,28	0
5	ACT	C	2009	4/4	0.81	0.22	29,31,31,31	0
4	NO3	A	503	4/4	0.84	0.19	29,30,31,33	0
5	ACT	C	2006	4/4	0.86	0.16	50,50,50,50	0
5	ACT	C	2007	4/4	0.88	0.13	28,29,29,30	0
6	TRS	A	2001	7/8	0.91	0.13	24,25,26,28	0
4	NO3	B	503	4/4	0.92	0.16	29,29,29,30	0
4	NO3	C	503	4/4	0.93	0.14	33,33,34,35	0
5	ACT	A	2010	4/4	0.96	0.09	20,20,21,22	0
5	ACT	B	2003	4/4	0.97	0.10	23,25,25,26	0
5	ACT	C	2008	4/4	0.97	0.07	19,20,20,20	0
5	ACT	B	2005	4/4	0.98	0.09	20,21,22,23	0
2	CU1	C	501	1/1	0.99	0.04	23,23,23,23	0
3	CU	B	502	1/1	1.00	0.03	20,20,20,20	0
2	CU1	B	501	1/1	1.00	0.04	20,20,20,20	0
2	CU1	A	501	1/1	1.00	0.04	18,18,18,18	0
3	CU	A	502	1/1	1.00	0.02	17,17,17,17	0
3	CU	C	502	1/1	1.00	0.04	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.