



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 08:28 am BST

PDB ID : 2PPC  
Title : Oxidized wild type AfNiR exposed to NO (nitrite bound)  
Authors : Tocheva, E.I.; Murphy, M.E.P.  
Deposited on : 2007-04-28  
Resolution : 1.58 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

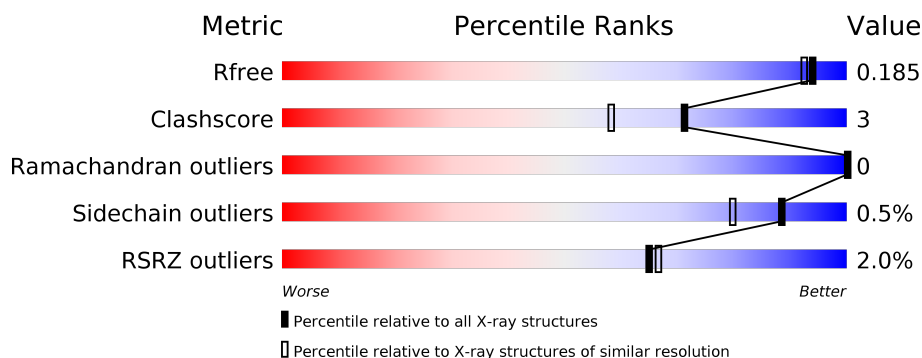
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.58 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	341	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>93%</span> <span>5% •</span> </div> </div>
1	B	341	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>2%</span> <span>94%</span> <span>5% •</span> </div> </div>
1	C	341	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 1%, green 93%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>3%</span> <span>93%</span> <span>6% •</span> </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
5	ACT	B	1506	-	-	X	-
5	ACT	B	504	-	-	X	-
5	ACT	C	504	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8641 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	2	0
			2576	1647	432	486	11			
1	C	336	Total	C	N	O	S	0	2	0
			2574	1646	434	483	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

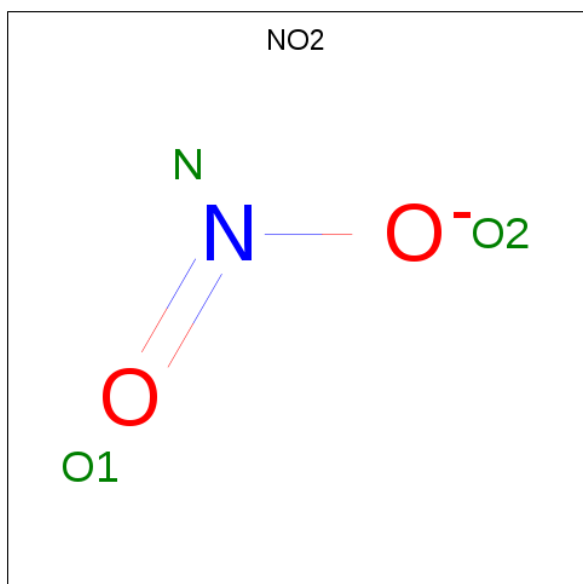
- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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 NITRITE ION (three-letter code: NO2) (formula: NO<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			3	1	2		
4	B	1	Total	N	O	0	0
			3	1	2		
4	C	1	Total	N	O	0	0
			3	1	2		

- 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	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
			6	3	3		

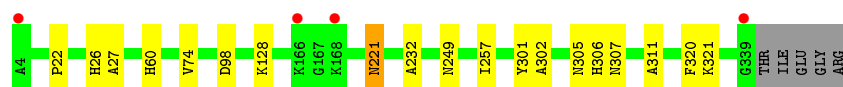
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	299	Total	O	0	0
			299	299		
7	B	293	Total	O	0	0
			293	293		
7	C	244	Total	O	0	0
			244	244		

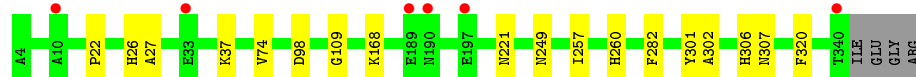
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

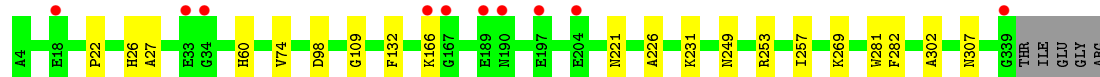
- Molecule 1: Copper-containing nitrite reductase



- Molecule 1: Copper-containing nitrite reductase



- Molecule 1: Copper-containing nitrite reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.11Å 101.83Å 145.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.58 29.90 – 1.58	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-1.58) 93.1 (29.90-1.58)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.161 , 0.182 0.163 , 0.185	Depositor DCC
$R_{free}$ test set	5827 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.5	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8641	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 3.87% 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: TRS, CU, NO2, 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	0.47	0/2665	0.63	1/3634 (0.0%)
1	B	0.46	0/2652	0.63	0/3617
1	C	0.46	0/2650	0.60	0/3613
All	All	0.46	0/7967	0.62	1/10864 (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
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ASP	CB-CG-OD2	5.38	123.14	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	HIS	Peptide
1	B	306	HIS	Peptide

## 5.2 Too-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 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	13	0
1	B	2576	0	2496	19	0
1	C	2574	0	2497	21	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	3	0	0	0	0
4	B	3	0	0	1	0
4	C	3	0	0	0	0
5	A	4	0	3	0	0
5	B	20	0	15	10	0
5	C	16	0	12	7	0
6	A	6	0	0	4	0
7	A	299	0	0	1	0
7	B	293	0	0	0	0
7	C	244	0	0	1	0
All	All	8641	0	7547	53	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 53 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:B:98[B]:ASP:OD1	5:B:504:ACT:H1	1.54	1.08
1:C:26:HIS:HE1	1:C:74:VAL:H	1.22	0.87
1:A:26:HIS:HE1	1:A:74:VAL:H	1.29	0.80
1:B:26:HIS:HE1	1:B:74:VAL:H	1.29	0.77
1:B:98[A]:ASP:OD1	5:B:504:ACT:OXT	2.05	0.75

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	338/341 (99%)	336 (99%)	2 (1%)	0	100	100
1	B	337/341 (99%)	335 (99%)	2 (1%)	0	100	100
1	C	336/341 (98%)	332 (99%)	4 (1%)	0	100	100
All	All	1011/1023 (99%)	1003 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	268/268 (100%)	267 (100%)	1 (0%)	91	84
1	B	267/268 (100%)	265 (99%)	2 (1%)	84	72
1	C	266/268 (99%)	265 (100%)	1 (0%)	91	84
All	All	801/804 (100%)	797 (100%)	4 (0%)	88	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	B	37	LYS
1	B	168	LYS
1	C	166	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 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\# Z  > 2$
4	NO2	C	503	3	1,2,2	4.59	1 (100%)	0,1,1	0.00	-
5	ACT	B	1506	-	1,3,3	0.94	0	0,3,3	0.00	-
4	NO2	A	503	3	1,2,2	4.50	1 (100%)	0,1,1	0.00	-
4	NO2	B	503	3	1,2,2	4.46	1 (100%)	0,1,1	0.00	-
5	ACT	B	504	3	1,3,3	1.59	0	0,3,3	0.00	-
5	ACT	C	1507	-	1,3,3	1.32	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ACT	B	1504	-	1,3,3	1.43	0	0,3,3	0.00	-
5	ACT	B	1505	-	1,3,3	1.47	0	0,3,3	0.00	-
6	TRS	A	1501	-	3,3,7	0.07	0	-		
5	ACT	C	504	3	1,3,3	1.54	0	0,3,3	0.00	-
5	ACT	A	1510	-	1,3,3	1.34	0	0,3,3	0.00	-
5	ACT	B	1503	-	1,3,3	0.90	0	0,3,3	0.00	-
5	ACT	C	1508	-	1,3,3	1.51	0	0,3,3	0.00	-
5	ACT	C	1509	-	1,3,3	0.77	0	0,3,3	0.00	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	NO2	O1-N	4.59	1.45	1.22
4	A	503	NO2	O1-N	4.50	1.45	1.22
4	B	503	NO2	O1-N	4.46	1.44	1.22

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1506	ACT	3	0
4	B	503	NO2	1	0
5	B	504	ACT	7	0
6	A	1501	TRS	4	0
5	C	504	ACT	7	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%)	-0.29	4 (1%) 79 80	12, 16, 26, 39	0
1	B	337/341 (98%)	-0.23	6 (1%) 68 70	12, 16, 30, 38	0
1	C	336/341 (98%)	-0.06	10 (2%) 50 51	13, 20, 30, 39	0
All	All	1009/1023 (98%)	-0.19	20 (1%) 65 66	12, 17, 29, 39	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	LYS	4.5
1	C	34	GLY	3.7
1	B	33	GLU	3.6
1	A	339	GLY	3.6
1	B	197	GLU	3.5

### 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	504	4/4	0.81	0.31	19,19,20,20	4
6	TRS	A	1501	6/8	0.83	0.15	24,24,25,30	0
5	ACT	C	504	4/4	0.83	0.22	19,19,19,20	4
5	ACT	C	1507	4/4	0.85	0.14	32,32,32,33	0
5	ACT	B	1506	4/4	0.88	0.19	50,50,50,50	0
5	ACT	C	1509	4/4	0.90	0.18	26,28,28,28	0
4	NO2	C	503	3/3	0.91	0.17	19,19,19,20	3
5	ACT	B	1504	4/4	0.92	0.18	23,23,23,23	0
4	NO2	B	503	3/3	0.92	0.28	20,20,21,21	3
5	ACT	A	1510	4/4	0.94	0.17	23,23,24,24	0
4	NO2	A	503	3/3	0.95	0.13	34,34,35,35	0
5	ACT	C	1508	4/4	0.96	0.07	22,23,23,23	0
5	ACT	B	1503	4/4	0.96	0.10	23,25,25,26	0
5	ACT	B	1505	4/4	0.97	0.11	20,22,22,22	0
2	CU1	C	501	1/1	0.99	0.04	19,19,19,19	0
2	CU1	A	501	1/1	1.00	0.02	14,14,14,14	0
3	CU	B	502	1/1	1.00	0.03	15,15,15,15	0
3	CU	A	502	1/1	1.00	0.03	13,13,13,13	0
2	CU1	B	501	1/1	1.00	0.04	16,16,16,16	0
3	CU	C	502	1/1	1.00	0.04	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.