



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2025 – 01:27 pm BST

PDB ID : 9FNF / pdb\_00009fnf  
Title : The glycoside hydrolase family 71 (GH71) member AnGH71C from *Aspergillus nidulans*.  
Authors : Mazurkewich, S.; Widen, T.; Branden, G.; Larsbrink, J.  
Deposited on : 2024-06-10  
Resolution : 1.33 Å(reported)

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

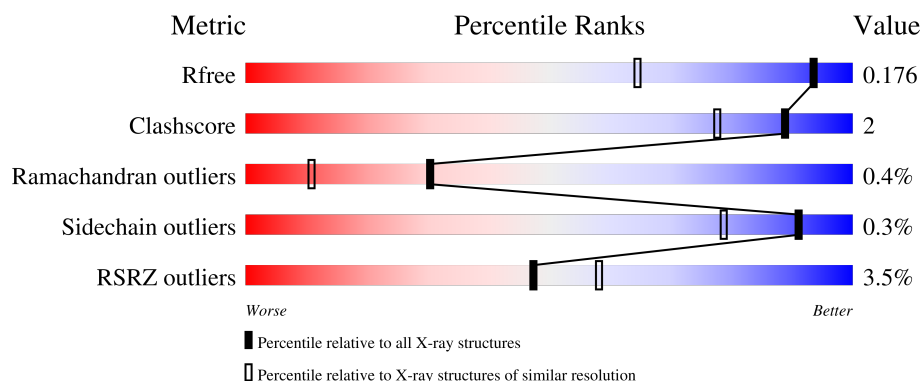
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.33 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))
$R_{free}$	164625	1904 (1.36-1.32)
Clashscore	180529	2038 (1.36-1.32)
Ramachandran outliers	177936	2016 (1.36-1.32)
Sidechain outliers	177891	2016 (1.36-1.32)
RSRZ outliers	164620	1903 (1.36-1.32)

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  $\geq 3$ , 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	430	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>5%</div> <div>7%</div> </div> </div>
1	B	430	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>•</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7971 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 Glycoside hydrolase family 71.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	18	0
			3314	2113	535	652	14			
1	B	397	Total	C	N	O	S	0	17	0
			3283	2096	529	644	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP G5EB58
A	3	GLY	-	expression tag	UNP G5EB58
A	4	SER	-	expression tag	UNP G5EB58
A	5	SER	-	expression tag	UNP G5EB58
A	6	HIS	-	expression tag	UNP G5EB58
A	7	HIS	-	expression tag	UNP G5EB58
A	8	HIS	-	expression tag	UNP G5EB58
A	9	HIS	-	expression tag	UNP G5EB58
A	10	HIS	-	expression tag	UNP G5EB58
A	11	HIS	-	expression tag	UNP G5EB58
A	12	SER	-	expression tag	UNP G5EB58
A	13	SER	-	expression tag	UNP G5EB58
A	14	GLU	-	expression tag	UNP G5EB58
A	15	ASN	-	expression tag	UNP G5EB58
A	16	LEU	-	expression tag	UNP G5EB58
A	17	TYR	-	expression tag	UNP G5EB58
A	18	PHE	-	expression tag	UNP G5EB58
A	19	GLN	-	expression tag	UNP G5EB58
A	20	GLY	-	expression tag	UNP G5EB58
A	21	HIS	-	expression tag	UNP G5EB58
B	2	MET	-	initiating methionine	UNP G5EB58
B	3	GLY	-	expression tag	UNP G5EB58
B	4	SER	-	expression tag	UNP G5EB58
B	5	SER	-	expression tag	UNP G5EB58
B	6	HIS	-	expression tag	UNP G5EB58

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP G5EB58
B	8	HIS	-	expression tag	UNP G5EB58
B	9	HIS	-	expression tag	UNP G5EB58
B	10	HIS	-	expression tag	UNP G5EB58
B	11	HIS	-	expression tag	UNP G5EB58
B	12	SER	-	expression tag	UNP G5EB58
B	13	SER	-	expression tag	UNP G5EB58
B	14	GLU	-	expression tag	UNP G5EB58
B	15	ASN	-	expression tag	UNP G5EB58
B	16	LEU	-	expression tag	UNP G5EB58
B	17	TYR	-	expression tag	UNP G5EB58
B	18	PHE	-	expression tag	UNP G5EB58
B	19	GLN	-	expression tag	UNP G5EB58
B	20	GLY	-	expression tag	UNP G5EB58
B	21	HIS	-	expression tag	UNP G5EB58

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			28	16	2	10		
3	A	1	Total	C	N	O	0	1
			28	16	2	10		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	1
			28	16	2	10		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

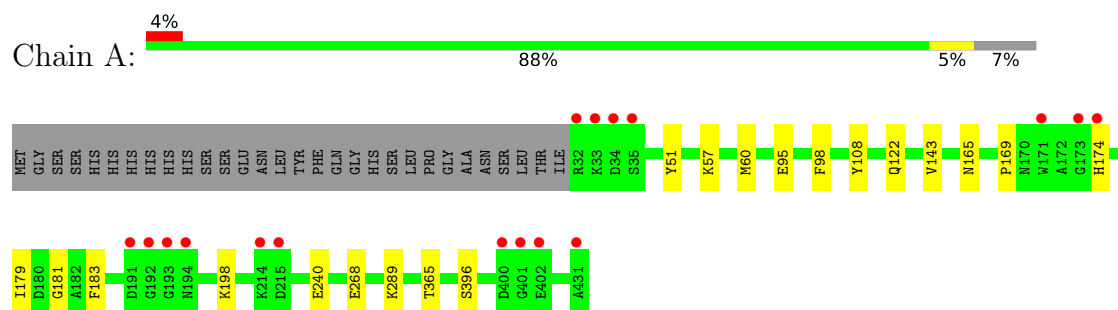
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	603	Total	O	0	0
			603	603		
5	B	653	Total	O	0	0
			653	653		

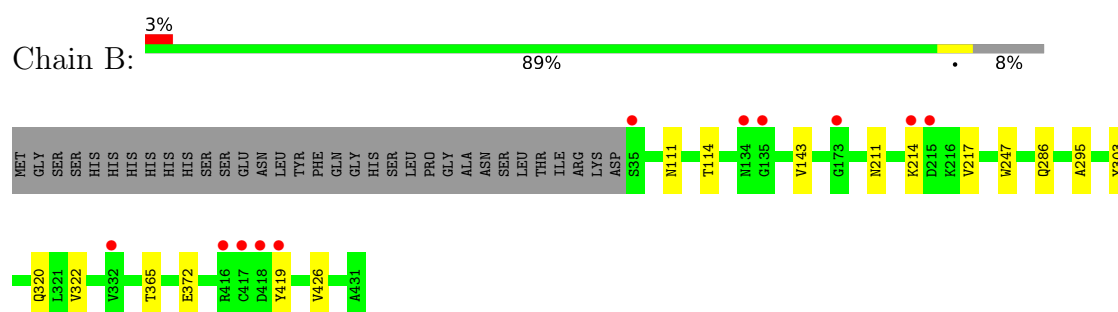
### 3 Residue-property plots [i](#)

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: Glycoside hydrolase family 71



- Molecule 1: Glycoside hydrolase family 71



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.19Å 84.75Å 103.32Å 90.00° 130.85° 90.00°	Depositor
Resolution (Å)	39.08 – 1.33 39.08 – 1.33	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.08-1.33) 99.5 (39.08-1.33)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 1.33Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.159 , 0.176 0.159 , 0.176	Depositor DCC
$R_{free}$ test set	189141 reflections (7.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.5	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7971	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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, NA, BTB

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	0.37	1/3416 (0.0%)	0.54	0/4663
1	B	0.42	1/3385 (0.0%)	0.57	0/4624
All	All	0.40	2/6801 (0.0%)	0.55	0/9287

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	PRO	C-O	-7.22	1.14	1.24
1	B	322	VAL	C-O	-5.24	1.18	1.24

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	3314	0	3052	12	0
1	B	3283	0	3023	8	0
2	A	5	0	0	0	0
3	A	70	0	95	4	0
3	B	42	0	57	1	0
4	B	1	0	0	0	0
5	A	603	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	653	0	0	3	0
All	All	7971	0	6227	23	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 2.

The worst 5 of 23 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:60:MET:HG2	1:A:98:PHE:CD2	2.24	0.72
1:B:111:ASN:O	1:B:114[B]:THR:HG23	1.96	0.66
1:A:174[A]:HIS:CE1	5:A:1024:HOH:O	2.59	0.55
1:B:372:GLU:HB3	5:B:660:HOH:O	2.11	0.50
1:A:289:LYS:NZ	5:A:613:HOH:O	2.43	0.50

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	416/430 (97%)	405 (97%)	9 (2%)	2 (0%)	25	6
1	B	412/430 (96%)	402 (98%)	9 (2%)	1 (0%)	44	19
All	All	828/860 (96%)	807 (98%)	18 (2%)	3 (0%)	30	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	VAL
1	B	143	VAL
1	A	240	GLU

### 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	356/364 (98%)	355 (100%)	1 (0%)	91	79
1	B	352/364 (97%)	350 (99%)	2 (1%)	84	64
All	All	708/728 (97%)	705 (100%)	3 (0%)	91	76

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TYR
1	B	217[A]	VAL
1	B	217[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	212	ASN
1	B	320	GLN
1	A	254	GLN
1	A	320	GLN
1	B	36	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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
3	BTB	A	502[B]	-	13,13,13	0.94	1 (7%)	7,16,16	0.38	0
3	BTB	A	503[A]	-	13,13,13	0.82	0	7,16,16	0.50	0
3	BTB	B	501	-	13,13,13	0.90	1 (7%)	7,16,16	0.40	0
3	BTB	B	502[A]	-	13,13,13	0.87	1 (7%)	7,16,16	0.49	0
3	BTB	A	503[B]	-	13,13,13	0.74	0	7,16,16	0.56	0
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.16	0
3	BTB	A	504	-	13,13,13	0.73	0	7,16,16	0.35	0
3	BTB	B	502[B]	-	13,13,13	0.89	1 (7%)	7,16,16	0.60	0
3	BTB	A	502[A]	-	13,13,13	0.81	0	7,16,16	0.27	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	BTB	A	502[B]	-	-	0/21/21/21	-
3	BTB	A	503[A]	-	-	0/21/21/21	-
3	BTB	B	501	-	-	1/21/21/21	-
3	BTB	B	502[A]	-	-	0/21/21/21	-
3	BTB	A	504	-	-	0/21/21/21	-
3	BTB	A	503[B]	-	-	0/21/21/21	-
3	BTB	B	502[B]	-	-	1/21/21/21	-
3	BTB	A	502[A]	-	-	0/21/21/21	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	BTB	C2-N	2.42	1.53	1.48
3	A	502[B]	BTB	C2-N	2.19	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502[B]	BTB	C2-N	2.07	1.52	1.48
3	B	502[A]	BTB	C2-N	2.05	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502[B]	BTB	C4-C2-C3-O3
3	B	501	BTB	N-C7-C8-O8

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503[B]	BTB	1	0
3	A	504	BTB	3	0
3	B	502[B]	BTB	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	400/430 (93%)	0.07	17 (4%)	40 50	6, 13, 26, 58	18 (4%)
1	B	397/430 (92%)	-0.03	11 (2%)	55 65	6, 13, 24, 49	17 (4%)
All	All	797/860 (92%)	0.02	28 (3%)	47 58	6, 13, 25, 58	35 (4%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417[A]	CYS	10.5
1	B	419[A]	TYR	5.2
1	A	194	ASN	4.9
1	A	215[A]	ASP	4.7
1	A	34	ASP	4.1

### 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 oligosaccharides 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
3	BTB	B	502[A]	14/14	0.77	0.17	20,29,33,34	14
3	BTB	B	502[B]	14/14	0.77	0.17	20,29,34,34	14
2	SO4	A	501	5/5	0.91	0.11	25,32,34,37	0
3	BTB	A	503[A]	14/14	0.94	0.07	10,13,18,19	14
3	BTB	A	503[B]	14/14	0.94	0.07	10,12,22,27	14
3	BTB	A	504	14/14	0.94	0.08	15,22,27,30	0
3	BTB	A	502[A]	14/14	0.94	0.06	10,12,13,13	14
3	BTB	A	502[B]	14/14	0.94	0.06	11,12,13,14	14
3	BTB	B	501	14/14	0.96	0.07	12,13,19,20	0
4	NA	B	503	1/1	0.97	0.06	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.