



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 29, 2024 – 10:09 AM JST

PDB ID : 8KAP
Title : Glycoside hydrolase family 1 beta-glucosidase from *Streptomyces griseus* (ligand-free)
Authors : Kumakura, H.; Motouchi, S.; Nakai, H.; Nakajima, M.
Deposited on : 2023-08-03
Resolution : 2.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

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 : 2.37.1
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) : 2.37.1

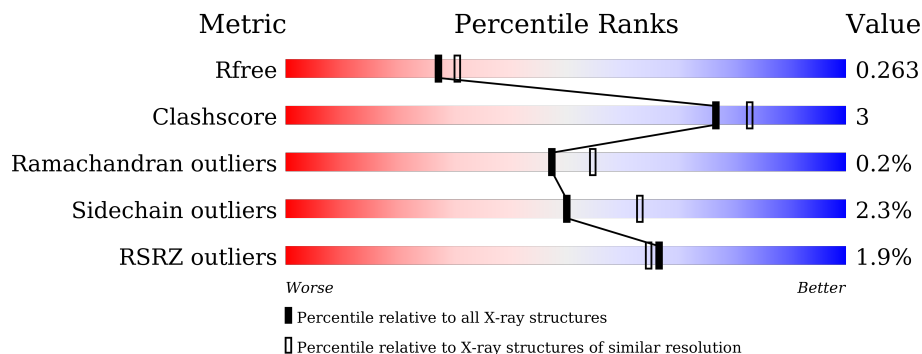
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

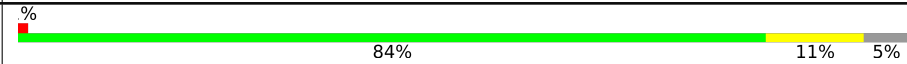
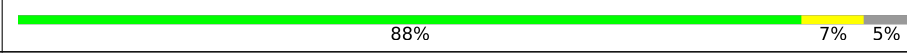
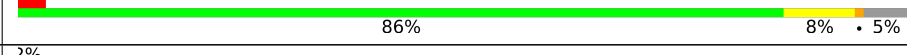
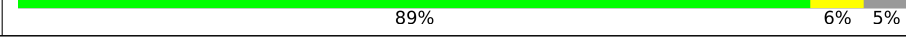
The reported resolution of this entry is 2.20 Å.

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 ≥ 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	414	 2% 84% 11% 5%
1	B	414	 88% 7% 5%
1	C	414	 3% 86% 8% 5%
1	D	414	 2% 89% 6% 5%

2 Entry composition [i](#)

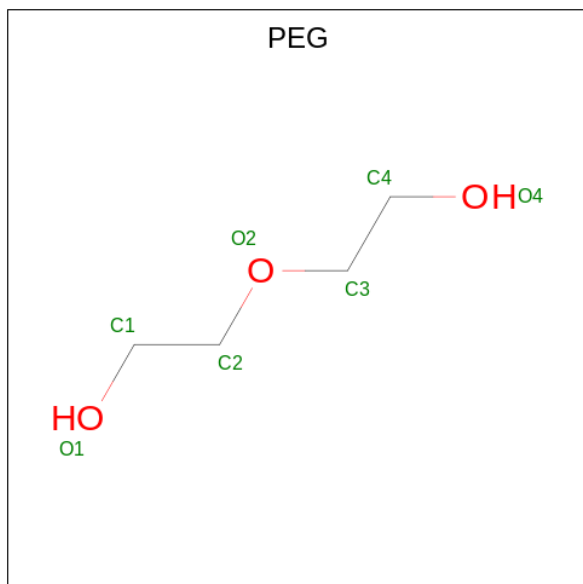
There are 6 unique types of molecules in this entry. The entry contains 12655 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SGR_2426.

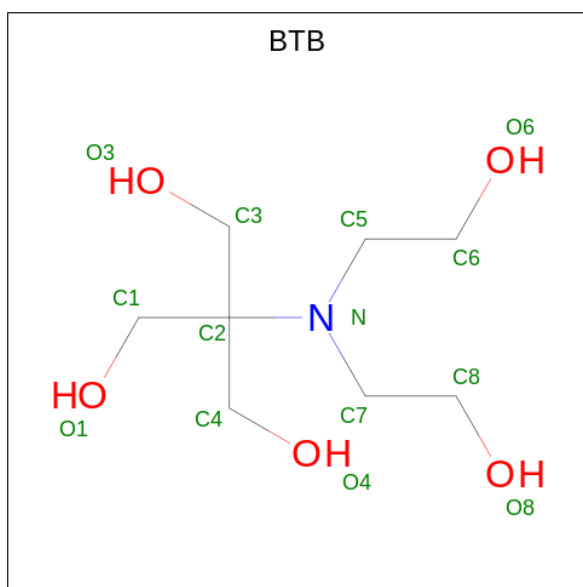
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	395	Total 3072	C 1942	N 538	O 584	S 8	0	0	0
1	B	393	Total 3056	C 1932	N 535	O 581	S 8	0	0	0
1	C	393	Total 3056	C 1932	N 535	O 581	S 8	0	0	0
1	D	393	Total 3056	C 1932	N 535	O 581	S 8	0	0	0

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



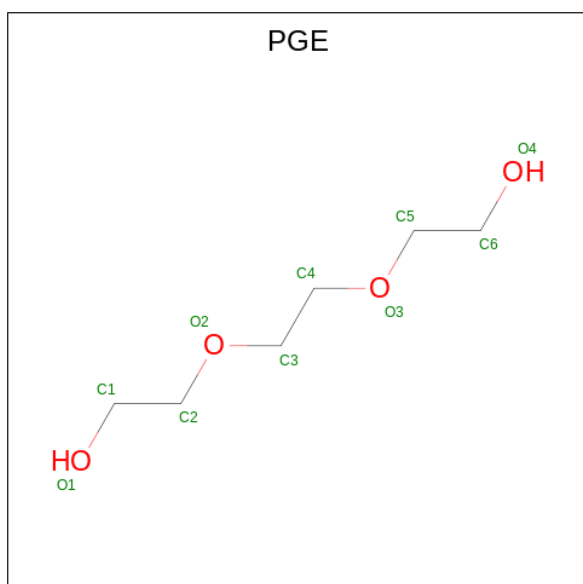
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 7	C 4	O 3	0	0

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



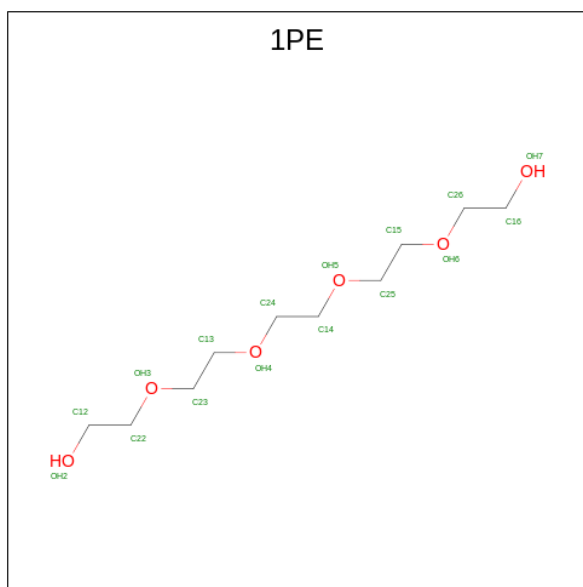
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total	O	0	0
			78	78		
6	B	80	Total	O	0	0
			80	80		
6	C	65	Total	O	0	0
			65	65		
6	D	79	Total	O	0	0
			79	79		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.86Å 97.76Å 184.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.26 – 2.20 46.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.26-2.20) 100.0 (46.22-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.232 , 0.257 0.238 , 0.263	Depositor DCC
R_{free} test set	4438 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtrriage
Anisotropy	0.124	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.035 for k,h,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12655	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PGE, BTB, PEG, 1PE

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	0.27	0/3161	0.49	0/4326
1	B	0.27	0/3145	0.50	0/4305
1	C	0.27	0/3145	0.52	0/4305
1	D	0.27	0/3145	0.50	0/4305
All	All	0.27	0/12596	0.50	0/17241

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	3072	0	2907	23	0
1	B	3056	0	2887	14	0
1	C	3056	0	2887	20	0
1	D	3056	0	2887	13	0
2	A	7	0	10	1	0
3	A	14	0	19	0	0
3	B	14	0	19	0	0
3	C	28	0	38	4	0
3	D	14	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	14	0	0
4	D	10	0	14	0	0
5	B	16	0	22	0	0
6	A	78	0	0	0	0
6	B	80	0	0	0	0
6	C	65	0	0	0	0
6	D	79	0	0	0	0
All	All	12655	0	11723	71	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 71 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:214:ARG:NH1	1:A:260:ASP:OD1	2.34	0.61
1:C:314:LEU:HB2	1:C:350:ILE:HG22	1.86	0.56
1:D:271:ARG:HD2	1:D:278:ILE:HD11	1.89	0.55
1:B:64:TRP:N	1:B:65:PRO:CD	2.72	0.53
1:C:64:TRP:N	1:C:65:PRO:CD	2.71	0.52

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	393/414 (95%)	377 (96%)	15 (4%)	1 (0%)	41 46
1	B	391/414 (94%)	382 (98%)	9 (2%)	0	100 100
1	C	391/414 (94%)	375 (96%)	14 (4%)	2 (0%)	29 31
1	D	391/414 (94%)	375 (96%)	16 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1566/1656 (95%)	1509 (96%)	54 (3%)	3 (0%)	47 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	GLY
1	C	235	PRO
1	C	249	GLU

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	307/323 (95%)	299 (97%)	8 (3%)	46 58
1	B	305/323 (94%)	301 (99%)	4 (1%)	69 81
1	C	305/323 (94%)	294 (96%)	11 (4%)	35 45
1	D	305/323 (94%)	300 (98%)	5 (2%)	62 76
All	All	1222/1292 (95%)	1194 (98%)	28 (2%)	50 63

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	160	VAL
1	D	269	ARG
1	C	235	PRO
1	D	186	PHE
1	C	224	TRP

Sometimes 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](#)

9 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	BTB	C	501	-	13,13,13	1.31	3 (23%)	7,16,16	0.47	0
2	PEG	A	501	-	6,6,6	0.14	0	5,5,5	0.11	0
3	BTB	A	502	-	13,13,13	1.13	2 (15%)	7,16,16	0.54	0
4	PGE	B	501	-	9,9,9	0.16	0	8,8,8	0.12	0
4	PGE	D	501	-	9,9,9	0.20	0	8,8,8	0.13	0
5	1PE	B	503	-	15,15,15	0.20	0	14,14,14	0.11	0
3	BTB	C	502	-	13,13,13	1.07	2 (15%)	7,16,16	0.21	0
3	BTB	D	502	-	13,13,13	1.14	3 (23%)	7,16,16	0.27	0
3	BTB	B	502	-	13,13,13	1.00	1 (7%)	7,16,16	0.18	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	C	501	-	-	8/21/21/21	-
2	PEG	A	501	-	-	4/4/4/4	-
3	BTB	A	502	-	-	4/21/21/21	-
4	PGE	B	501	-	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	D	501	-	-	4/7/7/7	-
5	1PE	B	503	-	-	4/13/13/13	-
3	BTB	C	502	-	-	2/21/21/21	-
3	BTB	D	502	-	-	2/21/21/21	-
3	BTB	B	502	-	-	5/21/21/21	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	BTB	C2-N	3.27	1.55	1.48
3	D	502	BTB	C2-N	2.78	1.54	1.48
3	C	502	BTB	C2-N	2.51	1.53	1.48
3	A	502	BTB	C2-N	2.45	1.53	1.48
3	C	501	BTB	C7-N	2.43	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	BTB	C1-C2-C3-O3
3	A	502	BTB	C8-C7-N-C5
3	B	502	BTB	O1-C1-C2-C4
3	C	501	BTB	C1-C2-N-C5
3	C	501	BTB	C1-C2-N-C7

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	BTB	4	0
2	A	501	PEG	1	0

5.7 Other polymers [i](#)

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 [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, 95th 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 ²)	Q<0.9
1	A	395/414 (95%)	0.05	6 (1%) 73 72	17, 23, 47, 54	0
1	B	393/414 (94%)	-0.13	2 (0%) 91 90	17, 23, 36, 48	0
1	C	393/414 (94%)	0.13	12 (3%) 49 47	17, 27, 49, 63	0
1	D	393/414 (94%)	0.06	10 (2%) 57 55	16, 25, 45, 57	0
All	All	1574/1656 (95%)	0.03	30 (1%) 66 65	16, 24, 45, 63	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	235	PRO	4.8
1	C	186	PHE	4.3
1	D	282	ASP	3.9
1	D	278	ILE	3.5
1	A	275	GLU	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 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, 95th 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(\AA^2)	Q<0.9
4	PGE	D	501	10/10	0.69	0.23	38,39,39,39	0
3	BTB	A	502	14/14	0.77	0.29	29,31,33,33	0
5	1PE	B	503	16/16	0.80	0.21	49,51,52,52	0
3	BTB	B	502	14/14	0.81	0.19	31,32,34,35	0
3	BTB	C	501	14/14	0.84	0.17	29,29,31,31	0
4	PGE	B	501	10/10	0.86	0.16	27,28,28,28	0
3	BTB	C	502	14/14	0.90	0.12	26,27,27,27	0
2	PEG	A	501	7/7	0.90	0.16	28,28,28,28	0
3	BTB	D	502	14/14	0.92	0.12	28,28,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.