



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 03:32 AM EDT

PDB ID : 1XQI / pdb_00001xqi
Title : Crystal Structure Analysis of an NDP kinase from *Pyrobaculum aerophilum*
Authors : Pedelacq, J.D.; Waldo, G.S.; Cabantous, S.; Liong, E.C.; Berendzen, J.; Terwilliger, T.C.
Deposited on : 2004-10-12
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

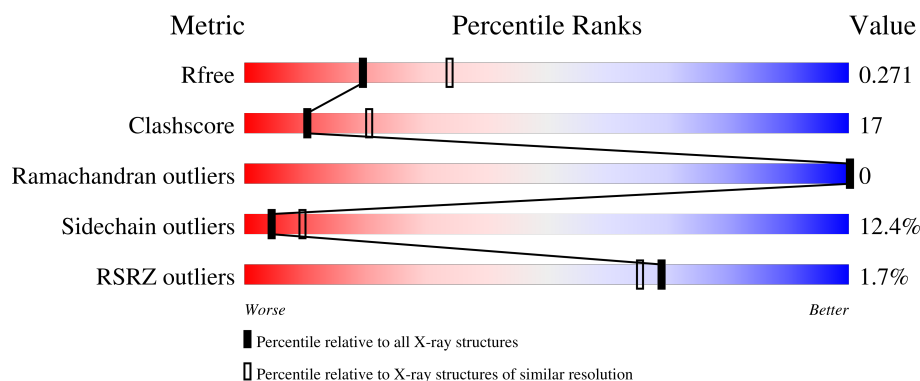
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	195	0% 65% 26% 7%
1	B	195	2% 60% 29% 5% 7%
1	C	195	2% 58% 31% 7%

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
3	PGE	A	500	-	-	X	-
3	PGE	B	600	-	-	X	-
3	PGE	C	700	-	X	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4454 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	Se	0	0	0
			1414	900	246	265	3			
1	B	182	Total	C	N	O	Se	0	0	0
			1414	900	246	265	3			
1	C	182	Total	C	N	O	Se	0	0	0
			1414	900	246	265	3			

There are 33 discrepancies between the modelled and reference sequences:

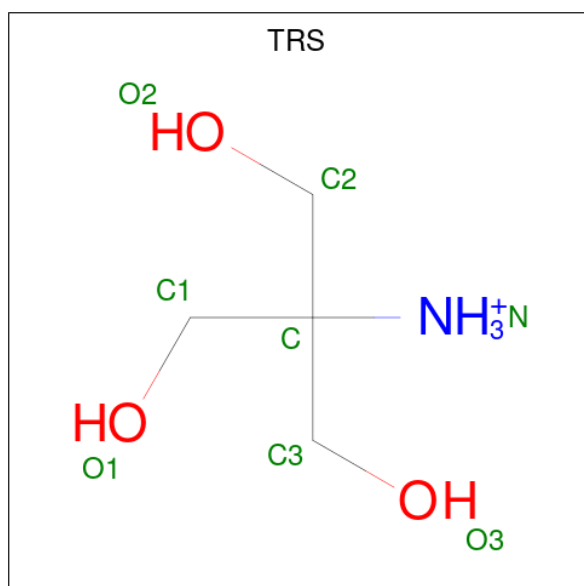
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8ZWY4
A	10	ASP	ALA	engineered mutation	UNP Q8ZWY4
A	13	MSE	MET	modified residue	UNP Q8ZWY4
A	33	ASP	GLY	engineered mutation	UNP Q8ZWY4
A	40	LYS	GLU	engineered mutation	UNP Q8ZWY4
A	51	MSE	MET	modified residue	UNP Q8ZWY4
A	71	GLN	ARG	engineered mutation	UNP Q8ZWY4
A	107	ASN	SER	engineered mutation	UNP Q8ZWY4
A	112	MSE	MET	modified residue	UNP Q8ZWY4
A	117	ASN	ILE	engineered mutation	UNP Q8ZWY4
A	120	MSE	MET	modified residue	UNP Q8ZWY4
B	1	MSE	MET	modified residue	UNP Q8ZWY4
B	10	ASP	ALA	engineered mutation	UNP Q8ZWY4
B	13	MSE	MET	modified residue	UNP Q8ZWY4
B	33	ASP	GLY	engineered mutation	UNP Q8ZWY4
B	40	LYS	GLU	engineered mutation	UNP Q8ZWY4
B	51	MSE	MET	modified residue	UNP Q8ZWY4
B	71	GLN	ARG	engineered mutation	UNP Q8ZWY4
B	107	ASN	SER	engineered mutation	UNP Q8ZWY4
B	112	MSE	MET	modified residue	UNP Q8ZWY4
B	117	ASN	ILE	engineered mutation	UNP Q8ZWY4
B	120	MSE	MET	modified residue	UNP Q8ZWY4
C	1	MSE	MET	modified residue	UNP Q8ZWY4

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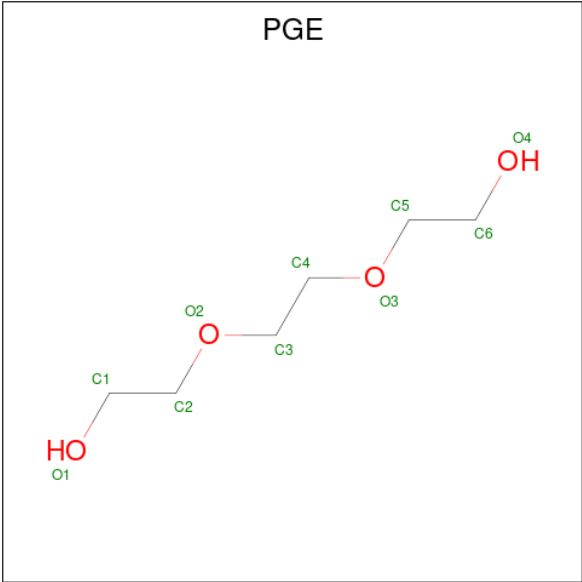
Chain	Residue	Modelled	Actual	Comment	Reference
C	10	ASP	ALA	engineered mutation	UNP Q8ZWHY4
C	13	MSE	MET	modified residue	UNP Q8ZWHY4
C	33	ASP	GLY	engineered mutation	UNP Q8ZWHY4
C	40	LYS	GLU	engineered mutation	UNP Q8ZWHY4
C	51	MSE	MET	modified residue	UNP Q8ZWHY4
C	71	GLN	ARG	engineered mutation	UNP Q8ZWHY4
C	107	ASN	SER	engineered mutation	UNP Q8ZWHY4
C	112	MSE	MET	modified residue	UNP Q8ZWHY4
C	117	ASN	ILE	engineered mutation	UNP Q8ZWHY4
C	120	MSE	MET	modified residue	UNP Q8ZWHY4

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	57	Total	O	0	0
			57	57		
4	C	55	Total	O	0	0
			55	55		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.02Å 72.04Å 104.99Å 90.00° 133.30° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (25.00-2.50) 86.7 (25.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.260 0.205 , 0.271	Depositor DCC
R_{free} test set	1513 reflections (6.45%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4454	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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, TRS

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	1.13	3/1438 (0.2%)	1.14	2/1942 (0.1%)
1	B	1.15	8/1438 (0.6%)	1.20	10/1942 (0.5%)
1	C	1.13	5/1438 (0.3%)	1.17	4/1942 (0.2%)
All	All	1.14	16/4314 (0.4%)	1.17	16/5826 (0.3%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	144	PRO	CA-C	8.67	1.56	1.51
1	C	51	MSE	SE-CE	-8.03	1.71	1.95
1	A	120	MSE	SE-CE	-6.51	1.75	1.95
1	C	120	MSE	SE-CE	-6.50	1.75	1.95
1	A	51	MSE	SE-CE	-6.42	1.76	1.95

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	51	MSE	CG-SE-CE	-7.17	83.16	98.92
1	C	176	SER	N-CA-C	6.23	113.74	108.13
1	B	128	VAL	N-CA-C	-6.20	104.47	110.42
1	C	192	GLU	N-CA-C	-5.94	105.61	114.64
1	B	138	THR	N-CA-C	5.75	118.32	111.71

There are no chirality outliers.

There are no planarity outliers.

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	1414	0	1443	53	0
1	B	1414	0	1443	32	1
1	C	1414	0	1443	63	0
2	A	8	0	12	3	0
2	B	8	0	12	1	0
2	C	8	0	12	2	0
3	A	10	0	14	14	0
3	B	10	0	14	7	0
3	C	10	0	14	18	0
4	A	46	0	0	11	0
4	B	57	0	0	4	0
4	C	55	0	0	7	0
All	All	4454	0	4407	148	1

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 17.

The worst 5 of 148 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:69:TRP:HE1	3:C:700:PGE:H6	1.26	0.99
1:A:172:HIS:CE1	3:A:500:PGE:H1	1.97	0.98
1:C:172:HIS:CE1	3:C:700:PGE:H1	2.02	0.95
2:A:200:TRS:H21	3:A:500:PGE:O4	1.67	0.94
1:B:32:VAL:HG23	4:B:647:HOH:O	1.75	0.86

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:NH2	1:B:95:ASP:OD2[2_757]	2.12	0.08

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	180/195 (92%)	176 (98%)	4 (2%)	0	100	100
1	B	180/195 (92%)	173 (96%)	7 (4%)	0	100	100
1	C	180/195 (92%)	174 (97%)	6 (3%)	0	100	100
All	All	540/585 (92%)	523 (97%)	17 (3%)	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	153/162 (94%)	137 (90%)	16 (10%)	6	14
1	B	153/162 (94%)	132 (86%)	21 (14%)	3	7
1	C	153/162 (94%)	133 (87%)	20 (13%)	4	8
All	All	459/486 (94%)	402 (88%)	57 (12%)	4	9

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	122	LEU
1	C	169	ASN
1	B	191	GLU
1	C	162	GLU
1	C	130	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	169	ASN
1	C	75	GLN
1	C	169	ASN
1	A	169	ASN
1	A	117	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	PGE	A	500	-	9,9,9	1.39	2 (22%)	8,8,8	1.93	3 (37%)
2	TRS	B	300	-	7,7,7	0.43	0	9,9,9	1.17	1 (11%)
3	PGE	C	700	-	9,9,9	1.40	1 (11%)	8,8,8	1.54	2 (25%)
2	TRS	A	200	-	7,7,7	0.56	0	9,9,9	0.91	0
3	PGE	B	600	-	9,9,9	1.29	0	8,8,8	1.86	3 (37%)
2	TRS	C	400	-	7,7,7	0.49	0	9,9,9	1.16	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	PGE	A	500	-	-	3/7/7/7	-
2	TRS	B	300	-	-	6/9/9/9	-
3	PGE	C	700	-	-	7/7/7/7	-
2	TRS	A	200	-	-	5/9/9/9	-
3	PGE	B	600	-	-	3/7/7/7	-
2	TRS	C	400	-	-	9/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	700	PGE	O2-C3	2.70	1.53	1.42
3	A	500	PGE	O2-C3	2.28	1.51	1.42
3	A	500	PGE	O3-C4	2.06	1.51	1.42

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	PGE	O2-C2-C1	3.47	125.40	110.11
3	A	500	PGE	O2-C2-C1	3.34	124.82	110.11
3	A	500	PGE	O3-C5-C6	3.13	123.89	110.11
3	C	700	PGE	O2-C2-C1	2.90	122.89	110.11
3	B	600	PGE	O2-C3-C4	2.69	122.59	110.35

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	300	TRS	C1-C-C3-O3
2	C	400	TRS	C1-C-C3-O3
3	A	500	PGE	C1-C2-O2-C3
3	C	700	PGE	C6-C5-O3-C4
3	B	600	PGE	C6-C5-O3-C4

There are no ring outliers.

6 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	PGE	14	0
2	B	300	TRS	1	0
3	C	700	PGE	18	0
2	A	200	TRS	3	0
3	B	600	PGE	7	0
2	C	400	TRS	2	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, 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	179/195 (91%)	-0.03	2 (1%) 78 75	20, 33, 53, 67	0
1	B	179/195 (91%)	0.03	3 (1%) 69 65	22, 34, 65, 76	0
1	C	179/195 (91%)	-0.00	4 (2%) 62 58	20, 34, 59, 70	0
All	All	537/585 (91%)	0.00	9 (1%) 69 65	20, 34, 59, 76	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14	PRO	4.1
1	A	14	PRO	3.6
1	B	195	GLU	3.5
1	C	185	ARG	2.8
1	B	194	LEU	2.5

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 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, 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($\text{\AA}^2$)	Q<0.9
2	TRS	A	200	8/8	0.73	0.18	46,51,54,58	0
3	PGE	C	700	10/10	0.74	0.23	62,65,70,71	0
3	PGE	B	600	10/10	0.77	0.24	72,74,78,79	0
2	TRS	B	300	8/8	0.80	0.18	53,54,59,60	0
2	TRS	C	400	8/8	0.82	0.16	52,56,58,64	0
3	PGE	A	500	10/10	0.87	0.15	47,52,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.