



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3GYB / pdb_00003gyb
Title : Crystal structure of a LacI-family transcriptional regulatory protein from *Corynebacterium glutamicum*
Authors : Palani, K.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-04-03
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

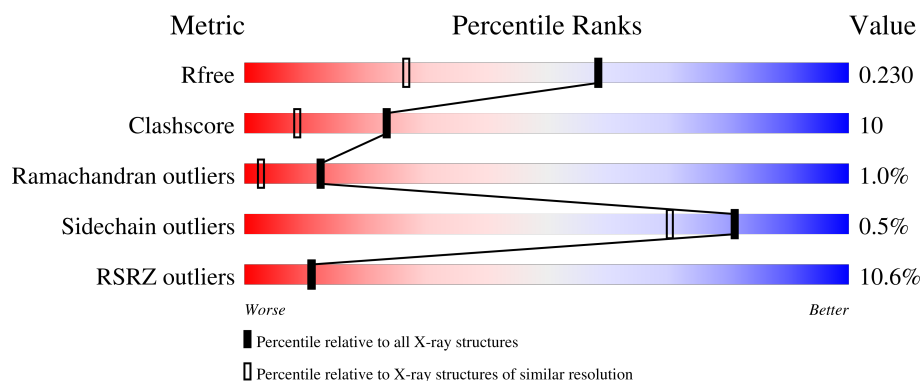
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	280	9% 78% 14% 7%
1	B	280	10% 68% 19% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4144 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 Transcriptional regulators (LACI-FAMILY TRANSCRIPTIONAL REGULATORY PROTEIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	Se	0	0	0
			1980	1247	342	386	1	4			
1	B	246	Total	C	N	O	S	Se	0	0	0
			1865	1176	316	368	1	4			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MSE	-	expression tag	UNP Q8NTY1
A	60	SER	-	expression tag	UNP Q8NTY1
A	61	LEU	-	expression tag	UNP Q8NTY1
A	331	GLU	-	expression tag	UNP Q8NTY1
A	332	GLY	-	expression tag	UNP Q8NTY1
A	333	HIS	-	expression tag	UNP Q8NTY1
A	334	HIS	-	expression tag	UNP Q8NTY1
A	335	HIS	-	expression tag	UNP Q8NTY1
A	336	HIS	-	expression tag	UNP Q8NTY1
A	337	HIS	-	expression tag	UNP Q8NTY1
A	338	HIS	-	expression tag	UNP Q8NTY1
B	59	MSE	-	expression tag	UNP Q8NTY1
B	60	SER	-	expression tag	UNP Q8NTY1
B	61	LEU	-	expression tag	UNP Q8NTY1
B	331	GLU	-	expression tag	UNP Q8NTY1
B	332	GLY	-	expression tag	UNP Q8NTY1
B	333	HIS	-	expression tag	UNP Q8NTY1
B	334	HIS	-	expression tag	UNP Q8NTY1
B	335	HIS	-	expression tag	UNP Q8NTY1
B	336	HIS	-	expression tag	UNP Q8NTY1
B	337	HIS	-	expression tag	UNP Q8NTY1
B	338	HIS	-	expression tag	UNP Q8NTY1

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total 152	O 152	0	0
3	B	145	Total 145	O 145	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.07Å 61.88Å 65.60Å 115.83° 106.37° 90.50°	Depositor
Resolution (Å)	32.55 – 1.60 32.55 – 1.60	Depositor EDS
% Data completeness (in resolution range)	90.4 (32.55-1.60) 90.5 (32.55-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.231 0.214 , 0.230	Depositor DCC
R_{free} test set	3089 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l 0.016 for -h,k,-k-l 0.007 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4144	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.01% 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: MG

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	0.36	0/2014	0.86	6/2742 (0.2%)
1	B	0.35	0/1894	0.87	6/2576 (0.2%)
All	All	0.36	0/3908	0.87	12/5318 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ILE	N-CA-C	6.48	116.97	110.23
1	B	79	ILE	N-CA-C	6.43	116.92	110.23
1	A	89	LEU	N-CA-C	6.32	119.46	111.69
1	A	282	LEU	N-CA-C	5.50	118.59	109.46
1	B	282	LEU	N-CA-C	5.36	118.35	109.46
1	B	89	LEU	N-CA-C	5.33	118.25	111.69
1	A	305	ASP	CA-C-N	5.26	124.92	119.56
1	A	305	ASP	C-N-CA	5.26	124.92	119.56
1	B	98	VAL	N-CA-C	5.22	116.10	108.53
1	A	283	THR	N-CA-C	-5.21	102.15	109.96
1	B	75	ASN	CA-C-N	5.04	126.14	119.84
1	B	75	ASN	C-N-CA	5.04	126.14	119.84

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	1980	0	1974	34	0
1	B	1865	0	1855	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	152	0	0	1	0
3	B	145	0	0	3	0
All	All	4144	0	3829	78	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 10.

All (78) 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:65:LEU:HB3	1:A:117:MSE:HE2	1.22	1.12
1:B:312:GLU:HG2	1:B:313:ILE:H	1.30	0.97
1:A:65:LEU:HB3	1:A:117:MSE:CE	2.04	0.87
1:A:65:LEU:HD13	1:A:117:MSE:HE3	1.58	0.85
1:A:65:LEU:CB	1:A:117:MSE:HE2	2.10	0.77
1:B:128:ILE:HG23	1:B:129:PRO:HD3	1.73	0.70
1:B:133:VAL:C	3:B:451:HOH:O	2.34	0.69
1:A:311:PRO:HG2	1:A:313:ILE:HD11	1.74	0.69
1:A:65:LEU:HD22	1:A:117:MSE:CE	2.24	0.67
1:A:295:ASN:ND2	1:A:314:MSE:H	1.92	0.67
1:B:128:ILE:HG13	1:B:187:GLY:N	2.10	0.67
1:B:312:GLU:HG2	1:B:313:ILE:N	2.09	0.66
1:B:128:ILE:O	1:B:187:GLY:HA3	1.97	0.65
1:B:216:ALA:HB1	1:B:242:ASN:HD21	1.62	0.64
1:A:65:LEU:HD22	1:A:117:MSE:HE1	1.78	0.64
1:A:65:LEU:HD13	1:A:117:MSE:CE	2.27	0.64
1:B:300:LEU:O	1:B:304:LEU:HD13	1.97	0.63
1:A:65:LEU:HD21	1:B:116:SER:OG	1.99	0.62
1:B:128:ILE:CG2	1:B:129:PRO:HD3	2.30	0.61
1:A:184:VAL:HG21	1:A:242:ASN:ND2	2.17	0.59
1:B:97:SER:OG	1:B:117:MSE:HE1	2.02	0.59
1:A:92:LYS:HE2	3:A:364:HOH:O	2.02	0.59
1:B:65:LEU:CD2	1:B:117:MSE:SE	3.01	0.58
1:A:158:ASN:HD22	1:A:319:PRO:HB3	1.69	0.57
1:A:115:LEU:HD21	1:A:137:LEU:HD12	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HA	3:B:451:HOH:O	2.04	0.57
1:A:184:VAL:HG21	1:A:242:ASN:HD21	1.71	0.55
1:B:184:VAL:HG23	1:B:189:GLY:HA3	1.89	0.55
1:B:176:HIS:HD2	1:B:236:THR:OG1	1.89	0.55
1:A:213:LEU:H	1:A:213:LEU:HD23	1.70	0.54
1:B:92:LYS:HE3	1:B:301:LEU:HD21	1.90	0.53
1:A:269:TYR:O	1:A:270:ASP:CB	2.56	0.53
1:B:70:ILE:O	1:B:100:ASP:HA	2.08	0.53
1:B:206:GLU:OE1	1:B:207:PRO:HD2	2.09	0.53
1:B:70:ILE:C	1:B:126:GLN:HG2	2.35	0.52
1:B:133:VAL:HG13	1:B:154:ASP:O	2.09	0.52
1:A:271:ASN:HA	1:A:284:THR:HG21	1.92	0.51
1:B:330:ARG:HH11	1:B:330:ARG:HG3	1.74	0.51
1:A:149:GLN:HG3	1:A:150:ALA:N	2.25	0.51
1:B:216:ALA:CB	1:B:242:ASN:HD21	2.23	0.51
1:B:65:LEU:HD21	1:B:117:MSE:SE	2.60	0.51
1:B:269:TYR:O	1:B:270:ASP:CB	2.59	0.50
1:B:108:THR:C	1:B:110:PRO:HD3	2.37	0.50
1:A:149:GLN:HG3	1:A:150:ALA:H	1.77	0.50
1:B:312:GLU:CG	1:B:313:ILE:H	2.09	0.49
1:A:147:ILE:HG22	1:A:149:GLN:HG2	1.94	0.49
1:A:70:ILE:O	1:A:100:ASP:HA	2.13	0.49
1:A:62:ARG:NH2	1:A:94:TYR:OH	2.46	0.48
1:B:137:LEU:HB3	1:B:138:PRO:HD3	1.94	0.48
1:A:269:TYR:O	1:A:270:ASP:CG	2.57	0.48
1:B:90:THR:OG1	1:B:91:PRO:HD3	2.13	0.47
1:B:269:TYR:O	1:B:270:ASP:CG	2.57	0.47
1:B:158:ASN:HD22	1:B:319:PRO:HB3	1.80	0.46
1:B:81:LEU:C	1:B:81:LEU:HD23	2.41	0.46
1:B:184:VAL:HG21	3:B:384:HOH:O	2.16	0.46
1:A:117:MSE:HB2	1:B:117:MSE:HB2	1.98	0.45
1:B:97:SER:OG	1:B:117:MSE:SE	2.84	0.45
1:A:190:LEU:O	1:A:194:GLU:HG3	2.16	0.45
1:B:164:ALA:HB3	1:B:195:SER:HB3	1.99	0.45
1:B:271:ASN:HA	1:B:284:THR:HG21	1.99	0.44
1:B:329:PRO:O	1:B:330:ARG:HB2	2.16	0.44
1:A:126:GLN:HE21	1:A:128:ILE:HD11	1.83	0.44
1:A:269:TYR:O	1:A:270:ASP:HB2	2.18	0.44
1:B:131:PHE:O	1:B:132:THR:CB	2.65	0.43
1:B:128:ILE:HG13	1:B:187:GLY:CA	2.48	0.43
1:B:128:ILE:N	1:B:129:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:HB3	1:B:126:GLN:CD	2.42	0.43
1:B:137:LEU:H	1:B:138:PRO:CD	2.32	0.42
1:A:305:ASP:OD2	1:A:308:ALA:HB2	2.19	0.42
1:A:114:ALA:O	1:A:117:MSE:HG2	2.20	0.42
1:A:81:LEU:C	1:A:81:LEU:HD23	2.45	0.42
1:A:164:ALA:HB3	1:A:195:SER:HB3	2.01	0.42
1:B:176:HIS:CD2	1:B:237:ALA:HB2	2.55	0.42
1:A:110:PRO:HG3	1:A:126:GLN:HE22	1.85	0.41
1:B:134:PRO:HD2	1:B:154:ASP:O	2.21	0.41
1:A:63:THR:O	1:A:64:GLN:HB2	2.20	0.41
1:B:330:ARG:HG3	1:B:330:ARG:NH1	2.36	0.41
1:B:131:PHE:CZ	1:B:157:ALA:HB1	2.56	0.40

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	257/280 (92%)	251 (98%)	5 (2%)	1 (0%)	30	14
1	B	240/280 (86%)	230 (96%)	6 (2%)	4 (2%)	7	1
All	All	497/560 (89%)	481 (97%)	11 (2%)	5 (1%)	12	3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	137	LEU
1	A	270	ASP
1	B	270	ASP
1	B	132	THR
1	B	129	PRO

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	216/229 (94%)	215 (100%)	1 (0%)	81	70
1	B	205/229 (90%)	204 (100%)	1 (0%)	81	70
All	All	421/458 (92%)	419 (100%)	2 (0%)	81	70

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	LEU
1	B	261	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	149	GLN
1	A	158	ASN
1	A	232	HIS
1	A	295	ASN
1	B	64	GLN
1	B	158	ASN
1	B	176	HIS
1	B	232	HIS
1	B	242	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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	257/280 (91%)	0.48	24 (9%) 14 14	10, 17, 34, 50	0
1	B	242/280 (86%)	0.75	29 (11%) 9 8	10, 17, 40, 56	0
All	All	499/560 (89%)	0.61	53 (10%) 11 11	10, 17, 35, 56	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	PHE	14.8
1	B	128	ILE	14.4
1	B	133	VAL	12.0
1	B	129	PRO	10.5
1	B	137	LEU	8.6
1	B	136	SER	8.2
1	A	213	LEU	7.5
1	B	138	PRO	6.3
1	B	132	THR	6.1
1	B	134	PRO	5.9
1	A	150	ALA	5.8
1	B	330	ARG	5.6
1	B	130	ASP	5.5
1	A	330	ARG	5.3
1	B	135	ASP	5.1
1	A	147	ILE	4.8
1	B	211	ASP	4.6
1	A	313	ILE	4.5
1	B	304	LEU	4.5
1	A	211	ASP	4.4
1	B	127	ASP	4.4
1	A	144	GLY	4.3
1	A	128	ILE	4.2
1	A	62	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	151	SER	4.0
1	A	112	THR	4.0
1	A	149	GLN	4.0
1	A	212	TYR	3.9
1	A	307	GLU	3.7
1	A	145	THR	3.3
1	B	301	LEU	3.3
1	B	185	GLY	3.2
1	B	154	ASP	3.1
1	A	312	GLU	3.1
1	B	63	THR	2.9
1	B	212	TYR	2.9
1	A	190	LEU	2.8
1	B	313	ILE	2.8
1	A	148	THR	2.6
1	B	118	ARG	2.6
1	B	65	LEU	2.4
1	B	206	GLU	2.4
1	B	312	GLU	2.4
1	A	311	PRO	2.4
1	B	191	ARG	2.4
1	B	64	GLN	2.3
1	A	107	GLY	2.2
1	A	63	THR	2.2
1	B	228	LEU	2.1
1	B	161	PHE	2.1
1	A	127	ASP	2.0
1	A	310	HIS	2.0
1	A	305	ASP	2.0

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	MG	B	2	1/1	0.98	0.04	12,12,12,12	0
2	MG	A	1	1/1	0.99	0.03	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.