



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 06:58 PM BST

PDB ID : 6XS4
Title : Crystal structure of glycyl radical enzyme ECL_02896 from *Enterobacter cloacae* subsp. *cloacae*
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Deposited on : 2020-07-14
Resolution : 2.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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	:	2.13.1
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)	:	2.13.1

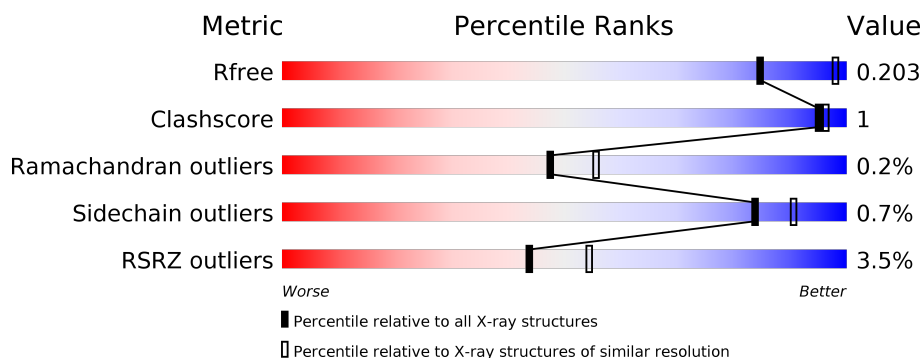
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 on 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	811	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	B	811	<div> <div>5%</div> <div> <div></div> <div>97%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13427 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.

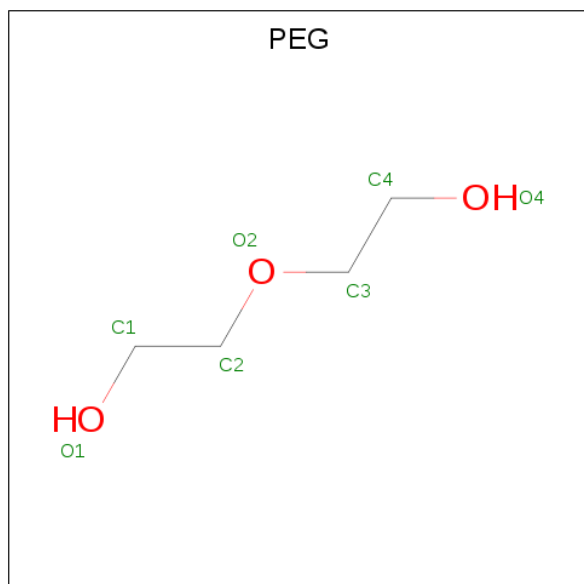
- Molecule 1 is a protein called Formate C-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	810	Total	C	N	O	S	0	0	0
			6341	3998	1116	1196	31			
1	B	810	Total	C	N	O	S	0	0	0
			6341	3998	1116	1196	31			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A0H3CPF7
B	0	GLY	-	expression tag	UNP A0A0H3CPF7

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



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

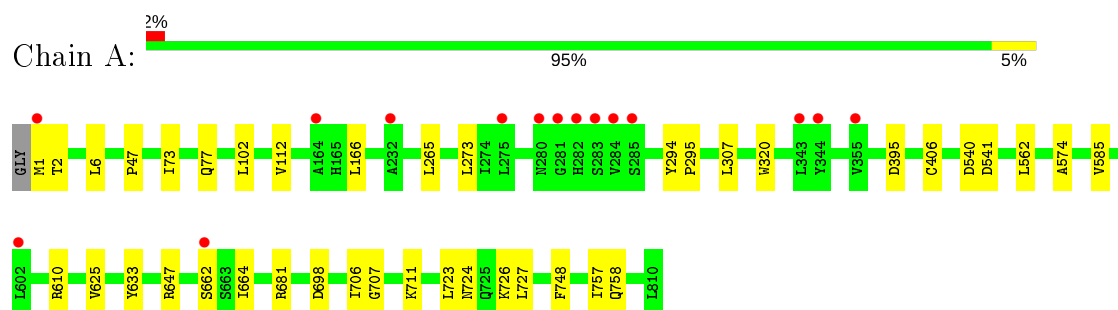
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	349	Total	O	0	0
			349	349		
4	B	373	Total	O	0	0
			373	373		

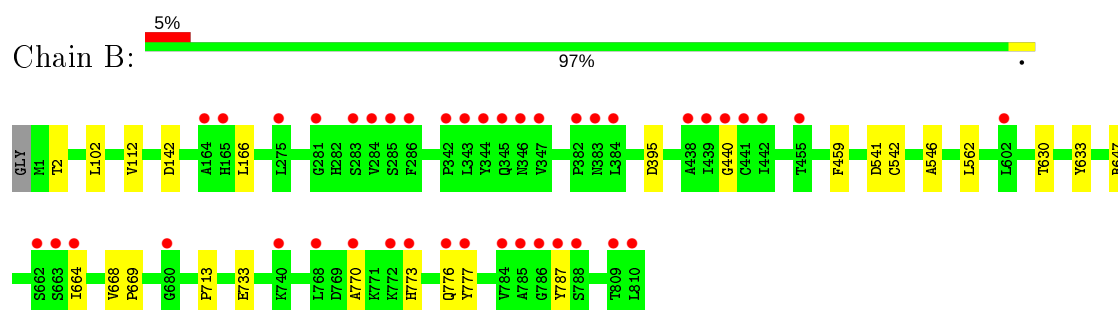
3 Residue-property plots [i](#)

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: Formate C-acetyltransferase



- Molecule 1: Formate C-acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	283.10Å 60.97Å 118.95Å 90.00° 107.65° 90.00°	Depositor
Resolution (Å)	39.72 – 2.33 39.72 – 2.33	Depositor EDS
% Data completeness (in resolution range)	95.2 (39.72-2.33) 95.2 (39.72-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.179 , 0.203 0.179 , 0.203	Depositor DCC
R_{free} test set	1996 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.778	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13427	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO

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	0.26	0/6471	0.43	0/8772
1	B	0.28	0/6471	0.44	0/8772
All	All	0.27	0/12942	0.43	0/17544

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

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	6341	0	6271	19	0
1	B	6341	0	6271	11	0
2	A	7	0	10	0	0
3	A	4	0	6	1	0
3	B	12	0	18	0	0
4	A	349	0	0	1	0
4	B	373	0	0	0	0
All	All	13427	0	12576	30	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 1.

All (30) 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:773:HIS:HB2	1:B:776:GLN:HG3	1.82	0.61
1:A:102:LEU:HD12	1:A:112:VAL:HG21	1.90	0.54
1:B:102:LEU:HD12	1:B:112:VAL:HG21	1.92	0.51
1:B:668:VAL:HB	1:B:669:PRO:HD3	1.93	0.50
1:A:47:PRO:HB3	3:A:902:EDO:H12	1.92	0.49
1:B:773:HIS:CB	1:B:776:GLN:HG3	2.43	0.49
1:B:787:TYR:N	1:B:787:TYR:CD1	2.81	0.47
1:B:770:ALA:HA	1:B:777:TYR:CD2	2.49	0.47
1:A:726:LYS:O	1:A:727:LEU:HD23	2.15	0.47
1:A:6:LEU:HD13	1:A:406:CYS:SG	2.54	0.47
1:B:166:LEU:C	1:B:166:LEU:HD12	2.35	0.47
1:A:166:LEU:HD12	1:A:166:LEU:C	2.35	0.46
1:A:585:VAL:HG12	1:A:610:ARG:HH12	1.81	0.46
1:A:77:GLN:HA	1:A:273:LEU:HD11	1.98	0.46
1:A:707:GLY:O	1:A:711:LYS:HG3	2.16	0.45
1:B:459:PHE:CE1	1:B:562:LEU:HD23	2.51	0.44
1:A:73:ILE:HD11	1:A:265:LEU:HD23	1.99	0.44
1:A:698:ASP:N	1:A:698:ASP:OD1	2.45	0.44
1:A:294:TYR:N	1:A:295:PRO:CD	2.82	0.43
1:A:2:THR:N	1:A:395:ASP:OD2	2.52	0.43
1:A:562:LEU:HD22	1:A:662:SER:C	2.39	0.43
1:B:630:THR:HG23	1:B:713:PRO:HD3	2.01	0.42
1:B:2:THR:N	1:B:395:ASP:OD1	2.47	0.42
1:A:724:ASN:OD1	1:A:758:GLN:NE2	2.53	0.42
1:A:574:ALA:HB2	1:A:625:VAL:HG23	2.02	0.42
1:B:542:CYS:O	1:B:546:ALA:N	2.52	0.42
1:A:540:ASP:HA	1:A:541:ASP:HA	1.84	0.41
1:A:723:LEU:HD23	1:A:757:ILE:HD12	2.02	0.41
1:A:706:ILE:HB	1:A:748:PHE:CD1	2.55	0.40
1:A:1:MET:N	4:A:1017:HOH:O	2.49	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	808/811 (100%)	779 (96%)	28 (4%)	1 (0%)	51	62
1	B	808/811 (100%)	779 (96%)	27 (3%)	2 (0%)	47	55
All	All	1616/1622 (100%)	1558 (96%)	55 (3%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	664	ILE
1	B	664	ILE
1	B	440	GLY

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	674/674 (100%)	669 (99%)	5 (1%)	84	90
1	B	674/674 (100%)	669 (99%)	5 (1%)	84	90
All	All	1348/1348 (100%)	1338 (99%)	10 (1%)	84	90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	LEU
1	A	320	TRP
1	A	633	TYR
1	A	647	ARG
1	A	681	ARG
1	B	142	ASP
1	B	541	ASP
1	B	633	TYR
1	B	647	ARG
1	B	733	GLU

Some 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](#)

5 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	EDO	B	901	-	3,3,3	0.57	0	2,2,2	0.31	0
3	EDO	B	903	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	A	902	-	3,3,3	0.46	0	2,2,2	0.19	0
3	EDO	B	902	-	3,3,3	0.45	0	2,2,2	0.31	0
2	PEG	A	901	-	6,6,6	0.70	0	5,5,5	0.55	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	EDO	B	901	-	-	0/1/1/1	-
3	EDO	B	903	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	902	-	-	1/1/1/1	-
3	EDO	B	902	-	-	0/1/1/1	-
2	PEG	A	901	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	PEG	O1-C1-C2-O2
3	A	902	EDO	O1-C1-C2-O2
2	A	901	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	EDO	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 ⓘ

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	810/811 (99%)	-0.07	15 (1%) 66 75	34, 51, 80, 114	0
1	B	810/811 (99%)	0.02	42 (5%) 27 38	32, 49, 83, 110	0
All	All	1620/1622 (99%)	-0.02	57 (3%) 44 54	32, 50, 82, 114	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	344	TYR	4.6
1	B	786	GLY	4.4
1	B	602	LEU	3.9
1	B	343	LEU	3.9
1	B	662	SER	3.7
1	B	442	ILE	3.7
1	B	441	CYS	3.5
1	B	785	ALA	3.4
1	A	343	LEU	3.4
1	A	284	VAL	3.4
1	B	440	GLY	3.3
1	B	777	TYR	3.3
1	B	664	ILE	3.3
1	B	284	VAL	3.3
1	B	773	HIS	3.2
1	B	382	PRO	3.2
1	A	602	LEU	3.1
1	B	768	LEU	3.1
1	B	165	HIS	3.1
1	B	772	LYS	3.1
1	B	285	SER	3.1
1	B	787	TYR	3.0
1	A	344	TYR	3.0
1	A	285	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	282	HIS	3.0
1	B	810	LEU	3.0
1	A	283	SER	2.9
1	A	1	MET	2.9
1	B	439	ILE	2.8
1	B	770	ALA	2.8
1	B	342	PRO	2.8
1	B	346	ASN	2.8
1	B	283	SER	2.8
1	B	383	ASN	2.7
1	B	663	SER	2.6
1	B	164	ALA	2.5
1	A	164	ALA	2.5
1	B	345	GLN	2.5
1	B	740	LYS	2.5
1	B	286	PHE	2.5
1	B	438	ALA	2.4
1	A	280	ASN	2.3
1	A	281	GLY	2.3
1	B	776	GLN	2.2
1	B	788	SER	2.1
1	B	680	GLY	2.1
1	B	275	LEU	2.1
1	B	347	VAL	2.1
1	B	784	VAL	2.1
1	B	809	THR	2.1
1	A	232	ALA	2.1
1	B	384	LEU	2.1
1	B	455	THR	2.1
1	A	275	LEU	2.0
1	B	281	GLY	2.0
1	A	662	SER	2.0
1	A	355	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
3	EDO	B	903	4/4	0.90	0.23	52,53,53,54	0
2	PEG	A	901	7/7	0.92	0.18	72,72,72,72	0
3	EDO	B	901	4/4	0.94	0.19	47,47,48,48	0
3	EDO	B	902	4/4	0.97	0.21	53,53,53,53	0
3	EDO	A	902	4/4	0.97	0.12	53,53,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.