

wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 12:25 PM EST

PDB ID : 2O9A

Title : The crystal structure of the E.coli IclR C-terminal fragment in complex with

pyruvate.

Authors: Lunin, V.V.; Ezersky, A.; Evdokimova, E.; Kudritska, M.; Savchenko, A.

Deposited on : 2006-12-13

Resolution : 1.80 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 (i) 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 (1)) 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 : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

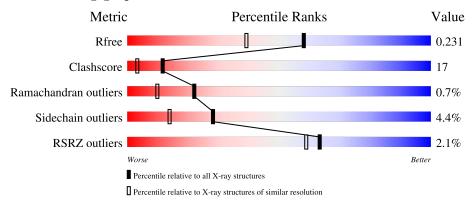
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.80 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	182	77%	17%	•
1	В	182	80%	15%	
1	С	182	82%	15%	
1	D	182	74%	20%	

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	PYR	С	907	-	X	-	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6553 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 Acetate operon repressor.

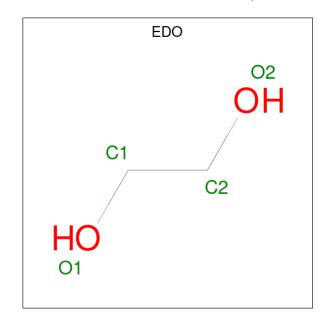
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	182	Total	С	N	О	S	0	6	0
1	A	102	1445	903	263	267	12	0	0	U
1	В	179	Total	С	N	О	S	0	3	0
1	Ъ	119	1399	873	254	260	12	U	3	U
1	С	182	Total	С	N	О	S	0	3	0
1		102	1417	886	259	261	11	0	3	U
1	1 D	D 100	Total	С	N	О	S	0	4	0
	180	1417	886	259	260	12		1	0	

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P16528
A	2	HIS	-	cloning artifact	UNP P16528
A	3	MET	-	cloning artifact	UNP P16528
A	181	GLY	-	cloning artifact	UNP P16528
A	182	SER	-	cloning artifact	UNP P16528
В	1	GLY	-	cloning artifact	UNP P16528
В	2	HIS	-	cloning artifact	UNP P16528
В	3	MET	-	cloning artifact	UNP P16528
В	181	GLY	-	cloning artifact	UNP P16528
В	182	SER	-	cloning artifact	UNP P16528
С	1	GLY	-	cloning artifact	UNP P16528
С	2	HIS	-	cloning artifact	UNP P16528
С	3	MET	-	cloning artifact	UNP P16528
С	181	GLY	-	cloning artifact	UNP P16528
С	182	SER	-	cloning artifact	UNP P16528
D	1	GLY	-	cloning artifact	UNP P16528
D	2	HIS	-	cloning artifact	UNP P16528
D	3	MET	-	cloning artifact	UNP P16528
D	181	GLY	-	cloning artifact	UNP P16528
D	182	SER	-	cloning artifact	UNP P16528

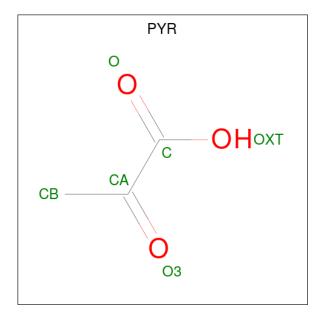


 \bullet Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	В	1	Total C O 4 2 2	0	0
2	С	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

 \bullet Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: $\mathrm{C_3H_4O_3}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	В	1	Total C O 6 3 3	0	0
3	С	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

• Molecule 4 is water.

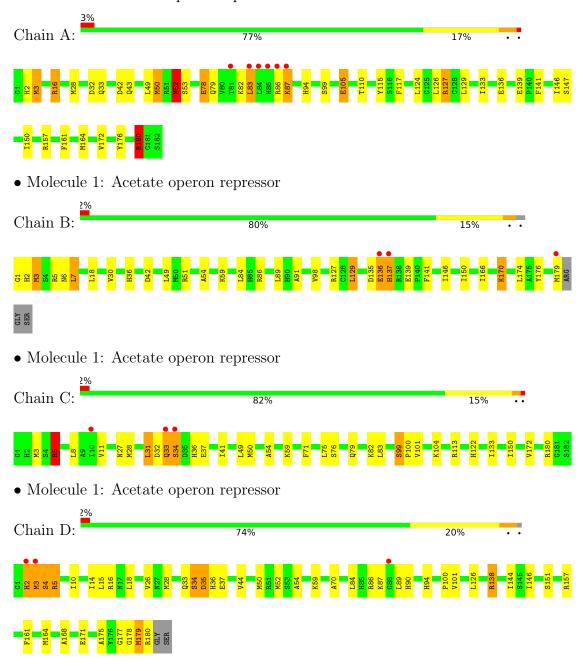
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	217	Total O 217 217	0	0
4	В	196	Total O 196 196	0	0
4	С	214	Total O 214 214	0	0
4	D	208	Total O 208 208	0	0



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: Acetate operon repressor





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	53.50Å 81.43Å 154.25Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.01 - 1.80	Depositor
rtesolution (A)	72.01 - 1.80	EDS
% Data completeness	97.8 (72.01-1.80)	Depositor
(in resolution range)	97.8 (72.01-1.80)	EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	3.99 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D.D.	0.173 , 0.232	Depositor
R, R_{free}	0.172 , 0.231	DCC
R_{free} test set	3131 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 55.4	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6553	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 23.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4893e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: EDO, PYR

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.79	0/1472	0.92	7/1980~(0.4%)	
1	В	0.89	0/1423	0.89	7/1918~(0.4%)	
1	С	1.00	0/1447	0.92	5/1947~(0.3%)	
1	D	0.84	0/1444	0.86	3/1945~(0.2%)	
All	All	0.88	0/5786	0.90	$22/7790 \ (0.3\%)$	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	С	0	1
1	D	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	В	129	LEU	CA-CB-CG	-7.94	97.04	115.30
1	D	35	ASP	N-CA-CB	-7.24	97.57	110.60
1	С	5[A]	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	С	5[B]	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	52	MET	CG-SD-CE	6.94	111.31	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	С	33	GLN	Peptide
1	D	179	MET	Peptide
1	D	33	GLN	Peptide

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	1445	0	1461	75	0
1	В	1399	0	1402	34	0
1	С	1417	0	1438	42	0
1	D	1417	0	1432	68	0
2	A	4	0	6	1	0
2	В	4	0	6	0	0
2	С	4	0	6	0	0
2	D	4	0	6	2	0
3	A	6	0	0	0	0
3	В	6	0	0	0	0
3	С	6	0	0	0	0
3	D	6	0	0	0	0
4	A	217	0	0	15	0
4	В	196	0	0	11	0
4	С	214	0	0	12	0
4	D	208	0	0	30	0
All	All	6553	0	5757	201	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 17.

The worst 5 of 201 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:86[A]:ARG:HB2	1:A:87[A]:LYS:CB	1.33	1.56
1:A:50[B]:MET:HE1	1:D:50[B]:MET:CE	1.18	1.54
1:A:50[B]:MET:CE	1:D:50[B]:MET:HE1	1.14	1.54
1:A:50[B]:MET:CE	1:D:50[B]:MET:CE	1.77	1.45
1:A:50[B]:MET:SD	1:D:50[B]:MET:CE	2.12	1.36



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	Perce	ntiles
1	A	186/182 (102%)	173 (93%)	10 (5%)	3 (2%)	9	2
1	В	180/182 (99%)	172 (96%)	7 (4%)	1 (1%)	25	12
1	С	183/182 (100%)	176 (96%)	6 (3%)	1 (0%)	29	15
1	D	182/182 (100%)	175 (96%)	6 (3%)	1 (0%)	29	15
All	All	731/728 (100%)	696 (95%)	29 (4%)	6 (1%)	22	7

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87[A]	LYS
1	A	87[B]	LYS
1	С	34	SER
1	A	180	ARG
1	В	137	HIS

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	154/148 (104%)	143 (93%)	11 (7%)	14 5
1	В	149/148 (101%)	142 (95%)	7 (5%)	26 12
1	С	151/148 (102%)	146 (97%)	5 (3%)	38 23

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percen	tiles
1	D	151/148 (102%)	145 (96%)	6 (4%)	31	16
All	All	$605/592 \; (102\%)$	576 (95%)	29 (5%)	28	11

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	141	PHE
1	D	101	VAL
1	В	179	MET
1	D	3	MET
1	В	174	LEU

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	С	79	GLN
1	D	90	HIS
1	В	36	HIS
1	В	102	HIS
1	В	137	HIS

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)

8 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	Tuno	Chain	Res	Link	В	ond leng	$_{ m gths}$	В	ond ang	gles
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	D	904	-	3,3,3	0.46	0	2,2,2	0.75	0
2	EDO	В	902	-	3,3,3	0.40	0	2,2,2	1.03	0
2	EDO	A	901	-	3,3,3	0.43	0	2,2,2	0.83	0
3	PYR	В	906	1	5,5,5	4.35	2 (40%)	3,6,6	1.86	1 (33%)
2	EDO	С	903	-	3,3,3	0.56	0	2,2,2	0.93	0
3	PYR	A	905	1	5,5,5	4.50	2 (40%)	3,6,6	1.68	1 (33%)
3	PYR	С	907	1	5,5,5	4.49	2 (40%)	3,6,6	2.58	2 (66%)
3	PYR	D	908	1	5,5,5	4.33	1 (20%)	3,6,6	2.03	1 (33%)

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
2	EDO	D	904	-	-	0/1/1/1	-
2	EDO	В	902	-	-	1/1/1/1	-
2	EDO	A	901	ı	-	1/1/1/1	ı
3	PYR	В	906	1	-	2/4/4/4	-
2	EDO	С	903	-	-	1/1/1/1	-
3	PYR	A	905	1	-	2/4/4/4	-
3	PYR	С	907	1	-	2/4/4/4	_
3	PYR	D	908	1	-	2/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

I	Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
	3	С	907	PYR	O3-CA	9.65	1.44	1.23
	3	В	906	PYR	O3-CA	9.37	1.43	1.23
	3	A	905	PYR	O3-CA	9.34	1.43	1.23
	3	D	908	PYR	O3-CA	9.27	1.43	1.23
	3	A	905	PYR	CB-CA	3.15	1.56	1.50

All (5) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
3	С	907	PYR	OXT-C-CA	3.17	122.64	113.97
3	С	907	PYR	O3-CA-CB	-3.10	112.86	119.73
3	D	908	PYR	O3-CA-CB	-3.03	113.02	119.73
3	В	906	PYR	O3-CA-CB	-2.52	114.15	119.73
3	A	905	PYR	OXT-C-CA	2.00	119.45	113.97

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	907	PYR	OXT-C-CA-CB
3	D	908	PYR	OXT-C-CA-CB
3	A	905	PYR	O-C-CA-CB
3	В	906	PYR	O-C-CA-CB
3	С	907	PYR	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	904	EDO	2	0
2	A	901	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 (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^{th} 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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	182/182 (100%)	-0.18	6 (3%) 46 40	11, 19, 41, 54	0
1	В	179/182~(98%)	-0.36	3 (1%) 70 66	11, 16, 34, 50	0
1	С	182/182 (100%)	-0.41	3 (1%) 72 68	10, 15, 27, 46	1 (0%)
1	D	180/182 (98%)	-0.24	3 (1%) 70 66	10, 18, 36, 50	0
All	All	723/728 (99%)	-0.30	15 (2%) 63 59	10, 17, 35, 54	1 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	HIS	5.9
1	D	2	HIS	4.1
1	A	84	LEU	4.1
1	A	86[A]	ARG	4.0
1	В	136	GLU	3.8

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	EDO	A	901	4/4	0.93	0.14	24,24,26,28	0
3	PYR	A	905	6/6	0.96	0.09	15,17,17,17	0
2	EDO	С	903	4/4	0.97	0.10	18,19,20,21	0
2	EDO	D	904	4/4	0.97	0.09	16,18,18,18	0
2	EDO	В	902	4/4	0.97	0.07	21,22,22,22	0
3	PYR	В	906	6/6	0.98	0.07	13,13,14,16	0
3	PYR	С	907	6/6	0.98	0.06	12,13,14,15	0
3	PYR	D	908	6/6	0.98	0.08	11,14,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.

