



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 07:29 am BST

PDB ID : 1KMP  
Title : Crystal structure of the Outer Membrane Transporter FecA Complexed with Ferric Citrate  
Authors : Ferguson, A.D.; Chakraborty, R.; Smith, B.S.; Esser, L.; van der Helm, D.; Deisenhofer, J.  
Deposited on : 2001-12-17  
Resolution : 2.50 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](mailto: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.

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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	:	2.11
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)	:	2.11

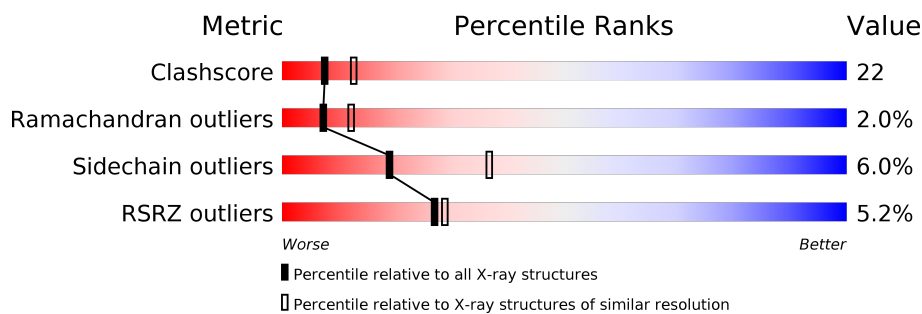
# 1 Overall quality at a glance

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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	774	

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
4	LDA	A	753	-	-	-	X
4	LDA	A	757	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5615 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.

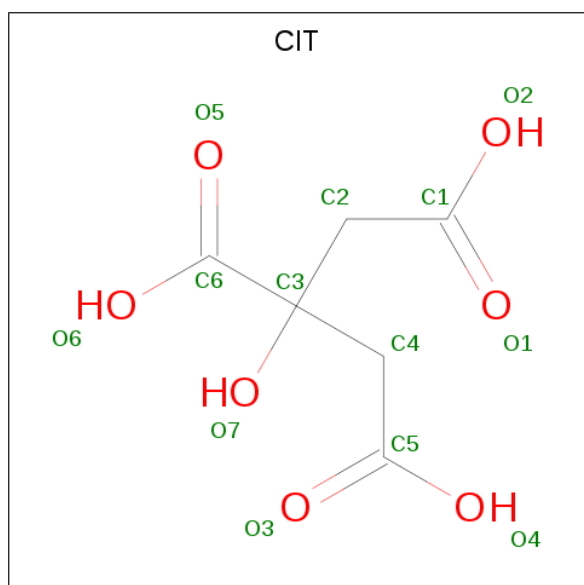
- Molecule 1 is a protein called IRON(III) DICITRATE TRANSPORT PROTEIN FECA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	647	Total	C	N	O	Se	0	0	0
			5079	3178	894	993	14			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

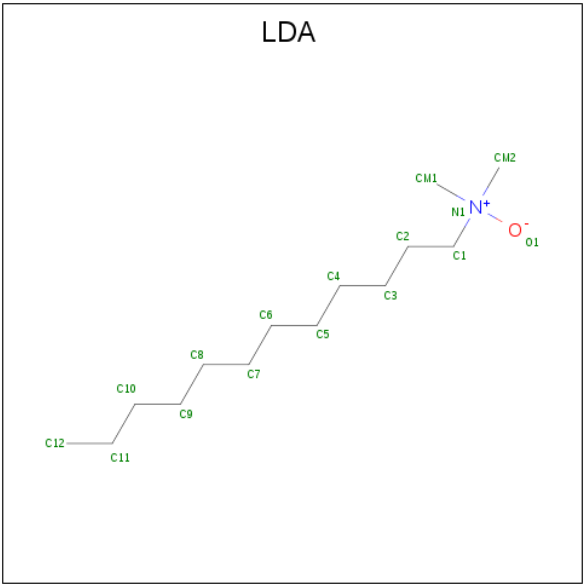
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	252	Total	O	0	0
			252	252		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.47Å 88.76Å 95.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.95 – 2.50 36.95 – 2.49	Depositor EDS
% Data completeness (in resolution range)	86.5 (36.95-2.50) 93.4 (36.95-2.49)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.242 , 0.282 0.240 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: LDA, FE, CIT

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	0.39	0/5194	0.64	0/7031

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	5079	0	4798	236	0
2	A	2	0	0	0	0
3	A	26	0	8	1	0
4	A	256	0	496	12	0
5	A	252	0	0	18	0
All	All	5615	0	5302	236	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 22.

The worst 5 of 236 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:567:ASP:HB2	1:A:576:THR:HB	1.46	0.98
1:A:519:GLN:H	1:A:522:GLN:HE21	1.13	0.91
1:A:225:ILE:HD11	1:A:250:VAL:HG13	1.57	0.84
1:A:533:GLU:HB3	1:A:534:PRO:HA	1.59	0.84
1:A:533:GLU:OE1	1:A:535:GLU:HG3	1.79	0.83

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	645/774 (83%)	581 (90%)	51 (8%)	13 (2%)	7	12

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	GLU
1	A	210	GLY
1	A	223	PHE
1	A	433	SER
1	A	521	SER

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	534/621 (86%)	502 (94%)	32 (6%)	19 37

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
1	A	559	LEU
1	A	712	ASP
1	A	536	LYS
1	A	562	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
1	A	522	GLN
1	A	569	ASN
1	A	412	ASN
1	A	565	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 for Mogul analysis.

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$
4	LDA	A	749	-	12,15,15	2.06	1 (8%)	14,17,17	1.69	4 (28%)
4	LDA	A	743	-	12,15,15	2.12	1 (8%)	14,17,17	1.62	4 (28%)
4	LDA	A	748	-	12,15,15	2.09	1 (8%)	14,17,17	1.64	4 (28%)
3	CIT	A	2003	2	3,12,12	2.74	1 (33%)	3,17,17	0.91	0
3	CIT	A	2001	2	3,12,12	1.91	1 (33%)	3,17,17	0.78	0
4	LDA	A	746	-	12,15,15	2.10	1 (8%)	14,17,17	1.75	4 (28%)
4	LDA	A	758	-	12,15,15	2.09	1 (8%)	14,17,17	1.74	4 (28%)
4	LDA	A	757	-	12,15,15	1.97	1 (8%)	14,17,17	1.76	4 (28%)
4	LDA	A	750	-	12,15,15	1.96	1 (8%)	14,17,17	1.69	4 (28%)
4	LDA	A	751	-	12,15,15	2.07	1 (8%)	14,17,17	1.64	4 (28%)
4	LDA	A	756	-	12,15,15	2.05	1 (8%)	14,17,17	1.71	4 (28%)
4	LDA	A	754	-	12,15,15	2.05	1 (8%)	14,17,17	1.64	4 (28%)
4	LDA	A	744	-	12,15,15	2.10	1 (8%)	14,17,17	1.65	4 (28%)
4	LDA	A	752	-	12,15,15	2.03	1 (8%)	14,17,17	1.65	4 (28%)
4	LDA	A	755	-	12,15,15	1.92	1 (8%)	14,17,17	1.65	4 (28%)
4	LDA	A	753	-	12,15,15	1.99	1 (8%)	14,17,17	1.68	4 (28%)
4	LDA	A	747	-	12,15,15	2.08	1 (8%)	14,17,17	1.67	5 (35%)
4	LDA	A	745	-	12,15,15	2.03	1 (8%)	14,17,17	1.72	4 (28%)

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
4	LDA	A	749	-	-	10/13/13/13	-
4	LDA	A	743	-	-	8/13/13/13	-
4	LDA	A	748	-	-	10/13/13/13	-
3	CIT	A	2003	2	-	0/6/16/16	-
3	CIT	A	2001	2	-	0/6/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	A	746	-	-	9/13/13/13	-
4	LDA	A	758	-	-	10/13/13/13	-
4	LDA	A	757	-	-	8/13/13/13	-
4	LDA	A	750	-	-	10/13/13/13	-
4	LDA	A	751	-	-	7/13/13/13	-
4	LDA	A	756	-	-	10/13/13/13	-
4	LDA	A	754	-	-	8/13/13/13	-
4	LDA	A	744	-	-	7/13/13/13	-
4	LDA	A	752	-	-	5/13/13/13	-
4	LDA	A	755	-	-	12/13/13/13	-
4	LDA	A	753	-	-	9/13/13/13	-
4	LDA	A	747	-	-	10/13/13/13	-
4	LDA	A	745	-	-	10/13/13/13	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	743	LDA	O1-N1	-7.00	1.25	1.42
4	A	744	LDA	O1-N1	-6.95	1.25	1.42
4	A	748	LDA	O1-N1	-6.94	1.25	1.42
4	A	746	LDA	O1-N1	-6.94	1.25	1.42
4	A	758	LDA	O1-N1	-6.92	1.26	1.42

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	746	LDA	CM1-N1-C1	-3.82	102.21	110.23
4	A	757	LDA	CM1-N1-C1	-3.65	102.56	110.23
4	A	745	LDA	CM1-N1-C1	-3.60	102.68	110.23
4	A	758	LDA	CM1-N1-C1	-3.58	102.70	110.23
4	A	753	LDA	CM1-N1-C1	-3.53	102.82	110.23

There are no chirality outliers.

5 of 143 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	746	LDA	C2-C3-C4-C5
4	A	748	LDA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	A	750	LDA	C3-C4-C5-C6
4	A	757	LDA	C11-C10-C9-C8
4	A	748	LDA	C3-C4-C5-C6

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	743	LDA	1	0
4	A	748	LDA	1	0
3	A	2001	CIT	1	0
4	A	758	LDA	1	0
4	A	757	LDA	1	0
4	A	756	LDA	3	0
4	A	755	LDA	1	0
4	A	753	LDA	1	0
4	A	747	LDA	1	0
4	A	745	LDA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	633/774 (81%)	0.27	33 (5%) 27 29	7, 21, 47, 82	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	694	PRO	6.1
1	A	693	GLY	4.8
1	A	697	ALA	4.6
1	A	527	VAL	4.6
1	A	741	PHE	4.5

### 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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	LDA	A	757	16/16	0.61	0.41	39,42,48,49	0
4	LDA	A	756	16/16	0.64	0.33	52,53,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	LDA	A	753	16/16	0.64	0.44	40,42,54,54	0
4	LDA	A	755	16/16	0.66	0.36	39,41,49,50	0
4	LDA	A	754	16/16	0.70	0.31	41,43,47,49	0
4	LDA	A	752	16/16	0.70	0.33	45,48,54,54	0
4	LDA	A	751	16/16	0.72	0.30	46,49,50,50	0
4	LDA	A	744	16/16	0.74	0.35	38,44,50,52	0
4	LDA	A	746	16/16	0.75	0.34	40,44,46,48	0
4	LDA	A	750	16/16	0.77	0.30	30,33,48,48	0
2	FE	A	2002	1/1	0.79	0.22	58,58,58,58	0
3	CIT	A	2003	13/13	0.79	0.30	53,55,58,60	0
4	LDA	A	743	16/16	0.80	0.30	40,45,47,51	0
3	CIT	A	2001	13/13	0.80	0.29	51,52,57,58	0
4	LDA	A	747	16/16	0.80	0.30	34,37,47,48	0
4	LDA	A	745	16/16	0.81	0.34	42,44,51,52	0
4	LDA	A	748	16/16	0.82	0.38	37,41,44,44	0
4	LDA	A	758	16/16	0.83	0.37	39,43,48,50	0
4	LDA	A	749	16/16	0.86	0.28	34,41,54,56	0
2	FE	A	2000	1/1	0.92	0.11	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.