



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:28 PM GMT

PDB ID : 4F2D
Title : Crystal Structure of Escherichia coli L-arabinose Isomerase (ECAI) complexed with Ribitol
Authors : Manjasetty, B.A.; Burley, S.K.; Almo, S.C.; Chance, M.R.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2012-05-07
Resolution : 2.30 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 <http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

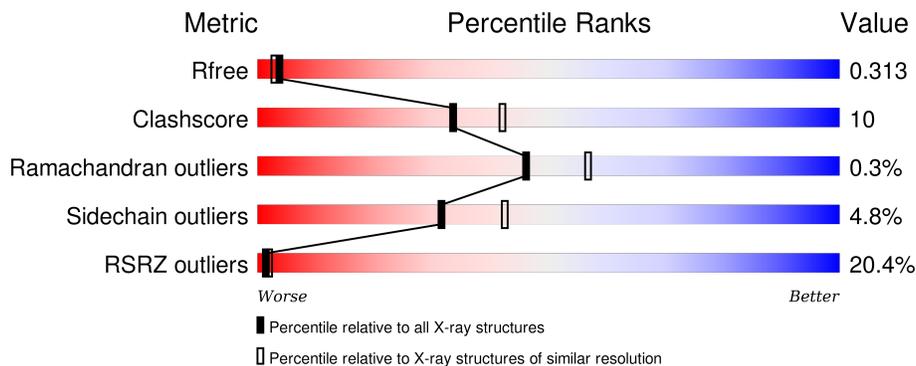
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	500	 11% 81% 16% •
1	B	500	 10% 81% 17% •
1	C	500	 37% 81% 16% •

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
2	MN	A	601	-	-	-	X
2	MN	B	601	-	-	-	X
3	RB0	A	602	-	-	-	X
3	RB0	B	602	-	-	-	X
3	RB0	C	602	-	-	-	X
4	ACY	B	603	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11787 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 L-arabinose isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	498	3861	2451	677	710	7	16	0	0	0
1	B	498	3901	2478	681	718	7	17	0	1	0
1	C	498	3767	2379	658	706	7	17	0	1	0

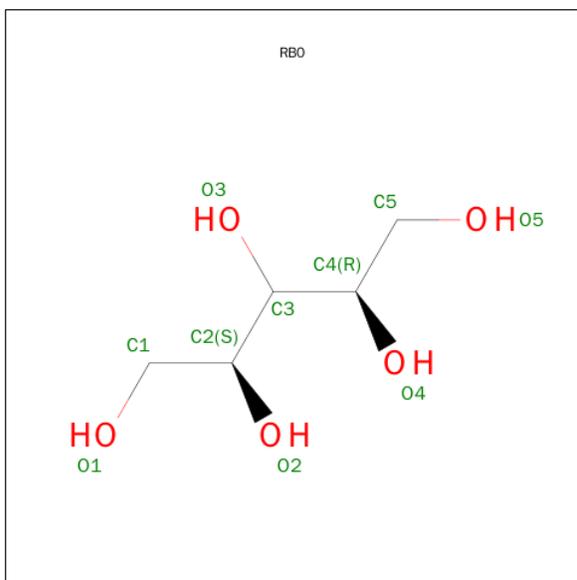
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLU	LYS	CONFLICT	UNP P08202
A	360	VAL	ALA	CONFLICT	UNP P08202
B	248	GLU	LYS	CONFLICT	UNP P08202
B	360	VAL	ALA	CONFLICT	UNP P08202
C	248	GLU	LYS	CONFLICT	UNP P08202
C	360	VAL	ALA	CONFLICT	UNP P08202

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

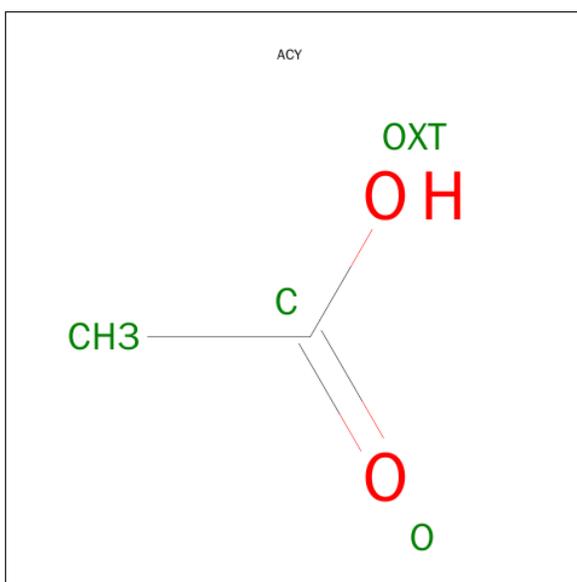
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is SUGAR (D-RIBULOSE) (three-letter code: RB0) (formula: C₅H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		

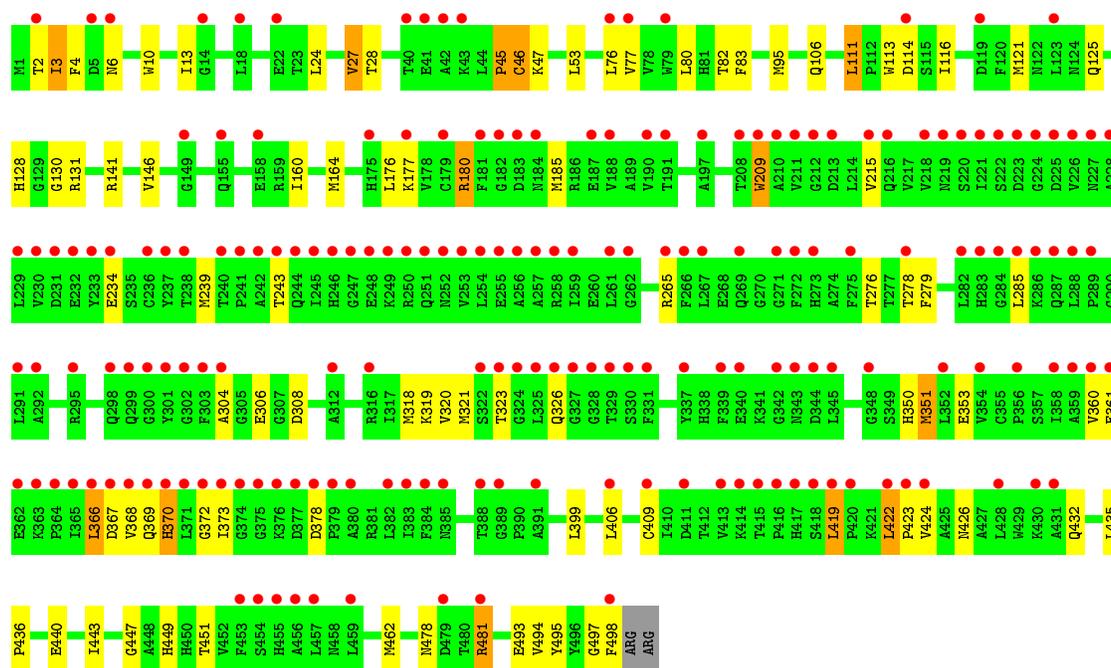
- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	92	Total O 92 92	0	0
5	B	95	Total O 95 95	0	0
5	C	34	Total O 34 34	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.47Å 116.47Å 214.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.30) 98.5 (19.76-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.212 , 0.255 0.281 , 0.313	Depositor DCC
R_{free} test set	3793 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.3	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 74254 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11787	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ACY, MN, RB0

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	0.53	1/3940 (0.0%)	0.61	4/5328 (0.1%)
1	B	0.52	2/3984 (0.1%)	0.59	2/5388 (0.0%)
1	C	0.53	0/3847	0.60	2/5203 (0.0%)
All	All	0.53	3/11771 (0.0%)	0.60	8/15919 (0.1%)

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	3
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	TRP	CD2-CE2	5.03	1.47	1.41
1	A	79	TRP	CD2-CE2	5.00	1.47	1.41
1	B	79	TRP	CD2-CE2	5.00	1.47	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	LYS	N-CA-C	-7.56	90.58	111.00
1	B	141	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	22	GLU	N-CA-C	6.24	127.86	111.00
1	C	370	HIS	N-CA-C	-6.19	94.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ASN	N-CA-C	6.02	127.26	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	PHE	Peptide
1	A	18	LEU	Peptide
1	A	21	PRO	Peptide
1	B	326	GLN	Peptide
1	C	46	CYS	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	3861	0	3723	76	0
1	B	3901	0	3790	94	0
1	C	3767	0	3524	90	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	10	0	11	1	0
3	B	10	0	11	1	0
3	C	10	0	12	0	0
4	B	4	0	3	6	0
5	A	92	0	0	2	0
5	B	95	0	0	1	0
5	C	34	0	0	5	0
All	All	11787	0	11074	230	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.

The worst 5 of 230 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:288:LEU:CD2	1:B:351:MSE:HE2	1.68	1.22
1:B:288:LEU:HD22	1:B:351:MSE:CE	1.75	1.17
1:C:2:THR:HG23	1:C:323:THR:HG21	1.20	1.16
1:A:122:ASN:HD21	1:C:373:ILE:HD11	1.09	1.12
1:C:239:MSE:HE3	1:C:366:LEU:HG	1.37	1.04

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	496/500 (99%)	480 (97%)	14 (3%)	2 (0%)	39	48
1	B	497/500 (99%)	484 (97%)	12 (2%)	1 (0%)	52	64
1	C	497/500 (99%)	479 (96%)	16 (3%)	2 (0%)	39	48
All	All	1490/1500 (99%)	1443 (97%)	42 (3%)	5 (0%)	46	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	B	20	GLY
1	C	372	GLY
1	A	351	MSE
1	C	351	MSE

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	401/402 (100%)	383 (96%)	18 (4%)	34	46
1	B	411/402 (102%)	389 (95%)	22 (5%)	27	36
1	C	379/402 (94%)	361 (95%)	18 (5%)	32	43
All	All	1191/1206 (99%)	1133 (95%)	58 (5%)	31	41

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	232	GLU
1	B	335	TYR
1	C	366	LEU
1	B	244	GLN
1	B	250	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	102	GLN
1	B	125	GLN
1	C	125	GLN
1	B	104	HIS
1	B	252	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
3	RB0	A	602	2	9,9,9	0.30	0	10,11,11	0.94	0
3	RB0	B	602	2	9,9,9	0.23	0	10,11,11	0.46	0
4	ACY	B	603	-	1,3,3	0.68	0	0,3,3	0.00	-
3	RB0	C	602	2	9,9,9	0.26	0	10,11,11	0.54	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	RB0	A	602	2	-	0/12/12/12	0/0/0/0
3	RB0	B	602	2	-	0/12/12/12	0/0/0/0
4	ACY	B	603	-	-	0/0/0/0	0/0/0/0
3	RB0	C	602	2	-	0/12/12/12	0/0/0/0

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.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	RB0	1	0
3	B	602	RB0	1	0
4	B	603	ACY	6	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	481/500 (96%)	0.85	56 (11%) 6 10	16, 26, 59, 77	2 (0%)
1	B	481/500 (96%)	0.79	51 (10%) 8 12	17, 27, 35, 60	1 (0%)
1	C	481/500 (96%)	2.13	187 (38%) 0 0	20, 43, 74, 81	1 (0%)
All	All	1443/1500 (96%)	1.26	294 (20%) 1 2	16, 29, 69, 81	4 (0%)

The worst 5 of 294 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	246	HIS	14.1
1	C	219	ASN	13.2
1	C	251	GLN	12.6
1	C	416	PRO	10.4
1	C	234	GLU	10.4

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	RB0	A	602	10/10	0.96	0.33	6.25	37,43,50,52	2
2	MN	A	601	1/1	0.97	0.25	4.76	45,45,45,45	0
2	MN	B	601	1/1	0.95	0.24	3.65	52,52,52,52	0
3	RB0	B	602	10/10	0.93	0.29	2.28	37,52,62,65	2
3	RB0	C	602	10/10	0.72	0.56	1.92	48,54,59,63	10
4	ACY	B	603	4/4	0.94	0.22	1.16	25,35,37,39	0
2	MN	C	601	1/1	0.95	0.25	0.26	80,80,80,80	1

6.5 Other polymers [i](#)

There are no such residues in this entry.