



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 25, 2024 – 03:36 PM EST

PDB ID : 1R43  
Title : Crystal structure of beta-alanine synthase from *Saccharomyces kluyveri* (selenomethionine substituted protein)  
Authors : Lundgren, S.; Gojkovic, Z.; Piskur, J.; Dobritsch, D.  
Deposited on : 2003-10-03  
Resolution : 2.80 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

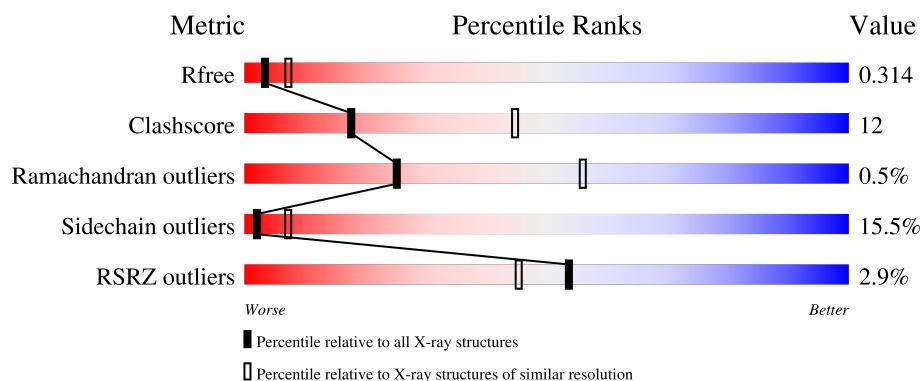
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	463	<div> <div></div> <div>63%</div> <div>26%</div> <div>5%</div> <div>5%</div> </div>
1	B	463	<div> <div>4%</div> <div>60%</div> <div>28%</div> <div>5%</div> <div>7%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6818 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 beta-alanine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	Se	0	0	0
			3379	2130	580	653	8	8			
1	B	432	Total	C	N	O	S	Se	0	0	0
			3337	2103	573	645	8	8			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q96W94
A	61	MSE	MET	modified residue	UNP Q96W94
A	73	MSE	MET	modified residue	UNP Q96W94
A	96	MSE	MET	modified residue	UNP Q96W94
A	187	MSE	MET	modified residue	UNP Q96W94
A	277	MSE	MET	modified residue	UNP Q96W94
A	281	MSE	MET	modified residue	UNP Q96W94
A	332	MSE	MET	modified residue	UNP Q96W94
A	410	MSE	MET	modified residue	UNP Q96W94
A	456	HIS	-	expression tag	UNP Q96W94
A	457	HIS	-	expression tag	UNP Q96W94
A	458	HIS	-	expression tag	UNP Q96W94
A	459	HIS	-	expression tag	UNP Q96W94
A	460	HIS	-	expression tag	UNP Q96W94
A	461	HIS	-	expression tag	UNP Q96W94
A	462	HIS	-	expression tag	UNP Q96W94
A	463	HIS	-	expression tag	UNP Q96W94
B	1	MSE	MET	modified residue	UNP Q96W94
B	61	MSE	MET	modified residue	UNP Q96W94
B	73	MSE	MET	modified residue	UNP Q96W94
B	96	MSE	MET	modified residue	UNP Q96W94
B	187	MSE	MET	modified residue	UNP Q96W94
B	277	MSE	MET	modified residue	UNP Q96W94
B	281	MSE	MET	modified residue	UNP Q96W94
B	332	MSE	MET	modified residue	UNP Q96W94

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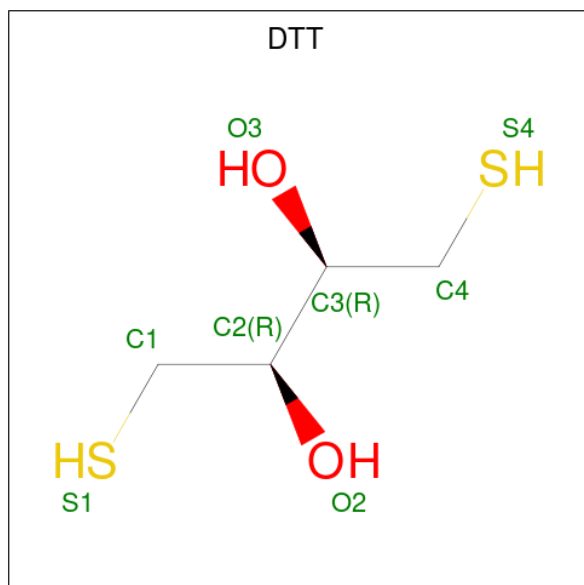
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Chain	Residue	Modelled	Actual	Comment	Reference
B	410	MSE	MET	modified residue	UNP Q96W94
B	456	HIS	-	expression tag	UNP Q96W94
B	457	HIS	-	expression tag	UNP Q96W94
B	458	HIS	-	expression tag	UNP Q96W94
B	459	HIS	-	expression tag	UNP Q96W94
B	460	HIS	-	expression tag	UNP Q96W94
B	461	HIS	-	expression tag	UNP Q96W94
B	462	HIS	-	expression tag	UNP Q96W94
B	463	HIS	-	expression tag	UNP Q96W94

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

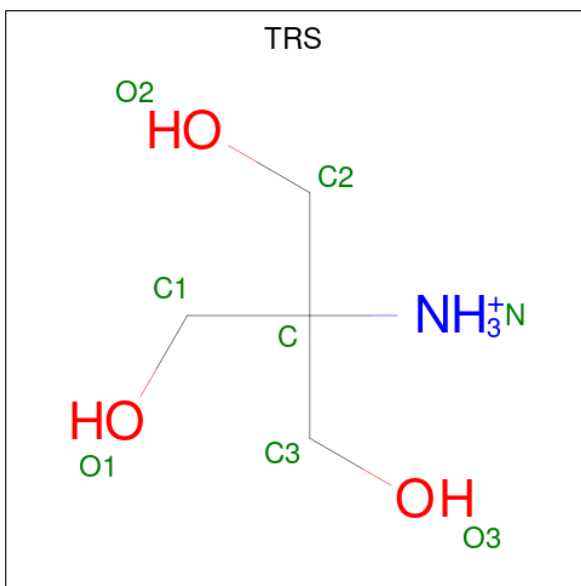
- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		

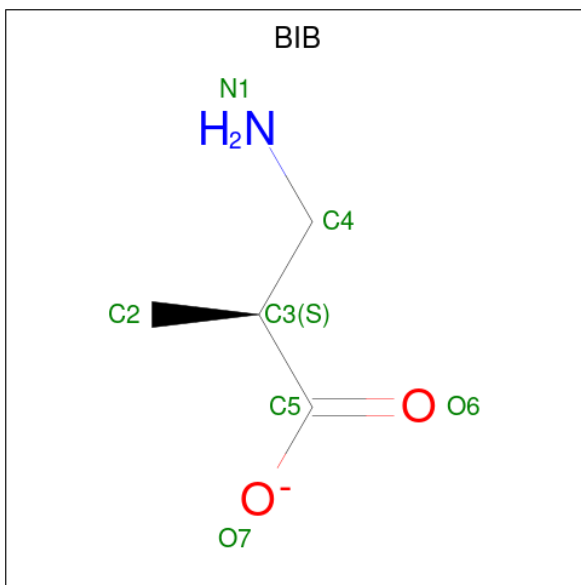
- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code:

TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is BETA-AMINO ISOBUTYRATE (three-letter code: BIB) (formula:  $C_4H_8NO_2$ ).

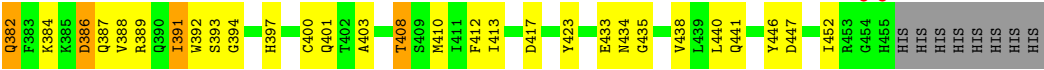


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			7	4	1	2		
5	B	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total 54	O 54	0	0
6	B	14	Total 14	O 14	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.43Å 77.63Å 110.57Å 90.00° 95.63° 90.00°	Depositor
Resolution (Å)	29.75 – 2.80 29.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.75-2.80) 99.1 (29.75-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.211 , 0.274 0.285 , 0.314	Depositor DCC
$R_{free}$ test set	1275 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 10.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	6818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: DTT, TRS, ZN, BIB

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	0.54	0/3449	0.79	9/4665 (0.2%)
1	B	0.43	0/3406	0.74	11/4605 (0.2%)
All	All	0.49	0/6855	0.76	20/9270 (0.2%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASP	CB-CG-OD2	7.15	124.73	118.30
1	B	320	ASP	CB-CG-OD2	6.36	124.03	118.30
1	A	220	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	192	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	386	ASP	CB-CG-OD2	6.10	123.79	118.30

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	3379	0	3263	87	0
1	B	3337	0	3219	80	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	9	0	0
4	A	8	0	12	0	0
5	A	7	0	8	0	0
5	B	7	0	8	0	0
6	A	54	0	0	2	0
6	B	14	0	0	1	0
All	All	6818	0	6519	162	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 12.

The worst 5 of 162 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:35:LEU:HB2	1:A:135:GLU:HG3	1.54	0.88
1:A:371:CYS:HB3	1:A:409:SER:HB2	1.57	0.87
1:A:323:HIS:CD2	1:A:332:MSE:HE1	2.14	0.83
1:A:240:ILE:HG12	1:A:438:VAL:HG21	1.61	0.80
1:B:108:PRO:HB2	1:B:152:CYS:HB3	1.67	0.76

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	436/463 (94%)	404 (93%)	30 (7%)	2 (0%)	25	56
1	B	430/463 (93%)	395 (92%)	33 (8%)	2 (0%)	25	56
All	All	866/926 (94%)	799 (92%)	63 (7%)	4 (0%)	25	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	B	237	ASN
1	B	25	ALA
1	A	158	ASN

### 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	360/375 (96%)	310 (86%)	50 (14%)	3	9
1	B	355/375 (95%)	294 (83%)	61 (17%)	1	5
All	All	715/750 (95%)	604 (84%)	111 (16%)	2	7

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	LYS
1	B	452	ILE
1	B	152	CYS
1	B	440	LEU
1	B	377	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	250	ASN
1	B	382	GLN
1	B	441	GLN
1	A	250	ASN
1	A	21	ASN

### 5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	$\# Z  > 2$
5	BIB	B	1505	-	5,6,6	0.99	0	5,7,7	0.57	0
4	TRS	A	504	-	7,7,7	0.36	0	9,9,9	0.58	0
3	DTT	A	503	1	7,7,7	0.49	0	4,8,8	1.34	0
5	BIB	A	505	-	5,6,6	0.90	0	5,7,7	0.91	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
5	BIB	B	1505	-	-	0/6/6/6	-
4	TRS	A	504	-	-	3/9/9/9	-
3	DTT	A	503	1	-	4/8/8/8	-
5	BIB	A	505	-	-	4/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	DTT	S1-C1-C2-O2
3	A	503	DTT	S1-C1-C2-C3
3	A	503	DTT	C2-C3-C4-S4
3	A	503	DTT	O3-C3-C4-S4
5	A	505	BIB	C5-C3-C4-N1

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

**Warning:** The R factor obtained from EDS is 0.2866, which does not match the depositor's R factor of 0.2106. Please interpret the results in this section carefully.

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	430/463 (92%)	0.35	6 (1%) 73 66	14, 20, 24, 31	0
1	B	424/463 (91%)	0.57	19 (4%) 39 31	16, 20, 22, 29	0
All	All	854/926 (92%)	0.46	25 (2%) 54 45	14, 20, 23, 31	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	GLY	3.3
1	B	25	ALA	3.1
1	A	386	ASP	3.1
1	B	145	TYR	3.1
1	A	19	THR	2.9

### 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<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( $\text{\AA}^2$ )	Q<0.9
4	TRS	A	504	8/8	0.70	0.17	19,20,20,20	0
5	BIB	A	505	7/7	0.72	0.14	15,18,18,18	0
5	BIB	B	1505	7/7	0.83	0.12	19,19,20,20	0
3	DTT	A	503	8/8	0.85	0.13	30,31,31,33	0
2	ZN	B	501	1/1	0.93	0.06	26,26,26,26	0
2	ZN	B	500	1/1	0.97	0.03	20,20,20,20	0
2	ZN	A	500	1/1	0.99	0.07	21,21,21,21	0
2	ZN	A	501	1/1	0.99	0.07	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.