

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 13, 2020 - 02:43 am BST

PDB ID	:	4Y0U
Title	:	Crystal Structure of 6Alpha-Hydroxymethylpenicillanate Complexed with
		OXA-58, a Carbapenem hydrolyzing Class D betalactamase from Acinetobac-
		ter baumanii.
Authors	:	Pratap, S.; Katiki, M.; Gill, P.; Golemi-Kotra, D.; Kumar, P.
Deposited on		
Resolution	:	2.60  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 following versions of software and data (see references (1)) were used in the production of this report:

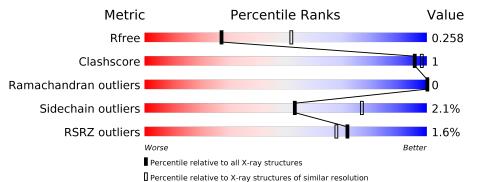
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455(2.60-2.60)
Sidechain outliers	138945	3455(2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	А	280	% • 84%	·	13%
1	В	280	% <b>8</b> 4%	•	13%
1	С	280	83%	•	14%
1	D	280	83%	••	13%



# 2 Entry composition (i)

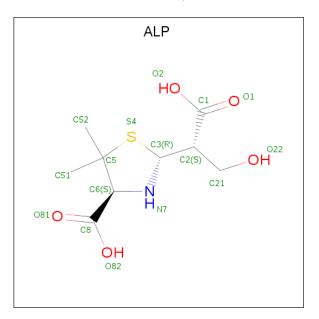
There are 3 unique types of molecules in this entry. The entry contains 8126 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	Δ	243	Total	С	Ν	Ο	S	0	0	0
	A	240	1943	1252	326	358	7	0	0	0
1	В	243	Total	С	Ν	Ο	S	0	0	0
	D	240	1943	1252	326	358	7	0	0	0
1	С	242	Total	С	Ν	Ο	S	0	1	0
	U	242	1946	1254	327	358	7	0	T	0
1	П	243	Total	С	Ν	Ο	S	0	1	0
		240	1952	1255	329	361	7			U

• Molecule 1 is a protein called Beta-lactamase.

• Molecule 2 is 2-(1-CARBOXY-2-HYDROXY-ETHYL)-5,5-DIMETHYL-THIAZOLIDINE-4-CARBOXYLIC ACID (three-letter code: ALP) (formula: C<sub>9</sub>H<sub>15</sub>NO<sub>5</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
0	Δ	1	Total	С	Ν	Ο	S	0	0	
	A	1	15	9	1	4	1	0	U	
0	р	1	Total	С	Ν	Ο	S	0	0	
	D	1	15	9	1	4	1		U	

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
0	C	1	Total	С	Ν	Ο	S	0	0
	U	L	15	9	1	4	1	0	0
0	Л	1	Total	С	Ν	Ο	S	0	0
	D	T	15	9	1	4	1	0	0

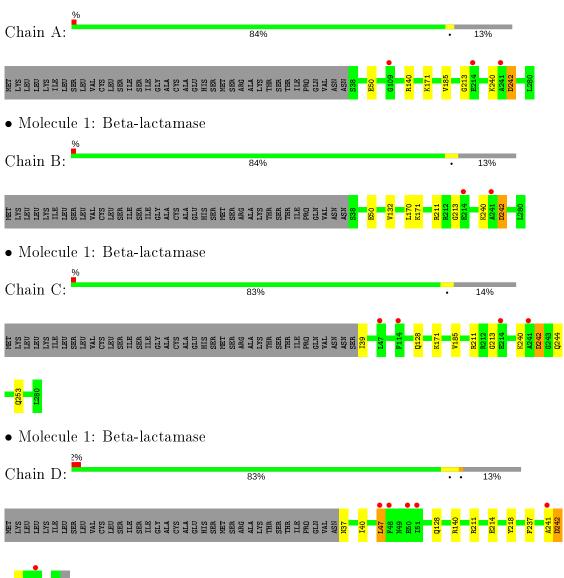
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	81	Total O 81 81	0	0
3	В	54	Total         O           54         54	0	0
3	С	82	TotalO8282	0	0
3	D	65	Total O 65 65	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Beta-lactamase





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	$36.94 \text{\AA}$ $65.66 \text{\AA}$ $191.59 \text{\AA}$	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $91.70^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	36.93 - 2.60	Depositor
Resolution (A)	36.93 - 2.60	EDS
% Data completeness	74.3 (36.93 - 2.60)	Depositor
(in resolution range)	74.3 (36.93-2.60)	EDS
R <sub>merge</sub>	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.68 ({\rm at} 2.61 {\rm \AA})$	Xtriage
Refinement program	REFMAC $5.8.0073$	Depositor
$R, R_{free}$	0.219 , $0.261$	Depositor
It, Itfree	0.222 , $0.258$	DCC
$R_{free}$ test set	983 reflections $(4.66\%)$	wwPDB-VP
Wilson B-factor ( $Å^2$ )	34.1	Xtriage
Anisotropy	1.158	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	$0.35 \;,  38.7$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8126	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 14.75% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: KCX, ALP

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.85	0/1974	0.88	2/2669~(0.1%)	
1	В	0.85	0/1974	0.89	2/2669~(0.1%)	
1	С	0.86	0/1977	0.90	2/2673~(0.1%)	
1	D	0.87	0/1983	0.88	2/2681~(0.1%)	
All	All	0.86	0/7908	0.89	8/10692~(0.1%)	

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	211	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	В	211	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	А	140	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	211	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	В	213	GLY	N-CA-C	-5.38	99.64	113.10

There are no chirality outliers.

There are no planarity outliers.

### 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	А	1943	0	1929	1	0
1	В	1943	0	1929	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	1946	0	1931	3	0
1	D	1952	0	1931	10	0
2	А	15	0	13	0	0
2	В	15	0	13	2	0
2	С	15	0	13	0	0
2	D	15	0	13	0	0
3	А	81	0	0	0	0
3	В	54	0	0	0	0
3	С	82	0	0	0	0
3	D	65	0	0	0	0
All	All	8126	0	7772	17	0

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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.

The worst 5 of 17 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:C:242:ASP:OD1	1:C:242:ASP:N	2.26	0.67
1:A:242:ASP:N	1:A:242:ASP:OD1	2.25	0.62
1:D:214:GLU:CB	1:D:241:ALA:HB2	2.30	0.62
1:B:242:ASP:N	1:B:242:ASP:OD1	2.35	0.59
1:D:214:GLU:HB3	1:D:241:ALA:HB2	1.84	0.58

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	А	240/280~(86%)	231 (96%)	9 (4%)	0	100	100
1	В	240/280~(86%)	233 (97%)	7(3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	С	240/280~(86%)	230~(96%)	10 (4%)	0	100 100	
1	D	241/280~(86%)	232~(96%)	9 (4%)	0	100 100	
All	All	961/1120~(86%)	926~(96%)	35~(4%)	0	100 100	

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There are no Ramachandran outliers to report.

#### 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	А	202/235~(86%)	197~(98%)	5(2%)	47 73
1	В	202/235~(86%)	198~(98%)	4 (2%)	55 78
1	С	202/235~(86%)	196~(97%)	6 (3%)	41 67
1	D	203/235~(86%)	201~(99%)	2(1%)	76 90
All	All	809/940~(86%)	792~(98%)	17 (2%)	53 77

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	240	LYS
1	В	242	ASP
1	С	242	ASP
1	В	171	LYS
1	С	253	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	43	ASN
1	С	43	ASN
1	С	152	GLN
1	С	244	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)

4 non-standard protein/DNA/RNA residues 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	Tune	Chain	Res	Link	B	ond leng	$_{ m gths}$	Bond angles		
	Type	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KCX	В	86	1	7,11,12	0.50	0	4,12,14	0.65	0
1	KCX	А	86	1	7,11,12	0.50	0	4,12,14	0.65	0
1	KCX	D	86	1	7,11,12	0.61	0	4,12,14	0.67	0
1	KCX	С	86	1	7,11,12	0.43	0	4,12,14	0.75	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	$\mathbf{Link}$	Chirals	Torsions	Rings
1	KCX	В	86	1	-	0/7/10/12	-
1	KCX	А	86	1	-	0/7/10/12	-
1	KCX	D	86	1	-	0/7/10/12	-
1	KCX	С	86	1	-	0/7/10/12	-

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.

No monomer is involved in short contacts.



#### 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry (i)

4 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).

Mal	Mol Type Chain Res			Link	B	Bond lengths			Bond angles		
	туре	Cham	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	ALP	А	301	1	$9,\!15,\!16$	1.73	2 (22%)	9,22,24	1.49	1 (11%)	
2	ALP	D	301	1	$9,\!15,\!16$	1.63	2 (22%)	9,22,24	1.49	1 (11%)	
2	ALP	В	301	1	$9,\!15,\!16$	2.66	3 (33%)	9,22,24	1.64	1 (11%)	
2	ALP	С	301	1	$9,\!15,\!16$	1.84	2 (22%)	$9,\!22,\!24$	1.64	1 (11%)	

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	ALP	А	301	1	-	2/4/27/29	0/1/1/1
2	ALP	D	301	1	-	2/4/27/29	0/1/1/1
2	ALP	В	301	1	-	2/4/27/29	0/1/1/1
2	ALP	С	301	1	-	2/4/27/29	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	В	301	ALP	C5-S4	-6.03	1.72	1.85
2	С	301	ALP	C5-S4	-4.09	1.77	1.85
2	В	301	ALP	C3-S4	-4.06	1.74	1.84
2	А	301	ALP	C5-S4	-3.80	1.77	1.85
2	D	301	ALP	C5-S4	-3.17	1.78	1.85



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	С	301	ALP	O1-C1-C2	-4.40	114.88	125.16
2	В	301	ALP	O1-C1-C2	-4.24	115.27	125.16
2	D	301	ALP	O1-C1-C2	-4.10	115.58	125.16
2	А	301	ALP	O1-C1-C2	-4.04	115.73	125.16

All (4) bond angle outliers are listed below:

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	301	ALP	C1-C2-C21-O22
2	А	301	ALP	C3-C2-C21-O22
2	D	301	ALP	C1-C2-C21-O22
2	D	301	ALP	C3-C2-C21-O22
2	В	301	ALP	C1-C2-C21-O22

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	301	ALP	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,  $95^{th}$  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	<RSRZ $>$	#RSRZ $>$ 2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$	
1	А	242/280~(86%)	-0.22	3 (1%)	79	76	$39,\ 50,\ 63,\ 82$	0
1	В	242/280~(86%)	-0.28	2(0%)	86	84	39,  50,  64,  79	0
1	С	241/280~(86%)	-0.16	4 (1%)	70	66	39, 52, 74, 106	0
1	D	242/280~(86%)	-0.08	6 (2%)	57	51	44, 57, 80, 92	0
All	All	967/1120~(86%)	-0.18	15 (1%)	72	68	39, 52, 72, 106	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	241	ALA	4.5
1	А	241	ALA	4.5
1	С	214	GLU	3.2
1	D	50	GLU	2.9
1	D	275	GLY	2.9

### 6.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
1	KCX	В	86	12/13	0.95	0.13	$40,\!43,\!48,\!48$	0
1	KCX	D	86	12/13	0.95	0.14	44,46,49,49	0
1	KCX	С	86	12/13	0.95	0.16	$39,\!41,\!44,\!45$	0
1	KCX	А	86	12/13	0.96	0.13	$40,\!41,\!43,\!43$	0



#### 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$Q{<}0.9$
2	ALP	D	301	15/16	0.92	0.18	$56,\!56,\!56,\!56$	0
2	ALP	А	301	15/16	0.93	0.16	$56,\!56,\!56,\!56$	0
2	ALP	В	301	15/16	0.93	0.14	56, 56, 56, 56	0
2	ALP	С	301	15/16	0.94	0.17	56, 56, 56, 56	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

