



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:51 AM GMT

PDB ID : 4HK5
Title : Crystal structure of Cordyceps militaris IDCase in apo form
Authors : Xu, S.; Zhu, J.; Ding, J.
Deposited on : 2012-10-15
Resolution : 1.90 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

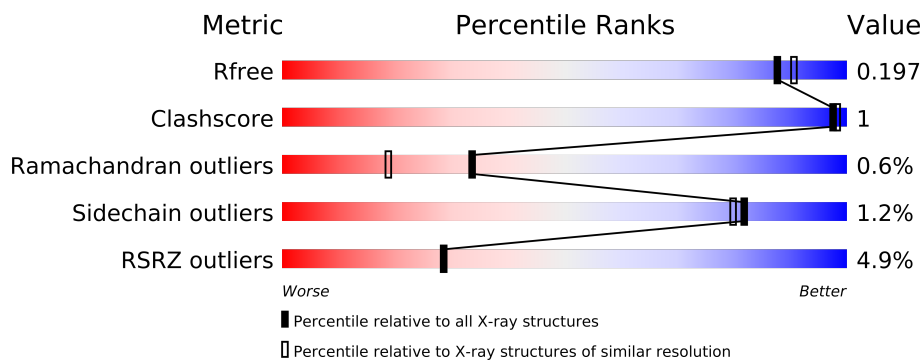
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	387	
1	B	387	
1	C	387	
1	D	387	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12209 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Uracil-5-carboxylate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2742	1769	469	490	14			
1	B	362	Total	C	N	O	S	0	0	0
			2781	1790	480	497	14			
1	C	370	Total	C	N	O	S	0	0	0
			2826	1819	483	510	14			
1	D	380	Total	C	N	O	S	0	1	0
			2924	1879	507	524	14			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP G3J531
A	-1	GLY	-	EXPRESSION TAG	UNP G3J531
A	0	SER	-	EXPRESSION TAG	UNP G3J531
A	377	LEU	-	EXPRESSION TAG	UNP G3J531
A	378	GLU	-	EXPRESSION TAG	UNP G3J531
A	379	HIS	-	EXPRESSION TAG	UNP G3J531
A	380	HIS	-	EXPRESSION TAG	UNP G3J531
A	381	HIS	-	EXPRESSION TAG	UNP G3J531
A	382	HIS	-	EXPRESSION TAG	UNP G3J531
A	383	HIS	-	EXPRESSION TAG	UNP G3J531
A	384	HIS	-	EXPRESSION TAG	UNP G3J531
B	-2	MET	-	EXPRESSION TAG	UNP G3J531
B	-1	GLY	-	EXPRESSION TAG	UNP G3J531
B	0	SER	-	EXPRESSION TAG	UNP G3J531
B	377	LEU	-	EXPRESSION TAG	UNP G3J531
B	378	GLU	-	EXPRESSION TAG	UNP G3J531
B	379	HIS	-	EXPRESSION TAG	UNP G3J531
B	380	HIS	-	EXPRESSION TAG	UNP G3J531
B	381	HIS	-	EXPRESSION TAG	UNP G3J531
B	382	HIS	-	EXPRESSION TAG	UNP G3J531
B	383	HIS	-	EXPRESSION TAG	UNP G3J531

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	384	HIS	-	EXPRESSION TAG	UNP G3J531
C	-2	MET	-	EXPRESSION TAG	UNP G3J531
C	-1	GLY	-	EXPRESSION TAG	UNP G3J531
C	0	SER	-	EXPRESSION TAG	UNP G3J531
C	377	LEU	-	EXPRESSION TAG	UNP G3J531
C	378	GLU	-	EXPRESSION TAG	UNP G3J531
C	379	HIS	-	EXPRESSION TAG	UNP G3J531
C	380	HIS	-	EXPRESSION TAG	UNP G3J531
C	381	HIS	-	EXPRESSION TAG	UNP G3J531
C	382	HIS	-	EXPRESSION TAG	UNP G3J531
C	383	HIS	-	EXPRESSION TAG	UNP G3J531
C	384	HIS	-	EXPRESSION TAG	UNP G3J531
D	-2	MET	-	EXPRESSION TAG	UNP G3J531
D	-1	GLY	-	EXPRESSION TAG	UNP G3J531
D	0	SER	-	EXPRESSION TAG	UNP G3J531
D	377	LEU	-	EXPRESSION TAG	UNP G3J531
D	378	GLU	-	EXPRESSION TAG	UNP G3J531
D	379	HIS	-	EXPRESSION TAG	UNP G3J531
D	380	HIS	-	EXPRESSION TAG	UNP G3J531
D	381	HIS	-	EXPRESSION TAG	UNP G3J531
D	382	HIS	-	EXPRESSION TAG	UNP G3J531
D	383	HIS	-	EXPRESSION TAG	UNP G3J531
D	384	HIS	-	EXPRESSION TAG	UNP G3J531

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	213	Total O 213 213	0	0

Continued on next page...

Continued from previous page...

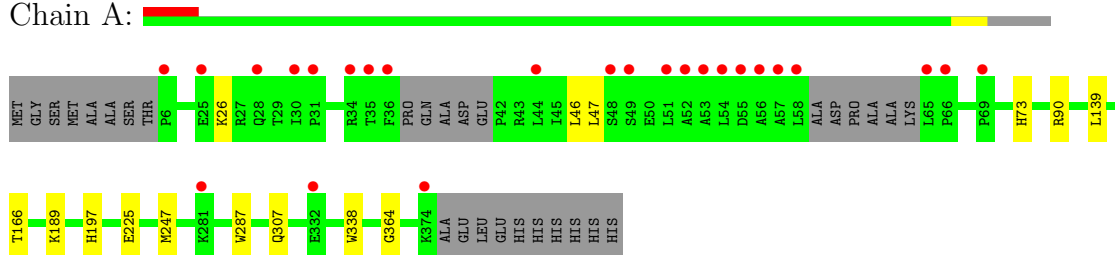
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	193	Total 193	O 193	0	0
3	C	234	Total 234	O 234	0	0
3	D	291	Total 291	O 291	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

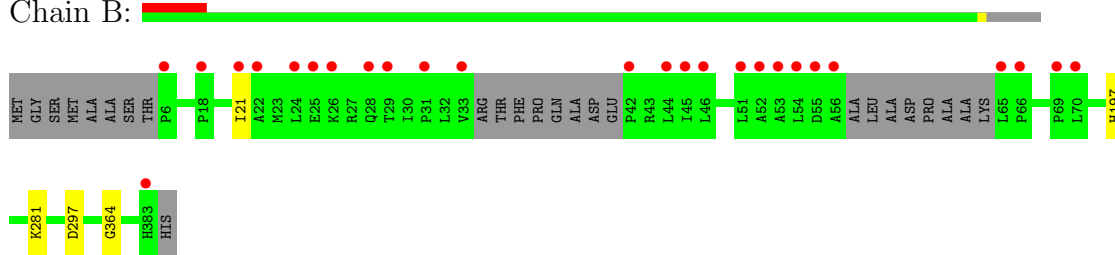
- Molecule 1: Uracil-5-carboxylate decarboxylase

Chain A:



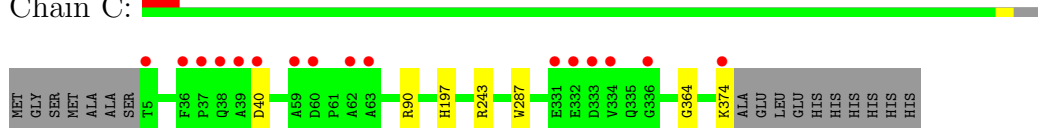
- Molecule 1: Uracil-5-carboxylate decarboxylase

Chain B:



- Molecule 1: Uracil-5-carboxylate decarboxylase

Chain C:



- Molecule 1: Uracil-5-carboxylate decarboxylase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.65Å 146.16Å 77.77Å 90.00° 96.52° 90.00°	Depositor
Resolution (Å)	77.27 – 1.90 48.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (77.27-1.90) 99.4 (48.77-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.157 , 0.197 0.157 , 0.197	Depositor DCC
R_{free} test set	6731 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.0	EDS
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 134917 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12209	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.45	2/2810 (0.1%)	0.53	0/3821
1	B	0.46	0/2853	0.50	0/3880
1	C	0.45	1/2898 (0.0%)	0.52	0/3948
1	D	0.48	2/3006 (0.1%)	0.53	0/4095
All	All	0.46	5/11567 (0.0%)	0.52	0/15744

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	338	TRP	CD2-CE2	5.28	1.47	1.41
1	D	287	TRP	CD2-CE2	5.17	1.47	1.41
1	A	338	TRP	CD2-CE2	5.08	1.47	1.41
1	C	287	TRP	CD2-CE2	5.08	1.47	1.41
1	A	287	TRP	CD2-CE2	5.08	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2742	0	0	3	0
1	B	2781	0	0	1	0
1	C	2826	0	0	1	0
1	D	2924	0	0	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	213	0	0	2	0
3	B	193	0	0	0	0
3	C	234	0	0	1	0
3	D	291	0	0	2	0
All	All	12209	0	0	9	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (9) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:380[A]:HIS:NE2	3:D:741:HOH:O	2.31	0.60
1:A:166:THR:OG1	1:A:225:GLU:OE1	2.25	0.54
1:D:307:GLN:NE2	3:D:765:HOH:O	2.43	0.51
1:C:90:ARG:NH2	3:C:732:HOH:O	2.44	0.51
1:A:307:GLN:NE2	3:A:667:HOH:O	2.48	0.46
1:B:297:ASP:OD1	1:B:297:ASP:C	2.55	0.45
1:A:73:HIS:CD2	3:A:661:HOH:O	2.71	0.44
1:D:264:GLU:OE1	1:D:283:ARG:NH2	2.52	0.41
1:D:297:ASP:C	1:D:297:ASP:OD1	2.59	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	352/387 (91%)	343 (97%)	7 (2%)	2 (1%)	33 19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	356/387 (92%)	346 (97%)	8 (2%)	2 (1%)	33	19
1	C	368/387 (95%)	359 (98%)	7 (2%)	2 (0%)	38	23
1	D	379/387 (98%)	371 (98%)	6 (2%)	2 (0%)	38	23
All	All	1455/1548 (94%)	1419 (98%)	28 (2%)	8 (0%)	33	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	197	HIS
1	D	197	HIS
1	A	197	HIS
1	B	197	HIS
1	A	364	GLY
1	B	364	GLY
1	D	364	GLY
1	C	364	GLY

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	292/313 (93%)	285 (98%)	7 (2%)	61	53
1	B	296/313 (95%)	294 (99%)	2 (1%)	91	90
1	C	300/313 (96%)	297 (99%)	3 (1%)	85	84
1	D	310/313 (99%)	308 (99%)	2 (1%)	92	92
All	All	1198/1252 (96%)	1184 (99%)	14 (1%)	82	80

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	46	LEU
1	A	47	LEU
1	A	90	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	139	LEU
1	A	189	LYS
1	A	247	MET
1	B	21	ILE
1	B	281	LYS
1	C	40	ASP
1	C	243	ARG
1	C	374	LYS
1	D	154	LYS
1	D	281	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	358/387 (92%)	0.12	25 (6%) 16 16	9, 19, 46, 69	0
1	B	362/387 (93%)	0.13	26 (7%) 15 14	10, 21, 55, 79	0
1	C	370/387 (95%)	-0.17	16 (4%) 34 34	8, 16, 37, 83	0
1	D	380/387 (98%)	-0.16	6 (1%) 68 70	9, 16, 35, 58	0
All	All	1470/1548 (94%)	-0.02	73 (4%) 28 28	8, 18, 46, 83	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	ILE	9.6
1	A	44	LEU	6.6
1	A	56	ALA	6.1
1	B	28	GLN	6.1
1	A	57	ALA	5.9
1	B	56	ALA	5.2
1	A	35	THR	5.2
1	C	39	ALA	5.2
1	A	34	ARG	5.2
1	A	52	ALA	5.2
1	B	66	PRO	4.7
1	B	51	LEU	4.7
1	B	24	LEU	4.7
1	A	28	GLN	4.5
1	D	5	THR	4.3
1	B	22	ALA	4.3
1	B	52	ALA	4.2
1	C	40	ASP	4.1
1	B	383	HIS	3.9
1	B	55	ASP	3.9
1	B	65	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	42	PRO	3.7
1	A	36	PHE	3.7
1	A	53	ALA	3.7
1	B	6	PRO	3.6
1	C	38	GLN	3.5
1	D	62	ALA	3.5
1	A	374	LYS	3.5
1	C	62	ALA	3.5
1	B	29	THR	3.4
1	B	31	PRO	3.3
1	C	60	ASP	3.2
1	A	25	GLU	3.2
1	B	46	LEU	3.1
1	A	55	ASP	3.1
1	C	59	ALA	2.9
1	C	333	ASP	2.9
1	A	65	LEU	2.8
1	C	334	VAL	2.8
1	B	26	LYS	2.8
1	A	48	SER	2.8
1	B	53	ALA	2.7
1	C	37	PRO	2.7
1	C	374	LYS	2.7
1	A	51	LEU	2.7
1	B	33	VAL	2.7
1	B	18	PRO	2.7
1	B	45	ILE	2.7
1	A	54	LEU	2.6
1	A	58	LEU	2.5
1	B	44	LEU	2.5
1	A	30	ILE	2.5
1	C	5	THR	2.5
1	A	49	SER	2.5
1	A	69	PRO	2.4
1	B	70	LEU	2.4
1	C	336	GLY	2.4
1	C	63	ALA	2.4
1	D	59	ALA	2.4
1	D	377	LEU	2.3
1	B	69	PRO	2.3
1	C	331	GLU	2.2
1	C	332	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	381	HIS	2.2
1	A	31	PRO	2.2
1	B	54	LEU	2.2
1	C	36	PHE	2.1
1	A	6	PRO	2.1
1	A	66	PRO	2.1
1	A	332	GLU	2.1
1	D	378	GLU	2.1
1	A	281	LYS	2.1
1	B	25	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	D	401	1/1	0.04	-2.99	16,16,16,16	0
2	ZN	A	401	1/1	0.04	-3.24	17,17,17,17	0
2	ZN	B	401	1/1	0.04	-3.64	21,21,21,21	0
2	ZN	C	401	1/1	0.03	-4.12	15,15,15,15	0
2	ZN	D	402	1/1	0.03	-4.34	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.