



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:54 AM GMT

PDB ID : 4L50  
Title : Crystal structures of the LsrR proteins complexed with phospho-AI-2 and its two different analogs reveal distinct mechanisms for ligand recognition  
Authors : Ryu, K.S.; Ha, J.H.; Eo, Y.  
Deposited on : 2013-06-10  
Resolution : 2.10 Å(reported)

This is a full wwPDB validation 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 <http://wwpdb.org/ValidationPDFNotes.html>

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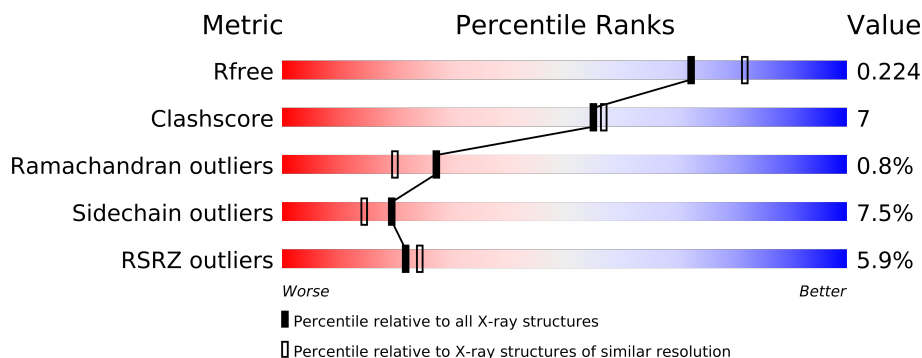
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.10 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	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. 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	266	
1	B	266	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3912 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.

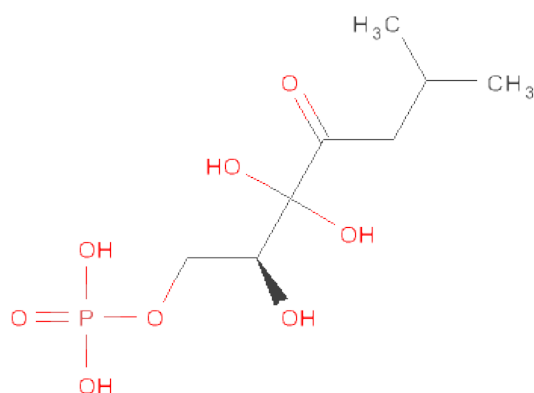
- Molecule 1 is a protein called Transcriptional regulator LsrR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	3	0
			1838	1151	329	348	10			
1	B	247	Total	C	N	O	S	0	3	0
			1825	1140	327	348	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	SER	-	EXPRESSION TAG	UNP P76141
B	52	SER	-	EXPRESSION TAG	UNP P76141

- Molecule 2 is (2S)-2,3,3-TRIHIDROXY-6-METHYL-4-OXOHEPTYLDIHYDROGEN PHOSPHATE (three-letter code: D8X) (formula: C<sub>8</sub>H<sub>17</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			17	8	8	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			17	8	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	113	Total	O	0	0
			113	113		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.81Å 116.81Å 79.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.52 – 2.10 34.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (34.52-2.10) 97.2 (34.50-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.166 , 0.218 0.177 , 0.224	Depositor DCC
$R_{free}$ test set	1781 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.1	EDS
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 35296 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: D8X

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	0.91	0/1859	0.99	5/2508 (0.2%)
1	B	0.91	0/1848	0.94	1/2493 (0.0%)
All	All	0.91	0/3707	0.97	6/5001 (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	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	80	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	134	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	279	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	279	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	250	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	93	LEU	CA-CB-CG	5.47	127.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152[B]	GLY	Peptide

## 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	1838	0	1893	23	0
1	B	1825	0	1880	27	0
2	A	17	0	17	3	0
2	B	17	0	16	2	0
3	A	102	0	0	2	0
3	B	113	0	0	3	0
All	All	3912	0	3806	50	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 7.

All (50) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:164:ASN:OD1	1:A:167:CYS:SG	2.46	0.73
1:A:314:ILE:O	1:A:317:SER:HB2	1.91	0.71
2:A:501:D8X:H17	2:A:501:D8X:O2	1.93	0.67
1:B:248:PHE:H	1:B:262:HIS:CE1	2.14	0.66
1:B:117:GLN:HA	1:B:143:GLN:O	1.99	0.63
2:B:401:D8X:O2	2:B:401:D8X:H17	1.98	0.63
1:B:212:ALA:H	1:B:215:GLN:HE21	1.47	0.63
1:A:92:GLY:H	1:A:308:GLN:HE21	1.46	0.62
1:A:124:PHE:CD2	2:A:501:D8X:H11	2.35	0.61
1:B:124:PHE:CD1	2:B:401:D8X:H11	2.37	0.60
1:B:163:LEU:HB3	1:B:167:CYS:SG	2.42	0.60
1:A:187:LEU:HD21	1:B:187:LEU:HD21	1.84	0.59
1:B:258:ASN:OD1	1:B:258:ASN:N	2.26	0.58
1:A:164:ASN:ND2	1:A:166:ALA:HB3	2.19	0.57
1:B:156:TYR:HB3	1:B:160:ILE:HD12	1.87	0.56
1:A:93:LEU:HD22	1:A:96:ALA:N	2.24	0.53
1:A:192:CYS:SG	1:B:175:PRO:HB3	2.49	0.53
1:A:153:VAL:O	1:A:156:TYR:HB2	2.10	0.52
1:B:248:PHE:H	1:B:262:HIS:HE1	1.55	0.52
1:A:163:LEU:HB3	1:A:167:CYS:SG	2.51	0.51
1:B:104:ILE:HD11	1:B:134:ARG:NH2	2.26	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:152[A]:GLY:O	1:A:154:GLY:N	2.45	0.50
1:A:92:GLY:H	1:A:308:GLN:NE2	2.11	0.48
1:A:93:LEU:HD22	1:A:93:LEU:C	2.34	0.48
1:B:100:GLY:HA2	1:B:130:ASN:HD21	1.79	0.48
1:B:178:ALA:HB2	1:B:266:ILE:HD11	1.97	0.47
1:B:91:PRO:O	1:B:101:ARG:NH2	2.48	0.47
1:B:84:LEU:CD1	1:B:87:VAL:HG22	2.45	0.47
1:A:86:HIS:CD2	1:A:113:LEU:HD21	2.50	0.47
1:A:68:PHE:O	1:A:69:GLU:HB2	2.15	0.46
1:A:116:PRO:HG3	1:A:142:GLN:NE2	2.31	0.46
1:A:258:ASN:N	1:A:258:ASN:OD1	2.48	0.45
1:B:126:GLU:HG2	3:B:544:HOH:O	2.16	0.45
1:A:173:PRO:O	1:B:175:PRO:HD3	2.17	0.44
1:B:260:LYS:HD3	3:B:520:HOH:O	2.17	0.44
1:A:117:GLN:HA	1:A:143:GLN:O	2.18	0.44
1:A:116:PRO:HG3	1:A:142:GLN:HE21	1.83	0.43
1:B:247:TYR:CD2	1:B:270:LEU:HD13	2.54	0.43
1:B:75:GLU:HG2	1:B:89:VAL:HG23	2.01	0.43
1:A:154:GLY:HA2	1:A:157:MET:CE	2.49	0.42
1:B:84:LEU:HD12	1:B:87:VAL:CG2	2.50	0.42
1:B:137:GLY:O	1:B:141:SER:HB3	2.20	0.42
1:B:154:GLY:HA2	1:B:157:MET:HG2	2.02	0.42
1:B:71:CYS:O	1:B:75:GLU:HG3	2.20	0.42
1:B:160:ILE:O	1:B:162:GLN:N	2.52	0.42
2:A:501:D8X:C22	2:A:501:D8X:O2	2.62	0.41
1:A:68:PHE:N	3:A:645:HOH:O	2.53	0.41
1:A:79[B]:ARG:HD2	3:A:666:HOH:O	2.20	0.41
1:B:194:LYS:HG3	3:B:536:HOH:O	2.21	0.40
1:B:152[A]:GLY:O	1:B:154:GLY:N	2.54	0.40

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	247/266 (93%)	239 (97%)	6 (2%)	2 (1%)	27	20
1	B	246/266 (92%)	238 (97%)	6 (2%)	2 (1%)	27	20
All	All	493/532 (93%)	477 (97%)	12 (2%)	4 (1%)	27	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	GLU
1	A	153	VAL
1	B	153	VAL
1	B	162	GLN

### 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	190/203 (94%)	175 (92%)	15 (8%)	18	13
1	B	189/203 (93%)	176 (93%)	13 (7%)	22	17
All	All	379/406 (93%)	351 (93%)	28 (7%)	19	15

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	PHE
1	A	72	LEU
1	A	93	LEU
1	A	116	PRO
1	A	135	LEU
1	A	136	SER
1	A	146	LEU
1	A	189	ASN
1	A	224	SER
1	A	237	ARG
1	A	243	ASP
1	A	258	ASN
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	287	ASN
1	A	317	SER
1	B	73	GLU
1	B	80	ARG
1	B	90	ILE
1	B	95	ASP
1	B	112	SER
1	B	136	SER
1	B	141	SER
1	B	146	LEU
1	B	194	LYS
1	B	243	ASP
1	B	258	ASN
1	B	268	LEU
1	B	270	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	142	GLN
1	A	287	ASN
1	A	308	GLN
1	B	130	ASN
1	B	142	GLN
1	B	164	ASN
1	B	191	ASN
1	B	215	GLN
1	B	262	HIS

### 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 ⓘ

2 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	D8X	A	501	-	16,16,16	1.12	1 (6%)	24,24,24	1.21	3 (12%)
2	D8X	B	401	-	16,16,16	1.70	3 (18%)	24,24,24	3.41	10 (41%)

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	D8X	A	501	-	-	1/19/22/22	0/0/0/0
2	D8X	B	401	-	-	1/19/22/22	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	D8X	C3-C2	4.18	1.60	1.54
2	B	401	D8X	P-O1P	-2.80	1.44	1.54
2	B	401	D8X	C1-C2	2.62	1.54	1.51
2	A	501	D8X	C1-C2	-2.28	1.49	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	D8X	O3'-C3-C2	-8.99	92.74	108.14
2	B	401	D8X	C5-C4-C3	-6.70	105.00	112.91
2	B	401	D8X	O3'-C3-C4	6.53	124.04	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	D8X	O3-C3-C2	-6.27	97.40	108.14
2	B	401	D8X	C4-C3-C2	-4.73	97.96	110.44
2	A	501	D8X	C1'-C1-C2	-3.57	106.65	115.43
2	B	401	D8X	O3'-C3-O3	3.34	117.49	111.59
2	B	401	D8X	O3-C3-C4	3.10	115.23	107.28
2	B	401	D8X	O4-C4-C3	2.60	114.75	109.43
2	B	401	D8X	P-O5-C5	2.48	125.36	118.19
2	A	501	D8X	O3-C3-C4	2.38	113.38	107.28
2	A	501	D8X	O3'-C3-O3	-2.25	107.60	111.59
2	B	401	D8X	C1-C2-C3	2.13	121.52	118.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	D8X	O3'-C3-C2-C1
2	A	501	D8X	O3-C3-C2-C1

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, 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	248/266 (93%)	-0.05	14 (5%) 24 26	19, 29, 81, 107	0
1	B	247/266 (92%)	-0.06	15 (6%) 21 23	19, 29, 79, 122	0
All	All	495/532 (93%)	-0.05	29 (5%) 22 24	19, 29, 82, 122	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ALA	7.8
1	B	69	GLU	7.6
1	B	167	CYS	5.7
1	B	96	ALA	5.6
1	B	165	ALA	5.4
1	A	165	ALA	5.4
1	B	166	ALA	5.3
1	A	97	ASP	4.9
1	B	97	ASP	4.7
1	A	166	ALA	4.7
1	A	167	CYS	4.6
1	A	164	ASN	4.2
1	B	70	GLY	4.1
1	B	161	GLY	3.8
1	A	68	PHE	3.7
1	A	162	GLN	3.7
1	B	164	ASN	3.7
1	B	317	SER	3.6
1	B	160	ILE	3.3
1	A	69	GLU	3.0
1	B	95	ASP	2.9
1	A	98	VAL	2.7
1	A	158	THR	2.7
1	A	161	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	92	GLY	2.4
1	B	162	GLN	2.4
1	A	317	SER	2.3
1	A	160	ILE	2.3
1	B	158	THR	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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	D8X	B	401	17/17	0.09	-0.55	23,29,46,50	0
2	D8X	A	501	17/17	0.09	-0.59	21,29,44,52	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.