wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2014 – 01:42 AM GMT

PDB ID : 2A92
Title : Crystal structure of lactate dehydrogenase from Plasmodium vivax: complex with NADH
Authors : Chaikuad, A.; Fairweather, V.; Conners, R.; Joseph-Horne, T.; Turgut-Balik, D.; Brady, R.L.
Deposited on : 2005-07-11
Resolution : 2.04 Å(reported)

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.04 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		9
Ramachandran outliers		2.1%
Sidechain outliers		3.2%
RSRZ outliers		7.4%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
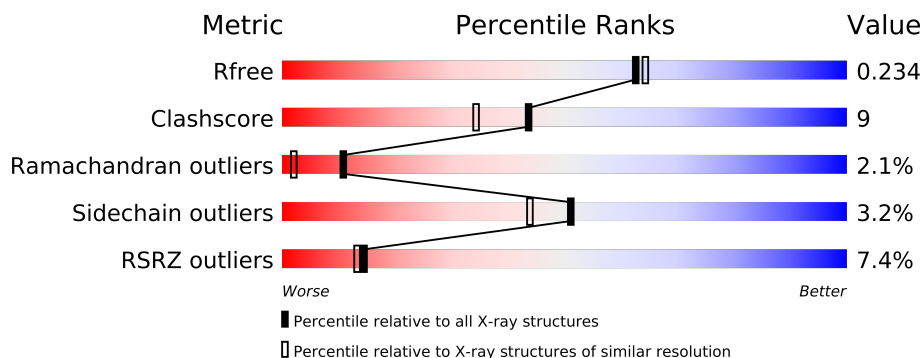
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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	321	
1	B	321	
1	C	321	
1	D	321	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10257 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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	4	0
			2404	1535	404	451	14			
1	B	315	Total	C	N	O	S	0	3	0
			2389	1526	400	449	14			
1	C	318	Total	C	N	O	S	0	4	0
			2419	1544	409	452	14			
1	D	315	Total	C	N	O	S	0	3	0
			2389	1526	400	449	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	HIS	-	EXPRESSION TAG	GB 66967948
A	331	HIS	-	EXPRESSION TAG	GB 66967948
A	332	HIS	-	EXPRESSION TAG	GB 66967948
A	333	HIS	-	EXPRESSION TAG	GB 66967948
A	334	HIS	-	EXPRESSION TAG	GB 66967948
A	335	HIS	-	EXPRESSION TAG	GB 66967948
B	330	HIS	-	EXPRESSION TAG	GB 66967948
B	331	HIS	-	EXPRESSION TAG	GB 66967948
B	332	HIS	-	EXPRESSION TAG	GB 66967948
B	333	HIS	-	EXPRESSION TAG	GB 66967948
B	334	HIS	-	EXPRESSION TAG	GB 66967948
B	335	HIS	-	EXPRESSION TAG	GB 66967948
C	330	HIS	-	EXPRESSION TAG	GB 66967948
C	331	HIS	-	EXPRESSION TAG	GB 66967948
C	332	HIS	-	EXPRESSION TAG	GB 66967948
C	333	HIS	-	EXPRESSION TAG	GB 66967948
C	334	HIS	-	EXPRESSION TAG	GB 66967948
C	335	HIS	-	EXPRESSION TAG	GB 66967948
D	330	HIS	-	EXPRESSION TAG	GB 66967948
D	331	HIS	-	EXPRESSION TAG	GB 66967948
D	332	HIS	-	EXPRESSION TAG	GB 66967948

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Chain	Residue	Modelled	Actual	Comment	Reference
D	333	HIS	-	EXPRESSION TAG	GB 66967948
D	334	HIS	-	EXPRESSION TAG	GB 66967948
D	335	HIS	-	EXPRESSION TAG	GB 66967948

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDEADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).
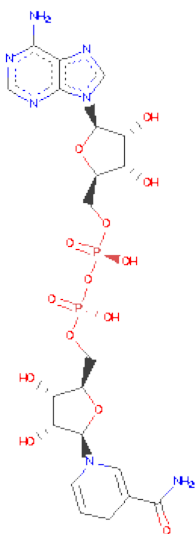
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total	O	0	0
			148	148		
3	B	130	Total	O	0	0
			130	130		
3	C	112	Total	O	0	0
			112	112		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	90	Total O 90 90		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.
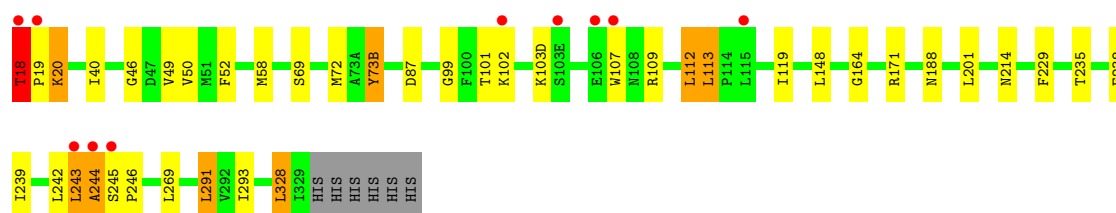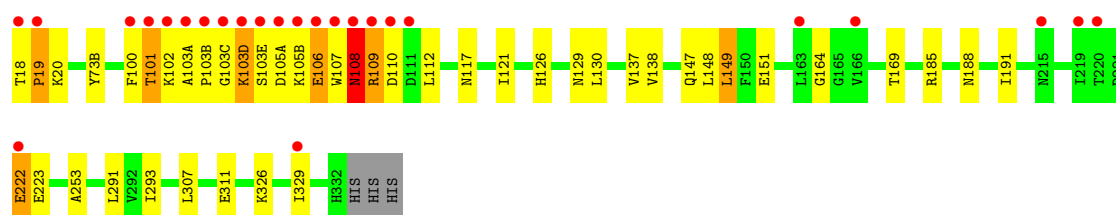
- Molecule 1: L-lactate dehydrogenase

Chain A:
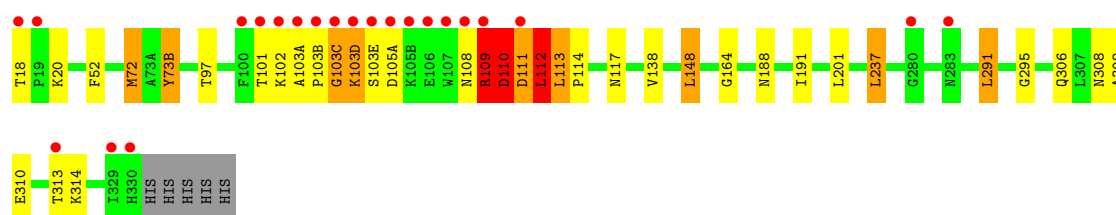
- Molecule 1: L-lactate dehydrogenase

Chain B:

- Molecule 1: L-lactate dehydrogenase

Chain C:

- Molecule 1: L-lactate dehydrogenase

Chain D:

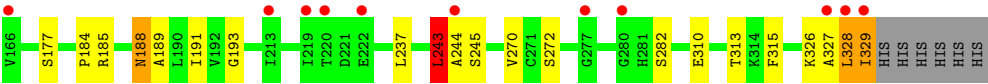V166 S177 P184 R185 N188 A189 L190 I191 V192 G193 I213 I219 T220 D221 E222 L237 L243 A244 S245 V270 C271 S272 G277 G280 H281 S282 E310 T313 K314 F315 K326 A327 L328 I329 HIS HIS HIS HIS HIS HIS
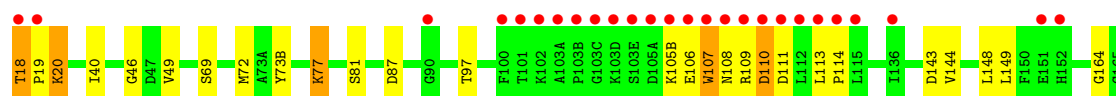
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.59Å 128.64Å 130.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 2.04 32.97 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.8 (91.29-2.04) 97.8 (32.97-2.04)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.236 0.195 , 0.234	Depositor DCC
R_{free} test set	4299 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.9	EDS
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 85849 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10257	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]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: NAI

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	0.73	0/2443	0.74	2/3308 (0.1%)
1	B	0.67	0/2424	0.69	2/3282 (0.1%)
1	C	0.67	0/2457	0.63	0/3327
1	D	0.59	0/2424	0.63	0/3282
All	All	0.67	0/9748	0.67	4/13199 (0.0%)

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	2
1	D	0	1
All	All	0	6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	291	LEU	CA-CB-CG	9.46	137.06	115.30
1	B	291	LEU	CA-CB-CG	7.43	132.40	115.30
1	A	113	LEU	N-CA-C	-6.92	92.33	111.00
1	B	112	LEU	CA-CB-CG	6.01	129.13	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Peptide
1	A	111	ASP	Peptide
1	A	112	LEU	Peptide
1	B	18	THR	Peptide
1	B	244	ALA	Peptide

5.2 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 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	2404	0	2496	43	0
1	B	2389	0	2483	37	0
1	C	2419	0	2502	68	0
1	D	2389	0	2483	33	0
2	A	44	0	27	3	0
2	B	44	0	27	1	0
2	C	44	0	27	1	0
2	D	44	0	27	1	0
3	A	148	0	0	2	0
3	B	130	0	0	2	0
3	C	112	0	0	1	0
3	D	90	0	0	1	0
All	All	10257	0	10072	173	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 9.

The worst 5 of 173 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:100:PHE:CG	1:C:101:THR:HB	1.42	1.55
1:C:103(C):GLY:HA3	1:C:103(D):LYS:CB	1.26	1.49
1:C:103(C):GLY:CA	1:C:103(D):LYS:HB2	1.27	1.39
1:C:100:PHE:HA	1:C:101:THR:CB	1.60	1.25
1:C:100:PHE:HA	1:C:101:THR:OG1	1.35	1.22

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	315/321 (98%)	297 (94%)	12 (4%)	6 (2%)	12	2
1	B	313/321 (98%)	304 (97%)	6 (2%)	3 (1%)	22	9
1	C	316/321 (98%)	294 (93%)	13 (4%)	9 (3%)	8	1
1	D	313/321 (98%)	295 (94%)	10 (3%)	8 (3%)	8	1
All	All	1257/1284 (98%)	1190 (95%)	41 (3%)	26 (2%)	11	2

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103(C)	GLY
1	A	103(D)	LYS
1	A	110	ASP
1	A	112	LEU
1	B	243	LEU

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	269/273 (98%)	260 (97%)	9 (3%)	50	42
1	B	267/273 (98%)	258 (97%)	9 (3%)	49	41
1	C	270/273 (99%)	263 (97%)	7 (3%)	59	54
1	D	267/273 (98%)	258 (97%)	9 (3%)	49	41
All	All	1073/1092 (98%)	1039 (97%)	34 (3%)	51	44

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	188	ASN
1	C	102	LYS
1	D	243	LEU
1	B	328	LEU
1	A	188	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	188	ASN
1	B	210(B)	GLN
1	C	234	ASN
1	A	306	GLN
1	B	178	GLN

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 ⓘ

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAI	A	601	-	48,48,48	1.77	6 (12%)	73,73,73	1.84	14 (19%)
2	NAI	B	701	-	48,48,48	1.68	8 (16%)	73,73,73	1.69	9 (12%)
2	NAI	C	501	-	48,48,48	1.72	7 (14%)	73,73,73	1.94	15 (20%)
2	NAI	D	801	-	48,48,48	1.70	7 (14%)	73,73,73	1.76	9 (12%)

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	NAI	A	601	-	-	0/30/72/72	0/3/5/5
2	NAI	B	701	-	-	0/30/72/72	0/3/5/5
2	NAI	C	501	-	-	0/30/72/72	0/3/5/5
2	NAI	D	801	-	-	0/30/72/72	0/3/5/5

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAI	O7N-C7N	6.31	1.41	1.24
2	A	601	NAI	O7N-C7N	6.20	1.40	1.24
2	D	801	NAI	O7N-C7N	5.90	1.39	1.24
2	B	701	NAI	O7N-C7N	5.75	1.39	1.24
2	D	801	NAI	C4N-C3N	-5.31	1.39	1.50

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	NAI	N3A-C2A-N1A	-11.34	119.22	128.71
2	A	601	NAI	N3A-C2A-N1A	-9.88	120.44	128.71
2	D	801	NAI	N3A-C2A-N1A	-9.85	120.48	128.71
2	B	701	NAI	N3A-C2A-N1A	-9.06	121.13	128.71
2	D	801	NAI	O4B-C1B-N9A	4.27	112.41	108.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	316/321 (98%)	0.43	22 (6%)	16	15	4, 9, 14, 20	31 (9%)
1	B	315/321 (98%)	-0.03	10 (3%)	45	45	3, 9, 15, 22	34 (10%)
1	C	318/321 (99%)	0.62	25 (7%)	13	12	4, 9, 15, 21	52 (16%)
1	D	315/321 (98%)	1.09	37 (11%)	5	5	2, 10, 16, 22	55 (17%)
All	All	1264/1284 (98%)	0.53	94 (7%)	14	13	2, 9, 15, 22	172 (13%)

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	107	TRP	27.7
1	A	103(B)	PRO	26.4
1	A	103(A)	ALA	25.1
1	D	108	ASN	23.9
1	D	100	PHE	21.0

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	NAI	A	601	44/44	0.10	-	3,7,12,17	0
2	NAI	C	501	44/44	0.10	-	2,6,9,11	0
2	NAI	B	701	44/44	0.13	-	8,13,22,25	0
2	NAI	D	801	44/44	0.13	-	12,17,22,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.