



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:29 PM GMT

PDB ID : 1P8L
Title : New Crystal Structure of Chlorella Virus DNA Ligase-Adenylate
Authors : Odell, M.; Malinina, L.; Teplova, M.; Shuman, S.
Deposited on : 2003-05-07
Resolution : 2.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

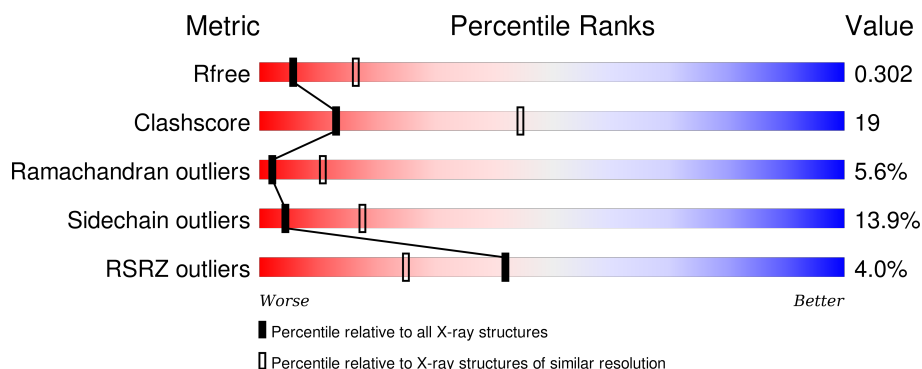
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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. 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 $\leq 5\%$. 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	A	304	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2252 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.

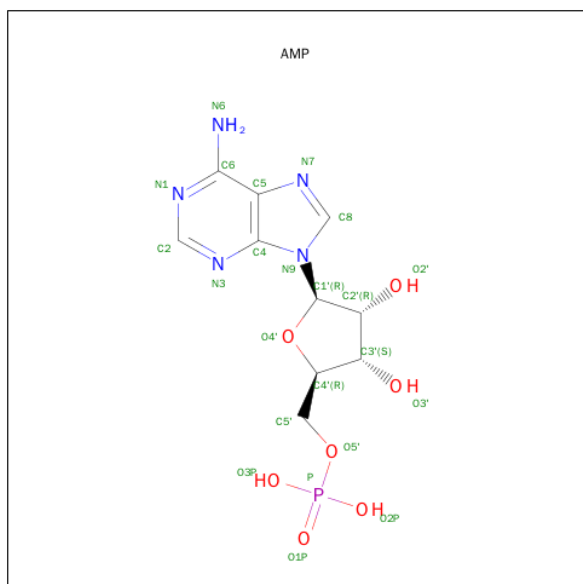
- Molecule 1 is a protein called PBCV-1 DNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2228	1433	365	417	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP O41026
A	-4	HIS	-	EXPRESSION TAG	UNP O41026
A	-3	HIS	-	EXPRESSION TAG	UNP O41026
A	-2	HIS	-	EXPRESSION TAG	UNP O41026
A	-1	HIS	-	EXPRESSION TAG	UNP O41026
A	0	HIS	-	EXPRESSION TAG	UNP O41026

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		

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 ($\text{RSRZ} > 2$). 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.

Chain A:

4% 47% 35% 8% 9%

HIS HIS HIS HIS HIS HIS MET A2 K5 A9 A10 T11 T12 E13 N14 I15 E16 D17 V18 Q19 F20 F21 T25 T26 D29 S33 V34 K35 Q36 T37 Q38 Q39 L40 L48 M52 M53 L56 T57 E58 L59 L60 P61 S64 D65 G66 I70 F75 Q76 D77 T78 T79 V62 V63 M64 T65 R66 R67 G68 Y69 Y90 A91 Y92 S94 S95 Y96 Y97 Y98 V101 T102 D103 D104 P105 L106 I110 E114 D115 M116 K117 T121 T126 L127 E128 H129 V132 K133 T134 P136 E141 T142 M143 N144 E147 L148 Y151 E152 R153 D154 V155 F160 V163 M164 T165 R166 P167 P168 D169 Y172 S177 K180 T183 L184 L185 M187 K188 Q189 F190 K191 D192 A193 A194 A195 I198 S199 M200 L203 T204 K205 C206 T208 T209 T210 T211 T212 T213 T214 T215 T216 T217 T218 T219 T220 T221 T222 T223 T224 T225 T226 T227 T228 T229 T230 T231 T232 T233 T234 T235 T236 T237 T238 T239 T240 T241 T242 T243 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255 T256 T257 T258 T259 T260 T261 T262 T263 T264 T265 T266 T267 T268 T269 T270 T271 T272 T273 T274 T275 T276 T277 T278 T279 T280 T281 T282 T283 T284 T285 T286 T287 T288 T289 T290 T291 T292 T293 T294 T295 T296 T297 T298 T299 T300 T301 T302 T303 T304 T305 T306 T307 T308 T309 T310 T311 T312 T313 T314 T315 T316 T317 T318 T319 T320 T321 T322 T323 T324 T325 T326 T327 T328 T329 T330 T331 T332 T333 T334 T335 T336 T337 T338 T339 T340 T341 T342 T343 T344 T345 T346 T347 T348 T349 T350 T351 T352 T353 T354 T355 T356 T357 T358 T359 T360 T361 T362 T363 T364 T365 T366 T367 T368 T369 T370 T371 T372 T373 T374 T375 T376 T377 T378 T379 T380 T381 T382 T383 T384 T385 T386 T387 T388 T389 T390 T391 T392 T393 T394 T395 T396 T397 T398 T399 T400 T401 T402 T403 T404 T405 T406 T407 T408 T409 T410 T411 T412 T413 T414 T415 T416 T417 T418 T419 T420 T421 T422 T423 T424 T425 T426 T427 T428 T429 T430 T431 T432 T433 T434 T435 T436 T437 T438 T439 T440 T441 T442 T443 T444 T445 T446 T447 T448 T449 T450 T451 T452 T453 T454 T455 T456 T457 T458 T459 T460 T461 T462 T463 T464 T465 T466 T467 T468 T469 T470 T471 T472 T473 T474 T475 T476 T477 T478 T479 T480 T481 T482 T483 T484 T485 T486 T487 T488 T489 T490 T491 T492 T493 T494 T495 T496 T497 T498 T499 T500 T501 T502 T503 T504 T505 T506 T507 T508 T509 T510 T511 T512 T513 T514 T515 T516 T517 T518 T519 T520 T521 T522 T523 T524 T525 T526 T527 T528 T529 T530 T531 T532 T533 T534 T535 T536 T537 T538 T539 T540 T541 T542 T543 T544 T545 T546 T547 T548 T549 T550 T551 T552 T553 T554 T555 T556 T557 T558 T559 T560 T561 T562 T563 T564 T565 T566 T567 T568 T569 T570 T571 T572 T573 T574 T575 T576 T577 T578 T579 T580 T581 T582 T583 T584 T585 T586 T587 T588 T589 T590 T591 T592 T593 T594 T595 T596 T597 T598 T599 T600 T601 T602 T603 T604 T605 T606 T607 T608 T609 T610 T611 T612 T613 T614 T615 T616 T617 T618 T619 T620 T621 T622 T623 T624 T625 T626 T627 T628 T629 T630 T631 T632 T633 T634 T635 T636 T637 T638 T639 T640 T641 T642 T643 T644 T645 T646 T647 T648 T649 T650 T651 T652 T653 T654 T655 T656 T657 T658 T659 T660 T661 T662 T663 T664 T665 T666 T667 T668 T669 T670 T671 T672 T673 T674 T675 T676 T677 T678 T679 T680 T681 T682 T683 T684 T685 T686 T687 T688 T689 T690 T691 T692 T693 T694 T695 T696 T697 T698 T699 T700 T701 T702 T703 T704 T705 T706 T707 T708 T709 T710 T711 T712 T713 T714 T715 T716 T717 T718 T719 T720 T721 T722 T723 T724 T725 T726 T727 T728 T729 T730 T731 T732 T733 T734 T735 T736 T737 T738 T739 T740 T741 T742 T743 T744 T745 T746 T747 T748 T749 T750 T751 T752 T753 T754 T755 T756 T757 T758 T759 T760 T761 T762 T763 T764 T765 T766 T767 T768 T769 T770 T771 T772 T773 T774 T775 T776 T777 T778 T779 T780 T781 T782 T783 T784 T785 T786 T787 T788 T789 T790 T791 T792 T793 T794 T795 T796 T797 T798 T799 T800 T801 T802 T803 T804 T805 T806 T807 T808 T809 T810 T811 T812 T813 T814 T815 T816 T817 T818 T819 T820 T821 T822 T823 T824 T825 T826 T827 T828 T829 T830 T831 T832 T833 T834 T835 T836 T837 T838 T839 T840 T841 T842 T843 T844 T845 T846 T847 T848 T849 T850 T851 T852 T853 T854 T855 T856 T857 T858 T859 T860 T861 T862 T863 T864 T865 T866 T867 T868 T869 T870 T871 T872 T873 T874 T875 T876 T877 T878 T879 T880 T881 T882 T883 T884 T885 T886 T887 T888 T889 T890 T891 T892 T893 T894 T895 T896 T897 T898 T899 T900 T901 T902 T903 T904 T905 T906 T907 T908 T909 T910 T911 T912 T913 T914 T915 T916 T917 T918 T919 T920 T921 T922 T923 T924 T925 T926 T927 T928 T929 T930 T931 T932 T933 T934 T935 T936 T937 T938 T939 T940 T941 T942 T943 T944 T945 T946 T947 T948 T949 T950 T951 T952 T953 T954 T955 T956 T957 T958 T959 T960 T961 T962 T963 T964 T965 T966 T967 T968 T969 T970 T971 T972 T973 T974 T975 T976 T977 T978 T979 T980 T981 T982 T983 T984 T985 T986 T987 T988 T989 T990 T991 T992 T993 T994 T995 T996 T997 T998 T999 T1000

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	91.06 Å 60.57 Å 70.27 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.95 14.99 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.9 (15.00-2.95) 96.9 (14.99-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.96 Å)	Xtriage
Refinement program	REFMAC 5.1.06	Depositor
R, R_{free}	0.263 , 0.304 0.250 , 0.302	Depositor DCC
R_{free} test set	680 reflections (8.97%)	DCC
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 39.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 8265 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2252	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: AMP

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	0.61	0/2275	0.91	10/3064 (0.3%)

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.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	192	ASP	CB-CG-OD2	7.43	124.99	118.30
1	A	104	ASP	CB-CG-OD2	6.89	124.50	118.30
1	A	297	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	282	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	241	ASP	CB-CG-OD2	6.16	123.85	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	PHE	Peptide

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	2228	0	2215	85	0
2	A	22	0	12	3	0
3	A	2	0	0	0	0
All	All	2252	0	2227	85	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 19.

The worst 5 of 85 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:15:ILE:HD12	1:A:189:GLN:HG3	1.69	0.75
1:A:93:PHE:CZ	1:A:132:VAL:HG22	2.23	0.72
1:A:38:GLN:HA	1:A:57:THR:HG21	1.70	0.71
1:A:52:MET:SD	1:A:82:VAL:HG22	2.33	0.68
1:A:117:LYS:O	1:A:121:THR:HG22	1.94	0.68

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	270/304 (89%)	234 (87%)	21 (8%)	15 (6%)	2 11

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	PHE
1	A	21	PRO
1	A	204	PHE
1	A	37	THR
1	A	126	ILE

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	245/273 (90%)	211 (86%)	34 (14%)	4 17

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

Mol	Chain	Res	Type
1	A	142	ILE
1	A	180	LYS
1	A	283	CYS
1	A	154	ASP
1	A	83	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	294	HIS
1	A	150	GLN
1	A	129	HIS
1	A	144	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	AMP	A	301	1	15,24,25	1.42	2 (13%)	16,35,38	3.29	3 (18%)

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	AMP	A	301	1	-	0/3/25/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	AMP	C2-N1	2.33	1.38	1.33
2	A	301	AMP	C2-N3	4.03	1.39	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	AMP	N3-C2-N1	-9.80	121.39	128.89
2	A	301	AMP	C2'-C1'-N9	-7.96	102.13	114.29

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	301	AMP	C4'-O4'-C1'	2.16	112.09	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	AMP	3	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, 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	276/304 (90%)	0.18	11 (3%) 42 25	8, 26, 40, 74	3 (1%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	ASP	4.5
1	A	193	ALA	3.0
1	A	278	MET	3.0
1	A	280	SER	3.0
1	A	230	GLU	2.8

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 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	AMP	A	301	22/23	0.92	0.18	-0.19	30,32,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.