



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:14 PM GMT

PDB ID : 3S8A
Title : Structure of Yeast Ribonucleotide Reductase R293A with dGTP
Authors : Ahmad, M.F.; Kaushal, P.S.; Wan, Q.; Wijeratna, S.R.; Huang, M.; Dealwis, C.D.
Deposited on : 2011-05-27
Resolution : 2.90 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>

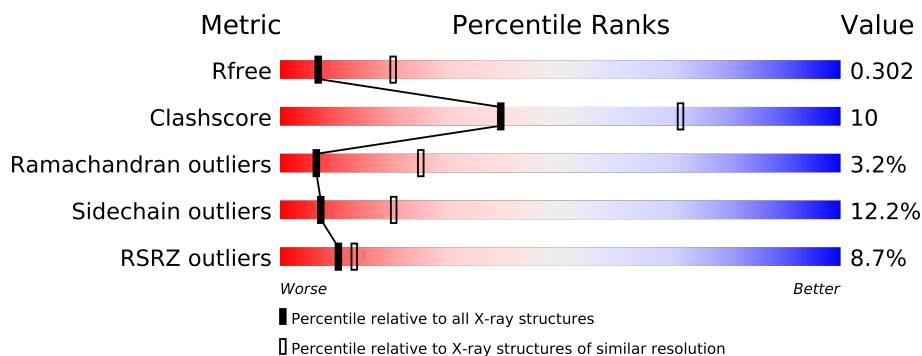
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	888	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	2001	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5341 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 Ribonucleoside-diphosphatereductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	664	5296	3373	899	993	31	0	0	0

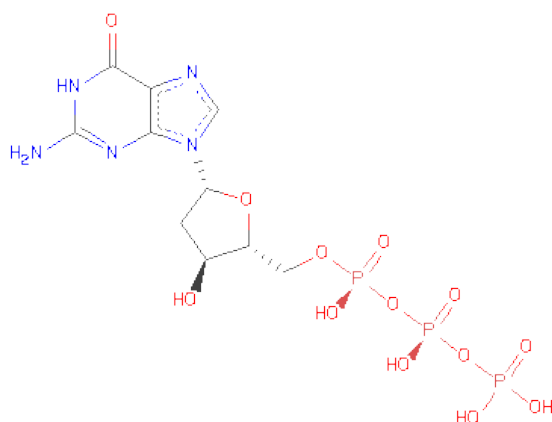
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	ALA	ARG	ENGINEERED MUTATION	UNP P21524

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.44Å 117.72Å 64.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.99-2.90) 96.5 (19.94-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.300 0.237 , 0.302	Depositor DCC
R_{free} test set	1834 reflections (11.15%)	DCC
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 18284 reflections (0.011%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5341	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: MG, DGT

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	0.68	1/5418 (0.0%)	0.79	3/7337 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	620	CYS	CB-SG	-7.81	1.69	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	LEU	CA-CB-CG	7.22	131.91	115.30
1	A	244	THR	N-CA-C	-6.13	94.44	111.00
1	A	507	LEU	CA-CB-CG	5.57	128.11	115.30

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	5296	0	0	51	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	0	0
4	A	13	0	0	0	0
All	All	5341	0	12	51	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 10.

All (51) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:461:LYS:C	1:A:462:THR:CG2	2.46	0.80
1:A:460:GLY:O	1:A:462:THR:CG2	2.30	0.79
1:A:461:LYS:O	1:A:462:THR:CG2	2.30	0.79
1:A:662:TYR:CD1	1:A:662:TYR:O	2.37	0.77
1:A:686:THR:CG2	1:A:688:TRP:CD1	2.67	0.77
1:A:482:ASN:OD1	1:A:503:ARG:NH1	2.27	0.67
1:A:168:GLN:NE2	1:A:190:TYR:OH	2.28	0.66
1:A:619:GLU:O	1:A:620:CYS:CB	2.46	0.64
1:A:244:THR:OG1	1:A:245:ALA:N	2.30	0.63
1:A:666:GLN:N	1:A:666:GLN:CD	2.53	0.62
1:A:709:SER:OG	1:A:710:HIS:N	2.34	0.60
1:A:159:ILE:CG2	1:A:160:ASN:N	2.65	0.60
1:A:261:TYR:OH	1:A:266:ASN:ND2	2.37	0.58
1:A:245:ALA:CB	1:A:288:GLN:CD	2.75	0.55
1:A:245:ALA:CB	1:A:288:GLN:OE1	2.55	0.55
1:A:329:PHE:CE1	1:A:742:TYR:OH	2.60	0.54
1:A:713:ASN:ND2	1:A:741:TYR:CD2	2.76	0.54
1:A:416:GLN:NE2	1:A:600:SER:OG	2.41	0.54
1:A:224:LYS:NZ	1:A:494:GLU:OE2	2.41	0.53
1:A:520:ARG:NH2	1:A:648:ASP:OD2	2.42	0.53
1:A:557:TYR:CE1	1:A:559:THR:CG2	2.91	0.53
1:A:413:LYS:NZ	1:A:735:GLY:O	2.42	0.52
1:A:94:PHE:CD1	1:A:169:HIS:CD2	2.97	0.52
1:A:537:GLU:OE1	1:A:585:TRP:NE1	2.43	0.52
1:A:384:LYS:O	1:A:385:ALA:C	2.49	0.52
1:A:160:ASN:C	1:A:162:GLN:N	2.64	0.51
1:A:459:ASP:C	1:A:459:ASP:OD2	2.49	0.51
1:A:459:ASP:O	1:A:459:ASP:OD2	2.30	0.50
1:A:571:GLN:CA	1:A:571:GLN:NE2	2.74	0.50
1:A:459:ASP:O	1:A:460:GLY:O	2.30	0.50
1:A:146:PHE:O	1:A:150:THR:OG1	2.30	0.49
1:A:461:LYS:O	1:A:462:THR:CB	2.58	0.49
1:A:343:GLU:OE2	1:A:733:LYS:NZ	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:304:TRP:CE3	1:A:304:TRP:C	2.86	0.49
1:A:246:GLY:C	1:A:247:GLY:O	2.50	0.48
1:A:648:ASP:OD2	1:A:684:TYR:OH	2.31	0.48
1:A:160:ASN:O	1:A:162:GLN:N	2.46	0.48
1:A:745:THR:OG1	1:A:746:GLN:N	2.46	0.47
1:A:471:HIS:NE2	1:A:541:HIS:ND1	2.63	0.46
1:A:319:GLY:O	1:A:320:LYS:C	2.52	0.46
1:A:265:THR:O	1:A:266:ASN:C	2.54	0.46
1:A:406:TYR:N	1:A:737:LYS:O	2.49	0.45
1:A:246:GLY:O	1:A:247:GLY:O	2.35	0.45
1:A:456:THR:O	1:A:457:SER:O	2.35	0.45
1:A:534:GLN:O	1:A:538:THR:CG2	2.65	0.44
1:A:630:SER:CB	1:A:638:PHE:O	2.65	0.44
1:A:502:HIS:ND1	1:A:559:THR:CG2	2.81	0.44
1:A:243:LYS:C	1:A:244:THR:O	2.51	0.44
1:A:686:THR:O	1:A:689:GLU:N	2.50	0.44
1:A:665:THR:N	1:A:666:GLN:NE2	2.66	0.43
1:A:671:GLN:O	1:A:672:GLY:C	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	660/888 (74%)	587 (89%)	52 (8%)	21 (3%)	6 25

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ILE
1	A	320	LYS
1	A	457	SER
1	A	459	ASP
1	A	674	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	145	TYR
1	A	161	GLY
1	A	288	GLN
1	A	460	GLY
1	A	462	THR
1	A	687	VAL
1	A	375	GLU
1	A	584	ASP
1	A	620	CYS
1	A	672	GLY
1	A	211	PRO
1	A	314	ILE
1	A	78	ALA
1	A	292	LYS
1	A	135	ILE
1	A	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	573/760 (75%)	503 (88%)	70 (12%)	7 20

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	115	MET
1	A	119	ASP
1	A	131	LEU
1	A	138	ASP
1	A	145	TYR
1	A	146	PHE
1	A	154	SER
1	A	162	GLN
1	A	170	LEU
1	A	176	LEU
1	A	183	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	207	ASN
1	A	211	PRO
1	A	214	GLN
1	A	220	LEU
1	A	266	ASN
1	A	272	LEU
1	A	275	MET
1	A	314	ILE
1	A	317	ASN
1	A	318	HIS
1	A	320	LYS
1	A	322	GLU
1	A	323	ILE
1	A	326	ARG
1	A	333	TRP
1	A	337	LEU
1	A	359	LEU
1	A	383	ILE
1	A	388	LEU
1	A	401	THR
1	A	438	ASP
1	A	445	LEU
1	A	462	THR
1	A	463	SER
1	A	464	THR
1	A	473	ILE
1	A	475	LYS
1	A	505	ILE
1	A	507	LEU
1	A	512	LEU
1	A	518	LEU
1	A	520	ARG
1	A	530	LEU
1	A	534	GLN
1	A	538	THR
1	A	561	GLN
1	A	574	MET
1	A	594	LYS
1	A	606	MET
1	A	608	THR
1	A	610	SER
1	A	620	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	621	PHE
1	A	638	PHE
1	A	647	ARG
1	A	652	LEU
1	A	661	GLN
1	A	665	THR
1	A	666	GLN
1	A	673	LEU
1	A	679	GLU
1	A	686	THR
1	A	692	GLN
1	A	712	LEU
1	A	720	THR
1	A	721	MET
1	A	726	SER
1	A	743	LEU

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
3	DGT	A	1001	2	33,33,33	1.96	6 (18%)	49,52,52	2.99	14 (28%)

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
3	DGT	A	1001	2	-	0/20/34/34	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	DGT	C6-C5	5.20	1.49	1.41
3	A	1001	DGT	C2-N2	4.90	1.40	1.32
3	A	1001	DGT	C2-N3	4.80	1.39	1.33
3	A	1001	DGT	C5-C4	3.73	1.48	1.40
3	A	1001	DGT	C8-N7	2.88	1.40	1.34
3	A	1001	DGT	PG-O3B	2.31	1.64	1.60

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	DGT	C6-C5-N7	15.28	136.20	134.14
3	A	1001	DGT	N3-C4-N9	5.19	134.52	126.91
3	A	1001	DGT	C5-C4-N3	-4.82	118.96	125.94
3	A	1001	DGT	C2-N3-C4	4.55	121.48	115.09
3	A	1001	DGT	PA-O3A-PB	-4.24	119.25	131.68
3	A	1001	DGT	O3A-PB-O3B	-4.02	93.48	101.66
3	A	1001	DGT	C8-N9-C4	3.66	109.69	106.90
3	A	1001	DGT	C4-C5-N7	-3.55	106.48	109.52
3	A	1001	DGT	O2G-PG-O3G	2.83	119.68	110.44
3	A	1001	DGT	O1B-PB-O3B	2.40	116.53	105.14
3	A	1001	DGT	PB-O3B-PG	-2.36	124.76	131.68
3	A	1001	DGT	O1G-PG-O3G	2.33	118.07	110.44
3	A	1001	DGT	O4'-C1'-N9	-2.17	103.60	107.68
3	A	1001	DGT	O3B-PG-O3G	-2.02	97.22	111.00

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	664/888 (74%)	0.31	58 (8%) 10 13	57, 71, 108, 132	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	665	THR	8.5
1	A	638	PHE	7.4
1	A	291	ASN	7.2
1	A	319	GLY	5.6
1	A	318	HIS	5.5
1	A	77	LEU	5.2
1	A	461	LYS	5.1
1	A	629	TYR	4.9
1	A	138	ASP	4.7
1	A	293	ALA	4.6
1	A	145	TYR	4.5
1	A	320	LYS	4.4
1	A	322	GLU	4.2
1	A	647	ARG	4.2
1	A	460	GLY	3.9
1	A	321	GLU	3.9
1	A	89	GLN	3.8
1	A	746	GLN	3.7
1	A	718	ALA	3.6
1	A	462	THR	3.5
1	A	81	ILE	3.5
1	A	456	THR	3.4
1	A	717	ARG	3.4
1	A	459	ASP	3.4
1	A	153	ARG	3.4
1	A	390	TYR	3.2
1	A	457	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	78	ALA	3.2
1	A	80	ARG	3.1
1	A	129	ASP	3.1
1	A	662	TYR	3.0
1	A	133	SER	3.0
1	A	88	LYS	3.0
1	A	594	LYS	3.0
1	A	146	PHE	2.8
1	A	246	GLY	2.8
1	A	268	THR	2.8
1	A	468	LYS	2.6
1	A	264	GLY	2.6
1	A	85	ASN	2.5
1	A	76	THR	2.5
1	A	126	GLU	2.5
1	A	458	GLU	2.5
1	A	294	PRO	2.4
1	A	630	SER	2.4
1	A	733	LYS	2.4
1	A	610	SER	2.3
1	A	212	LYS	2.3
1	A	657	GLU	2.3
1	A	553	LYS	2.3
1	A	292	LYS	2.3
1	A	720	THR	2.3
1	A	561	GLN	2.3
1	A	160	ASN	2.2
1	A	489	TYR	2.2
1	A	619	GLU	2.2
1	A	628	MET	2.1
1	A	578	LYS	2.1

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	MG	A	2001	1/1	0.22	11.11	64,64,64,64	0
3	DGT	A	1001	31/31	0.17	-0.53	40,43,49,52	0

6.5 Other polymers

There are no such residues in this entry.