



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:14 pm BST

PDB ID : 6LDM  
Title : Structural basis of G-quadruplex DNA recognition by the yeast telomeric protein Rap1  
Authors : Traczyk, A.; Gill, D.J.; Chong, W.L.; Rhodes, D.  
Deposited on : 2019-11-22  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

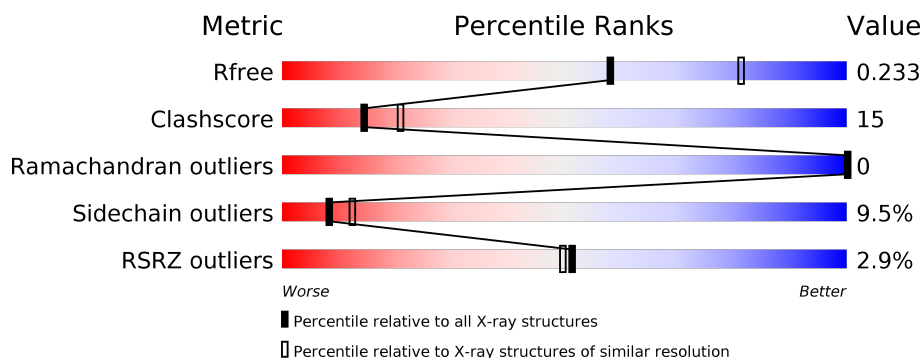
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 respectively. 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	291	<div> <div>2%</div> <div> <div>45%</div> <div>18%</div> <div>•</div> <div>34%</div> </div> </div>
2	B	19	<div> <div>84%</div> <div>5%</div> <div>5%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NA	A	603	-	-	-	X
5	NA	B	107	-	-	-	X
5	NA	B	111	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 2055 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 DNA-binding protein RAP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1598	1014	284	299	1			

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	HIS	-	expression tag	UNP P11938
A	308	HIS	-	expression tag	UNP P11938
A	309	HIS	-	expression tag	UNP P11938
A	310	HIS	-	expression tag	UNP P11938
A	311	HIS	-	expression tag	UNP P11938
A	312	HIS	-	expression tag	UNP P11938
A	313	SER	-	expression tag	UNP P11938
A	314	SER	-	expression tag	UNP P11938
A	315	GLY	-	expression tag	UNP P11938
A	316	LEU	-	expression tag	UNP P11938
A	317	VAL	-	expression tag	UNP P11938
A	318	PRO	-	expression tag	UNP P11938
A	319	ARG	-	expression tag	UNP P11938
A	320	GLY	-	expression tag	UNP P11938
A	321	SER	-	expression tag	UNP P11938
A	322	GLY	-	expression tag	UNP P11938
A	323	MET	-	expression tag	UNP P11938
A	324	LYS	-	expression tag	UNP P11938
A	325	GLU	-	expression tag	UNP P11938
A	326	THR	-	expression tag	UNP P11938
A	327	ALA	-	expression tag	UNP P11938
A	328	ALA	-	expression tag	UNP P11938
A	329	ALA	-	expression tag	UNP P11938
A	330	LYS	-	expression tag	UNP P11938
A	331	PHE	-	expression tag	UNP P11938
A	332	GLU	-	expression tag	UNP P11938
A	333	ARG	-	expression tag	UNP P11938

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	GLN	-	expression tag	UNP P11938
A	335	HIS	-	expression tag	UNP P11938
A	336	MET	-	expression tag	UNP P11938
A	337	ASP	-	expression tag	UNP P11938
A	338	SER	-	expression tag	UNP P11938
A	339	PRO	-	expression tag	UNP P11938
A	340	ASP	-	expression tag	UNP P11938
A	341	LEU	-	expression tag	UNP P11938
A	342	GLY	-	expression tag	UNP P11938
A	343	THR	-	expression tag	UNP P11938
A	344	GLY	-	expression tag	UNP P11938
A	345	SER	-	expression tag	UNP P11938
A	346	GLU	-	expression tag	UNP P11938
A	347	ASN	-	expression tag	UNP P11938
A	348	LEU	-	expression tag	UNP P11938
A	349	TYR	-	expression tag	UNP P11938
A	350	PHE	-	expression tag	UNP P11938
A	351	GLN	-	expression tag	UNP P11938
A	352	GLY	-	expression tag	UNP P11938
A	?	-	GLU	deletion	UNP P11938

- Molecule 2 is a DNA chain called G-guadruplex DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	P	0	0	0
			384	180	72	114	18			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	8	Total	Na	0	0
			8	8		
5	A	3	Total	Na	0	0
			3	3		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	5	Total	K	0	0
			5	5		

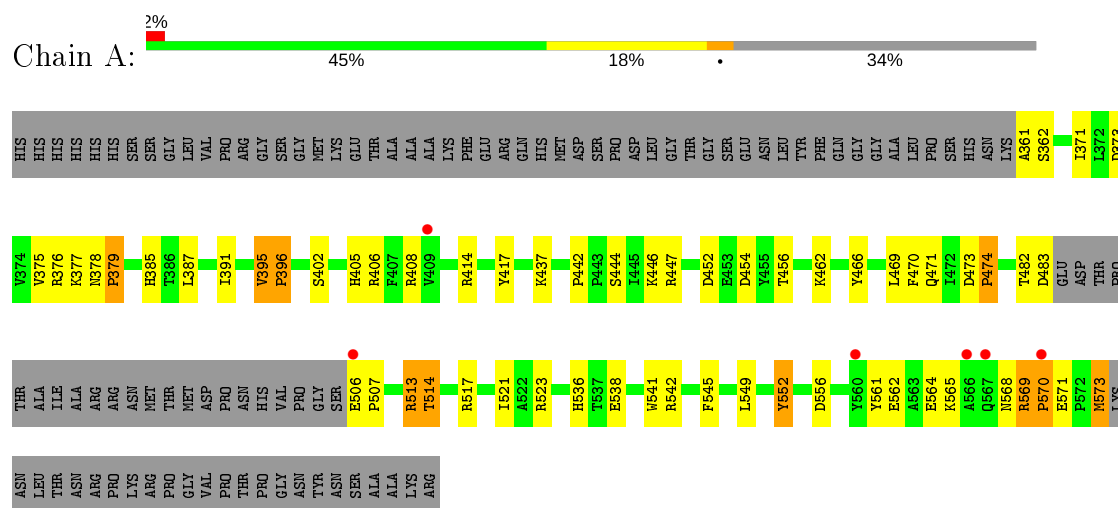
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	28	Total	O	0	0
			28	28		
7	B	15	Total	O	0	0
			15	15		

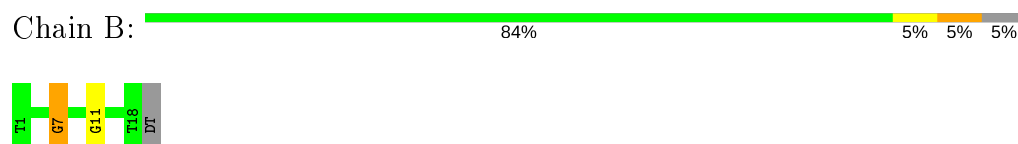
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: DNA-binding protein RAP1



- Molecule 2: G-guadruplex DNA





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.68Å 70.20Å 64.85Å 90.00° 97.72° 90.00°	Depositor
Resolution (Å)	35.09 – 2.40 32.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (35.09-2.40) 98.9 (32.13-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, $R_{free}$	0.203 , 0.233 0.218 , 0.233	Depositor DCC
$R_{free}$ test set	737 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.0	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, TRS, K, NA

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	0.94	8/1639 (0.5%)	0.82	4/2216 (0.2%)
2	B	1.10	1/431 (0.2%)	0.98	1/668 (0.1%)
All	All	0.97	9/2070 (0.4%)	0.86	5/2884 (0.2%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	570	PRO	N-CA	13.08	1.69	1.47
1	A	474	PRO	N-CA	13.00	1.69	1.47
1	A	396	PRO	N-CA	12.79	1.69	1.47
1	A	379	PRO	N-CA	12.78	1.69	1.47
1	A	569	ARG	C-N	5.92	1.45	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	PRO	CA-N-CD	-7.98	100.33	111.50
1	A	570	PRO	CA-N-CD	-7.67	100.77	111.50
1	A	474	PRO	CA-N-CD	-7.46	101.05	111.50
1	A	396	PRO	CA-N-CD	-7.30	101.28	111.50
2	B	7	DG	O4'-C4'-C3'	-5.76	102.20	104.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	1598	0	1520	56	0
2	B	384	0	205	2	0
3	A	6	0	8	1	0
4	A	8	0	12	1	0
5	A	3	0	0	0	0
5	B	8	0	0	0	0
6	B	5	0	0	0	0
7	A	28	0	0	1	0
7	B	15	0	0	0	0
All	All	2055	0	1745	58	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 15.

The worst 5 of 58 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:396:PRO:N	1:A:396:PRO:CA	1.69	1.41
1:A:379:PRO:N	1:A:379:PRO:CA	1.69	1.41
1:A:570:PRO:CA	1:A:570:PRO:N	1.69	1.41
1:A:474:PRO:N	1:A:474:PRO:CA	1.69	1.40
1:A:552:TYR:HB3	1:A:573:MET:HE1	1.42	0.99

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	187/291 (64%)	176 (94%)	11 (6%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	168/253 (66%)	152 (90%)	16 (10%)	<b>8</b> <b>12</b>

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	513	ARG
1	A	514	THR
1	A	552	TYR
1	A	483	ASP
1	A	556	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	471	GLN

### 5.3.3 RNA [i](#)

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

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 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	GOL	A	601	-	5,5,5	0.09	0	5,5,5	0.17	0
4	TRS	A	602	-	7,7,7	0.46	0	9,9,9	0.74	0

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	GOL	A	601	-	-	2/4/4/4	-
4	TRS	A	602	-	-	3/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	TRS	C3-C-C1-O1
3	A	601	GOL	O1-C1-C2-C3
4	A	602	TRS	C2-C-C1-O1
4	A	602	TRS	N-C-C1-O1
3	A	601	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	GOL	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	TRS	1	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, 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	191/291 (65%)	0.01	6 (3%) 49 47	46, 73, 109, 126	0
2	B	18/19 (94%)	0.18	0 100 100	56, 69, 106, 122	0
All	All	209/310 (67%)	0.03	6 (2%) 51 50	46, 72, 109, 126	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	567	GLN	3.4
1	A	506	GLU	2.9
1	A	570	PRO	2.7
1	A	566	ALA	2.5
1	A	560	TYR	2.3

### 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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	601	6/6	0.48	0.26	121,122,122,122	0
5	NA	A	603	1/1	0.61	0.55	92,92,92,92	0
5	NA	B	107	1/1	0.71	0.56	82,82,82,82	0
6	K	B	105	1/1	0.78	0.08	104,104,104,104	0
5	NA	B	111	1/1	0.80	0.44	85,85,85,85	0
5	NA	B	113	1/1	0.82	0.43	75,75,75,75	0
5	NA	B	112	1/1	0.84	1.04	92,92,92,92	0
5	NA	A	604	1/1	0.85	0.39	63,63,63,63	0
5	NA	B	108	1/1	0.88	0.94	79,79,79,79	0
4	TRS	A	602	8/8	0.89	0.21	55,56,58,59	0
5	NA	B	106	1/1	0.89	0.42	66,66,66,66	0
5	NA	A	605	1/1	0.90	0.64	79,79,79,79	0
5	NA	B	110	1/1	0.95	0.40	87,87,87,87	0
6	K	B	104	1/1	0.95	0.06	97,97,97,97	0
6	K	B	101	1/1	0.96	0.10	51,51,51,51	0
5	NA	B	109	1/1	0.97	0.38	73,73,73,73	0
6	K	B	103	1/1	0.97	0.09	45,45,45,45	1
6	K	B	102	1/1	0.97	0.08	48,48,48,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.