



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 11:26 AM UTC

PDB ID : 2MS6 / pdb_00002ms6
BMRB ID : 25107
Title : Human Telomeric G-quadruplex DNA sequence (TTAGGGT)₄ complexed with Flavonoid Quercetin
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Deposited on : 2014-07-24

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 10%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

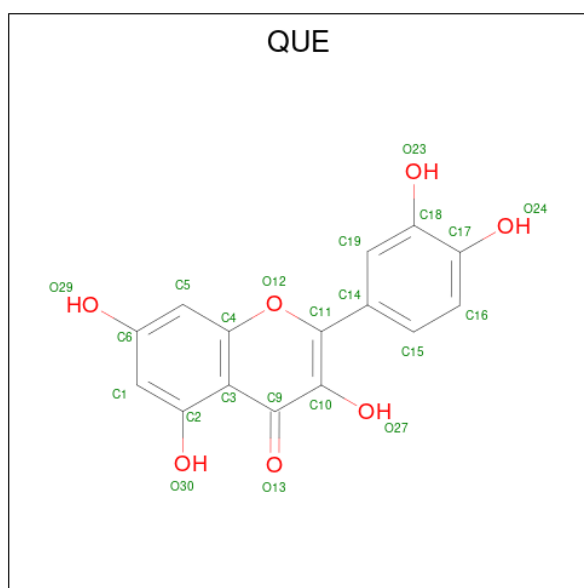
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 968 atoms, of which 348 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA_(5'-D(*TP*TP*AP*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
1	A	7	226	70	82	26	42	6	0
1	B	7	226	70	82	26	42	6	0
1	C	7	226	70	82	26	42	6	0
1	D	7	226	70	82	26	42	6	0

- Molecule 2 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (CCD ID: QUE) (formula: C₁₅H₁₀O₇).



Mol	Chain	Residues	Atoms			
			Total	C	H	O
2	C	1	32	15	10	7
2	D	1	32	15	10	7

4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: DNA_ (5'-D(*TP*TP*AP*GP*GP*GP*T)-3')

Chain A:  57% 43%



- Molecule 1: DNA_ (5'-D(*TP*TP*AP*GP*GP*GP*T)-3')

Chain B:  43% 57%



- Molecule 1: DNA_ (5'-D(*TP*TP*AP*GP*GP*GP*T)-3')

Chain C:  43% 57%



- Molecule 1: DNA_ (5'-D(*TP*TP*AP*GP*GP*GP*T)-3')

Chain D:  71% 29%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 1 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Discover	structure solution	
Discover	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	61
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	100%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 10% for the well-defined parts and 10% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	61
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 10%, i.e. 54 atoms were assigned a chemical shift out of a possible 548. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	43/336 (13%)	43/196 (22%)	0/140 (0%)	0/0 (—%)
Base	11/212 (5%)	11/128 (9%)	0/44 (0%)	0/40 (0%)
Overall	54/548 (10%)	54/324 (17%)	0/184 (0%)	0/40 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 54 atoms were assigned a chemical shift out of a possible 548. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Sugar	43/336 (13%)	43/196 (22%)	0/140 (0%)	0/0 (—%)
Base	11/212 (5%)	11/128 (9%)	0/44 (0%)	0/40 (0%)
Overall	54/548 (10%)	54/324 (17%)	0/184 (0%)	0/40 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins