



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 6FY7
Title : Concerted dynamics of metallo-base pairs in an A/B-form helical transition (minor species)
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This is a wwPDB NMR 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

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

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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

2 Ensemble composition and analysis

This entry contains 20 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 882 atoms, of which 316 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(*CP*GP*TP*CP*TP*CP*AP*TP*GP*AP*TP*AP*CP*G)-3')_minor.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
1	A	14	Total	C	H	N	O	P	0
			440	136	158	50	83	13	
1	B	14	Total	C	H	N	O	P	0
			440	136	158	50	83	13	

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).


Mol	Chain	Residues	Atoms	
2	A	2	Total	Hg
			2	2

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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(*CP*GP*TP*CP*TP*CP*AP*TP*GP*AP*TP*AP*CP*G)-3')_minor

Chain A:  79% 21%



- Molecule 1: DNA (5'-D(*CP*GP*TP*CP*TP*CP*AP*TP*GP*AP*TP*AP*CP*G)-3')_minor


Chain B:  71% 29%



4.2 Residue scores for the representative (author defined) model from the NMR ensemble


The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: DNA (5'-D(*CP*GP*TP*CP*TP*CP*AP*TP*GP*AP*TP*AP*CP*G)-3')_minor

Chain A:  79% 21%



- Molecule 1: DNA (5'-D(*CP*GP*TP*CP*TP*CP*AP*TP*GP*AP*TP*AP*CP*G)-3')_minor

Chain B:  79% 21%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 20 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
Xplor-NIH	refinement	2.46
Xplor-NIH	structure calculation	2.46

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	150
Number of shifts mapped to atoms	150
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	23%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
HG

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	282	158	158	7±4
1	B	282	158	158	8±4
All	All	11320	6320	6320	241

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 14.

5 of 76 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:15:DC:HO5'	1:B:15:DC:H6	0.89	0.90	14	10
1:A:1:DC:H6	1:A:1:DC:HO5'	0.88	0.90	14	6
1:A:1:DC:HO5'	1:A:1:DC:H6	0.87	0.88	16	8
1:B:15:DC:H6	1:B:15:DC:HO5'	0.85	1.14	6	3
1:A:3:DT:C4	1:A:4:DC:N4	0.77	2.53	10	3

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 23% for the well-defined parts and 23% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *chemical_shifts_minor_2_sr_adjusted_converted*

7.1.1 Bookkeeping [i](#)

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	150
Number of shifts mapped to atoms	150
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 [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 23%, i.e. 126 atoms were assigned a chemical shift out of a possible 550. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	126/550 (23%)	126/326 (39%)	0/190 (0%)	0/34 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (chemical_shifts_minor_2_sr_adjusted_converted). RCI is only applicable to proteins.