Mandatory tags (not three tags that should not be mandatory in Chemical shift referencing section)

Section

Field Tag

-------------------------------------------------------------------------------

Sample

Sample label

Sample type

Concentration value \_pdbx\_nmr\_exptl\_sample.concentration

|  |
| --- |
|  |

Sample conditions

pH

pH units

|  |
| --- |
| \_pdbx\_nmr\_exptl\_sample\_conditions.pH\_units |

Temperature

Temperature units

|  |
| --- |
| \_pdbx\_nmr\_exptl\_sample\_conditions.temperature\_units |

Software

Software Authors or vendor

|  |
| --- |
| \_pdbx\_nmr\_software.authors |

Chemical shift referencing

Referencing method

Referencing type

Indirect ratio

|  |
| --- |
| \_pdbx\_nmr\_chem\_shift\_ref.indirect\_shift\_ratio |

**Should not be mandatory**

Offset type

Affected atom type

Offset value

Chemical shift connection

Assigned chemical shift list label

Spectral peak lists

Sweep width

NMR constraints

Constraint file name

|  |
| --- |
| \_pdbx\_nmr\_constraint\_file.constraint\_filename |

Software file format

|  |
| --- |
| \_pdbx\_nmr\_constraint\_file.software\_name |

Number of constraints of this kind in the file

|  |
| --- |
| \_pdbx\_nmr\_constraint\_file.constraint\_number |

NMR refinement and conformer statistics

Total number of conformers calculated

|  |
| --- |
| \_pdbx\_nmr\_ensemble.conformers\_calculated\_total\_number |

Number of conformers submitted

|  |
| --- |
| \_pdbx\_nmr\_ensemble.conformers\_submitted\_total\_number |

Conformer selection criteria

|  |
| --- |
| \_pdbx\_nmr\_ensemble.conformer\_selection\_criteria |

Representative conformer

|  |
| --- |
| \_pdbx\_nmr\_ensemble.representative\_conformer |

Representative conformer selection criteria

|  |
| --- |
| \_pdbx\_nmr\_representative.selection\_criteria |

Refinement method

|  |
| --- |
| \_pdbx\_nmr\_refine.method |