Full wwPDB NMR Structure Validation Report

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PDB ID	:	2M6E
Title	:	NMR solution structure of cis (minor) form of In936 in Methanol
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Deposited on	:	2013-03-29

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 (i) 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 (i)) were used in the production of this report:

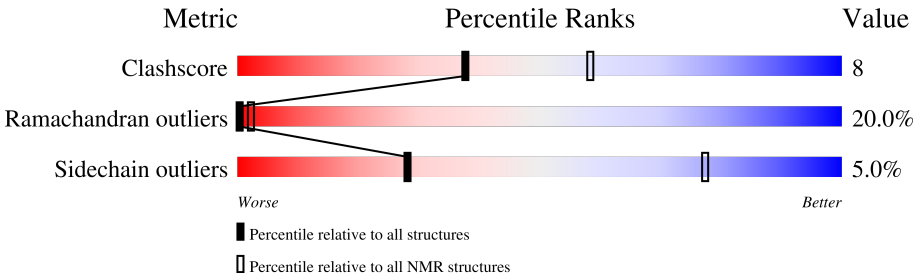
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.29
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 62%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	8	62% 38%

2 Ensemble composition and analysis (i)

This entry contains 10 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (6) was below the domain threshold value (8).

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 121 atoms, of which 57 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Contryphan-In.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	8	121	44	57	9	9	2	0

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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: Contryphan-In

Chain A: 

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Contryphan-In

Chain A: 

4.2.2 Score per residue for model 2

• Molecule 1: Contryphan-In

Chain A: 

4.2.3 Score per residue for model 3

• Molecule 1: Contryphan-In

Chain A: 

4.2.4 Score per residue for model 4

• Molecule 1: Contryphan-In

Chain A: 

4.2.5 Score per residue for model 5

• Molecule 1: Contryphan-In

Chain A: 

4.2.6 Score per residue for model 6

• Molecule 1: Contryphan-In

Chain A: 

4.2.7 Score per residue for model 7

• Molecule 1: Contryphan-In

Chain A: 

4.2.8 Score per residue for model 8

• Molecule 1: Contryphan-In

Chain A: 

4.2.9 Score per residue for model 9

• Molecule 1: Contryphan-In

Chain A: 

4.2.10 Score per residue for model 10

• Molecule 1: Contryphan-In

Chain A: 

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 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
CYANA	structure solution	3
CYANA	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	63
Number of shifts mapped to atoms	63
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	62%

6 Model quality

6.1 Standard geometry

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

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

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	64	57	58	1±0
All	All	640	570	598	10

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 8.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:TYR:HA	1:A:6:PRO:C	0.47	2.30	6	10

6.3 Torsion angles

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	5/8 (62%)	4±0 (80±0%)	0±0 (0±0%)	1±0 (20±0%)	0 2
All	All	50/80 (62%)	40 (80%)	0 (0%)	10 (20%)	0 2

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	3	VAL	10

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	6/6 (100%)	6±0 (95±8%)	0±0 (5±8%)	28 77
All	All	60/60 (100%)	57 (95%)	3 (5%)	28 77

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	7	TRP	3

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 62% for the well-defined parts and 62% 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	63
Number of shifts mapped to atoms	63
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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 62%, i.e. 50 atoms were assigned a chemical shift out of a possible 80. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	12/33 (36%)	11/13 (85%)	1/14 (7%)	0/6 (0%)
Sidechain	19/27 (70%)	16/17 (94%)	3/10 (30%)	0/0 (—%)
Aromatic	19/20 (95%)	10/10 (100%)	9/9 (100%)	0/1 (0%)
Overall	50/80 (62%)	37/40 (92%)	13/33 (39%)	0/7 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 62%, i.e. 50 atoms were assigned a chemical shift out of a possible 80. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	12/33 (36%)	11/13 (85%)	1/14 (7%)	0/6 (0%)
Sidechain	19/27 (70%)	16/17 (94%)	3/10 (30%)	0/0 (—%)
Aromatic	19/20 (95%)	10/10 (100%)	9/9 (100%)	0/1 (0%)
Overall	50/80 (62%)	37/40 (92%)	13/33 (39%)	0/7 (0%)

7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	6	PRO	CG	21.46	32.66 – 21.76	-5.3
1	A	6	PRO	HG3	0.20	3.56 – 0.26	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.