



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 26, 2016 – 09:14 PM BST

PDB ID : 2GLH
Title : Solution Conformation of Salmon Calcitonin in Sodium Dodecyl Sulfate Micelles
Authors : Andreotti, G.; Lopez-Mendez, B.; Amodeo, P.; Morelli, M.A.; Nakamuta, H.; Motta, A.
Deposited on : 2006-04-04

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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Percentile statistics : **NOT EXECUTED**
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

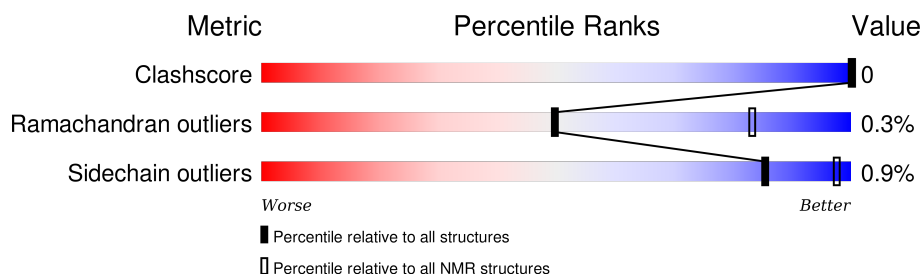
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	33	<div> <div style="width: 33%; background-color: red;"></div> <div style="width: 67%; background-color: cyan;"></div> </div> <div> <div style="width: 33%;"></div> <div style="width: 67%;"></div> </div>

2 Ensemble composition and analysis

This entry contains 100 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 82 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:13 (11)	0.12	82

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 13 clusters and 13 single-model clusters were found.

Cluster number	Models
1	14, 18, 22, 24, 25, 26, 27, 34, 35, 40, 42, 43, 44, 45, 47, 48, 49, 51, 56, 65, 66, 69, 71, 77, 85, 89, 90
2	16, 20, 23, 33, 46, 53, 54, 55, 63, 70, 72, 73, 79, 81, 82, 83, 87, 94, 97
3	4, 5, 6, 7, 8, 11, 15, 19, 30, 31, 84
4	52, 58, 59, 64, 93
5	37, 39, 41, 91
6	32, 74, 86, 95
7	96, 98, 100
8	67, 68, 80
9	3, 10, 12
10	60, 61
11	29, 76
12	57, 62
13	2, 9
Single-model clusters	1; 13; 17; 21; 28; 36; 38; 50; 75; 78; 88; 92; 99

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 480 atoms, of which 241 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcitonin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	33	Total	C	H	N	O	S	1
			480	145	241	44	48	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: Calcitonin-1



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

The representative model is number 82. Colouring as in section 4.1 above.

- Molecule 1: Calcitonin-1



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *restrained simulated annealing/energy minimization followed by unrestrained molecular dynamics*.

Of the 100 calculated structures, 100 were deposited, based on the following criterion: *periodically sampled unrestrained molecular dynamics structures*.

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

Software name	Classification	Version
AMBER	structure solution	6.0
AMBER	refinement	6.0

No chemical shift data was provided. 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: NH2

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
All	All	7700	8500	8500	-

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 -.

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 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 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	11/33 (33%)	11±0 (97±4%)	0±0 (3±4%)	0±0 (0±2%)	50	83
All	All	1100/3300 (33%)	1069 (97%)	28 (3%)	3 (0%)	50	83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	4	LEU	3

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	10/29 (34%)	10±0 (99±3%)	0±0 (1±3%)	85	97
All	All	1000/2900 (34%)	991 (99%)	9 (1%)	85	97

All 4 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	6	THR	4
1	A	13	SER	2
1	A	4	LEU	2
1	A	9	LEU	1

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](#)

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

No chemical shift data were provided