



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1B4M
Title : NMR STRUCTURE OF APO CELLULAR RETINOL-BINDING PROTEIN II, 24 STRUCTURES
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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

<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
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

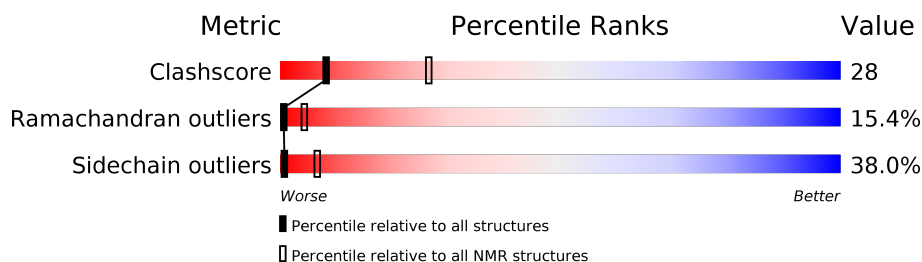
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

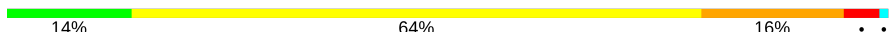
The overall completeness of chemical shifts assignment was not calculated.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	134	

2 Ensemble composition and analysis

This entry contains 24 models. Model 12 is the overall representative, medoid model (most similar to other models).

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:134 (132)	0.65	12

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 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	4, 6, 8, 11, 12, 15, 17, 21, 24
2	1, 2, 3, 5, 7, 10, 14, 18, 23
3	9, 19, 22
4	13, 20
Single-model clusters	16

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2168 atoms, of which 1073 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CELLULAR RETINOL-BINDING PROTEIN II.

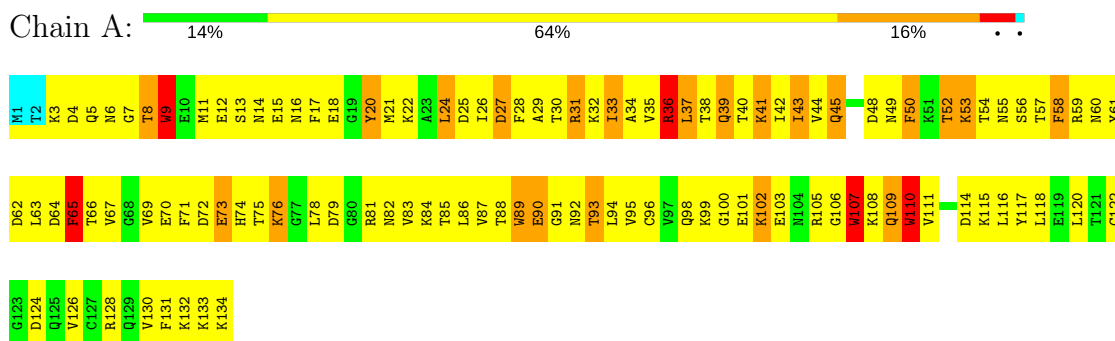
Mol	Chain	Residues	Atoms						Trace
1	A	134	Total	C	H	N	O	S	0
			2168	686	1073	189	214	6	

4 Residue-property plots

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.

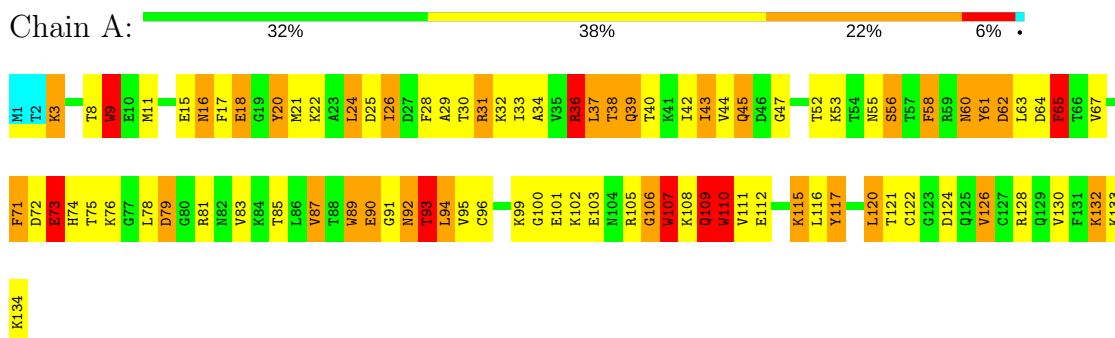
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



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

The representative model is number 12. Colouring as in section 4.1 above.

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING REFINEMENT*.

Of the 25 calculated structures, 24 were deposited, based on the following criterion: *FINAL PENALTY FUNCTION VALUES WITHIN 2 STANDARD DEVIATIONS FROM THE MEAN*.

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

Software name	Classification	Version
TINKER	refinement	
TINKER	structure solution	

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](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.07±0.01	6±1/1098 (0.6±0.1%)	2.28±0.05	48±4/1474 (3.3±0.2%)
All	All	1.07	145/26352 (0.6%)	2.29	1161/35376 (3.3%)

5 of 9 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	110	TRP	CD2-CE2	-7.11	1.32	1.41	13	22
1	A	110	TRP	CG-CD2	-6.83	1.32	1.43	23	18
1	A	107	TRP	CD2-CE2	-6.82	1.33	1.41	15	24
1	A	9	TRP	CD2-CE2	-6.75	1.33	1.41	2	17
1	A	89	TRP	CD2-CE2	-6.53	1.33	1.41	21	24

5 of 188 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	105	ARG	NE-CZ-NH1	23.54	132.07	120.30	22	9
1	A	9	TRP	CD1-CG-CD2	-14.72	94.52	106.30	16	24
1	A	89	TRP	CD1-CG-CD2	14.71	118.07	106.30	7	24
1	A	89	TRP	CG-CD1-NE1	-14.30	95.80	110.10	24	24
1	A	128	ARG	NE-CZ-NH1	14.08	127.34	120.30	6	13

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	1080	1055	1054	59±10
All	All	25920	25320	25296	1409

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 28.

5 of 735 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:HD11	1:A:107:TRP:CZ2	1.01	1.91	7	6
1:A:37:LEU:HD11	1:A:58:PHE:CE1	1.00	1.91	19	3
1:A:24:LEU:HD11	1:A:79:ASP:HB2	0.98	1.34	20	1
1:A:37:LEU:HD21	1:A:58:PHE:CE2	0.97	1.93	9	2
1:A:65:PHE:CD1	1:A:87:VAL:HG21	0.92	2.00	5	3

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	131/134 (98%)	78±4 (60±3%)	33±3 (25±3%)	20±3 (15±3%)	1	4
All	All	3144/3216 (98%)	1872 (60%)	788 (25%)	484 (15%)	1	4

5 of 85 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	111	VAL	20
1	A	36	ARG	17
1	A	25	ASP	15
1	A	126	VAL	15
1	A	12	GLU	14

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	118/120 (98%)	73±4 (62±3%)	45±4 (38±3%)	1	6
All	All	2832/2880 (98%)	1756 (62%)	1076 (38%)	1	6

5 of 111 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	9	TRP	24
1	A	52	THR	24
1	A	120	LEU	24
1	A	31	ARG	22
1	A	102	LYS	21

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided