



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2JZB  
Title : Solution structure of the complex between E.coli NusA-AR2 and RNAP-aCTD  
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Deposited on : 2008-01-02

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

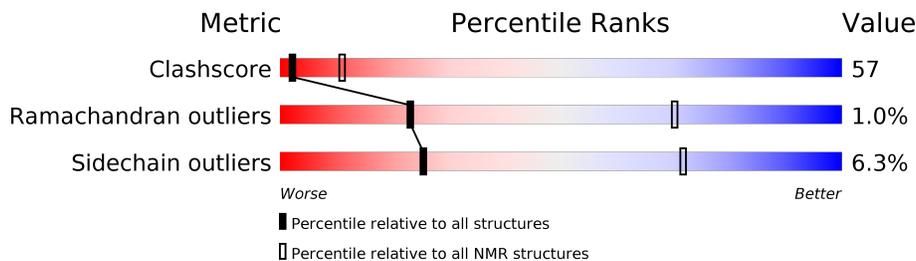
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 81%.

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  $\geq 3$ , 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	99	
2	B	74	

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:249-A:326, B:428-B:492 (143)	0.67	4

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 3 clusters and 3 single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2309 atoms, of which 1155 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	81	1287	400	655	108	122	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	GLY	-	EXPRESSION TAG	UNP P0A7Z4
A	232	PRO	-	EXPRESSION TAG	UNP P0A7Z4

- Molecule 2 is a protein called Transcription elongation protein nusA.

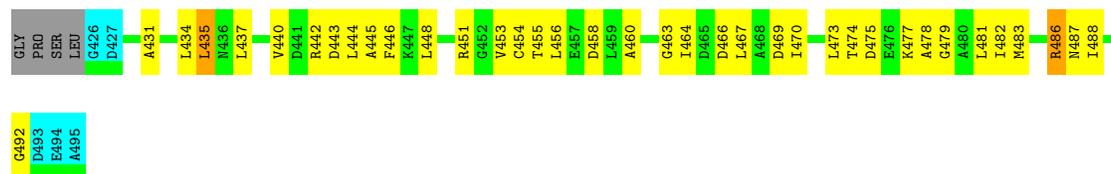
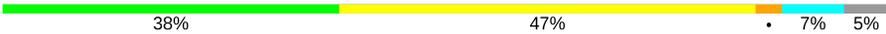
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	70	1022	321	500	87	111	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	422	GLY	-	EXPRESSION TAG	UNP P0AFF6
B	423	PRO	-	EXPRESSION TAG	UNP P0AFF6



## ● Molecule 2: Transcription elongation protein nusA

Chain B: 

## 5 Refinement protocol and experimental data overview

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

Of the 240 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
X-PLOR NIH	structure solution	
X-PLOR NIH	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)	BMRB entry 15614
Number of chemical shift lists	1
Total number of shifts	1886
Number of shifts mapped to atoms	1886
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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](#)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	5.0±0.0
2	B	0.0±0.0	2.7±0.5
All	All	0	154

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

5 of 8 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	255	ARG	Sidechain	20
1	A	317	ARG	Sidechain	20
1	A	284	ARG	Sidechain	20
1	A	310	ARG	Sidechain	20
1	A	265	ARG	Sidechain	20

### 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	609	640	639	80±8
2	B	487	478	478	56±7
All	All	21920	22360	22340	2503

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 57.

5 of 908 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:437:LEU:HD22	2:B:456:LEU:HD11	1.10	1.23	4	4
2:B:467:LEU:HD12	2:B:478:ALA:HB1	1.07	1.25	12	10
2:B:444:LEU:HD11	2:B:473:LEU:HD21	1.06	1.28	7	8
1:A:252:ILE:HD13	1:A:312:LEU:HD22	1.05	1.23	6	2
1:A:306:VAL:HG11	1:A:312:LEU:HD21	1.04	1.26	7	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	77/99 (78%)	70±1 (91±2%)	6±1 (7±2%)	1±1 (2±1%)	14	57
2	B	65/74 (88%)	63±1 (97±2%)	2±1 (3±2%)	0±0 (0±0%)	100	100
All	All	2840/3460 (82%)	2664 (94%)	148 (5%)	28 (1%)	23	70

All 4 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	321	TRP	18
1	A	262	LEU	5
1	A	322	PRO	3
1	A	313	SER	2

### 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	69/88 (78%)	64±2 (93±2%)	5±2 (7±2%)	22	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	49/55 (89%)	46±1 (95±2%)	3±1 (5±2%)	30 76
All	All	2360/2860 (83%)	2211 (94%)	149 (6%)	25 72

5 of 25 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)
2	B	455	THR	20
1	A	257	VAL	20
1	A	313	SER	13
2	B	435	LEU	12
1	A	312	LEU	11

### 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 81% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 15614

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 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	1886
Number of shifts mapped to atoms	1886
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](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	167	$-0.19 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	156	$0.14 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	159	$0.76 \pm 0.29$	Should be applied

#### 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 81%, i.e. 1391 atoms were assigned a chemical shift out of a possible 1720. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	557/703 (79%)	279/280 (100%)	141/286 (49%)	137/137 (100%)
Sidechain	792/951 (83%)	488/549 (89%)	296/362 (82%)	8/40 (20%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	42/66 (64%)	24/35 (69%)	16/28 (57%)	2/3 (67%)
Overall	1391/1720 (81%)	791/864 (92%)	453/676 (67%)	147/180 (82%)

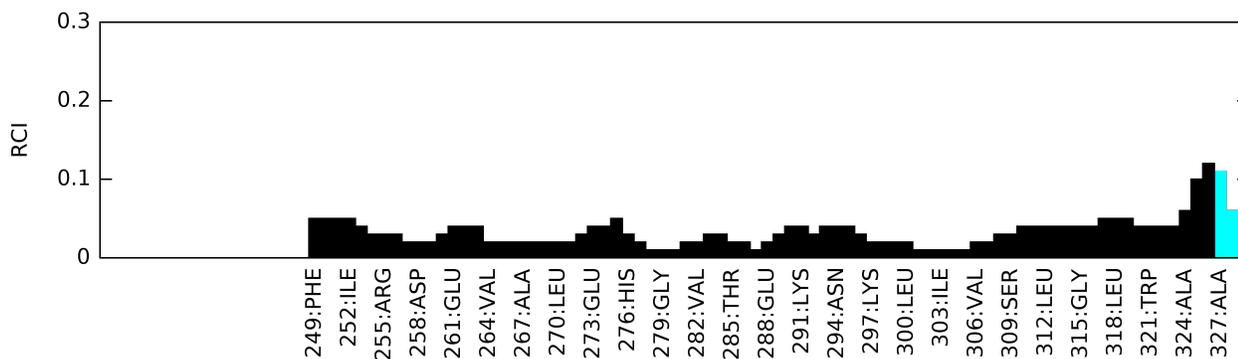
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

