



# Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 06:39 am BST

PDB ID : 5B88  
Title : RRM-like domain of DEAD-box protein, CsdA  
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Deposited on : 2016-06-13

This is a Full wwPDB NMR Structure Validation 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

<https://www.wwpdb.org/validation/2017/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 : 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 : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

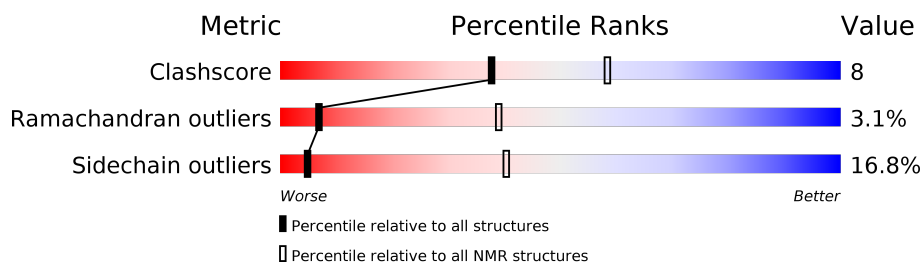
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 68%.

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  $\geq 3$ , 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	85	<div>67%28%...</div>

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:482-A:564 (83)	0.16	2

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 5 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1321 atoms, of which 662 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ATP-dependent RNA helicase DeaD.

Mol	Chain	Residues	Atoms						Trace
1	A	85	Total	C	H	N	O	S	0
			1321	410	662	120	124	5	

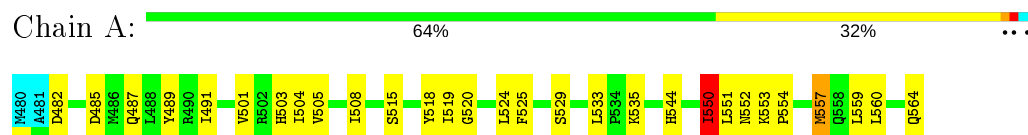
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	480	MET	-	expression tag	UNP P0A9P6
A	481	ALA	-	expression tag	UNP P0A9P6



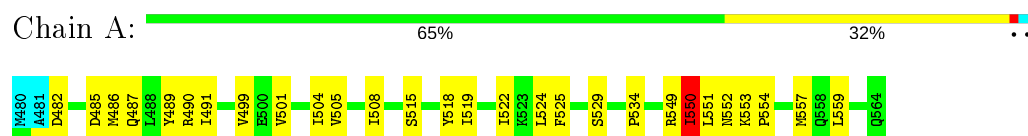
### 4.2.3 Score per residue for model 3

- Molecule 1: ATP-dependent RNA helicase DeaD



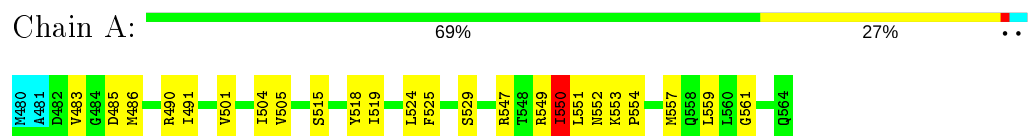
### 4.2.4 Score per residue for model 4

- Molecule 1: ATP-dependent RNA helicase DeaD



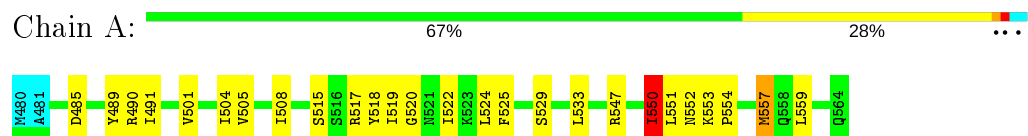
### 4.2.5 Score per residue for model 5

- Molecule 1: ATP-dependent RNA helicase DeaD



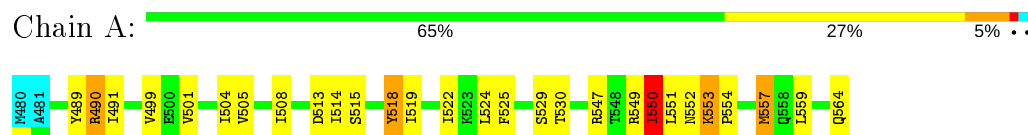
### 4.2.6 Score per residue for model 6

- Molecule 1: ATP-dependent RNA helicase DeaD



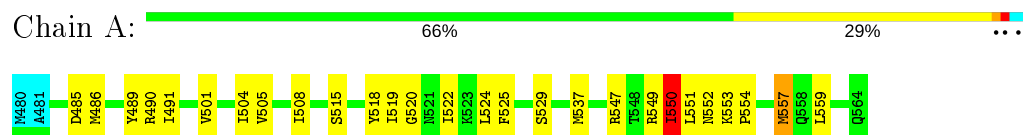
### 4.2.7 Score per residue for model 7

- Molecule 1: ATP-dependent RNA helicase DeaD



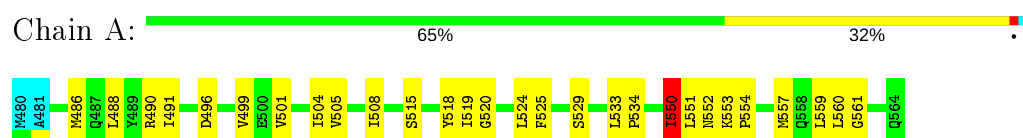
### 4.2.8 Score per residue for model 8

- Molecule 1: ATP-dependent RNA helicase DeaD



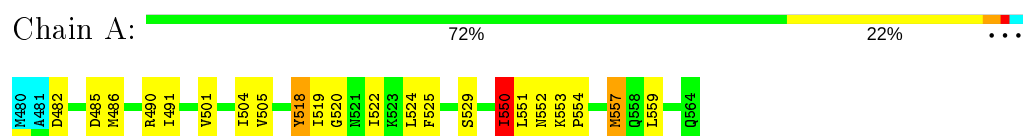
### 4.2.9 Score per residue for model 9

- Molecule 1: ATP-dependent RNA helicase DeaD



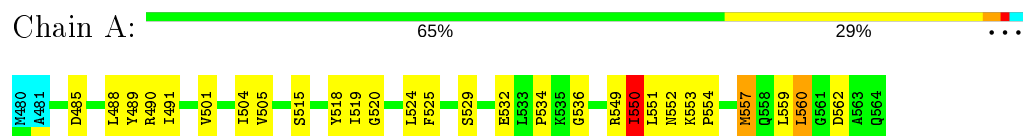
### 4.2.10 Score per residue for model 10

- Molecule 1: ATP-dependent RNA helicase DeaD



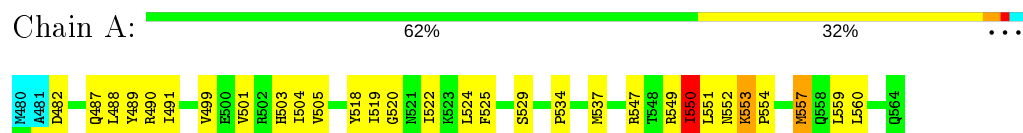
### 4.2.11 Score per residue for model 11

- Molecule 1: ATP-dependent RNA helicase DeaD



### 4.2.12 Score per residue for model 12

- Molecule 1: ATP-dependent RNA helicase DeaD

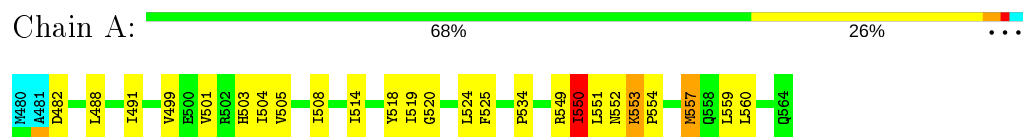






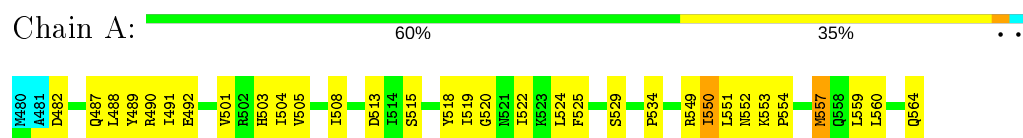
#### 4.2.18 Score per residue for model 18

- Molecule 1: ATP-dependent RNA helicase DeaD



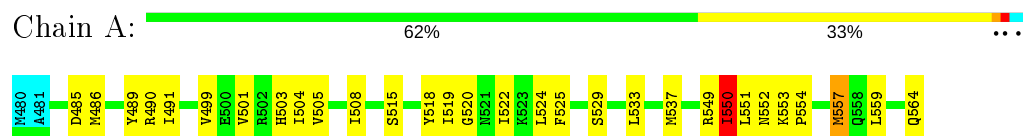
#### 4.2.19 Score per residue for model 19

- Molecule 1: ATP-dependent RNA helicase DeaD



#### 4.2.20 Score per residue for model 20

- Molecule 1: ATP-dependent RNA helicase DeaD



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	3.0

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	714
Number of shifts mapped to atoms	714
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	68%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

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	646	648	648	10±2
All	All	12920	12960	12960	209

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:488:LEU:HD23	1:A:560:LEU:HD21	0.62	1.70	18	7
1:A:505:VAL:HG13	1:A:519:ILE:CD1	0.61	2.25	17	20
1:A:503:HIS:CE1	1:A:551:LEU:HD11	0.60	2.31	18	5
1:A:508:ILE:HD13	1:A:533:LEU:HD11	0.56	1.75	9	6
1:A:508:ILE:HD11	1:A:519:ILE:HD11	0.56	1.77	13	6
1:A:505:VAL:HG13	1:A:519:ILE:HD13	0.55	1.79	7	11
1:A:499:VAL:HG23	1:A:551:LEU:HD13	0.55	1.77	12	7
1:A:489:TYR:CE2	1:A:559:LEU:HD23	0.53	2.39	13	1
1:A:491:ILE:HG22	1:A:557:MET:HB3	0.53	1.80	18	18
1:A:501:VAL:HG22	1:A:524:LEU:HB2	0.50	1.82	5	20
1:A:487:GLN:OE1	1:A:559:LEU:HD11	0.50	2.06	19	3
1:A:499:VAL:HG13	1:A:524:LEU:HD21	0.48	1.83	17	2
1:A:550:ILE:HG23	1:A:552:ASN:H	0.48	1.69	9	20
1:A:519:ILE:CG2	1:A:522:ILE:HD11	0.48	2.39	4	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:508:ILE:HD11	1:A:519:ILE:CD1	0.47	2.39	17	4
1:A:553:LYS:HB3	1:A:554:PRO:HD2	0.47	1.86	16	20
1:A:488:LEU:HD23	1:A:560:LEU:HD11	0.46	1.88	13	1
1:A:487:GLN:OE1	1:A:559:LEU:HD21	0.46	2.11	12	1
1:A:559:LEU:C	1:A:559:LEU:HD13	0.43	2.34	1	9
1:A:487:GLN:NE2	1:A:559:LEU:HD21	0.43	2.29	13	1
1:A:559:LEU:HD13	1:A:559:LEU:C	0.43	2.34	15	8
1:A:550:ILE:O	1:A:551:LEU:C	0.42	2.57	13	20
1:A:490:ARG:HB3	1:A:530:THR:HG22	0.42	1.91	7	1
1:A:487:GLN:NE2	1:A:559:LEU:HD11	0.42	2.29	13	1
1:A:559:LEU:HD11	1:A:561:GLY:O	0.41	2.15	17	3
1:A:508:ILE:CD1	1:A:514:ILE:HG21	0.41	2.46	7	2
1:A:487:GLN:CD	1:A:559:LEU:HD21	0.41	2.35	3	1

## 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	82/85 (96%)	63±2 (76±2%)	17±2 (21±2%)	3±1 (3±1%)	7	39
All	All	1640/1700 (96%)	1252 (76%)	337 (21%)	51 (3%)	7	39

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	550	ILE	20
1	A	520	GLY	17
1	A	485	ASP	13
1	A	483	VAL	1

### 6.3.2 Protein sidechains

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	70/71 (99%)	58±2 (83±3%)	12±2 (17±3%)	5	40
All	All	1400/1420 (99%)	1165 (83%)	235 (17%)	5	40

All 32 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	518	TYR	20
1	A	525	PHE	20
1	A	504	ILE	20
1	A	529	SER	19
1	A	490	ARG	18
1	A	550	ILE	17
1	A	515	SER	17
1	A	557	MET	15
1	A	549	ARG	14
1	A	489	TYR	13
1	A	486	MET	11
1	A	547	ARG	10
1	A	482	ASP	6
1	A	553	LYS	5
1	A	564	GLN	5
1	A	537	MET	4
1	A	560	LEU	3
1	A	517	ARG	2
1	A	503	HIS	2
1	A	513	ASP	2
1	A	496	ASP	1
1	A	555	MET	1
1	A	552	ASN	1
1	A	485	ASP	1
1	A	532	GLU	1
1	A	516	SER	1
1	A	556	ASN	1
1	A	492	GLU	1
1	A	562	ASP	1
1	A	544	HIS	1
1	A	497	ASP	1
1	A	535	LYS	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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 68% for the well-defined parts and 67% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

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

#### 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	714
Number of shifts mapped to atoms	714
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
$^{13}\text{C}_\alpha$	83	$-0.04 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	74	$-0.17 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	80	$0.37 \pm 0.28$	None needed ( $< 0.5$ ppm)

#### 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 68%, i.e. 694 atoms were assigned a chemical shift out of a possible 1021. 8 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	320/409 (78%)	157/163 (96%)	83/166 (50%)	80/80 (100%)
Sidechain	374/557 (67%)	216/325 (66%)	158/203 (78%)	0/29 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/55 (0%)	0/30 (0%)	0/22 (0%)	0/3 (0%)
Overall	694/1021 (68%)	373/518 (72%)	241/391 (62%)	80/112 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 67%, i.e. 694 atoms were assigned a chemical shift out of a possible 1041. 8 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	320/419 (76%)	157/167 (94%)	83/170 (49%)	80/82 (98%)
Sidechain	374/567 (66%)	216/331 (65%)	158/207 (76%)	0/29 (0%)
Aromatic	0/55 (0%)	0/30 (0%)	0/22 (0%)	0/3 (0%)
Overall	694/1041 (67%)	373/528 (71%)	241/399 (60%)	80/114 (70%)

#### 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 image below reports *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:

