

# wwPDB NMR Structure Validation Summary Report (i)

#### Aug 21, 2022 – 07:25 AM EDT

PDB ID : 1HKS

Title: SOLUTION STRUCTURE OF THE DNA-BINDING DOMAIN OF

DROSOPHILA HEAT SHOCK TRANSCRIPTION FACTOR

Authors: Vuister, G.W.; Kim, S.-J.; Orosz, A.; Marquardt, J.L.; Wu, C.; Bax, A.

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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
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 (i)

The following experimental techniques were used to determine the structure:  $SOLUTION\ NMR$ 

The overall completeness of chemical shifts assignment was not calculated.

There are no overall percentile quality scores available for this entry.

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	106	100%



# 2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.



### 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1741 atoms, of which 865 are hydrogens and 0 are deuteriums.

 $\bullet$  Molecule 1 is a protein called HEAT-SHOCK TRANSCRIPTION FACTOR.

Mol	Chain	Residues		Atoms								
1	Λ	106	Total	С	Н	N	О	S	0			
1	A	106	1741	563	865	157	153	3	U			



## 4 Residue-property plots (i)

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: HEAT-SHOCK TRANSCRIPTION FACTOR

C	'h	a	in	L	A	:																							10	0%	6																				l			
G43	S44	G45	V46	P47	A48	44.0 0 C	L50 A51	K52	1.53	W54	R55	156	V57	D58	DE9	A60	D61	T62	N63	R64	165	991	290	W68	T69	K70	D7.1	G72	<b>Q73</b>	S74	F75	V76	17.7 040	M70	080	A81	<b>0</b> 82	F83	A84	No TR R R	1.87	188	P89	1.90	N91	Y92	K93	MOR	96N	M9.7	A98	F100	1101	R102
-	_	_	-		┙.		H1 10		-		_	_	_	_	_	_	₩	⊣	₩	R124	$\rightarrow$	E126	$\leftarrow$	$\leftarrow$	F129	$\leftarrow$	H131	P132	F133	$\leftarrow$	÷.	R136	н,	4 +	F140	÷	÷	÷.	Q144	4 +		Ĥ												



#### Refinement protocol and experimental data overview (i) 5



Of the? calculated structures, 1 were deposited, based on the following criterion:?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.



### 6 Model quality (i)

#### 6.1 Standard geometry (i)

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		
1	A	0	0	0	0		
All	All	0	0	0	-		

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	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.



#### 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	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

#### 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 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 (i)

No chemical shift data were provided

