wwPDB NMR Structure Validation Summary Report (i)

Mar 3, 2022 – 07:36 AM EST

PDB ID	:	2HGH
Title	:	Transcription Factor IIIA zinc fingers 4-6 bound to 5S rRNA 55mer (NMR structure)
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Deposited on	:	2006-06-27

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 following versions of software and data (see references (i)) were used in the production of this report:

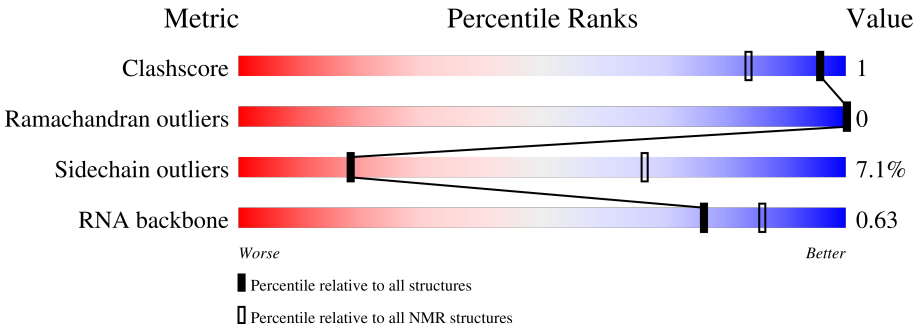
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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.

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
RNA backbone	4643	676

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	B	55	69% 25% 5%
2	A	87	84% 13% • •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:104-A:188 (85)	0.21	3

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. No single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3166 atoms, of which 1276 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 55-MER.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	55	1758	520	591	201	391	55	0

- Molecule 2 is a protein called Transcription factor IIIA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	A	87	1405	455	685	133	124	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MET	-	initiating methionine	UNP P03001

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	A	3	3	3

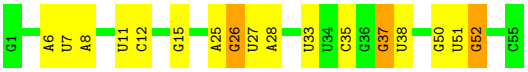
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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.

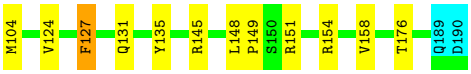
• Molecule 1: 55-MER

Chain B:



• Molecule 2: Transcription factor IIIA

Chain A:

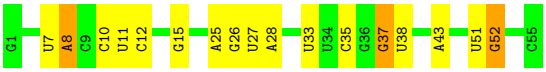


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

• Molecule 1: 55-MER

Chain B:



• Molecule 2: Transcription factor IIIA

Chain A:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics, molecular dynamics, generalized Born solvation model.*

Of the 200 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
DYANA	structure solution	1.5
Amber	refinement	8

No chemical shift data was provided.

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: ZN

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	B	1.31±0.00	0±0/1301 (0.0± 0.0%)	1.31±0.01	6±1/2025 (0.3± 0.1%)
2	A	0.79±0.00	0±0/727 (0.0± 0.0%)	1.00±0.02	6±1/977 (0.6± 0.1%)
All	All	1.15	0/40560 (0.0%)	1.21	231/60040 (0.4%)

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	B	0.0±0.0	11.4±1.6
2	A	0.0±0.0	0.8±0.8
All	All	0	246

There are no bond-length outliers.

5 of 27 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	154	ARG	NE-CZ-NH1	8.07	124.34	120.30	12	18
2	A	151	ARG	NE-CZ-NH1	8.00	124.30	120.30	7	15
1	B	25	A	C3'-C2'-C1'	-7.96	95.13	101.50	8	16
1	B	6	A	O4'-C4'-C3'	6.72	111.48	106.10	2	16
2	A	151	ARG	NE-CZ-NH2	-6.66	116.97	120.30	20	7

There are no chirality outliers.

5 of 22 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	B	33	U	Sidechain	20
1	B	35	C	Sidechain	20
1	B	37	G	Sidechain	20
1	B	51	U	Sidechain	20
1	B	52	G	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	B	1167	591	592	1±1
2	A	703	673	671	3±1
All	All	37460	25280	25260	58

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 1.

5 of 11 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:25:A:N3	2:A:118:LYS:HE2	0.55	2.16	5	5
2:A:124:VAL:HG21	2:A:148:LEU:HD23	0.55	1.78	4	8
2:A:124:VAL:HG21	2:A:148:LEU:HD13	0.53	1.79	19	10
1:B:26:G:O4'	2:A:118:LYS:HE3	0.52	2.04	9	7
2:A:124:VAL:HG21	2:A:148:LEU:CD2	0.49	2.38	18	8

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	
2	A	84/87 (97%)	80±1 (95±1%)	4±1 (5±1%)	0±0 (0±0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1680/1740 (97%)	1595 (95%)	85 (5%)	0 (0%)	100 100

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
2	A	78/80 (98%)	72±1 (93±1%)	6±1 (7±1%)	18 67
All	All	1560/1600 (98%)	1450 (93%)	110 (7%)	18 67

5 of 14 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	A	104	MET	20
2	A	127	PHE	20
2	A	176	THR	20
2	A	131	GLN	19
2	A	144	LYS	6

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	B	54/55 (98%)	4±0 (8±0%)	0±0 (0±0%)	0.63±0.01
All	All	1080/1100 (98%)	81 (8%)	1 (0%)	0.63

The overall RNA backbone suiteness is 0.63.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	12	C	20
1	B	26	G	20
1	B	52	G	20
1	B	15	G	17

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Mol	Chain	Res	Type	Models (Total)
1	B	14	U	4

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	14	U	1

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)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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