



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:27 AM UTC

PDB ID : 1A66 / pdb_00001a66
Title : SOLUTION NMR STRUCTURE OF THE CORE NFATC1/DNA COM-
PLEX, 18 STRUCTURES
Authors : Zhou, P.; Sun, L.J.; Doetsch, V.; Wagner, G.; Verdine, G.L.
Deposited on : 1998-03-06

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

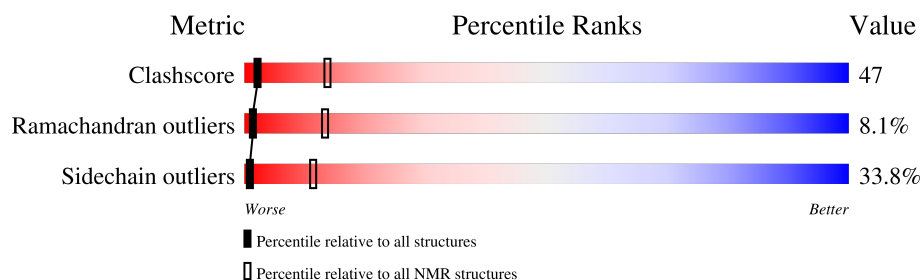
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	B	12	100%
2	C	12	100%
3	A	178	23% 56% 13% 8%

2 Ensemble composition and analysis

This entry contains 18 models. Model 3 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:10-A:40, A:45-A:177 (164)	1.34	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 2 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3595 atoms, of which 1704 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms						Trace
1	B	12	Total	C	H	N	O	P	0
			385	119	136	52	67	11	

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*AP*AP*TP*TP*TP*TP*CP*CP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms						Trace
2	C	12	Total	C	H	N	O	P	0
			376	116	139	37	73	11	

- Molecule 3 is a protein called CORE NFATC1.

Mol	Chain	Residues	Atoms						Trace
3	A	178	Total	C	H	N	O	S	0
			2834	875	1429	267	258	5	

There are 3 discrepancies between the modelled and reference sequences:

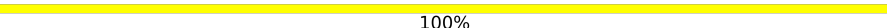
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	ALA	engineered mutation	UNP O95644
A	2	LYS	LEU	engineered mutation	UNP O95644
A	28	ARG	HIS	engineered mutation	UNP O95644

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

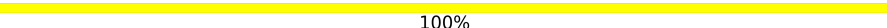
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')

Chain B:  100%

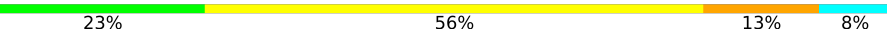
C315
C316
A317
G318
G319
A320
A321
A322
A323
T324
T325
G326

- Molecule 2: DNA (5'-D(*CP*AP*AP*TP*TP*TP*TP*CP*CP*TP*CP*G)-3')

Chain C:  100%

C340
A341
A342
T343
T344
T345
T346
C347
C348
T349
C350
G351

- Molecule 3: CORE NFATC1

Chain A:  23% 56% 13% 8%

M1 K2 D3 D4 G6 L6 P7 S8 H9 G11 G12 Y13 E14 L15 R16 L17 E18 V19 Q20 P21 K22 H25 R26 A27 R28 Y29 T31 T32 E32 G33 S34 R35 G36 A37 V38 K39 A40 S41 A42 G43 G44 H45 P46 L47 V48 Q49 L50 H51 G52 Y53 L54 E55 N56 F57 F58 L59 M60 L61

Q62 L63 F64 I65 G66 T67 A68 D69 D70 R71 L72 L73 R74 P75 H76 A77 F78 Y79 Q80 V81 H82 R83 I84 T85 G86 K87 T88 V89 T92 S93 H94 E95 A96 I97 L98 S99 M100 T101 K102 V103 L104 E105 I106 P107 L108 L109 P110 E111 N112 S113 M114 V117 I118 D119 C120 A121 G122 I123

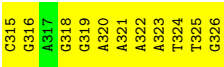
L124 K125 L126 R127 N128 S129 D130 I131 E132 L133 R134 K135 G136 E137 T138 D139 I140 G141 R142 K143 N144 T145 R146 V147 R148 L149 V150 F151 R152 V153 H154 V155 P156 Q157 P158 S159 G160 R161 T162 L163 S164 L165 Q166 V167 A168 S169 I172 E173 S176

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

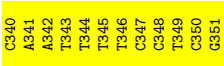
The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')

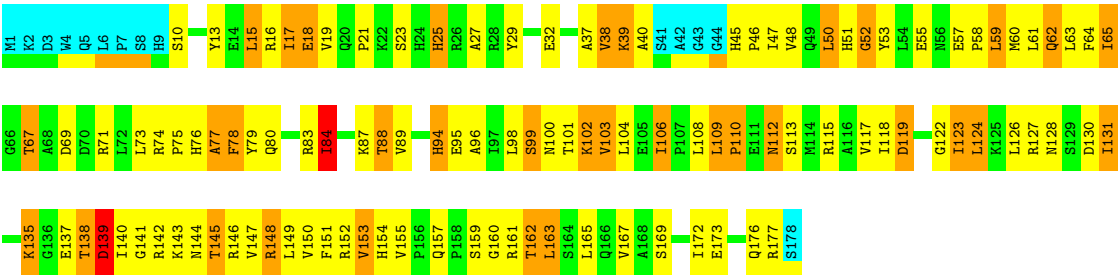
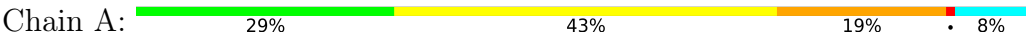
Chain B:  8% 92%



• Molecule 2: DNA (5'-D(*CP*AP*AP*TP*TP*TP*TP*CP*CP*TP*CP*G)-3')



• Molecule 3: CORE NFATC1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS AND SIMULATED ANNEALING*.

Of the 18 calculated structures, 18 were deposited, based on the following criterion: *NOE VIOLATION ≤ 0.4 ANGSTROM, DIHEDRAL ANGLE VIOLATION ≤ 5 DEGREE*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
DYANA-1.4	structure solution	
X-PLOR	structure solution	3.1

No chemical shift data was provided.

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	B	0.58±0.01	0±0/281 (0.0± 0.0%)	1.26±0.01	0±0/433 (0.0± 0.0%)
2	C	0.55±0.01	0±0/263 (0.0± 0.0%)	1.31±0.01	0±0/403 (0.0± 0.0%)
3	A	1.45±0.02	0±1/1325 (0.0± 0.1%)	1.14±0.01	0±0/1794 (0.0± 0.0%)
All	All	1.26	9/33642 (0.0%)	1.19	0/47340 (0.0%)

All 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
3	A	122	GLY	N-CA	7.03	1.50	1.44	14	4
3	A	106	ILE	N-CA	5.45	1.50	1.46	1	2
3	A	155	VAL	N-CA	5.43	1.50	1.45	12	2
3	A	141	GLY	N-CA	5.26	1.50	1.45	12	1

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	B	249	136	136	16±2
2	C	237	139	139	21±3
3	A	1300	1332	1332	132±14
All	All	32148	28926	28926	2867

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 47.

5 of 1022 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:61:LEU:HD13	3:A:153:VAL:HG22	1.11	1.11	14	18
3:A:15:LEU:HD13	3:A:153:VAL:HG21	1.09	1.23	10	18
3:A:37:ALA:HB2	3:A:123:ILE:HG22	1.05	1.17	14	6
3:A:79:TYR:CE2	3:A:126:LEU:HD21	1.04	1.87	13	7
3:A:47:ILE:HD12	3:A:117:VAL:HG13	1.00	1.34	17	12

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	
3	A	164/178 (92%)	114±5 (70±3%)	37±5 (22±3%)	13±3 (8±2%)	1	13
All	All	2952/3204 (92%)	2054 (70%)	659 (22%)	239 (8%)	1	13

5 of 49 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	99	SER	18
3	A	110	PRO	18
3	A	77	ALA	16
3	A	18	GLU	15
3	A	52	GLY	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	
3	A	145/156 (93%)	96±6 (66±4%)	49±6 (34±4%)	1	11
All	All	2610/2808 (93%)	1727 (66%)	883 (34%)	1	11

5 of 117 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)
3	A	65	ILE	18
3	A	167	VAL	18
3	A	15	LEU	17
3	A	62	GLN	16
3	A	84	ILE	16

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 oligosaccharides 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

No chemical shift data were provided