



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2HDC
Title : STRUCTURE OF TRANSCRIPTION FACTOR GENESIS/DNA COM-
PLEX
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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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

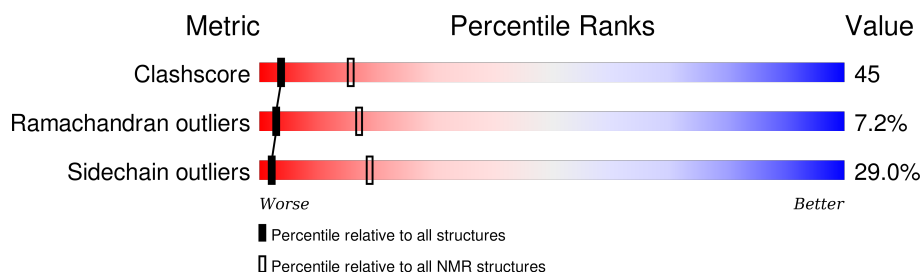
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	17	<div> <div>29%</div> <div>71%</div> </div>
2	C	17	<div> <div>18%</div> <div>82%</div> </div>
3	A	97	<div> <div>19%</div> <div>58%</div> <div>7%</div> <div>16%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:7-A:87 (81)	0.52	6

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. No single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2581 atoms, of which 1080 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	B	17	Total	C	H	N	O	P	0
			493	167	145	67	97	17	

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*AP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms						Trace
2	C	17	Total	C	H	N	O	P	0
			484	169	135	56	107	17	

- Molecule 3 is a protein called PROTEIN (TRANSCRIPTION FACTOR).

Mol	Chain	Residues	Atoms						Trace
3	A	97	Total	C	H	N	O	S	0
			1604	517	800	143	140	4	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

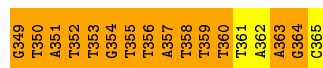
- Molecule 1: DNA (5'-D(P*GP*CP*TP*TP*AP*AP*AP*AP*TP*AP*AP*CP*AP*AP*TP*A P*C)-3')

Chain B: 



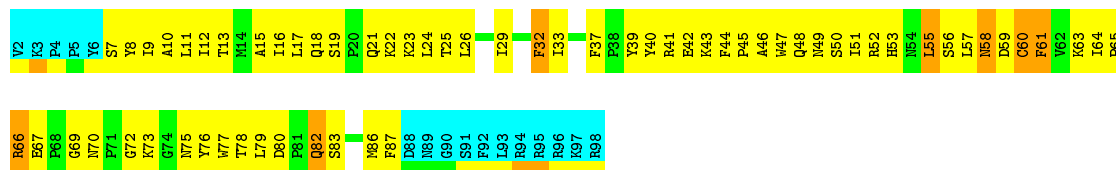
- Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*TP*AP*AP*G P*C)-3')

Chain C: 



- Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A: 



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

The representative model is number 6. Colouring as in section 4.1 above.

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

Chain B:  35% 65%


G249 C250 T251 T252 A253 A254 A255 A256 A257 A258 A259 C260 A261 A262 T263 A264 C265

- Molecule 2: DNA (5'-D(P*GP*TP*AP*TP*TP*GP*TP*TP*AP*TP*TP*TP*TP*AP*AP*G P*C)-3')

Chain C:  35% 65%

G349 T350 A351 T352 T353 G354 T355 T356 A357 T358 T359 T360 T361 A362 A363 G364 C365

- Molecule 3: PROTEIN (TRANSCRIPTION FACTOR)

Chain A:  22% 46% 13% • 16%

Y2 K3 P4 P5 Y6 S7 Y8 I9 A10 L11 I12 T13 M14 A15 Q18 S19 P20 Q21 R22 R23 L24 T25 L26 L29 F32 I33 S34 N35 R36 F37 Y39 Y40 R41 E42 R43 F44 P45 A46 W47 Q48 N49 S50 I51 R52 H53 N54 L55 S56 L57 N58 D59 C60 F61 V62 K63 I64
P65 R66 E67 P68 G69 N70 W71 G72 M75 Y76 W77 L78 L79 D80 P81 Q82 D85 D88 N89 G90 S91 P92 L93 R94 R95 R96 K97 R98

5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
DYANA	refinement	1.5
DYANA	structure solution	

No chemical shift data was provided. 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

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	4.98±2.25	13±1/391 (3.4±0.3%)	5.51±0.64	49±1/600 (8.1±0.2%)
2	C	3.59±0.38	12±2/389 (3.2±0.4%)	4.76±0.32	63±2/599 (10.4±0.3%)
3	A	0.72±0.00	0±0/685 (0.0±0.0%)	0.92±0.00	0±0/930 (0.0±0.0%)
All	All	3.42	513/29300 (1.8%)	3.93	2223/42580 (5.2%)

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	8.1±1.1	0.0±0.0
2	C	4.2±1.0	0.0±0.0
All	All	246	0

5 of 34 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
1	B	249	DG	C4'-O4'	277.59	4.22	1.45	20	15
2	C	359	DT	C4'-O4'	60.77	2.05	1.45	18	19
2	C	363	DA	C4'-O4'	44.67	1.89	1.45	9	7
1	B	260	DC	C4'-O4'	42.10	1.87	1.45	3	20
1	B	254	DA	C4'-O4'	-37.77	1.07	1.45	2	20

5 of 132 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(°)	Ideal(°)	Models	
								Worst	Total
1	B	249	DG	O4'-C4'-C3'	-121.26	33.25	106.00	20	12
1	B	249	DG	C1'-O4'-C4'	-79.09	31.00	110.10	20	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	359	DT	O4'-C4'-C3'	-56.61	72.04	106.00	18	14
2	C	363	DA	O4'-C4'-C3'	-48.22	77.07	106.00	9	19
1	B	260	DC	O4'-C4'-C3'	-45.03	78.98	106.00	11	20

5 of 28 unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	B	255	DA	C4'	20
1	B	260	DC	C4'	20
1	B	263	DT	C4'	18
2	C	359	DT	C4'	18
2	C	353	DT	C4'	16

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	B	348	145	192	26±6
2	C	349	135	197	22±5
3	A	664	652	652	72±13
All	All	27220	18640	20820	2141

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 45.

5 of 863 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:261:DA:O4'	1:B:261:DA:C4'	1.39	1.64	13	6
2:C:361:DT:C4'	2:C:361:DT:O4'	1.38	1.63	9	1
1:B:256:DA:O4'	1:B:256:DA:C4'	1.37	1.64	11	7
2:C:364:DG:C4'	2:C:364:DG:O4'	1.36	1.64	15	4
1:B:251:DT:O4'	1:B:251:DT:C4'	1.35	1.65	3	2

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	81/97 (84%)	62±2 (77±3%)	13±2 (16±2%)	6±1 (7±2%)	3	17
All	All	1620/1940 (84%)	1244 (77%)	260 (16%)	116 (7%)	3	17

5 of 16 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	58	ASN	20
3	A	82	GLN	17
3	A	66	ARG	14
3	A	46	ALA	14
3	A	60	CYS	13

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	74/89 (83%)	53±4 (71±5%)	21±4 (29±5%)	2	19
All	All	1480/1780 (83%)	1051 (71%)	429 (29%)	2	19

5 of 61 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	32	PHE	19
3	A	63	LYS	18
3	A	61	PHE	16
3	A	55	LEU	14
3	A	21	GLN	13

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

No chemical shift data were provided