



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1ZGW
Title : NMR structure of E. Coli Ada protein in complex with DNA
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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 : 1.7.1 (RC1), CSD as537be (2016)
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

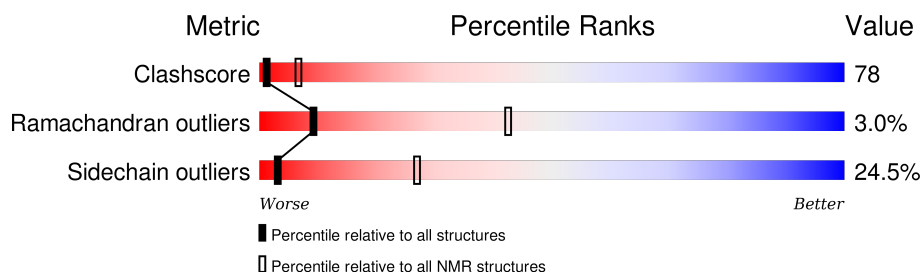
1 Overall quality at a glance

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	18	6% 89% 6%
2	C	18	22% 72% 6%
3	A	139	17% 60% 18% 6%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 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:8-A:37, A:39-A:139 (131)	0.60	1

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 6 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3364 atoms, of which 1517 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	B	18	Total	C	H	N	O	P	0
			573	177	202	78	99	17	

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

Mol	Chain	Residues	Atoms						Trace
2	C	18	Total	C	H	N	O	P	0
			570	176	209	55	113	17	

- Molecule 3 is a protein called Ada polypeptide.

Mol	Chain	Residues	Atoms						Trace
3	A	139	Total	C	H	N	O	S	0
			2220	692	1106	219	194	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	SMC	CYS	MODIFIED RESIDUE	UNP P06134

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
4	A	1	Total	Zn
			1	1

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: 5'-D(*GP*CP*AP*AP*AP*TP*TP*AP*AP*AP*GP*CP*GP*CP*AP*AP*GP*A)-3'

Chain B: 



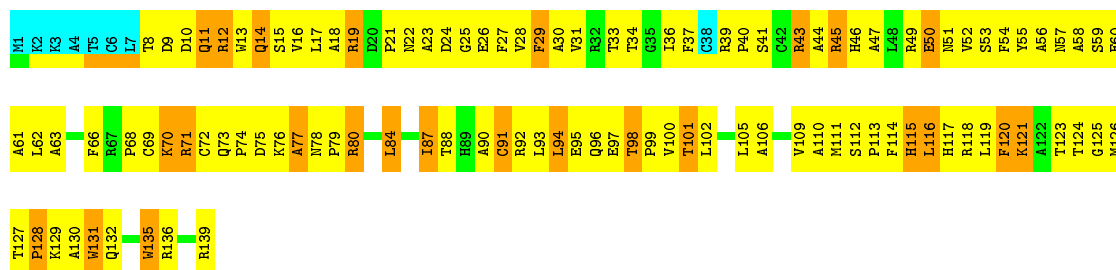
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 



- Molecule 3: Ada polypeptide

Chain A: 



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

The representative model is number 1. Colouring as in section 4.1 above.

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

Chain B: 

G190 C191 A192 A193 A194 T195 T196 A197 A198 A199 G200 C201 G202 C203 A204 A205 G206 A207

- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

T221 C222 T223 T224 G225 C226 G227 C228 T229 T230 T231 A232 A233 T234 T235 T236 G237 C238

- Molecule 3: Ada polypeptide

Chain A: 

M1 K2 K3 A4 T5 C6 L7 T8 D9 Q10 R11 R12 W13 Q14 S15 V16 L17 A18 R19 N22 A23 D24 G25 E26 F27 V28 F29 A30 V31 R32 T33 T34 I36 F37 C38 R39 P40 S41 C42 R43 A44 R45 H46 A47 L48 R49 E50 N51 V52 S53 F54 Y55 A56 N57 A58 S59 E60 A61

L62 A63 A64 G65 F66 R67 P68 C69 R70 R71 C72 Q73 P74 D75 K76 A77 N78 P79 R80 R81 H82 R83 L84 D85 K86 T87 T88 H89 A90 C91 R92 L93 L94 R95 Q96 E97 T98 P99 V100 T101 L102 L105 A106 D107 Q108 V109 A110 M111 S112 F113 F114 H115 L116 H117 R118 L119 F120 K121 A122

T123 T124 G125 M126 T127 P128 K129 A130 W131 Q132 W135 R136 R139

5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 40 calculated structures, 20 were deposited, based on the following criterion: *The submitted conformer models have no restraint violations and lowest energies*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
Procheck nmr	structure solution	3.5.4

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 ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SMC

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	2.70±0.01	37±0/419 (8.8±0.1%)	2.86±0.00	55±1/645 (8.6±0.1%)
2	C	2.74±0.01	37±1/401 (9.1±0.2%)	2.75±0.01	53±2/617 (8.6±0.3%)
3	A	1.02±0.01	0±0/1080 (0.0±0.0%)	1.34±0.01	4±1/1459 (0.3±0.1%)
All	All	1.95	1469/38000 (3.9%)	2.15	2250/54420 (4.1%)

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	1.0±0.0
2	C	0.0±0.0	1.0±0.0
All	All	0	40

5 of 79 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	191	DC	C3'-C2'	-9.80	1.40	1.52	19	20
2	C	233	DA	C3'-C2'	-9.75	1.40	1.52	16	20
1	B	190	DG	C3'-C2'	-9.57	1.40	1.52	12	20
2	C	221	DT	C3'-C2'	-9.55	1.40	1.52	6	20
1	B	201	DC	C3'-C2'	-9.35	1.41	1.52	7	20

5 of 126 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($^{\circ}$)	Ideal($^{\circ}$)	Models	
								Worst	Total
1	B	204	DA	C3'-C2'-C1'	11.15	115.88	102.50	15	20
2	C	235	DT	C3'-C2'-C1'	10.97	115.66	102.50	6	20
1	B	199	DA	C3'-C2'-C1'	10.70	115.34	102.50	7	20
2	C	227	DG	C3'-C2'-C1'	10.68	115.31	102.50	15	20
1	B	192	DA	C3'-C2'-C1'	10.63	115.26	102.50	7	20

There are no chirality outliers.

All 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	200	DG	Sidechain	20
2	C	227	DG	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	371	202	202	28 \pm 5
2	C	361	209	209	36 \pm 6
3	A	1055	1034	1034	221 \pm 17
All	All	35760	28900	28900	5071

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 78.

5 of 1049 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(\AA)	Distance(\AA)	Models	
				Worst	Total
2:C:235:DT:OP1	3:A:46:HIS:O	1.18	1.62	13	5
3:A:97:GLU:OE2	3:A:101:THR:OG1	1.12	1.65	1	3
2:C:224:DT:OP2	3:A:129:LYS:HB3	1.06	1.50	11	19
2:C:234:DT:O3'	3:A:46:HIS:O	1.05	1.75	18	17
3:A:102:LEU:HD23	3:A:116:LEU:HD23	1.02	1.23	1	3

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	130/139 (94%)	113±2 (87±1%)	13±2 (10±1%)	4±1 (3±1%)	9	42
All	All	2600/2780 (94%)	2266 (87%)	256 (10%)	78 (3%)	9	42

5 of 10 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	128	PRO	20
3	A	98	THR	20
3	A	70	LYS	16
3	A	77	ALA	9
3	A	9	ASP	4

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	108/114 (95%)	82±4 (76±4%)	26±4 (24±4%)	3	27
All	All	2160/2280 (95%)	1631 (76%)	529 (24%)	3	27

5 of 60 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	120	PHE	20
3	A	131	TRP	20
3	A	29	PHE	20
3	A	135	TRP	20
3	A	101	THR	20

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	SMC	A	38	3,4	4,6,7	0.90±0.14	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	SMC	A	38	3,4	2,6,8	2.20±0.29	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SMC	A	38	3,4	-	0±0,3,5,7	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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

No chemical shift data were provided