



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1XS9 / pdb_00001xs9
Title : A MODEL OF THE TERNARY COMPLEX FORMED BETWEEN MARA,
THE ALPHA-CTD OF RNA POLYMERASE AND DNA
Authors : Dangi, B.; Gronenborn, A.M.; Rosner, J.L.; Martin, R.G.
Deposited on : 2004-10-18

This is a Full wwPDB NMR Structure Validation 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

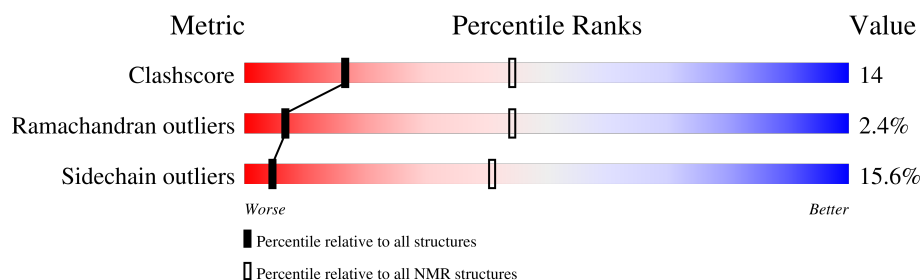
1 Overall quality at a glance

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	20	5% 95%
2	C	20	35% 60% 5%
3	A	132	70% 25% . .
4	D	84	56% 35% 6% .

2 Ensemble composition and analysis ⓘ

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

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4720 atoms, of which 2181 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(P*GP*AP*TP*TP*TP*AP*GP*CP*AP*AP*AP*AP*CP*GP*TP*GP*GP*CP*AP*T)-3'.

Mol	Chain	Residues	Atoms						Trace
1	B	20	Total	C	H	N	O	P	0
			642	197	227	79	119	20	

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

Mol	Chain	Residues	Atoms						Trace
2	C	20	Total	C	H	N	O	P	0
			636	195	229	69	123	20	

- Molecule 3 is a protein called Multiple antibiotic resistance protein marA.

Mol	Chain	Residues	Atoms						Trace
3	A	129	Total	C	H	N	O	S	0
			2154	682	1069	195	202	6	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P0ACH5
A	-1	SER	-	cloning artifact	UNP P0ACH5
A	0	HIS	-	cloning artifact	UNP P0ACH5

- Molecule 4 is a protein called DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms						Trace
4	D	81	Total	C	H	N	O	S	0
			1288	400	656	108	122	2	

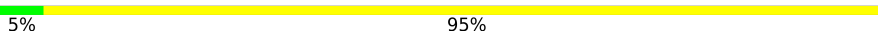
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	246	GLY	-	cloning artifact	UNP P0A7Z4
D	247	SER	-	cloning artifact	UNP P0A7Z4
D	248	HIS	-	cloning artifact	UNP P0A7Z4

4 Residue-property plots

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: 5'-D(P*GP*AP*TP*TP*TP*AP*GP*CP*AP*AP*AP*AP*CP*GP*TP*GP*GP*CP*AP*T)-3'

Chain B:  5% 95%

G404
A405
T406
T407
A408
G409
G410
C411
A412
A413
A414
A415
C416
G417
T418
G420
C421
A422
T423

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

Chain C:  35% 60% 5%

A428
T429
A433
C434
G435
T436
T437
T438
T439
G440
C441
T442
A443
A444
A445
T446
C447

- Molecule 3: Multiple antibiotic resistance protein marA

Chain A:  70% 25% . .

GLY
SER
HIS
M1
T8
T13
M19
I20
E21
D22
N23
L24
E25
S26
P27
E31
K32
R36
S40
Q45
R46
M47
E51
L56
Y59
I60
R63
R64
M65
T66
S75
E84
R85
K99
D103
Y104
P105
R110
M111
Q115
P123
L124

N125
H126
Y127
N128
S129

- Molecule 4: DNA-directed RNA polymerase alpha chain

Chain D:  56% 35% 6% .

GLY
SER
HIS
F249
I252
R255
P256
V257
L260
E261
L262
T263
V264
R265
S266
C269
L270
K271
A272
E273
A274
L275
H276
Y277
I278
G279
D280
Q283
R284
T285
E286
N284
T301
R310
G311
L312
S313
L314
G315
M316
R317
W321
P322
P323
I326
A327
D328
E329

5 Refinement protocol and experimental data overview

The models were refined using the following method: *MODEL BASED ON CHEMICAL SHIFT PERTURBATION MAPPING*.

Of the 200 calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
HADDOCK	refinement	
NMRPipe	structure solution	
XwinNMR	structure solution	
HADDOCK	structure solution	

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	0.33	1/466 (0.2%)	0.49	0/716 (0.0%)
2	C	0.34	1/454 (0.2%)	0.53	0/696 (0.0%)
3	A	0.35	0/1111 (0.0%)	0.71	0/1492 (0.0%)
4	D	0.37	0/641 (0.0%)	0.70	0/868 (0.0%)
All	All	0.35	2/2672 (0.1%)	0.64	0/3772 (0.0%)

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	428	DA	OP3-P	5.68	1.59	1.48
1	B	404	DG	OP3-P	5.62	1.59	1.48

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	415	227	226	24
2	C	407	229	228	11
3	A	1085	1069	1065	20
4	D	632	656	654	19
All	All	2539	2181	2173	66

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 14.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:414:DA:H2'	1:B:415:DA:O4'	0.71	1.86
1:B:419:DG:H2'	1:B:420:DG:O4'	0.70	1.86
1:B:415:DA:H2'	1:B:416:DC:O4'	0.70	1.85
2:C:437:DT:H2'	2:C:438:DT:O4'	0.65	1.91
2:C:442:DT:H2'	2:C:443:DA:O4'	0.61	1.95
4:D:252:ILE:HA	4:D:255:ARG:HD3	0.61	1.71
3:A:26:SER:HB2	3:A:27:PRO:HD3	0.60	1.73
3:A:111:MET:HA	3:A:111:MET:HE2	0.60	1.73
3:A:65:MET:HE2	3:A:65:MET:HA	0.57	1.76
4:D:321:TRP:H	4:D:322:PRO:CD	0.56	2.13
1:B:413:DA:C2	1:B:414:DA:C4	0.56	2.94
1:B:412:DA:C2	1:B:413:DA:C4	0.55	2.92
4:D:257:VAL:HG12	4:D:278:ILE:HD13	0.55	1.76
1:B:415:DA:C2	1:B:416:DC:C2	0.55	2.95
2:C:439:DT:H2'	2:C:440:DG:C8	0.51	2.40
4:D:312:LEU:HD22	4:D:316:MET:HE1	0.50	1.82
3:A:21:GLU:HG3	3:A:123:PRO:HB3	0.50	1.84
2:C:444:DA:C2	2:C:445:DA:C4	0.50	3.00
1:B:417:DG:H2'	1:B:418:DT:O4'	0.50	2.06
3:A:26:SER:HA	3:A:85:ARG:O	0.49	2.06
3:A:31:GLU:HG2	3:A:45:GLN:HG3	0.49	1.84
3:A:13:ILE:HD11	3:A:47:MET:HB3	0.49	1.84
1:B:414:DA:C6	1:B:415:DA:C6	0.48	3.00
1:B:414:DA:C2'	1:B:415:DA:O4'	0.47	2.62
4:D:271:LYS:HA	4:D:275:ILE:O	0.47	2.09
4:D:260:LEU:HD23	4:D:262:LEU:HD11	0.47	1.86
1:B:407:DT:C5'	3:A:105:PRO:HB3	0.47	2.40
1:B:422:DA:H2'	1:B:423:DT:O4'	0.46	2.10
3:A:127:TYR:C	3:A:129:SER:H	0.46	2.19
4:D:283:GLN:HA	4:D:315:GLY:HA2	0.46	1.87
4:D:321:TRP:H	4:D:322:PRO:HD2	0.46	1.70
3:A:19:TRP:HA	4:D:265:ARG:HG3	0.46	1.87
3:A:56:LEU:O	3:A:60:ILE:HG12	0.46	2.11
3:A:31:GLU:HG2	3:A:45:GLN:CG	0.46	2.41
1:B:414:DA:N1	1:B:415:DA:C2	0.45	2.84
2:C:434:DC:H2'	2:C:435:DG:O4'	0.45	2.09
2:C:433:DA:H2'	2:C:434:DC:C6	0.45	2.46
3:A:21:GLU:HB2	4:D:264:VAL:HG11	0.45	1.87
3:A:20:ILE:HG22	3:A:24:LEU:HD23	0.45	1.88
4:D:265:ARG:HG2	4:D:269:CYS:SG	0.45	2.51

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
4:D:321:TRP:CG	4:D:322:PRO:HD3	0.44	2.47
1:B:409:DA:C2	1:B:410:DG:C4	0.44	3.04
1:B:415:DA:C2	1:B:416:DC:H1'	0.44	2.47
4:D:275:ILE:HG23	4:D:280:ASP:HB3	0.44	1.89
1:B:420:DG:C2	1:B:421:DC:C2	0.44	3.06
1:B:417:DG:C4	2:C:435:DG:N2	0.44	2.86
1:B:405:DA:C2	1:B:406:DT:C2	0.44	3.06
1:B:409:DA:C5	2:C:443:DA:C2	0.44	3.05
4:D:265:ARG:CZ	4:D:265:ARG:HB3	0.44	2.43
1:B:418:DT:H2'	1:B:419:DG:C8	0.43	2.48
4:D:255:ARG:O	4:D:278:ILE:HG12	0.43	2.13
3:A:31:GLU:HG3	3:A:56:LEU:HD13	0.43	1.90
3:A:59:TYR:CE1	3:A:125:ASN:HB2	0.43	2.49
4:D:286:GLU:HG3	4:D:314:LEU:HD11	0.43	1.90
4:D:265:ARG:HB3	4:D:265:ARG:NH1	0.42	2.29
2:C:428:DA:C2	2:C:429:DT:C2	0.42	3.08
1:B:409:DA:H2'	1:B:410:DG:O4'	0.42	2.15
3:A:99:LYS:O	3:A:103:ASP:HA	0.42	2.15
1:B:411:DC:H2'	1:B:412:DA:O4'	0.42	2.14
1:B:413:DA:C2	2:C:439:DT:O2	0.42	2.73
3:A:124:LEU:HD21	3:A:127:TYR:HD2	0.42	1.75
3:A:19:TRP:HA	4:D:265:ARG:HB2	0.41	1.91
1:B:412:DA:C2	2:C:440:DG:C2	0.41	3.08
4:D:321:TRP:N	4:D:322:PRO:CD	0.41	2.81
1:B:414:DA:C2	1:B:415:DA:N3	0.41	2.89
3:A:13:ILE:HB	3:A:51:GLU:HG3	0.41	1.93

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	127/132 (96%)	112 (88%)	14 (11%)	1 (1%)	18	68
4	D	79/84 (94%)	69 (87%)	6 (8%)	4 (5%)	3	23
All	All	206/216 (95%)	181 (88%)	20 (10%)	5 (2%)	7	44

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

Mol	Chain	Res	Type
3	A	26	SER
4	D	266	SER
4	D	294	ASN
4	D	321	TRP
4	D	323	PRO

6.3.2 Protein sidechains ⓘ

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	121/123 (98%)	106 (88%)	15 (12%)	7	48
4	D	71/73 (97%)	56 (79%)	15 (21%)	3	31
All	All	192/196 (98%)	162 (84%)	30 (16%)	4	41

All 30 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
3	A	1	MET
3	A	8	THR
3	A	23	ASN
3	A	32	LYS
3	A	36	ARG
3	A	40	SER
3	A	56	LEU
3	A	63	ARG
3	A	66	THR
3	A	75	SER
3	A	84	GLU
3	A	85	ARG
3	A	110	ARG
3	A	111	MET
3	A	115	GLN
4	D	249	PHE
4	D	263	THR

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Mol	Chain	Res	Type
4	D	265	ARG
4	D	269	CYS
4	D	271	LYS
4	D	273	GLU
4	D	277	TYR
4	D	285	THR
4	D	301	THR
4	D	310	ARG
4	D	313	SER
4	D	314	LEU
4	D	317	ARG
4	D	326	ILE
4	D	328	ASP

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