

# Full wwPDB NMR Structure Validation Report (i)

### Jun 2, 2020 - 12:06 pm BST

PDB ID	:	5OR5
Title	:	NMR structure of the complex formed by an engineered region 2 of sigmaE in
		complex with GTAAAA
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Deposited on	:	2017-08-15
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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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

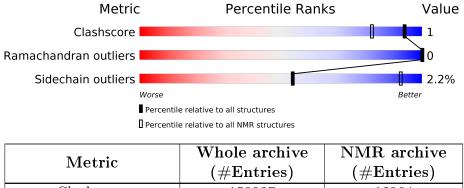
Cyrange	:	Kirchner and Güntert (2011)
$\operatorname{NmrClust}$	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{RCI}$	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
${ m ShiftChecker}$	:	2.11
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 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 is 85%.

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	$(\# { m Entries})$	$(\# { m Entries})$
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	А	95	78%	• 18%
2	В	6	67%	33%



# 2 Ensemble composition and analysis (i)

This entry contains 13 models. Model 9 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:7-A:84 (78)	0.10	9			

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 and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 6, 7, 9, 11, 12
2	3, 10, 13
3	4, 8
Single-model clusters	5



# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1761 atoms, of which 862 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called ECF RNA polymerase sigma-E factor, ECF RNA polymerase sigma factor SigW, ECF RNA polymerase sigma-E factor.

Mol	Chain	Residues		Atoms					Trace
1	Λ	05	Total	С	Н	Ν	0	S	0
	. A	A 95	1569	495	793	139	141	1	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	SER	-	linker	UNP Q45585
A	93	LEU	-	expression tag	UNP P0AGB6
A	94	GLU	-	expression tag	UNP P0AGB6
A	95	LEU	-	expression tag	UNP P0AGB6

• Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*TP\*AP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					Trace	
0	D	6	Total	С	Η	Ν	0	Р	0
	2 В	0	192	60	69	27	31	5	0



# 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: ECF RNA polymerase sigma-E factor,ECF RNA polymerase sigma factor SigW,ECF RNA polymerase sigma-E factor

Chain A:	78%	• 18%
20 20 20 20 20 20 20 20 20 20 20 20 20 2	744 785 785 783 783 783 783 783 783 783 783 783 783	
• Molecule 2:	DNA $(5'-D(*GP*TP*AP*AP*AP*A)-3')$	
Chain B:	67%	33%
796 197 100 101		

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

Chain A: 77%	5%	18%
M1 52 52 53 15 15 75 783 783 785 193 693 193 193 193 193 193 193 193 193 193 1		
• Molecule 2: DNA (5'-D(*GP*TP*AP*AP*AP*A)-3')		
Chain B: 83%		17%





#### 4.2.2 Score per residue for model 2

• Molecule 1: ECF RNA polymerase sigma-E factor,ECF RNA polymerase sigma factor SigW,ECF RNA polymerase sigma-E factor

Chain A:	78%	•	18%
M1 S2 L5 L5 K20 K20	K32 V46 C90 C90 C90 C93 C93 C93 C93 C93 C93 C93 C93 C93 C93		
• Molecule	2: DNA (5'-D(*GP*TP*AP*AP*AP*A)-3')		
Chain B:	83%		17%
796 197 A101			

### 4.2.3 Score per residue for model 3

 $\bullet$  Molecule 1: ECF RNA polymerase sigma-E factor, ECF RNA polymerase sigma factor SigW, ECF RNA polymerase sigma-E factor

Chain A:	77%	5% 18%
M 22 19 19 19 19 19 19 19 19 19 19 19 19 19	A8 18 19 19 19 19 19 19 19 19 19 19 19 19 19	
• Molecule 2: DN	A (5'-D(*GP*TP*AP*AP*AP*A)-3	')
Chain B:	67%	33%
796 197 A100 A101		

### 4.2.4 Score per residue for model 4

Chain A:	79%	•	18%
M1 83 83 83 83 83 84 84 88 88 88 89 89 89 89 89 89 89 89 89 89			
	PROTEIN DATA BANK		

• Molecule 2: DNA (5'-D(\*GP\*TP\*AP\*AP\*AP\*A)-3')

Chain B:	83%	17%
197 197 A 101		

### 4.2.5 Score per residue for model 5

• Molecule 1: ECF RNA polymerase sigma-E factor, ECF RNA polymerase sigma factor SigW, ECF RNA polymerase sigma-E factor

Chain A:	79%		•	18%
M1 83 15 16 16 16 16 76	P 44 7 48 7 48 1 88 1 88 1 89 1 99 1 99 1 99 1 99 1 9			
• Molecule 2	2: DNA (5'-D(*GP*TP*AP*AP*AP*A)-3')			
Chain B:	50%	50%		
796 197 4100 4101				

### 4.2.6 Score per residue for model 6

• Molecule 1: ECF RNA polymerase sigma-E factor,ECF RNA polymerase sigma factor SigW,ECF RNA polymerase sigma-E factor

Chain A:	78%	•	18%
전 12 12 12 12 12 12 12 12 12 12 12 12 12	K32 K32 K32 K32 K32 K32 K32 K32 K32 K32		
• Molecule	e 2: DNA (5'-D(*GP*TP*AP*A	P*AP*A)-3')	
Chain B:	50%	50%	
797 197 100 101			

### 4.2.7 Score per residue for model 7



Chain A:	77%		5%	18%
표 25 8 8 2 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	K32 K32 K32 K32 K85 K87 K87 K87 K87 K87 K87 K87 K87 K87 K87			
• Molecul	e 2: DNA (5'-D(*GP*TP*AP*A	P*AP*A)-3')		
Chain B:	50%	50%		
796 197 8100 8101				

#### 4.2.8 Score per residue for model 8

 $\bullet$  Molecule 1: ECF RNA polymerase sigma-E factor, ECF RNA polymerase sigma factor SigW, ECF RNA polymerase sigma-E factor

Chain A:	75%	7%	18%
표 <u>양 명 </u> 중 명 원 <mark>현</mark>	K32 K32 K32 K32 K32 K32 K33 K33 K33 K33		
• Molecule	e 2: DNA (5'-D(*GP*TP*AP*AP*AP*A)-3')		
Chain B:	67%	17%	17%
796 197 A100 A101			

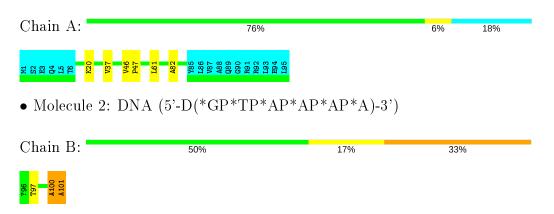
### 4.2.9 Score per residue for model 9 (medoid)

Chain A:	77%	5% 18%
M1 S2 C2 F5 F5 F5 F5 F5 F5 F5 F5 F5 F5 F5 F5 F5	V 46 P 47 A 82 A 83 A 83 A 83 C 94 C 93 C 93 C 93 C 93 C 93 C 93 C 93 C 93	
• Molecule 2:	DNA $(5'-D(*GP*TP*AP*AP*AP*A)-3')$	
Chain B:	67%	33%
796 197 100 100 101		



### 4.2.10 Score per residue for model 10

• Molecule 1: ECF RNA polymerase sigma-E factor,ECF RNA polymerase sigma factor SigW,ECF RNA polymerase sigma-E factor



### 4.2.11 Score per residue for model 11

• Molecule 1: ECF RNA polymerase sigma-E factor, ECF RNA polymerase sigma factor SigW, ECF RNA polymerase sigma-E factor

Chain A:	78%	•	18%
M1 S2 G4 T6 T6 X20 X20	K32 K32 V46 V46 R91 R91 R91 R91 R91 C95 E93 E93 C95 C95 C95 C95 C95 C95 C95 C95 C95 C95		
• Molecule	e 2: DNA (5'-D(*GP*TP*AP*AP*AP*A)-3')		
Chain B:	83%		17%
796 101 A101			

### 4.2.12 Score per residue for model 12

Chain A:	78%	•	18%
44 155 155 155 155 155 155 155 155 155 1	P47 1865 1865 193 193 193 193 193 193		
• Molecule 2: D	$\mathbf{DNA} (5'-\mathbf{D}(^{*}\mathbf{GP}^{*}\mathbf{TP}^{*}\mathbf{AP}^{*}\mathbf{AP}^{*}\mathbf{AP}^{*}\mathbf{A})-3')$		
Chain B:	83%		17%



### 4.2.13 Score per residue for model 13

Chain A:	76%	6%	18%
M1 82 83 83 83 83 83 15 75 83 83 83 847 947	A82 186 186 188 189 193 193 193 193 193		
• Molecule 2: DNA (	5'-D(*GP*TP*AP*AP*AP*A)-3')		
Chain B:	83%		17%
796 197 A101			



# 5 Refinement protocol and experimental data overview (i)

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

Of the 30 calculated structures, 13 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
Amber	refinement	
CYANA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1256
Number of shifts mapped to atoms	1256
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

## 5.1 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	А	636	646	646	2±0
2	В	123	69	69	0±0
All	All	9867	9295	9295	23

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.

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



Atom-1	Atom-2	$Clack(\lambda)$	Distance(Å)	Models	
Atom-1	Atom-2	$\cdot 2 \qquad Clash(Å) \ Distance(Å)$		Worst	Total
1:A:37:VAL:HG23	1:A:82:ALA:HB2	0.48	1.84	10	6
2:B:100:DA:C8	2:B:100:DA:H5"	0.45	2.46	8	1
1:A:46:VAL:N	1:A:47:PRO:HD2	0.43	2.27	11	13
1:A:32:LYS:HA	1:A:32:LYS:HE2	0.42	1.90	11	1
1:A:32:LYS:HE2	1:A:32:LYS:HA	0.41	1.92	12	1
2:B:100:DA:H1'	2:B:101:DA:O5'	0.41	2.16	10	1

## 5.2 Torsion angles (i)

### 5.2.1 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	Perce	entiles
1	А	78/95~(82%)	78±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1014/1235~(82%)	1014~(100%)	0  (0%)	0  (0%)	100	100

There are no Ramachandran outliers.

### 5.2.2 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	Percen	tiles
1	А	69/84~(82%)	$67 \pm 1 (98 \pm 1\%)$	$2\pm1 (2\pm1\%)$	54	92
All	All	897/1092 (82%)	877 (98%)	20 (2%)	54	92

All 3 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)
1	А	20	LYS	12
1	А	32	LYS	6
1	А	61	LEU	2



### 5.2.3 RNA (i)

There are no RNA molecules in this entry.

### 5.3 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.4 Carbohydrates (i)

There are no carbohydrates in this entry.

### 5.5 Ligand geometry (i)

There are no ligands in this entry.

## 5.6 Other polymers (i)

There are no such molecules in this entry.

## 5.7 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 83% for the entire structure.

## 6.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *complex.str* 

### 6.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1256
Number of shifts mapped to atoms	1256
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

### 6.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	${\bf Correction}\pm{\bf precision},ppm$	Suggested action
$^{13}C_{\alpha}$	92	$-0.43 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}C_{\beta}$	89	$0.39 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}C'$	84	$-0.22 \pm 0.12$	None needed ( $< 0.5$ ppm)
<sup>15</sup> N	90	$0.47 \pm 0.34$	None needed ( $< 0.5$ ppm)

### 6.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 85%, i.e. 948 atoms were assigned a chemical shift out of a possible 1111. 18 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	380/386~(98%)	154/154~(100%)	150/156~(96%)	76/76~(100%)
Sidechain	459/540~(85%)	282/314~(90%)	168/193~(87%)	9/33~(27%)

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	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}\mathbf{N}$
Aromatic	68/87~(78%)	44/46~(96%)	23/39~(59%)	1/2~(50%)
Overall	948/1111 (85%)	521/572~(91%)	341/423~(81%)	86/116 (74%)

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The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1106 atoms were assigned a chemical shift out of a possible 1336. 21 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}$ N
Backbone	448/471~(95%)	182/188~(97%)	176/190~(93%)	90/93~(97%)
Sidechain	543/672~(81%)	335/391~(86%)	197/240~(82%)	11/41~(27%)
Aromatic	74/95~(78%)	48/50~(96%)	25/43~(58%)	1/2~(50%)
Overall	1106/1336~(83%)	606/687~(88%)	398/508~(78%)	102/141~(72%)

### 6.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

### 6.1.5 Random Coil Index (RCI) plots (1)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

