

# Full wwPDB NMR Structure Validation Report (i)

#### Feb 9, 2022 – 07:53 AM EST

PDB ID	:	1EDL
Title	:	STAPHYLOCOCCAL PROTEIN A E-DOMAIN (-60), NMR, 22 STRUC-
		TURES
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Deposited on	:	1996-07-22

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

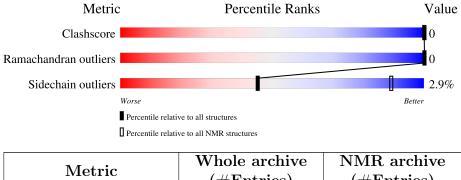
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

## 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 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	(#Entries)	(#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	Qualit	ty of chain	
1	А	56	57%	•	41%



## 2 Ensemble composition and analysis (i)

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:19-A:36 (18)	0.14	1		
2	A:39-A:53 (15)	0.09	14		

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



## 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 844 atoms, of which 408 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called STAPHYLOCOCCAL PROTEIN A.

Mol	Chain	Residues	Atoms			Trace			
1	٨	56	Total	С	Η	Ν	Ο	S	0
	A	56	844	263	408	80	92	1	0

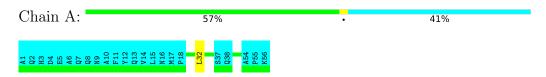


## 4 Residue-property plots (i)

### 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: STAPHYLOCOCCAL PROTEIN A

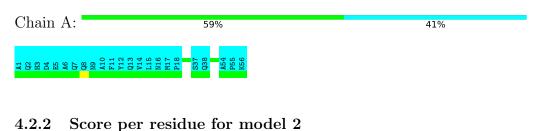


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1 (medoid)

### • Molecule 1: STAPHYLOCOCCAL PROTEIN A







### 4.2.3 Score per residue for model 3

• Molecule 1: STAPHYLOCOCCAL PROTEIN A

Chain A:	57% .	41%
A1 Q2 Q2 Q3 Q3 Q3 F11 F11 V12 V13 V13	L15 N16 M17 M17 8337 8337 855 K56 K56	
4.2.4 Score per	residue for model 4	
• Molecule 1: STA	PHYLOCOCCAL PROTEIN A	
Chain A:	55% •	41%
A1 92 93 94 95 97 97 710 712 712 712	L15 L15 M16 M16 M16 M18 C33 C33 A54 A54 A55 K56	
4.2.5 Score per	residue for model 5	
• Molecule 1: STA	PHYLOCOCCAL PROTEIN A	
Chain A:	59%	41%
A1 41 42 42 443 46 46 41 40 41 41 41 41 41 41 41 41 41 41 41 41 41	L15 M16 M17 M17 M18 M18 M18 M18 M18 M18 M18 M18 M18 M18	
4.2.6 Score per	residue for model 6	
• Molecule 1: STA	PHYLOCOCCAL PROTEIN A	
Chain A:	59%	41%
A1 Q2 Q2 Q4 Q4 Q1 V12 V12 V12 V13	L15 M16 M17 M17 833 P55 P555 K56	
4.2.7 Score per	residue for model 7	
• Molecule 1: STA	PHYLOCOCCAL PROTEIN A	
Chain A:	57% •	41%
A1 42 43 45 46 46 46 410 712 712 712 713 713	L15 L15 M16 M17 M17 L32 Q38 Q38 Q38 Q38 C56 K56	

D W I D E D B DATA BANK

### 4.2.8 Score per residue for model 8

Chain A	A:	57% •	41%
A 1 Q 2 D 4 3 5 5 5 7 4 3 5 5 5 5 5 5 5 5 6 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7	47 47 48 410 413 413 413 413 413 713 713 713 713 713 713 713 713 713 7	L32 337 A64 F55 K566	
4.2.9	Score per resid	lue for model 9	
• Mole	cule 1: STAPHYL	LOCOCCAL PROTEIN	А
Chain A	A:	59%	41%
A1 A2 A2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	40 48 410 410 411 411 411 411 411 411 718 718 718	837 938 944 755 755	
4.2.10	Score per resi	idue for model 10	
• Mole	cule 1: STAPHYL	OCOCCAL PROTEIN	А
Chain A	A:	57% •	41%
A1 Q2 55 55 55	AC 470 481 410 411 411 411 411 718 718 718	L32 337 A54 K56 K56	
4.2.11	Score per resi	idue for model 11	
• Moleo	cule 1: STAPHYL	OCOCCAL PROTEIN	А
Chain A	A:	57% •	41%
A1 0 4 5 5 5 5 7 4 2 4 2 4 2 4 2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	40 40 41 41 41 41 41 41 41 41 41 41 41 41 41	132 337 854 A54 K56 K56	
4.2.12	Score per resi	idue for model 12	
• Moleo	cule 1: STAPHYL	OCOCCAL PROTEIN	А
Chain A	A:	59%	41%
A1 Q2 D4 D4 35	47 47 410 410 411 411 411 411 711 711 711 718 718	837 938 755 755 755	



### 4.2.13 Score per residue for model 13

Chain A:	57%	• 41%
A1 42 43 46 46 46 410 88 711 711 711 711 711	V14 L15 N17 P18 P18 P18 P18 P18 P18 P18 P18	
4.2.14 Score p	er residue for model 14	
• Molecule 1: STA	APHYLOCOCCAL PROTEIN	N A
Chain A:	57%	• 41%
A1 42 43 43 45 46 46 47 410 712 712 712 712	V14 N15 N17 N17 N17 N17 N17 N17 N16 N16 N16 N16 N16 N16 N16 N16 N16 N16	
4.2.15 Score p	er residue for model 15	
• Molecule 1: STA	APHYLOCOCCAL PROTEIN	N A
Chain A:	55% •	41%
A1 41 42 42 46 46 46 46 46 41 41 41 41 41 41 32 41 32 41 32 41 32 41 41 41 41 41 41 41 41 41 41 41 41 41	V14 N16 M17 M17 M17 233 233 233 755 755 755 755 755 755 755 755 755 7	
4.2.16 Score p	er residue for model 16	
• Molecule 1: STA	APHYLOCOCCAL PROTEIN	N A
Chain A:	59%	41%
A1 42 43 44 44 46 46 46 46 47 11 711 712 713 713 713 713 713 713 713 713 713 713	V14 M17 M17 R117 R137 R55 K55 K55	
4.2.17 Score p	er residue for model 17	
• Molecule 1: STA	APHYLOCOCCAL PROTEIN	N A
Chain A:	57%	• 41%
A1 42 43 46 46 46 410 88 711 711 711 711 713	V14 L15 N17 837 237 238 438 454 K56 K56	



### 4.2.18 Score per residue for model 18

Chain A:	57%	·	41%	_
A1 42 42 43 46 46 43 41 43 41 41 41 41 41 41 41 41 41 41 41 41 41	P 18 537 337 454 755 755 755 755			
4.2.19 Score per re	esidue for model	19		
• Molecule 1: STAPHY	LOCOCCAL PRO	DTEIN A		
Chain A:	57%	·	41%	_
A1 42 42 45 46 46 46 710 712 711 711 711 711 711 711 712 711 712 711 712 711 712 713	P18 337 337 454 855 855 855 855			
4.2.20 Score per re	esidue for model	20		
• Molecule 1: STAPHY	YLOCOCCAL PRO	DTEIN A		
Chain A:	57%	·	41%	_
A1 Q2 H3 E5 A6 Q7 Q7 A10 M16 M15 M17 M17	P18 132 132 132 132 132 132 132 132			



## 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DG FOLLOWED BY RESTRAINED MOLECULAR DYNAMICS*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *LOWEST RESTRAINT VIOLATION ENERGY*.

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

Software name	Classification	Version
Discover	refinement	
DGII	structure solution	
DISCOVER (BIOSYM)	structure solution	(BIOSYM)

No chemical shift data was provided.



## 6 Model quality (i)

## 6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

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	А	252	239	239	0±0
All	All	5040	4780	4780	-

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 -.

There are no clashes.

### 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	Favoured Allowed		Percentiles
1	А	33/56~(59%)	$33 \pm 0 (99 \pm 1\%)$	0±0 (1±1%)	0±0 (0±0%)	100 100
All	All	660/1120~(59%)	656~(99%)	4 (1%)	0 (0%)	100 100

There are no Ramachandran outliers.



#### 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	
1	А	28/47~(60%)	$27 \pm 1 (97 \pm 2\%)$	$1\pm1 (3\pm2\%)$	45 8	39
All	All	560/940~(60%)	544 (97%)	16 (3%)	45 8	39

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	32	LEU	13
1	А	48	LYS	2
1	А	47	GLN	1

#### 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 monosaccharides 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 (i)

No chemical shift data were provided

