



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 20, 2024 – 07:17 PM EDT

PDB ID : 2KQW  
Title : SARS coronavirus-unique domain (SUD): Three-domain molecular architecture in solution and RNA binding. II: Structure of the SUD-C domain of SUD-MC  
Authors : Johnson, M.A.; Chatterjee, A.; Wuthrich, K.; Joint Center for Structural Genomics (JCSG)  
Deposited on : 2009-11-19

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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) : 2.36.2

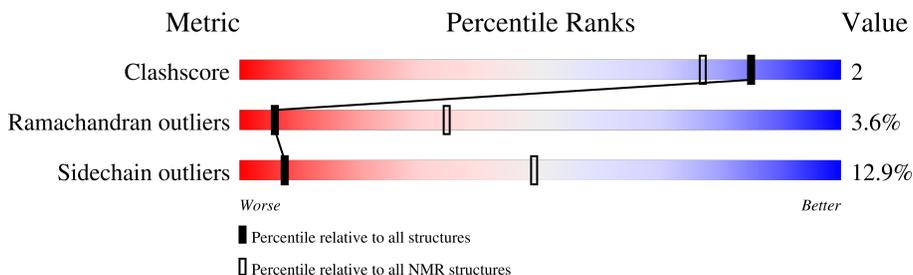
# 1 Overall quality at a glance

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	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  $\geq 3$ , 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	A	198	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:132-A:198 (67)	0.70	10

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 4 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1062 atoms, of which 523 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Non-structural protein 3.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	67	1062	343	523	88	108	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P0C6U8
A	2	SER	-	expression tag	UNP P0C6U8
A	3	HIS	-	expression tag	UNP P0C6U8
A	4	MET	-	expression tag	UNP P0C6U8





Chain A:  27% 6% 66%

GLY SER HIS MET GLY THR VAL SER TRP ASN LEU ARG MET LEU HIS ALA ALA GLU THR ARG LYS LEU MET PRO ILE TYR CYS MET ASP VAL ARG ALA ILE MET LEU ALA THR ILE GLN ARG LYS TYR MET LYS GLY ILE LYS LEU THR VAL ASP TYR VAL ARG PHE THR

TYR THR SER LYS GLU TYR VAL ALA SER TRP ILE ASN LEU THR LYS LEU ASN LEU ASN ALA GLU PRO LEU VAL THR LYS MET PRO ILE GLY TYR VAL THR HIS VAL PHE ASN LEU MET LEU GLU ALA THR ILE ASN LEU ALA ARG CYS MET ARG SER LEU LYS THR VAL ASP TYR VAL ARG PHE THR

THR TYR ASN GLY TYR LEU THR SER SER SER LYS T132 S133 E134 E135 V141 F163 L164 R165 R166 K169 S177 S189 L190 D191 K192 L193 K194 S195 L196 L197 S198

#### 4.2.6 Score per residue for model 6

- Molecule 1: Non-structural protein 3

Chain A:  30% 66%

GLY SER HIS MET THR VAL SER TRP ASN LEU ARG MET LEU HIS ALA ALA GLU THR ARG LYS LEU MET PRO ILE TYR CYS MET THR ASP VAL ARG ALA ILE MET LEU ALA THR ILE GLN ARG LYS TYR LYS ILE LYS LEU THR VAL ASP TYR VAL ARG PHE THR

TYR THR SER LYS GLU TYR VAL ALA SER TRP ILE ASN LEU THR LYS LEU ASN LEU ASN ALA GLU PRO LEU VAL THR LYS MET PRO ILE GLY TYR VAL THR HIS VAL PHE ASN LEU MET LEU GLU ALA THR ILE ASN LEU ALA ARG CYS MET ARG SER LEU LYS THR VAL ASP TYR VAL ARG PHE THR

THR TYR ASN GLY TYR LEU THR SER SER SER LYS T132 R166 H173 S177 P178 V179 D184 S195 L196 L197 S198

#### 4.2.7 Score per residue for model 7

- Molecule 1: Non-structural protein 3

Chain A:  27% 7% 66%

GLY SER HIS MET THR VAL SER TRP ASN LEU ARG MET LEU HIS ALA ALA GLU THR ARG LYS LEU MET PRO ILE TYR CYS MET THR ASP VAL ARG ALA ILE MET LEU ALA THR ILE GLN ARG LYS TYR LYS ILE LYS LEU THR VAL ASP TYR VAL ARG PHE THR

TYR THR SER LYS GLU TYR VAL ALA SER TRP ILE ASN LEU THR LYS LEU ASN LEU ASN ALA GLU PRO LEU VAL THR LYS MET PRO ILE GLY TYR VAL THR HIS VAL PHE ASN LEU MET LEU GLU ALA THR ILE ASN LEU ALA ARG CYS MET ARG SER LEU LYS THR VAL ASP TYR VAL ARG PHE THR

THR TYR ASN GLY TYR LEU THR SER SER SER LYS T132 S146 Y147 R148 S153 G154 Q155 R156 R166 H173 T174 L175 E176 S177 P178 H182 L190 S195 L196 L197 S198

#### 4.2.8 Score per residue for model 8

- Molecule 1: Non-structural protein 3

Chain A:  29% 66%



THR THR SER LYS PRO VAL ALA SER SER ILE ILE THR LYS LEU ASN SER SER ASN LEU LEU ASN GLU PRO LEU VAL THR MET PRO ILE GLY TYR VAL THR HIS GLY PHE ASN LEU GLU ALA ALA ARG CYS MET ARG SER LEU LYS ALA PRO ALA VAL SER VAL SER PRO ASP ALA VAL THR



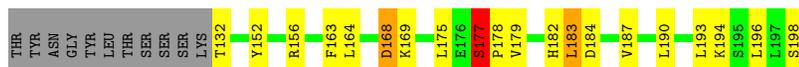
#### 4.2.12 Score per residue for model 12

- Molecule 1: Non-structural protein 3



GLY SER HIS MET GLY TYR THR VAL SER TRP ASN LEU ILE ILE THR ARG GLU MET LEU ASN SER ALA HIS LEU ASN ALA ALA GLU GLU THR LEU VAL ARG THR LYS LEU MET PRO ILE GLY TYR CYS MET THR ASP VAL ARG ALA ILE MET LEU ALA THR ILE GLN ARG LYS TYR LYS GLY ILE LYS ALA ILE ILE PRO GLN GLU GLY ILE ILE SER VAL ASP TYR SER SER GLY VAL ARG PHE PHE

THR THR SER LYS PRO VAL ALA SER SER ILE ILE THR LYS LEU ASN SER ALA HIS LEU ASN ALA ALA GLU PRO LEU VAL THR MET PRO ILE GLY TYR VAL THR ASP HIS VAL ARG ALA ILE ASN LEU GLU ALA THR ILE ALA ARG CYS MET TYR LYS ARG SER LEU ILE LYS ALA ILE ILE PRO GLN GLU VAL VAL SER VAL VAL TYR SER SER PRO ASP ARG PHE PHE



#### 4.2.13 Score per residue for model 13

- Molecule 1: Non-structural protein 3



GLY SER HIS MET GLY TYR THR VAL SER TRP ASN LEU ILE ILE THR ARG GLU MET LEU ASN SER ALA HIS LEU ASN ALA ALA GLU GLU THR LEU VAL ARG THR LYS LEU MET PRO ILE GLY TYR CYS MET THR ASP VAL ARG ALA ILE MET LEU ALA THR ILE ALA ARG CYS LYS TYR LYS ARG SER LEU ILE LYS ALA ILE ILE PRO GLN GLU VAL VAL SER VAL ASP TYR SER SER GLY VAL ARG PHE PHE

THR THR SER LYS PRO VAL ALA SER SER ILE ILE THR LYS LEU ASN SER ALA HIS LEU ASN ALA ALA GLU PRO LEU VAL THR MET PRO ILE GLY TYR VAL THR ASP HIS VAL ARG ALA ILE ASN LEU GLU ALA THR ILE ALA ARG CYS LYS TYR LYS ARG SER LEU ILE LYS ALA ILE ILE PRO GLN GLU VAL VAL SER VAL VAL TYR SER SER PRO ASP ARG PHE PHE



#### 4.2.14 Score per residue for model 14

- Molecule 1: Non-structural protein 3



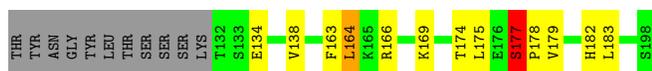
GLY SER HIS MET GLY TYR THR VAL SER TRP ASN LEU ILE ILE THR ARG GLU MET LEU ASN SER ALA HIS LEU ASN ALA ALA GLU GLU THR LEU VAL ARG THR LYS LEU MET PRO ILE GLY TYR CYS MET THR ASP VAL ARG ALA ILE MET LEU ALA THR ILE ALA ARG CYS LYS TYR LYS ARG SER LEU ILE LYS ALA ILE ILE PRO GLN GLU VAL VAL SER VAL ASP TYR SER SER GLY VAL ARG PHE PHE

THR THR SER LYS PRO VAL ALA SER SER ILE ILE THR LYS LEU ASN SER ALA HIS LEU ASN ALA ALA GLU PRO LEU VAL THR MET PRO ILE GLY TYR VAL THR ASP HIS VAL ARG ALA ILE ASN LEU GLU ALA THR ILE ALA ARG CYS MET TYR LYS ARG SER LEU ILE LYS ALA ILE ILE PRO GLN GLU VAL VAL SER VAL VAL TYR SER SER PRO ASP ARG PHE PHE



#### 4.2.15 Score per residue for model 15

- Molecule 1: Non-structural protein 3



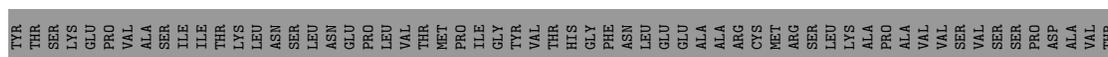
#### 4.2.16 Score per residue for model 16

- Molecule 1: Non-structural protein 3



#### 4.2.17 Score per residue for model 17

- Molecule 1: Non-structural protein 3





## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
UNIO	refinement	
CANDID	refinement	
OPALp	refinement	

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	A	0.62±0.01	0±0/550 ( 0.0± 0.0%)	1.10±0.05	1±1/742 ( 0.1± 0.1%)
All	All	0.62	0/11000 ( 0.0%)	1.10	16/14840 ( 0.1%)

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	A	0.0±0.0	1.0±1.0
All	All	0	20

There are no bond-length outliers.

All 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	A	197	LEU	CB-CG-CD2	8.44	125.34	111.00	8	2
1	A	166	ARG	NE-CZ-NH2	-6.36	117.12	120.30	7	2
1	A	193	LEU	CD1-CG-CD2	6.13	128.89	110.50	16	3
1	A	197	LEU	CD1-CG-CD2	6.08	128.75	110.50	17	1
1	A	148	ARG	NE-CZ-NH2	-6.03	117.29	120.30	20	1
1	A	173	HIS	CA-CB-CG	5.42	122.81	113.60	17	2
1	A	156	ARG	NE-CZ-NH2	-5.28	117.66	120.30	11	1
1	A	147	TYR	CB-CG-CD2	-5.26	117.84	121.00	18	1
1	A	152	TYR	CB-CG-CD2	-5.24	117.86	121.00	12	1
1	A	148	ARG	NE-CZ-NH1	5.18	122.89	120.30	14	1
1	A	166	ARG	NE-CZ-NH1	5.06	122.83	120.30	7	1

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	A	148	ARG	Sidechain	6
1	A	166	ARG	Sidechain	6
1	A	152	TYR	Sidechain	4
1	A	156	ARG	Sidechain	3
1	A	163	PHE	Sidechain	1

## 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	A	539	523	522	2±2
All	All	10780	10460	10440	46

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:LEU:HD13	1:A:184:ASP:HB3	0.64	1.67	12	1
1:A:193:LEU:CD1	1:A:197:LEU:HD21	0.57	2.29	20	3
1:A:182:HIS:CD2	1:A:187:VAL:HG22	0.57	2.35	12	2
1:A:141:VAL:HG11	1:A:164:LEU:HD11	0.56	1.77	4	1
1:A:174:THR:HG23	1:A:180:GLU:OE1	0.55	2.02	14	1
1:A:174:THR:HG23	1:A:180:GLU:CD	0.54	2.23	14	1
1:A:163:PHE:CD2	1:A:164:LEU:HD23	0.52	2.38	5	3
1:A:188:LEU:HD12	1:A:196:LEU:HD11	0.48	1.85	13	1
1:A:175:LEU:H	1:A:175:LEU:HD22	0.48	1.69	11	1
1:A:197:LEU:H	1:A:197:LEU:HD22	0.47	1.70	17	1
1:A:141:VAL:HG11	1:A:164:LEU:HD21	0.47	1.86	5	1
1:A:163:PHE:CG	1:A:164:LEU:HD23	0.47	2.45	5	1
1:A:138:VAL:HA	1:A:163:PHE:CZ	0.46	2.45	14	5
1:A:188:LEU:CD1	1:A:196:LEU:HD11	0.46	2.40	13	1
1:A:193:LEU:O	1:A:197:LEU:HD22	0.46	2.10	13	2
1:A:194:LYS:HA	1:A:197:LEU:CD2	0.46	2.41	17	1
1:A:169:LYS:HB3	1:A:183:LEU:HD11	0.44	1.90	15	2
1:A:177:SER:N	1:A:178:PRO:HA	0.43	2.28	12	12
1:A:197:LEU:HD22	1:A:197:LEU:H	0.42	1.75	16	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:PHE:CE2	1:A:164:LEU:CD2	0.41	3.02	15	1
1:A:137:PHE:CD1	1:A:194:LYS:HE2	0.41	2.49	18	1
1:A:190:LEU:HD11	1:A:194:LYS:HE3	0.41	1.92	12	1
1:A:160:GLY:HA2	1:A:175:LEU:HD21	0.41	1.92	3	1
1:A:179:VAL:HG12	1:A:181:PHE:CZ	0.40	2.51	8	1

## 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	
1	A	65/198 (33%)	55±2 (85±3%)	8±2 (12±3%)	2±1 (4±1%)	6	34
All	All	1300/3960 (33%)	1099 (85%)	154 (12%)	47 (4%)	6	34

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	177	SER	20
1	A	179	VAL	15
1	A	174	THR	4
1	A	148	ARG	2
1	A	153	SER	1
1	A	168	ASP	1
1	A	134	GLU	1
1	A	189	SER	1
1	A	160	GLY	1
1	A	185	GLY	1

### 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	A	61/174 (35%)	53±3 (87±4%)	8±3 (13±4%)	7	49
All	All	1220/3480 (35%)	1063 (87%)	157 (13%)	7	49

All 37 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	A	177	SER	20
1	A	156	ARG	14
1	A	196	LEU	13
1	A	132	THR	8
1	A	166	ARG	8
1	A	151	SER	7
1	A	184	ASP	7
1	A	195	SER	7
1	A	175	LEU	6
1	A	193	LEU	6
1	A	135	GLU	4
1	A	153	SER	4
1	A	169	LYS	4
1	A	180	GLU	4
1	A	164	LEU	4
1	A	189	SER	4
1	A	149	ASP	3
1	A	191	ASP	3
1	A	190	LEU	3
1	A	146	SER	2
1	A	155	GLN	2
1	A	165	LYS	2
1	A	194	LYS	2
1	A	133	SER	2
1	A	198	SER	2
1	A	173	HIS	2
1	A	182	HIS	2
1	A	140	THR	2
1	A	168	ASP	2
1	A	139	GLU	1
1	A	152	TYR	1
1	A	183	LEU	1
1	A	158	GLU	1
1	A	197	LEU	1
1	A	147	TYR	1
1	A	148	ARG	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	192	LYS	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

No chemical shift data were provided