



# wwPDB X-ray Structure Validation Summary Report

Oct 11, 2023 – 03:03 PM EDT

PDB ID : 8UFL  
Title : Crystal Structure of SARS-Unique Domain (SUD) of Nsp3 from SARS coronavirus  
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Deposited on : 2023-10-04  
Resolution : 2.51 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

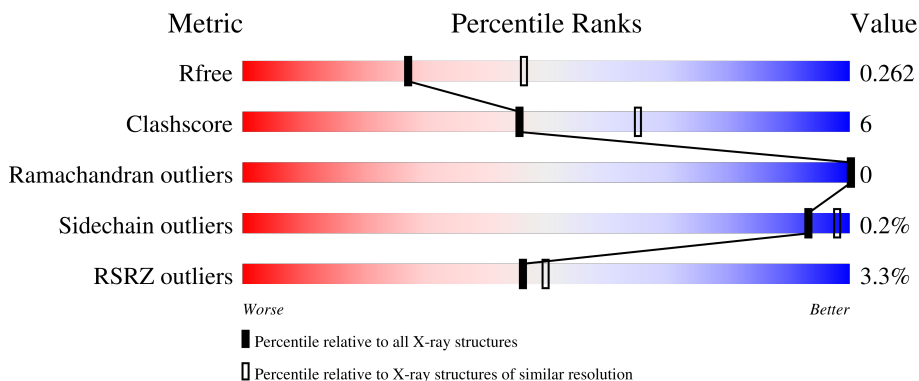
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

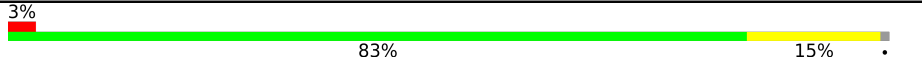
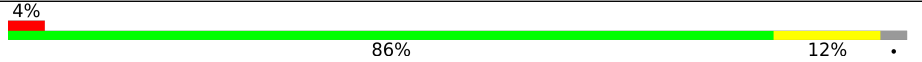
The reported resolution of this entry is 2.51 Å.

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	267	 3% 83% 15%
1	B	267	 4% 86% 12%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4268 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Papain-like protease nsp3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2058	1311	337	393	17	0	3	0
1	B	260	2018	1286	329	387	16	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	SER	-	expression tag	UNP P0C6U8
A	387	ASN	-	expression tag	UNP P0C6U8
A	388	ALA	-	expression tag	UNP P0C6U8
B	386	SER	-	expression tag	UNP P0C6U8
B	387	ASN	-	expression tag	UNP P0C6U8
B	388	ALA	-	expression tag	UNP P0C6U8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	Cl	0	0
			9	9		
2	B	7	Total	Cl	0	0
			7	7		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

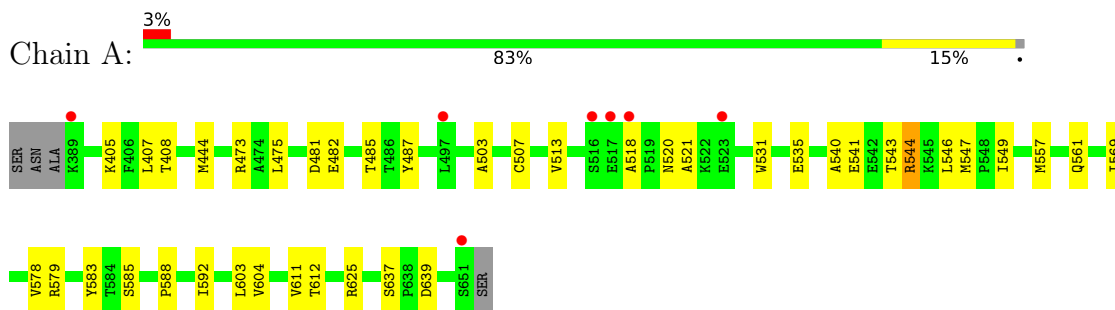
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	75	Total O 75 75	0	2
4	B	50	Total O 51 51	0	1

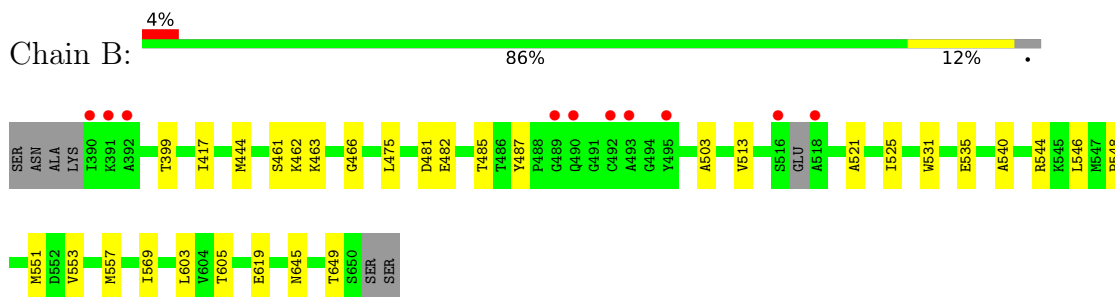
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Papain-like protease nsp3



- Molecule 1: Papain-like protease nsp3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.70Å 84.86Å 93.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 2.51 29.80 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.80-2.51) 99.7 (29.80-2.51)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.213 , 0.267 0.213 , 0.262	Depositor DCC
$R_{free}$ test set	928 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtrriage
Anisotropy	0.089	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL

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 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	0.66	0/2094	0.77	0/2830
1	B	0.66	0/2053	0.77	0/2777
All	All	0.66	0/4147	0.77	0/5607

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2058	0	2105	34	0
1	B	2018	0	2053	28	0
2	A	9	0	0	1	0
2	B	7	0	0	1	0
3	A	25	0	0	0	0
3	B	25	0	0	1	0
4	A	75	0	0	0	0
4	B	51	0	0	0	0
All	All	4268	0	4158	53	0

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 6.

The worst 5 of 53 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LEU:HD12	1:B:503:ALA:HB1	1.68	0.75
1:B:525:ILE:HD11	1:B:649:THR:HG23	1.72	0.71
1:A:444:MET:CE	1:B:553:VAL:HG22	2.21	0.69
1:B:525:ILE:HG23	1:B:645:ASN:ND2	2.09	0.68
1:A:585:SER:HB2	1:B:417:ILE:HG13	1.76	0.67

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	264/267 (99%)	249 (94%)	15 (6%)	0	100	100
1	B	257/267 (96%)	244 (95%)	13 (5%)	0	100	100
All	All	521/534 (98%)	493 (95%)	28 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	229/229 (100%)	228 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	224/229 (98%)	224 (100%)	0	100	100
All	All	453/458 (99%)	452 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 16 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	B	710	-	4,4,4	0.34	0	6,6,6	0.05	0
3	SO4	A	711	-	4,4,4	0.38	0	6,6,6	0.06	0
3	SO4	A	713	-	4,4,4	0.38	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	708	-	4,4,4	0.38	0	6,6,6	0.07	0
3	SO4	B	709	-	4,4,4	0.38	0	6,6,6	0.06	0
3	SO4	A	714	-	4,4,4	0.38	0	6,6,6	0.05	0
3	SO4	A	710	-	4,4,4	0.38	0	6,6,6	0.07	0
3	SO4	B	711	-	4,4,4	0.38	0	6,6,6	0.05	0
3	SO4	B	712	-	4,4,4	0.37	0	6,6,6	0.06	0
3	SO4	A	712	-	4,4,4	0.39	0	6,6,6	0.05	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	712	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	263/267 (98%)	-0.07	7 (2%) 54 58	24, 41, 72, 107	0
1	B	260/267 (97%)	0.24	10 (3%) 40 43	26, 56, 96, 125	0
All	All	523/534 (97%)	0.09	17 (3%) 46 50	24, 47, 88, 125	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	GLN	7.2
1	B	390	ILE	5.8
1	B	391	LYS	4.9
1	B	392	ALA	4.3
1	B	495	TYR	3.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	702	1/1	0.68	0.23	74,74,74,74	0
2	CL	A	701	1/1	0.70	0.19	85,85,85,85	0
3	SO4	A	713	5/5	0.71	0.28	98,103,118,119	0
3	SO4	B	712	5/5	0.77	0.24	54,101,110,112	0
2	CL	A	703	1/1	0.82	0.14	73,73,73,73	0
2	CL	A	708	1/1	0.82	0.10	75,75,75,75	0
3	SO4	A	714	5/5	0.88	0.29	71,71,92,109	0
2	CL	A	706	1/1	0.91	0.07	60,60,60,60	0
2	CL	B	705	1/1	0.91	0.11	72,72,72,72	0
3	SO4	B	708	5/5	0.91	0.14	66,75,93,105	0
3	SO4	A	712	5/5	0.91	0.25	86,96,97,98	0
2	CL	B	706	1/1	0.92	0.23	72,72,72,72	0
2	CL	B	704	1/1	0.92	0.22	70,70,70,70	0
3	SO4	B	709	5/5	0.93	0.17	55,68,70,74	0
3	SO4	B	711	5/5	0.93	0.13	82,84,92,94	0
2	CL	B	702	1/1	0.93	0.17	60,60,60,60	0
2	CL	A	709	1/1	0.94	0.26	57,57,57,57	0
2	CL	A	707	1/1	0.94	0.07	67,67,67,67	0
2	CL	A	704	1/1	0.94	0.27	63,63,63,63	0
3	SO4	B	710	5/5	0.95	0.13	48,52,62,78	0
2	CL	A	705	1/1	0.96	0.27	77,77,77,77	0
3	SO4	A	711	5/5	0.96	0.18	55,61,75,81	0
2	CL	B	701	1/1	0.97	0.04	62,62,62,62	0
2	CL	B	703	1/1	0.97	0.06	67,67,67,67	0
3	SO4	A	710	5/5	0.98	0.09	37,38,44,46	0
2	CL	B	707	1/1	0.98	0.29	64,64,64,64	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.