

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 15, 2023 – 03:26 PM EDT

PDB ID : 7U1R

Title: SARS-CoV-2 Spike-derived peptide S1185-1193 K1191N mutant (RL-

NEVANNL) presented by HLA-A\*02:01

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Deposited on : 2022-02-22

Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

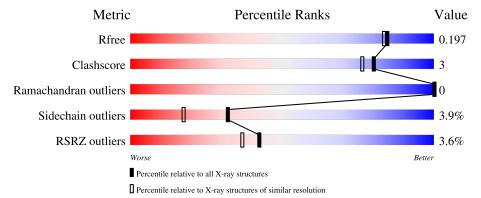
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.80 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 >=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 <=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	٨	0.05	2%						
1	А	365	69%	6%	24%				
	D	100	5%						
2	В	100	91%		8% •				
			11%						
3	С	9	56%	33%	11%				



# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 3458 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 HLA class I antigen.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	276	Total 2318	C 1454	N 421	O 434	S 9	0	9	0

• Molecule 2 is a protein called Beta-2-microglobulin.

$\mathbf{Mol}$	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	100	Total 844	C 539	N 141	O 160	S 4	0	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	0	MET	-	initiating methionine	UNP P61769

• Molecule 3 is a protein called Spike protein S2' peptide.

N	/Iol	Chain	Residues	1	Ator	$\mathbf{n}\mathbf{s}$		ZeroOcc	AltConf	Trace
	3	С	9	Total 78	C 46	N 16	O 16	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
С	7	ASN	LYS	engineered mutation	UNP P0DTC2	

• Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cd 1 1	0	0

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

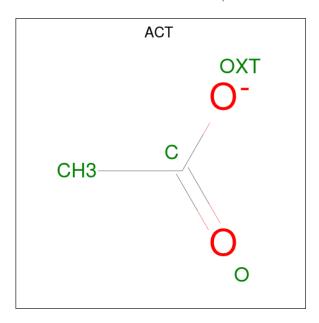


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0

• Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0

• Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	В	1	Total C 4 2	O 2	0	0

• Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	1	Total Cl 1 1	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	149	Total O 149 149	0	0

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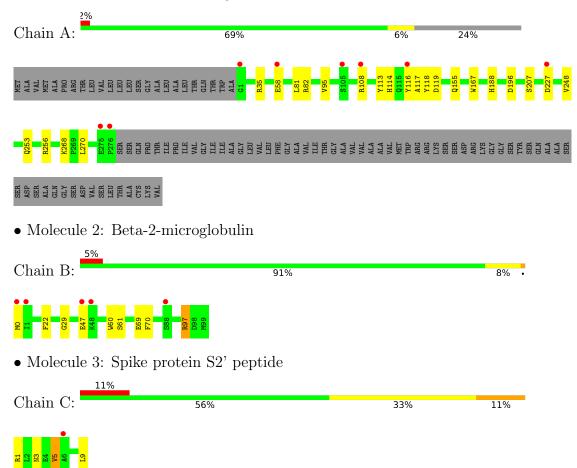
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	57	Total O 57 57	0	0
9	С	4	Total O 4 4	0	0



# 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: HLA class I antigen





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	59.59Å 78.54Å 111.26Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.27 - 1.80	Depositor
rtesolution (A)	26.27 - 1.80	EDS
% Data completeness	100.0 (26.27-1.80)	Depositor
(in resolution range)	100.0 (26.27-1.80)	EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.79 (at 1.80Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
D D.	0.183 , 0.196	Depositor
$R, R_{free}$	0.184 , 0.197	DCC
$R_{free}$ test set	2460 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36, 46.8	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3458	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.43% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, ZN, ACT, CD

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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.52	0/2404	0.65	0/3264	
2	В	0.51	0/873	0.64	0/1180	
3	С	0.55	0/80	0.84	0/106	
All	All	0.52	0/3357	0.65	0/4550	

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 (i)

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	2318	0	2181	13	0
2	В	844	0	817	5	0
3	С	78	0	81	4	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	В	4	0	3	0	0
8	В	1	0	0	0	0
9	A	149	0	0	2	0
9	В	57	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	С	4	0	0	0	0
All	All	3458	0	3082	17	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 3.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	$overlap (\AA)$
1:A:116[A]:TYR:CE1	3:C:9:LEU:HD11	2.33	0.64
1:A:114:HIS:HE1	1:A:116[B]:TYR:CE1	2.17	0.63
2:B:97:ARG:HD2	9:B:242:HOH:O	2.04	0.57
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.41	0.56
1:A:167:TRP:CE2	3:C:1:ARG:HD2	2.42	0.55
1:A:58[A]:GLU:HG2	9:A:553:HOH:O	2.07	0.53
1:A:253:GLN:O	1:A:256:ARG:HG3	2.10	0.52
1:A:188:HIS:HD2	9:A:562:HOH:O	1.94	0.50
1:A:114:HIS:CE1	1:A:116[B]:TYR:CE1	2.99	0.49
1:A:155:GLN:HB3	3:C:5:VAL:HG11	1.97	0.46
1:A:119:ASP:HB3	2:B:0:MET:HA	1.98	0.46
1:A:227:ASP:HB3	1:A:248[A]:VAL:CG1	2.46	0.45
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.53	0.43
1:A:227:ASP:HB3	1:A:248[A]:VAL:HG12	2.00	0.43
3:C:3[A]:ASN:OD1	3:C:5:VAL:HG13	2.18	0.43
2:B:29:GLY:HA2	2:B:61[B]:SER:HB3	2.01	0.42
2:B:22:PHE:CE2	2:B:69:GLU:HG2	2.56	0.40

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	Perce	entiles
1	A	$283/365 \ (78\%)$	279 (99%)	4 (1%)	0	100	100
2	В	100/100 (100%)	100 (100%)	0	0	100	100
3	С	8/9 (89%)	8 (100%)	0	0	100	100
All	All	391/474 (82%)	387 (99%)	4 (1%)	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	Rotameric Outliers	
1	A	241/299 (81%)	231 (96%)	10 (4%)	30 16
2	В	97/95 (102%)	94 (97%)	3 (3%)	40 25
3	С	9/8 (112%)	8 (89%)	1 (11%)	6 1
All	All	347/402 (86%)	333 (96%)	14 (4%)	32 16

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	82	ARG
1	A	95[A]	VAL
1	A	95[B]	VAL
1	A	108	ARG
1	A	113	TYR
1	A	196	ASP
1	A	207	SER
1	A	268	LYS
1	A	270	LEU
2	В	47	GLU
2	В	70	PHE
2	В	97	ARG
3	С	5	VAL



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	188	HIS
3	С	7	ASN

#### 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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	В	ond leng	$_{ m gths}$	E	Bond ang	gles
MIOI	Type	Chain	n nes	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
7	ACT	В	101	-	3,3,3	1.25	0	3,3,3	0.71	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.



No monomer is involved in short contacts.

# 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,  $95^{th}$  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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	$276/365\ (75\%)$	-0.12	8 (2%) 51 46	19, 28, 50, 76	0
2	В	100/100 (100%)	0.02	5 (5%) 28 23	21, 30, 60, 74	0
3	С	9/9 (100%)	0.82	1 (11%) 5 4	23, 47, 55, 56	0
All	All	385/474 (81%)	-0.06	14 (3%) 42 37	19, 29, 54, 76	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	A	276	PRO	4.2	
2	В	0	MET	4.2	
2	В	48	LYS	3.8	
3	С	6	ALA	3.6	
1	A	275	GLU	3.4	
2	В	1	ILE	2.8	
1	A	116[A]	TYR	2.8	
2	В	88	SER	2.8	
1	A	1	GLY	2.7	
1	A	105	SER	2.6	
2	В	47	GLU	2.5	
1	A	108	ARG	2.4	
1	A	58[A]	GLU	2.1	
1	A	227	ASP	2.0	

### 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,  $95^{th}$  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	$\operatorname{B-factors}(\mathrm{\AA}^2)$	Q<0.9
7	ACT	В	101	4/4	0.83	0.11	51,54,55,55	0
8	CL	В	102	1/1	0.92	0.07	50,50,50,50	0
6	NA	A	403	1/1	0.95	0.13	39,39,39,39	0
5	ZN	A	402	1/1	0.97	0.03	44,44,44,44	0
4	CD	A	401	1/1	1.00	0.05	27,27,27,27	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

