



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2021 – 02:07 PM JST

PDB ID : 7EU2  
Title : Complex structure of HLA0201 with recognizing SARS-CoV-2 epitope S1  
Authors : Deng, S.; Jin, T.  
Deposited on : 2021-05-15  
Resolution : 2.80 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.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
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) : 2.23.1

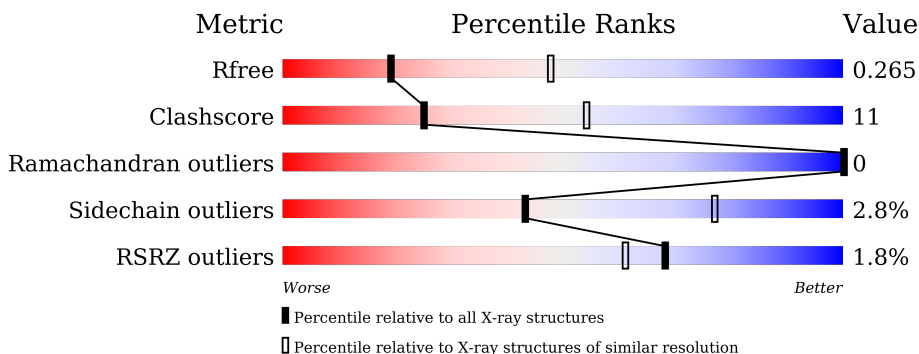
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	308	<div> <div>0%</div> <div>71%</div> <div>19%</div> <div>• 9%</div> </div>
1	D	308	<div> <div>2%</div> <div>69%</div> <div>20%</div> <div>• 9%</div> </div>
2	B	104	<div> <div>0%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>
2	E	104	<div> <div>4%</div> <div>68%</div> <div>25%</div> <div>• 5%</div> </div>
3	C	9	<div> <div>11%</div> <div>56%</div> <div>44%</div> </div>
3	F	9	<div> <div>33%</div> <div>56%</div> <div>11%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6379 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2282	1424	415	434	9			
1	D	279	Total	C	N	O	S	0	0	0
			2275	1419	414	433	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP A0A5H2UU57
A	-3	ASN	-	expression tag	UNP A0A5H2UU57
A	-2	SER	-	expression tag	UNP A0A5H2UU57
A	-1	VAL	-	expression tag	UNP A0A5H2UU57
A	0	ASP	-	expression tag	UNP A0A5H2UU57
A	277	GLY	-	expression tag	UNP A0A5H2UU57
A	278	SER	-	expression tag	UNP A0A5H2UU57
A	279	GLY	-	expression tag	UNP A0A5H2UU57
A	280	LEU	-	expression tag	UNP A0A5H2UU57
A	281	ASN	-	expression tag	UNP A0A5H2UU57
A	282	ASP	-	expression tag	UNP A0A5H2UU57
A	283	ILE	-	expression tag	UNP A0A5H2UU57
A	284	PHE	-	expression tag	UNP A0A5H2UU57
A	285	GLU	-	expression tag	UNP A0A5H2UU57
A	286	ALA	-	expression tag	UNP A0A5H2UU57
A	287	GLN	-	expression tag	UNP A0A5H2UU57
A	288	LYS	-	expression tag	UNP A0A5H2UU57
A	289	ILE	-	expression tag	UNP A0A5H2UU57
A	290	GLU	-	expression tag	UNP A0A5H2UU57
A	291	TRP	-	expression tag	UNP A0A5H2UU57
A	292	HIS	-	expression tag	UNP A0A5H2UU57
A	293	ALA	-	expression tag	UNP A0A5H2UU57
A	294	ALA	-	expression tag	UNP A0A5H2UU57
A	295	ALA	-	expression tag	UNP A0A5H2UU57
A	296	LEU	-	expression tag	UNP A0A5H2UU57

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Chain	Residue	Modelled	Actual	Comment	Reference
A	297	GLU	-	expression tag	UNP A0A5H2UU57
A	298	HIS	-	expression tag	UNP A0A5H2UU57
A	299	HIS	-	expression tag	UNP A0A5H2UU57
A	300	HIS	-	expression tag	UNP A0A5H2UU57
A	301	HIS	-	expression tag	UNP A0A5H2UU57
A	302	HIS	-	expression tag	UNP A0A5H2UU57
A	303	HIS	-	expression tag	UNP A0A5H2UU57
D	-4	MET	-	initiating methionine	UNP A0A5H2UU57
D	-3	ASN	-	expression tag	UNP A0A5H2UU57
D	-2	SER	-	expression tag	UNP A0A5H2UU57
D	-1	VAL	-	expression tag	UNP A0A5H2UU57
D	0	ASP	-	expression tag	UNP A0A5H2UU57
D	277	GLY	-	expression tag	UNP A0A5H2UU57
D	278	SER	-	expression tag	UNP A0A5H2UU57
D	279	GLY	-	expression tag	UNP A0A5H2UU57
D	280	LEU	-	expression tag	UNP A0A5H2UU57
D	281	ASN	-	expression tag	UNP A0A5H2UU57
D	282	ASP	-	expression tag	UNP A0A5H2UU57
D	283	ILE	-	expression tag	UNP A0A5H2UU57
D	284	PHE	-	expression tag	UNP A0A5H2UU57
D	285	GLU	-	expression tag	UNP A0A5H2UU57
D	286	ALA	-	expression tag	UNP A0A5H2UU57
D	287	GLN	-	expression tag	UNP A0A5H2UU57
D	288	LYS	-	expression tag	UNP A0A5H2UU57
D	289	ILE	-	expression tag	UNP A0A5H2UU57
D	290	GLU	-	expression tag	UNP A0A5H2UU57
D	291	TRP	-	expression tag	UNP A0A5H2UU57
D	292	HIS	-	expression tag	UNP A0A5H2UU57
D	293	ALA	-	expression tag	UNP A0A5H2UU57
D	294	ALA	-	expression tag	UNP A0A5H2UU57
D	295	ALA	-	expression tag	UNP A0A5H2UU57
D	296	LEU	-	expression tag	UNP A0A5H2UU57
D	297	GLU	-	expression tag	UNP A0A5H2UU57
D	298	HIS	-	expression tag	UNP A0A5H2UU57
D	299	HIS	-	expression tag	UNP A0A5H2UU57
D	300	HIS	-	expression tag	UNP A0A5H2UU57
D	301	HIS	-	expression tag	UNP A0A5H2UU57
D	302	HIS	-	expression tag	UNP A0A5H2UU57
D	303	HIS	-	expression tag	UNP A0A5H2UU57

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	E	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			

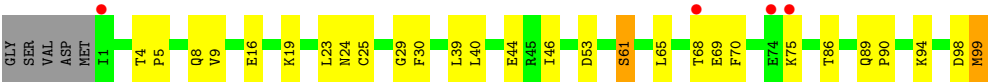
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P61769
B	-3	SER	-	expression tag	UNP P61769
B	-2	VAL	-	expression tag	UNP P61769
B	-1	ASP	-	expression tag	UNP P61769
B	0	MET	-	expression tag	UNP P61769
E	-4	GLY	-	expression tag	UNP P61769
E	-3	SER	-	expression tag	UNP P61769
E	-2	VAL	-	expression tag	UNP P61769
E	-1	ASP	-	expression tag	UNP P61769
E	0	MET	-	expression tag	UNP P61769

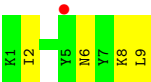
- Molecule 3 is a protein called SARS-CoV-2 T-cell Epitope S1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			79	53	12	14			
3	F	9	Total	C	N	O	0	0	0
			79	53	12	14			

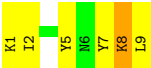




● Molecule 3: SARS-CoV-2 T-cell Epitope S1



● Molecule 3: SARS-CoV-2 T-cell Epitope S1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.49Å 103.34Å 128.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.13 – 2.80 43.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.13-2.80) 91.0 (43.13-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.231 , 0.266 0.231 , 0.265	Depositor DCC
$R_{free}$ test set	1186 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.4	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 31.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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 [i](#)

### 5.1 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 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	0.28	0/2348	0.49	0/3189
1	D	0.35	0/2340	0.54	1/3177 (0.0%)
2	B	0.27	0/859	0.52	0/1162
2	E	0.31	0/851	0.55	0/1152
3	C	0.29	0/80	0.54	0/106
3	F	0.38	0/80	0.78	0/106
All	All	0.31	0/6558	0.53	1/8892 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	ARG	N-CA-C	-5.40	96.42	111.00

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	2282	0	2127	51	0
1	D	2275	0	2120	76	0
2	B	836	0	803	8	0
2	E	828	0	794	19	0
3	C	79	0	83	4	0
3	F	79	0	83	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6379	0	6010	132	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 11.

The worst 5 of 132 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:D:73:THR:HA	3:F:8:LYS:HZ1	1.14	1.08
1:D:73:THR:CA	3:F:8:LYS:HZ1	1.75	0.98
1:D:73:THR:HG23	3:F:8:LYS:NZ	1.83	0.94
1:D:73:THR:HG23	3:F:8:LYS:HZ3	1.33	0.92
1:D:73:THR:HA	3:F:8:LYS:NZ	1.85	0.91

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	278/308 (90%)	269 (97%)	9 (3%)	0	100	100
1	D	277/308 (90%)	267 (96%)	10 (4%)	0	100	100
2	B	98/104 (94%)	93 (95%)	5 (5%)	0	100	100
2	E	97/104 (93%)	92 (95%)	5 (5%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	764/842 (91%)	735 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	236/258 (92%)	232 (98%)	4 (2%)	60	87
1	D	235/258 (91%)	227 (97%)	8 (3%)	37	71
2	B	95/98 (97%)	94 (99%)	1 (1%)	73	92
2	E	94/98 (96%)	89 (95%)	5 (5%)	22	54
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	7 (88%)	1 (12%)	4	14
All	All	676/728 (93%)	657 (97%)	19 (3%)	43	77

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	70	PHE
2	E	99	MET
3	F	8	LYS
2	E	94	LYS
1	D	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	155	GLN
1	D	174	ASN
2	E	8	GLN
2	B	89	GLN
3	C	6	ASN

### 5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

## 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	280/308 (90%)	0.01	3 (1%) 80 75	35, 54, 88, 115	0
1	D	279/308 (90%)	0.10	5 (1%) 68 61	36, 63, 98, 165	0
2	B	100/104 (96%)	0.01	1 (1%) 82 77	36, 51, 77, 130	0
2	E	99/104 (95%)	0.48	4 (4%) 38 28	50, 81, 110, 116	0
3	C	9/9 (100%)	0.65	1 (11%) 5 3	46, 67, 92, 105	0
3	F	9/9 (100%)	0.73	0 100 100	65, 85, 102, 112	0
All	All	776/842 (92%)	0.12	14 (1%) 68 61	35, 60, 102, 165	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	0	MET	6.0
1	D	17	ARG	4.3
1	D	18	GLY	4.2
1	A	197	HIS	3.4
2	E	1	ILE	3.1

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.