



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 28, 2022 – 04:04 PM EDT

PDB ID : 7SL5  
Title : Crystal Structure of VP12E7 Fab in complex with SARS-CoV-2 S fusion peptide  
Authors : Tortorici, M.A.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2021-10-22  
Resolution : 2.50 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
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

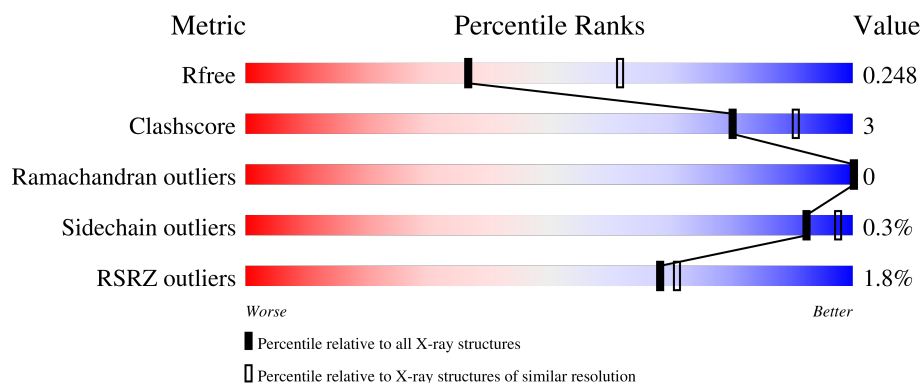
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.



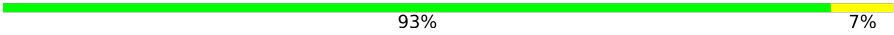
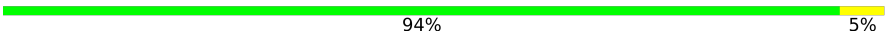

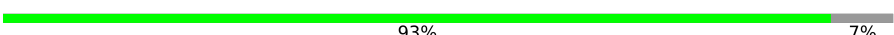


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	235	<div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	D	235	<div> <div>2%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	G	235	<div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	J	235	<div> <div>6%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
2	B	215	<div> <div>93%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	215	 93%7%
2	H	215	 94%5%
2	K	215	 3%92%8%
3	C	15	 7%80%13%7%
3	F	15	 93%7%
3	I	15	 7%67%20%13%
3	L	15	 13%80%20%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14157 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 Heavy chain VP12E7 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	1	0
			1678	1053	286	333	6			
1	D	228	Total	C	N	O	S	0	0	0
			1639	1036	278	319	6			
1	G	229	Total	C	N	O	S	0	2	0
			1700	1069	289	336	6			
1	J	227	Total	C	N	O	S	0	1	0
			1561	981	264	310	6			

- Molecule 2 is a protein called Light chain VP12E7 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1621	1019	268	329	5			
2	E	215	Total	C	N	O	S	0	0	0
			1607	1011	264	326	6			
2	H	215	Total	C	N	O	S	0	1	0
			1642	1030	270	336	6			
2	K	214	Total	C	N	O	S	0	0	0
			1574	993	258	318	5			

- Molecule 3 is a protein called PRO-SER-LYS-ARG-SER-PHE-ILE-GLU-ASP-LEU-LEU-PHE-ASN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	0	0	0
			119	78	20	21			
3	F	14	Total	C	N	O	0	0	0
			119	78	20	21			
3	I	13	Total	C	N	O	0	0	0
			106	69	17	20			
3	L	12	Total	C	N	O	0	0	0
			95	63	16	16			


- Molecule 4 is water.

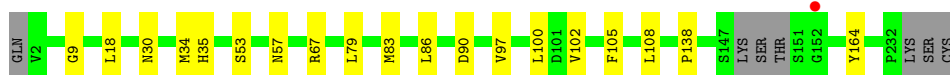
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total 95	O 95	0	0
4	B	94	Total 94	O 94	0	0
4	C	3	Total 3	O 3	0	0
4	D	53	Total 53	O 53	0	0
4	E	82	Total 82	O 82	0	0
4	F	3	Total 3	O 3	0	0
4	G	152	Total 152	O 152	0	0
4	H	124	Total 124	O 124	0	0
4	I	3	Total 3	O 3	0	0
4	J	27	Total 27	O 27	0	0
4	K	59	Total 59	O 59	0	0
4	L	1	Total 1	O 1	0	0

### 3 Residue-property plots

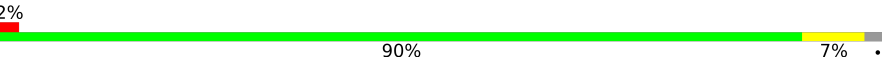
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Heavy chain VP12E7 Fab

Chain A: 




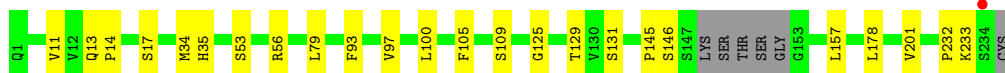
- Molecule 1: Heavy chain VP12E7 Fab

Chain D: 




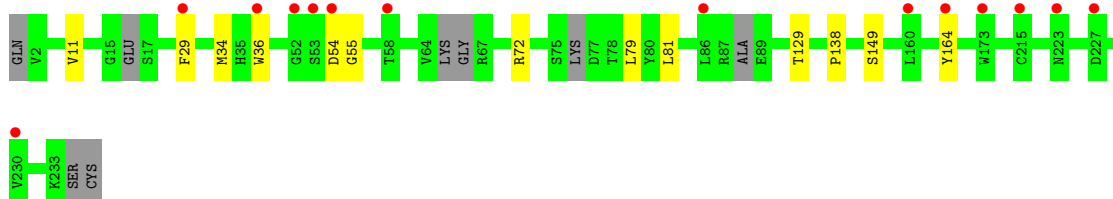
- Molecule 1: Heavy chain VP12E7 Fab

Chain G: 



- Molecule 1: Heavy chain VP12E7 Fab

Chain J: 



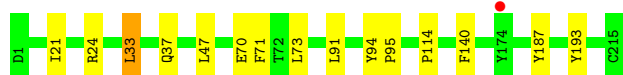
- Molecule 2: Light chain VP12E7 Fab

Chain B: 



- Molecule 2: Light chain VP12E7 Fab

Chain E: 93% 7%



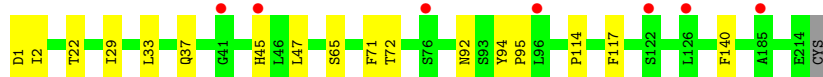
- Molecule 2: Light chain VP12E7 Fab

Chain H: 94% 5%



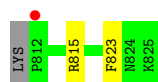
- Molecule 2: Light chain VP12E7 Fab

Chain K: 92% 3% 8%



- Molecule 3: PRO-SER-LYS-ARG-SER-PHE-ILE-GLU-ASP-LEU-LEU-PHE-ASN

Chain C: 80% 7% 13% 7%



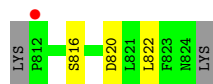
- Molecule 3: PRO-SER-LYS-ARG-SER-PHE-ILE-GLU-ASP-LEU-LEU-PHE-ASN

Chain F: 93% 7%



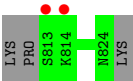
- Molecule 3: PRO-SER-LYS-ARG-SER-PHE-ILE-GLU-ASP-LEU-LEU-PHE-ASN

Chain I: 67% 7% 20% 13%



- Molecule 3: PRO-SER-LYS-ARG-SER-PHE-ILE-GLU-ASP-LEU-LEU-PHE-ASN

Chain L: 80% 13% 20%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.15Å 81.36Å 95.65Å 90.34° 95.96° 100.65°	Depositor
Resolution (Å)	48.20 – 2.50 48.20 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.20-2.50) 97.9 (48.20-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.210 , 0.251 0.207 , 0.248	Depositor DCC
$R_{free}$ test set	3567 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.5	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	0.94	EDS
Total number of atoms	14157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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

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	0/1715	0.52	0/2341
1	D	0.27	0/1676	0.51	0/2290
1	G	0.32	0/1740	0.58	0/2373
1	J	0.27	0/1595	0.48	0/2184
2	B	0.29	0/1659	0.52	0/2263
2	E	0.28	0/1645	0.50	0/2247
2	H	0.30	0/1680	0.53	0/2291
2	K	0.27	0/1612	0.49	0/2209
3	C	0.28	0/121	0.46	0/159
3	F	0.27	0/121	0.43	0/159
3	I	0.30	0/108	0.44	0/144
3	L	0.27	0/96	0.41	0/128
All	All	0.29	0/13768	0.51	0/18788

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 outliers	#Planarity outliers
1	G	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	146	SER	Mainchain
1	G	232	PRO	Mainchain
1	G	233[A]	LYS	Mainchain
1	G	233[B]	LYS	Mainchain

## 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	1678	0	1582	11	0
1	D	1639	0	1520	9	0
1	G	1700	0	1622	14	0
1	J	1561	0	1312	7	0
2	B	1621	0	1534	8	0
2	E	1607	0	1499	8	0
2	H	1642	0	1556	8	0
2	K	1574	0	1431	9	0
3	C	119	0	123	2	0
3	F	119	0	123	0	0
3	I	106	0	99	3	0
3	L	95	0	86	0	0
4	A	95	0	0	0	0
4	B	94	0	0	0	0
4	C	3	0	0	0	0
4	D	53	0	0	0	0
4	E	82	0	0	0	1
4	F	3	0	0	0	0
4	G	152	0	0	0	0
4	H	124	0	0	1	1
4	I	3	0	0	0	0
4	J	27	0	0	0	0
4	K	59	0	0	0	0
4	L	1	0	0	0	0
All	All	14157	0	12487	69	1

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.

The worst 5 of 69 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)
2:E:21:ILE:HD11	2:E:73:LEU:HD23	1.67	0.76
1:A:67:ARG:NH2	1:A:90:ASP:OD2	2.20	0.69
1:G:56:ARG:NH2	3:I:820:ASP:OD2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:MET:HB3	1:D:79:LEU:HD22	1.81	0.62
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.82	0.62

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:362:HOH:O	4:H:406:HOH:O[1_545]	2.13	0.07

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	225/235 (96%)	220 (98%)	5 (2%)	0	100	100
1	D	224/235 (95%)	220 (98%)	4 (2%)	0	100	100
1	G	227/235 (97%)	223 (98%)	4 (2%)	0	100	100
1	J	218/235 (93%)	213 (98%)	5 (2%)	0	100	100
2	B	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
2	E	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
2	H	214/215 (100%)	210 (98%)	4 (2%)	0	100	100
2	K	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
3	C	12/15 (80%)	12 (100%)	0	0	100	100
3	F	12/15 (80%)	12 (100%)	0	0	100	100
3	I	11/15 (73%)	11 (100%)	0	0	100	100
3	L	10/15 (67%)	10 (100%)	0	0	100	100
All	All	1790/1860 (96%)	1752 (98%)	38 (2%)	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	182/200 (91%)	182 (100%)	0	100	100
1	D	168/200 (84%)	168 (100%)	0	100	100
1	G	186/200 (93%)	186 (100%)	0	100	100
1	J	141/200 (70%)	141 (100%)	0	100	100
2	B	180/188 (96%)	179 (99%)	1 (1%)	86	95
2	E	175/188 (93%)	174 (99%)	1 (1%)	86	95
2	H	185/188 (98%)	184 (100%)	1 (0%)	88	96
2	K	164/188 (87%)	163 (99%)	1 (1%)	86	95
3	C	14/15 (93%)	14 (100%)	0	100	100
3	F	14/15 (93%)	14 (100%)	0	100	100
3	I	12/15 (80%)	12 (100%)	0	100	100
3	L	9/15 (60%)	9 (100%)	0	100	100
All	All	1430/1612 (89%)	1426 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	69	THR
2	E	33	LEU
2	H	214	GLU
2	K	22	THR

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

### 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	228/235 (97%)	0.12	1 (0%) 92 93	26, 40, 71, 93	0
1	D	228/235 (97%)	0.24	4 (1%) 68 71	36, 52, 78, 92	0
1	G	229/235 (97%)	0.01	1 (0%) 92 93	23, 35, 53, 80	1 (0%)
1	J	227/235 (96%)	0.75	14 (6%) 20 21	43, 68, 86, 98	0
2	B	214/215 (99%)	-0.03	0 100 100	24, 38, 55, 70	0
2	E	215/215 (100%)	0.09	1 (0%) 91 91	31, 43, 60, 73	0
2	H	215/215 (100%)	0.01	1 (0%) 91 91	25, 35, 49, 108	0
2	K	214/215 (99%)	0.38	7 (3%) 46 50	37, 53, 75, 82	0
3	C	14/15 (93%)	0.18	1 (7%) 16 16	38, 42, 55, 73	1 (7%)
3	F	14/15 (93%)	-0.15	0 100 100	32, 40, 50, 61	4 (28%)
3	I	13/15 (86%)	0.03	1 (7%) 13 13	35, 42, 60, 82	5 (38%)
3	L	12/15 (80%)	1.36	2 (16%) 1 1	53, 64, 74, 77	3 (25%)
All	All	1823/1860 (98%)	0.20	33 (1%) 68 71	23, 44, 76, 108	14 (0%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	234	SER	4.4
3	C	812	PRO	4.0
1	J	173	TRP	3.9
3	L	813	SER	3.7
2	K	126	LEU	3.5

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.