wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 1, 2022 – 12:07 PM JST

PDB ID	:	7WVL
Title	:	Structure of P4A2 Fab in complex with Spike-RBD from SARS-CoV-2
Authors	:	Narayanan, N.; Nair, D.T.
Deposited on	:	2022-02-10
Resolution	:	3.00 Å(reported)

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

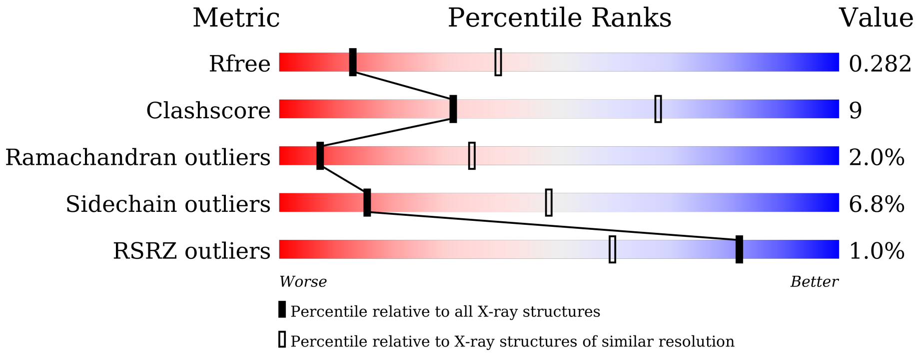
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

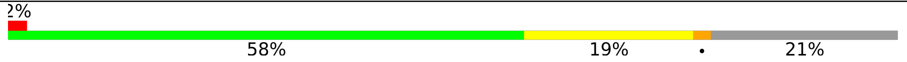
The reported resolution of this entry is 3.00 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	L	218	
2	H	212	
3	F	223	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4627 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 P4A2 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	216	1660	1034	288	331	7	0	0	0

- Molecule 2 is a protein called P4A2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	212	1566	984	253	321	8	0	0	0

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	177	1341	847	230	259	5	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	533	GLY	-	expression tag	UNP P0DTC2
F	534	SER	-	expression tag	UNP P0DTC2
F	535	LEU	-	expression tag	UNP P0DTC2
F	536	GLU	-	expression tag	UNP P0DTC2
F	537	VAL	-	expression tag	UNP P0DTC2
F	538	LEU	-	expression tag	UNP P0DTC2
F	539	PHE	-	expression tag	UNP P0DTC2
F	540	GLN	-	expression tag	UNP P0DTC2
F	541	GLY	-	expression tag	UNP P0DTC2
F	542	PRO	-	expression tag	UNP P0DTC2
F	543	GLY	-	expression tag	UNP P0DTC2
F	544	SER	-	expression tag	UNP P0DTC2
F	545	HIS	-	expression tag	UNP P0DTC2
F	546	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	547	HIS	-	expression tag	UNP P0DTC2
F	548	HIS	-	expression tag	UNP P0DTC2
F	549	HIS	-	expression tag	UNP P0DTC2
F	550	HIS	-	expression tag	UNP P0DTC2
F	551	HIS	-	expression tag	UNP P0DTC2
F	552	HIS	-	expression tag	UNP P0DTC2
F	553	HIS	-	expression tag	UNP P0DTC2
F	554	HIS	-	expression tag	UNP P0DTC2

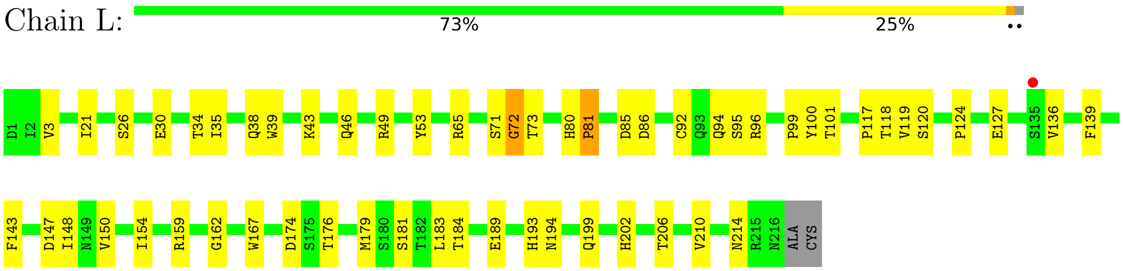
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	23	Total O 23 23	0	0
4	H	25	Total O 25 25	0	0
4	F	12	Total O 12 12	0	0

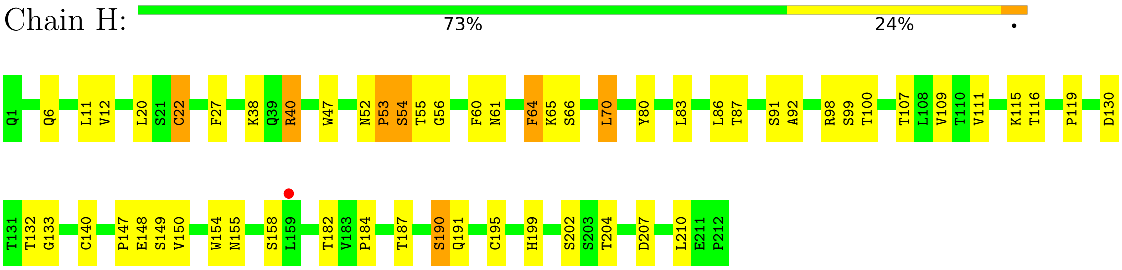
3 Residue-property plots ⓘ

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.

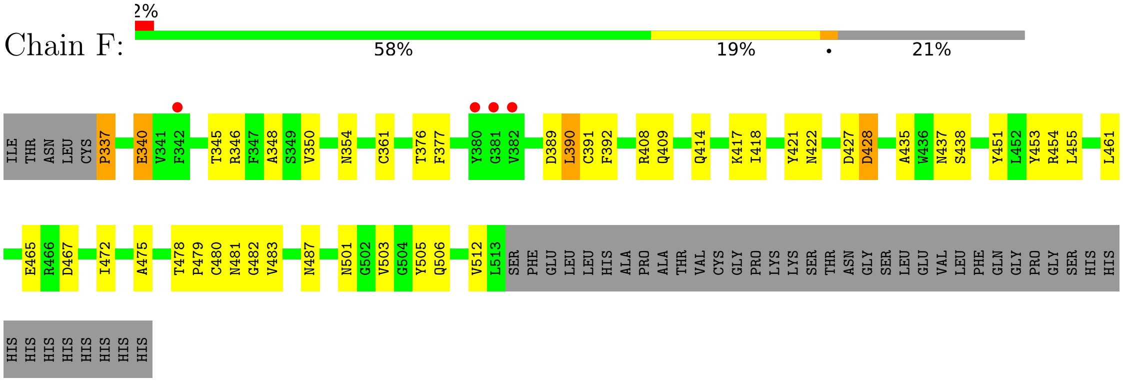
- Molecule 1: P4A2 Fab Light Chain



- Molecule 2: P4A2 Fab heavy chain



- Molecule 3: Spike protein S1



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	85.31Å 85.31Å 205.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	73.88 – 3.00 73.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (73.88-3.00) 99.7 (73.88-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.233 , 0.279 0.235 , 0.282	Depositor DCC
R_{free} test set	1375 reflections (7.65%)	wwPDB-VP
Wilson B-factor (Å^2)	93.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.9	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.49, $< L^2 >$ = 0.32	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4627	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] 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.

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	L	0.27	0/1697	0.51	0/2305
2	H	0.26	0/1605	0.51	0/2197
3	F	0.30	0/1375	0.54	1/1875 (0.1%)
All	All	0.28	0/4677	0.52	1/6377 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	337	PRO	N-CA-CB	5.84	110.31	103.30

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	L	1660	0	1603	28	0
2	H	1566	0	1507	29	0
3	F	1341	0	1192	26	0
4	F	12	0	0	1	0
4	H	25	0	0	3	0
4	L	23	0	0	1	0
All	All	4627	0	4302	81	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 9.

The worst 5 of 81 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:H:91:SER:HB3	2:H:111:VAL:HG12	1.65	0.78
1:L:124:PRO:HD3	1:L:136:VAL:HG22	1.69	0.75
1:L:3:VAL:HG22	1:L:26:SER:HB3	1.67	0.75
2:H:52:ASN:O	2:H:54:SER:N	2.24	0.70
1:L:167:TRP:CD1	1:L:179:MET:HG3	2.32	0.65

There are no symmetry-related clashes.

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	L	214/218 (98%)	200 (94%)	12 (6%)	2 (1%)	17	55
2	H	210/212 (99%)	185 (88%)	19 (9%)	6 (3%)	4	24
3	F	175/223 (78%)	143 (82%)	28 (16%)	4 (2%)	6	30
All	All	599/653 (92%)	528 (88%)	59 (10%)	12 (2%)	7	34

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	72	GLY
2	H	54	SER
2	H	149	SER
3	F	391	CYS
3	F	392	PHE

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	L	187/190 (98%)	174 (93%)	13 (7%)	15	47
2	H	179/183 (98%)	163 (91%)	16 (9%)	9	35
3	F	133/193 (69%)	128 (96%)	5 (4%)	33	69
All	All	499/566 (88%)	465 (93%)	34 (7%)	16	48

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	207	ASP
3	F	340	GLU
3	F	427	ASP
1	L	206	THR
1	L	189	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	17	GLN
1	L	94	GLN
2	H	199	HIS
3	F	422	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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^{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>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	216/218 (99%)	-0.08	1 (0%)	91	75	52, 76, 115, 135	0
2	H	212/212 (100%)	0.06	1 (0%)	91	75	52, 79, 125, 141	0
3	F	177/223 (79%)	-0.04	4 (2%)	60	31	72, 114, 185, 206	0
All	All	605/653 (92%)	-0.02	6 (0%)	82	59	52, 85, 155, 206	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	381	GLY	4.5
2	H	159	LEU	3.3
3	F	382	VAL	2.4
3	F	380	TYR	2.3
1	L	135	SER	2.2

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.