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wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 10:04 am BST

PDB ID	:	8BSF
Title	:	CRYSTAL STRUCTURE OF SARS-COV-2 RECEPTOR BINDING DO-MAIN (RBD-beta variant) in complex with 3D2 Fab
Authors	:	Welin, M.; Kimbung, Y.R.; Focht, D.; Pisitkun, T.
Deposited on	:	2022-11-25
Resolution	:	2.20 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*
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.

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

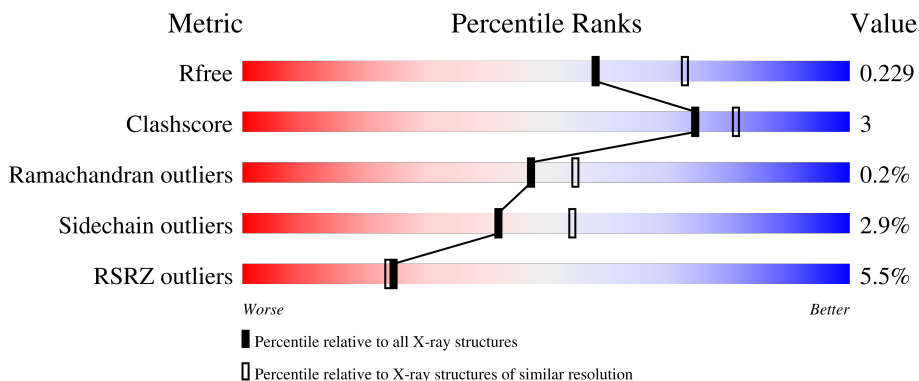|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.20 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	Percentile Ranks	Value
Rfree		0.229
Clashscore		3
Ramachandran outliers		0.2%
Sidechain outliers		2.9%
RSRZ outliers		5.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	A	231	13% / 65% 10% 26%
2	H	231	% / 87% 8% ·
3	L	216	93% 6% ·

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 4789 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1369	879	227	255	8			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	ASN	LYS	engineered mutation	UNP P0DTC2
A	484	LYS	GLU	engineered mutation	UNP P0DTC2
A	501	TYR	ASN	engineered mutation	UNP P0DTC2
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called 3D2 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1660	1057	273	324	6			

- Molecule 3 is a protein called 3D2 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	3	0
			1599	1002	263	330	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

O6
OH

O5
O1
HO   O
C1(R)   C5(R)   C6
C2(R)   C4(S)
N2   C3(R)
HN   OH
O4
C7   OH
C8   O   O3
O7

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3
OH O3

C1   C2

HO   OH
O1   O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total 6	C 3	O 3	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total 18	O 18	0	0
6	H	39	Total 39	O 39	0	0
6	L	66	Total 66	O 66	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.
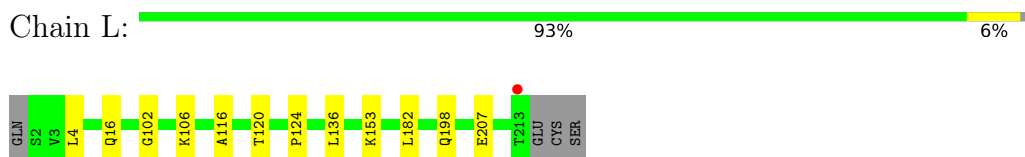
• Molecule 1: Spike protein S1
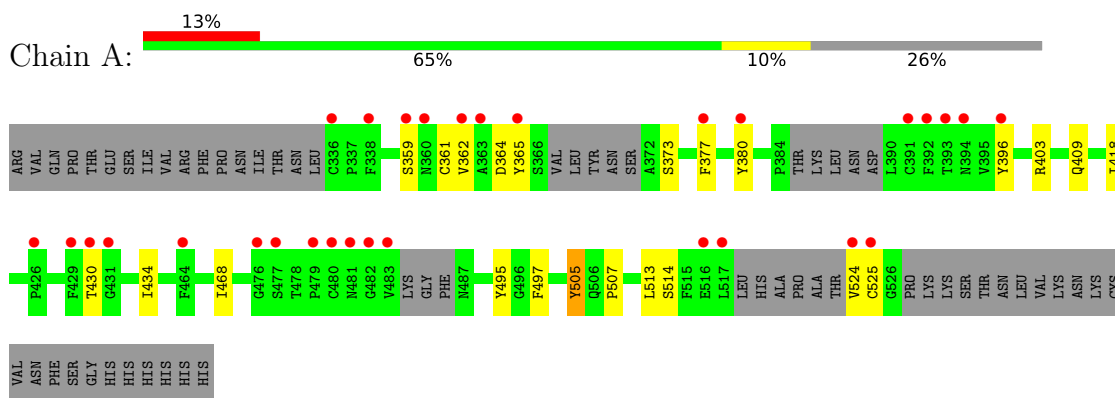
• Molecule 2: 3D2 FAB HEAVY CHAIN
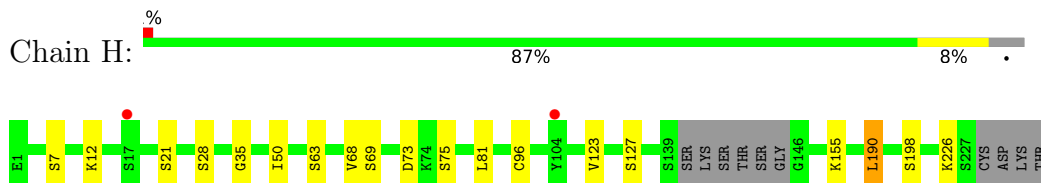
• Molecule 3: 3D2 FAB LIGHT CHAIN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	104.69Å 71.20Å 121.25Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	48.07 – 2.20 48.07 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.07-2.20) 98.7 (48.07-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.66 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.196 , 0.229 0.201 , 0.229	Depositor DCC
R_{free} test set	2189 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.8	EDS
L-test for twinning[2]	$<\|L\|>$ = 0.50, $<L^2>$ = 0.33	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4789	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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   ⓘ

5.1   Standard geometry   ⓘ

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

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	0.70	0/1405	0.81	0/1905
2	H	0.69	0/1706	0.89	0/2325
3	L	0.73	0/1638	0.89	0/2242
All	All	0.71	0/4749	0.87	0/6472

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	1369	0	1279	10	0
2	H	1660	0	1625	10	0
3	L	1599	0	1548	9	0
4	A	14	0	13	0	0
5	H	6	0	8	0	0
5	L	18	0	24	2	0
6	A	18	0	0	0	0
6	H	39	0	0	1	0
6	L	66	0	0	2	0
All	All	4789	0	4497	29	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.

The worst 5 of 29 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:68:VAL:HG11	2:H:81:LEU:HD11	1.66	0.77
2:H:155:LYS:NZ	6:H:401:HOH:O	2.19	0.73
2:H:68:VAL:CG1	2:H:81:LEU:HD11	2.26	0.64
2:H:190:LEU:C	2:H:190:LEU:HD12	2.17	0.64
3:L:4:LEU:HB2	3:L:102:GLY:HA2	1.84	0.59

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	A	162/231 (70%)	153 (94%)	8 (5%)	1 (1%)	25	26
2	H	217/231 (94%)	210 (97%)	7 (3%)	0	100	100
3	L	213/216 (99%)	208 (98%)	5 (2%)	0	100	100
All	All	592/678 (87%)	571 (96%)	20 (3%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	CYS

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	148/203 (73%)	143 (97%)	5 (3%)	37	47
2	H	187/196 (95%)	178 (95%)	9 (5%)	25	32
3	L	181/182 (100%)	180 (99%)	1 (1%)	86	93
All	All	516/581 (89%)	501 (97%)	15 (3%)	42	54

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	28	SER
2	H	226	LYS
2	H	63	SER
3	L	106	LYS
2	H	190	LEU

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 ⓘ

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 ⓘ

5 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
5	GOL	L	303	-	5,5,5	0.21	0	5,5,5	0.49	0
5	GOL	H	301	-	5,5,5	0.19	0	5,5,5	0.42	0
5	GOL	L	302	-	5,5,5	0.23	0	5,5,5	0.40	0
4	NAG	A	601	1	14,14,15	1.17	2 (14%)	17,19,21	2.95	4 (23%)
5	GOL	L	301	-	5,5,5	0.12	0	5,5,5	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	L	303	-	-	2/4/4/4	-
5	GOL	H	301	-	-	4/4/4/4	-
5	GOL	L	302	-	-	0/4/4/4	-
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
5	GOL	L	301	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	O5-C1	2.31	1.47	1.43
4	A	601	NAG	O5-C5	2.08	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C1-O5-C5	10.16	125.95	112.19
4	A	601	NAG	C2-N2-C7	3.68	128.15	122.90
4	A	601	NAG	O5-C5-C6	2.56	111.22	107.20
4	A	601	NAG	O7-C7-N2	2.07	125.75	121.95

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	301	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	H	301	GOL	C1-C2-C3-O3
5	L	301	GOL	O1-C1-C2-C3
5	L	301	GOL	O2-C2-C3-O3
5	L	303	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	303	GOL	1	0
5	L	302	GOL	1	0

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, 95th 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	A	172/231 (74%)	0.90	30 (17%)	1	1	43, 73, 130, 151	0
2	H	221/231 (95%)	-0.15	2 (0%)	84	83	34, 51, 76, 97	0
3	L	212/216 (98%)	-0.16	1 (0%)	91	90	29, 41, 61, 99	0
All	All	605/678 (89%)	0.14	33 (5%)	25	24	29, 51, 110, 151	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	TYR	6.5
1	A	483	VAL	5.7
1	A	524	VAL	5.6
1	A	481	ASN	5.5
1	A	359	SER	5.2

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 ⓘ

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, 95th 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	H	301	6/6	0.63	0.16	71,79,80,86	0
4	NAG	A	601	14/15	0.70	0.16	81,92,105,106	0
5	GOL	L	303	6/6	0.79	0.24	57,81,90,92	0
5	GOL	L	302	6/6	0.85	0.23	55,57,65,65	0
5	GOL	L	301	6/6	0.92	0.21	44,63,67,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

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