



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 17, 2021 – 07:22 PM JST

PDB ID : 7CHF
Title : Crystal structure of the SARS-CoV-2 RBD in complex with BD-604 Fab and BD-368-2 Fab
Authors : Xiao, J.; Zhu, Q.
Deposited on : 2020-07-05
Resolution : 2.67 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 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	:	2.18
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)	:	2.18

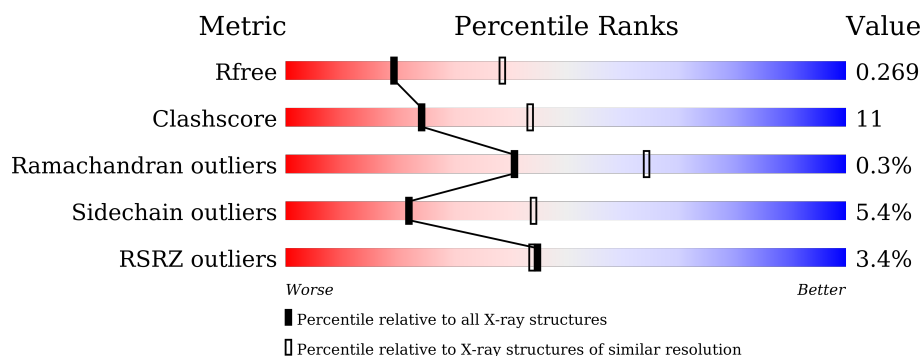
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 $\leq 5\%$. 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	H	222	
2	L	214	
3	R	223	
4	A	230	
5	B	219	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8008 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 BD-604 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	210	Total	C	N	O	S	0	0	0
			1556	983	259	307	7			

- Molecule 2 is a protein called BD-604 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1615	1012	270	329	4			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	189	Total	C	N	O	S	0	0	0
			1498	958	249	283	8			

- Molecule 4 is a protein called BD-368-2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	226	Total	C	N	O	S	0	0	0
			1680	1058	286	330	6			


- Molecule 5 is a protein called BD-368-2 Fab light chain.

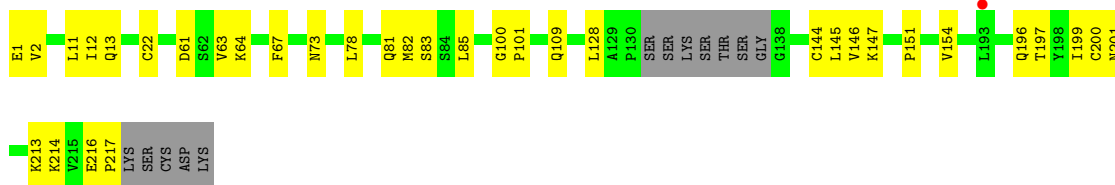
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	216	Total	C	N	O	S	0	0	0
			1659	1038	281	334	6			

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.

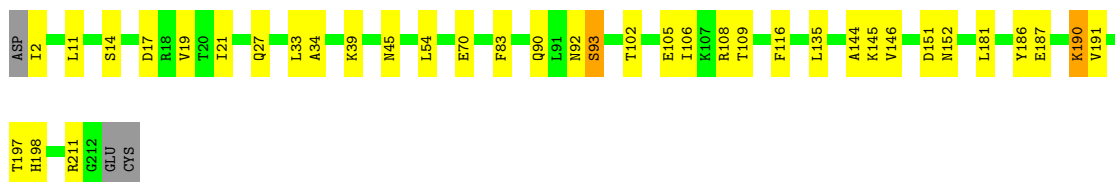
- Molecule 1: BD-604 Fab heavy chain

Chain H: 



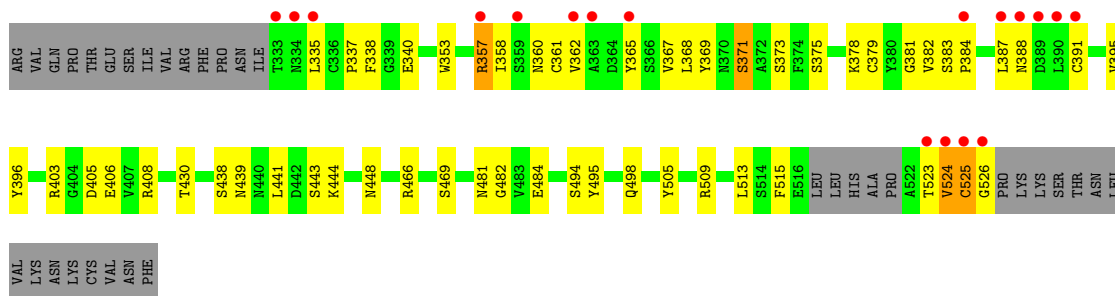
- Molecule 2: BD-604 Fab light chain

Chain L: 




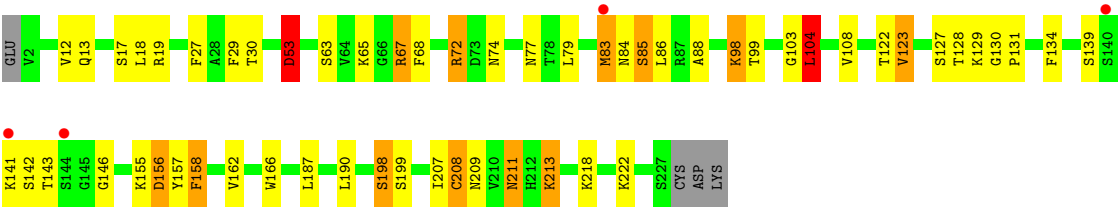
- Molecule 3: Spike protein S1

Chain R: 

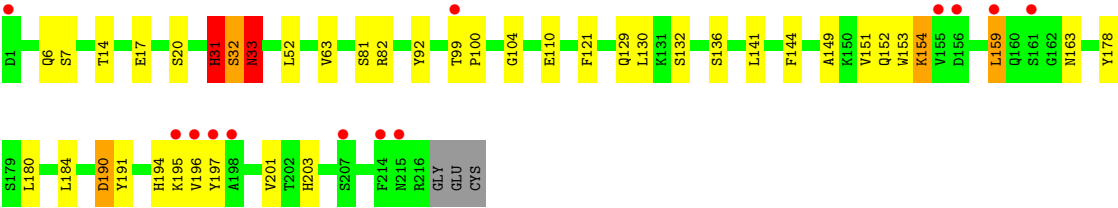
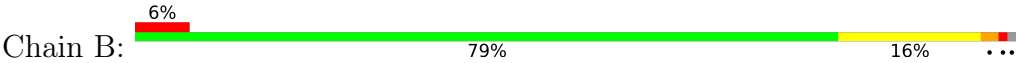


- Molecule 4: BD-368-2 Fab heavy chain

Chain A: 



● Molecule 5: BD-368-2 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.85Å 116.22Å 115.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.87 – 2.67 50.08 – 2.67	Depositor EDS
% Data completeness (in resolution range)	96.0 (45.87-2.67) 92.6 (50.08-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.220 , 0.270 0.221 , 0.269	Depositor DCC
R_{free} test set	1868 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8008	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	H	0.60	0/1591	0.70	0/2169
2	L	0.63	0/1648	0.73	1/2238 (0.0%)
3	R	0.68	2/1538 (0.1%)	0.84	3/2090 (0.1%)
4	A	0.77	4/1720 (0.2%)	0.89	3/2341 (0.1%)
5	B	0.54	1/1695 (0.1%)	0.72	2/2303 (0.1%)
All	All	0.65	7/8192 (0.1%)	0.78	9/11141 (0.1%)

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
4	A	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	213	LYS	C-N	8.67	1.50	1.34
3	R	498	GLN	C-N	8.28	1.50	1.34
4	A	130	GLY	C-N	7.99	1.49	1.34
4	A	158	PHE	C-N	7.86	1.49	1.34
5	B	32	SER	CA-CB	-6.56	1.43	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	357	ARG	NE-CZ-NH1	-13.31	113.64	120.30
2	L	151	ASP	CB-CA-C	8.30	126.99	110.40
4	A	53	ASP	CB-CA-C	-7.08	96.25	110.40
5	B	33	ASN	CB-CA-C	-6.94	96.53	110.40
4	A	104	LEU	N-CA-C	-5.58	95.93	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	53	ASP	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	H	1556	0	1534	25	0
2	L	1615	0	1573	29	0
3	R	1498	0	1413	47	1
4	A	1680	0	1642	48	2
5	B	1659	0	1618	29	1
All	All	8008	0	7780	173	2

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 173 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)
4:A:68:PHE:CE1	4:A:83:MET:HB3	1.50	1.44
4:A:68:PHE:HE1	4:A:83:MET:CB	1.39	1.34
2:L:187:GLU:HA	2:L:211:ARG:HH11	1.06	1.15
3:R:369:TYR:CE2	3:R:384:PRO:HG3	1.87	1.09
4:A:72:ARG:NH1	4:A:74:ASN:OD1	1.90	1.04

All (2) 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:A:84:ASN:OD1	5:B:82:ARG:NH1[4_555]	1.39	0.81
3:R:375:SER:OG	4:A:199:SER:OG[3_645]	2.01	0.19

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	H	206/222 (93%)	199 (97%)	7 (3%)	0	100	100
2	L	209/214 (98%)	199 (95%)	10 (5%)	0	100	100
3	R	185/223 (83%)	171 (92%)	14 (8%)	0	100	100
4	A	224/230 (97%)	201 (90%)	22 (10%)	1 (0%)	34	58
5	B	214/219 (98%)	203 (95%)	9 (4%)	2 (1%)	17	37
All	All	1038/1108 (94%)	973 (94%)	62 (6%)	3 (0%)	41	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	33	ASN
5	B	31	HIS
4	A	156	ASP

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	H	175/186 (94%)	170 (97%)	5 (3%)	42	69
2	L	184/187 (98%)	179 (97%)	5 (3%)	44	71
3	R	163/196 (83%)	153 (94%)	10 (6%)	18	38
4	A	184/188 (98%)	163 (89%)	21 (11%)	5	12
5	B	190/192 (99%)	183 (96%)	7 (4%)	34	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	896/949 (94%)	848 (95%)	48 (5%)	22	44

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	85	SER
4	A	155	LYS
4	A	98	LYS
4	A	123	VAL
4	A	208	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	35	ASN
4	A	211	ASN
5	B	6	GLN
4	A	216	ASN
3	R	498	GLN

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 [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, 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	H	210/222 (94%)	-0.04	1 (0%) 91 92	19, 40, 59, 74	0
2	L	211/214 (98%)	-0.12	0 100 100	15, 33, 54, 67	0
3	R	189/223 (84%)	0.41	18 (9%) 8 6	16, 36, 89, 113	0
4	A	226/230 (98%)	0.09	4 (1%) 68 69	20, 42, 73, 86	0
5	B	216/219 (98%)	0.27	13 (6%) 21 20	15, 39, 72, 77	0
All	All	1052/1108 (94%)	0.11	36 (3%) 45 44	15, 38, 74, 113	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	333	THR	8.5
3	R	387	LEU	4.5
5	B	196	VAL	4.5
3	R	526	GLY	4.4
3	R	365	TYR	4.3

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.