

Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 02:56 am GMT

PDB ID : 8Q94

Title : Crystal structure of The SARS-COV-2 BA.2.75 RBD with neutralizing-VHHs

Re32D03 and Ma3B12

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Deposited on : 2023-08-19

Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467 Xtriage (Phenix): 1.13

EDS : 2.36

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)

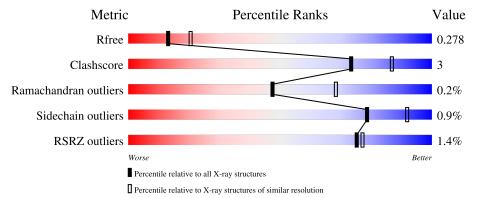
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
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 >=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	187	86%	7% 7%
2	В	131	87%	11%
3	С	132	88%	8% •



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3336 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.

\mathbf{Mol}	Chain	Residues					ZeroOcc	AltConf	Trace	
1	A	174	Total 1370	C 884	N 230	O 249	S 7	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	GLU	-	expression tag	UNP P0DTC2
A	332	GLY	-	expression tag	UNP P0DTC2
A	333	SER	-	expression tag	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	343	ASP	ASN	conflict	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	391	SER	CYS	conflict	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2

• Molecule 2 is a protein called Nanobody Ma3B12.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	128	Total 980	C 617	N 163	O 197	S 3	0	0	0

• Molecule 3 is a protein called Nanobody Re32D03.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	197	Total	С	N	О	S	0	0	0
5		121	958	604	162	185	7	U	0	U

\bullet Molecule 4 is water.

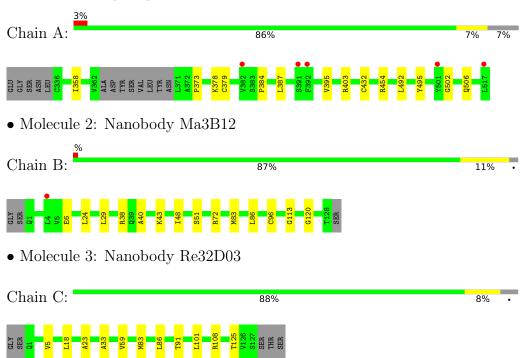
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	В	6	Total O 6 6	0	0
4	С	9	Total O 9 9	0	0



3 Residue-property plots (i)

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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	67.16Å 67.16Å 224.90Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 - 2.50	Depositor
rtesolution (A)	47.49 - 2.50	EDS
% Data completeness	99.9 (47.49-2.50)	Depositor
(in resolution range)	100.0 (47.49-2.50)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.11 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
D.D.	0.220 , 0.277	Depositor
R, R_{free}	0.218 , 0.278	DCC
R_{free} test set	935 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 39.1	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3336	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.25	0/1413	0.47	0/1924	
2	В	0.25	0/1005	0.49	0/1367	
3	С	0.25	0/980	0.50	0/1331	
All	All	0.25	0/3398	0.49	0/4622	

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 (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	1370	0	1267	9	0
2	В	980	0	909	9	0
3	С	958	0	935	5	0
4	A	13	0	0	0	0
4	В	6	0	0	0	0
4	С	9	0	0	0	0
All	All	3336	0	3111	21	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.

All (21) 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:A:379:CYS:SG	1:A:432[A]:CYS:HB3	2.39	0.62
1:A:384:PRO:HA	1:A:387:LEU:HD23	1.86	0.56
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.91	0.52
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.91	0.52
3:C:5:VAL:HG23	3:C:23:ALA:HB3	1.91	0.52
2:B:24:LEU:HD12	2:B:29:LEU:HA	1.93	0.50
3:C:33:ALA:HB2	3:C:101:LEU:HD22	1.94	0.49
1:A:492:LEU:O	3:C:108:ARG:NH2	2.46	0.49
3:C:83:MET:HB3	3:C:86:LEU:HD21	1.96	0.48
2:B:51:SER:O	2:B:72:ARG:NH2	2.49	0.45
1:A:379:CYS:HA	1:A:432[A]:CYS:HA	1.99	0.44
1:A:378:LYS:NZ	2:B:113:GLY:O	2.46	0.44
1:A:379:CYS:HA	1:A:432[B]:CYS:HA	1.99	0.44
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.53	0.44
2:B:6:GLU:CD	2:B:120:GLY:H	2.23	0.42
1:A:502:GLY:O	1:A:506:GLN:HG3	2.20	0.42
2:B:6:GLU:HG3	2:B:96:CYS:SG	2.59	0.42
2:B:40:ALA:HB3	2:B:43:LYS:HD3	2.01	0.42
2:B:38:ARG:HB3	2:B:48:ILE:HD11	2.01	0.41
2:B:38:ARG:HD3	2:B:48:ILE:HD11	2.03	0.41
3:C:91:THR:HG23	3:C:125:THR:HA	2.03	0.41

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 Outlie		Outliers	Perce	entiles	
1	A	171/187 (91%)	162 (95%)	8 (5%)	1 (1%)	25	43
2	В	126/131 (96%)	122 (97%)	4 (3%)	0	100	100
3	С	$125/132\ (95\%)$	125 (100%)	0	0	100	100
All	All	422/450 (94%)	409 (97%)	12 (3%)	1 (0%)	47	68



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	PRO

5.3.2 Protein sidechains (i)

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	Percer	ntiles
1	A	142/163 (87%)	141 (99%)	1 (1%)	84	94
2	В	102/108 (94%)	102 (100%)	0	100	100
3	С	103/107 (96%)	101 (98%)	2 (2%)	57	80
All	All	347/378 (92%)	344 (99%)	3 (1%)	78	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	454	ARG
3	С	18	LEU
3	С	59	VAL

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

5.3.3 RNA (i)

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^{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>	$\#\mathrm{RSRZ}{>}2$	$ ext{OWAB}(ext{Å}^2)$	Q<0.9
1	A	174/187 (93%)	0.21	5 (2%) 51 55	42, 55, 110, 139	0
2	В	128/131 (97%)	0.08	1 (0%) 86 87	47, 61, 76, 93	0
3	С	127/132 (96%)	0.00	0 100 100	43, 54, 75, 102	0
All	All	429/450 (95%)	0.11	6 (1%) 75 77	42, 56, 89, 139	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	392	PHE	6.3
1	A	391	SER	4.0
1	A	517	LEU	3.6
1	A	501	TYR	2.7
1	A	382	VAL	2.1
2	В	4	LEU	2.0

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.

