



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 06:41 PM JST

PDB ID : 7X63
Title : SARS-CoV-2-Beta-RBD and BD-236-GWP/P-VK antibody complex
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Deposited on : 2022-03-06
Resolution : 2.24 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.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
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

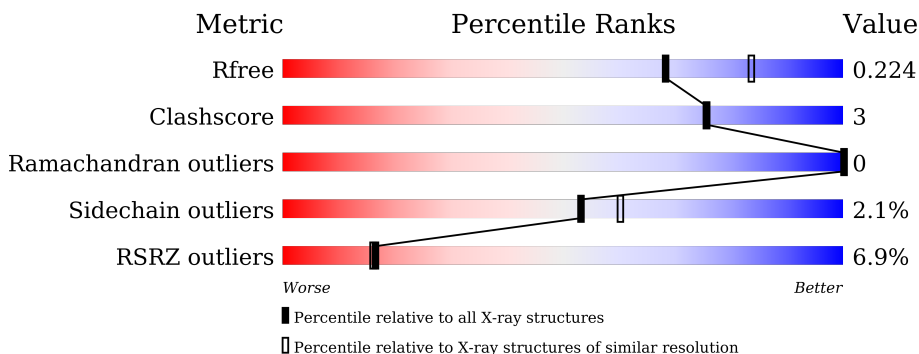
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	223	 7% 91% 6% .
2	L	215	 % 86% 12% ..
3	R	227	 11% 75% 10% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5040 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-236 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	215	1582	996	267	312	7	0	0	0

- Molecule 2 is a protein called BD-236 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	212	1611	1012	270	325	4	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	R	194	1537	987	256	286	8	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	417	ASN	LYS	variant	UNP P0DTC2
R	484	LYS	GLU	variant	UNP P0DTC2
R	501	TYR	ASN	variant	UNP P0DTC2
R	538	HIS	-	expression tag	UNP P0DTC2
R	539	HIS	-	expression tag	UNP P0DTC2
R	540	HIS	-	expression tag	UNP P0DTC2
R	541	HIS	-	expression tag	UNP P0DTC2
R	542	HIS	-	expression tag	UNP P0DTC2
R	543	HIS	-	expression tag	UNP P0DTC2
R	544	HIS	-	expression tag	UNP P0DTC2
R	545	HIS	-	expression tag	UNP P0DTC2

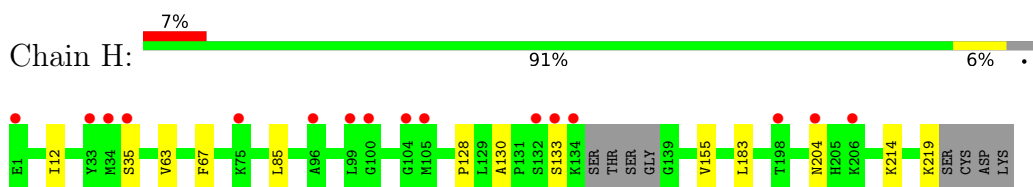
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	116	Total 116	O 116	0	0
4	L	113	Total 113	O 113	0	0
4	R	81	Total 81	O 81	0	0

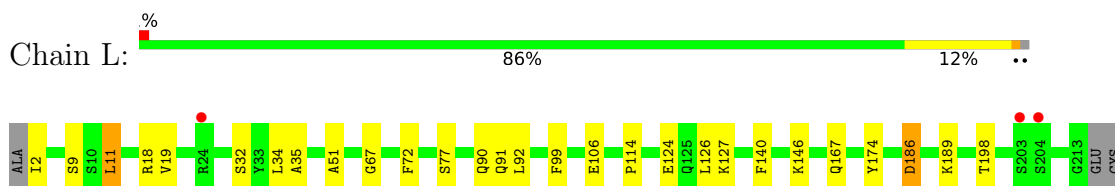
3 Residue-property plots [i](#)

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.

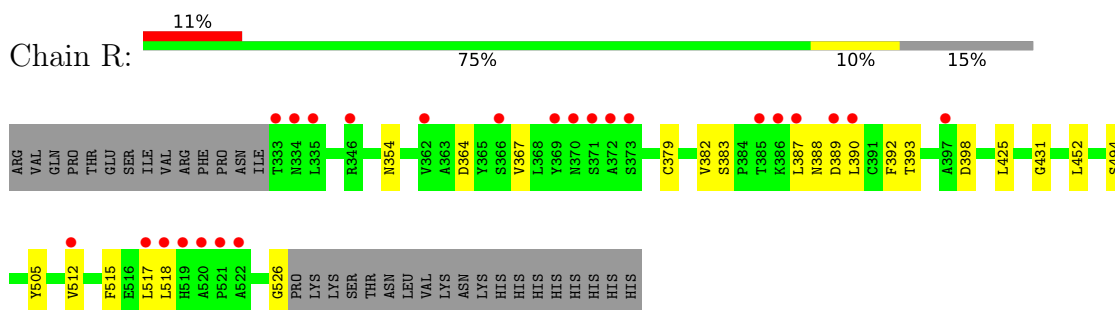
- Molecule 1: BD-236 Fab heavy chain



- Molecule 2: BD-236 Fab light chain



- Molecule 3: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.68Å 84.72Å 57.78Å 90.00° 99.65° 90.00°	Depositor
Resolution (Å)	30.38 – 2.24 30.38 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.38-2.24) 98.0 (30.38-2.24)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.24Å)	Xtrriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.193 , 0.224 0.192 , 0.224	Depositor DCC
R_{free} test set	1976 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtrriage
Anisotropy	0.546	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5040	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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 [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	H	0.37	0/1617	0.62	1/2203 (0.0%)
2	L	0.37	0/1647	0.60	0/2239
3	R	0.36	0/1581	0.56	0/2152
All	All	0.37	0/4845	0.59	1/6594 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	H	183	LEU	CA-CB-CG	5.15	127.15	115.30

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	H	1582	0	1555	4	0
2	L	1611	0	1576	14	0
3	R	1537	0	1451	12	0
4	H	116	0	0	0	0
4	L	113	0	0	0	0
4	R	81	0	0	0	0
All	All	5040	0	4582	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.

All (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)
3:R:387:LEU:HA	3:R:390:LEU:HD12	1.53	0.90
1:H:63:VAL:HG13	1:H:67:PHE:HB2	1.74	0.68
1:H:130:ALA:HB2	1:H:219:LYS:HE2	1.78	0.64
2:L:124:GLU:HA	2:L:127:LYS:HD2	1.81	0.62
2:L:18:ARG:HD3	2:L:77:SER:HA	1.82	0.61
2:L:167:GLN:HG3	2:L:174:TYR:CZ	2.38	0.59
2:L:114:PRO:HB3	2:L:140:PHE:HB3	1.91	0.52
3:R:364:ASP:OD2	3:R:367:VAL:HG13	2.10	0.52
3:R:388:ASN:O	3:R:526:GLY:HA3	2.11	0.50
3:R:383:SER:O	3:R:387:LEU:HG	2.14	0.48
2:L:2:ILE:HG13	3:R:505:TYR:OH	2.15	0.46
1:H:12:ILE:HG21	1:H:85:LEU:HD13	1.98	0.45
1:H:128:PRO:HD3	1:H:214:LYS:HE2	1.98	0.45
3:R:354:ASN:O	3:R:398:ASP:HA	2.16	0.45
3:R:379:CYS:HB3	3:R:382:VAL:HG23	1.98	0.45
3:R:392:PHE:HD1	3:R:517:LEU:HG	1.81	0.45
2:L:32:SER:HA	2:L:51:ALA:HA	1.99	0.44
2:L:146:LYS:HB3	2:L:198:THR:HB	2.00	0.43
3:R:452:LEU:HD23	3:R:494:SER:HA	2.00	0.43
2:L:11:LEU:HD21	2:L:19:VAL:CG1	2.49	0.42
3:R:425:LEU:HD21	3:R:512:VAL:HG11	2.02	0.42
2:L:186:ASP:HA	2:L:189:LYS:HD3	2.02	0.41
2:L:67:GLY:HA3	2:L:72:PHE:HA	2.02	0.41
2:L:11:LEU:HD21	2:L:19:VAL:HG13	2.02	0.41
2:L:126:LEU:HD23	2:L:126:LEU:HA	1.94	0.41
2:L:35:ALA:HB2	2:L:92:LEU:HD11	2.03	0.41
3:R:393:THR:HG21	3:R:518:LEU:HB2	2.02	0.40
2:L:90:GLN:HG3	2:L:99:PHE:CE1	2.57	0.40
3:R:431:GLY:HA2	3:R:515:PHE:CE2	2.57	0.40

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	H	211/223 (95%)	207 (98%)	4 (2%)	0	100	100
2	L	210/215 (98%)	203 (97%)	7 (3%)	0	100	100
3	R	192/227 (85%)	185 (96%)	7 (4%)	0	100	100
All	All	613/665 (92%)	595 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	Percentiles	
1	H	175/184 (95%)	171 (98%)	4 (2%)	50	57
2	L	183/185 (99%)	177 (97%)	6 (3%)	38	43
3	R	166/200 (83%)	165 (99%)	1 (1%)	86	90
All	All	524/569 (92%)	513 (98%)	11 (2%)	53	60

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	35	SER
1	H	133	SER
1	H	155	VAL
1	H	204	ASN
2	L	9	SER
2	L	11	LEU
2	L	34	LEU
2	L	91	GLN
2	L	106	GLU
2	L	186	ASP
3	R	389	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	204	ASN

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

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	H	215/223 (96%)	0.18	16 (7%) 14 14	32, 41, 56, 88	0
2	L	212/215 (98%)	-0.06	3 (1%) 75 76	32, 42, 55, 61	0
3	R	194/227 (85%)	0.43	24 (12%) 4 3	30, 46, 85, 94	0
All	All	621/665 (93%)	0.18	43 (6%) 16 16	30, 43, 72, 94	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	133	SER	6.9
3	R	372	ALA	4.8
3	R	371	SER	4.5
3	R	387	LEU	4.1
3	R	390	LEU	4.1
3	R	334	ASN	4.0
3	R	519	HIS	4.0
1	H	134	LYS	3.8
3	R	521	PRO	3.8
3	R	370	ASN	3.8
3	R	373	SER	3.7
1	H	96	ALA	3.6
3	R	335	LEU	3.6
1	H	1	GLU	3.5
3	R	386	LYS	3.4
3	R	369	TYR	3.4
3	R	333	THR	3.3
3	R	517	LEU	3.3
3	R	346	ARG	3.0
3	R	520	ALA	2.9
3	R	522	ALA	2.7
3	R	362	VAL	2.7
1	H	99	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	204	SER	2.6
1	H	33	TYR	2.6
1	H	105	MET	2.6
3	R	389	ASP	2.6
2	L	203	SER	2.5
3	R	385	THR	2.5
2	L	24	ARG	2.4
3	R	366	SER	2.4
1	H	104	GLY	2.4
1	H	198	THR	2.3
1	H	132	SER	2.3
1	H	35	SER	2.3
3	R	518	LEU	2.2
1	H	100	GLY	2.2
1	H	34	MET	2.2
1	H	75	LYS	2.1
1	H	204	ASN	2.1
3	R	397	ALA	2.1
1	H	206	LYS	2.1
3	R	512	VAL	2.1

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.