



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 30, 2024 – 05:44 pm BST

PDB ID : 8R80
Title : SARS-CoV-2 Delta RBD in complex with XBB-9 Fab and an anti-Fab nanobody
Authors : Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2023-11-27
Resolution : 4.03 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
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

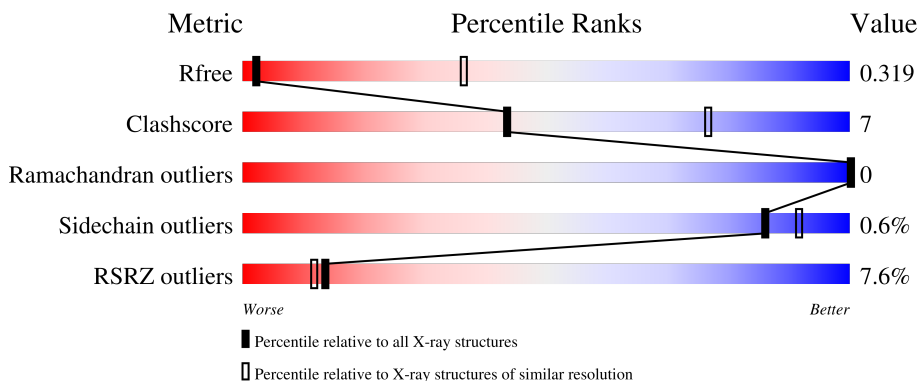
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.03 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.



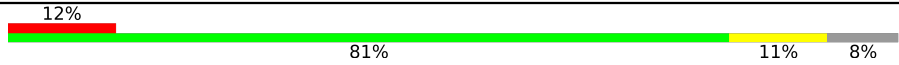

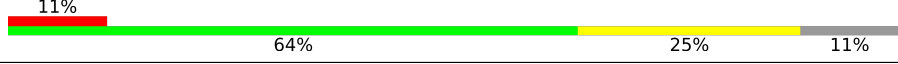
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1105 (4.38-3.70)
Clashscore	141614	1005 (4.36-3.72)
Ramachandran outliers	138981	1125 (4.38-3.70)
Sidechain outliers	138945	1115 (4.38-3.70)
RSRZ outliers	127900	1003 (4.40-3.68)

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	A	224	
1	H	224	
2	B	214	
2	L	214	
3	E	202	

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Mol	Chain	Length	Quality of chain
3	R	202	
4	J	135	
4	N	135	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11366 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 XBB-9 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	220	Total 1615	C 1013	N 274	O 320	S 8	0	0	0
1	A	220	Total 1615	C 1013	N 274	O 320	S 8	0	0	0

- Molecule 2 is a protein called XBB-9 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	Total 1653	C 1043	N 275	O 330	S 5	0	0	0
2	B	213	Total 1647	C 1040	N 274	O 329	S 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	E	186	Total 1493	C 957	N 250	O 279	S 7	0	1	0
3	R	186	Total 1493	C 957	N 250	O 279	S 7	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	452	ARG	LEU	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	527	LYS	-	expression tag	UNP P0DTC2
E	528	LYS	-	expression tag	UNP P0DTC2
R	327	HIS	-	expression tag	UNP P0DTC2
R	328	HIS	-	expression tag	UNP P0DTC2
R	329	HIS	-	expression tag	UNP P0DTC2
R	330	HIS	-	expression tag	UNP P0DTC2
R	331	HIS	-	expression tag	UNP P0DTC2
R	332	HIS	-	expression tag	UNP P0DTC2
R	452	ARG	LEU	variant	UNP P0DTC2
R	478	LYS	THR	variant	UNP P0DTC2
R	527	LYS	-	expression tag	UNP P0DTC2
R	528	LYS	-	expression tag	UNP P0DTC2

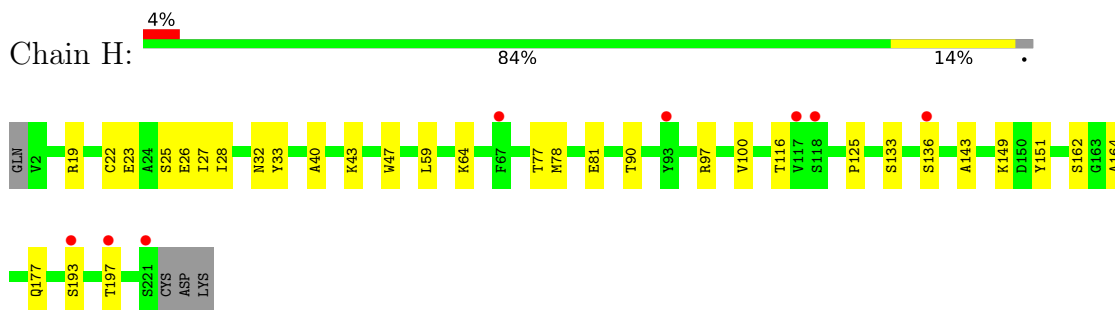
- Molecule 4 is a protein called anti-Fab nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	N	120	925	574	163	184	4	0	0	0
4	J	120	925	574	163	184	4	0	0	0

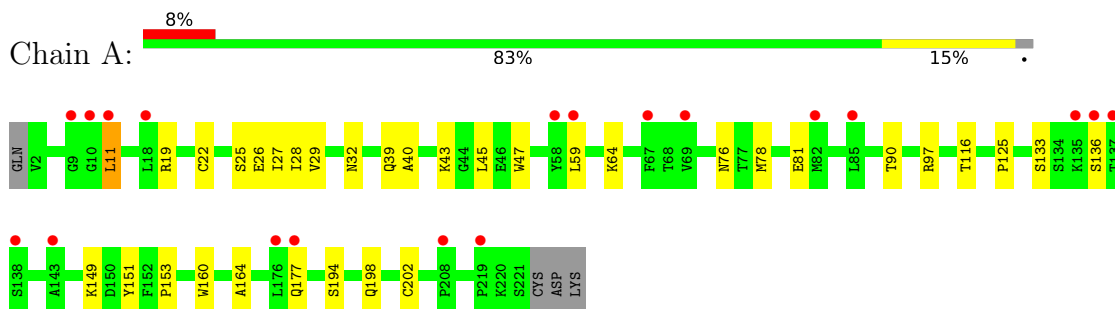
3 Residue-property plots [i](#)

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.

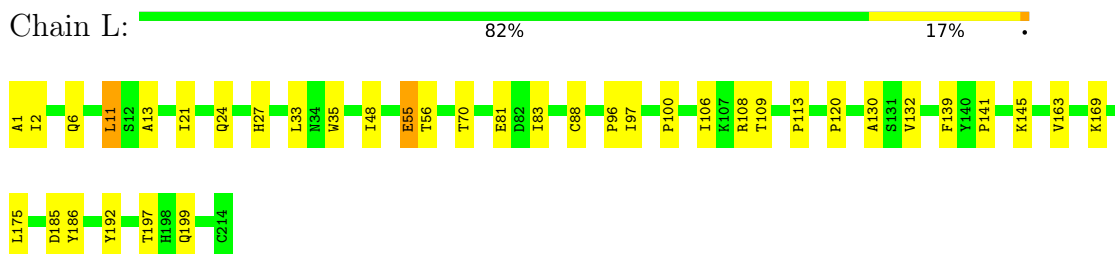
- Molecule 1: XBB-9 Fab heavy chain



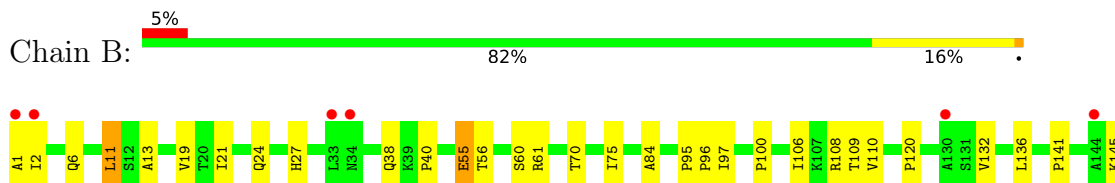
- Molecule 1: XBB-9 Fab heavy chain

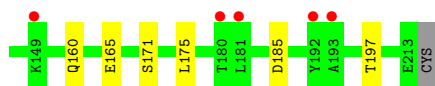


- Molecule 2: XBB-9 Fab light chain

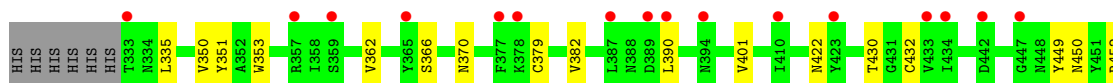
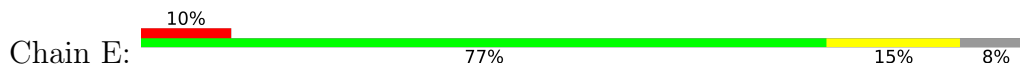


- Molecule 2: XBB-9 Fab light chain

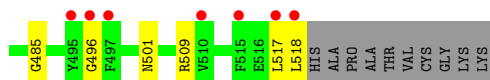
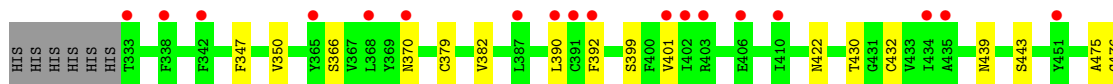
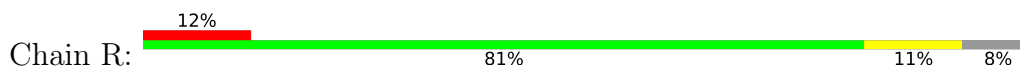




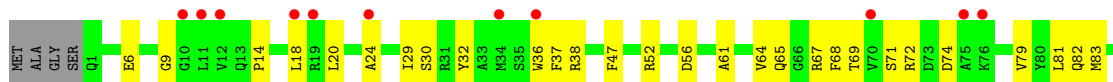
- Molecule 3: Spike protein S1



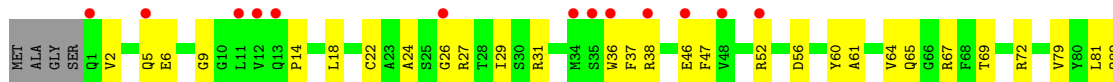
- Molecule 3: Spike protein S1



- Molecule 4: anti-Fab nanobody



- Molecule 4: anti-Fab nanobody



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.54Å 126.40Å 164.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.64 – 4.03 65.64 – 4.03	Depositor EDS
% Data completeness (in resolution range)	99.4 (65.64-4.03) 99.5 (65.64-4.03)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 4.01Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.268 , 0.313 0.270 , 0.319	Depositor DCC
R_{free} test set	945 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	166.8	Xtrriage
Anisotropy	0.243	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 189.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11366	wwPDB-VP
Average B, all atoms (Å ²)	203.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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	A	0.25	0/1648	0.50	0/2246
1	H	0.25	0/1648	0.50	0/2246
2	B	0.26	0/1686	0.48	0/2293
2	L	0.26	0/1692	0.48	0/2301
3	E	0.26	0/1537	0.47	0/2087
3	R	0.26	0/1537	0.47	0/2087
4	J	0.28	0/944	0.54	0/1276
4	N	0.26	0/944	0.51	0/1276
All	All	0.26	0/11636	0.49	0/15812

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	1615	0	1609	21	0
1	H	1615	0	1609	21	0
2	B	1647	0	1605	25	0
2	L	1653	0	1610	25	0
3	E	1493	0	1420	19	0
3	R	1493	0	1420	13	0
4	J	925	0	873	26	0
4	N	925	0	873	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11366	0	11019	150	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 7.

The worst 5 of 150 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:430:THR:HG21	3:R:517:LEU:HD11	1.64	0.78
1:H:164:ALA:HB2	3:E:484:GLU:HB2	1.68	0.76
3:E:476:GLY:HA2	1:A:27:ILE:HA	1.69	0.75
2:L:6:GLN:HB3	2:L:100:PRO:HD2	1.68	0.75
3:R:485:GLY:HA3	1:A:164:ALA:HB1	1.69	0.74

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	Outliers	Percentiles	
1	A	218/224 (97%)	211 (97%)	7 (3%)	0	100	100
1	H	218/224 (97%)	211 (97%)	7 (3%)	0	100	100
2	B	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
2	L	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
3	E	185/202 (92%)	174 (94%)	11 (6%)	0	100	100
3	R	185/202 (92%)	173 (94%)	12 (6%)	0	100	100
4	J	118/135 (87%)	107 (91%)	11 (9%)	0	100	100
4	N	118/135 (87%)	107 (91%)	11 (9%)	0	100	100
All	All	1465/1550 (94%)	1388 (95%)	77 (5%)	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	A	183/187 (98%)	182 (100%)	1 (0%)	88	93
1	H	183/187 (98%)	183 (100%)	0	100	100
2	B	188/189 (100%)	185 (98%)	3 (2%)	62	79
2	L	189/189 (100%)	186 (98%)	3 (2%)	62	79
3	E	163/175 (93%)	162 (99%)	1 (1%)	86	91
3	R	163/175 (93%)	163 (100%)	0	100	100
4	J	96/108 (89%)	96 (100%)	0	100	100
4	N	96/108 (89%)	96 (100%)	0	100	100
All	All	1261/1318 (96%)	1253 (99%)	8 (1%)	86	91

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	185	ASP
2	B	55	GLU
1	A	11	LEU
3	E	468	ILE
2	B	11	LEU

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

Mol	Chain	Res	Type
2	B	160	GLN

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, 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	220/224 (98%)	0.61	19 (8%) 10 9	144, 198, 296, 561	0
1	H	220/224 (98%)	0.39	8 (3%) 42 34	139, 184, 270, 341	0
2	B	213/214 (99%)	0.42	11 (5%) 27 24	135, 179, 238, 281	0
2	L	214/214 (100%)	0.19	0 100 100	134, 175, 232, 264	0
3	E	186/202 (92%)	0.62	20 (10%) 5 5	160, 208, 315, 473	0
3	R	186/202 (92%)	0.86	25 (13%) 3 4	150, 207, 310, 382	0
4	J	120/135 (88%)	0.72	14 (11%) 4 5	157, 215, 299, 348	0
4	N	120/135 (88%)	0.65	15 (12%) 3 5	163, 226, 283, 308	0
All	All	1479/1550 (95%)	0.53	112 (7%) 13 12	134, 197, 292, 561	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	J	1	GLN	8.6
3	E	333	THR	7.9
3	R	391	CYS	7.9
1	A	136	SER	6.3
4	J	13	GLN	6.2

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.