



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8YK4 / pdb_00008yk4
Title : Structure of SARS-CoV-2 RBD and antibody NT-108
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Deposited on : 2024-03-04
Resolution : 3.20 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

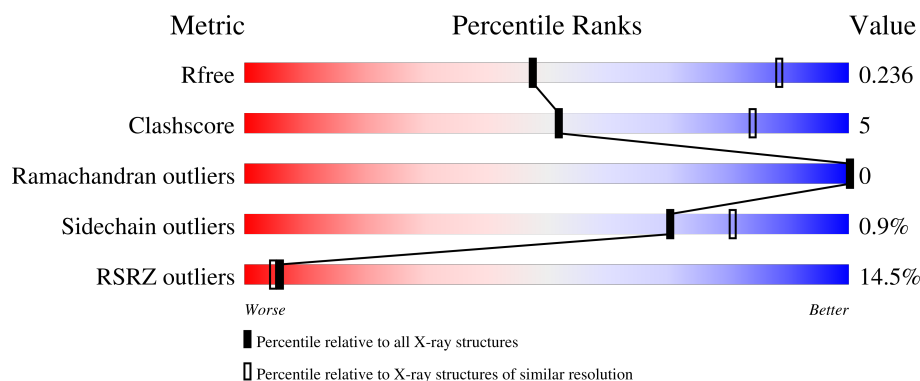
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	282	5% 72% 9% 18%
2	C	215	20% 67% 16% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3179 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 antibody NT-108, single chain Fv fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1761	1111	299	345	6			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	178	Total	C	N	O	S	0	0	0
			1418	908	237	267	6			

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	55.15Å 149.64Å 253.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 3.20 48.35 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.35-3.20) 99.3 (48.35-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.243 , 0.267 (Not available) , 0.236	Depositor DCC
R_{free} test set	862 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3179	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% 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	0.08	0/1803	0.25	0/2452
2	C	0.07	0/1455	0.24	0/1974
All	All	0.07	0/3258	0.25	0/4426

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	1761	0	1707	14	0
2	C	1418	0	1339	18	0
All	All	3179	0	3046	32	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 5.

All (32) 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:C:381:GLY:HA3	2:C:430:THR:HA	1.76	0.67
1:A:39:GLN:HB2	1:A:49:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:O	1:A:179:ARG:NH1	2.35	0.60
2:C:412:PRO:HB3	2:C:427:ASP:HA	1.84	0.60
2:C:350:VAL:HG11	2:C:418:ILE:HD12	1.85	0.58
2:C:401:VAL:HG22	2:C:509:ARG:HG2	1.89	0.55
2:C:357:ARG:NH2	2:C:396:TYR:OH	2.40	0.54
1:A:217:THR:HG23	1:A:243:THR:HA	1.94	0.49
1:A:90:CYS:O	1:A:100:GLY:N	2.44	0.49
2:C:444:LYS:H	2:C:448:ASN:HB2	1.79	0.48
1:A:13:SER:HB3	1:A:108:LYS:HE3	1.94	0.48
2:C:376:THR:HB	2:C:435:ALA:HB3	1.97	0.47
2:C:403:ARG:HG2	2:C:404:GLY:H	1.82	0.45
1:A:67:SER:HG	1:A:74:THR:HG1	1.62	0.45
2:C:368:LEU:HB3	2:C:374:PHE:HE2	1.81	0.45
1:A:177:TYR:HD2	1:A:179:ARG:HE	1.62	0.45
2:C:382:VAL:HG11	2:C:387:LEU:HD21	1.97	0.44
1:A:129:GLN:NE2	1:A:240:THR:HG22	2.32	0.44
1:A:193:ARG:HB2	1:A:210:ASN:HB3	2.00	0.42
2:C:466:ARG:HG2	2:C:468:ILE:HD11	2.01	0.42
2:C:502:GLY:O	2:C:506:GLN:HG3	2.19	0.42
1:A:162:ILE:HD11	1:A:233:PHE:CE1	2.55	0.42
1:A:32:SER:OG	1:A:93:TYR:O	2.36	0.41
1:A:162:ILE:O	1:A:221:PHE:N	2.41	0.41
2:C:418:ILE:HA	2:C:422:ASN:HD22	1.85	0.41
2:C:453:TYR:CE2	2:C:455:LEU:HD23	2.54	0.41
1:A:81:GLU:HB3	1:A:83:GLU:HG2	2.01	0.41
2:C:403:ARG:HB3	2:C:406:GLU:HG2	2.03	0.41
2:C:409:GLN:HB3	2:C:419:ALA:HB2	2.02	0.41
1:A:85:PHE:CD1	1:A:106:GLU:HA	2.56	0.41
2:C:367:VAL:HG13	2:C:368:LEU:HG	2.03	0.40
2:C:472:ILE:HD13	2:C:484:GLU:HB3	2.03	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	A	226/282 (80%)	212 (94%)	14 (6%)	0	100	100
2	C	172/215 (80%)	159 (92%)	13 (8%)	0	100	100
All	All	398/497 (80%)	371 (93%)	27 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	194/228 (85%)	192 (99%)	2 (1%)	68	80
2	C	153/188 (81%)	152 (99%)	1 (1%)	76	83
All	All	347/416 (83%)	344 (99%)	3 (1%)	70	81

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

Mol	Chain	Res	Type
1	A	35	LEU
1	A	81	GLU
2	C	362	VAL

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 [i](#)

There are no oligosaccharides 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	A	230/282 (81%)	0.64	15 (6%) 25 16	30, 51, 84, 109	0
2	C	178/215 (82%)	1.39	44 (24%) 2 2	47, 92, 145, 198	0
All	All	408/497 (82%)	0.97	59 (14%) 6 5	30, 67, 135, 198	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	365	TYR	6.9
2	C	369	TYR	5.8
1	A	210	ASN	5.2
1	A	123	SER	4.8
1	A	211	SER	4.1
2	C	394	ASN	4.0
2	C	385	THR	4.0
2	C	522	ALA	3.9
2	C	361	CYS	3.8
1	A	78	SER	3.8
2	C	338	PHE	3.8
1	A	246	SER	3.8
1	A	33	THR	3.4
1	A	56	MET	3.2
1	A	108	LYS	3.1
2	C	340	GLU	3.1
2	C	362	VAL	3.1
2	C	383	SER	3.0
1	A	180	SER	3.0
2	C	388	ASN	3.0
2	C	406	GLU	3.0
2	C	384	PRO	2.9
1	A	227	SER	2.9
1	A	98	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	90	CYS	2.9
2	C	349	SER	2.8
2	C	371	SER	2.8
2	C	426	PRO	2.8
2	C	368	LEU	2.8
2	C	364	ASP	2.7
2	C	514	SER	2.7
2	C	380	TYR	2.6
2	C	516	GLU	2.6
2	C	433	VAL	2.6
2	C	445	VAL	2.6
2	C	525	CYS	2.5
2	C	354	ASN	2.5
2	C	430	THR	2.5
2	C	464	PHE	2.4
2	C	370	ASN	2.4
1	A	85	PHE	2.4
1	A	79	ARG	2.3
2	C	356	LYS	2.3
2	C	436	TRP	2.2
2	C	523	THR	2.2
1	A	69	SER	2.2
2	C	444	LYS	2.2
2	C	357	ARG	2.2
2	C	373	SER	2.1
2	C	415	THR	2.1
2	C	363	ALA	2.1
2	C	377	PHE	2.1
2	C	423	TYR	2.1
2	C	367	VAL	2.0
2	C	432	CYS	2.0
2	C	481	ASN	2.0
2	C	372	ALA	2.0
2	C	482	GLY	2.0
2	C	402	ILE	2.0

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 [i](#)

There are no oligosaccharides 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.