



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:31 PM UTC

PDB ID : 8SIR / pdb_00008sir
Title : Crystal structure of SARS-CoV-2 spike receptor-binding domain in complex with broadly neutralizing antibody CC25.54 Fab
Authors : Liu, H.; Wilson, I.A.
Deposited on : 2023-04-16
Resolution : 3.30 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
Mogul : 2022.3.0, CSD as543be (2022)
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

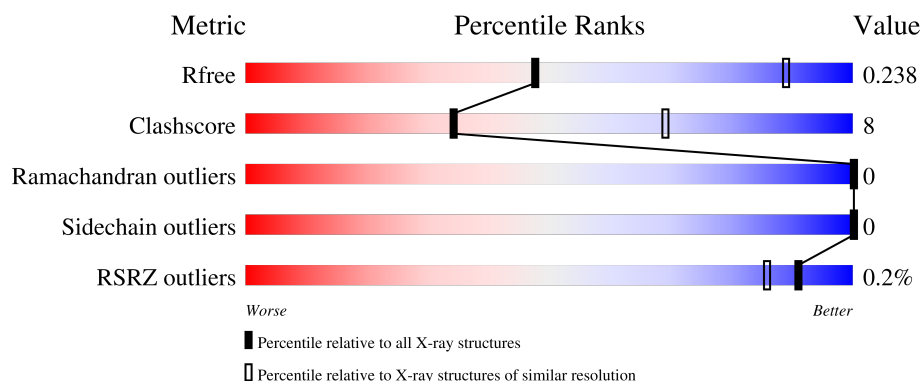
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	205	 80% 15% 5%
2	H	242	 76% 18% 7%
3	L	215	 82% 16% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4803 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1497	959	248	282	8			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2

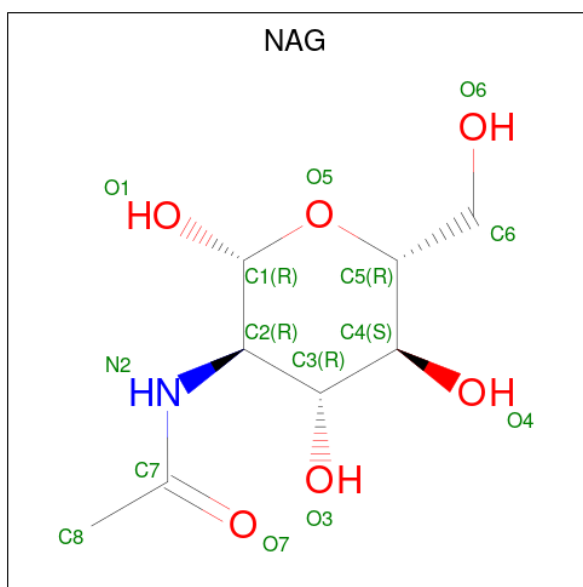
- Molecule 2 is a protein called CC25.54 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1683	1064	277	337	5			

- Molecule 3 is a protein called CC25.54 Fab light chain.

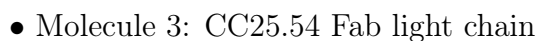
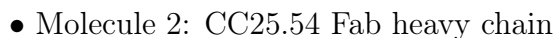
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1609	1008	266	330	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

- Molecule 1: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.87Å 135.87Å 87.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.76 – 3.30 48.76 – 3.30	Depositor EDS
% Data completeness (in resolution range)	78.5 (48.76-3.30) 78.4 (48.76-3.30)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.208 , 0.236 0.208 , 0.238	Depositor DCC
R_{free} test set	542 reflections (3.80%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.092 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4803	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.11	0/1540	0.31	0/2104
2	H	0.10	0/1726	0.28	0/2363
3	L	0.11	0/1647	0.34	0/2246
All	All	0.11	0/4913	0.31	0/6713

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

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	1497	0	1360	21	0
2	H	1683	0	1612	32	0
3	L	1609	0	1523	24	0
4	A	14	0	13	0	0
All	All	4803	0	4508	71	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 8.

All (71) 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:H:87:THR:HG22	2:H:111:VAL:H	1.39	0.87
1:A:402:ILE:HD11	1:A:418:ILE:HG13	1.57	0.83
1:A:360:ASN:H	1:A:523:THR:HB	1.48	0.77
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.68	0.74
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.72	0.72
2:H:12:VAL:HG21	2:H:18:LEU:HD12	1.75	0.68
1:A:402:ILE:HG13	1:A:403:ARG:H	1.60	0.66
1:A:350:VAL:HG21	1:A:402:ILE:HD12	1.78	0.65
2:H:59:TYR:HE1	2:H:69:MET:HB2	1.62	0.65
3:L:33:LEU:HD11	3:L:88:CYS:HB2	1.82	0.62
3:L:11:LEU:HD23	3:L:19:VAL:HG13	1.82	0.61
3:L:137:ASN:O	3:L:174:SER:OG	2.17	0.61
2:H:2:VAL:HG21	2:H:94:ARG:HH11	1.65	0.60
2:H:18:LEU:HD11	2:H:109:VAL:HG11	1.85	0.57
2:H:36:TRP:HB3	2:H:48:ILE:HD12	1.88	0.56
1:A:413:GLY:HA3	2:H:34:PHE:HZ	1.71	0.56
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.88	0.54
3:L:34:ALA:HB1	3:L:46:LEU:HD11	1.90	0.54
1:A:484:GLU:HG2	1:A:489:TYR:HA	1.90	0.54
2:H:8:GLY:HA3	2:H:20:LEU:HD13	1.90	0.53
2:H:41:PRO:HD3	2:H:88:ALA:HA	1.90	0.53
2:H:66:ARG:HH22	2:H:86:ASP:CG	2.17	0.53
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.92	0.52
2:H:18:LEU:O	2:H:81:LYS:HA	2.10	0.52
2:H:181:VAL:HG21	3:L:135:LEU:HD11	1.92	0.52
2:H:126:PRO:HG2	2:H:213:PRO:HG3	1.91	0.52
1:A:350:VAL:HG12	1:A:422:ASN:HB3	1.91	0.51
1:A:360:ASN:N	1:A:523:THR:HB	2.22	0.51
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.92	0.51
1:A:353:TRP:H	1:A:353:TRP:CD1	2.30	0.50
1:A:359:SER:OG	1:A:394:ASN:OD1	2.25	0.50
2:H:47:LEU:HD12	3:L:96:TRP:HB2	1.93	0.50
3:L:39:LYS:HG2	3:L:84:ALA:HB2	1.94	0.49
2:H:108:THR:HB	2:H:149:PRO:HD3	1.94	0.49
1:A:379:CYS:SG	1:A:384:PRO:HG3	2.53	0.49
2:H:66:ARG:NE	2:H:82(A):GLY:O	2.34	0.48
1:A:444:LYS:O	1:A:499:PRO:HD3	2.13	0.48
2:H:53:LYS:NZ	2:H:55:ARG:O	2.44	0.48
3:L:115:VAL:HA	3:L:135:LEU:O	2.13	0.48
2:H:66:ARG:HB2	2:H:82(A):GLY:H	1.79	0.48
2:H:53:LYS:C	2:H:55:ARG:H	2.22	0.48
3:L:113:PRO:HB3	3:L:139:PHE:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:6:GLN:NE2	3:L:86:TYR:O	2.45	0.47
3:L:46:LEU:HD23	3:L:55:GLU:OE1	2.15	0.46
3:L:63:SER:O	3:L:73:LEU:HD22	2.16	0.46
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.51	0.46
3:L:91:TYR:HA	3:L:96:TRP:CE3	2.51	0.46
2:H:122:PHE:CE2	3:L:124:GLN:HG3	2.51	0.46
2:H:18:LEU:HG	2:H:20:LEU:HD23	1.98	0.45
1:A:402:ILE:HG13	1:A:403:ARG:N	2.29	0.45
3:L:50:LYS:C	3:L:52:SER:H	2.24	0.45
3:L:18:SER:HA	3:L:75:ILE:O	2.17	0.45
2:H:2:VAL:HG21	2:H:94:ARG:NH1	2.31	0.44
3:L:36:TYR:CE1	3:L:46:LEU:HB2	2.53	0.44
2:H:52(B):SER:H	2:H:54:SER:HB3	1.83	0.43
2:H:39:GLN:HB2	2:H:45:LEU:HD23	2.00	0.43
3:L:113:PRO:HD2	3:L:201:LEU:HG	2.01	0.43
3:L:19:VAL:O	3:L:74:THR:HA	2.18	0.43
2:H:4:LEU:HD21	2:H:35(A):TRP:HZ3	1.83	0.43
2:H:166:PHE:CD1	3:L:164:THR:HG23	2.53	0.42
1:A:461:LEU:HD22	1:A:465:GLU:CD	2.45	0.42
1:A:366:SER:HA	1:A:369:TYR:CZ	2.55	0.42
1:A:404:GLY:C	1:A:406:GLU:H	2.28	0.42
1:A:413:GLY:HA3	2:H:34:PHE:CZ	2.53	0.41
1:A:412:PRO:HG3	1:A:429:PHE:HB3	2.01	0.41
2:H:12:VAL:HG21	2:H:18:LEU:CD1	2.48	0.41
2:H:71:VAL:HG22	2:H:78:VAL:HG22	2.01	0.41
1:A:347:PHE:HB3	1:A:401:VAL:HG23	2.03	0.41
2:H:138:LEU:HB2	2:H:211:VAL:HG11	2.02	0.40
2:H:100(A):ARG:H	2:H:100(A):ARG:HG2	1.51	0.40
3:L:50:LYS:HG3	3:L:50:LYS:O	2.21	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	193/205 (94%)	181 (94%)	12 (6%)	0	100	100
2	H	220/242 (91%)	209 (95%)	11 (5%)	0	100	100
3	L	209/215 (97%)	200 (96%)	9 (4%)	0	100	100
All	All	622/662 (94%)	590 (95%)	32 (5%)	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	154/177 (87%)	154 (100%)	0	100	100
2	H	191/211 (90%)	191 (100%)	0	100	100
3	L	181/190 (95%)	181 (100%)	0	100	100
All	All	526/578 (91%)	526 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	GLN
1	A	437	ASN
1	A	448	ASN
1	A	487	ASN
2	H	32	HIS
2	H	58	ASN
2	H	199	ASN
3	L	79	GLN
3	L	137	ASN
3	L	147	GLN
3	L	210	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	601	1	14,14,15	1.01	1 (7%)	17,19,21	1.19	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	601	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	O5-C1	3.31	1.49	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	601	NAG	C1-O5-C5	4.68	118.46	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	A	601	NAG	C8-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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	195/205 (95%)	-0.18	0 100 100	43, 66, 110, 148	0
2	H	226/242 (93%)	-0.38	1 (0%) 88 79	38, 62, 91, 111	0
3	L	211/215 (98%)	-0.34	0 100 100	42, 69, 92, 113	0
All	All	632/662 (95%)	-0.30	1 (0%) 91 86	38, 66, 95, 148	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	52(A)	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	601	14/15	0.87	0.12	63,84,101,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.