



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 1, 2022 – 03:01 PM EST

PDB ID : 8DW9
Title : Crystal structure of neutralizing antibody D29 Fab in complex with SARS-CoV-2 spike receptor binding domain (RBD)
Authors : Reddem, E.R.; Shapiro, L.
Deposited on : 2022-08-01
Resolution : 4.00 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	:	2.31.2
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)	:	2.31.2

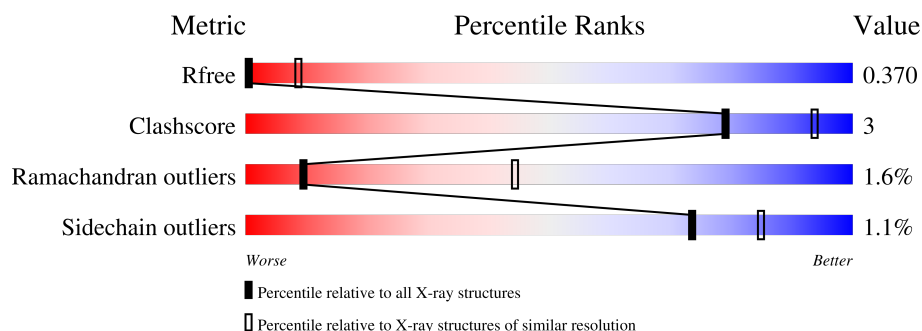
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	195	80% 9% • 11%
1	B	195	82% 7% • 11%
2	C	219	91% 8% •
2	H	219	89% 10% •
3	D	211	92% 6% •
3	L	211	92% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9236 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	174	Total	C	N	O	S	0	1	0
			1378	886	232	254	6			
1	B	174	Total	C	N	O	S	0	1	0
			1378	886	232	254	6			

- Molecule 2 is a protein called D29 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	219	Total	C	N	O	S	0	3	0
			1640	1043	265	326	6			
2	H	219	Total	C	N	O	S	0	3	0
			1640	1043	265	326	6			


- Molecule 3 is a protein called D29 Fab light chain.

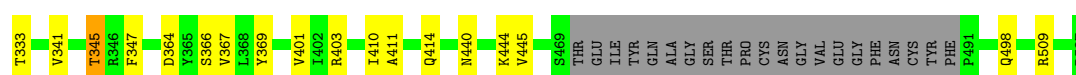
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	2	0
			1600	1010	269	317	4			
3	L	211	Total	C	N	O	S	0	2	0
			1600	1010	269	317	4			

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. 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. 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.

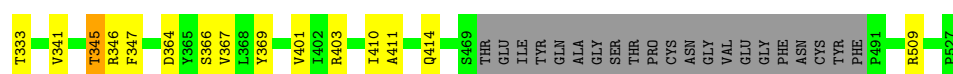
- Molecule 1: Spike protein S1

Chain A:  80% 9% 11%




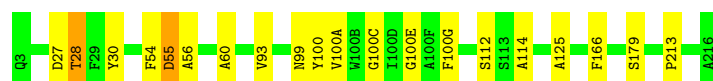
- Molecule 1: Spike protein S1

Chain B:  82% 7% 11%




- Molecule 2: D29 Heavy chain

Chain C:  91% 8% 1%



- Molecule 2: D29 Heavy chain

Chain H:  89% 10% 1%



- Molecule 3: D29 Fab light chain

Chain D:  92% 6% 2%



- Molecule 3: D29 Fab light chain

Chain L:  92% 8% 0%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.17Å 106.71Å 207.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.09 – 4.00 94.91 – 4.00	Depositor EDS
% Data completeness (in resolution range)	82.0 (95.09-4.00) 82.0 (94.91-4.00)	Depositor EDS
R_{merge}	0.96	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 4.01Å)	Xtriage
Refinement program	PHENIX Refine	Depositor
R, R_{free}	0.300 , 0.381 0.345 , 0.370	Depositor DCC
R_{free} test set	639 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	88.9	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	9236	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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

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	0.38	0/1416	0.56	0/1925
1	B	0.38	0/1416	0.56	0/1925
2	C	0.36	0/1684	0.58	0/2298
2	H	0.37	0/1684	0.59	0/2298
3	D	0.35	0/1642	0.58	0/2238
3	L	0.35	0/1642	0.59	0/2238
All	All	0.36	0/9484	0.58	0/12922

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	1378	0	1314	9	0
1	B	1378	0	1314	7	0
2	C	1640	0	1592	14	0
2	H	1640	0	1592	16	0
3	D	1600	0	1556	10	0
3	L	1600	0	1556	9	0
All	All	9236	0	8924	51	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 (51) 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:445:VAL:HG21	2:H:64:GLN:HE22	1.38	0.88
1:B:333:THR:N	2:H:28:THR:HG1	1.74	0.86
2:C:93:VAL:HG11	2:C:100(G):PHE:HB3	1.67	0.76
1:A:333:THR:N	2:C:28:THR:HG1	2.04	0.55
1:A:345:THR:HG21	2:H:32:PHE:CE2	2.42	0.55
2:H:11:VAL:HG13	2:H:110:THR:OG1	2.06	0.55
2:H:93:VAL:HG11	2:H:100(G):PHE:HB3	1.89	0.54
2:H:100:TYR:HB3	2:H:100(C):GLY:HA3	1.89	0.54
2:H:93:VAL:HG11	2:H:100(G):PHE:CD2	2.43	0.53
2:H:54:PHE:O	2:H:56:ALA:N	2.42	0.53
2:H:166:PHE:HB3	3:L:163:THR:HG21	1.91	0.52
3:L:114:PRO:HB2	3:L:137:ILE:HG23	1.92	0.51
2:C:54:PHE:O	2:C:56:ALA:N	2.43	0.50
2:H:112:SER:O	2:H:114:ALA:N	2.44	0.50
2:C:112:SER:O	2:C:114:ALA:N	2.45	0.50
3:D:33:LEU:HD23	3:D:89:GLN:O	2.12	0.49
2:C:100(E):GLY:HA3	3:D:91:TYR:CD1	2.47	0.49
3:D:114:PRO:HB2	3:D:137:ILE:HG23	1.94	0.49
1:B:345:THR:HG22	2:C:99:ASN:HB3	1.94	0.48
3:D:164:LYS:HB3	3:D:165:PRO:HD2	1.93	0.48
1:B:411:ALA:HB3	1:B:414:GLN:HG2	1.95	0.48
3:L:107:LYS:HA	3:L:141:TYR:OH	2.14	0.48
3:D:107:LYS:HA	3:D:141:TYR:OH	2.14	0.47
1:B:366:SER:HA	1:B:369:TYR:CE2	2.50	0.47
2:C:100:TYR:HB3	2:C:100(C):GLY:HA3	1.97	0.47
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.98	0.46
3:L:164:LYS:HB3	3:L:165:PRO:HD2	1.98	0.46
2:C:166:PHE:HB3	3:D:163:THR:HG21	1.97	0.46
1:A:366:SER:HA	1:A:369:TYR:CE2	2.50	0.45
3:L:33:LEU:HD23	3:L:34:ALA:N	2.31	0.45
2:C:100:TYR:CG	2:C:100(A):VAL:N	2.85	0.45
1:A:444:LYS:HE2	2:H:56:ALA:HB1	1.98	0.44
2:H:125:ALA:HB1	2:H:213:PRO:HA	1.98	0.44
2:C:125:ALA:HB1	2:C:213:PRO:HA	2.00	0.44
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.99	0.44
3:D:164:LYS:HB3	3:D:165:PRO:CD	2.48	0.43
1:A:364:ASP:O	1:A:367:VAL:HG12	2.18	0.43
2:H:100:TYR:CG	2:H:100(A):VAL:N	2.86	0.42
2:C:93:VAL:CG1	2:C:100(G):PHE:HB3	2.42	0.42
2:C:60:ALA:HA	3:D:95:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ASP:O	1:B:367:VAL:HG12	2.19	0.42
1:B:346:ARG:HD2	2:C:54:PHE:CE2	2.54	0.42
1:B:401:VAL:HG22	1:B:509:ARG:HG2	2.01	0.41
2:C:179:SER:HG	3:D:178:TYR:HE2	1.63	0.41
3:L:164:LYS:HB3	3:L:165:PRO:CD	2.51	0.41
2:H:32:PHE:O	2:H:52(A):PRO:HD2	2.21	0.41
3:L:149:TRP:O	3:L:155:PRO:HA	2.20	0.41
3:D:149:TRP:O	3:D:155:PRO:HA	2.20	0.41
2:H:124:LEU:HB3	3:L:119:PHE:CD2	2.56	0.41
1:A:440:ASN:HB3	3:L:93:ASP:HA	2.03	0.40
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.02	0.40

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	170/195 (87%)	148 (87%)	18 (11%)	4 (2%)	6	36
1	B	170/195 (87%)	148 (87%)	18 (11%)	4 (2%)	6	36
2	C	214/219 (98%)	194 (91%)	17 (8%)	3 (1%)	11	46
2	H	214/219 (98%)	194 (91%)	18 (8%)	2 (1%)	17	55
3	D	208/211 (99%)	192 (92%)	13 (6%)	3 (1%)	11	46
3	L	208/211 (99%)	191 (92%)	14 (7%)	3 (1%)	11	46
All	All	1184/1250 (95%)	1067 (90%)	98 (8%)	19 (2%)	9	44

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	55	ASP

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Mol	Chain	Res	Type
2	H	55	ASP
1	A	345	THR
1	B	345	THR
2	H	30	TYR
1	A	403	ARG
1	B	403	ARG
2	C	30	TYR
2	C	27	ASP
3	D	56	THR
3	D	165	PRO
3	L	165	PRO
3	L	56	THR
1	B	341	VAL
1	A	341	VAL
1	A	410	ILE
1	B	410	ILE
3	L	44	PRO
3	D	44	PRO

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	149/168 (89%)	147 (99%)	2 (1%)	69	82
1	B	149/168 (89%)	148 (99%)	1 (1%)	84	90
2	C	184/184 (100%)	182 (99%)	2 (1%)	73	85
2	H	184/184 (100%)	182 (99%)	2 (1%)	73	85
3	D	175/177 (99%)	173 (99%)	2 (1%)	73	85
3	L	175/177 (99%)	173 (99%)	2 (1%)	73	85
All	All	1016/1058 (96%)	1005 (99%)	11 (1%)	73	85

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

Mol	Chain	Res	Type
1	A	347	PHE
1	A	498	GLN
1	B	347	PHE
2	C	28	THR
2	C	55	ASP
3	D	33	LEU
3	D	89	GLN
2	H	28	THR
2	H	55	ASP
3	L	7	SER
3	L	154	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	GLN
1	B	440	ASN
2	H	61	GLN
2	H	64	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	2
2	C	2
3	D	1
3	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	127:SER	C	134:GLY	N	13.16
1	C	127:SER	C	134:GLY	N	11.03
1	C	113:SER	C	114:ALA	N	4.75
1	H	113:SER	C	114:ALA	N	4.74
1	D	107:LYS	C	108:GLY	N	3.73
1	L	107:LYS	C	108:GLY	N	3.73

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.