



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2023 – 06:17 AM EDT

PDB ID : 7L7E  
Title : Crystal structure of SARS-CoV-2 spike RBD in complex with human monoclonal antibodies AZD8895 and AZD1061  
Authors : Dong, J.; Crowe, J.E.  
Deposited on : 2020-12-28  
Resolution : 3.00 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

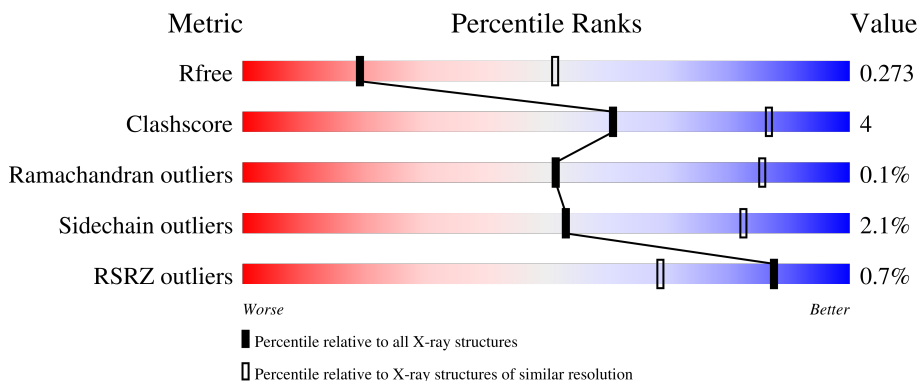
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	225	 89% 8%
1	H	225	 81% 16%
1	I	225	 85% 12%
1	T	225	 87% 10%
2	B	216	 88% 10%

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Mol	Chain	Length	Quality of chain
2	J	216	 84% 14%
2	L	216	 90% 9%
2	U	216	 85% 14%
3	C	236	 89% 11%
3	E	236	 84% 15%
3	M	236	 86% 14%
3	O	236	 85% 14%
4	D	219	 85% 15%
4	F	219	 86% 14%
4	N	219	 83% 17%
4	P	219	 88% 12%
5	G	215	 79% 12% 9%
5	K	215	 76% 13% 10%
5	S	215	 79% 12% 10%
5	b	215	 88% 10%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 32879 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 heavy chain of human monoclonal antibody AZD8895.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	219	1614	1016	273	315	10	0	0	0
1	H	218	1603	1012	273	308	10	0	0	0
1	I	218	1608	1013	272	313	10	0	0	0
1	T	217	1608	1013	272	313	10	0	0	0

- Molecule 2 is a protein called light chain of human monoclonal antibody Fab AZD8895.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	1614	1010	276	324	4	0	0	0
2	J	213	1618	1013	279	322	4	0	0	0
2	L	214	1607	1004	275	324	4	0	0	0
2	U	213	1605	1003	275	323	4	0	0	0

- Molecule 3 is a protein called heavy chain of human monoclonal antibody Fab AZD1061.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	236	1754	1110	291	346	7	0	0	0
3	E	234	1739	1101	288	343	7	0	0	0
3	M	235	1737	1099	287	344	7	0	0	0
3	O	234	1734	1097	287	343	7	0	0	0

- Molecule 4 is a protein called light chain of human monoclonal antibody Fab AZD1061.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	219	Total	C	N	O	S	0	0	0
			1685	1056	283	339	7			
4	F	219	Total	C	N	O	S	0	0	0
			1693	1061	284	341	7			
4	N	219	Total	C	N	O	S	0	0	0
			1688	1056	282	343	7			
4	P	219	Total	C	N	O	S	0	0	0
			1685	1055	282	341	7			

- Molecule 5 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	G	195	Total	C	N	O	S	0	0	0
			1522	978	255	281	8			
5	K	194	Total	C	N	O	S	0	0	0
			1508	964	254	282	8			
5	S	194	Total	C	N	O	S	0	0	0
			1517	971	254	284	8			
5	b	194	Total	C	N	O	S	0	0	0
			1500	959	252	281	8			

There are 60 discrepancies between the modelled and reference sequences:

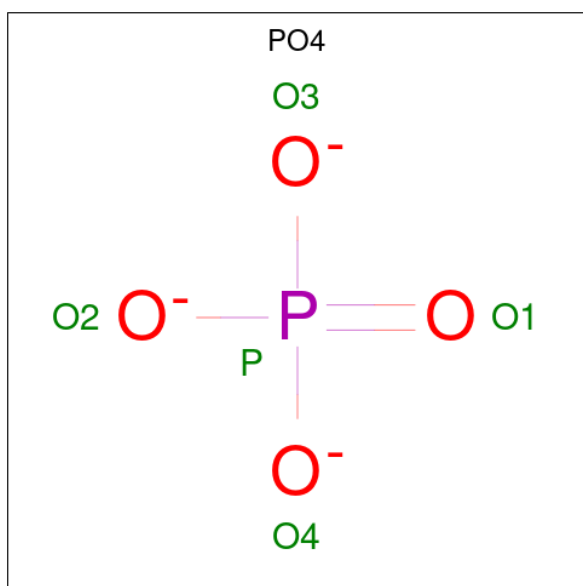
Chain	Residue	Modelled	Actual	Comment	Reference
G	530	GLY	-	expression tag	UNP P0DTC2
G	531	LEU	-	expression tag	UNP P0DTC2
G	532	VAL	-	expression tag	UNP P0DTC2
G	533	PRO	-	expression tag	UNP P0DTC2
G	534	ARG	-	expression tag	UNP P0DTC2
G	535	GLY	-	expression tag	UNP P0DTC2
G	536	SER	-	expression tag	UNP P0DTC2
G	537	HIS	-	expression tag	UNP P0DTC2
G	538	HIS	-	expression tag	UNP P0DTC2
G	539	HIS	-	expression tag	UNP P0DTC2
G	540	HIS	-	expression tag	UNP P0DTC2
G	541	HIS	-	expression tag	UNP P0DTC2
G	542	HIS	-	expression tag	UNP P0DTC2
G	543	HIS	-	expression tag	UNP P0DTC2
G	544	HIS	-	expression tag	UNP P0DTC2
K	530	GLY	-	expression tag	UNP P0DTC2
K	531	LEU	-	expression tag	UNP P0DTC2
K	532	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	533	PRO	-	expression tag	UNP P0DTC2
K	534	ARG	-	expression tag	UNP P0DTC2
K	535	GLY	-	expression tag	UNP P0DTC2
K	536	SER	-	expression tag	UNP P0DTC2
K	537	HIS	-	expression tag	UNP P0DTC2
K	538	HIS	-	expression tag	UNP P0DTC2
K	539	HIS	-	expression tag	UNP P0DTC2
K	540	HIS	-	expression tag	UNP P0DTC2
K	541	HIS	-	expression tag	UNP P0DTC2
K	542	HIS	-	expression tag	UNP P0DTC2
K	543	HIS	-	expression tag	UNP P0DTC2
K	544	HIS	-	expression tag	UNP P0DTC2
S	530	GLY	-	expression tag	UNP P0DTC2
S	531	LEU	-	expression tag	UNP P0DTC2
S	532	VAL	-	expression tag	UNP P0DTC2
S	533	PRO	-	expression tag	UNP P0DTC2
S	534	ARG	-	expression tag	UNP P0DTC2
S	535	GLY	-	expression tag	UNP P0DTC2
S	536	SER	-	expression tag	UNP P0DTC2
S	537	HIS	-	expression tag	UNP P0DTC2
S	538	HIS	-	expression tag	UNP P0DTC2
S	539	HIS	-	expression tag	UNP P0DTC2
S	540	HIS	-	expression tag	UNP P0DTC2
S	541	HIS	-	expression tag	UNP P0DTC2
S	542	HIS	-	expression tag	UNP P0DTC2
S	543	HIS	-	expression tag	UNP P0DTC2
S	544	HIS	-	expression tag	UNP P0DTC2
b	530	GLY	-	expression tag	UNP P0DTC2
b	531	LEU	-	expression tag	UNP P0DTC2
b	532	VAL	-	expression tag	UNP P0DTC2
b	533	PRO	-	expression tag	UNP P0DTC2
b	534	ARG	-	expression tag	UNP P0DTC2
b	535	GLY	-	expression tag	UNP P0DTC2
b	536	SER	-	expression tag	UNP P0DTC2
b	537	HIS	-	expression tag	UNP P0DTC2
b	538	HIS	-	expression tag	UNP P0DTC2
b	539	HIS	-	expression tag	UNP P0DTC2
b	540	HIS	-	expression tag	UNP P0DTC2
b	541	HIS	-	expression tag	UNP P0DTC2
b	542	HIS	-	expression tag	UNP P0DTC2
b	543	HIS	-	expression tag	UNP P0DTC2
b	544	HIS	-	expression tag	UNP P0DTC2

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	H	1	Total O P 5 4 1	0	0
6	I	1	Total O P 5 4 1	0	0
6	J	1	Total O P 5 4 1	0	0
6	L	1	Total O P 5 4 1	0	0
6	T	1	Total O P 5 4 1	0	0
6	U	1	Total O P 5 4 1	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	G	1	14	8	1	5	0	0
7	K	1	14	8	1	5	0	0
7	S	1	14	8	1	5	0	0
7	b	1	14	8	1	5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	14	14	14	0	0
8	B	5	5	5	0	0
8	C	16	16	16	0	0
8	D	20	20	20	0	0
8	E	7	7	7	0	0
8	F	9	9	9	0	0
8	H	7	7	7	0	0
8	I	3	3	3	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
8	L	2	Total O 2 2	0	0
8	M	8	Total O 8 8	0	0
8	N	13	Total O 13 13	0	0
8	O	5	Total O 5 5	0	0
8	P	8	Total O 8 8	0	0
8	T	4	Total O 4 4	0	0
8	U	2	Total O 2 2	0	0
8	G	6	Total O 6 6	0	0
8	K	7	Total O 7 7	0	0
8	S	3	Total O 3 3	0	0
8	b	5	Total O 5 5	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.

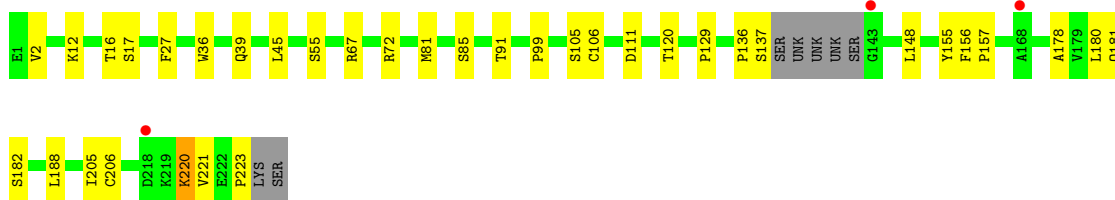
- Molecule 1: heavy chain of human monoclonal antibody AZD8895

Chain A:  89% 8%




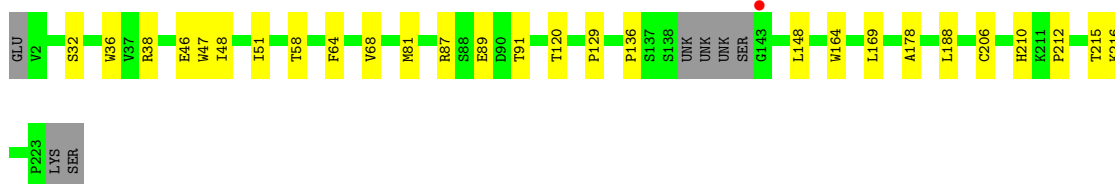
- Molecule 1: heavy chain of human monoclonal antibody AZD8895

Chain H:  81% 16%




- Molecule 1: heavy chain of human monoclonal antibody AZD8895

Chain I:  85% 12%




- Molecule 1: heavy chain of human monoclonal antibody AZD8895

Chain T:  87% 10%

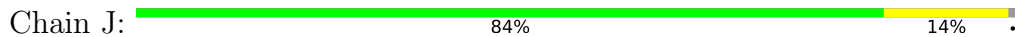


- Molecule 2: light chain of human monoclonal antibody Fab AZD8895

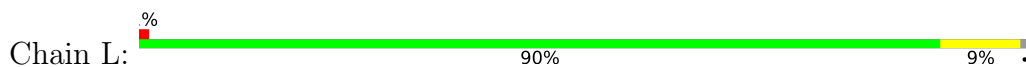
Chain B:  88% 10%



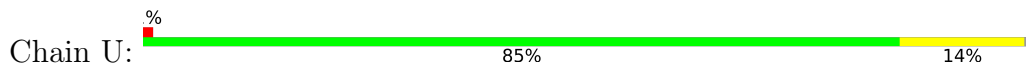
- Molecule 2: light chain of human monoclonal antibody Fab AZD8895



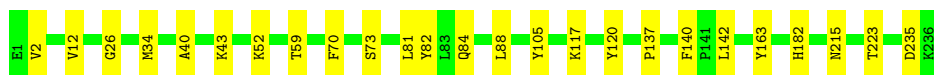
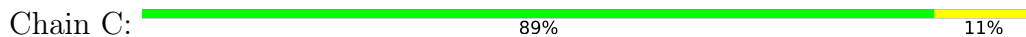
- Molecule 2: light chain of human monoclonal antibody Fab AZD8895



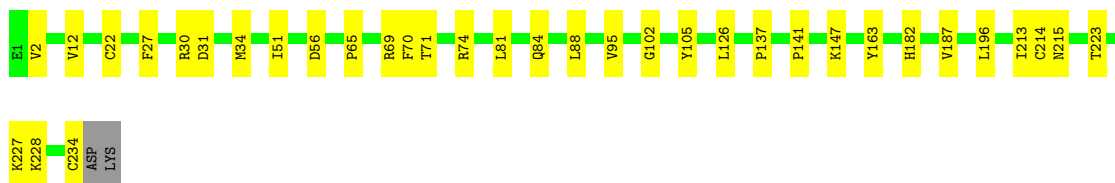
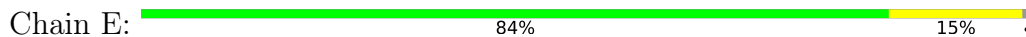
- Molecule 2: light chain of human monoclonal antibody Fab AZD8895



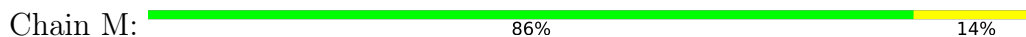
- Molecule 3: heavy chain of human monoclonal antibody Fab AZD1061



- Molecule 3: heavy chain of human monoclonal antibody Fab AZD1061



- Molecule 3: heavy chain of human monoclonal antibody Fab AZD1061





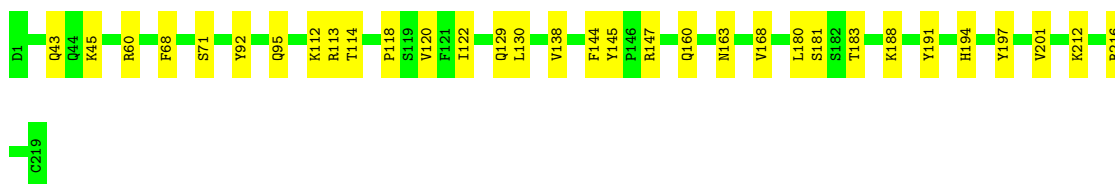
- Molecule 3: heavy chain of human monoclonal antibody Fab AZD1061

Chain O: 85% 14%



- Molecule 4: light chain of human monoclonal antibody Fab AZD1061

Chain D: 85% 15%



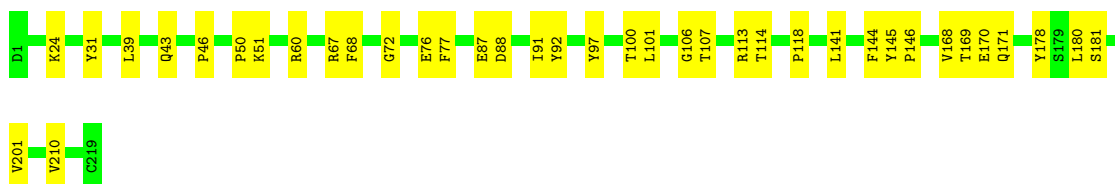
- Molecule 4: light chain of human monoclonal antibody Fab AZD1061

Chain F: 86% 14%



- Molecule 4: light chain of human monoclonal antibody Fab AZD1061

Chain N: 83% 17%

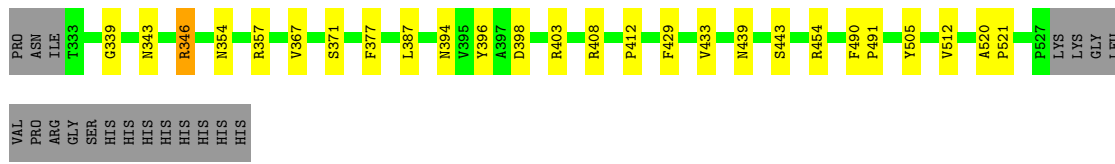
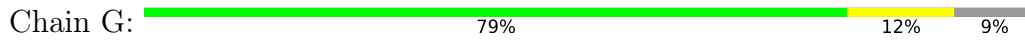


- Molecule 4: light chain of human monoclonal antibody Fab AZD1061

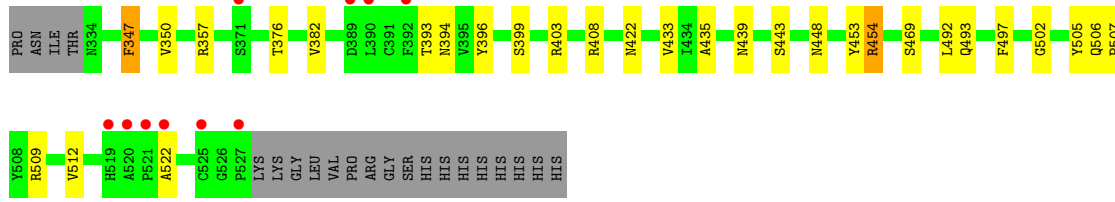
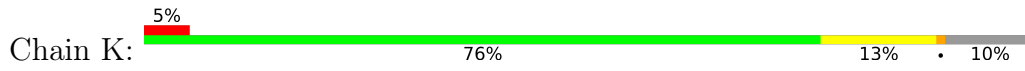
Chain P: 88% 12%



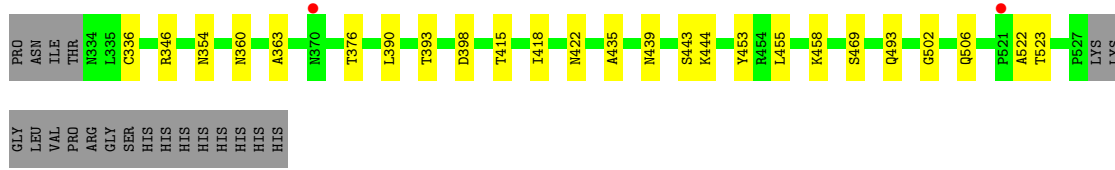
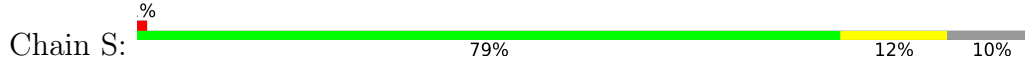
- Molecule 5: Spike protein S1



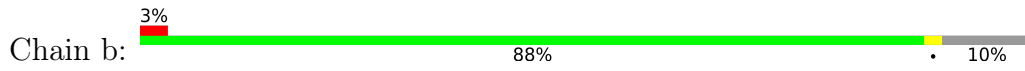
• Molecule 5: Spike protein S1



• Molecule 5: Spike protein S1



• Molecule 5: Spike protein S1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.15Å 152.53Å 199.24Å 90.00° 94.74° 90.00°	Depositor
Resolution (Å)	34.78 – 3.00 34.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.78-3.00) 100.0 (34.78-3.00)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 3.00Å)	Xtrriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, $R_{free}$	0.215 , 0.273 0.217 , 0.273	Depositor DCC
$R_{free}$ test set	5632 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtrriage
Anisotropy	0.937	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2505e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, 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	0.26	0/1651	0.49	0/2250
1	H	0.25	0/1640	0.48	0/2234
1	I	0.26	0/1645	0.49	0/2241
1	T	0.26	0/1645	0.48	0/2240
2	B	0.25	0/1651	0.46	0/2247
2	J	0.25	0/1655	0.45	0/2250
2	L	0.25	0/1643	0.47	0/2236
2	U	0.25	0/1642	0.46	0/2234
3	C	0.26	0/1797	0.49	0/2447
3	E	0.26	0/1782	0.48	0/2428
3	M	0.25	0/1780	0.48	0/2427
3	O	0.25	0/1777	0.49	0/2422
4	D	0.26	0/1721	0.49	0/2337
4	F	0.26	0/1729	0.48	0/2346
4	N	0.25	0/1724	0.47	0/2342
4	P	0.25	0/1721	0.47	0/2338
5	G	0.26	0/1565	0.47	0/2131
5	K	0.25	0/1551	0.44	0/2111
5	S	0.26	0/1560	0.45	0/2124
5	b	0.26	0/1543	0.44	0/2101
All	All	0.25	0/33422	0.47	0/45486

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	1614	0	1541	7	0
1	H	1603	0	1530	23	0
1	I	1608	0	1536	13	0
1	T	1608	0	1545	10	0
2	B	1614	0	1516	12	0
2	J	1618	0	1530	14	0
2	L	1607	0	1497	10	0
2	U	1605	0	1497	16	0
3	C	1754	0	1715	12	0
3	E	1739	0	1703	18	0
3	M	1737	0	1685	17	0
3	O	1734	0	1690	18	0
4	D	1685	0	1628	18	0
4	F	1693	0	1643	17	0
4	N	1688	0	1623	21	0
4	P	1685	0	1621	16	0
5	G	1522	0	1408	14	0
5	K	1508	0	1378	15	0
5	S	1517	0	1404	14	0
5	b	1500	0	1358	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	H	5	0	0	0	0
6	I	5	0	0	0	0
6	J	5	0	0	0	0
6	L	5	0	0	0	0
6	T	5	0	0	0	0
6	U	5	0	0	0	0
7	G	14	0	13	0	0
7	K	14	0	13	0	0
7	S	14	0	13	0	0
7	b	14	0	13	0	0
8	A	14	0	0	0	0
8	B	5	0	0	0	0
8	C	16	0	0	0	0
8	D	20	0	0	2	0
8	E	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	9	0	0	0	0
8	G	6	0	0	2	0
8	H	7	0	0	0	0
8	I	3	0	0	0	0
8	K	7	0	0	0	0
8	L	2	0	0	0	0
8	M	8	0	0	0	0
8	N	13	0	0	0	0
8	O	5	0	0	0	0
8	P	8	0	0	0	0
8	S	3	0	0	0	0
8	T	4	0	0	0	0
8	U	2	0	0	0	0
8	b	5	0	0	0	0
All	All	32879	0	31100	271	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 4.

The worst 5 of 271 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:H:220:LYS:H	1:H:220:LYS:HD2	1.37	0.88
2:U:122:PRO:HD3	2:U:134:VAL:HG12	1.63	0.80
2:J:110:ARG:HH11	2:J:113:ALA:HB2	1.53	0.74
1:I:136:PRO:HG3	1:I:148:LEU:HB3	1.70	0.73
2:U:134:VAL:HG22	2:U:181:LEU:HB3	1.72	0.72

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	215/225 (96%)	206 (96%)	8 (4%)	1 (0%)	29	68
1	H	214/225 (95%)	204 (95%)	10 (5%)	0	100	100
1	I	214/225 (95%)	206 (96%)	8 (4%)	0	100	100
1	T	213/225 (95%)	205 (96%)	8 (4%)	0	100	100
2	B	212/216 (98%)	201 (95%)	11 (5%)	0	100	100
2	J	211/216 (98%)	196 (93%)	14 (7%)	1 (0%)	29	68
2	L	212/216 (98%)	204 (96%)	8 (4%)	0	100	100
2	U	211/216 (98%)	199 (94%)	11 (5%)	1 (0%)	29	68
3	C	234/236 (99%)	225 (96%)	8 (3%)	1 (0%)	34	72
3	E	232/236 (98%)	223 (96%)	9 (4%)	0	100	100
3	M	233/236 (99%)	228 (98%)	5 (2%)	0	100	100
3	O	232/236 (98%)	223 (96%)	9 (4%)	0	100	100
4	D	217/219 (99%)	206 (95%)	11 (5%)	0	100	100
4	F	217/219 (99%)	208 (96%)	9 (4%)	0	100	100
4	N	217/219 (99%)	206 (95%)	11 (5%)	0	100	100
4	P	217/219 (99%)	208 (96%)	9 (4%)	0	100	100
5	G	193/215 (90%)	180 (93%)	13 (7%)	0	100	100
5	K	192/215 (89%)	183 (95%)	8 (4%)	1 (0%)	29	68
5	S	192/215 (89%)	182 (95%)	10 (5%)	0	100	100
5	b	192/215 (89%)	178 (93%)	14 (7%)	0	100	100
All	All	4270/4444 (96%)	4071 (95%)	194 (4%)	5 (0%)	51	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	153	ASP
1	A	145	THR
3	C	235	ASP
2	U	171	LYS
5	K	382	VAL

### 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	175/190 (92%)	170 (97%)	5 (3%)	42	76
1	H	171/190 (90%)	166 (97%)	5 (3%)	42	76
1	I	175/190 (92%)	171 (98%)	4 (2%)	50	80
1	T	176/190 (93%)	173 (98%)	3 (2%)	60	85
2	B	172/186 (92%)	169 (98%)	3 (2%)	60	85
2	J	173/186 (93%)	169 (98%)	4 (2%)	50	80
2	L	170/186 (91%)	165 (97%)	5 (3%)	42	76
2	U	170/186 (91%)	166 (98%)	4 (2%)	49	79
3	C	194/197 (98%)	191 (98%)	3 (2%)	65	87
3	E	193/197 (98%)	188 (97%)	5 (3%)	46	78
3	M	191/197 (97%)	185 (97%)	6 (3%)	40	75
3	O	192/197 (98%)	189 (98%)	3 (2%)	62	86
4	D	189/192 (98%)	186 (98%)	3 (2%)	62	86
4	F	191/192 (100%)	188 (98%)	3 (2%)	62	86
4	N	190/192 (99%)	188 (99%)	2 (1%)	73	90
4	P	189/192 (98%)	187 (99%)	2 (1%)	73	90
5	G	157/186 (84%)	154 (98%)	3 (2%)	57	84
5	K	155/186 (83%)	151 (97%)	4 (3%)	46	78
5	S	159/186 (86%)	156 (98%)	3 (2%)	57	84
5	b	152/186 (82%)	147 (97%)	5 (3%)	38	73
All	All	3534/3804 (93%)	3459 (98%)	75 (2%)	53	82

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	U	34	LEU
5	b	369	TYR
2	U	153	ASP
5	K	408	ARG
1	H	182	SER

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

Mol	Chain	Res	Type
4	D	95	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](#)

12 ligands are 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	$\# Z  > 2$
6	PO4	L	301	-	4,4,4	0.91	0	6,6,6	0.43	0
7	NAG	K	601	5	14,14,15	0.27	0	17,19,21	0.46	0
7	NAG	S	601	5	14,14,15	0.33	0	17,19,21	0.55	0
6	PO4	B	301	-	4,4,4	0.91	0	6,6,6	0.45	0
6	PO4	J	301	-	4,4,4	0.91	0	6,6,6	0.45	0
6	PO4	H	301	-	4,4,4	0.93	0	6,6,6	0.39	0
7	NAG	b	601	5	14,14,15	0.22	0	17,19,21	0.49	0
6	PO4	U	301	-	4,4,4	0.91	0	6,6,6	0.48	0
7	NAG	G	601	5	14,14,15	0.28	0	17,19,21	0.40	0
6	PO4	A	301	-	4,4,4	0.92	0	6,6,6	0.45	0
6	PO4	T	301	-	4,4,4	0.91	0	6,6,6	0.45	0
6	PO4	I	301	-	4,4,4	0.93	0	6,6,6	0.46	0

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
7	NAG	K	601	5	-	2/6/23/26	0/1/1/1
7	NAG	S	601	5	-	2/6/23/26	0/1/1/1
7	NAG	b	601	5	-	2/6/23/26	0/1/1/1
7	NAG	G	601	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	601	NAG	O5-C5-C6-O6
7	K	601	NAG	O5-C5-C6-O6
7	b	601	NAG	O5-C5-C6-O6
7	G	601	NAG	C4-C5-C6-O6
7	b	601	NAG	C4-C5-C6-O6

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	219/225 (97%)	-0.42	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	20, 38, 86, 120	0
1	H	218/225 (96%)	-0.11	3 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">49</span>	35, 59, 104, 128	0
1	I	218/225 (96%)	-0.29	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">75</span>	37, 57, 91, 114	0
1	T	217/225 (96%)	-0.45	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	23, 40, 83, 103	0
2	B	214/216 (99%)	-0.25	2 (0%) <span style="border: 1px solid blue; padding: 2px;">84</span> <span style="border: 1px solid blue; padding: 2px;">63</span>	24, 53, 89, 109	0
2	J	213/216 (98%)	-0.07	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	40, 66, 100, 113	0
2	L	214/216 (99%)	-0.08	3 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">49</span>	39, 70, 101, 109	0
2	U	213/216 (98%)	-0.20	3 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">49</span>	25, 55, 97, 110	0
3	C	236/236 (100%)	-0.49	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	23, 34, 52, 81	0
3	E	234/236 (99%)	-0.52	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	24, 34, 52, 74	0
3	M	235/236 (99%)	-0.32	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	42, 53, 69, 86	0
3	O	234/236 (99%)	-0.41	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	37, 52, 73, 89	0
4	D	219/219 (100%)	-0.55	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	21, 34, 54, 93	0
4	F	219/219 (100%)	-0.49	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	22, 34, 56, 73	0
4	N	219/219 (100%)	-0.42	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	40, 50, 74, 92	0
4	P	219/219 (100%)	-0.36	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	37, 53, 74, 104	0
5	G	195/215 (90%)	-0.38	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	21, 38, 91, 108	0
5	K	194/215 (90%)	-0.10	10 (5%) <span style="border: 1px solid red; padding: 2px;">27</span> <span style="border: 1px solid red; padding: 2px;">10</span>	34, 57, 106, 121	0
5	S	194/215 (90%)	-0.09	2 (1%) <span style="border: 1px solid blue; padding: 2px;">82</span> <span style="border: 1px solid blue; padding: 2px;">59</span>	44, 59, 102, 125	0
5	b	194/215 (90%)	-0.26	6 (3%) <span style="border: 1px solid blue; padding: 2px;">49</span> <span style="border: 1px solid red; padding: 2px;">21</span>	24, 40, 101, 116	0
All	All	4318/4444 (97%)	-0.32	30 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">69</span>	20, 49, 92, 128	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	K	520	ALA	3.7
5	b	521	PRO	3.5
5	b	519	HIS	3.5
5	K	527	PRO	3.3
5	S	370	ASN	3.1

## 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	NAG	S	601	14/15	0.77	0.26	58,66,90,91	0
7	NAG	K	601	14/15	0.82	0.22	65,93,108,109	0
6	PO4	A	301	5/5	0.82	0.25	67,75,83,92	0
6	PO4	I	301	5/5	0.86	0.21	85,96,99,103	0
6	PO4	J	301	5/5	0.87	0.20	72,74,80,87	0
6	PO4	H	301	5/5	0.88	0.23	96,97,107,109	0
6	PO4	B	301	5/5	0.89	0.22	62,64,75,93	0
6	PO4	T	301	5/5	0.90	0.21	77,81,84,90	0
7	NAG	b	601	14/15	0.90	0.31	47,77,90,91	0
6	PO4	U	301	5/5	0.91	0.19	78,80,80,85	0
7	NAG	G	601	14/15	0.92	0.15	63,69,77,89	0
6	PO4	L	301	5/5	0.92	0.19	83,84,85,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.