wwPDB EM Validation Summary Report ⓘ

Mar 12, 2024 – 06:53 PM JST

PDB ID	:	8WRO
EMDB ID	:	EMD-37784
Title	:	XBB.1.5.10 spike protein in complex with ACE2
Authors	:	Feng, L.L.; Feng, L.L.
Deposited on	:	2023-10-15
Resolution	:	3.90 Å(reported)

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

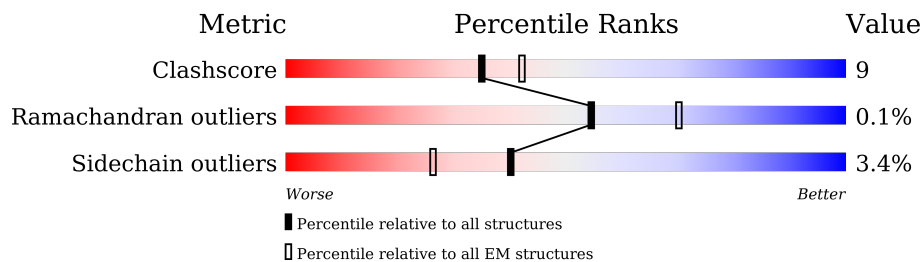|		
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1　Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	Percentile Ranks	Value
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		3.4%

Worse　　　　　　　　　　　　　　　　　　　*Better*

▌ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1318	62%　　　　18%　·　19%
1	B	1318	62%　　　　17%　·　20%
1	C	1318	60%　　　　19%　·　20%
2	D	594	77%　　　　22%　·

2   Entity composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 29807 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 glycoprotein,Spike glycoprotein,Spike glycoprotein,Fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1067	Total	C	N	O	S	0	0
			8364	5347	1397	1581	39		
1	B	1059	Total	C	N	O	S	0	0
			8295	5304	1384	1568	39		
1	C	1060	Total	C	N	O	S	0	0
			8303	5310	1385	1569	39		

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	24	SER	ALA	variant	UNP P0DTC2
A	80	ALA	VAL	variant	UNP P0DTC2
A	139	ASP	GLY	variant	UNP P0DTC2
A	143	GLN	HIS	variant	UNP P0DTC2
A	180	GLU	GLN	variant	UNP P0DTC2
A	210	GLU	VAL	variant	UNP P0DTC2
A	249	VAL	GLY	variant	UNP P0DTC2
A	336	HIS	GLY	variant	UNP P0DTC2
A	343	THR	ARG	variant	UNP P0DTC2
A	365	ILE	LEU	variant	UNP P0DTC2
A	368	PHE	SER	variant	UNP P0DTC2
A	370	PRO	SER	variant	UNP P0DTC2
A	372	PHE	SER	variant	UNP P0DTC2
A	373	ALA	THR	variant	UNP P0DTC2
A	402	ASN	ASP	variant	UNP P0DTC2
A	405	SER	ARG	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	variant	UNP P0DTC2
A	442	PRO	VAL	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	443	SER	GLY	variant	UNP P0DTC2
A	453	LEU	PHE	variant	UNP P0DTC2
A	457	LYS	ASN	variant	UNP P0DTC2
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	variant	UNP P0DTC2
A	483	PRO	PHE	conflict	UNP P0DTC2
A	487	SER	PHE	variant	UNP P0DTC2
A	495	ARG	GLN	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	variant	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	680	SER	ARG	conflict	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	761	LYS	ASN	variant	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	814	PRO	PHE	conflict	UNP P0DTC2
A	826	THR	ALA	conflict	UNP P0DTC2
A	833	LYS	GLN	conflict	UNP P0DTC2
A	889	PRO	ALA	conflict	UNP P0DTC2
A	896	PRO	ALA	conflict	UNP P0DTC2
A	939	PRO	ALA	conflict	UNP P0DTC2
A	951	HIS	GLN	variant	UNP P0DTC2
A	966	LYS	ASN	variant	UNP P0DTC2
A	983	PRO	LYS	variant	UNP P0DTC2
A	984	PRO	VAL	variant	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	24	SER	ALA	variant	UNP P0DTC2
B	80	ALA	VAL	variant	UNP P0DTC2
B	139	ASP	GLY	variant	UNP P0DTC2
B	143	GLN	HIS	variant	UNP P0DTC2
B	180	GLU	GLN	variant	UNP P0DTC2
B	210	GLU	VAL	variant	UNP P0DTC2
B	249	VAL	GLY	variant	UNP P0DTC2
B	336	HIS	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	343	THR	ARG	variant	UNP P0DTC2
B	365	ILE	LEU	variant	UNP P0DTC2
B	368	PHE	SER	variant	UNP P0DTC2
B	370	PRO	SER	variant	UNP P0DTC2
B	372	PHE	SER	variant	UNP P0DTC2
B	373	ALA	THR	variant	UNP P0DTC2
B	402	ASN	ASP	variant	UNP P0DTC2
B	405	SER	ARG	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	437	LYS	ASN	variant	UNP P0DTC2
B	442	PRO	VAL	variant	UNP P0DTC2
B	443	SER	GLY	variant	UNP P0DTC2
B	453	LEU	PHE	variant	UNP P0DTC2
B	457	LYS	ASN	variant	UNP P0DTC2
B	474	ASN	SER	variant	UNP P0DTC2
B	475	LYS	THR	variant	UNP P0DTC2
B	481	ALA	GLU	variant	UNP P0DTC2
B	483	PRO	PHE	conflict	UNP P0DTC2
B	487	SER	PHE	variant	UNP P0DTC2
B	495	ARG	GLN	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	502	HIS	TYR	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	652	TYR	HIS	variant	UNP P0DTC2
B	676	LYS	ASN	variant	UNP P0DTC2
B	678	HIS	PRO	variant	UNP P0DTC2
B	679	GLY	ARG	conflict	UNP P0DTC2
B	680	SER	ARG	conflict	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	761	LYS	ASN	variant	UNP P0DTC2
B	793	TYR	ASP	variant	UNP P0DTC2
B	814	PRO	PHE	conflict	UNP P0DTC2
B	826	THR	ALA	conflict	UNP P0DTC2
B	833	LYS	GLN	conflict	UNP P0DTC2
B	889	PRO	ALA	conflict	UNP P0DTC2
B	896	PRO	ALA	conflict	UNP P0DTC2
B	939	PRO	ALA	conflict	UNP P0DTC2
B	951	HIS	GLN	variant	UNP P0DTC2
B	966	LYS	ASN	variant	UNP P0DTC2
B	983	PRO	LYS	variant	UNP P0DTC2
B	984	PRO	VAL	variant	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	24	SER	ALA	variant	UNP P0DTC2
C	80	ALA	VAL	variant	UNP P0DTC2
C	139	ASP	GLY	variant	UNP P0DTC2
C	143	GLN	HIS	variant	UNP P0DTC2
C	180	GLU	GLN	variant	UNP P0DTC2
C	210	GLU	VAL	variant	UNP P0DTC2
C	249	VAL	GLY	variant	UNP P0DTC2
C	336	HIS	GLY	variant	UNP P0DTC2
C	343	THR	ARG	variant	UNP P0DTC2
C	365	ILE	LEU	variant	UNP P0DTC2
C	368	PHE	SER	variant	UNP P0DTC2
C	370	PRO	SER	variant	UNP P0DTC2
C	372	PHE	SER	variant	UNP P0DTC2
C	373	ALA	THR	variant	UNP P0DTC2
C	402	ASN	ASP	variant	UNP P0DTC2
C	405	SER	ARG	variant	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	437	LYS	ASN	variant	UNP P0DTC2
C	442	PRO	VAL	variant	UNP P0DTC2
C	443	SER	GLY	variant	UNP P0DTC2
C	453	LEU	PHE	variant	UNP P0DTC2
C	457	LYS	ASN	variant	UNP P0DTC2
C	474	ASN	SER	variant	UNP P0DTC2
C	475	LYS	THR	variant	UNP P0DTC2
C	481	ALA	GLU	variant	UNP P0DTC2
C	483	PRO	PHE	conflict	UNP P0DTC2
C	487	SER	PHE	variant	UNP P0DTC2
C	495	ARG	GLN	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	502	HIS	TYR	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	652	TYR	HIS	variant	UNP P0DTC2
C	676	LYS	ASN	variant	UNP P0DTC2
C	678	HIS	PRO	variant	UNP P0DTC2
C	679	GLY	ARG	conflict	UNP P0DTC2
C	680	SER	ARG	conflict	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	761	LYS	ASN	variant	UNP P0DTC2
C	793	TYR	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	814	PRO	PHE	conflict	UNP P0DTC2
C	826	THR	ALA	conflict	UNP P0DTC2
C	833	LYS	GLN	conflict	UNP P0DTC2
C	889	PRO	ALA	conflict	UNP P0DTC2
C	896	PRO	ALA	conflict	UNP P0DTC2
C	939	PRO	ALA	conflict	UNP P0DTC2
C	951	HIS	GLN	variant	UNP P0DTC2
C	966	LYS	ASN	variant	UNP P0DTC2
C	983	PRO	LYS	variant	UNP P0DTC2
C	984	PRO	VAL	variant	UNP P0DTC2

- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

| Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	594	4845	3099	803	914	29	0	0

3   Residue-property plots ⓘ

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 glycoprotein,Spike glycoprotein,Spike glycoprotein,Fusion protein
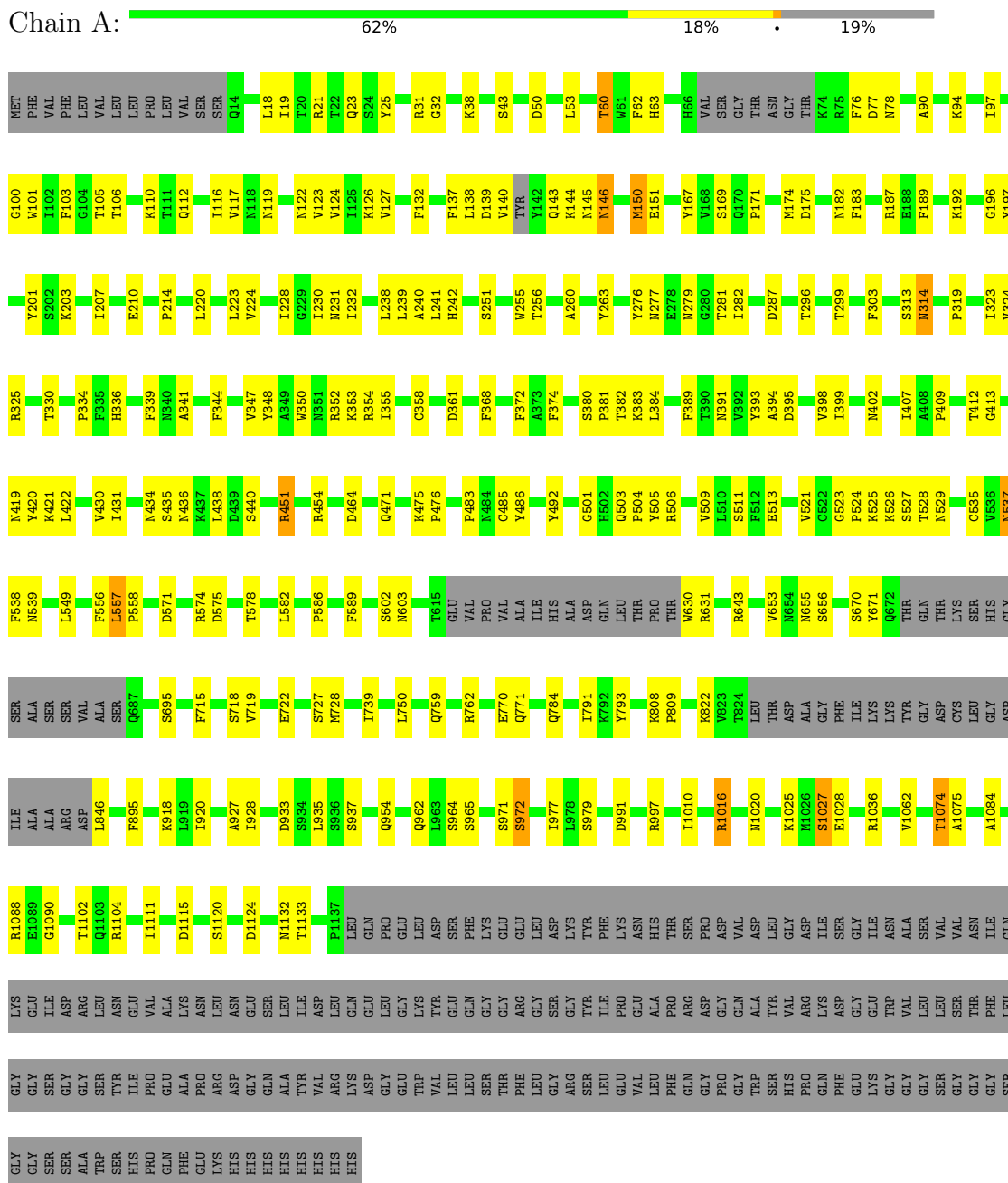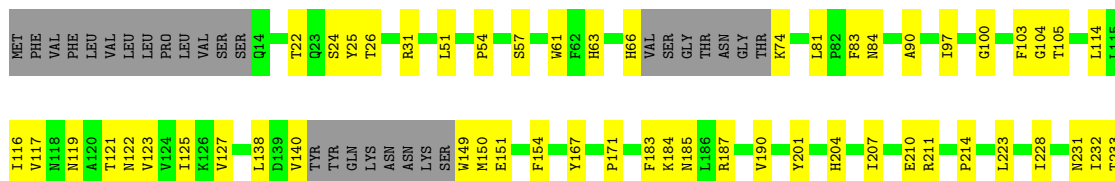
• Molecule 1: Spike glycoprotein,Spike glycoprotein,Spike glycoprotein,Fusion protein
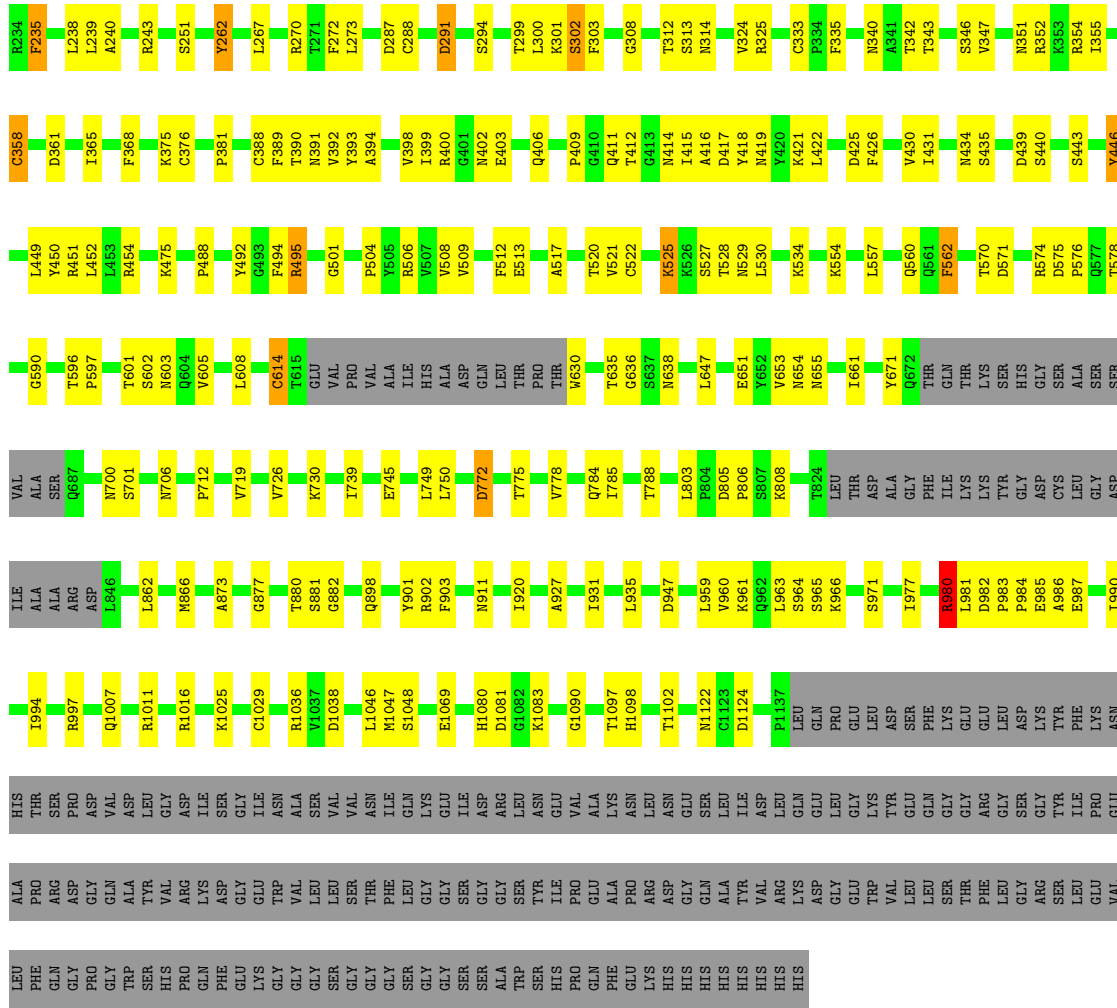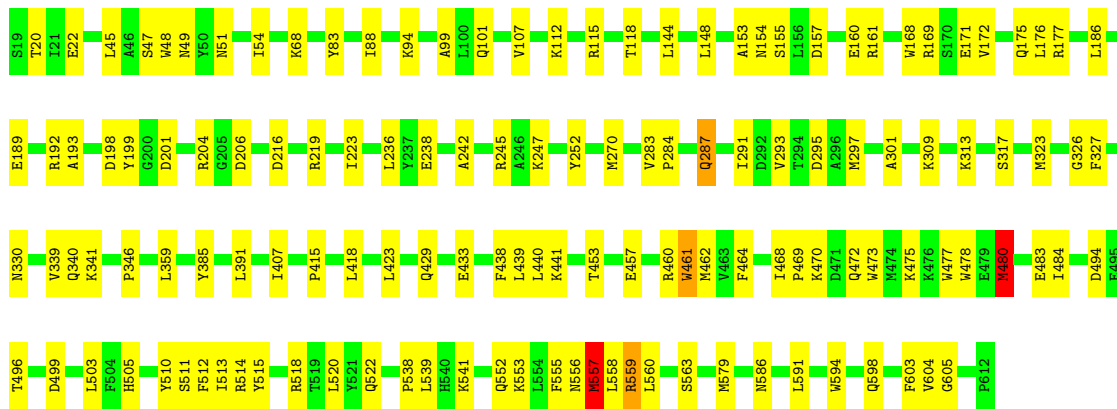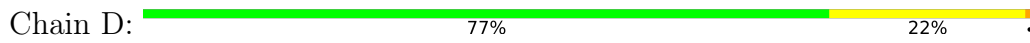
Chain B:

62%   17%   •   20%
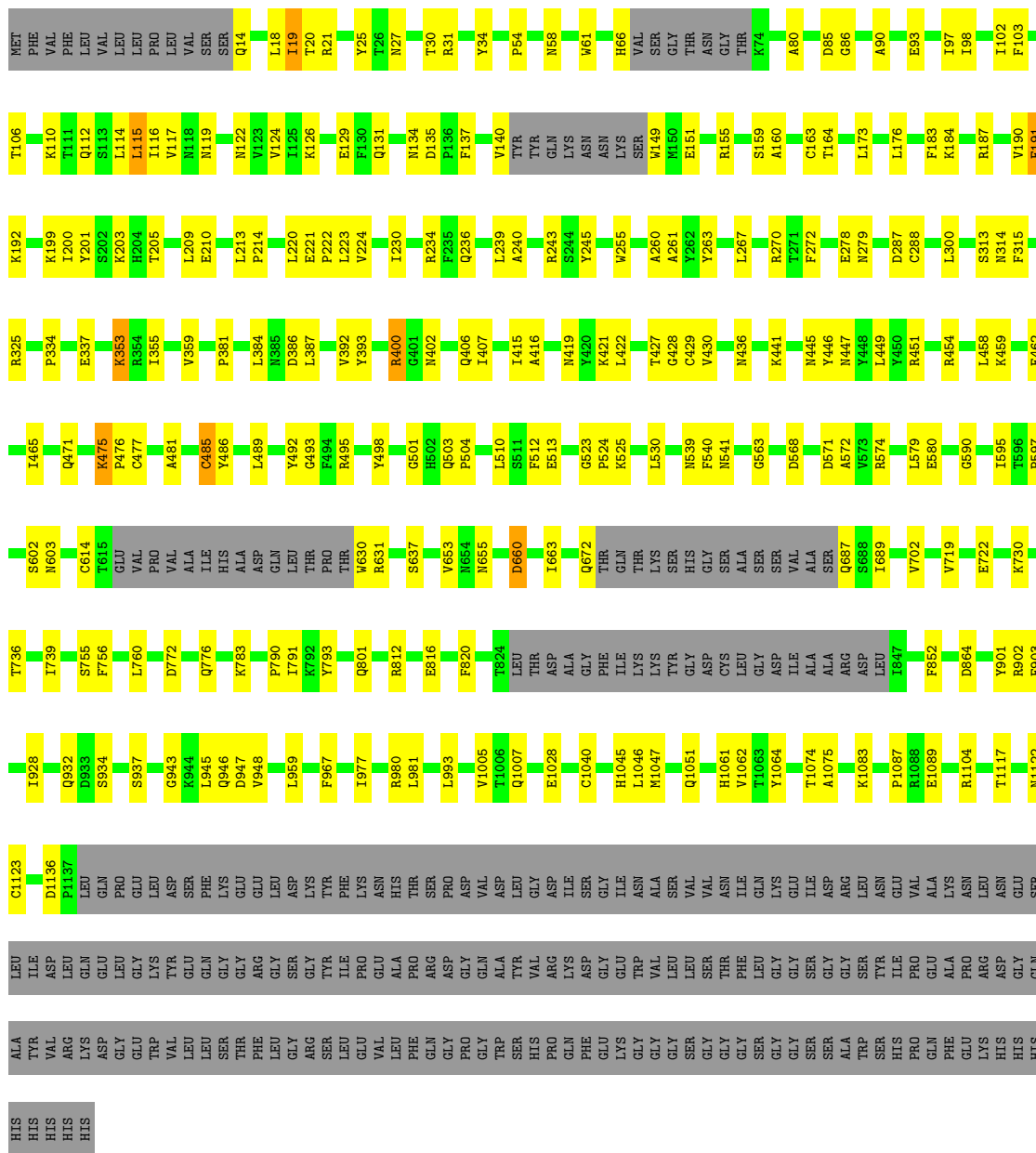
• Molecule 1: Spike glycoprotein,Spike glycoprotein,Spike glycoprotein,Fusion protein

Chain C:

60%   19%   •   20%

• Molecule 2: Processed angiotensin-converting enzyme 2

Chain D:

4　Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76881	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	52	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

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	0.29	0/8565	0.55	3/11656 (0.0%)
1	B	0.30	0/8495	0.54	1/11563 (0.0%)
1	C	0.30	0/8503	0.55	1/11574 (0.0%)
2	D	0.26	0/4981	0.53	4/6767 (0.1%)
All	All	0.29	0/30544	0.54	9/41560 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	19	ILE	CG1-CB-CG2	-7.42	95.07	111.40
1	A	150	MET	CA-CB-CG	6.09	123.65	113.30
1	A	991	ASP	CB-CG-OD1	5.64	123.38	118.30
2	D	462	MET	CA-CB-CG	5.54	122.72	113.30
1	A	557	LEU	CA-CB-CG	5.48	127.90	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	980	ARG	Sidechain

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	8364	0	8184	146	0
1	B	8295	0	8111	136	0
1	C	8303	0	8124	156	0
2	D	4845	0	4625	82	0
All	All	29807	0	29044	509	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 9.

The worst 5 of 509 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:117:VAL:O	1:A:123:VAL:HA	1.74	0.86
1:C:1025:LYS:O	1:C:1029:CYS:HB2	1.83	0.78
1:B:90:ALA:HB3	1:B:263:TYR:HB2	1.71	0.72
1:A:1084:ALA:HB3	1:A:1120:SER:O	1.89	0.72
2:D:480:MET:O	2:D:484:ILE:HB	1.90	0.72

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 PDB entries followed by that with respect to all EM entries.

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	1055/1318 (80%)	956 (91%)	98 (9%)	1 (0%)	51	84
1	B	1047/1318 (79%)	959 (92%)	88 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1048/1318 (80%)	942 (90%)	103 (10%)	3 (0%)	41	75
2	D	592/594 (100%)	565 (95%)	27 (5%)	0	100	100
All	All	3742/4548 (82%)	3422 (91%)	316 (8%)	4 (0%)	54	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	C	980	ARG
1	C	151	GLU
1	C	251	SER

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 PDB entries followed by that with respect to all EM entries.

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	935/1140 (82%)	902 (96%)	33 (4%)	36	62
1	B	927/1140 (81%)	896 (97%)	31 (3%)	38	63
1	C	928/1140 (81%)	894 (96%)	34 (4%)	34	60
2	D	525/525 (100%)	509 (97%)	16 (3%)	41	64
All	All	3315/3945 (84%)	3201 (97%)	114 (3%)	40	62

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	864	ASP
2	D	461	TRP
1	C	272	PHE
2	D	441	LYS
2	D	199	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	277	ASN
1	C	898	GLN
2	D	472	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 ⓘ

There are no chain breaks in this entry.