



wwPDB EM Validation Summary Report ⓘ

Feb 19, 2025 – 03:09 pm GMT

PDB ID : 8C5R
EMDB ID : EMD-16441
Title : Omicron B.1.1.529 2 RBD up conformation
Authors : Raghavan, S.S.R.; Walker, M.R.; Salanti, A.; Barfod, L.K.; Wang, K.T.
Deposited on : 2023-01-10
Resolution : 3.70 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

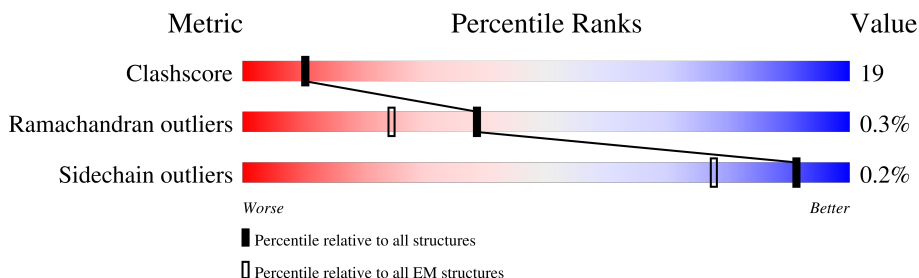
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1060	87% 12%
1	B	1060	86% 13%
1	C	1060	87% 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24969 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1060	Total	C	N	O	S	0	0
			8328	5331	1387	1572	38		
1	B	1060	Total	C	N	O	S	0	0
			8328	5331	1387	1572	38		
1	C	1058	Total	C	N	O	S	0	0
			8313	5322	1384	1569	38		

There are 318 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP A0A6M4AIH4
A	?	-	HIS	deletion	UNP A0A6M4AIH4
A	?	-	VAL	deletion	UNP A0A6M4AIH4
A	?	-	SER	deletion	UNP A0A6M4AIH4
A	?	-	GLY	deletion	UNP A0A6M4AIH4
A	?	-	THR	deletion	UNP A0A6M4AIH4
A	?	-	ASN	deletion	UNP A0A6M4AIH4
A	?	-	GLY	deletion	UNP A0A6M4AIH4
A	?	-	THR	deletion	UNP A0A6M4AIH4
A	69	SER	LYS	conflict	UNP A0A6M4AIH4
A	142	ASP	GLY	conflict	UNP A0A6M4AIH4
A	211	ILE	ASN	conflict	UNP A0A6M4AIH4
A	212	VAL	LEU	conflict	UNP A0A6M4AIH4
A	213	PRO	VAL	conflict	UNP A0A6M4AIH4
A	214	GLU	ARG	conflict	UNP A0A6M4AIH4
A	?	-	TYR	deletion	UNP A0A6M4AIH4
A	?	-	LEU	deletion	UNP A0A6M4AIH4
A	?	-	THR	deletion	UNP A0A6M4AIH4
A	?	-	PRO	deletion	UNP A0A6M4AIH4
A	?	-	GLY	deletion	UNP A0A6M4AIH4
A	?	-	ASP	deletion	UNP A0A6M4AIH4
A	?	-	SER	deletion	UNP A0A6M4AIH4
A	339	ASP	GLY	conflict	UNP A0A6M4AIH4
A	371	LEU	SER	conflict	UNP A0A6M4AIH4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	373	PRO	SER	conflict	UNP A0A6M4AIH4
A	375	PHE	SER	conflict	UNP A0A6M4AIH4
A	417	ASN	LYS	conflict	UNP A0A6M4AIH4
A	439	LYS	ASN	conflict	UNP A0A6M4AIH4
A	446	SER	GLY	conflict	UNP A0A6M4AIH4
A	477	ASN	SER	conflict	UNP A0A6M4AIH4
A	478	LYS	THR	conflict	UNP A0A6M4AIH4
A	484	ALA	GLU	conflict	UNP A0A6M4AIH4
A	493	ARG	GLN	conflict	UNP A0A6M4AIH4
A	496	SER	GLY	conflict	UNP A0A6M4AIH4
A	498	ARG	GLN	conflict	UNP A0A6M4AIH4
A	501	TYR	ASN	conflict	UNP A0A6M4AIH4
A	505	HIS	TYR	conflict	UNP A0A6M4AIH4
A	547	LYS	THR	conflict	UNP A0A6M4AIH4
A	?	-	PRO	deletion	UNP A0A6M4AIH4
A	?	-	VAL	deletion	UNP A0A6M4AIH4
A	?	-	ALA	deletion	UNP A0A6M4AIH4
A	?	-	ILE	deletion	UNP A0A6M4AIH4
A	?	-	HIS	deletion	UNP A0A6M4AIH4
A	?	-	ALA	deletion	UNP A0A6M4AIH4
A	?	-	ASP	deletion	UNP A0A6M4AIH4
A	?	-	GLN	deletion	UNP A0A6M4AIH4
A	?	-	LEU	deletion	UNP A0A6M4AIH4
A	?	-	THR	deletion	UNP A0A6M4AIH4
A	?	-	PRO	deletion	UNP A0A6M4AIH4
A	?	-	THR	deletion	UNP A0A6M4AIH4
A	?	-	TRP	deletion	UNP A0A6M4AIH4
A	?	-	ARG	deletion	UNP A0A6M4AIH4
A	?	-	VAL	deletion	UNP A0A6M4AIH4
A	?	-	TYR	deletion	UNP A0A6M4AIH4
A	?	-	SER	deletion	UNP A0A6M4AIH4
A	?	-	THR	deletion	UNP A0A6M4AIH4
A	?	-	GLY	deletion	UNP A0A6M4AIH4
A	?	-	SER	deletion	UNP A0A6M4AIH4
A	655	TYR	HIS	conflict	UNP A0A6M4AIH4
A	?	-	GLN	deletion	UNP A0A6M4AIH4
A	?	-	THR	deletion	UNP A0A6M4AIH4
A	?	-	ASN	deletion	UNP A0A6M4AIH4
A	?	-	SER	deletion	UNP A0A6M4AIH4
A	?	-	PRO	deletion	UNP A0A6M4AIH4
A	?	-	ARG	deletion	UNP A0A6M4AIH4
A	?	-	ARG	deletion	UNP A0A6M4AIH4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP A0A6M4AIH4
A	?	-	ARG	deletion	UNP A0A6M4AIH4
A	?	-	SER	deletion	UNP A0A6M4AIH4
A	?	-	VAL	deletion	UNP A0A6M4AIH4
A	?	-	ALA	deletion	UNP A0A6M4AIH4
A	764	LYS	ASN	conflict	UNP A0A6M4AIH4
A	796	TYR	ASP	conflict	UNP A0A6M4AIH4
A	?	-	PRO	deletion	UNP A0A6M4AIH4
A	?	-	LEU	deletion	UNP A0A6M4AIH4
A	?	-	ALA	deletion	UNP A0A6M4AIH4
A	?	-	ASP	deletion	UNP A0A6M4AIH4
A	?	-	ALA	deletion	UNP A0A6M4AIH4
A	?	-	GLY	deletion	UNP A0A6M4AIH4
A	?	-	PHE	deletion	UNP A0A6M4AIH4
A	?	-	ILE	deletion	UNP A0A6M4AIH4
A	?	-	LYS	deletion	UNP A0A6M4AIH4
A	?	-	GLN	deletion	UNP A0A6M4AIH4
A	?	-	TYR	deletion	UNP A0A6M4AIH4
A	?	-	GLY	deletion	UNP A0A6M4AIH4
A	?	-	ASP	deletion	UNP A0A6M4AIH4
A	?	-	CYS	deletion	UNP A0A6M4AIH4
A	?	-	LEU	deletion	UNP A0A6M4AIH4
A	?	-	GLY	deletion	UNP A0A6M4AIH4
A	?	-	ASP	deletion	UNP A0A6M4AIH4
A	?	-	ILE	deletion	UNP A0A6M4AIH4
A	?	-	ALA	deletion	UNP A0A6M4AIH4
A	?	-	ALA	deletion	UNP A0A6M4AIH4
A	?	-	ARG	deletion	UNP A0A6M4AIH4
A	?	-	ASP	deletion	UNP A0A6M4AIH4
A	?	-	LEU	deletion	UNP A0A6M4AIH4
A	?	-	ILE	deletion	UNP A0A6M4AIH4
A	?	-	CYS	deletion	UNP A0A6M4AIH4
A	?	-	ALA	deletion	UNP A0A6M4AIH4
A	?	-	GLN	deletion	UNP A0A6M4AIH4
A	856	LYS	ASN	conflict	UNP A0A6M4AIH4
A	954	HIS	GLN	conflict	UNP A0A6M4AIH4
A	969	LYS	ASN	conflict	UNP A0A6M4AIH4
A	981	PHE	LEU	conflict	UNP A0A6M4AIH4
A	986	PRO	LYS	conflict	UNP A0A6M4AIH4
A	987	PRO	VAL	conflict	UNP A0A6M4AIH4
B	67	VAL	ALA	conflict	UNP A0A6M4AIH4
B	?	-	HIS	deletion	UNP A0A6M4AIH4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	deletion	UNP A0A6M4AIH4
B	?	-	SER	deletion	UNP A0A6M4AIH4
B	?	-	GLY	deletion	UNP A0A6M4AIH4
B	?	-	THR	deletion	UNP A0A6M4AIH4
B	?	-	ASN	deletion	UNP A0A6M4AIH4
B	?	-	GLY	deletion	UNP A0A6M4AIH4
B	?	-	THR	deletion	UNP A0A6M4AIH4
B	69	SER	LYS	conflict	UNP A0A6M4AIH4
B	142	ASP	GLY	conflict	UNP A0A6M4AIH4
B	211	ILE	ASN	conflict	UNP A0A6M4AIH4
B	212	VAL	LEU	conflict	UNP A0A6M4AIH4
B	213	PRO	VAL	conflict	UNP A0A6M4AIH4
B	214	GLU	ARG	conflict	UNP A0A6M4AIH4
B	?	-	TYR	deletion	UNP A0A6M4AIH4
B	?	-	LEU	deletion	UNP A0A6M4AIH4
B	?	-	THR	deletion	UNP A0A6M4AIH4
B	?	-	PRO	deletion	UNP A0A6M4AIH4
B	?	-	GLY	deletion	UNP A0A6M4AIH4
B	?	-	ASP	deletion	UNP A0A6M4AIH4
B	?	-	SER	deletion	UNP A0A6M4AIH4
B	339	ASP	GLY	conflict	UNP A0A6M4AIH4
B	371	LEU	SER	conflict	UNP A0A6M4AIH4
B	373	PRO	SER	conflict	UNP A0A6M4AIH4
B	375	PHE	SER	conflict	UNP A0A6M4AIH4
B	417	ASN	LYS	conflict	UNP A0A6M4AIH4
B	439	LYS	ASN	conflict	UNP A0A6M4AIH4
B	446	SER	GLY	conflict	UNP A0A6M4AIH4
B	477	ASN	SER	conflict	UNP A0A6M4AIH4
B	478	LYS	THR	conflict	UNP A0A6M4AIH4
B	484	ALA	GLU	conflict	UNP A0A6M4AIH4
B	493	ARG	GLN	conflict	UNP A0A6M4AIH4
B	496	SER	GLY	conflict	UNP A0A6M4AIH4
B	498	ARG	GLN	conflict	UNP A0A6M4AIH4
B	501	TYR	ASN	conflict	UNP A0A6M4AIH4
B	505	HIS	TYR	conflict	UNP A0A6M4AIH4
B	547	LYS	THR	conflict	UNP A0A6M4AIH4
B	?	-	PRO	deletion	UNP A0A6M4AIH4
B	?	-	VAL	deletion	UNP A0A6M4AIH4
B	?	-	ALA	deletion	UNP A0A6M4AIH4
B	?	-	ILE	deletion	UNP A0A6M4AIH4
B	?	-	HIS	deletion	UNP A0A6M4AIH4
B	?	-	ALA	deletion	UNP A0A6M4AIH4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP A0A6M4AIH4
B	?	-	GLN	deletion	UNP A0A6M4AIH4
B	?	-	LEU	deletion	UNP A0A6M4AIH4
B	?	-	THR	deletion	UNP A0A6M4AIH4
B	?	-	PRO	deletion	UNP A0A6M4AIH4
B	?	-	THR	deletion	UNP A0A6M4AIH4
B	?	-	TRP	deletion	UNP A0A6M4AIH4
B	?	-	ARG	deletion	UNP A0A6M4AIH4
B	?	-	VAL	deletion	UNP A0A6M4AIH4
B	?	-	TYR	deletion	UNP A0A6M4AIH4
B	?	-	SER	deletion	UNP A0A6M4AIH4
B	?	-	THR	deletion	UNP A0A6M4AIH4
B	?	-	GLY	deletion	UNP A0A6M4AIH4
B	?	-	SER	deletion	UNP A0A6M4AIH4
B	655	TYR	HIS	conflict	UNP A0A6M4AIH4
B	?	-	GLN	deletion	UNP A0A6M4AIH4
B	?	-	THR	deletion	UNP A0A6M4AIH4
B	?	-	ASN	deletion	UNP A0A6M4AIH4
B	?	-	SER	deletion	UNP A0A6M4AIH4
B	?	-	PRO	deletion	UNP A0A6M4AIH4
B	?	-	ARG	deletion	UNP A0A6M4AIH4
B	?	-	ARG	deletion	UNP A0A6M4AIH4
B	?	-	ALA	deletion	UNP A0A6M4AIH4
B	?	-	ARG	deletion	UNP A0A6M4AIH4
B	?	-	SER	deletion	UNP A0A6M4AIH4
B	?	-	VAL	deletion	UNP A0A6M4AIH4
B	?	-	ALA	deletion	UNP A0A6M4AIH4
B	764	LYS	ASN	conflict	UNP A0A6M4AIH4
B	796	TYR	ASP	conflict	UNP A0A6M4AIH4
B	?	-	PRO	deletion	UNP A0A6M4AIH4
B	?	-	LEU	deletion	UNP A0A6M4AIH4
B	?	-	ALA	deletion	UNP A0A6M4AIH4
B	?	-	ASP	deletion	UNP A0A6M4AIH4
B	?	-	ALA	deletion	UNP A0A6M4AIH4
B	?	-	GLY	deletion	UNP A0A6M4AIH4
B	?	-	PHE	deletion	UNP A0A6M4AIH4
B	?	-	ILE	deletion	UNP A0A6M4AIH4
B	?	-	LYS	deletion	UNP A0A6M4AIH4
B	?	-	GLN	deletion	UNP A0A6M4AIH4
B	?	-	TYR	deletion	UNP A0A6M4AIH4
B	?	-	GLY	deletion	UNP A0A6M4AIH4
B	?	-	ASP	deletion	UNP A0A6M4AIH4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	CYS	deletion	UNP A0A6M4AIH4
B	?	-	LEU	deletion	UNP A0A6M4AIH4
B	?	-	GLY	deletion	UNP A0A6M4AIH4
B	?	-	ASP	deletion	UNP A0A6M4AIH4
B	?	-	ILE	deletion	UNP A0A6M4AIH4
B	?	-	ALA	deletion	UNP A0A6M4AIH4
B	?	-	ALA	deletion	UNP A0A6M4AIH4
B	?	-	ARG	deletion	UNP A0A6M4AIH4
B	?	-	ASP	deletion	UNP A0A6M4AIH4
B	?	-	LEU	deletion	UNP A0A6M4AIH4
B	?	-	ILE	deletion	UNP A0A6M4AIH4
B	?	-	CYS	deletion	UNP A0A6M4AIH4
B	?	-	ALA	deletion	UNP A0A6M4AIH4
B	?	-	GLN	deletion	UNP A0A6M4AIH4
B	856	LYS	ASN	conflict	UNP A0A6M4AIH4
B	954	HIS	GLN	conflict	UNP A0A6M4AIH4
B	969	LYS	ASN	conflict	UNP A0A6M4AIH4
B	981	PHE	LEU	conflict	UNP A0A6M4AIH4
B	986	PRO	LYS	conflict	UNP A0A6M4AIH4
B	987	PRO	VAL	conflict	UNP A0A6M4AIH4
C	67	VAL	ALA	conflict	UNP A0A6M4AIH4
C	?	-	HIS	deletion	UNP A0A6M4AIH4
C	?	-	VAL	deletion	UNP A0A6M4AIH4
C	?	-	SER	deletion	UNP A0A6M4AIH4
C	?	-	GLY	deletion	UNP A0A6M4AIH4
C	?	-	THR	deletion	UNP A0A6M4AIH4
C	?	-	ASN	deletion	UNP A0A6M4AIH4
C	?	-	GLY	deletion	UNP A0A6M4AIH4
C	?	-	THR	deletion	UNP A0A6M4AIH4
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C	211	ILE	ASN	conflict	UNP A0A6M4AIH4
C	212	VAL	LEU	conflict	UNP A0A6M4AIH4
C	213	PRO	VAL	conflict	UNP A0A6M4AIH4
C	214	GLU	ARG	conflict	UNP A0A6M4AIH4
C	?	-	TYR	deletion	UNP A0A6M4AIH4
C	?	-	LEU	deletion	UNP A0A6M4AIH4
C	?	-	THR	deletion	UNP A0A6M4AIH4
C	?	-	PRO	deletion	UNP A0A6M4AIH4
C	?	-	GLY	deletion	UNP A0A6M4AIH4
C	?	-	ASP	deletion	UNP A0A6M4AIH4
C	?	-	SER	deletion	UNP A0A6M4AIH4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	339	ASP	GLY	conflict	UNP A0A6M4AIH4
C	371	LEU	SER	conflict	UNP A0A6M4AIH4
C	373	PRO	SER	conflict	UNP A0A6M4AIH4
C	375	PHE	SER	conflict	UNP A0A6M4AIH4
C	417	ASN	LYS	conflict	UNP A0A6M4AIH4
C	439	LYS	ASN	conflict	UNP A0A6M4AIH4
C	446	SER	GLY	conflict	UNP A0A6M4AIH4
C	477	ASN	SER	conflict	UNP A0A6M4AIH4
C	478	LYS	THR	conflict	UNP A0A6M4AIH4
C	484	ALA	GLU	conflict	UNP A0A6M4AIH4
C	493	ARG	GLN	conflict	UNP A0A6M4AIH4
C	496	SER	GLY	conflict	UNP A0A6M4AIH4
C	498	ARG	GLN	conflict	UNP A0A6M4AIH4
C	501	TYR	ASN	conflict	UNP A0A6M4AIH4
C	505	HIS	TYR	conflict	UNP A0A6M4AIH4
C	547	LYS	THR	conflict	UNP A0A6M4AIH4
C	?	-	PRO	deletion	UNP A0A6M4AIH4
C	?	-	VAL	deletion	UNP A0A6M4AIH4
C	?	-	ALA	deletion	UNP A0A6M4AIH4
C	?	-	ILE	deletion	UNP A0A6M4AIH4
C	?	-	HIS	deletion	UNP A0A6M4AIH4
C	?	-	ALA	deletion	UNP A0A6M4AIH4
C	?	-	ASP	deletion	UNP A0A6M4AIH4
C	?	-	GLN	deletion	UNP A0A6M4AIH4
C	?	-	LEU	deletion	UNP A0A6M4AIH4
C	?	-	THR	deletion	UNP A0A6M4AIH4
C	?	-	PRO	deletion	UNP A0A6M4AIH4
C	?	-	THR	deletion	UNP A0A6M4AIH4
C	?	-	TRP	deletion	UNP A0A6M4AIH4
C	?	-	ARG	deletion	UNP A0A6M4AIH4
C	?	-	VAL	deletion	UNP A0A6M4AIH4
C	?	-	TYR	deletion	UNP A0A6M4AIH4
C	?	-	SER	deletion	UNP A0A6M4AIH4
C	?	-	THR	deletion	UNP A0A6M4AIH4
C	?	-	GLY	deletion	UNP A0A6M4AIH4
C	?	-	SER	deletion	UNP A0A6M4AIH4
C	655	TYR	HIS	conflict	UNP A0A6M4AIH4
C	?	-	GLN	deletion	UNP A0A6M4AIH4
C	?	-	THR	deletion	UNP A0A6M4AIH4
C	?	-	ASN	deletion	UNP A0A6M4AIH4
C	?	-	SER	deletion	UNP A0A6M4AIH4
C	?	-	PRO	deletion	UNP A0A6M4AIH4

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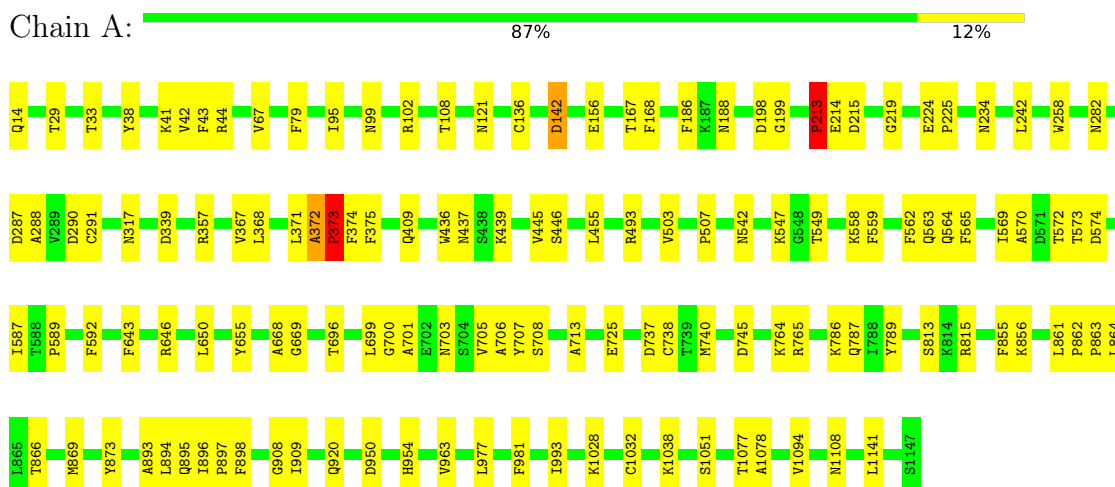
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP A0A6M4AIH4
C	?	-	ARG	deletion	UNP A0A6M4AIH4
C	?	-	ALA	deletion	UNP A0A6M4AIH4
C	?	-	ARG	deletion	UNP A0A6M4AIH4
C	?	-	SER	deletion	UNP A0A6M4AIH4
C	?	-	VAL	deletion	UNP A0A6M4AIH4
C	?	-	ALA	deletion	UNP A0A6M4AIH4
C	764	LYS	ASN	conflict	UNP A0A6M4AIH4
C	796	TYR	ASP	conflict	UNP A0A6M4AIH4
C	?	-	PRO	deletion	UNP A0A6M4AIH4
C	?	-	LEU	deletion	UNP A0A6M4AIH4
C	?	-	ALA	deletion	UNP A0A6M4AIH4
C	?	-	ASP	deletion	UNP A0A6M4AIH4
C	?	-	ALA	deletion	UNP A0A6M4AIH4
C	?	-	GLY	deletion	UNP A0A6M4AIH4
C	?	-	PHE	deletion	UNP A0A6M4AIH4
C	?	-	ILE	deletion	UNP A0A6M4AIH4
C	?	-	LYS	deletion	UNP A0A6M4AIH4
C	?	-	GLN	deletion	UNP A0A6M4AIH4
C	?	-	TYR	deletion	UNP A0A6M4AIH4
C	?	-	GLY	deletion	UNP A0A6M4AIH4
C	?	-	ASP	deletion	UNP A0A6M4AIH4
C	?	-	CYS	deletion	UNP A0A6M4AIH4
C	?	-	LEU	deletion	UNP A0A6M4AIH4
C	?	-	GLY	deletion	UNP A0A6M4AIH4
C	?	-	ASP	deletion	UNP A0A6M4AIH4
C	?	-	ILE	deletion	UNP A0A6M4AIH4
C	?	-	ALA	deletion	UNP A0A6M4AIH4
C	?	-	ALA	deletion	UNP A0A6M4AIH4
C	?	-	ARG	deletion	UNP A0A6M4AIH4
C	?	-	ASP	deletion	UNP A0A6M4AIH4
C	?	-	LEU	deletion	UNP A0A6M4AIH4
C	?	-	ILE	deletion	UNP A0A6M4AIH4
C	?	-	CYS	deletion	UNP A0A6M4AIH4
C	?	-	ALA	deletion	UNP A0A6M4AIH4
C	?	-	GLN	deletion	UNP A0A6M4AIH4
C	856	LYS	ASN	conflict	UNP A0A6M4AIH4
C	954	HIS	GLN	conflict	UNP A0A6M4AIH4
C	969	LYS	ASN	conflict	UNP A0A6M4AIH4
C	981	PHE	LEU	conflict	UNP A0A6M4AIH4
C	986	PRO	LYS	conflict	UNP A0A6M4AIH4
C	987	PRO	VAL	conflict	UNP A0A6M4AIH4

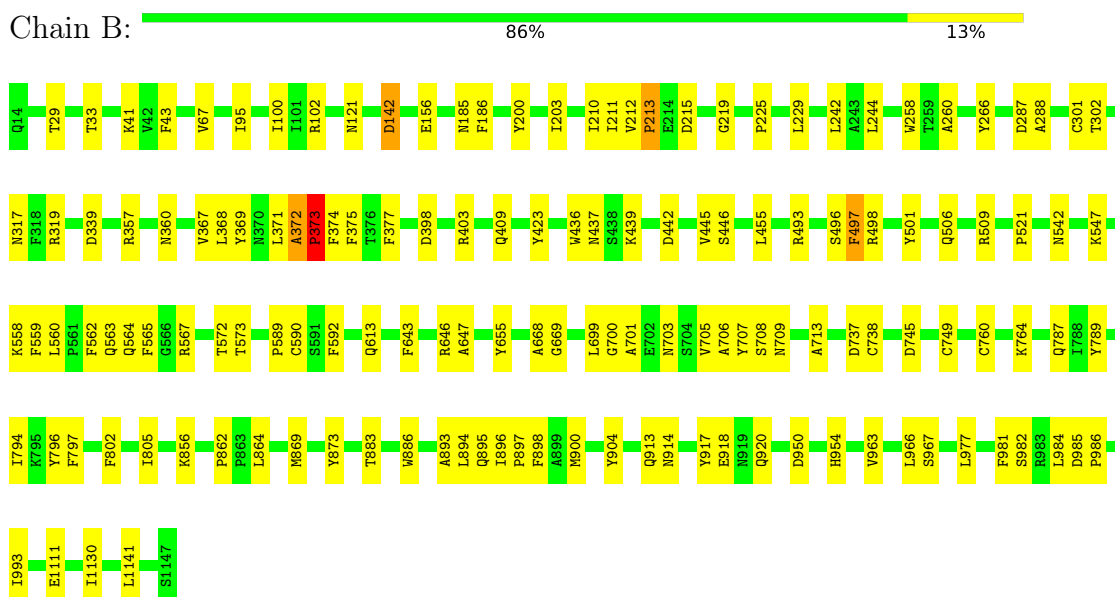
3 Residue-property plots

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.

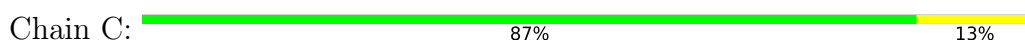
- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein



V1128	F855	I598	Q14
V1129	K856	D339	T33
I1130	G857	V367	Y38
	L858	L368	P39
L1141	T859	L371	D40
S1147	P863	A372	K41
	L864	P373	V42
	L865	F374	F43
	T866	F375	L48
	D867	V382	V67
	E868	S383	S94
	M869	K386	I95
	Y873	L390	E96
	A893	Y423	I100
	L894	W436	T108
	Q895	N437	D142
	I896	S438	E166
	T897	K439	N165
	F898	S443	F186
	Y904	V445	P213
		S446	E214
		L455	G219
	G908	K478	P225
	D950	R493	N234
	H954	R498	L242
	N960	Y501	A243
	V963	G502	L244
	K964	V503	W288
	Q965	Q506	T259
	L966	E516	A260
	L977	K547	Y266
	F981	K557	L276
	I993	F562	N280
	K1038	Q563	T284
	H1064	D568	D287
	E1072	I569	A288
	A1078	A570	
	P1079	D571	
	F1089	F592	
	P1090		
	R1107		
	S1123		
		LYS	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (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	0.26	0/8524	0.47	4/11592 (0.0%)
1	B	0.26	0/8524	0.48	4/11592 (0.0%)
1	C	0.26	0/8509	0.48	4/11573 (0.0%)
All	All	0.26	0/25557	0.48	12/34757 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	213	PRO	CA-N-CD	-8.90	99.04	111.50
1	C	373	PRO	CA-N-CD	-8.79	99.20	111.50
1	C	213	PRO	CA-N-CD	-8.77	99.22	111.50
1	A	373	PRO	CA-N-CD	-8.77	99.23	111.50
1	B	213	PRO	CA-N-CD	-8.75	99.26	111.50

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	8328	0	8145	428	0
1	B	8328	0	8143	515	0
1	C	8313	0	8128	440	0
All	All	24969	0	24416	921	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 19.

The worst 5 of 921 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:572:THR:HG23	1:C:856:LYS:CE	1.11	1.54
1:B:977:LEU:CD1	1:B:981:PHE:CE2	1.87	1.52
1:B:455:LEU:HD11	1:B:493:ARG:CD	1.04	1.49
1:B:455:LEU:HD13	1:B:493:ARG:CZ	1.02	1.48
1:B:977:LEU:CG	1:B:981:PHE:HE2	1.22	1.47

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 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	1046/1060 (99%)	1011 (97%)	32 (3%)	3 (0%)	37	67
1	B	1046/1060 (99%)	1010 (97%)	33 (3%)	3 (0%)	37	67
1	C	1044/1060 (98%)	1009 (97%)	32 (3%)	3 (0%)	37	67
All	All	3136/3180 (99%)	3030 (97%)	97 (3%)	9 (0%)	38	67

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	PRO
1	C	213	PRO
1	C	373	PRO
1	A	213	PRO
1	B	213	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 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	930/930 (100%)	930 (100%)	0	100	100
1	B	930/930 (100%)	926 (100%)	4 (0%)	89	93
1	C	928/930 (100%)	927 (100%)	1 (0%)	92	96
All	All	2788/2790 (100%)	2783 (100%)	5 (0%)	91	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	301	CYS
1	B	377	PHE
1	B	497	PHE
1	B	760	CYS
1	C	423	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	954	HIS
1	C	954	HIS
1	A	907	ASN
1	A	954	HIS
1	B	317	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 [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	6
1	A	6
1	C	4

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	827:THR	C	854:LYS	N	16.01
1	A	827:THR	C	854:LYS	N	15.89
1	A	620:VAL	C	641:ASN	N	15.78
1	B	620:VAL	C	641:ASN	N	14.50
1	C	620:VAL	C	641:ASN	N	14.48