W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Nov 4, 2024 – 07:55 AM JST

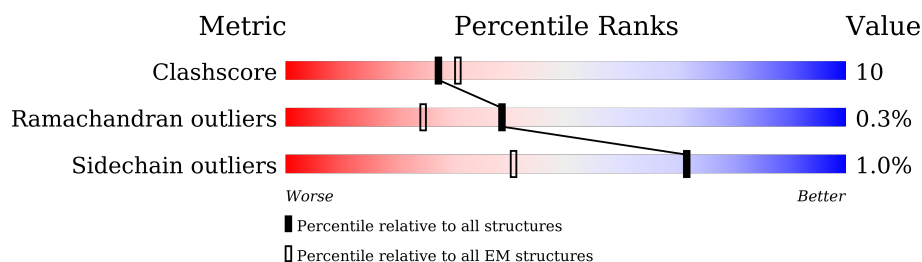|		
PDB ID	:	7WT7
EMDB ID	:	EMD-32770
Title	:	SARS-CoV-2 Omicron variant spike in complex with Fab 9A8 (State 1)
Authors	:	Wang, X.; Wang, L.
Deposited on	:	2022-02-04
Resolution	:	3.40 Å(reported)

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 3.40 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		10
Ramachandran outliers		0.3%
Sidechain outliers		1.0%

Worse   *Better*

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

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1270	21% / 66% 20% 14%
1	B	1270	31% / 68% 18% 14%
1	C	1270	18% / 68% 18% • 14%
2	H	122	95% / 70% 28% •
3	D	107	97% / 63% 36% •
4	E	3	67% / 100%
5	F	2	100% / 50% 50%
5	G	2	50% / 100%

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Mol	Chain	Length	Quality of chain
5	I	2	

2 Entity composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 28322 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	1098	Total 8632	C 5526	N 1438	O 1629	S 39	0	0
1	B	1098	Total 8632	C 5526	N 1438	O 1629	S 39	0	0
1	C	1098	Total 8630	C 5525	N 1438	O 1628	S 39	0	0

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	208	ILE	LEU	variant	UNP P0DTC2
A	211	GLU	-	insertion	UNP P0DTC2
A	212	PRO	-	insertion	UNP P0DTC2
A	213	GLU	-	insertion	UNP P0DTC2
A	336	ASP	GLY	variant	UNP P0DTC2
A	368	LEU	SER	variant	UNP P0DTC2
A	370	PRO	SER	variant	UNP P0DTC2
A	372	PHE	SER	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	variant	UNP P0DTC2
A	443	SER	GLY	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	490	ARG	GLN	variant	UNP P0DTC2
A	493	SER	GLY	variant	UNP P0DTC2

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W O R L D W I D E
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PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
A	495	ARG	GLN	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	variant	UNP P0DTC2
A	544	LYS	THR	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	680	ALA	ARG	variant	UNP P0DTC2
A	682	ALA	ARG	variant	UNP P0DTC2
A	761	LYS	ASN	variant	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	814	PRO	PHE	engineered mutation	UNP P0DTC2
A	853	LYS	ASN	variant	UNP P0DTC2
A	889	PRO	ALA	engineered mutation	UNP P0DTC2
A	896	PRO	ALA	engineered mutation	UNP P0DTC2
A	939	PRO	ALA	engineered mutation	UNP P0DTC2
A	951	HIS	GLN	variant	UNP P0DTC2
A	966	LYS	ASN	variant	UNP P0DTC2
A	978	PHE	LEU	variant	UNP P0DTC2
A	983	PRO	LYS	engineered mutation	UNP P0DTC2
A	984	PRO	VAL	engineered mutation	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	208	ILE	LEU	variant	UNP P0DTC2
B	211	GLU	-	insertion	UNP P0DTC2
B	212	PRO	-	insertion	UNP P0DTC2
B	213	GLU	-	insertion	UNP P0DTC2
B	336	ASP	GLY	variant	UNP P0DTC2
B	368	LEU	SER	variant	UNP P0DTC2
B	370	PRO	SER	variant	UNP P0DTC2
B	372	PHE	SER	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	437	LYS	ASN	variant	UNP P0DTC2
B	443	SER	GLY	variant	UNP P0DTC2
B	474	ASN	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	475	LYS	THR	variant	UNP P0DTC2
B	481	ALA	GLU	variant	UNP P0DTC2
B	490	ARG	GLN	variant	UNP P0DTC2
B	493	SER	GLY	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	544	LYS	THR	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	680	ALA	ARG	variant	UNP P0DTC2
B	682	ALA	ARG	variant	UNP P0DTC2
B	761	LYS	ASN	variant	UNP P0DTC2
B	793	TYR	ASP	variant	UNP P0DTC2
B	814	PRO	PHE	engineered mutation	UNP P0DTC2
B	853	LYS	ASN	variant	UNP P0DTC2
B	889	PRO	ALA	engineered mutation	UNP P0DTC2
B	896	PRO	ALA	engineered mutation	UNP P0DTC2
B	939	PRO	ALA	engineered mutation	UNP P0DTC2
B	951	HIS	GLN	variant	UNP P0DTC2
B	966	LYS	ASN	variant	UNP P0DTC2
B	978	PHE	LEU	variant	UNP P0DTC2
B	983	PRO	LYS	engineered mutation	UNP P0DTC2
B	984	PRO	VAL	engineered mutation	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	208	ILE	LEU	variant	UNP P0DTC2
C	211	GLU	-	insertion	UNP P0DTC2
C	212	PRO	-	insertion	UNP P0DTC2
C	213	GLU	-	insertion	UNP P0DTC2
C	334	ASP	GLY	variant	UNP P0DTC2
C	366	LEU	SER	variant	UNP P0DTC2
C	368	PRO	SER	variant	UNP P0DTC2
C	370	PHE	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	412	ASN	LYS	variant	UNP P0DTC2
C	435	LYS	ASN	variant	UNP P0DTC2
C	441	SER	GLY	variant	UNP P0DTC2
C	472	ASN	SER	variant	UNP P0DTC2
C	473	LYS	THR	variant	UNP P0DTC2
C	479	ALA	GLU	variant	UNP P0DTC2
C	488	ARG	GLN	variant	UNP P0DTC2
C	491	SER	GLY	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	TYR	ASN	variant	UNP P0DTC2
C	500	HIS	TYR	variant	UNP P0DTC2
C	542	LYS	THR	variant	UNP P0DTC2
C	609	GLY	ASP	variant	UNP P0DTC2
C	650	TYR	HIS	variant	UNP P0DTC2
C	674	LYS	ASN	variant	UNP P0DTC2
C	676	HIS	PRO	variant	UNP P0DTC2
C	678	ALA	ARG	variant	UNP P0DTC2
C	680	ALA	ARG	variant	UNP P0DTC2
C	759	LYS	ASN	variant	UNP P0DTC2
C	791	TYR	ASP	variant	UNP P0DTC2
C	812	PRO	PHE	engineered mutation	UNP P0DTC2
C	851	LYS	ASN	variant	UNP P0DTC2
C	887	PRO	ALA	engineered mutation	UNP P0DTC2
C	894	PRO	ALA	engineered mutation	UNP P0DTC2
C	937	PRO	ALA	engineered mutation	UNP P0DTC2
C	949	HIS	GLN	variant	UNP P0DTC2
C	964	LYS	ASN	variant	UNP P0DTC2
C	976	PHE	LEU	variant	UNP P0DTC2
C	981	PRO	LYS	engineered mutation	UNP P0DTC2
C	982	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of Fab 9A8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	122	900	558	154	183	5	0	0

- Molecule 3 is a protein called Light chain of Fab 9A8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	107	831	520	137	171	3	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
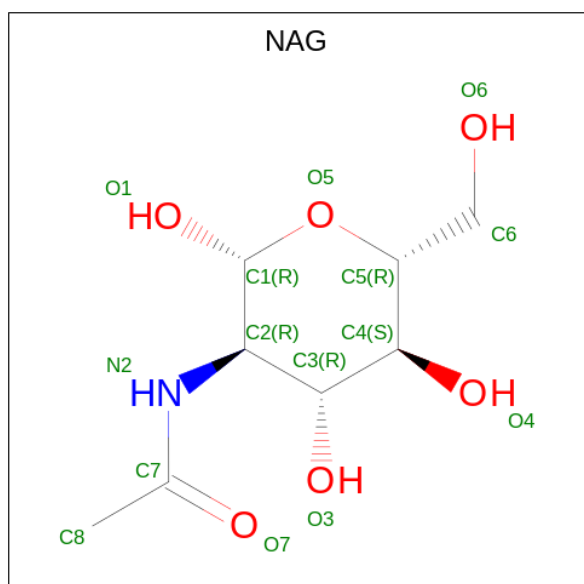

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	3	Total C N O 39 22 2 15				0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	2	Total C N O 28 16 2 10				0	0
5	G	2	Total C N O 28 16 2 10				0	0
5	I	2	Total C N O 28 16 2 10				0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0

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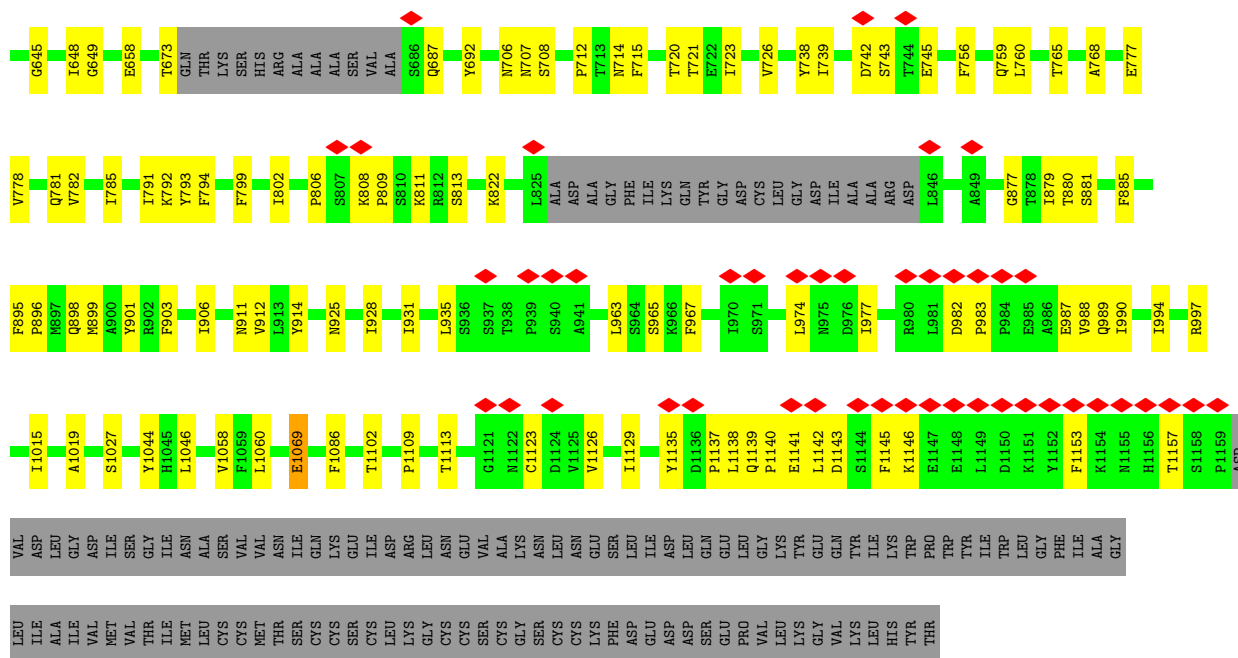| Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.
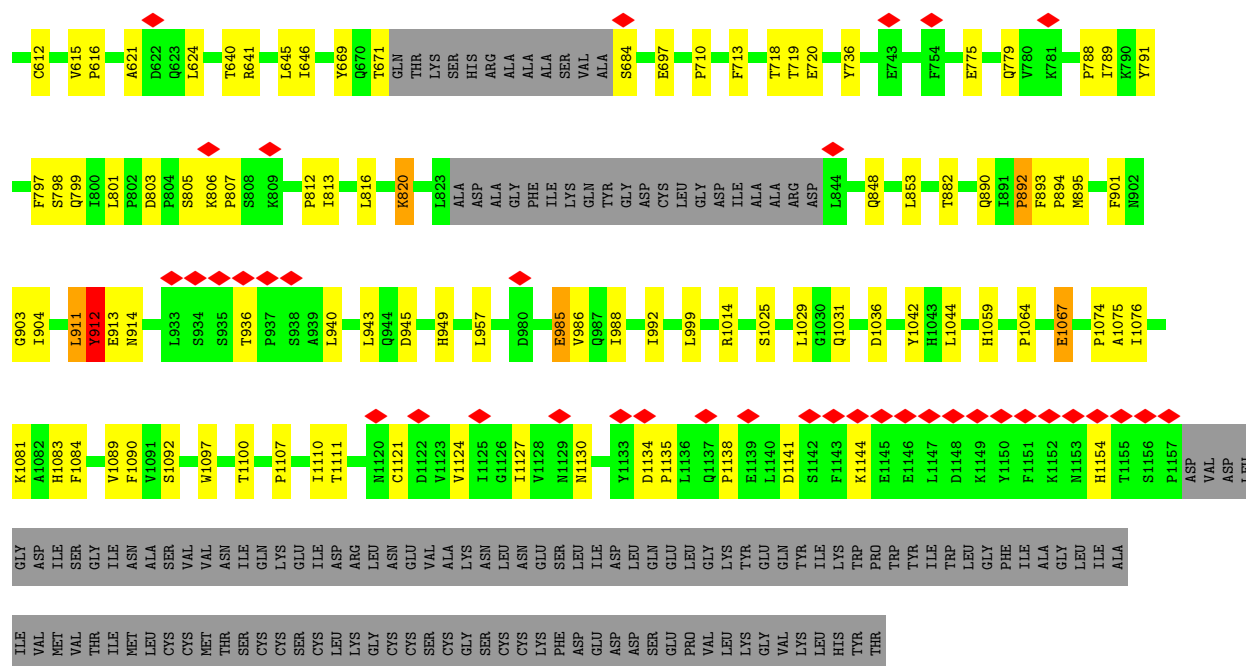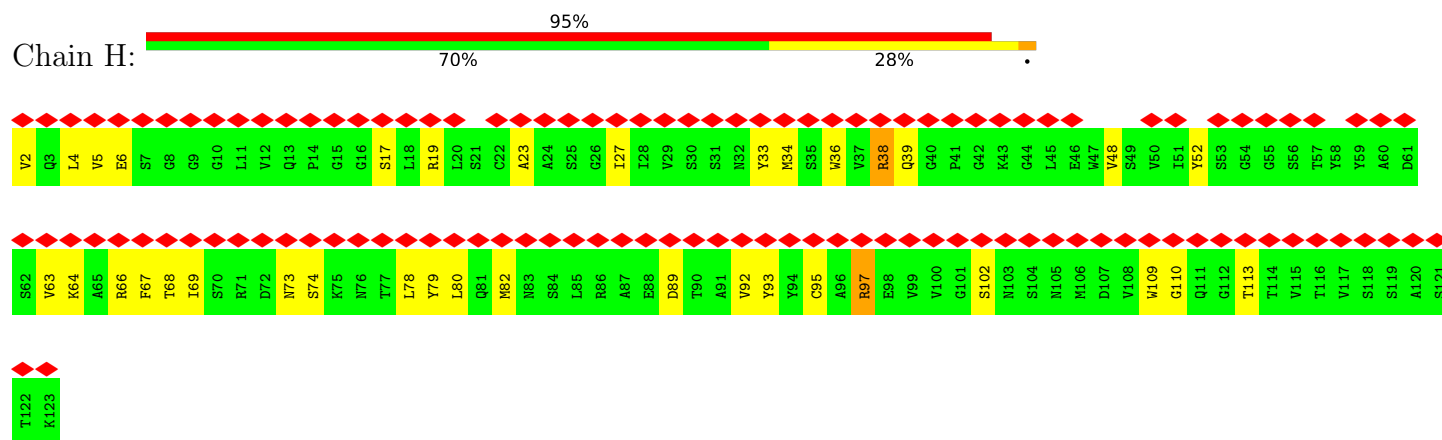
• Molecule 1: Spike glycoprotein
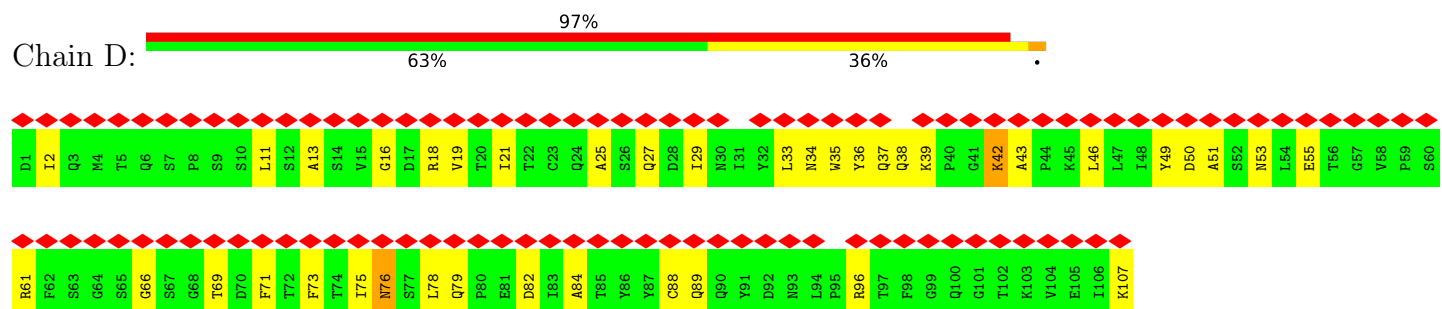
• Molecule 1: Spike glycoprotein

Chain B:

• Molecule 1: Spike glycoprotein

Chain C:

18%

68%   18% • 14%

C612 V615 P616 A621 D622 Q623 L624 T640 R641 L645 I646 Y669 Q670 T671 GLN THR LYS SER HIS ARG ALA ALA ALA SER VAL ALA S684 E697 P710 F713 T718 T719 E720 Y736 E743 F754 E775 Q779 V780 K781 P788 I789 K790 Y791

F797 S798 Q799 I800 L801 P802 D803 P804 S805 K806 P807 S808 K809 P812 I813 L816 K820 L823 ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP L844 Q848 L853 T882 Q890 I891 P892 F893 F894 M895 F901 N902

G903 I904 L911 Y912 E913 N914 L933 S934 S935 T936 P937 S938 A939 L940 L943 Q944 D945 H949 L957 D980 E985 V986 Q987 I988 I992 L999 R1014 S1025 L1029 G1030 Q1031 D1036 Y1042 H1043 L1044 H1059 P1064 E1067 P1074 A1075 I1076

K1081 A1082 H1083 F1084 V1089 F1090 V1091 S1092 W1097 T1100 P1107 I1110 T1111 N1120 C1121 D1122 V1123 V1124 I1125 G1126 I1127 V1128 N1129 N1130 Y1133 D1134 P1135 L1136 Q1137 P1138 E1139 L1140 D1141 S1142 F1143 K1144 E1145 E1146 L1147 D1148 K1149 Y1150 F1151 K1152 N1153 H1154 T1155 S1156 P1157 ASP VAL ASP LEU

GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN TYR ILE LYS TRP PRO TRP TYR ILE TRP LEU GLY PHE ILE ALA GLY LEU ILE ALA

ILE VAL MET VAL THR ILE MET LEU CYS CYS MET THR SER CYS CYS SER CYS LEU LYS GLY CYS CYS SER CYS GLY SER CYS CYS LYS PHE ASP GLU ASP ASP SER GLU PRO VAL LEU LYS GLY VAL LYS LEU HIS TYR THR

- Molecule 2: Heavy chain of Fab 9A8

Chain H:

95%
70% 28%

V2 Q3 L4 V5 E6 S7 G8 G9 G10 L11 V12 Q13 P14 G15 G16 S17 L18 R19 L20 S21 C22 A23 A24 S25 G26 I27 I28 V29 S30 S31 N32 Y33 M34 S35 W36 V37 R38 Q39 G40 P41 G42 K43 G44 L45 E46 W47 V48 S49 V50 I51 Y52 S53 G54 G55 T56 T57 Y58 Y59 A60 D61

S62 V63 K64 A65 R66 F67 T68 I69 S70 R71 D72 N73 S74 K75 N76 T77 L78 Y79 L80 Q81 M82 N83 S84 L85 R86 A87 E88 D89 T90 A91 V92 Y93 Y94 C95 A96 R97 E98 V99 V100 G101 S102 N103 S104 N105 M106 D107 V108 W109 G110 Q111 G112 T113 T114 V115 T116 V117 S118 S119 A120 S121

T122 K123

- Molecule 3: Light chain of Fab 9A8

Chain D:

97%
63% 36%

D1 I2 Q3 M4 T5 Q6 S7 P8 S9 S10 L11 S12 A13 S14 V15 G16 D17 R18 V19 T20 I21 T22 C23 Q24 A25 S26 Q27 D28 I29 N30 I31 Y32 L33 N34 W35 Y36 Q37 Q38 K39 P40 G41 K42 A43 P44 K45 L46 L47 I48 Y49 D50 A51 S52 N53 L54 E55 T56 G57 V58 P59 S60

R61 F62 S63 G64 S65 G66 S67 G68 T69 D70 F71 T72 F73 T74 I75 N76 S77 L78 Q79 P80 E81 D82 I83 A84 T85 Y86 Y87 C88 Q89 Q90 Y91 D92 N93 L94 P95 R96 T97 F98 G99 Q100 G101 T102 K103 V104 E105 I106 K107

- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain E:

67%
100%

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	494849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.552	Depositor
Minimum map value	-1.854	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.676	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.32	0/8842	0.56	4/12033 (0.0%)
1	B	0.32	0/8842	0.55	1/12033 (0.0%)
1	C	0.32	0/8840	0.55	2/12030 (0.0%)
2	H	0.27	0/915	0.59	0/1243
3	D	0.25	0/848	0.54	0/1151
All	All	0.32	0/28287	0.55	7/38490 (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	A	0	2
1	B	0	1
1	C	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	894	PRO	N-CA-CB	-7.93	93.79	103.30
1	C	892	PRO	N-CA-CB	-7.07	94.82	103.30
1	C	912	TYR	CB-CA-C	5.73	121.86	110.40
1	B	618	PRO	CA-N-CD	-5.67	103.56	111.50
1	A	1067	ALA	N-CA-CB	-5.33	102.64	110.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Res	Type	Group
1	A	145	ASN	Peptide
1	A	937	SER	Mainchain
1	B	142	ASP	Peptide
1	C	142	ASP	Peptide
1	C	612	CYS	Peptide

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	8632	0	8443	181	0
1	B	8632	0	8443	162	0
1	C	8630	0	8437	166	0
2	H	900	0	865	26	0
3	D	831	0	801	34	0
4	E	39	0	34	0	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0
5	I	28	0	25	0	0
6	A	168	0	155	2	0
6	B	210	0	195	0	0
6	C	196	0	182	4	0
All	All	28322	0	27630	535	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 10.

The worst 5 of 535 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:C:141:LEU:HB2	1:C:242:ALA:HB1	1.42	0.98
1:A:723:ILE:HG12	1:A:1058:VAL:HG22	1.55	0.89
1:A:938:THR:HG23	1:A:941:ALA:HB2	1.61	0.80
1:B:706:ASN:OD1	1:B:707:ASN:ND2	2.17	0.78
1:B:552:SER:HB2	1:B:583:ASP:HB2	1.65	0.78

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	1088/1270 (86%)	1010 (93%)	76 (7%)	2 (0%)	44	72
1	B	1088/1270 (86%)	1014 (93%)	72 (7%)	2 (0%)	44	72
1	C	1088/1270 (86%)	1005 (92%)	77 (7%)	6 (1%)	22	50
2	H	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
3	D	105/107 (98%)	91 (87%)	14 (13%)	0	100	100
All	All	3489/4039 (86%)	3231 (93%)	248 (7%)	10 (0%)	38	66

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	ILE
1	C	329	ASN
1	B	150	MET
1	C	214	ASP
1	C	911	LEU

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	967/1113 (87%)	962 (100%)	5 (0%)	86	91
1	B	967/1113 (87%)	960 (99%)	7 (1%)	81	88
1	C	966/1113 (87%)	951 (98%)	15 (2%)	58	75
2	H	98/100 (98%)	96 (98%)	2 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	94/94 (100%)	92 (98%)	2 (2%)	48	69
All	All	3092/3533 (88%)	3061 (99%)	31 (1%)	71	83

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	151	GLU
2	H	38	ARG
1	C	323	ARG
3	D	42	LYS
1	C	936	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	501	GLN
1	C	757	GLN
3	D	34	ASN
1	C	848	GLN
1	B	1033	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 ⓘ

9 monosaccharides 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
4	NAG	E	1	4,1	14,14,15	0.24	0	17,19,21	0.48	0
4	NAG	E	2	4	14,14,15	0.27	0	17,19,21	0.40	0
4	BMA	E	3	4	11,11,12	0.60	0	15,15,17	0.77	0
5	NAG	F	1	1,5	14,14,15	0.77	1 (7%)	17,19,21	0.80	0
5	NAG	F	2	5	14,14,15	0.24	0	17,19,21	0.49	0
5	NAG	G	1	1,5	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	G	2	5	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	I	1	1,5	14,14,15	0.29	0	17,19,21	0.50	0
5	NAG	I	2	5	14,14,15	0.21	0	17,19,21	0.43	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
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1	NAG	O5-C1	-2.70	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings
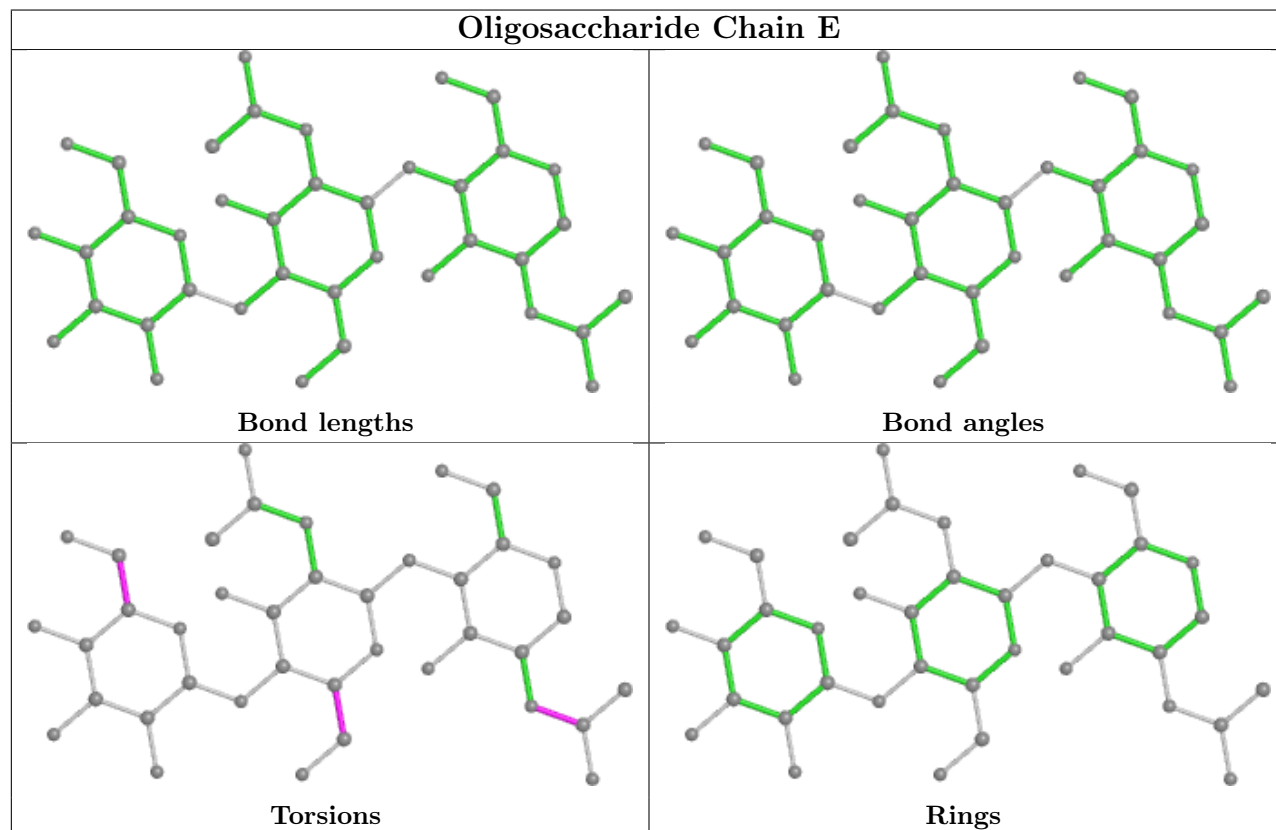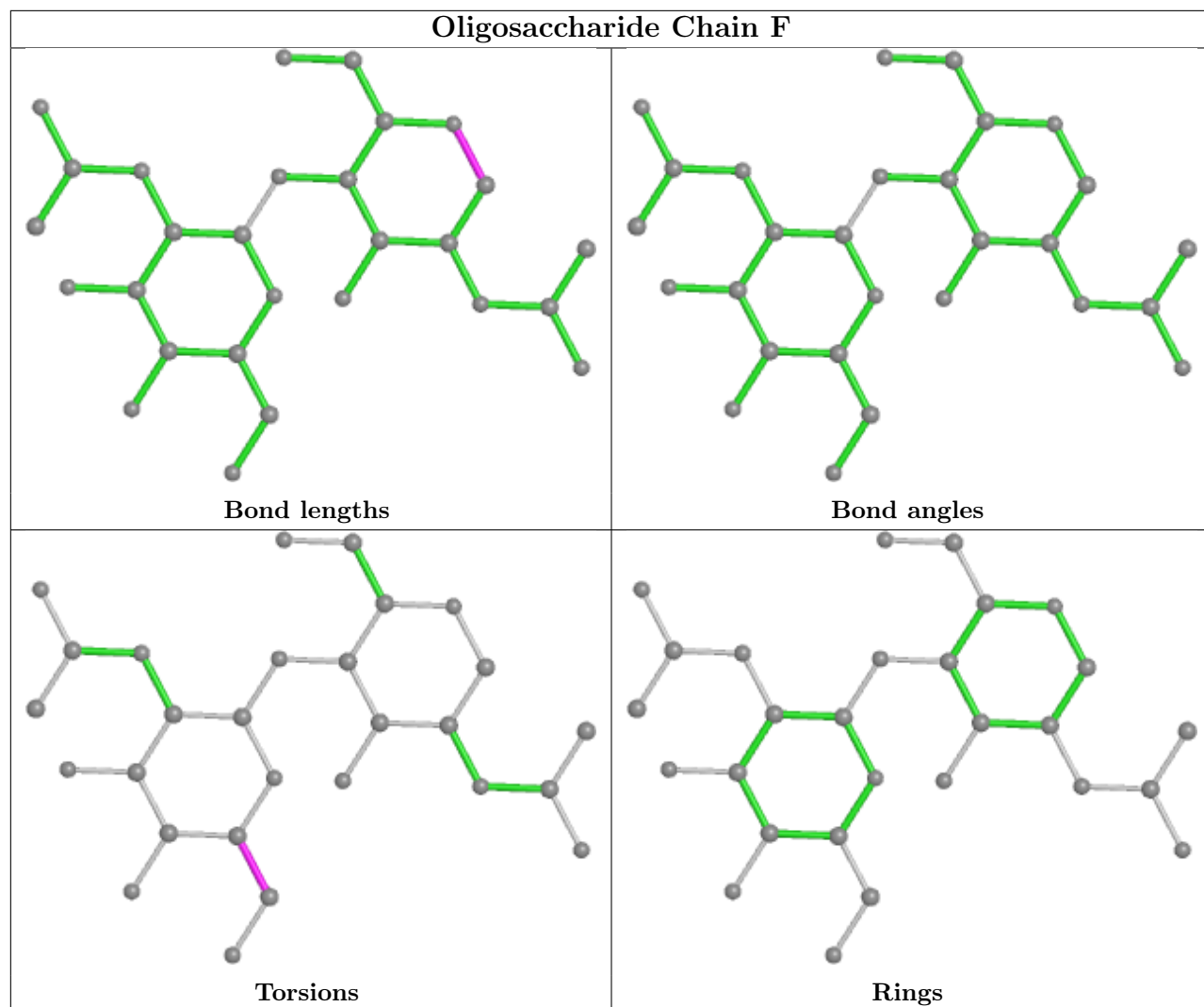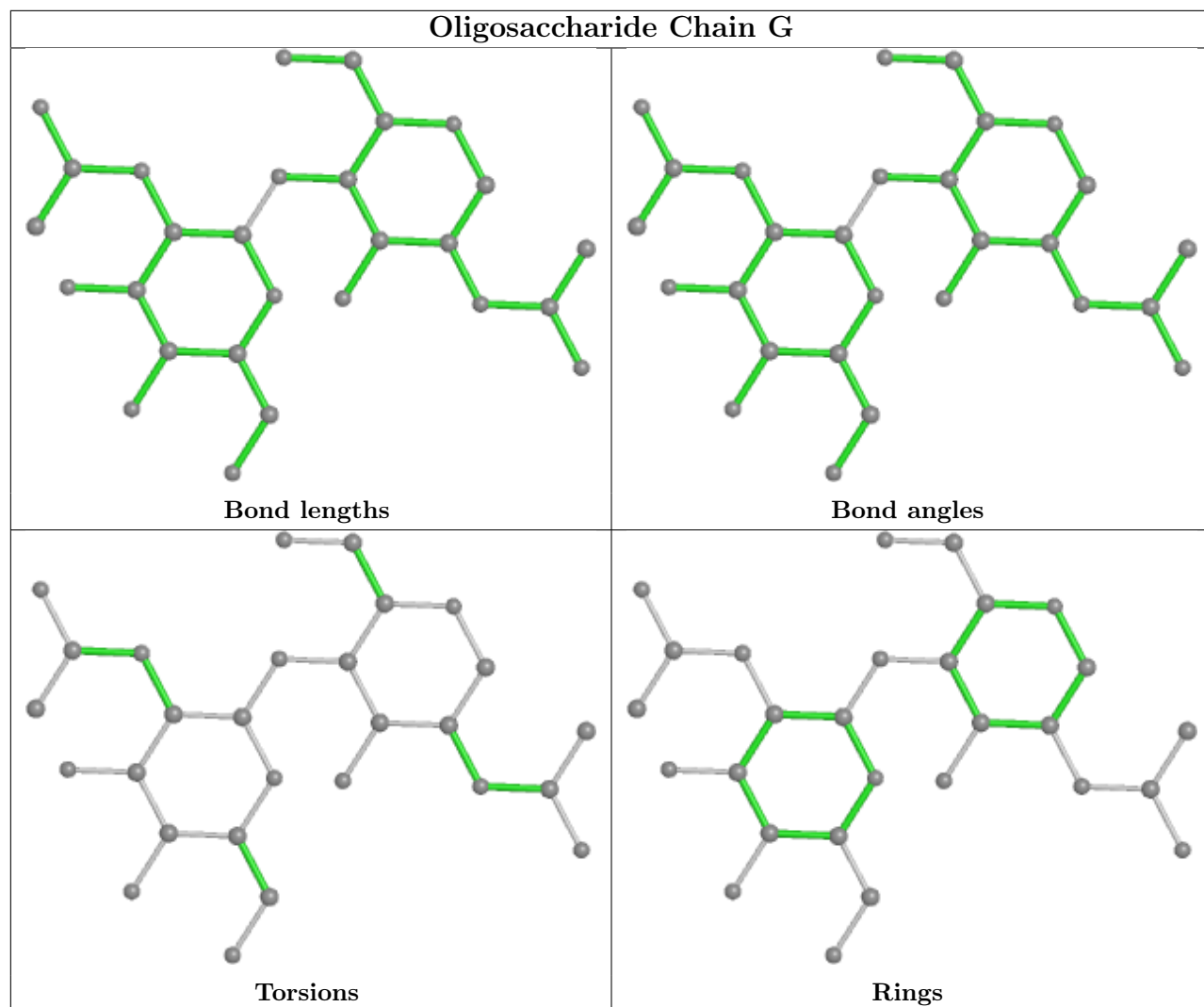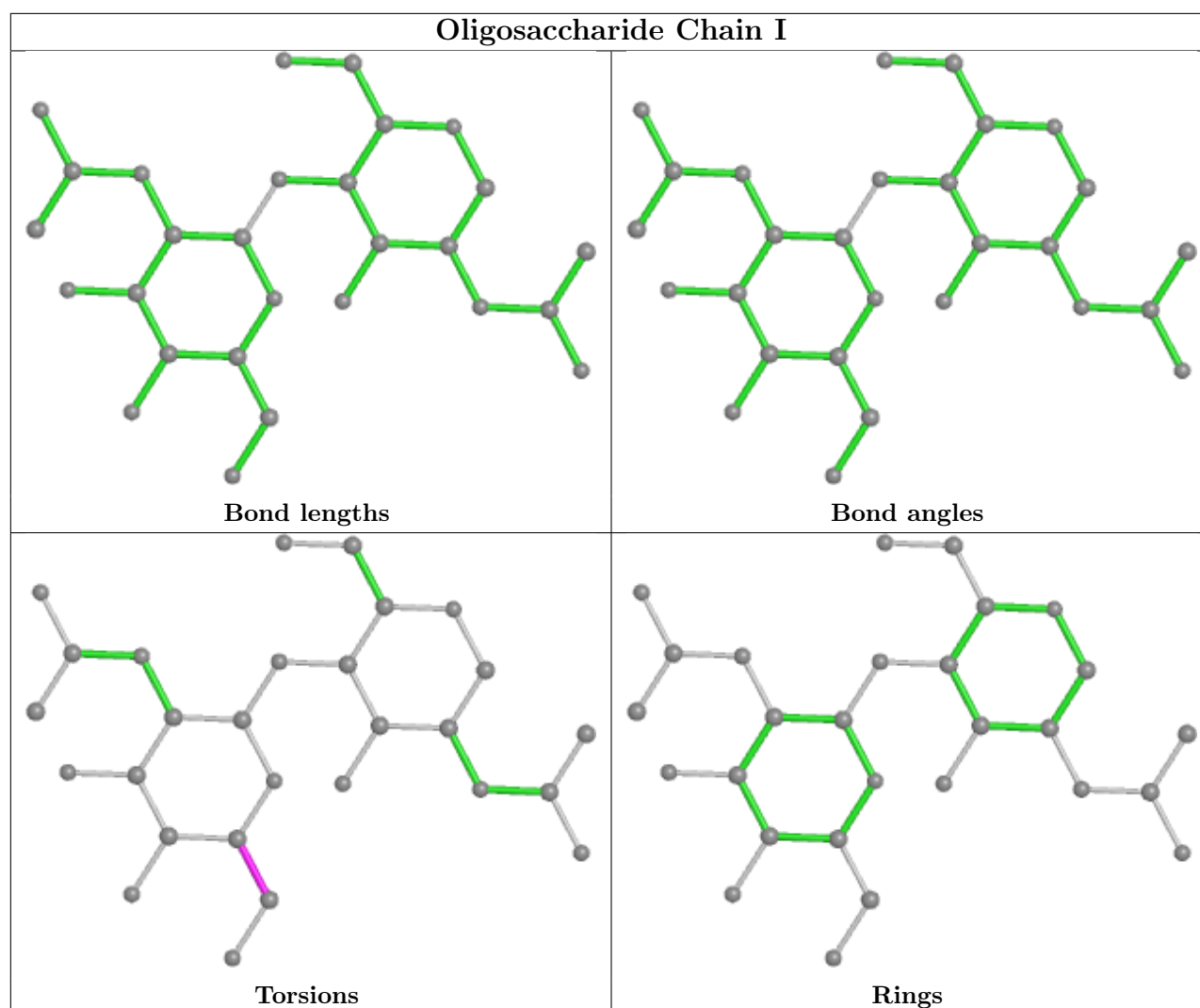
5.6   Ligand geometry ⓘ

41 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	NAG	C	1301	1	14,14,15	0.51	0	17,19,21	0.58	0
6	NAG	B	1315	1	14,14,15	0.17	0	17,19,21	0.39	0
6	NAG	A	1308	1	14,14,15	0.19	0	17,19,21	0.45	0
6	NAG	C	1314	1	14,14,15	0.21	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
6	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.45	0
6	NAG	B	1308	1	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	C	1308	1	14,14,15	0.38	0	17,19,21	0.54	0
6	NAG	B	1305	1	14,14,15	0.19	0	17,19,21	0.42	0
6	NAG	B	1313	1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	A	1309	1	14,14,15	0.25	0	17,19,21	0.48	0
6	NAG	B	1304	1	14,14,15	0.23	0	17,19,21	0.37	0
6	NAG	B	1312	1	14,14,15	0.21	0	17,19,21	0.39	0
6	NAG	B	1314	1	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	B	1309	1	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	A	1301	1	14,14,15	0.29	0	17,19,21	0.33	0
6	NAG	C	1310	1	14,14,15	0.22	0	17,19,21	0.49	0
6	NAG	C	1309	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	C	1312	1	14,14,15	0.31	0	17,19,21	0.48	0
6	NAG	C	1304	1	14,14,15	0.18	0	17,19,21	0.43	0
6	NAG	B	1303	1	14,14,15	0.40	0	17,19,21	0.33	0
6	NAG	C	1313	1	14,14,15	0.25	0	17,19,21	0.44	0
6	NAG	B	1310	1	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	A	1302	1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	A	1306	1	14,14,15	0.26	0	17,19,21	0.41	0
6	NAG	A	1310	1	14,14,15	0.21	0	17,19,21	0.40	0
6	NAG	B	1311	1	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.56	0
6	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.47	0
6	NAG	C	1307	1	14,14,15	0.26	0	17,19,21	0.36	0
6	NAG	C	1305	1	14,14,15	0.22	0	17,19,21	0.40	0
6	NAG	A	1311	1	14,14,15	0.20	0	17,19,21	0.38	0
6	NAG	A	1305	1	14,14,15	0.25	0	17,19,21	0.47	0
6	NAG	C	1306	1	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	C	1311	1	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	B	1301	1	14,14,15	0.27	0	17,19,21	0.49	0
6	NAG	A	1304	1	14,14,15	0.28	0	17,19,21	0.56	0
6	NAG	A	1312	1	14,14,15	0.19	0	17,19,21	0.45	0
6	NAG	C	1302	1	14,14,15	0.22	0	17,19,21	0.52	0
6	NAG	A	1307	1	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	B	1307	1	14,14,15	0.27	0	17,19,21	0.52	0
6	NAG	A	1303	1	14,14,15	0.29	0	17,19,21	0.45	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
6	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1315	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1308	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1314	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1311	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1303	1	-	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 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1303	NAG	C4-C5-C6-O6
6	C	1313	NAG	C4-C5-C6-O6
6	B	1304	NAG	C4-C5-C6-O6
6	B	1306	NAG	O5-C5-C6-O6
6	B	1308	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1301	NAG	1	0
6	C	1308	NAG	1	0
6	C	1310	NAG	1	0
6	C	1305	NAG	1	0
6	A	1312	NAG	1	0
6	A	1303	NAG	1	0

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.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-32770. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

| X | Y | Z |
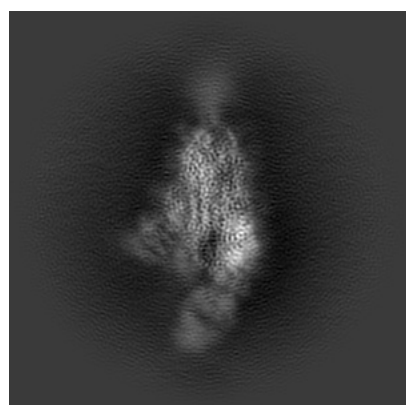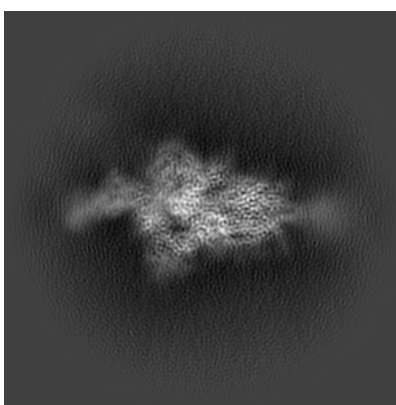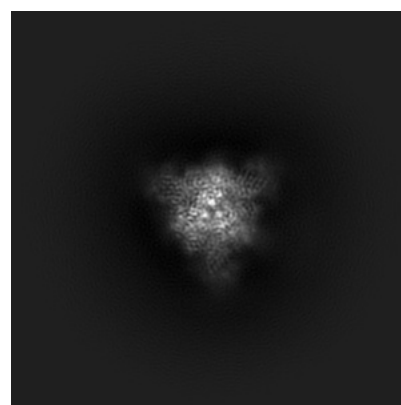
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
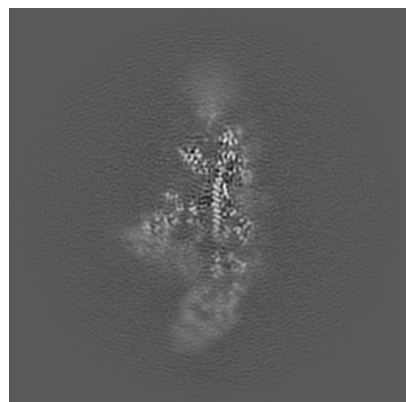
6.2.1 Primary map
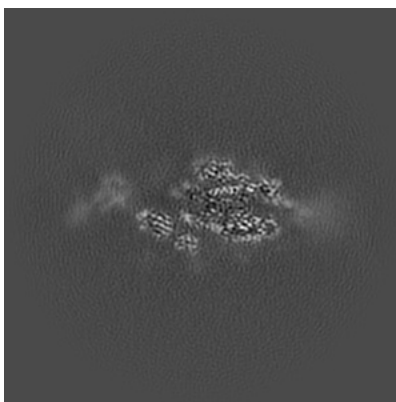
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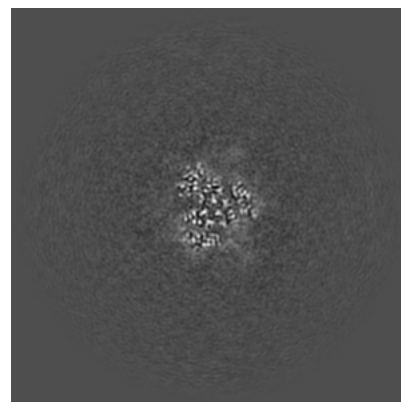
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices   ⓘ
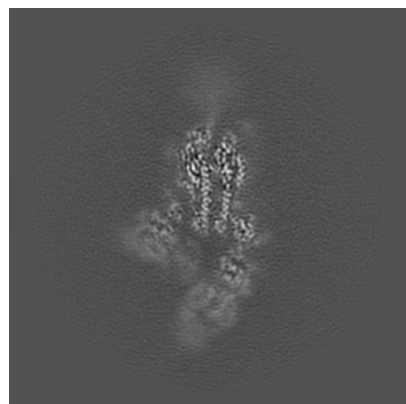
6.3.1   Primary map
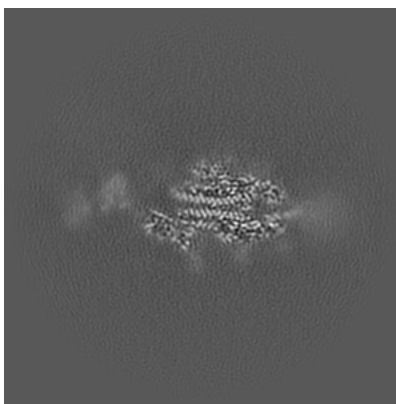
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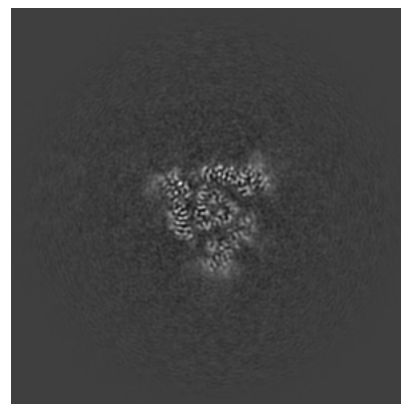
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal standard-deviation projections (False-color)   ⓘ

6.4.1   Primary map

| X | Y | Z |
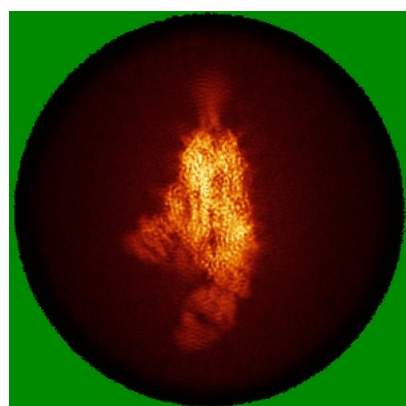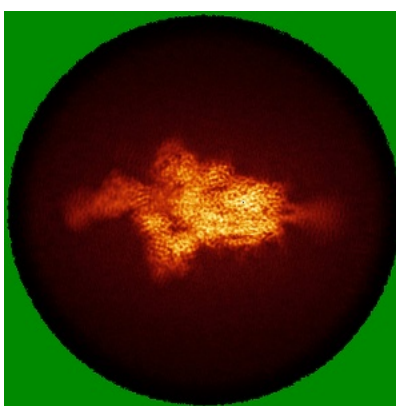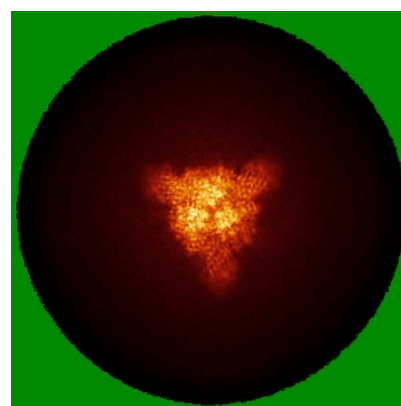
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z
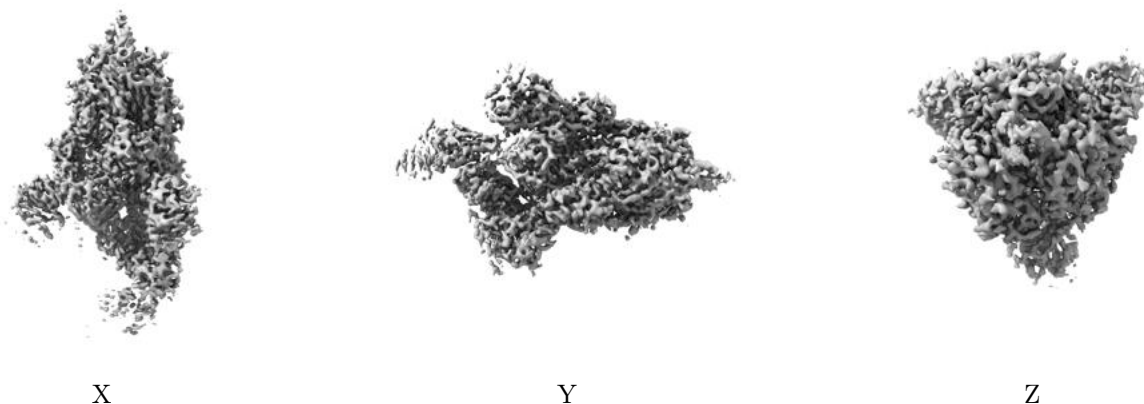
The images above show the 3D surface view of the map at the recommended contour level 0.676. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7   Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1   Map-value distribution ⓘ
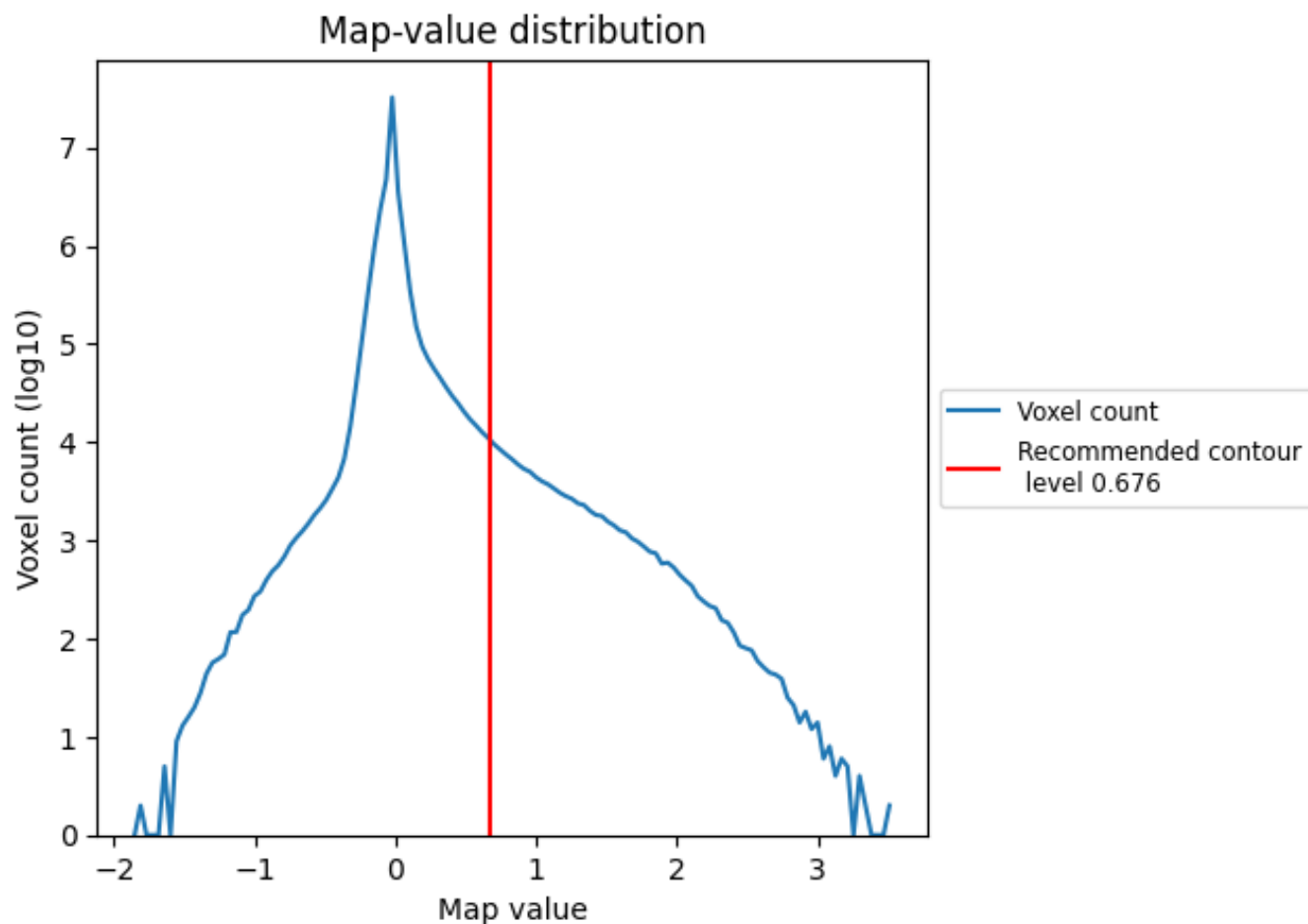
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
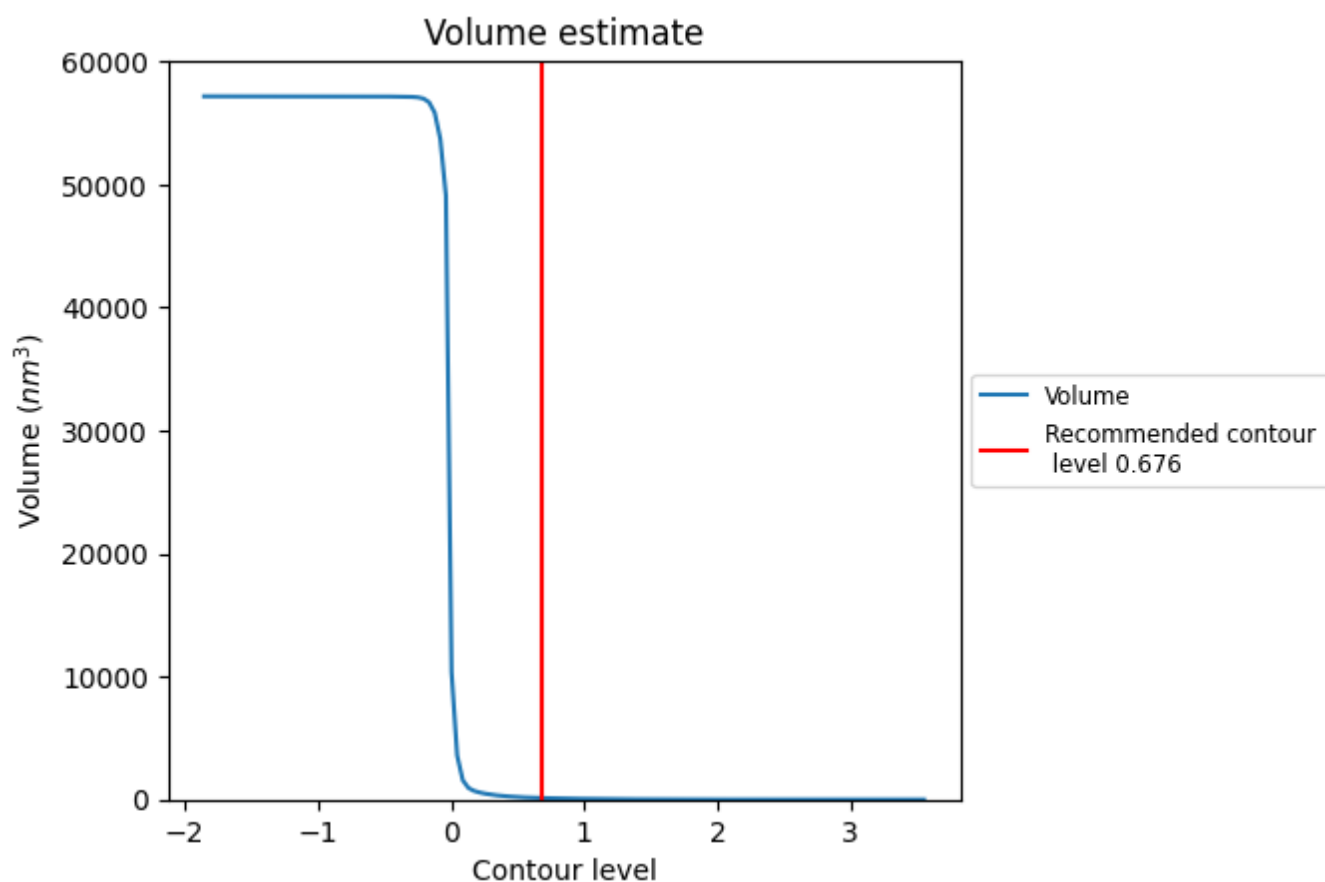
The volume at the recommended contour level is 127 nm^3; this corresponds to an approximate mass of 115 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3   Rotationally averaged power spectrum ⓘ
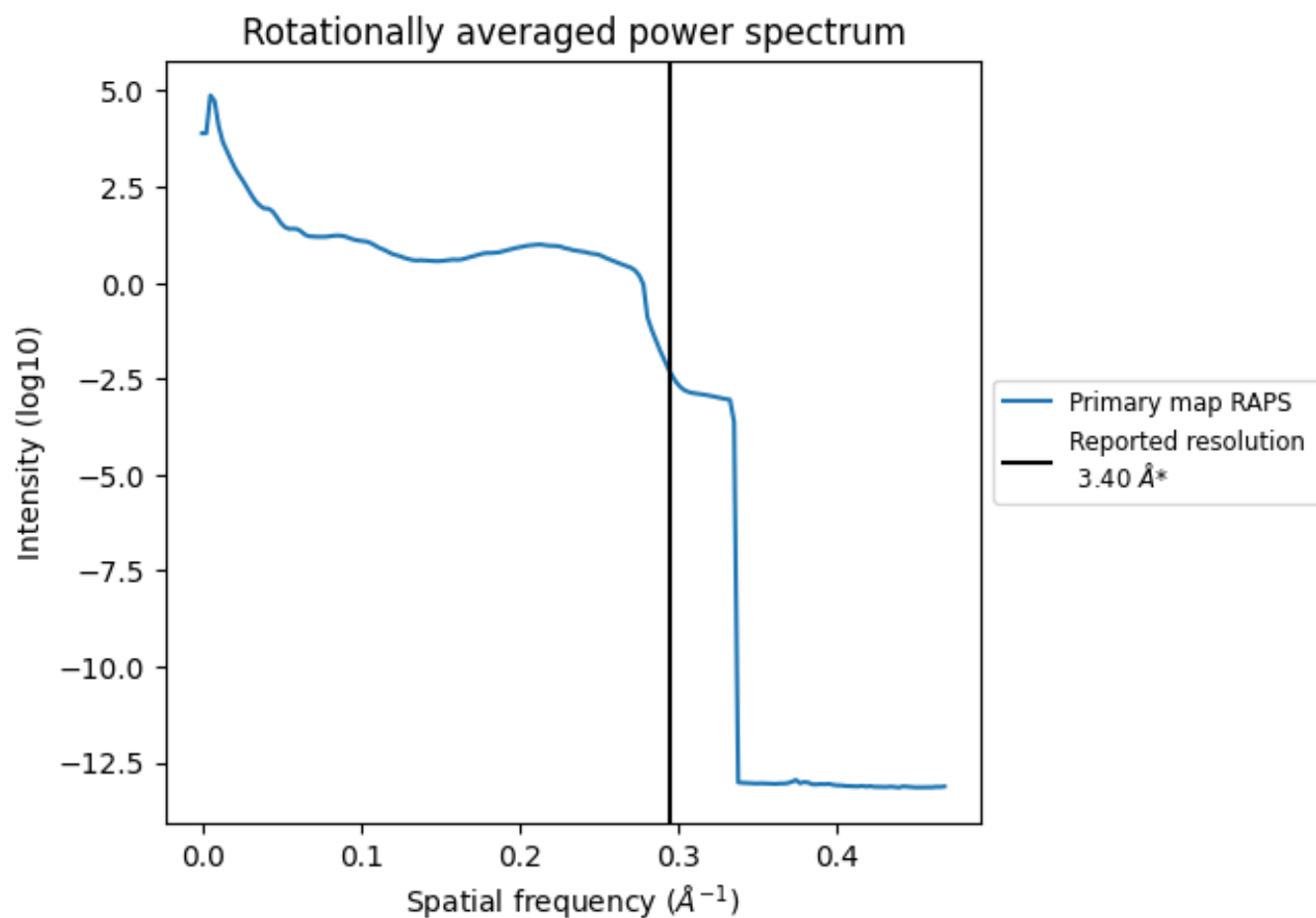
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-32770 and PDB model 7WT7. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay ⓘ

X   Y   Z
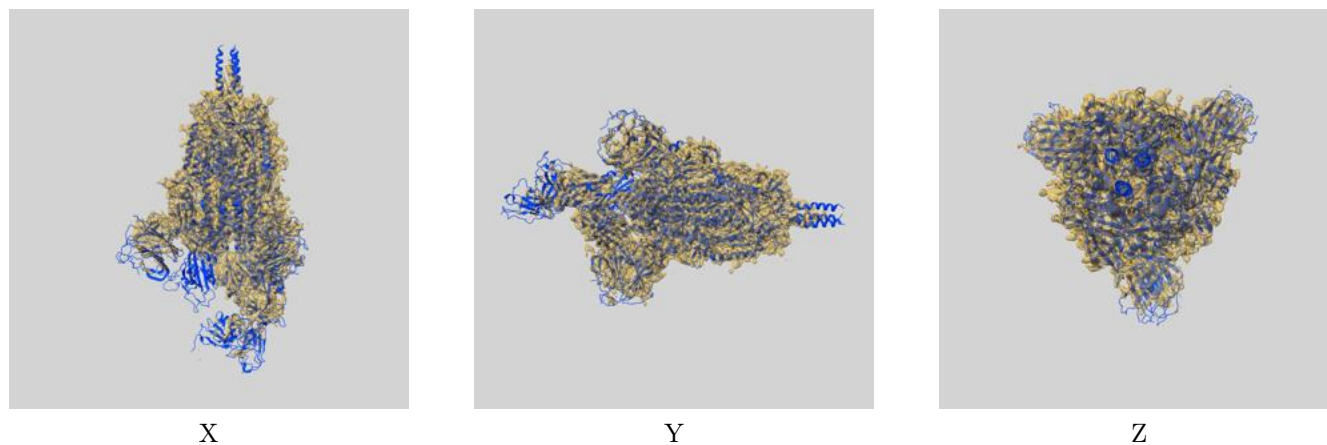
The images above show the 3D surface view of the map at the recommended contour level 0.676 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model   ⓘ
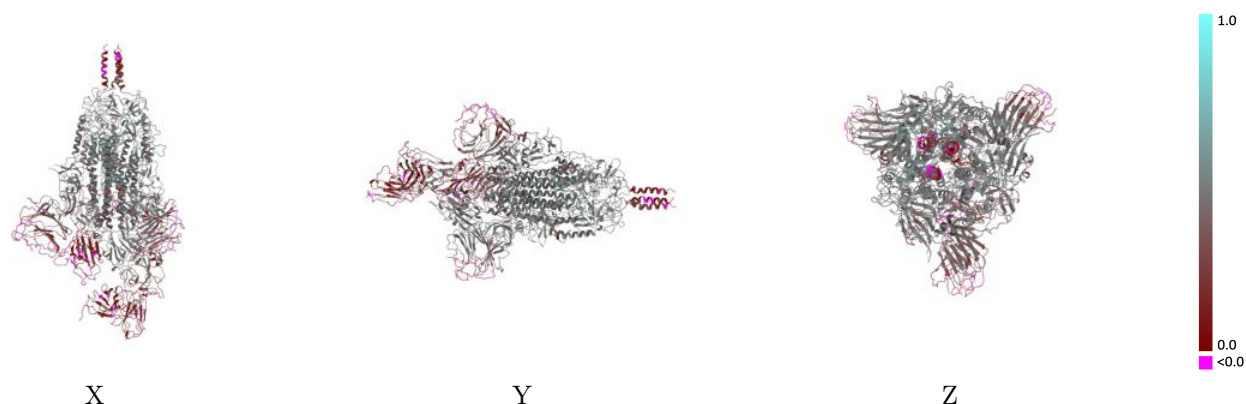
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3   Atom inclusion mapped to coordinate model   ⓘ
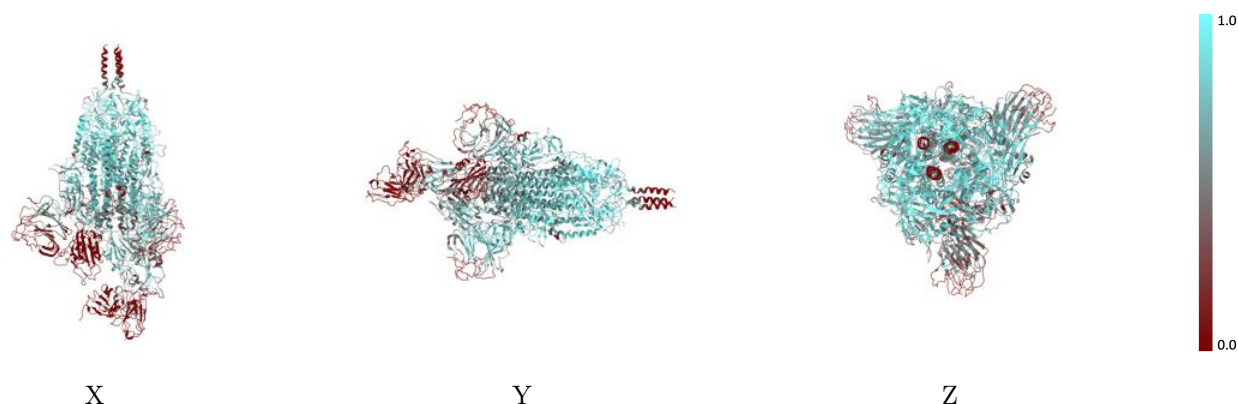
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.676).

9.4   Atom inclusion   ⓘ
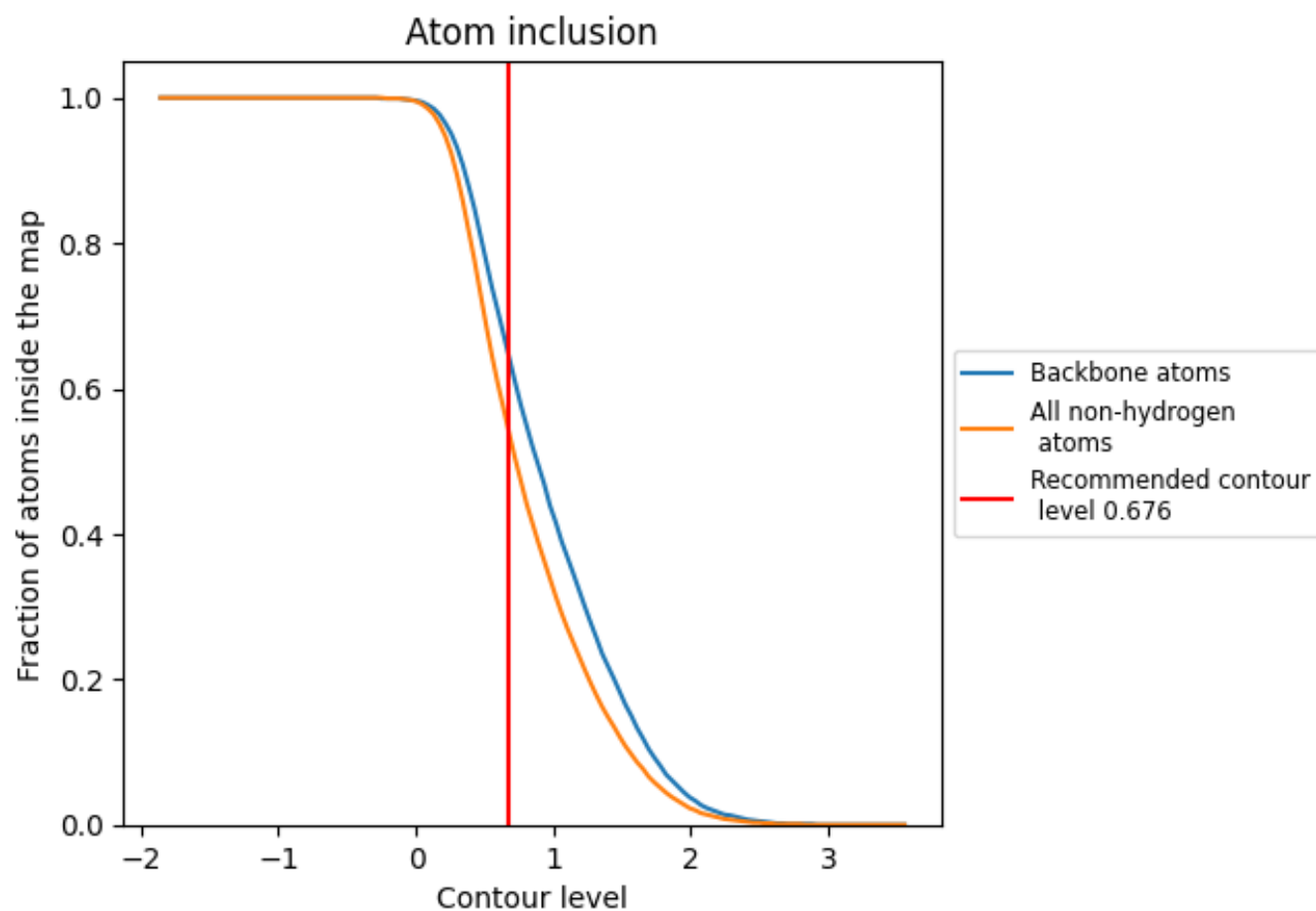
At the recommended contour level, 64% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.676) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5410	0.3850
A	0.5930	0.4090
B	0.5020	0.3640
C	0.6240	0.4220
D	0.0670	0.1930
E	0.2050	0.2810
F	0.1430	0.1680
G	0.4640	0.4890
H	0.0620	0.1670
I	0.4640	0.4060

1.0

0.0
<0.0