WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Sep 28, 2022 – 03:46 pm BST

PDB ID	:	7Z85
EMDB ID	:	EMD-14543
Title	:	CRYO-EM STRUCTURE OF SARS-COV-2 SPIKE : H11-B5 nanobody complex
Authors	:	Weckener, M.; Naismith, J.H.
Deposited on	:	2022-03-16
Resolution	:	3.10 Å(reported)
Based on initial model	:	6ZHD

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

|		
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.10 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		5
Ramachandran outliers		0.0%
Sidechain outliers		0.8%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
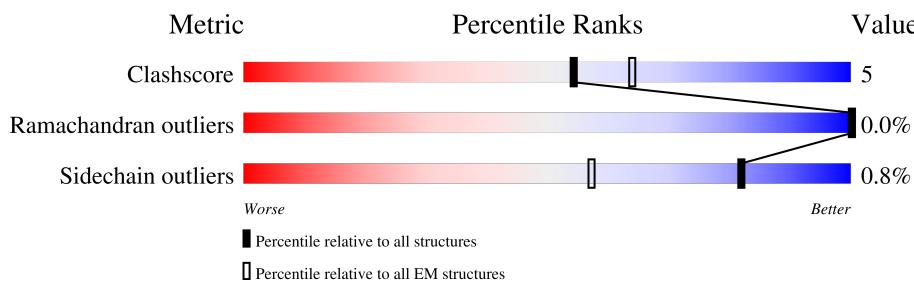
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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% 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	1260	13% / 67% 11% 22%
1	B	1260	· / 68% 10% 21%
1	C	1260	8% / 68% 11% 21%
2	D	134	93% / 81% 12% · 7%
2	E	134	80% / 78% 13% · 7%
2	F	134	92% / 80% 13% · 7%
3	G	2	100% / 100%
3	H	2	50% / 100%
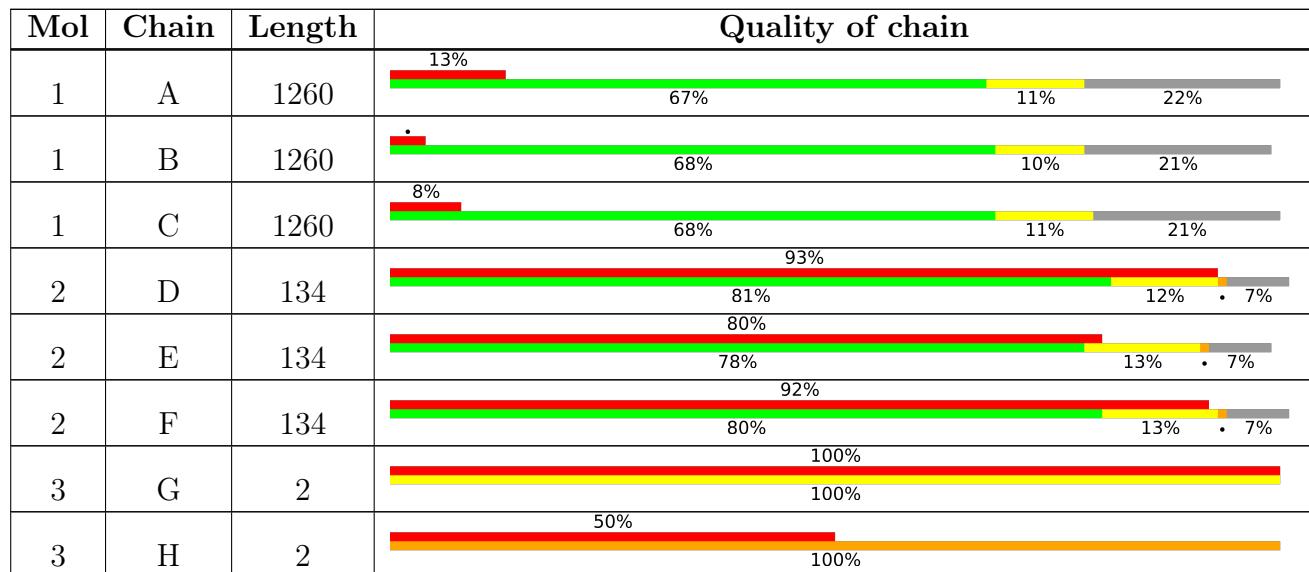
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Mol	Chain	Length	Quality of chain
3	I	2	50% 50% 50%
3	J	2	50% 100%
3	K	2	50% 50%
3	L	2	100%
3	M	2	50% 50% 50%
3	N	2	50% 50%
3	O	2	50% 50%
3	P	2	100%
3	Q	2	50% 50%
3	R	2	50% 50% 50%
3	S	2	50% 50% 50%
3	T	2	50% 100%
3	U	2	50% 50% 50%
3	V	2	100%
3	W	2	50% 100%
3	X	2	50% 100%
3	Y	2	50% 50%
3	Z	2	50% 50%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 26834 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	987	Total	C	N	O	S	0	0
			7646	4893	1271	1448	34		
1	B	992	Total	C	N	O	S	0	0
			7677	4912	1280	1451	34		
1	C	990	Total	C	N	O	S	0	0
			7659	4900	1278	1447	34		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1232	LEU	PHE	conflict	UNP P10104
A	1239	LEU	-	expression tag	UNP P10104
A	1240	LEU	-	expression tag	UNP P10104
A	1241	ASN	-	expression tag	UNP P10104
A	1242	ASP	-	expression tag	UNP P10104
A	1243	ILE	-	expression tag	UNP P10104
A	1244	PHE	-	expression tag	UNP P10104
A	1245	GLU	-	expression tag	UNP P10104
A	1246	ALA	-	expression tag	UNP P10104
A	1247	GLN	-	expression tag	UNP P10104
A	1248	LYS	-	expression tag	UNP P10104
A	1249	ILE	-	expression tag	UNP P10104
A	1250	GLU	-	expression tag	UNP P10104
A	1251	TRP	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	GLU	-	expression tag	UNP P10104
A	1254	LYS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	HIS	-	expression tag	UNP P10104
A	1259	HIS	-	expression tag	UNP P10104
A	1260	HIS	-	expression tag	UNP P10104
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1232	LEU	PHE	conflict	UNP P10104
B	1239	LEU	-	expression tag	UNP P10104
B	1240	LEU	-	expression tag	UNP P10104
B	1241	ASN	-	expression tag	UNP P10104
B	1242	ASP	-	expression tag	UNP P10104
B	1243	ILE	-	expression tag	UNP P10104
B	1244	PHE	-	expression tag	UNP P10104
B	1245	GLU	-	expression tag	UNP P10104
B	1246	ALA	-	expression tag	UNP P10104
B	1247	GLN	-	expression tag	UNP P10104
B	1248	LYS	-	expression tag	UNP P10104
B	1249	ILE	-	expression tag	UNP P10104
B	1250	GLU	-	expression tag	UNP P10104
B	1251	TRP	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104
B	1253	GLU	-	expression tag	UNP P10104
B	1254	LYS	-	expression tag	UNP P10104
B	1255	HIS	-	expression tag	UNP P10104
B	1256	HIS	-	expression tag	UNP P10104
B	1257	HIS	-	expression tag	UNP P10104
B	1258	HIS	-	expression tag	UNP P10104
B	1259	HIS	-	expression tag	UNP P10104
B	1260	HIS	-	expression tag	UNP P10104
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1210	SER	-	linker	UNP P0DTC2
C	1232	LEU	PHE	conflict	UNP P10104
C	1239	LEU	-	expression tag	UNP P10104
C	1240	LEU	-	expression tag	UNP P10104
C	1241	ASN	-	expression tag	UNP P10104
C	1242	ASP	-	expression tag	UNP P10104
C	1243	ILE	-	expression tag	UNP P10104
C	1244	PHE	-	expression tag	UNP P10104
C	1245	GLU	-	expression tag	UNP P10104
C	1246	ALA	-	expression tag	UNP P10104
C	1247	GLN	-	expression tag	UNP P10104
C	1248	LYS	-	expression tag	UNP P10104
C	1249	ILE	-	expression tag	UNP P10104
C	1250	GLU	-	expression tag	UNP P10104
C	1251	TRP	-	expression tag	UNP P10104
C	1252	HIS	-	expression tag	UNP P10104
C	1253	GLU	-	expression tag	UNP P10104
C	1254	LYS	-	expression tag	UNP P10104
C	1255	HIS	-	expression tag	UNP P10104
C	1256	HIS	-	expression tag	UNP P10104
C	1257	HIS	-	expression tag	UNP P10104
C	1258	HIS	-	expression tag	UNP P10104
C	1259	HIS	-	expression tag	UNP P10104
C	1260	HIS	-	expression tag	UNP P10104

- Molecule 2 is a protein called Nanobody H11-B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	125	Total	C	N	O	S	2	0
			976	617	167	185	7		
2	D	125	Total	C	N	O	S	2	0
			976	617	167	185	7		
2	E	125	Total	C	N	O	S	2	0
			976	617	167	185	7		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	2	Total 28	C 16	N 2	O 10	0	0
3	H	2	Total 28	C 16	N 2	O 10	0	0
3	I	2	Total 28	C 16	N 2	O 10	0	0
3	J	2	Total 28	C 16	N 2	O 10	0	0
3	K	2	Total 28	C 16	N 2	O 10	0	0
3	L	2	Total 28	C 16	N 2	O 10	0	0
3	M	2	Total 28	C 16	N 2	O 10	0	0
3	N	2	Total 28	C 16	N 2	O 10	0	0
3	O	2	Total 28	C 16	N 2	O 10	0	0
3	P	2	Total 28	C 16	N 2	O 10	0	0
3	Q	2	Total 28	C 16	N 2	O 10	0	0
3	R	2	Total 28	C 16	N 2	O 10	0	0
3	S	2	Total 28	C 16	N 2	O 10	0	0
3	T	2	Total 28	C 16	N 2	O 10	0	0
3	U	2	Total 28	C 16	N 2	O 10	0	0
3	V	2	Total 28	C 16	N 2	O 10	0	0
3	W	2	Total 28	C 16	N 2	O 10	0	0
3	X	2	Total 28	C 16	N 2	O 10	0	0
3	Y	2	Total 28	C 16	N 2	O 10	0	0
3	Z	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
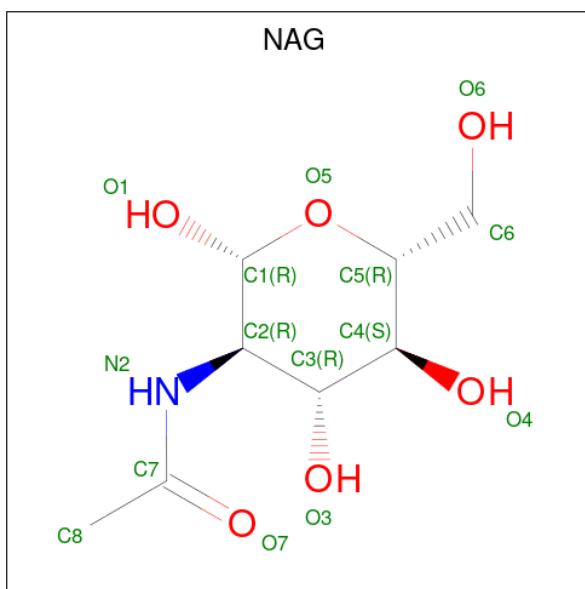
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	

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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	

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,Fibritin

I1018 K1028 M1029 S1030 E1031 C1032 G1035 Q1036 S1037 K1038 R1039 F1042 K1045 H1048 L1049 P1057 V1061 V1065 N1074 C1082 V1094 F1103 R1107 E1111 D1127 N1134 S1147 PHE LYS GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP

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

VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU SER LEU LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU LYS HIS HIS HIS HIS HIS HIS

• Molecule 1: Spike glycoprotein,Fibritin

Chain B:

68% 10% 21%

MET PHE VAL PHE LEU VAL LEU LEU PRO LEU VAL SER SER GLN CYS VAL ASN LEU THR THR ARG THR GLN LEU PRO PRO A27 S31 F32 T33 R34 P39 F43 R44 T51 V62 T63 W64 I68 H69 VAL SER GLY THR ASN GLY THR LYS ARG PHE ASP ASN P82

P85 T95 E96 K97 S98 I105 T108 D111 S112 K113 THR GLN S116 L117 N122 A123 T124 N125 E132 F135 C136 N137 D138 V143 TYR TYR HIS LYS ASN ASN LYS SER TRP MET GLU SER GLU PHE ARG VAL TYR SER SER ALA ASN ASN C166 S172 GLN PRO PHE

LEU MET ASP LEU GLU GLY LYS GLN GLY ASN F186 E191 D198 G199 Y200 F201 N211 L212 V213 R214 D215 F220 L229 P230 I231 G232 I233 R237 L241 L242 ALA LEU HIS ARG SER TYR LEU THR PRO GLY ASP SER SER SER GLY TRP THR ALA GLY ALA A263 A264

Y269 G283 D287 A288 N317 F318 R319 I326 V327 R328 R346 I358 S371 A372 C379 F392 T393 N394 V395 V401 I402 R403 K417 I418 A419 K424 G431 C432 N439 N440 L441 D442 S443 K444 V445 G446 G447 L455 E471 I472 S477 T478

N481 G482 V483 E484 G485 C488 G496 F497 Q498 P499 T500 N501 Y505 Q506 P507 Y508 R509 F515 E516 L517 L518 H519 A520 P521 T531 N532 L533 V539 L546 E554 T573 R577 Q580 I584 L585 V620 PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO

THR TRP ARG VAL TYR SER THR GLY SER N641 V642 I651 T676 GLN THR ASN SER PRO GLY SER ALA SER SER VAL ALA SER Q690 N703 N709 P715 V722 I726 M731 T732 K733 F759 L763 I770 Q774 D775 Q787 I788 Y789 F802 I805

K825 V826 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN LYS F855 E868 M869 W886 L894 A903 Y904 R905 T912 Q913 L916 I923 S943 D950 Q954 K964 L984

E988 L996 L1004 L1012 I1018 K1028 C1032 R1039 V1040 D1041 F1042 L1049 V1061 V1065 P1069 N1074 K1086 G1093 R1107 V1122 S1147 PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO 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 GLY SER GLY TYR VAL ARG LYS ASP GLY

GLU TRP VAL LEU LEU SER THR PHE LEU SER LEU LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU LYS HIS HIS HIS HIS HIS HIS

• Molecule 1: Spike glycoprotein,Fibritin

Chain C:

8%

68% 11% 21%

MET PHE VAL LEU VAL LEU LEU PRO LEU VAL SER SER GLN CYS VAL ASN LEU THR THR ARG THR GLN LEU PRO PRO A27 S31 F43 R44 V47 P57 V62 H66 ALA ILE HIS VAL SER GLY THR ASN GLY THR LYS ARG PHE ASP N81 E96 K97 S98

R102 I105 L110 D111 S112 K113 T114 Q115 S116 L117 N121 N122 N125 I128 K129 V130 C131 E132 N137 D138 L141 G142 V143 TYR TYR HIS ASN ASN LYS SER TRP MET GLU SER GLU PHE ARG VAL TYR SER SER ALA ASN N165 S172 GLN PRO PHE LEU MET ASP

LEU GLU GLY LYS GLN GLY ASN PHE K187 E191 D198 F201 S205 I210 N211 L212 V213 R214 D215 L216 P217 D228 L229 P230 I231 G232 I233 L241 L242 ALA LEU HIS ARG SER TYR LEU THR PRO GLY ASP SER SER GLY TRP THR ALA GLY ALA A264 R273

T299 V308 E309 K310 S316 N317 I326 V327 R328 F329 P330 N331 I332 T333 A344 T345 R346 F347 I358 Y365 Y369 N370 S371 A372 S373 F374 S375 C379 L387 F392 T393 N394 V395 R403 G404 D405 E406 V407 R408 G413 D420 Y421 N422 G431 C432

W436 N437 S438 N439 N440 L441 D442 S443 K444 V445 G446 G447 N448 Y449 L452 Y453 R454 L455 F456 R457 K458 S459 N460 D467 I468 S469 T470 E471 I472 Y473 Q474 A475 G476 S477 T478 P479 C480 N481 G482 V483 E484 G485 F486 N487 C488 Y489 F490 P491 L492 Q493 S494 Y495 G496 F497 Q498 P499 T500

N501 G502 V503 G504 Y505 Q506 R509 F515 E516 L517 L518 H519 A520 P521 A522 K529 L533 V534 V539 N540 F541 N544 G545 L546 E554 K557 I569 A570 D571 T572 T573 D574 A575 V576 R577 D578 P579 Q580 T581 L582 L585 D586 I587 T599 P600 G601 T602 V620

PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER THR GLY SER N641 V642 R646 I651 A668 T676 GLN THR ASN SER PRO GLY SER ALA SER SER VAL ALA SER Q690 N703 P715 S721 V722 I726 M731 V736 D737 C738

F759 L763 I770 Q774 Y789 K790 T791 P792 K795 F802 S803 Q804 I805 P809 K814 K825 V826 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN LYS PHE N856 L894 Q895

R905 L916 I923 Q935 A942 L959 I973 E988 Q992 L1004 Q1011 L1012 I1013 R1014 I1018 K1028 C1032 S1037 F1042 H1048 L1049 V1061 V1065 T1066 K1086 F1103 V1122 Q1142 L1145 D1146 S1147 PHE LYS GLU GLU LEU ASP

LYS TYR PHE LYS ASN HIS THR SER PRO 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 GLN GLY SER GLY TYR ILE

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

• **Molecule 2: Nanobody H11-B5**

Chain F:

GLN V2 Q3 L4 V5 E6 S7 G8 G9 G10 L11 M12 Q13 A14 G15 G16 S17 L18 R19 L20 S21 C22 A23 V24 S25 G26 R27 T28 F29 S30 T31 A32 A33 M34 G35 W36 F37 R38 Q39 A40 P41 G42 K43 E44 R45 E46 F47 V48 A49 A50 I51 R52 W53 S54 G55 G56 S57 A58 Y59 Y60

A61 D62 S63 V64 K65 G66 R67 F68 T69 I70 S71 R72 D73 K74 A75 K76 N77 T78 V79 Y80 L81 Q82 M83 N84 S85 L86 K87 Y88 E89 D90 T91 A92 V93 Y94 Y95 C96 A97 S98 Y99 Q100 A101 T102 R103 S104 L105 L106 S107 D108 Y109 A110 T111 W112 P113 Y114 D115 Y116 W117 G118 Q119 G120

T121 Q122 V123 T124 V125 S126 SER LYS HIS HIS HIS HIS HIS HIS

• Molecule 2: Nanobody H11-B5

93%

Chain D:

81% 12% • 7%

GLN V2 Q3 L4 V5 E6 S7 G8 G9 G10 L11 M12 Q13 A14 G15 G16 S17 L18 R19 L20 S21 C22 A23 V24 S25 G26 R27 T28 F29 S30 T31 A32 A33 M34 G35 W36 F37 R38 Q39 A40 P41 G42 K43 E44 R45 E46 F47 V48 A49 A50 I51 R52 W53 S54 G55 G56 S57 A58 Y59 Y60

A61 D62 S63 V64 K65 G66 R67 F68 T69 I70 S71 R72 D73 K74 A75 K76 N77 T78 V79 Y80 L81 Q82 M83 N84 S85 L86 K87 Y88 E89 D90 T91 A92 V93 Y94 Y95 C96 A97 S98 Y99 Q100 A101 T102 R103 S104 L105 L106 S107 D108 Y109 A110 T111 W112 P113 Y114 D115 Y116 W117 G118 Q119 G120

T121 Q122 V123 T124 V125 S126 SER LYS HIS HIS HIS HIS HIS HIS

• Molecule 2: Nanobody H11-B5

80%

Chain E:

78% 13% • 7%

GLN V2 Q3 L4 V5 E6 S7 G8 G9 G10 L11 M12 Q13 A14 G15 G16 S17 L18 R19 L20 S21 C22 A23 V24 S25 G26 R27 T28 F29 S30 T31 M34 G35 W36 F37 R38 Q39 A40 P41 G42 K43 E44 R45 E46 F47 V48 A49 A50 I51 R52 W53 S54 G55 G56 S57 A58 Y59 Y60 A61

D62 S63 V64 K65 G66 R67 F68 T69 I70 S71 R72 D73 K74 A75 K76 N77 T78 V79 Y80 L81 Q82 M83 N84 S85 L86 K87 Y88 E89 D90 T91 A92 V93 Y94 Y95 C96 A97 S98 Y99 Q100 A101 T102 L105 L106 S107 A110 T111 W112 P113 Y114 D115 Y116 W117 G118 Q119 G120 T121 Q122 V123

T124 V125 S126 SER LYS HIS HIS HIS HIS HIS HIS

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

100%

Chain G:

100%

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

50%

Chain H:

100%

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain U:

Chain V:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain V:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain W:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain X:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain Y:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain Z:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	318816	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.224	Depositor
Minimum map value	-0.159	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	275.59998, 275.59998, 275.59998	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/7818	0.52	0/10642
1	B	0.38	0/7849	0.52	0/10684
1	C	0.38	0/7831	0.52	1/10665 (0.0%)
2	D	0.26	0/1005	0.49	0/1360
2	E	0.27	0/1005	0.50	0/1360
2	F	0.27	0/1005	0.53	0/1360
All	All	0.37	0/26513	0.52	1/36071 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	110	LEU	CA-CB-CG	5.85	128.75	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	543	PHE	Peptide

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	7646	0	7408	88	0
1	B	7677	0	7463	86	0
1	C	7659	0	7429	93	0
2	D	976	0	936	10	0
2	E	976	0	936	14	0
2	F	976	0	936	14	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	1	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	1	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	1	0
3	Z	28	0	25	1	0
4	A	112	0	104	0	0
4	B	140	0	130	0	0
4	C	112	0	104	3	0
All	All	26834	0	25946	283	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 5.

The worst 5 of 283 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:B:64:TRP:HE1	1:B:264:ALA:HB1	1.48	0.76
1:C:393:THR:HG21	1:C:518:LEU:HB2	1.68	0.76
1:B:328:ARG:NH2	1:B:580:GLN:OE1	2.18	0.75
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.21	0.73
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.72	0.71

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	967/1260 (77%)	928 (96%)	38 (4%)	1 (0%)	51	83
1	B	974/1260 (77%)	938 (96%)	36 (4%)	0	100	100
1	C	974/1260 (77%)	937 (96%)	37 (4%)	0	100	100
2	D	125/134 (93%)	122 (98%)	3 (2%)	0	100	100
2	E	125/134 (93%)	122 (98%)	3 (2%)	0	100	100
2	F	125/134 (93%)	123 (98%)	2 (2%)	0	100	100
All	All	3290/4182 (79%)	3170 (96%)	119 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	528	LYS

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	844/1098 (77%)	837 (99%)	7 (1%)	81	92
1	B	847/1098 (77%)	845 (100%)	2 (0%)	93	97
1	C	843/1098 (77%)	838 (99%)	5 (1%)	86	94
2	D	100/107 (94%)	98 (98%)	2 (2%)	55	80
2	E	100/107 (94%)	97 (97%)	3 (3%)	41	71
2	F	100/107 (94%)	97 (97%)	3 (3%)	41	71
All	All	2834/3615 (78%)	2812 (99%)	22 (1%)	82	92

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	29	PHE
2	D	27	ARG
2	F	114	TYR
2	D	72	ARG
1	A	1107	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1048	HIS
1	C	901	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 ⓘ

40 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	#$|Z| > 2$
3	NAG	G	1	1,3	14,14,15	1.01	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	G	2	3	14,14,15	0.39	0	17,19,21	1.02	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.70	1 (7%)	17,19,21	0.59	0
3	NAG	H	2	3	14,14,15	0.47	0	17,19,21	0.92	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.41	0	17,19,21	0.81	1 (5%)
3	NAG	I	2	3	14,14,15	0.29	0	17,19,21	0.47	0
3	NAG	J	1	1,3	14,14,15	0.26	0	17,19,21	1.29	1 (5%)
3	NAG	J	2	3	14,14,15	0.69	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.55	0	17,19,21	0.85	1 (5%)
3	NAG	K	2	3	14,14,15	0.55	0	17,19,21	0.60	0
3	NAG	L	1	1,3	14,14,15	0.45	0	17,19,21	0.56	0
3	NAG	L	2	3	14,14,15	0.23	0	17,19,21	0.57	0
3	NAG	M	1	1,3	14,14,15	0.44	0	17,19,21	0.45	0
3	NAG	M	2	3	14,14,15	0.54	0	17,19,21	0.62	0
3	NAG	N	1	1,3	14,14,15	0.44	0	17,19,21	0.71	1 (5%)
3	NAG	N	2	3	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	O	1	1,3	14,14,15	0.30	0	17,19,21	1.10	1 (5%)
3	NAG	O	2	3	14,14,15	0.26	0	17,19,21	0.50	0
3	NAG	P	1	1,3	14,14,15	1.48	2 (14%)	17,19,21	0.85	1 (5%)
3	NAG	P	2	3	14,14,15	0.70	1 (7%)	17,19,21	0.96	2 (11%)
3	NAG	Q	1	1,3	14,14,15	0.50	0	17,19,21	0.69	1 (5%)
3	NAG	Q	2	3	14,14,15	0.52	0	17,19,21	0.53	0
3	NAG	R	1	1,3	14,14,15	0.51	0	17,19,21	0.41	0
3	NAG	R	2	3	14,14,15	0.44	0	17,19,21	0.69	1 (5%)
3	NAG	S	1	1,3	14,14,15	0.58	0	17,19,21	0.71	0
3	NAG	S	2	3	14,14,15	0.26	0	17,19,21	0.91	1 (5%)
3	NAG	T	1	1,3	14,14,15	0.87	1 (7%)	17,19,21	0.62	0
3	NAG	T	2	3	14,14,15	0.20	0	17,19,21	0.91	1 (5%)
3	NAG	U	1	1,3	14,14,15	0.66	1 (7%)	17,19,21	0.65	1 (5%)
3	NAG	U	2	3	14,14,15	0.38	0	17,19,21	0.69	0
3	NAG	V	1	1,3	14,14,15	0.28	0	17,19,21	0.76	1 (5%)
3	NAG	V	2	3	14,14,15	0.37	0	17,19,21	1.19	1 (5%)
3	NAG	W	1	1,3	14,14,15	0.46	0	17,19,21	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	W	2	3	14,14,15	0.42	0	17,19,21	0.93	1 (5%)
3	NAG	X	1	1,3	14,14,15	1.00	1 (7%)	17,19,21	1.39	2 (11%)
3	NAG	X	2	3	14,14,15	0.40	0	17,19,21	1.55	2 (11%)
3	NAG	Y	1	1,3	14,14,15	0.79	1 (7%)	17,19,21	0.68	0
3	NAG	Y	2	3	14,14,15	0.61	1 (7%)	17,19,21	0.42	0
3	NAG	Z	1	1,3	14,14,15	0.61	1 (7%)	17,19,21	0.93	2 (11%)
3	NAG	Z	2	3	14,14,15	0.42	0	17,19,21	0.63	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
3	NAG	G	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1	NAG	O5-C1	-4.86	1.35	1.43
3	G	1	NAG	O5-C1	-3.59	1.38	1.43
3	X	1	NAG	O5-C1	-3.18	1.38	1.43
3	T	1	NAG	O5-C1	-2.88	1.39	1.43
3	Y	1	NAG	O5-C1	-2.81	1.39	1.43

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	2	NAG	C1-O5-C5	5.66	119.86	112.19
3	J	1	NAG	C1-O5-C5	4.99	118.95	112.19
3	X	1	NAG	C1-O5-C5	4.39	118.14	112.19
3	V	2	NAG	C1-O5-C5	4.27	117.98	112.19
3	O	1	NAG	C1-O5-C5	4.03	117.65	112.19

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	2	NAG	C4-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	1	NAG	1	0
3	H	2	NAG	1	0
3	P	2	NAG	1	0
3	Y	1	NAG	1	0
3	Z	2	NAG	1	0
3	H	1	NAG	1	0
3	P	1	NAG	1	0
3	M	1	NAG	1	0

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 G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain O

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain P

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain Q

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain R

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain S

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain T

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain U

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain V

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain W

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain X

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain Y

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain Z

5.6 Ligand geometry ⓘ

26 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	$\#|Z| > 2$
4	NAG	A	1304	1	14,14,15	0.36	0	17,19,21	0.53	0
4	NAG	A	1305	1	14,14,15	0.59	0	17,19,21	0.64	1 (5%)
4	NAG	B	1307	1	14,14,15	0.65	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	B	1303	1	14,14,15	0.65	1 (7%)	17,19,21	1.93	1 (5%)
4	NAG	B	1301	1	14,14,15	0.83	1 (7%)	17,19,21	0.66	0
4	NAG	C	1407	1	14,14,15	0.23	0	17,19,21	1.03	1 (5%)
4	NAG	B	1310	1	14,14,15	0.28	0	17,19,21	0.38	0
4	NAG	B	1306	1	14,14,15	0.53	0	17,19,21	1.14	1 (5%)
4	NAG	C	1408	1	14,14,15	0.91	2 (14%)	17,19,21	1.69	1 (5%)
4	NAG	B	1304	1	14,14,15	0.29	0	17,19,21	0.61	1 (5%)
4	NAG	C	1403	1	14,14,15	0.35	0	17,19,21	0.73	1 (5%)
4	NAG	C	1404	1	14,14,15	0.42	0	17,19,21	0.78	1 (5%)
4	NAG	B	1305	1	14,14,15	0.55	0	17,19,21	0.69	0
4	NAG	C	1405	1	14,14,15	0.40	0	17,19,21	1.41	3 (17%)
4	NAG	C	1402	1	14,14,15	0.68	1 (7%)	17,19,21	1.42	1 (5%)
4	NAG	A	1303	1	14,14,15	0.49	0	17,19,21	1.42	1 (5%)
4	NAG	A	1306	1	14,14,15	0.37	0	17,19,21	0.67	1 (5%)
4	NAG	B	1308	1	14,14,15	0.32	0	17,19,21	1.08	1 (5%)
4	NAG	C	1401	1	14,14,15	0.45	0	17,19,21	0.99	1 (5%)
4	NAG	A	1302	1	14,14,15	0.72	1 (7%)	17,19,21	1.06	1 (5%)
4	NAG	A	1308	1	14,14,15	0.25	0	17,19,21	0.91	1 (5%)
4	NAG	C	1406	1	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
4	NAG	B	1302	1	14,14,15	0.35	0	17,19,21	0.88	1 (5%)
4	NAG	A	1301	1	14,14,15	0.68	0	17,19,21	0.75	1 (5%)
4	NAG	B	1309	1	14,14,15	0.20	0	17,19,21	0.66	1 (5%)
4	NAG	A	1307	1	14,14,15	0.41	0	17,19,21	0.83	1 (5%)

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	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1301	NAG	O5-C1	-2.92	1.39	1.43
4	A	1302	NAG	C1-C2	2.43	1.56	1.52
4	C	1408	NAG	C1-C2	2.38	1.55	1.52
4	B	1303	NAG	O5-C1	2.31	1.47	1.43
4	C	1408	NAG	O5-C1	2.30	1.47	1.43

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
4	B	1303	NAG	C1-O5-C5	7.67	122.58	112.19
4	C	1408	NAG	C1-O5-C5	6.80	121.41	112.19
4	A	1303	NAG	C1-O5-C5	5.61	119.79	112.19
4	C	1402	NAG	C1-O5-C5	5.45	119.58	112.19
4	C	1405	NAG	C2-N2-C7	4.39	129.15	122.90

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1403	NAG	O5-C5-C6-O6
4	C	1407	NAG	C4-C5-C6-O6
4	C	1403	NAG	C4-C5-C6-O6
4	C	1407	NAG	O5-C5-C6-O6
4	C	1402	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1404	NAG	2	0
4	C	1405	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-14543. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1   Orthogonal projections ⓘ
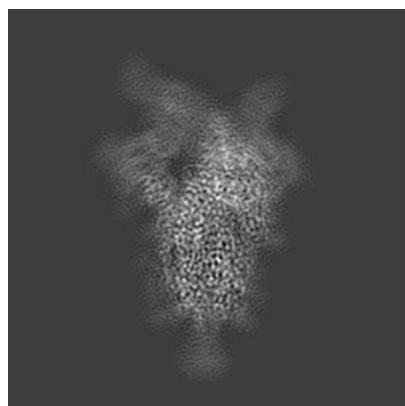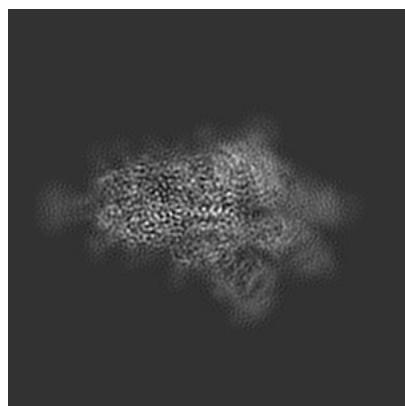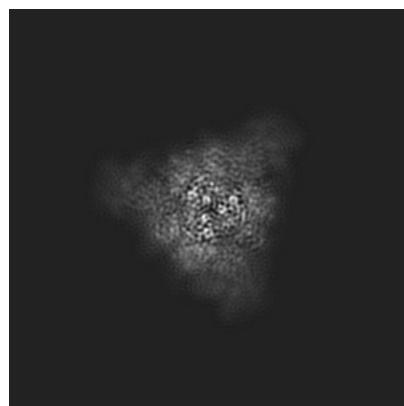
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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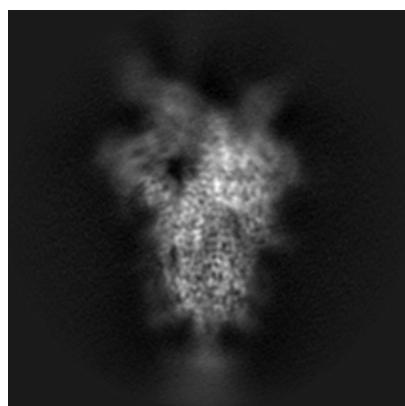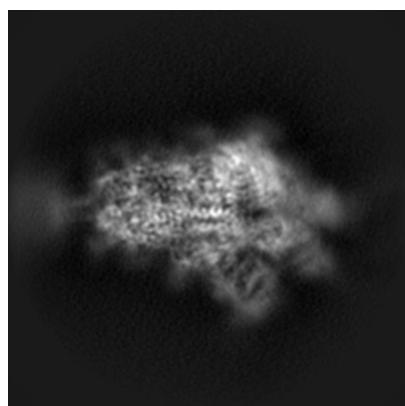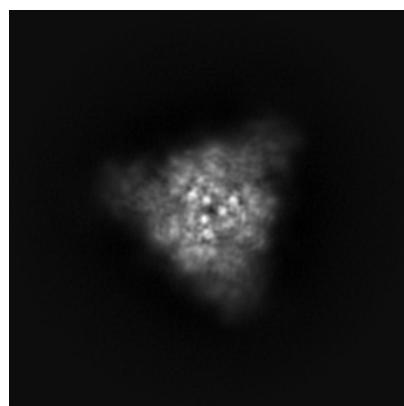
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
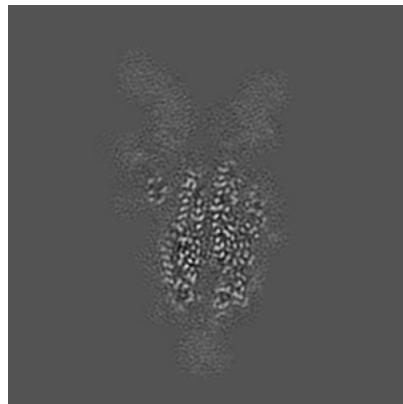
6.2.1 Primary map
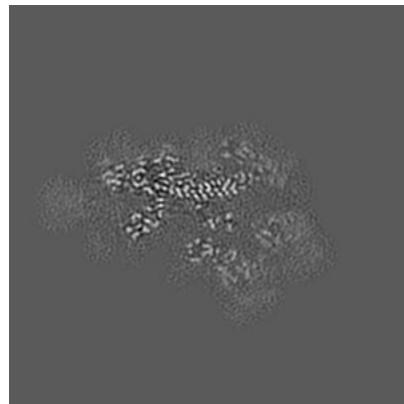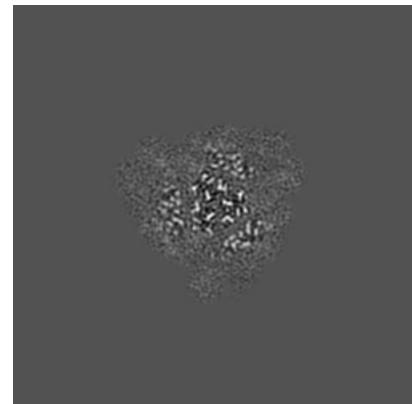
| X Index: 130 | Y Index: 130 | Z Index: 130 |

6.2.2 Raw map
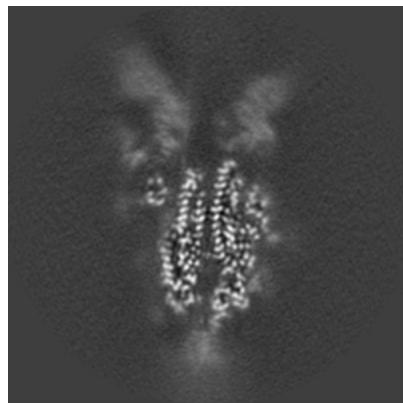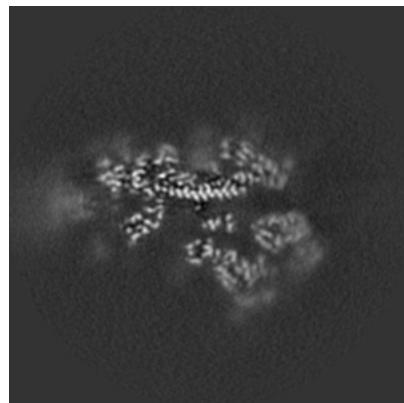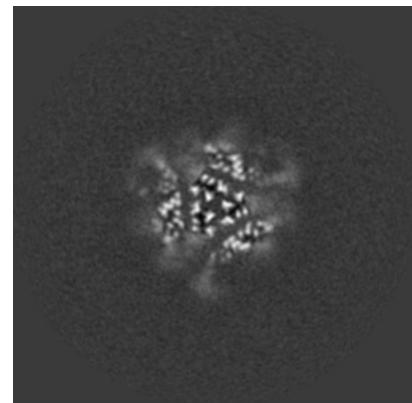
| X Index: 130 | Y Index: 130 | Z Index: 130 |

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
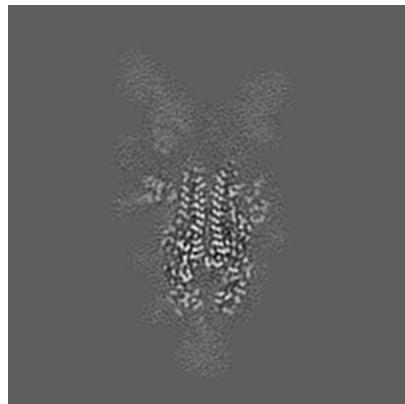
6.3.1 Primary map
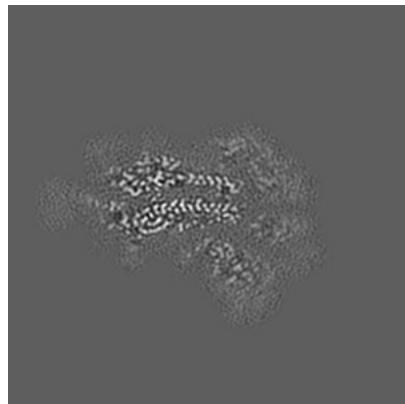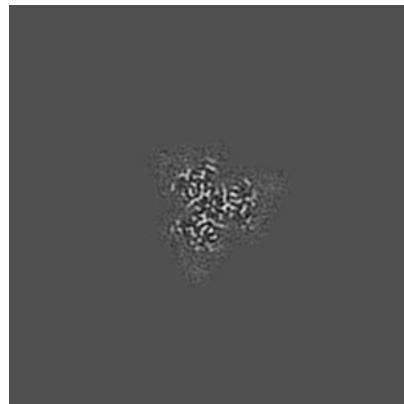
| X Index: 127 | Y Index: 136 | Z Index: 96 |

6.3.2 Raw map
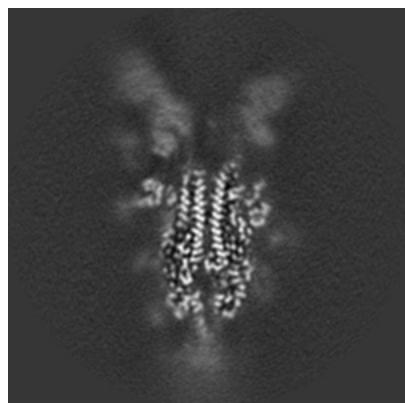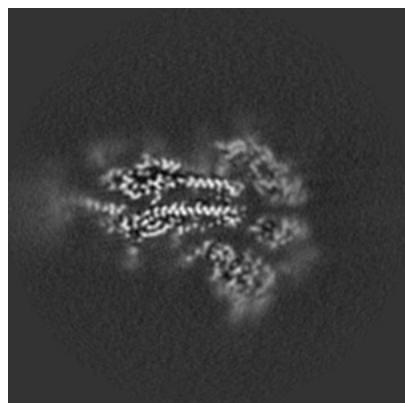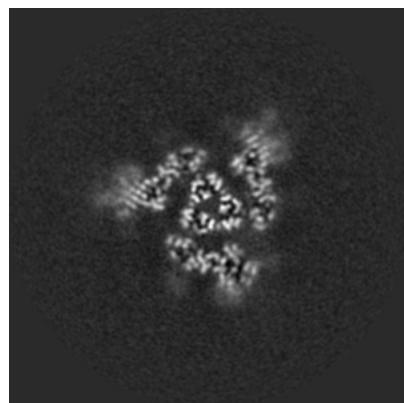
| X Index: 127 | Y Index: 136 | Z Index: 146 |

The images above show the largest variance slices of the map in three orthogonal directions.

6.4　Orthogonal surface views (i)

6.4.1　Primary map

X　　　　　　　　　　　Y　　　　　　　　　　　Z
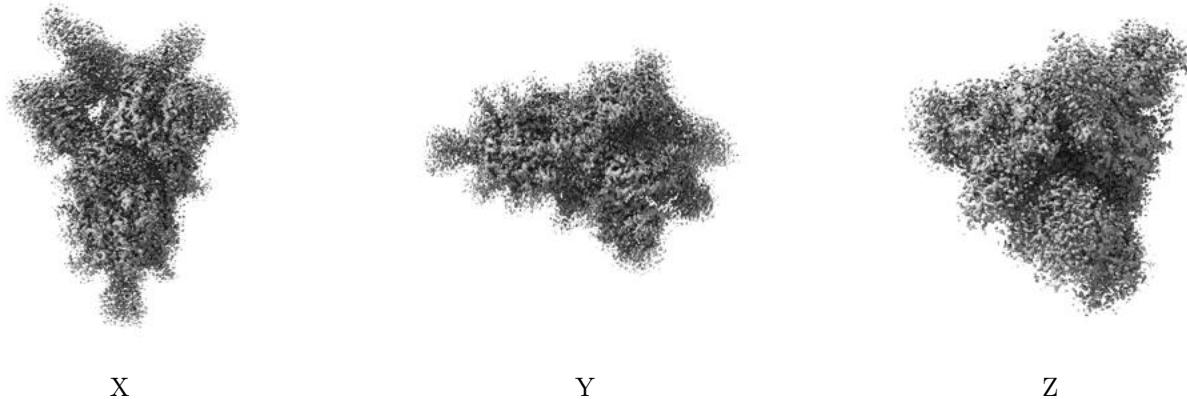
The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2　Raw map

X　　　　　　　　　　　Y　　　　　　　　　　　Z
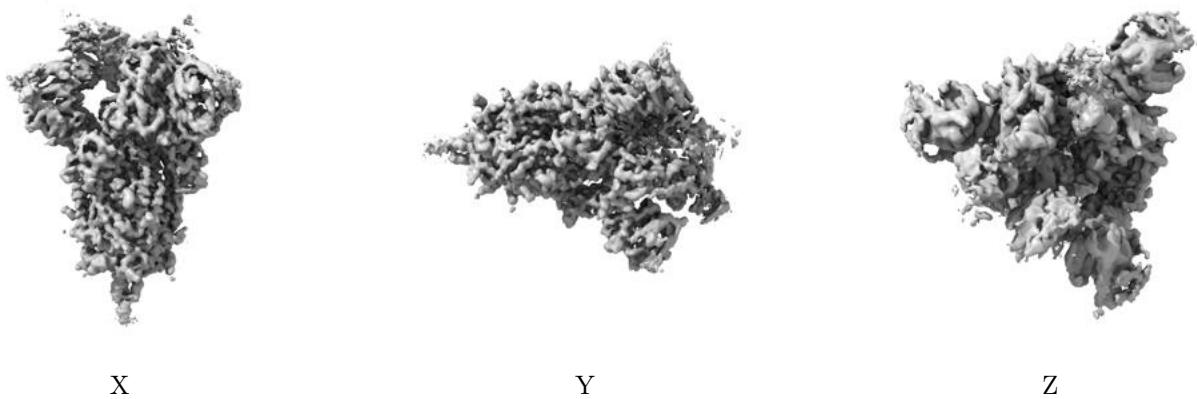
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.5.1 emd_14543_msk_1.map (i)

X   Y   Z
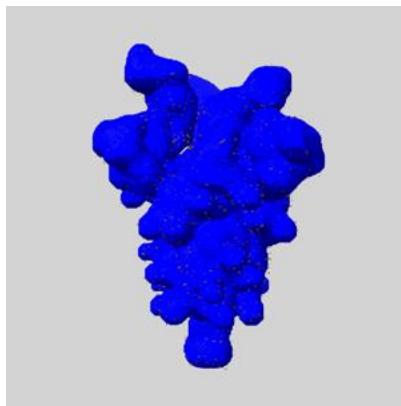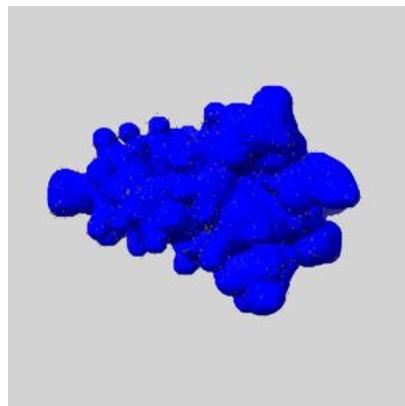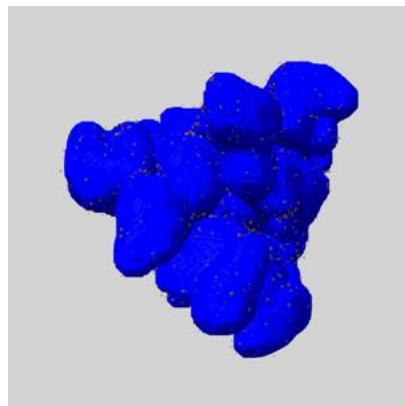
7 Map analysis ⓘ

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

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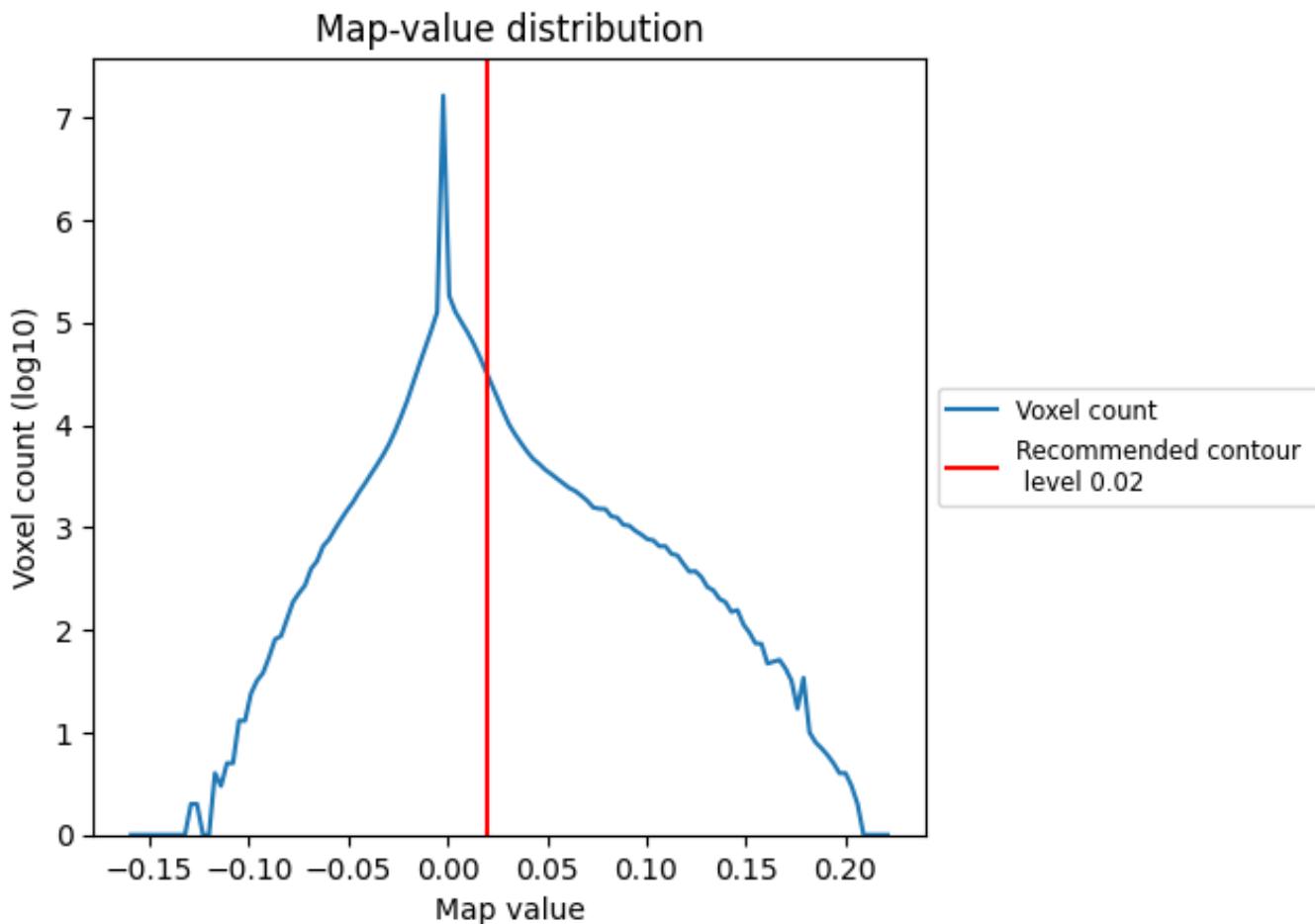
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
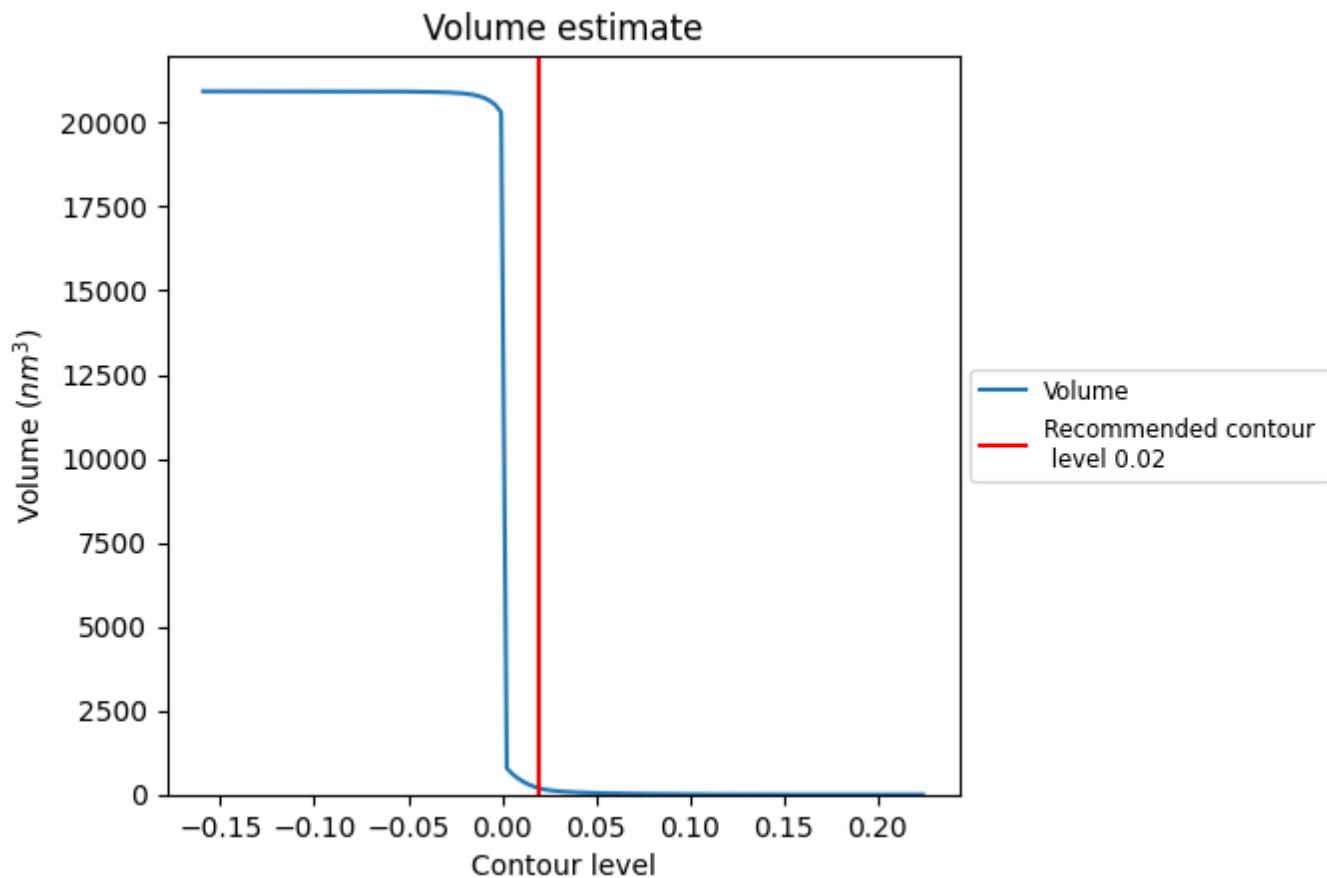
The volume at the recommended contour level is 189 nm^3; this corresponds to an approximate mass of 170 kDa.

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 ⓘ
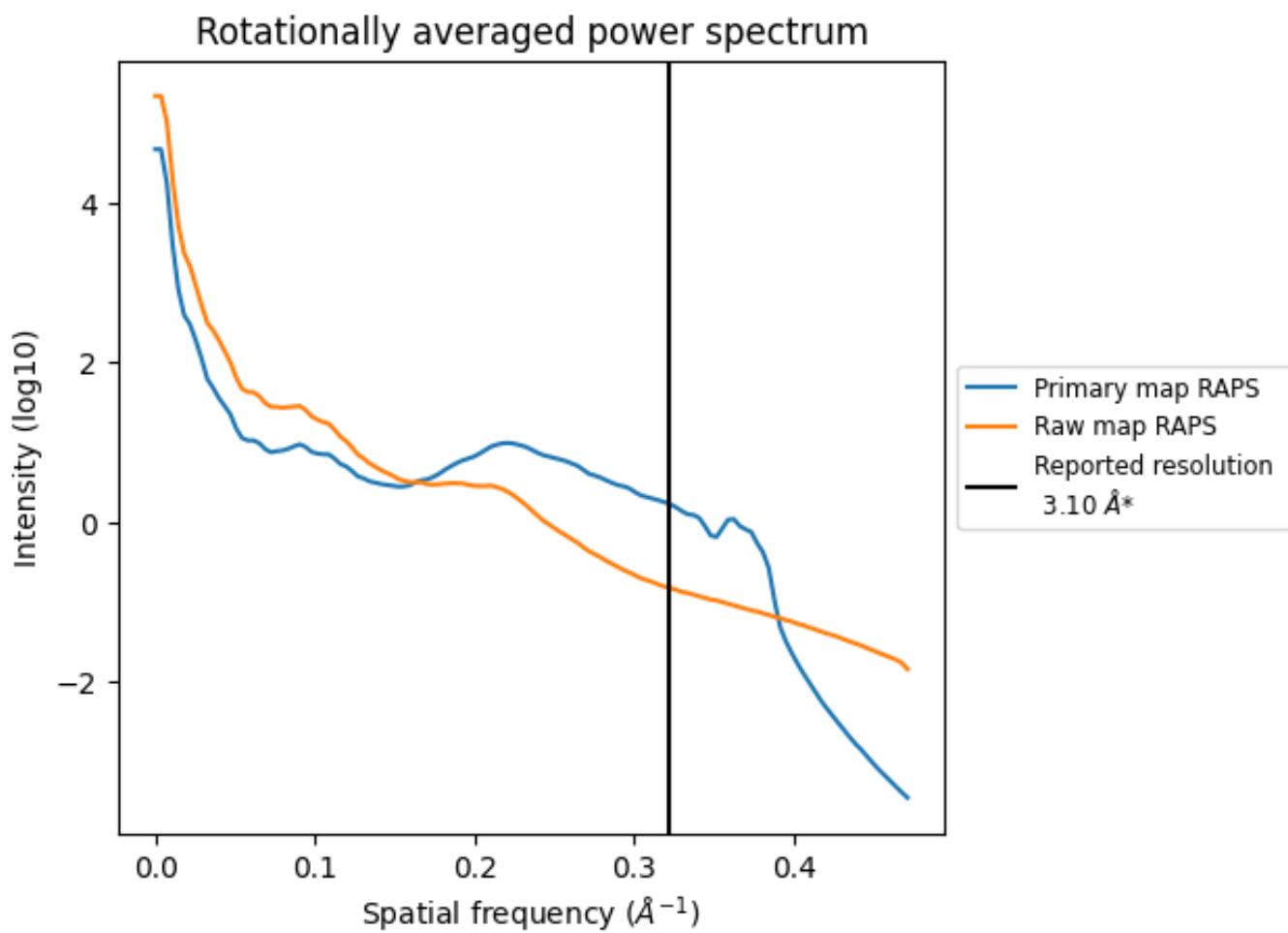
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ
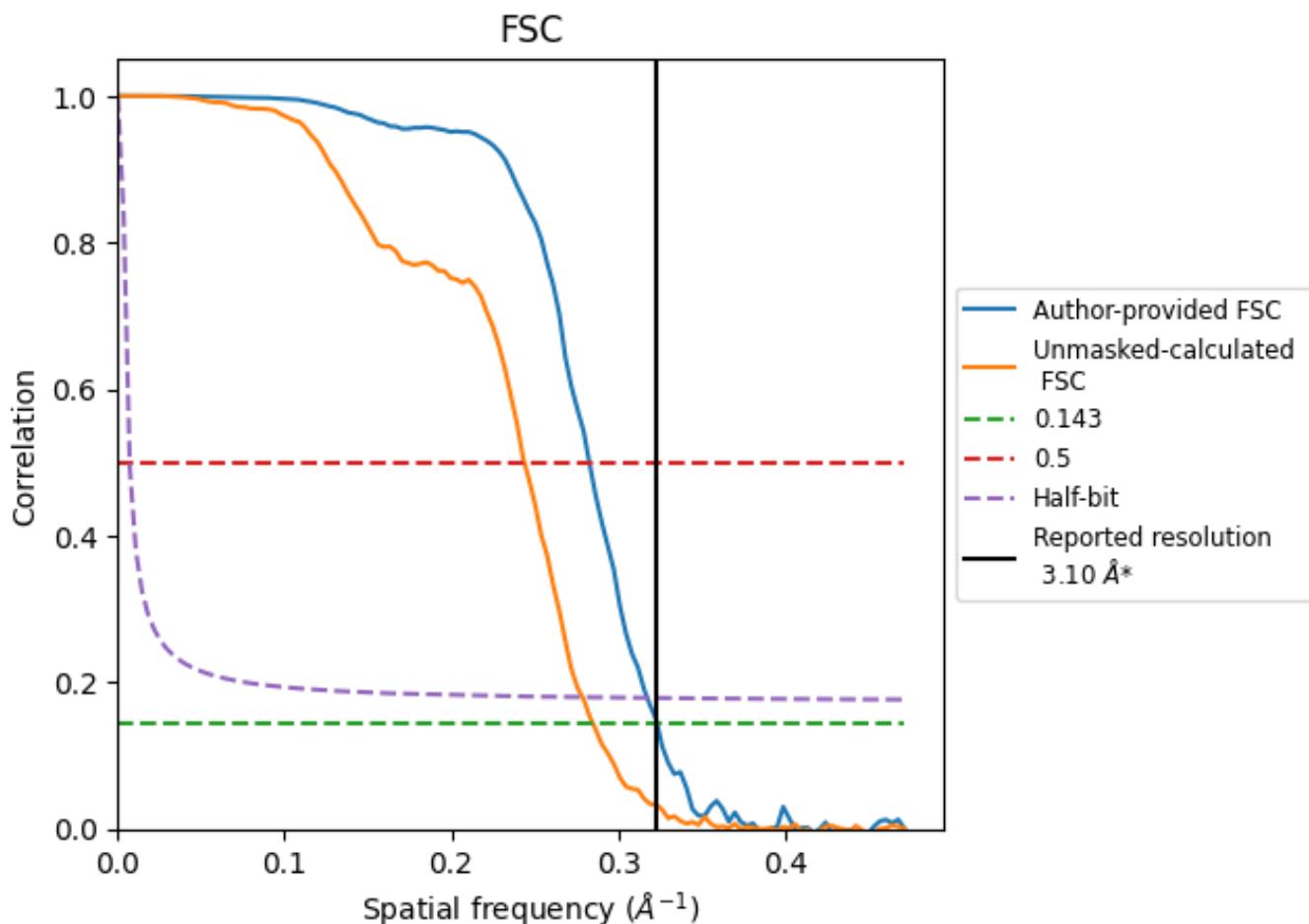
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.54	3.15
Unmasked-calculated*	3.51	4.10	3.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 3.1 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-14543 and PDB model 7Z85. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay ⓘ

| X | Y | Z |
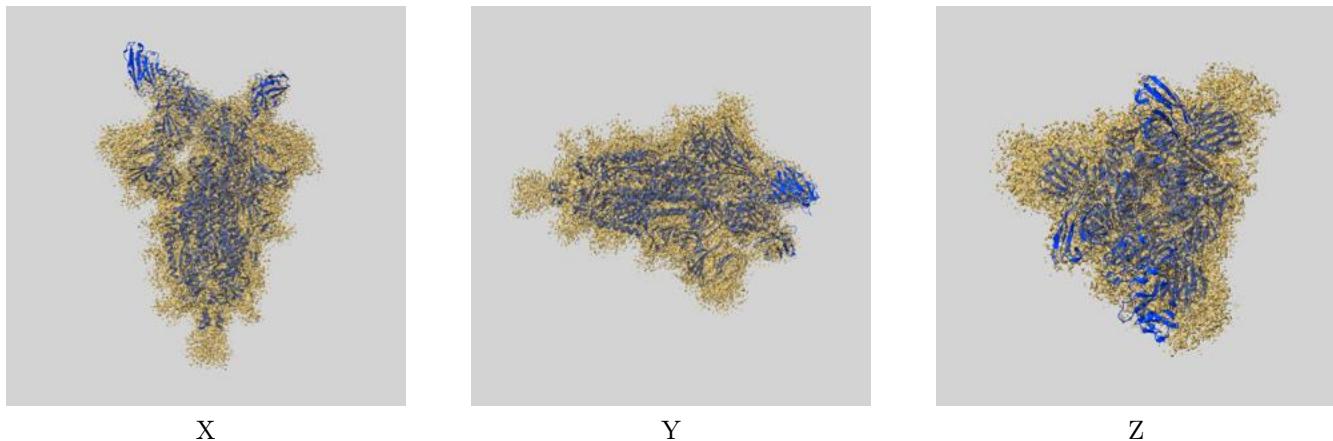
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z
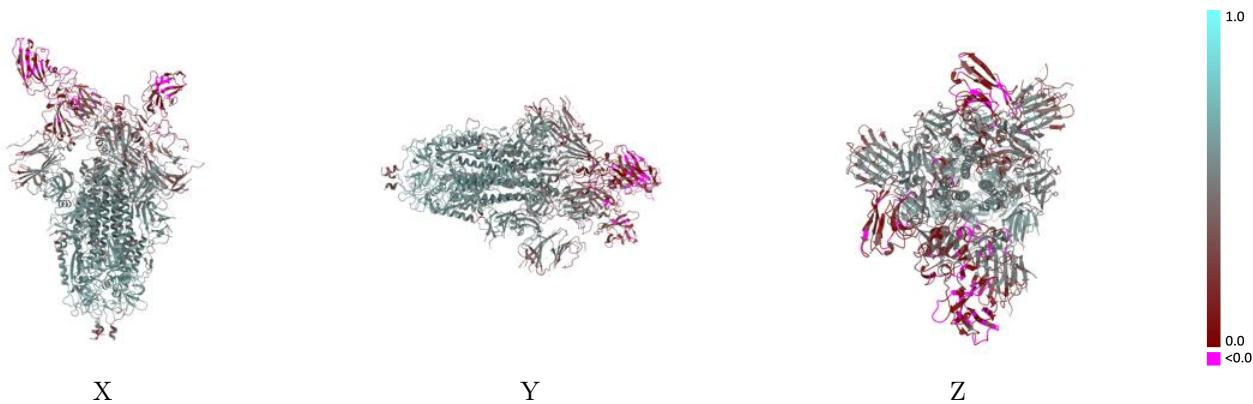
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ

X   Y   Z
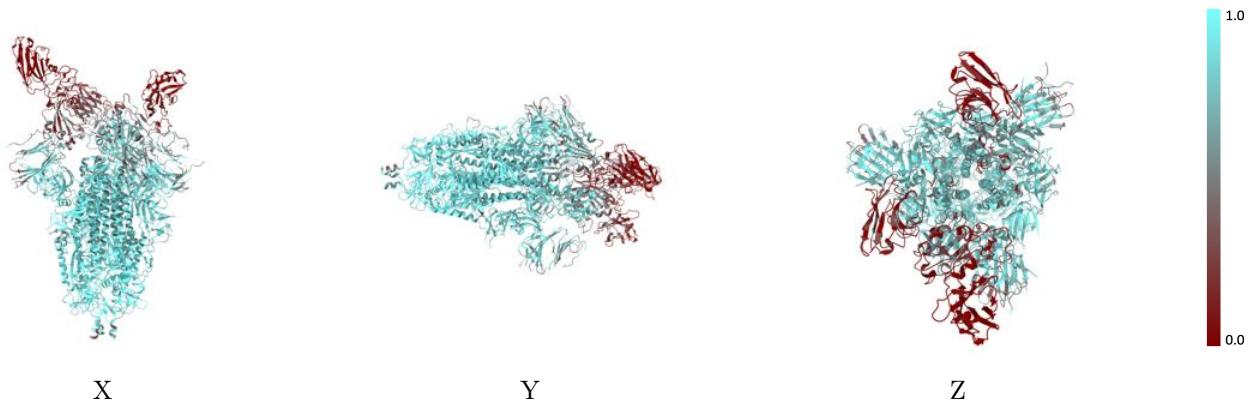
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4   Atom inclusion ⓘ
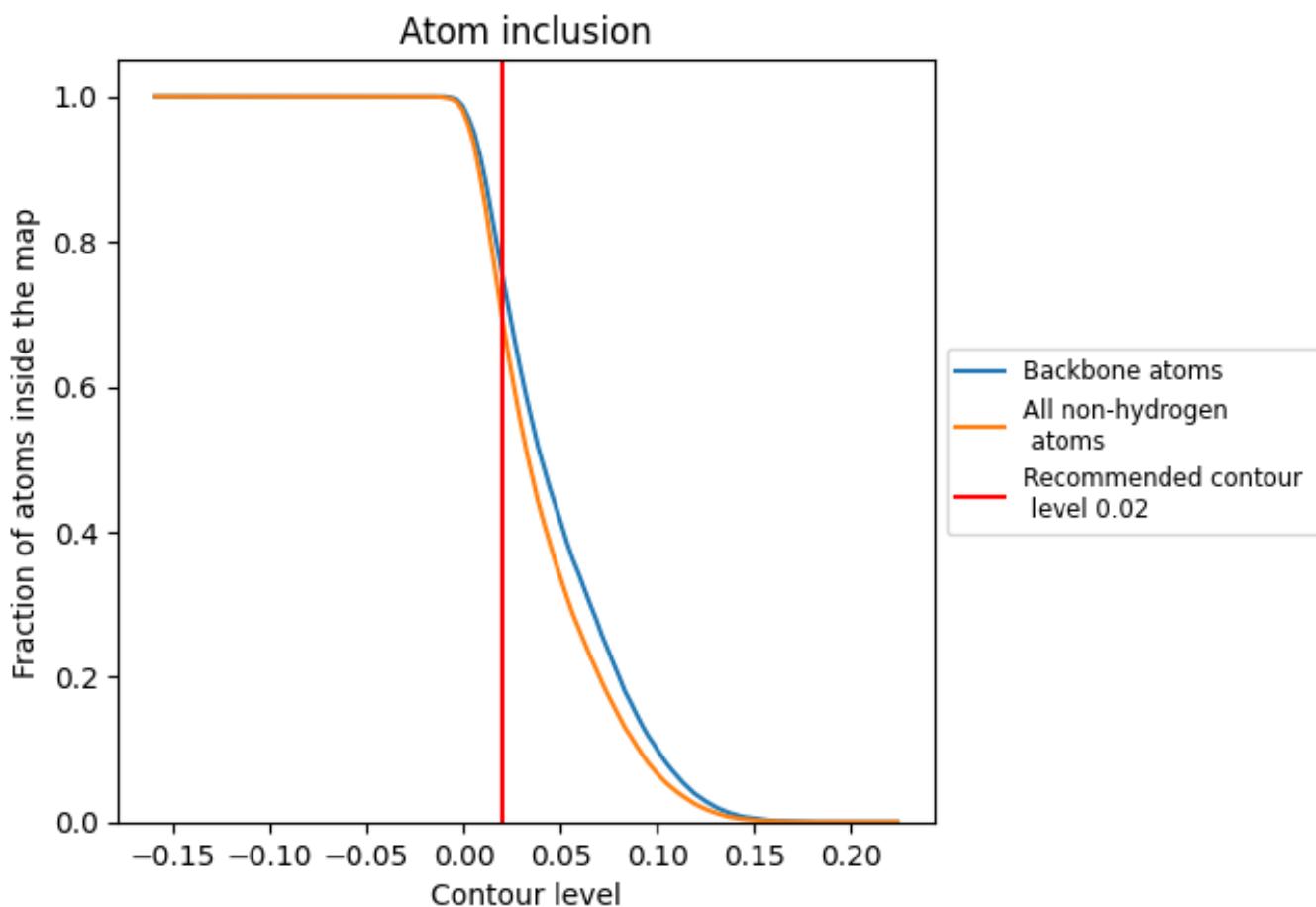
At the recommended contour level, 76% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6970	0.4470
A	0.7411	0.4730
B	0.7992	0.4980
C	0.7733	0.4880
D	0.0245	0.0800
E	0.2245	0.2070
F	0.0926	0.1200
G	0.2857	0.2080
H	0.3214	0.2920
I	0.4286	0.3890
J	0.4286	0.4370
K	0.8571	0.5130
L	0.7143	0.4270
M	0.6071	0.4180
N	0.6786	0.4770
O	0.8214	0.4610
P	0.7143	0.3540
Q	0.6786	0.4840
R	0.5714	0.3590
S	0.3214	0.3290
T	0.2500	0.2240
U	0.5357	0.4190
V	0.8571	0.5120
W	0.5714	0.3880
X	0.4643	0.4000
Y	0.8214	0.5100
Z	0.6786	0.4270

1.0

0.0
<0.0