Full wwPDB EM Validation Report ⓘ

Dec 31, 2024 – 09:24 PM EST

PDB ID	:	8PSD
EMDB ID	:	EMD-17850
Title	:	SARS-CoV-2 XBB 1.0 closed conformation.
Authors	:	Duhoo, Y.; Lau, K.
Deposited on	:	2023-07-13
Resolution	:	2.90 Å(reported)
Based on initial model	:	.

This is a Full wwPDB EM Validation 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:

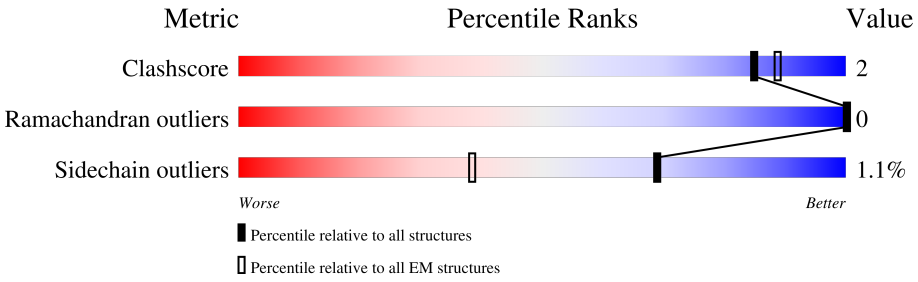
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	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	1204	79% 6% 15%
1	B	1204	79% 5% 16%
1	C	1204	81% 5% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 48535 atoms, of which 23966 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	C	1032	Total	C	H	N	O	S	0	0
			15987	5179	7894	1345	1534	35		
1	A	1027	Total	C	H	N	O	S	0	0
			15865	5135	7839	1333	1522	36		
1	B	1017	Total	C	H	N	O	S	0	0
			15711	5089	7765	1318	1504	35		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ILE	THR	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	24	SER	ALA	conflict	UNP P0DTC2
C	80	ALA	VAL	conflict	UNP P0DTC2
C	139	ASP	GLY	conflict	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	142	GLN	HIS	conflict	UNP P0DTC2
C	179	GLU	GLN	conflict	UNP P0DTC2
C	209	GLU	VAL	conflict	UNP P0DTC2
C	248	VAL	GLY	conflict	UNP P0DTC2
C	335	HIS	GLY	conflict	UNP P0DTC2
C	342	THR	ARG	conflict	UNP P0DTC2
C	364	ILE	LEU	conflict	UNP P0DTC2
C	367	PHE	SER	conflict	UNP P0DTC2
C	369	PRO	SER	conflict	UNP P0DTC2
C	371	PHE	SER	conflict	UNP P0DTC2
C	372	ALA	THR	conflict	UNP P0DTC2
C	401	ASN	ASP	conflict	UNP P0DTC2
C	404	SER	ARG	conflict	UNP P0DTC2
C	413	ASN	LYS	conflict	UNP P0DTC2
C	436	LYS	ASN	conflict	UNP P0DTC2
C	441	PRO	VAL	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	442	SER	GLY	conflict	UNP P0DTC2
C	456	LYS	ASN	conflict	UNP P0DTC2
C	473	ASN	SER	conflict	UNP P0DTC2
C	474	LYS	THR	conflict	UNP P0DTC2
C	480	ALA	GLU	conflict	UNP P0DTC2
C	482	SER	PHE	conflict	UNP P0DTC2
C	486	SER	PHE	conflict	UNP P0DTC2
C	494	ARG	GLN	conflict	UNP P0DTC2
C	497	TYR	ASN	conflict	UNP P0DTC2
C	501	HIS	TYR	conflict	UNP P0DTC2
C	610	GLY	ASP	conflict	UNP P0DTC2
C	651	TYR	HIS	conflict	UNP P0DTC2
C	675	LYS	ASN	conflict	UNP P0DTC2
C	677	HIS	PRO	conflict	UNP P0DTC2
C	678	GLY	ARG	conflict	UNP P0DTC2
C	679	SER	ARG	conflict	UNP P0DTC2
C	681	SER	ARG	conflict	UNP P0DTC2
C	760	LYS	ASN	conflict	UNP P0DTC2
C	792	TYR	ASP	conflict	UNP P0DTC2
C	950	HIS	GLN	conflict	UNP P0DTC2
C	965	LYS	ASN	conflict	UNP P0DTC2
C	982	PRO	LYS	conflict	UNP P0DTC2
C	983	PRO	VAL	conflict	UNP P0DTC2
C	1204	GLN	-	expression tag	UNP P0DTC2
A	19	ILE	THR	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	24	SER	ALA	conflict	UNP P0DTC2
A	80	ALA	VAL	conflict	UNP P0DTC2
A	139	ASP	GLY	conflict	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	142	GLN	HIS	conflict	UNP P0DTC2
A	179	GLU	GLN	conflict	UNP P0DTC2
A	209	GLU	VAL	conflict	UNP P0DTC2
A	248	VAL	GLY	conflict	UNP P0DTC2
A	335	HIS	GLY	conflict	UNP P0DTC2
A	342	THR	ARG	conflict	UNP P0DTC2
A	364	ILE	LEU	conflict	UNP P0DTC2
A	367	PHE	SER	conflict	UNP P0DTC2
A	369	PRO	SER	conflict	UNP P0DTC2
A	371	PHE	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	THR	conflict	UNP P0DTC2
A	401	ASN	ASP	conflict	UNP P0DTC2
A	404	SER	ARG	conflict	UNP P0DTC2
A	413	ASN	LYS	conflict	UNP P0DTC2
A	436	LYS	ASN	conflict	UNP P0DTC2
A	441	PRO	VAL	conflict	UNP P0DTC2
A	442	SER	GLY	conflict	UNP P0DTC2
A	456	LYS	ASN	conflict	UNP P0DTC2
A	473	ASN	SER	conflict	UNP P0DTC2
A	474	LYS	THR	conflict	UNP P0DTC2
A	480	ALA	GLU	conflict	UNP P0DTC2
A	482	SER	PHE	conflict	UNP P0DTC2
A	486	SER	PHE	conflict	UNP P0DTC2
A	494	ARG	GLN	conflict	UNP P0DTC2
A	497	TYR	ASN	conflict	UNP P0DTC2
A	501	HIS	TYR	conflict	UNP P0DTC2
A	610	GLY	ASP	conflict	UNP P0DTC2
A	651	TYR	HIS	conflict	UNP P0DTC2
A	675	LYS	ASN	conflict	UNP P0DTC2
A	677	HIS	PRO	conflict	UNP P0DTC2
A	678	GLY	ARG	conflict	UNP P0DTC2
A	679	SER	ARG	conflict	UNP P0DTC2
A	681	SER	ARG	conflict	UNP P0DTC2
A	760	LYS	ASN	conflict	UNP P0DTC2
A	792	TYR	ASP	conflict	UNP P0DTC2
A	950	HIS	GLN	conflict	UNP P0DTC2
A	965	LYS	ASN	conflict	UNP P0DTC2
A	982	PRO	LYS	conflict	UNP P0DTC2
A	983	PRO	VAL	conflict	UNP P0DTC2
A	1204	GLN	-	expression tag	UNP P0DTC2
B	19	ILE	THR	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	24	SER	ALA	conflict	UNP P0DTC2
B	80	ALA	VAL	conflict	UNP P0DTC2
B	139	ASP	GLY	conflict	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	142	GLN	HIS	conflict	UNP P0DTC2
B	179	GLU	GLN	conflict	UNP P0DTC2
B	209	GLU	VAL	conflict	UNP P0DTC2
B	248	VAL	GLY	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	335	HIS	GLY	conflict	UNP P0DTC2
B	342	THR	ARG	conflict	UNP P0DTC2
B	364	ILE	LEU	conflict	UNP P0DTC2
B	367	PHE	SER	conflict	UNP P0DTC2
B	369	PRO	SER	conflict	UNP P0DTC2
B	371	PHE	SER	conflict	UNP P0DTC2
B	372	ALA	THR	conflict	UNP P0DTC2
B	401	ASN	ASP	conflict	UNP P0DTC2
B	404	SER	ARG	conflict	UNP P0DTC2
B	413	ASN	LYS	conflict	UNP P0DTC2
B	436	LYS	ASN	conflict	UNP P0DTC2
B	441	PRO	VAL	conflict	UNP P0DTC2
B	442	SER	GLY	conflict	UNP P0DTC2
B	456	LYS	ASN	conflict	UNP P0DTC2
B	473	ASN	SER	conflict	UNP P0DTC2
B	474	LYS	THR	conflict	UNP P0DTC2
B	480	ALA	GLU	conflict	UNP P0DTC2
B	482	SER	PHE	conflict	UNP P0DTC2
B	486	SER	PHE	conflict	UNP P0DTC2
B	494	ARG	GLN	conflict	UNP P0DTC2
B	497	TYR	ASN	conflict	UNP P0DTC2
B	501	HIS	TYR	conflict	UNP P0DTC2
B	610	GLY	ASP	conflict	UNP P0DTC2
B	651	TYR	HIS	conflict	UNP P0DTC2
B	675	LYS	ASN	conflict	UNP P0DTC2
B	677	HIS	PRO	conflict	UNP P0DTC2
B	678	GLY	ARG	conflict	UNP P0DTC2
B	679	SER	ARG	conflict	UNP P0DTC2
B	681	SER	ARG	conflict	UNP P0DTC2
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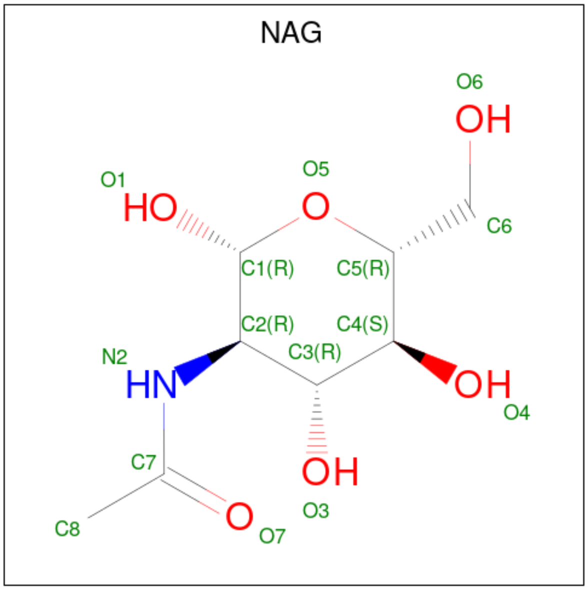
B	950	HIS	GLN	conflict	UNP P0DTC2
B	965	LYS	ASN	conflict	UNP P0DTC2
B	982	PRO	LYS	conflict	UNP P0DTC2
B	983	PRO	VAL	conflict	UNP P0DTC2
B	1204	GLN	-	expression tag	UNP P0DTC2

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



Mol	Chain	Residues	Atoms	AltConf
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	C	1	Total C H N O 27 8 13 1 5	0
2	A	1	Total C H N O 27 8 13 1 5	0

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 27	C 8	H 13	N 1	O 5	0
2	A	1	Total 27	C 8	H 13	N 1	O 5	0
2	A	1	Total 27	C 8	H 13	N 1	O 5	0
2	A	1	Total 27	C 8	H 13	N 1	O 5	0
2	A	1	Total 27	C 8	H 13	N 1	O 5	0
2	A	1	Total 27	C 8	H 13	N 1	O 5	0
2	A	1	Total 27	C 8	H 13	N 1	O 5	0
2	A	1	Total 27	C 8	H 13	N 1	O 5	0
2	A	1	Total 27	C 8	H 13	N 1	O 5	0
2	A	1	Total 27	C 8	H 13	N 1	O 5	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0
2	B	1	Total 27	C 8	H 13	N 1	O 5	0

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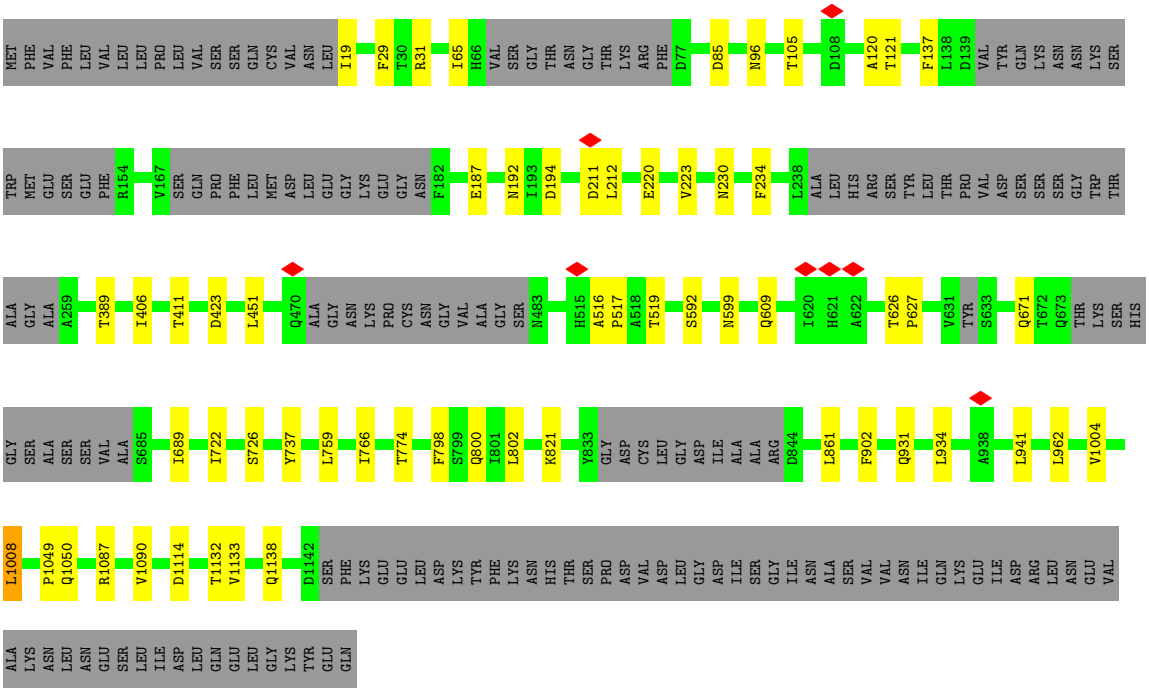
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	H	N	O	0
			27	8	13	1	5	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

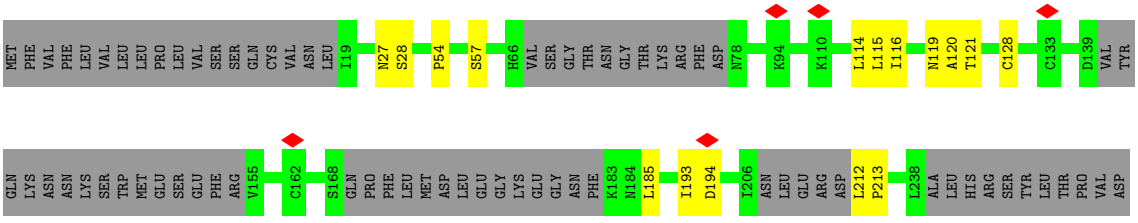
• Molecule 1: Spike glycoprotein

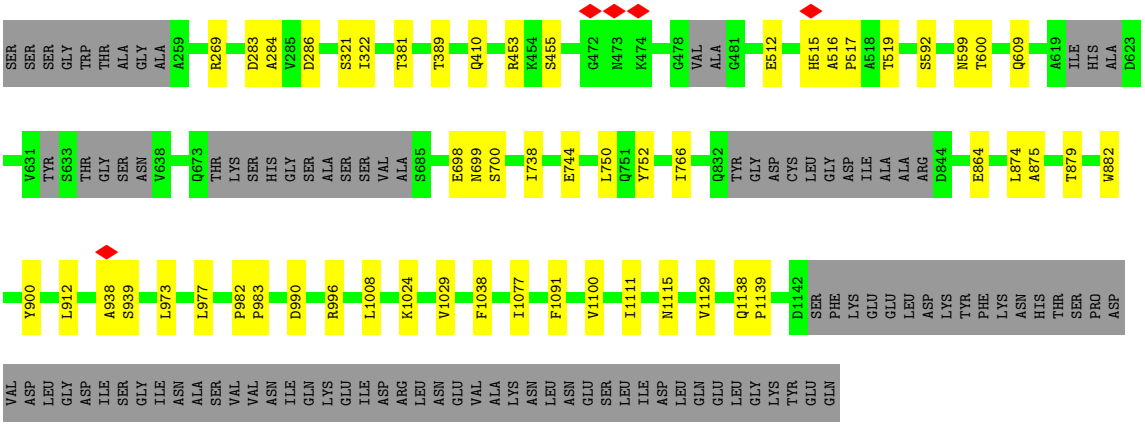
Chain C:



• Molecule 1: Spike glycoprotein

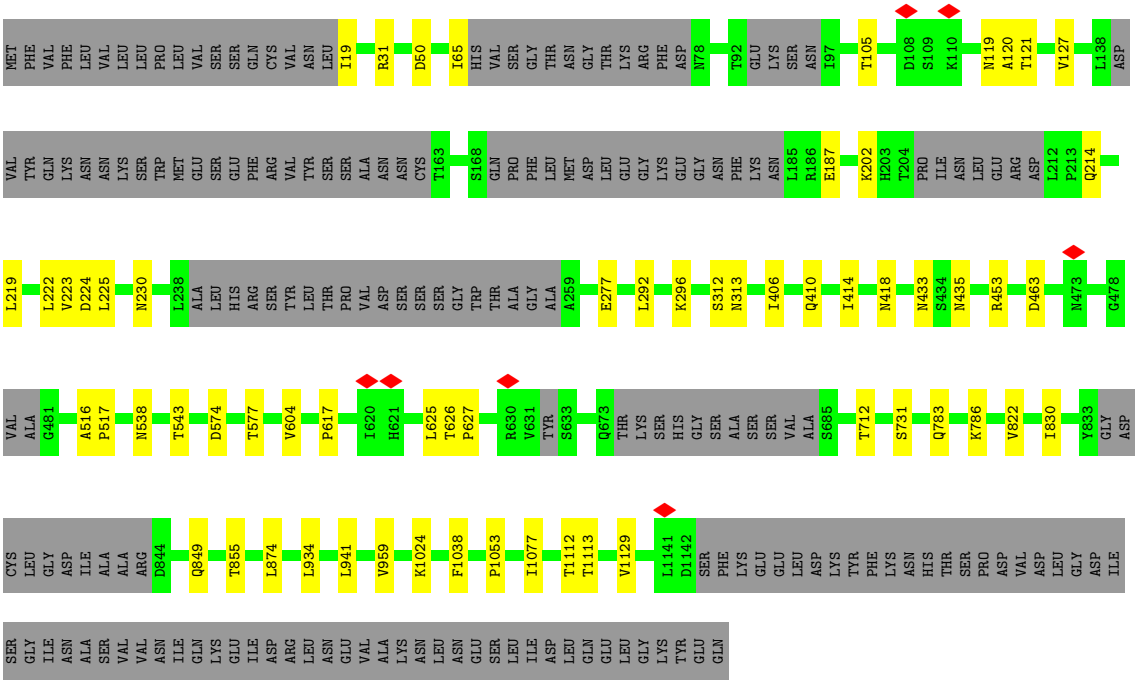
Chain A:





• Molecule 1: Spike glycoprotein

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65015	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.115	Depositor
Minimum map value	-1.245	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	456.51602, 456.51602, 456.51602	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2681, 1.2681, 1.2681	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	0.26	0/8210	0.47	0/11170
1	B	0.26	0/8130	0.47	0/11064
1	C	0.26	0/8281	0.47	0/11270
All	All	0.26	0/24621	0.47	0/33504

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	8026	7839	7854	35	0
1	B	7946	7765	7782	34	0
1	C	8093	7894	7916	29	0
2	A	154	143	143	3	0
2	B	168	156	156	5	0
2	C	182	169	169	3	0
All	All	24569	23966	24020	104	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 2.

All (104) 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:269:ARG:NH1	1:A:286:ASP:OD2	2.22	0.72
1:C:19:ILE:N	1:C:65:ILE:O	2.23	0.71
2:A:1306:NAG:H83	2:A:1306:NAG:H3	1.74	0.69
1:A:120:ALA:O	1:A:121:THR:OG1	2.07	0.69
2:C:1307:NAG:H83	2:C:1307:NAG:H3	1.73	0.69
1:B:119:ASN:OD1	1:B:120:ALA:N	2.26	0.69
1:C:766:ILE:HD11	1:C:1008:LEU:HD12	1.75	0.69
1:A:119:ASN:OD1	1:A:120:ALA:N	2.27	0.67
1:A:752:TYR:OH	1:A:990:ASP:OD1	2.12	0.67
1:B:214:GLN:N	1:B:214:GLN:OE1	2.27	0.67
1:C:220:GLU:OE1	1:C:220:GLU:N	2.29	0.65
1:C:31:ARG:NH1	1:C:187:GLU:OE2	2.29	0.65
1:B:120:ALA:O	1:B:121:THR:OG1	2.12	0.64
2:B:1304:NAG:O3	2:B:1304:NAG:O7	2.14	0.64
1:A:698:GLU:OE2	1:B:786:LYS:NZ	2.26	0.63
1:A:389:THR:O	1:A:519:THR:OG1	2.16	0.63
1:C:411:THR:HG22	1:A:381:THR:HB	1.83	0.61
2:B:1307:NAG:C1	2:B:1307:NAG:H82	2.31	0.60
1:B:230:ASN:OD1	2:B:1302:NAG:O4	2.07	0.60
1:B:453:ARG:NH1	1:B:463:ASP:OD2	2.36	0.58
1:C:120:ALA:O	1:C:121:THR:OG1	2.14	0.57
1:B:202:LYS:HB3	1:B:219:LEU:HD22	1.88	0.56
1:B:277:GLU:N	1:B:277:GLU:OE1	2.38	0.56
1:C:1087:ARG:NH1	1:C:1114:ASP:O	2.40	0.55
1:A:875:ALA:O	1:A:879:THR:HG22	2.07	0.55
1:C:798:PHE:O	1:C:802:LEU:HD23	2.07	0.55
1:A:699:ASN:OD1	1:A:700:SER:N	2.41	0.53
1:A:864:GLU:OE1	1:A:864:GLU:N	2.39	0.52
2:B:1307:NAG:C1	2:B:1307:NAG:C8	2.87	0.52
1:A:27:ASN:OD1	1:A:28:SER:N	2.44	0.50
1:A:1138:GLN:HB2	1:A:1139:PRO:HD3	1.93	0.50
1:A:699:ASN:ND2	1:B:783:GLN:OE1	2.42	0.50
1:C:211:ASP:OD1	1:C:212:LEU:N	2.44	0.50
1:C:821:LYS:NZ	1:C:934:LEU:O	2.36	0.49
1:C:1138:GLN:OE1	1:C:1138:GLN:N	2.44	0.49
1:C:96:ASN:O	1:C:96:ASN:ND2	2.44	0.49
1:A:592:SER:OG	1:A:609:GLN:OE1	2.29	0.49
1:B:1112:THR:HG22	1:B:1113:THR:H	1.76	0.49
1:B:105:THR:OG1	1:B:230:ASN:O	2.30	0.49
1:C:406:ILE:HG22	1:C:406:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:LEU:HD22	1:C:1004:VAL:HG21	1.94	0.49
1:B:1024:LYS:NZ	1:B:1038:PHE:O	2.45	0.48
1:A:453:ARG:NE	1:A:455:SER:O	2.45	0.48
1:B:617:PRO:HB2	1:B:625:LEU:HD11	1.95	0.48
1:B:222:LEU:HG	1:B:223:VAL:N	2.29	0.48
1:B:712:THR:HG22	1:B:712:THR:O	2.13	0.47
1:A:283:ASP:OD1	1:A:284:ALA:N	2.47	0.47
1:A:1024:LYS:NZ	1:A:1038:PHE:O	2.47	0.47
1:B:1077:ILE:HG22	1:B:1129:VAL:CG2	2.45	0.47
1:C:592:SER:OG	1:C:609:GLN:OE1	2.30	0.47
1:A:512:GLU:OE1	1:A:515:HIS:NE2	2.48	0.47
1:C:105:THR:OG1	1:C:230:ASN:O	2.33	0.46
1:B:941:LEU:N	1:B:941:LEU:HD12	2.30	0.46
1:A:766:ILE:HD11	1:A:1008:LEU:HD23	1.97	0.46
1:C:389:THR:O	1:C:519:THR:OG1	2.30	0.46
1:B:31:ARG:NH2	1:B:187:GLU:OE2	2.40	0.46
1:A:744:GLU:OE1	1:A:744:GLU:N	2.44	0.46
1:A:114:LEU:HD23	1:A:115:LEU:N	2.31	0.45
1:A:738:ILE:O	1:A:996:ARG:NH1	2.50	0.45
1:A:1100:VAL:HG23	1:A:1111:ILE:HG12	1.98	0.45
1:B:202:LYS:CB	1:B:219:LEU:HD22	2.46	0.45
1:A:1077:ILE:HD13	1:A:1129:VAL:CG2	2.46	0.45
1:B:406:ILE:HG22	1:B:406:ILE:O	2.17	0.45
1:B:822:VAL:HG13	1:B:1053:PRO:HG2	1.98	0.45
1:C:726:SER:OG	1:C:774:THR:OG1	2.34	0.45
1:B:538:ASN:ND2	1:B:543:THR:HG22	2.30	0.45
1:B:19:ILE:N	1:B:65:ILE:O	2.50	0.44
1:B:414:ILE:HD13	1:B:418:ASN:HD22	1.82	0.44
1:A:599:ASN:OD1	1:A:600:THR:N	2.50	0.44
2:C:1307:NAG:H3	2:C:1307:NAG:C8	2.46	0.44
1:B:433:ASN:OD1	1:B:435:ASN:N	2.50	0.44
1:A:973:LEU:O	1:A:977:LEU:HD23	2.18	0.44
1:C:737:TYR:CE1	1:C:962:LEU:HD13	2.53	0.43
1:A:1115:ASN:OD1	1:A:1115:ASN:N	2.52	0.43
1:B:292:LEU:HD11	1:B:296:LYS:HE3	2.01	0.43
1:B:223:VAL:HG22	1:B:225:LEU:CD1	2.48	0.43
1:A:1091:PHE:CE1	1:A:1100:VAL:HG22	2.53	0.43
2:A:1306:NAG:H3	2:A:1306:NAG:C8	2.48	0.43
1:B:127:VAL:O	1:B:127:VAL:HG12	2.19	0.43
2:B:1307:NAG:H83	2:B:1307:NAG:H3	2.01	0.43
1:C:85:ASP:OD1	1:C:85:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1132:THR:HG22	1:C:1133:VAL:N	2.34	0.42
1:C:800:GLN:OE1	1:C:931:GLN:NE2	2.53	0.42
1:B:312:SER:OG	1:B:313:ASN:N	2.53	0.42
1:B:849:GLN:HG2	1:B:959:VAL:HG21	2.01	0.42
1:C:766:ILE:HD11	1:C:1008:LEU:CD1	2.46	0.42
1:A:212:LEU:N	1:A:213:PRO:HD2	2.35	0.42
1:A:54:PRO:O	1:A:57:SER:OG	2.33	0.42
2:C:1306:NAG:O7	2:C:1306:NAG:O3	2.33	0.42
1:B:731:SER:OG	1:B:855:THR:OG1	2.38	0.42
1:C:722:ILE:HD13	1:C:941:LEU:HD23	2.01	0.41
1:C:626:THR:HB	1:C:627:PRO:HD3	2.03	0.41
1:B:574:ASP:OD2	1:B:577:THR:HG22	2.21	0.41
1:C:516:ALA:HB1	1:C:517:PRO:HD2	2.03	0.41
1:C:1049:PRO:O	1:C:1050:GLN:NE2	2.52	0.41
1:B:626:THR:HB	1:B:627:PRO:HD3	2.03	0.41
1:C:1090:VAL:HG11	1:A:900:TYR:OH	2.21	0.41
1:A:321:SER:C	1:A:322:ILE:HD12	2.41	0.41
1:B:516:ALA:HB1	1:B:517:PRO:HD2	2.03	0.40
1:A:516:ALA:HB1	1:A:517:PRO:HD2	2.03	0.40
1:A:938:ALA:O	1:A:939:SER:OG	2.31	0.40
1:A:982:PRO:N	1:A:983:PRO:CD	2.84	0.40
1:C:671:GLN:HG3	1:C:689:ILE:HD11	2.02	0.40
2:A:1306:NAG:H82	2:A:1306:NAG:C1	2.51	0.40

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	1007/1204 (84%)	971 (96%)	36 (4%)	0	100	100
1	B	999/1204 (83%)	953 (95%)	46 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1016/1204 (84%)	968 (95%)	48 (5%)	0	100	100
All	All	3022/3612 (84%)	2892 (96%)	130 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	897/1050 (85%)	886 (99%)	11 (1%)	67	89
1	B	886/1050 (84%)	879 (99%)	7 (1%)	79	93
1	C	904/1050 (86%)	892 (99%)	12 (1%)	65	88
All	All	2687/3150 (85%)	2657 (99%)	30 (1%)	69	90

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	PHE
1	C	137	PHE
1	C	192	ASN
1	C	194	ASP
1	C	223	VAL
1	C	234	PHE
1	C	423	ASP
1	C	451	LEU
1	C	599	ASN
1	C	861	LEU
1	C	902	PHE
1	C	1008	LEU
1	A	116	ILE
1	A	128	CYS
1	A	185	LEU
1	A	193	ILE
1	A	194	ASP

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Mol	Chain	Res	Type
1	A	410	GLN
1	A	750	LEU
1	A	874	LEU
1	A	882	TRP
1	A	912	LEU
1	A	1029	VAL
1	B	50	ASP
1	B	224	ASP
1	B	410	GLN
1	B	604	VAL
1	B	830	ILE
1	B	874	LEU
1	B	934	LEU

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

Mol	Chain	Res	Type
1	A	203	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

36 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	$\#\|Z\| > 2$
2	NAG	C	1311	1	14,14,15	0.22	0	17,19,21	0.47	0
2	NAG	C	1309	-	14,14,15	0.19	0	17,19,21	0.44	0
2	NAG	A	1311	1	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	C	1313	-	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	C	1312	1	14,14,15	0.53	0	17,19,21	1.19	1 (5%)
2	NAG	A	1302	1	14,14,15	0.19	0	17,19,21	0.40	0
2	NAG	A	1305	1	14,14,15	0.22	0	17,19,21	0.47	0
2	NAG	C	1302	-	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.58	0
2	NAG	A	1304	1	14,14,15	0.23	0	17,19,21	0.48	0
2	NAG	A	1307	1	14,14,15	0.24	0	17,19,21	0.53	0
2	NAG	B	1312	1	14,14,15	0.24	0	17,19,21	0.52	0
2	NAG	A	1310	1	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	B	1309	1	14,14,15	0.18	0	17,19,21	0.52	0
2	NAG	C	1304	1	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	B	1303	1	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.48	0
2	NAG	C	1310	1	14,14,15	0.26	0	17,19,21	0.60	0
2	NAG	B	1305	1	14,14,15	0.18	0	17,19,21	0.50	0
2	NAG	C	1306	1	14,14,15	0.30	0	17,19,21	0.45	0
2	NAG	A	1306	1	14,14,15	0.25	0	17,19,21	0.98	1 (5%)
2	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	C	1301	1	14,14,15	0.21	0	17,19,21	0.56	0
2	NAG	A	1301	1	14,14,15	0.26	0	17,19,21	0.53	0
2	NAG	C	1305	1	14,14,15	0.23	0	17,19,21	0.54	0
2	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.45	0
2	NAG	B	1311	-	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	A	1303	1	14,14,15	0.19	0	17,19,21	0.47	0
2	NAG	C	1307	1	14,14,15	0.24	0	17,19,21	0.93	1 (5%)
2	NAG	B	1304	1	14,14,15	0.30	0	17,19,21	0.43	0
2	NAG	B	1301	1	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	A	1308	-	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	B	1302	-	14,14,15	0.42	0	17,19,21	0.79	1 (5%)
2	NAG	B	1307	1	14,14,15	0.28	0	17,19,21	0.91	1 (5%)
2	NAG	B	1310	1	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	B	1308	1	14,14,15	0.29	0	17,19,21	0.54	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
2	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1309	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1313	-	-	2/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1302	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1312	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1310	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	6/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1311	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	6/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1308	-	-	4/6/23/26	0/1/1/1
2	NAG	B	1302	-	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1307	1	-	5/6/23/26	0/1/1/1
2	NAG	B	1310	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1312	NAG	C1-O5-C5	4.60	118.35	112.19
2	C	1307	NAG	C2-N2-C7	2.94	126.83	122.90
2	A	1306	NAG	C2-N2-C7	2.91	126.80	122.90
2	B	1302	NAG	C1-O5-C5	2.87	116.03	112.19
2	B	1307	NAG	C2-N2-C7	2.73	126.56	122.90

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1304	NAG	C1-C2-N2-C7
2	B	1302	NAG	C1-C2-N2-C7
2	B	1307	NAG	C1-C2-N2-C7
2	A	1304	NAG	C4-C5-C6-O6
2	B	1308	NAG	C4-C5-C6-O6
2	A	1303	NAG	C4-C5-C6-O6
2	C	1309	NAG	O5-C5-C6-O6
2	C	1306	NAG	O5-C5-C6-O6
2	A	1302	NAG	O5-C5-C6-O6
2	C	1308	NAG	C4-C5-C6-O6
2	C	1313	NAG	C4-C5-C6-O6
2	A	1301	NAG	O5-C5-C6-O6
2	A	1305	NAG	O5-C5-C6-O6
2	B	1303	NAG	O5-C5-C6-O6
2	B	1306	NAG	O5-C5-C6-O6
2	A	1302	NAG	C4-C5-C6-O6
2	C	1307	NAG	O5-C5-C6-O6
2	C	1305	NAG	O5-C5-C6-O6
2	B	1306	NAG	C4-C5-C6-O6
2	B	1302	NAG	O5-C5-C6-O6
2	A	1304	NAG	O5-C5-C6-O6
2	B	1307	NAG	O5-C5-C6-O6
2	B	1308	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	1306	NAG	C4-C5-C6-O6
2	C	1309	NAG	C4-C5-C6-O6
2	B	1303	NAG	C4-C5-C6-O6
2	C	1307	NAG	C4-C5-C6-O6
2	B	1307	NAG	C4-C5-C6-O6
2	C	1308	NAG	O5-C5-C6-O6
2	C	1313	NAG	O5-C5-C6-O6
2	B	1302	NAG	C4-C5-C6-O6
2	A	1308	NAG	O5-C5-C6-O6
2	C	1310	NAG	O5-C5-C6-O6
2	A	1303	NAG	O5-C5-C6-O6
2	A	1308	NAG	C4-C5-C6-O6
2	C	1311	NAG	O5-C5-C6-O6
2	C	1310	NAG	C4-C5-C6-O6
2	A	1305	NAG	C4-C5-C6-O6
2	B	1312	NAG	O5-C5-C6-O6
2	A	1301	NAG	C4-C5-C6-O6
2	C	1307	NAG	C8-C7-N2-C2
2	C	1307	NAG	O7-C7-N2-C2
2	C	1310	NAG	C8-C7-N2-C2
2	C	1310	NAG	O7-C7-N2-C2
2	C	1312	NAG	C8-C7-N2-C2
2	C	1312	NAG	O7-C7-N2-C2
2	A	1306	NAG	C8-C7-N2-C2
2	A	1306	NAG	O7-C7-N2-C2
2	A	1309	NAG	C8-C7-N2-C2
2	A	1309	NAG	O7-C7-N2-C2
2	B	1307	NAG	C8-C7-N2-C2
2	B	1307	NAG	O7-C7-N2-C2
2	B	1309	NAG	C8-C7-N2-C2
2	B	1309	NAG	O7-C7-N2-C2
2	B	1312	NAG	C8-C7-N2-C2
2	B	1312	NAG	O7-C7-N2-C2
2	A	1306	NAG	O5-C5-C6-O6
2	C	1311	NAG	C4-C5-C6-O6
2	A	1306	NAG	C4-C5-C6-O6
2	C	1305	NAG	C4-C5-C6-O6
2	B	1310	NAG	O5-C5-C6-O6
2	A	1311	NAG	O5-C5-C6-O6
2	B	1304	NAG	C4-C5-C6-O6
2	B	1304	NAG	O5-C5-C6-O6
2	C	1307	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	A	1306	NAG	C1-C2-N2-C7
2	A	1307	NAG	C1-C2-N2-C7
2	A	1311	NAG	C1-C2-N2-C7
2	B	1304	NAG	C1-C2-N2-C7
2	C	1301	NAG	C3-C2-N2-C7
2	C	1306	NAG	C3-C2-N2-C7
2	A	1301	NAG	C3-C2-N2-C7
2	A	1307	NAG	C3-C2-N2-C7
2	A	1311	NAG	C3-C2-N2-C7
2	B	1301	NAG	C3-C2-N2-C7
2	B	1302	NAG	C3-C2-N2-C7
2	B	1304	NAG	C3-C2-N2-C7
2	B	1312	NAG	C4-C5-C6-O6
2	C	1301	NAG	C1-C2-N2-C7
2	A	1301	NAG	C1-C2-N2-C7
2	A	1308	NAG	C1-C2-N2-C7
2	B	1301	NAG	C1-C2-N2-C7
2	C	1304	NAG	C3-C2-N2-C7
2	C	1307	NAG	C3-C2-N2-C7
2	C	1308	NAG	C3-C2-N2-C7
2	A	1306	NAG	C3-C2-N2-C7
2	A	1308	NAG	C3-C2-N2-C7
2	B	1303	NAG	C3-C2-N2-C7
2	C	1301	NAG	C4-C5-C6-O6
2	C	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1306	NAG	1	0
2	A	1306	NAG	3	0
2	C	1307	NAG	2	0
2	B	1304	NAG	1	0
2	B	1302	NAG	1	0
2	B	1307	NAG	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

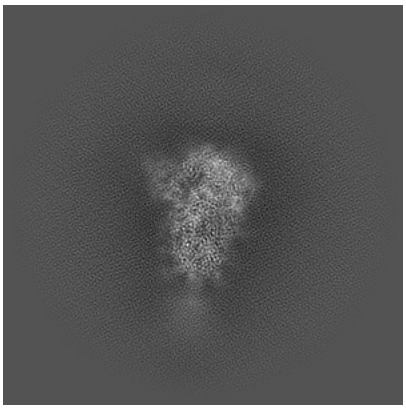
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17850. These allow visual inspection of the internal detail of the map and identification of artifacts.

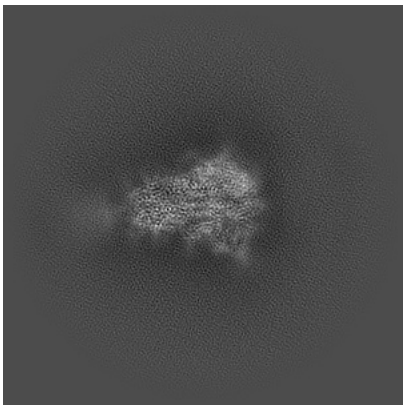
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

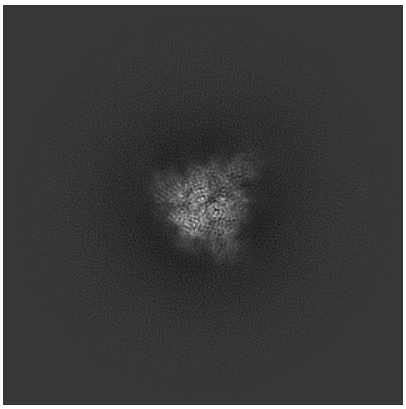
6.1.1 Primary map



X

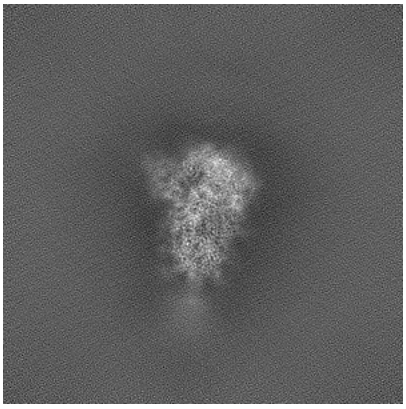


Y

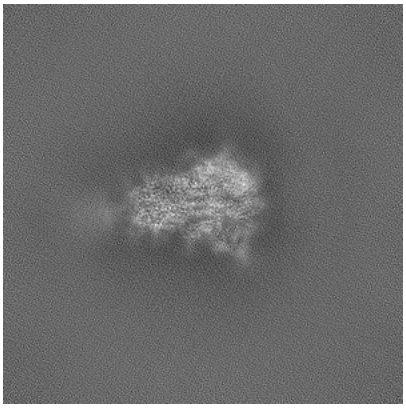


Z

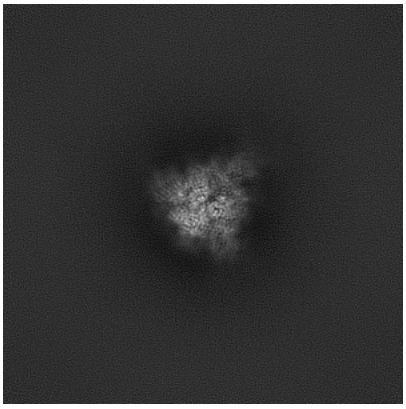
6.1.2 Raw map



X



Y

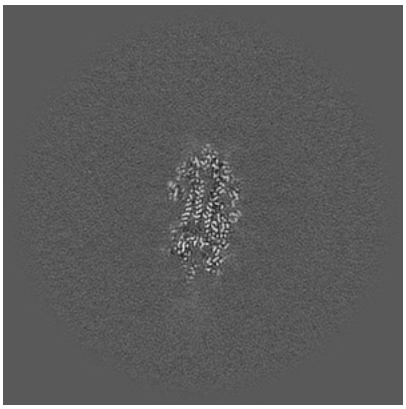


Z

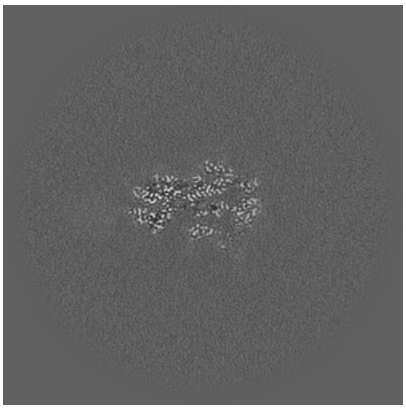
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

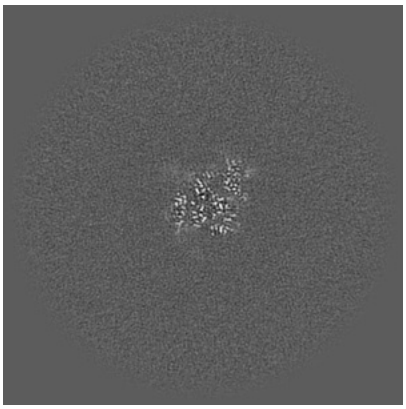
6.2.1 Primary map



X Index: 180

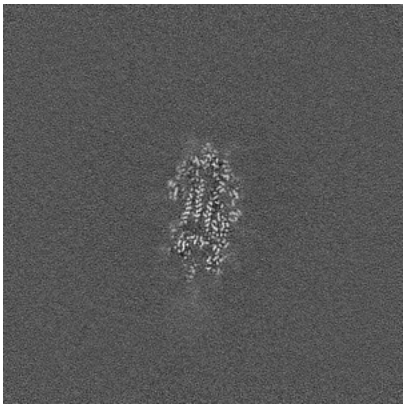


Y Index: 180

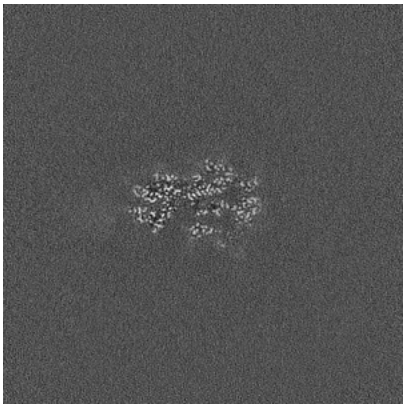


Z Index: 180

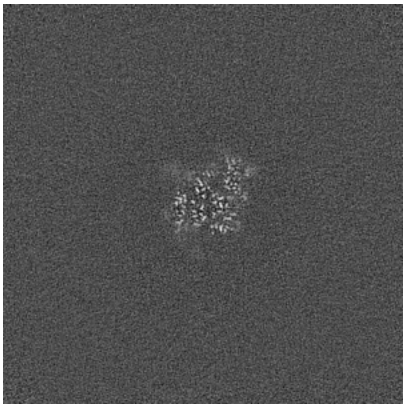
6.2.2 Raw map



X Index: 180



Y Index: 180

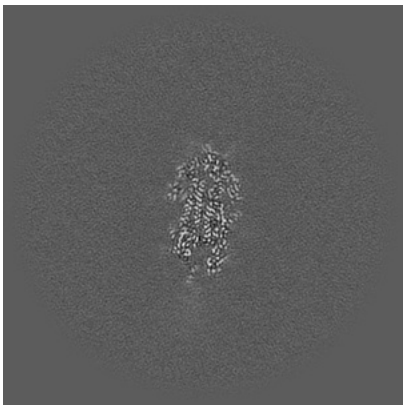


Z Index: 180

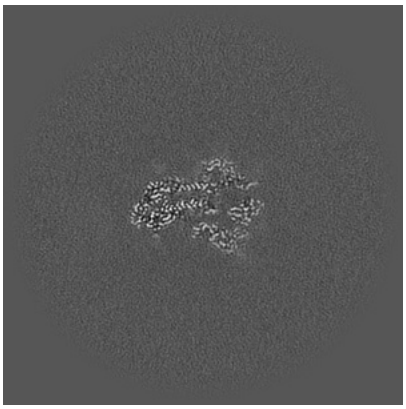
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

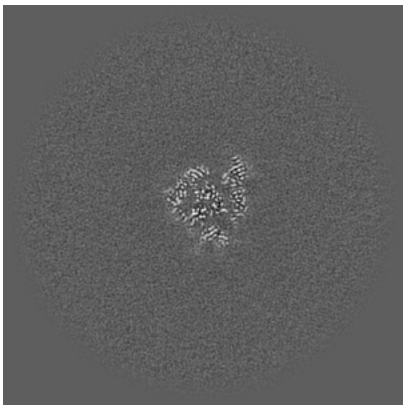
6.3.1 Primary map



X Index: 179

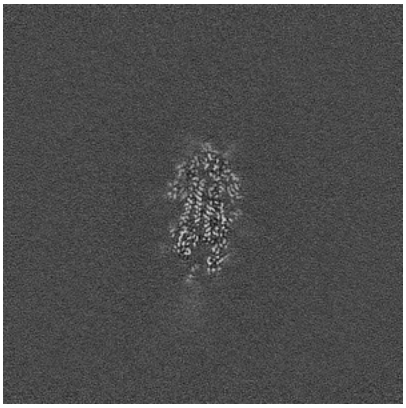


Y Index: 184

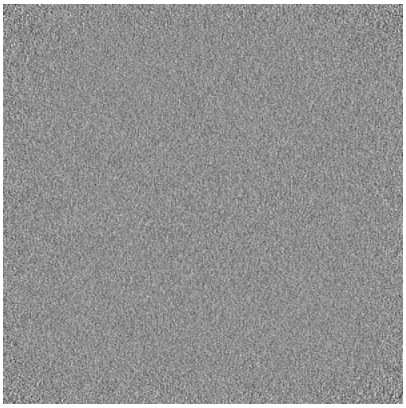


Z Index: 186

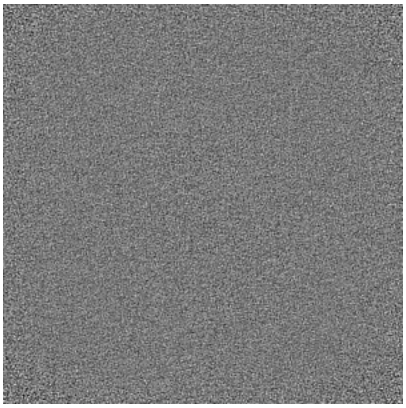
6.3.2 Raw map



X Index: 179



Y Index: 0

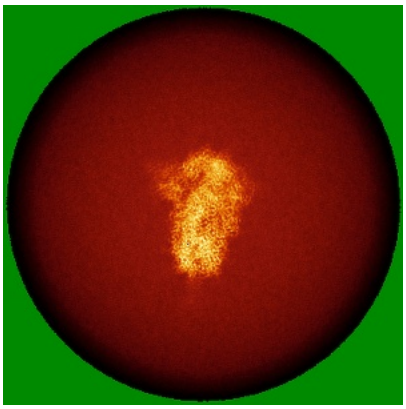


Z Index: 0

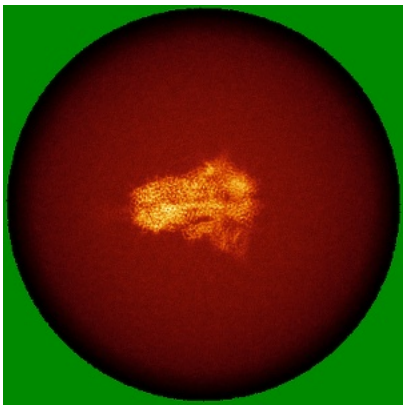
The images above show the largest variance slices of the map in three orthogonal directions.

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

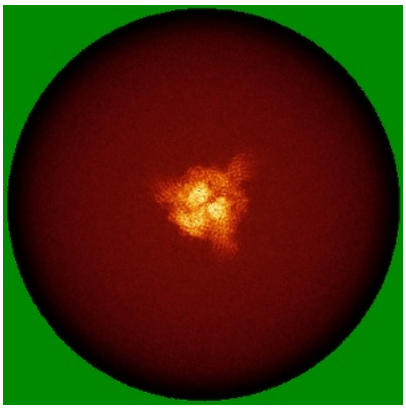
6.4.1 Primary map



X

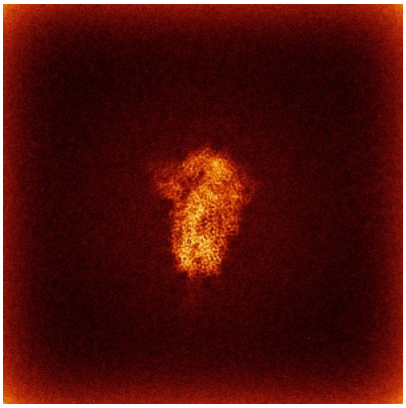


Y

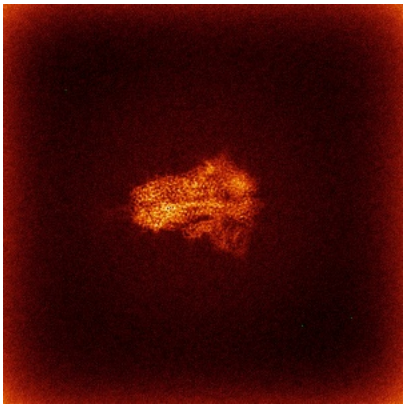


Z

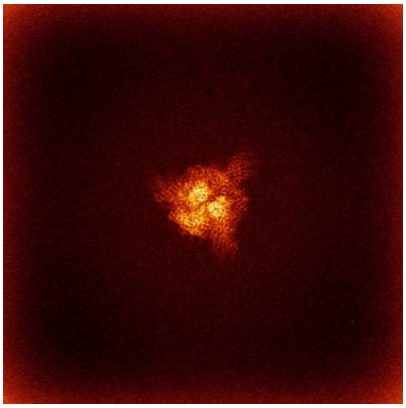
6.4.2 Raw map



X



Y

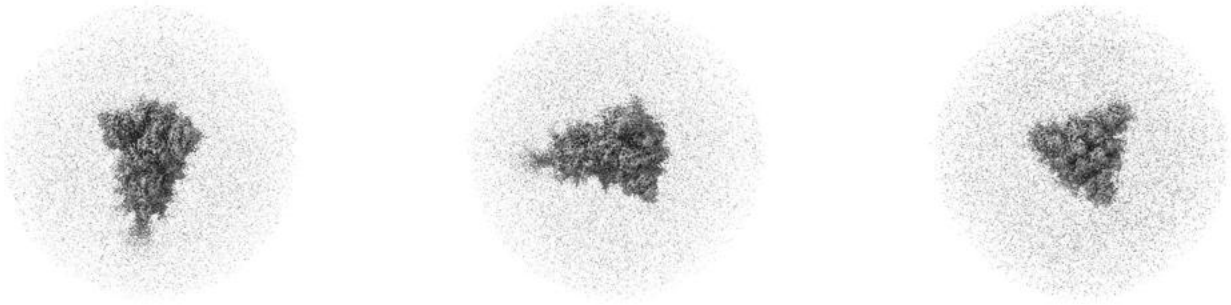


Z

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 (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

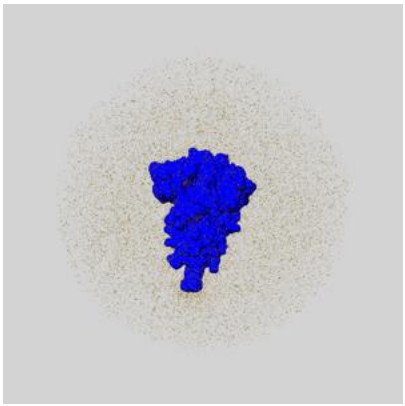
6.6 Mask visualisation (i)

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

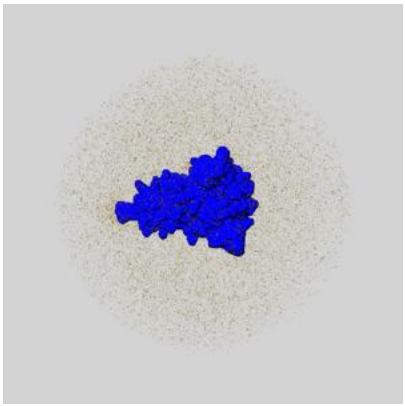
A mask typically either:

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

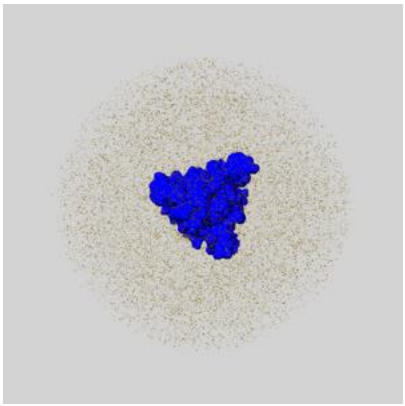
6.6.1 emd_17850_msk_1.map (i)



X



Y

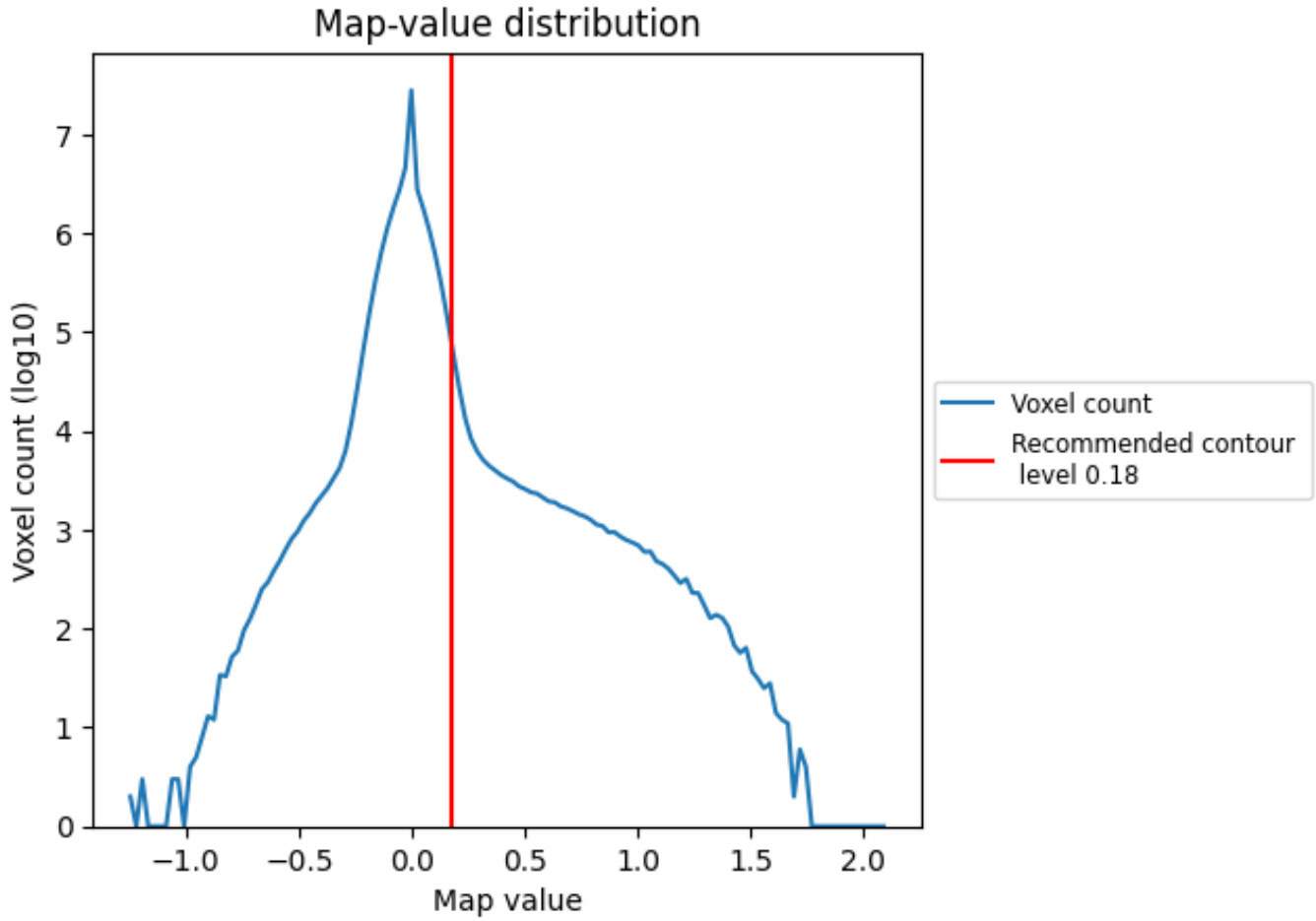


Z

7 Map analysis

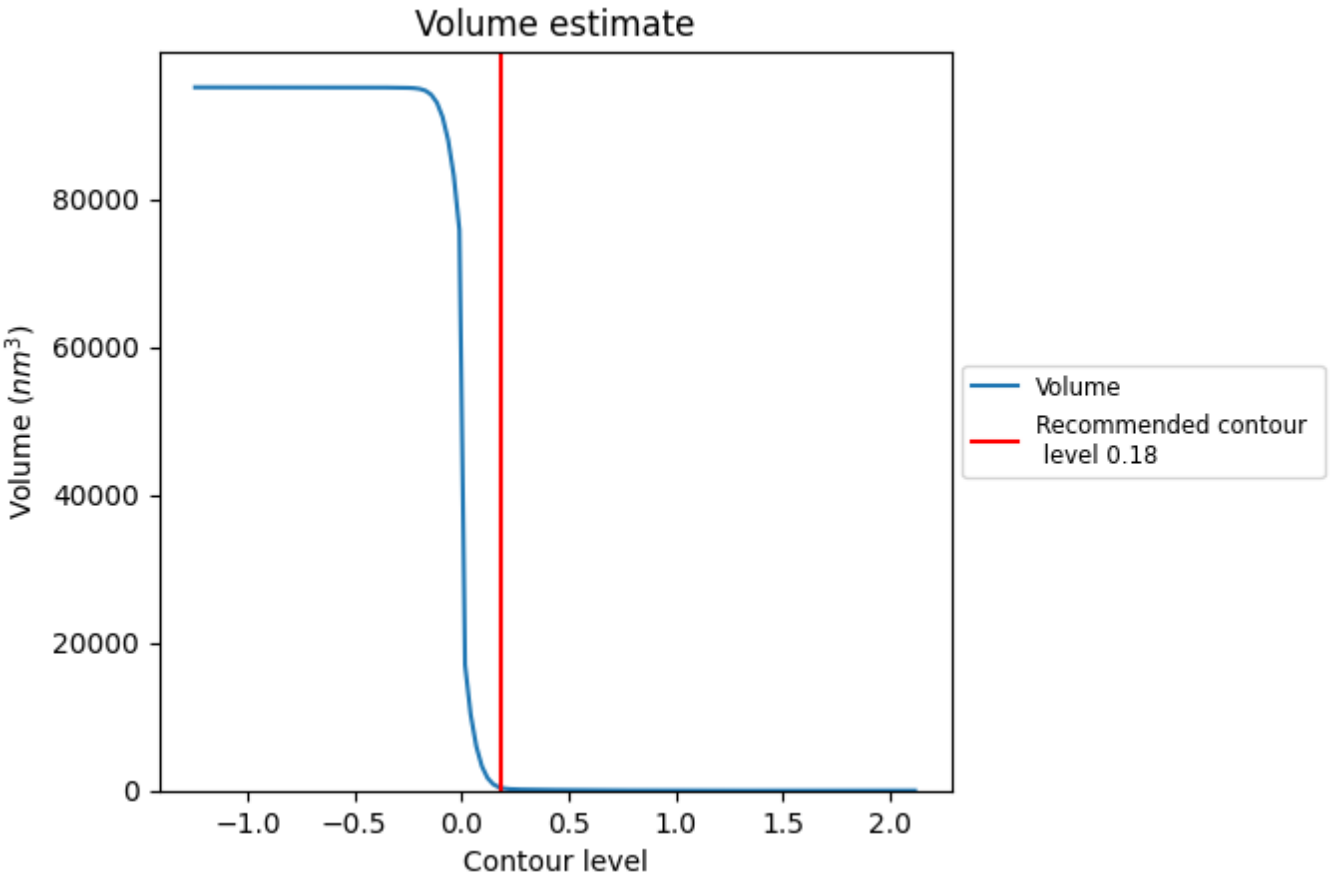
This section contains the results of statistical analysis of the map.

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.

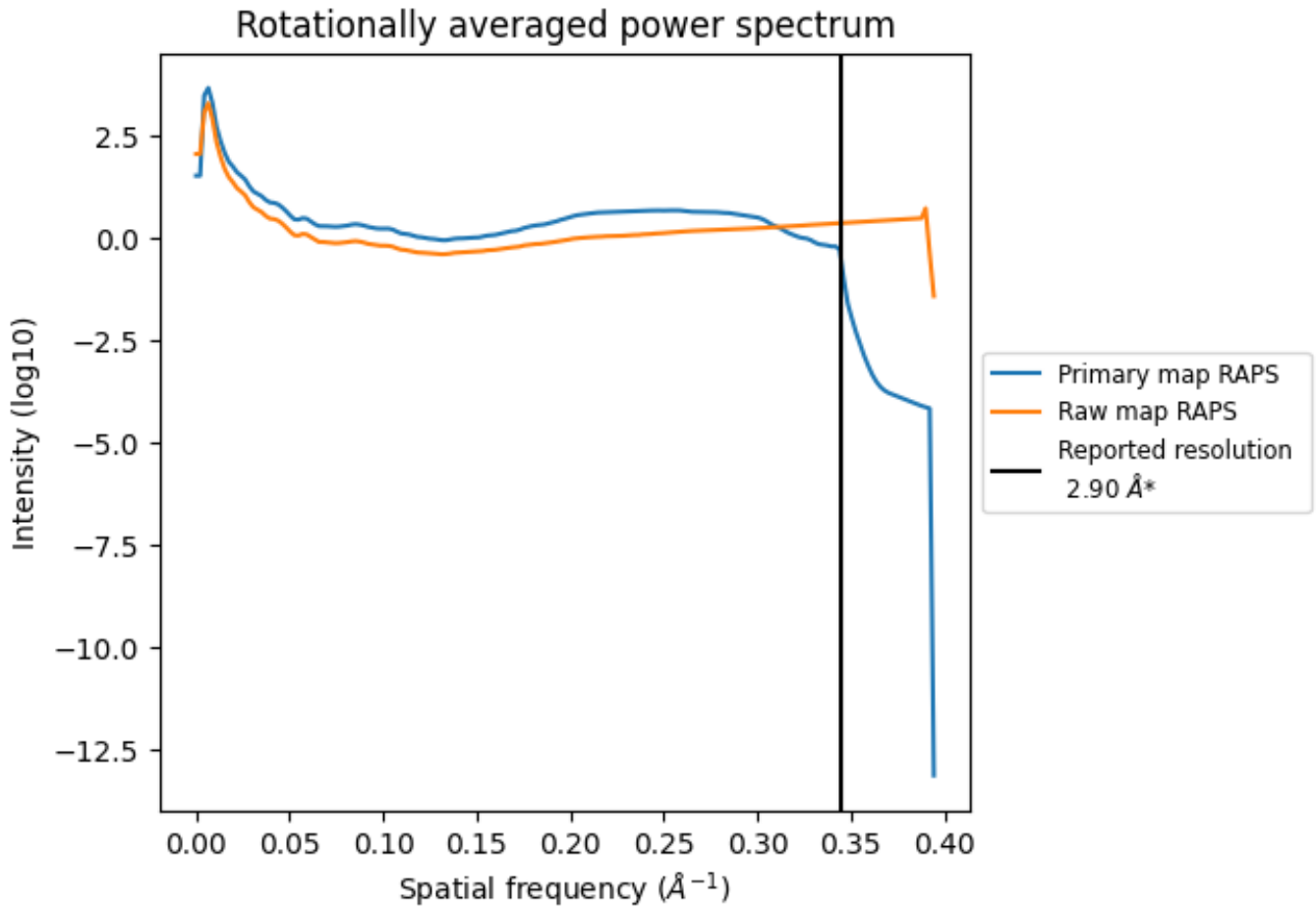
7.2 Volume estimate



The volume at the recommended contour level is 408 nm^3; this corresponds to an approximate mass of 369 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 (i)

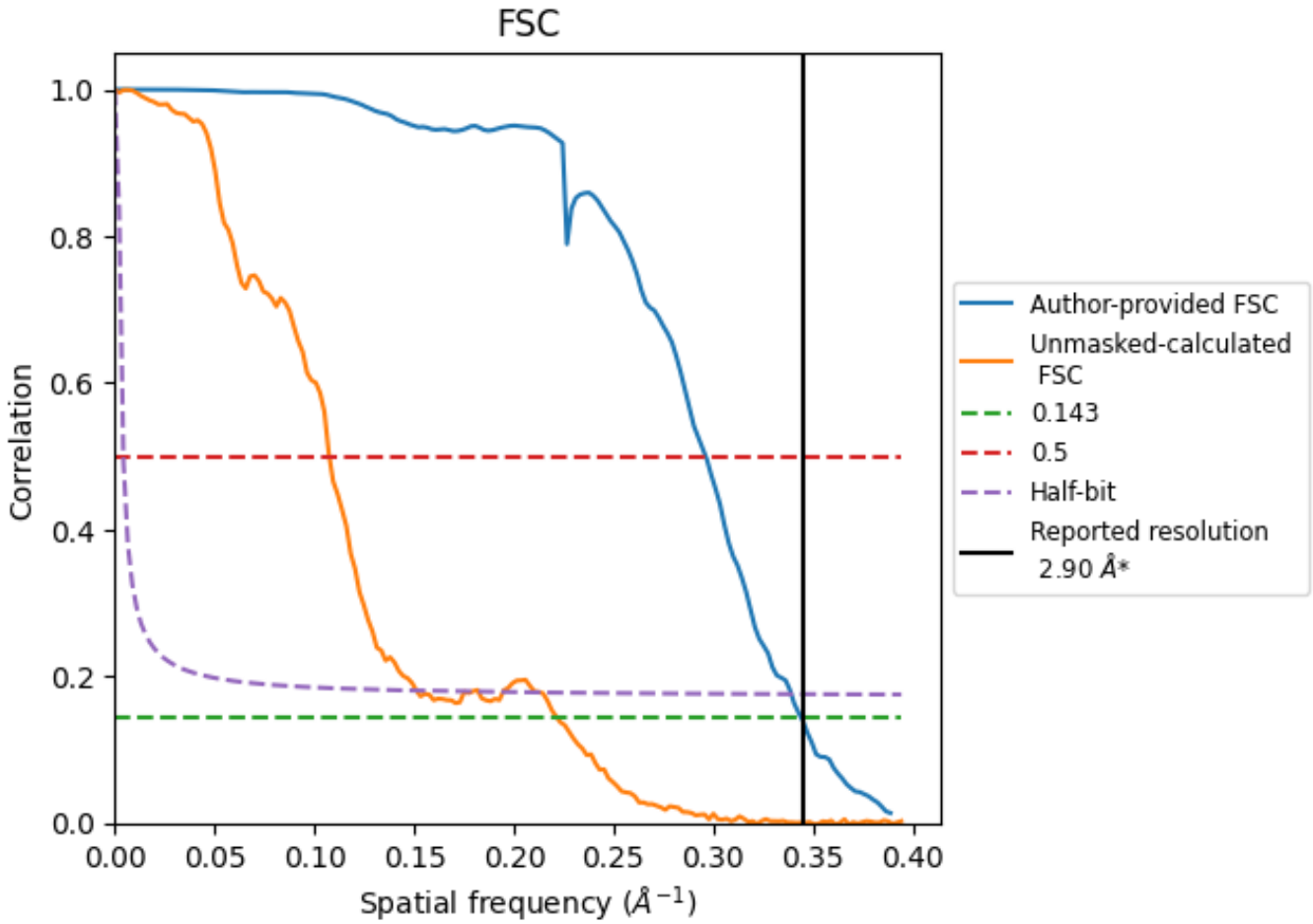


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

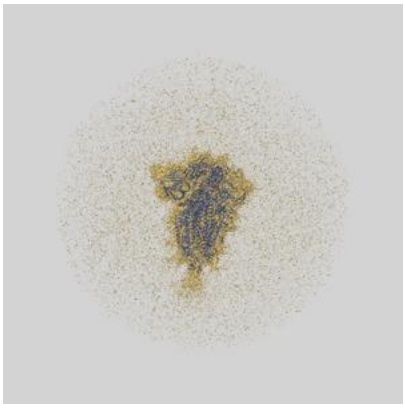
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.38	2.95
Unmasked-calculated*	4.51	9.29	6.61

*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 4.51 differs from the reported value 2.9 by more than 10 %

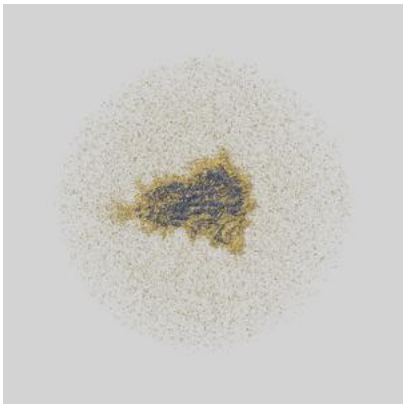
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17850 and PDB model 8PSD. Per-residue inclusion information can be found in section 3 on page 10.

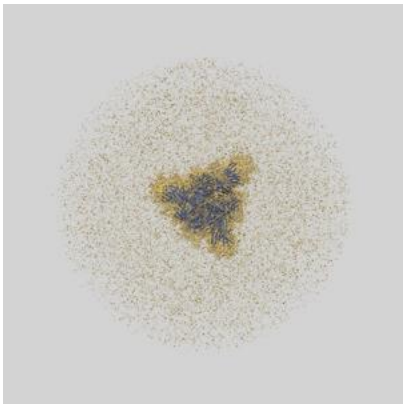
9.1 Map-model overlay



X



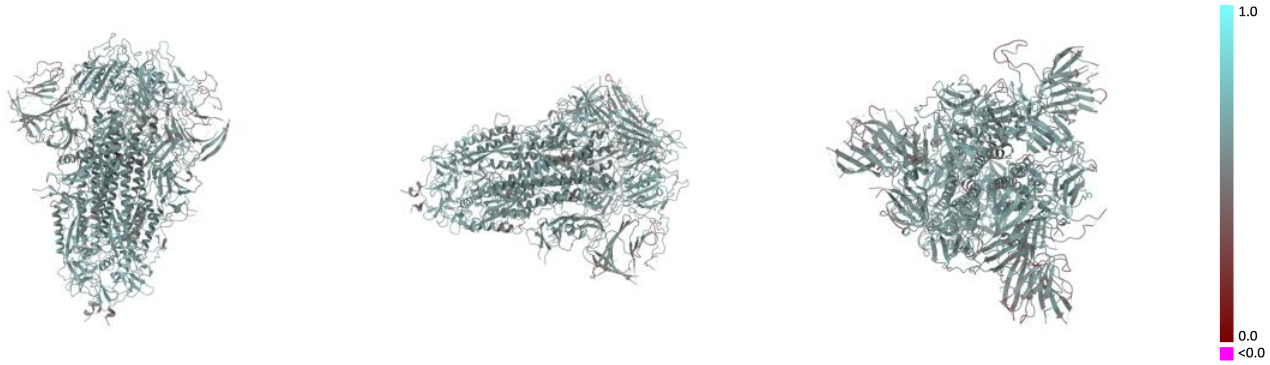
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18 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.

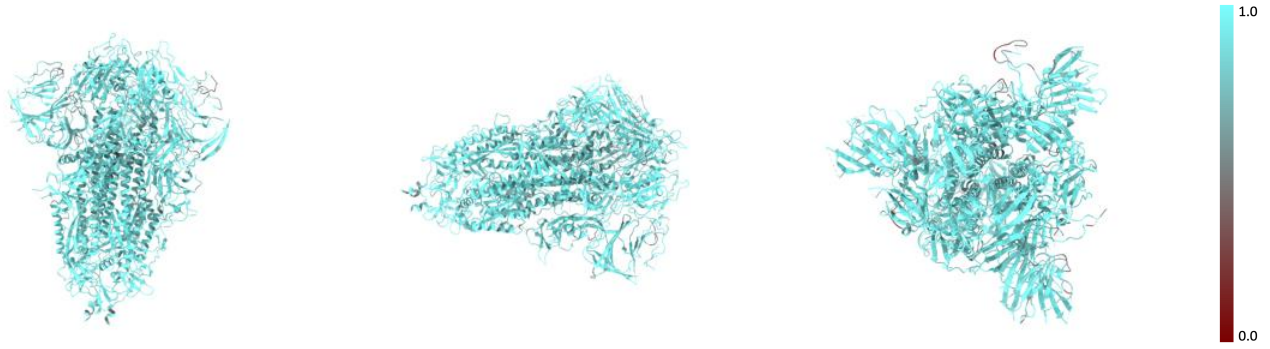
9.2 Q-score mapped to coordinate model (i)



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.

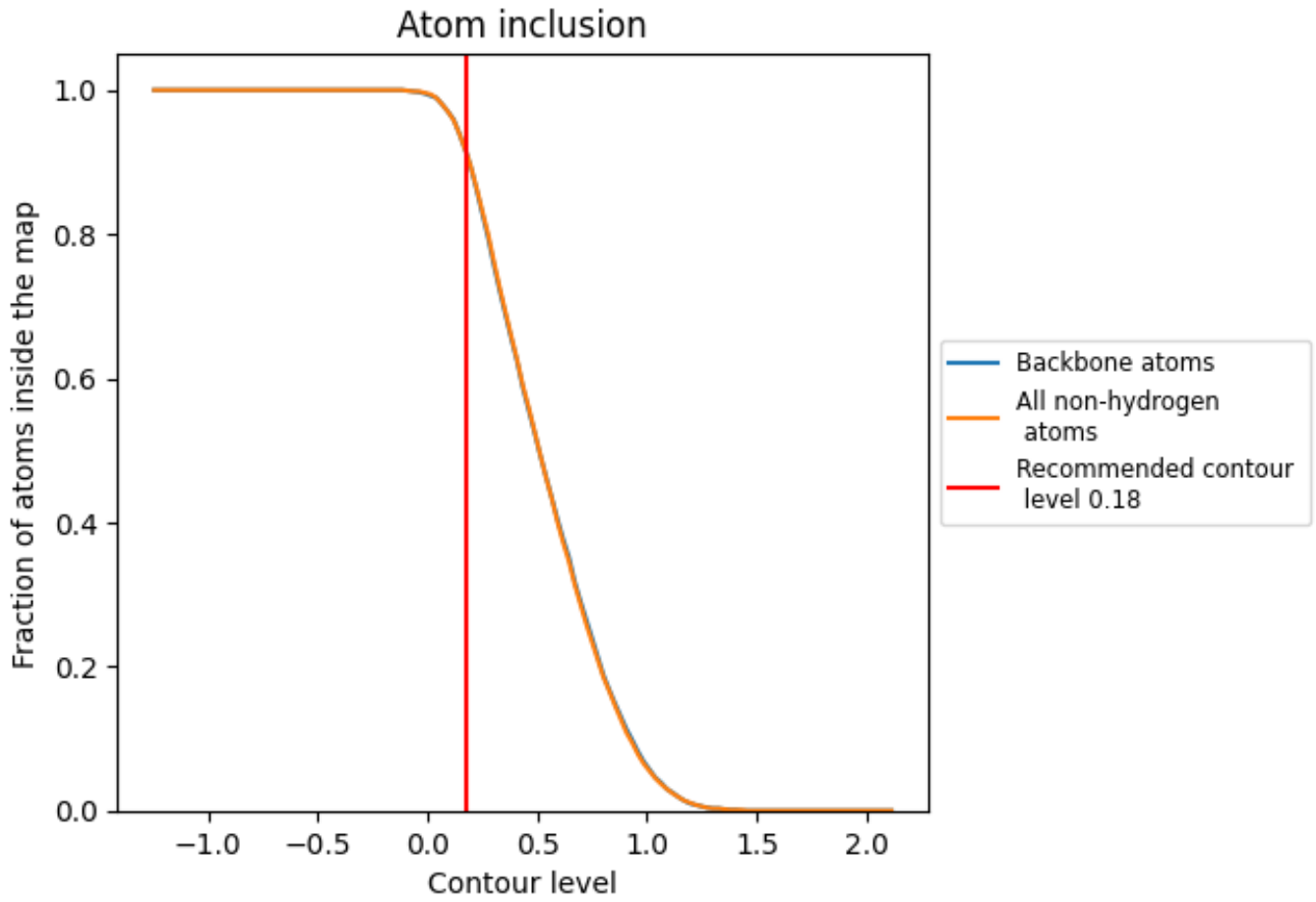
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.18).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9110	0.5620
A	0.9080	0.5600
B	0.9210	0.5650
C	0.9140	0.5610