



Full wwPDB EM Validation Report ⓘ

May 21, 2026 – 12:49 AM EDT

PDB ID : 11HN / pdb_000011hn
EMDB ID : EMD-75697
Title : SARS-CoV-2 spike S2 trimer stabilized in the early fusion intermediate conformation (E-FICs-v3) bound to C77G12 (S2 local refinement)
Authors : McCallum, M.; Seattle Structural Genomics Center for Infectious Disease (SS-GCID); Veesler, D.
Deposited on : 2026-02-24
Resolution : 2.70 Å(reported)

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

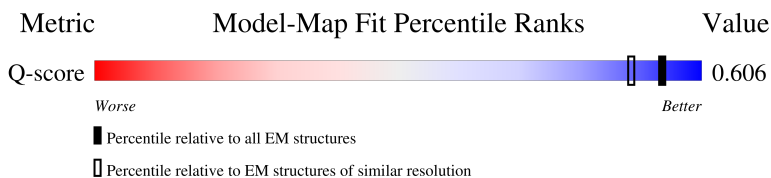
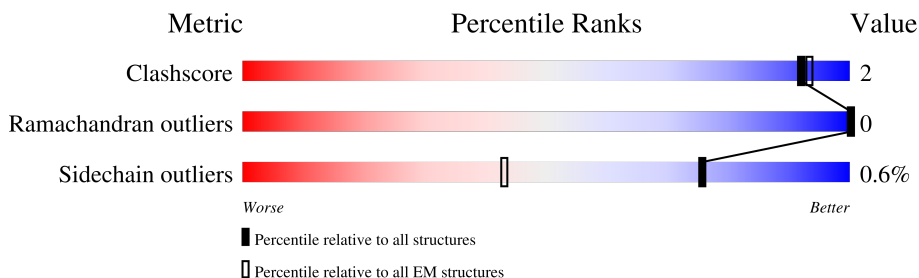
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	605	
1	B	605	
1	C	605	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5178 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 protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	226	Total	C	N	O	S	0	0
			1649	1053	291	296	9		
1	C	226	Total	C	N	O	S	0	0
			1649	1053	291	296	9		
1	A	226	Total	C	N	O	S	0	0
			1649	1053	291	296	9		

There are 489 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	755	MET	-	initiating methionine	UNP Q12306
B	756	THR	-	expression tag	UNP Q12306
B	757	ARG	-	expression tag	UNP Q12306
B	758	LEU	-	expression tag	UNP Q12306
B	759	THR	-	expression tag	UNP Q12306
B	760	VAL	-	expression tag	UNP Q12306
B	761	LEU	-	expression tag	UNP Q12306
B	762	ALA	-	expression tag	UNP Q12306
B	763	LEU	-	expression tag	UNP Q12306
B	764	LEU	-	expression tag	UNP Q12306
B	765	ALA	-	expression tag	UNP Q12306
B	766	GLY	-	expression tag	UNP Q12306
B	767	LEU	-	expression tag	UNP Q12306
B	768	LEU	-	expression tag	UNP Q12306
B	769	ALA	-	expression tag	UNP Q12306
B	770	SER	-	expression tag	UNP Q12306
B	771	SER	-	expression tag	UNP Q12306
B	772	ARG	-	expression tag	UNP Q12306
B	773	ALA	-	expression tag	UNP Q12306
B	774	SER	-	expression tag	UNP Q12306
B	869	ASN	-	linker	UNP Q12306
B	870	ASP	-	linker	UNP Q12306
B	871	ASP	-	linker	UNP Q12306
B	872	ASP	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	873	ASP	-	linker	UNP Q12306
B	874	LYS	-	linker	UNP Q12306
B	875	THR	-	linker	UNP Q12306
B	876	GLY	-	linker	UNP Q12306
B	877	THR	-	linker	UNP Q12306
B	878	GLY	-	linker	UNP Q12306
B	879	SER	-	linker	UNP Q12306
B	880	GLN	-	linker	UNP Q12306
B	881	SER	-	linker	UNP Q12306
B	882	ASN	-	linker	UNP Q12306
B	883	ALA	-	linker	UNP Q12306
B	884	GLU	-	linker	UNP Q12306
B	885	SER	-	linker	UNP Q12306
B	886	VAL	-	linker	UNP Q12306
B	887	GLN	-	linker	UNP Q12306
B	888	ASN	-	linker	UNP Q12306
B	889	HIS	-	linker	UNP Q12306
B	890	THR	-	linker	UNP Q12306
B	891	PHE	-	linker	UNP Q12306
B	892	GLU	-	linker	UNP Q12306
B	893	VAL	-	linker	UNP Q12306
B	894	LEU	-	linker	UNP Q12306
B	895	ASN	-	linker	UNP Q12306
B	896	ASN	-	linker	UNP Q12306
B	897	THR	-	linker	UNP Q12306
B	898	ILE	-	linker	UNP Q12306
B	899	ARG	-	linker	UNP Q12306
B	900	ALA	-	linker	UNP Q12306
B	901	LEU	-	linker	UNP Q12306
B	902	GLU	-	linker	UNP Q12306
B	903	LEU	-	linker	UNP Q12306
B	904	ILE	-	linker	UNP Q12306
B	905	LEU	-	linker	UNP Q12306
B	906	ARG	-	linker	UNP Q12306
B	907	LYS	-	linker	UNP Q12306
B	908	LEU	-	linker	UNP Q12306
B	909	GLU	-	linker	UNP Q12306
B	910	ILE	-	linker	UNP Q12306
B	911	LEU	-	linker	UNP Q12306
B	912	TYR	-	linker	UNP Q12306
B	913	GLU	-	linker	UNP Q12306
B	914	MET	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	915	ILE	-	linker	UNP Q12306
B	916	LEU	-	linker	UNP Q12306
B	917	GLN	-	linker	UNP Q12306
B	918	LEU	-	linker	UNP Q12306
B	919	HIS	-	linker	UNP Q12306
B	920	GLU	-	linker	UNP Q12306
B	921	GLU	-	linker	UNP Q12306
B	922	VAL	-	linker	UNP Q12306
B	923	GLU	-	linker	UNP Q12306
B	924	ALA	-	linker	UNP Q12306
B	925	ILE	-	linker	UNP Q12306
B	926	GLN	-	linker	UNP Q12306
B	927	LYS	-	linker	UNP Q12306
B	928	ALA	-	linker	UNP Q12306
B	929	ILE	-	linker	UNP Q12306
B	1001	ALA	ASP	conflict	UNP P0DTC2
B	1702	THR	-	linker	UNP P0DTC2
B	1834	THR	-	expression tag	UNP P0DTC2
B	1835	ILE	-	expression tag	UNP P0DTC2
B	1836	ASP	-	expression tag	UNP P0DTC2
B	1837	LYS	-	expression tag	UNP P0DTC2
B	1838	GLU	-	expression tag	UNP P0DTC2
B	1839	LYS	-	expression tag	UNP P0DTC2
B	1840	TRP	-	expression tag	UNP P0DTC2
B	1841	LYS	-	expression tag	UNP P0DTC2
B	1842	GLU	-	expression tag	UNP P0DTC2
B	1843	TRP	-	expression tag	UNP P0DTC2
B	1844	ARG	-	expression tag	UNP P0DTC2
B	1845	LYS	-	expression tag	UNP P0DTC2
B	1846	GLU	-	expression tag	UNP P0DTC2
B	1847	MET	-	expression tag	UNP P0DTC2
B	1848	GLU	-	expression tag	UNP P0DTC2
B	1849	ASN	-	expression tag	UNP P0DTC2
B	1850	LEU	-	expression tag	UNP P0DTC2
B	1851	THR	-	expression tag	UNP P0DTC2
B	1852	LYS	-	expression tag	UNP P0DTC2
B	1853	GLU	-	expression tag	UNP P0DTC2
B	1854	ILE	-	expression tag	UNP P0DTC2
B	1855	LYS	-	expression tag	UNP P0DTC2
B	1856	GLU	-	expression tag	UNP P0DTC2
B	1857	THR	-	expression tag	UNP P0DTC2
B	1858	LEU	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1859	GLU	-	expression tag	UNP P0DTC2
B	1860	GLU	-	expression tag	UNP P0DTC2
B	1861	ALA	-	expression tag	UNP P0DTC2
B	1862	ARG	-	expression tag	UNP P0DTC2
B	1863	LYS	-	expression tag	UNP P0DTC2
B	1864	THR	-	expression tag	UNP P0DTC2
B	1865	LEU	-	expression tag	UNP P0DTC2
B	1866	LYS	-	expression tag	UNP P0DTC2
B	1867	GLN	-	expression tag	UNP P0DTC2
B	1868	ALA	-	expression tag	UNP P0DTC2
B	1869	GLU	-	expression tag	UNP P0DTC2
B	1870	GLU	-	expression tag	UNP P0DTC2
B	1871	THR	-	expression tag	UNP P0DTC2
B	1872	PHE	-	expression tag	UNP P0DTC2
B	1873	LYS	-	expression tag	UNP P0DTC2
B	1874	THR	-	expression tag	UNP P0DTC2
B	1875	PRO	-	expression tag	UNP P0DTC2
B	1876	SER	-	expression tag	UNP P0DTC2
B	1877	SER	-	expression tag	UNP P0DTC2
B	1878	GLY	-	expression tag	UNP P0DTC2
B	1879	GLY	-	expression tag	UNP P0DTC2
B	1880	THR	-	expression tag	UNP P0DTC2
B	1881	ASP	-	expression tag	UNP P0DTC2
B	1882	ASP	-	expression tag	UNP P0DTC2
B	1883	ASP	-	expression tag	UNP P0DTC2
B	1884	ASP	-	expression tag	UNP P0DTC2
B	1885	LYS	-	expression tag	UNP P0DTC2
B	1886	THR	-	expression tag	UNP P0DTC2
B	1887	GLY	-	expression tag	UNP P0DTC2
B	1888	SER	-	expression tag	UNP P0DTC2
B	1889	LEU	-	expression tag	UNP P0DTC2
B	1890	ASN	-	expression tag	UNP P0DTC2
B	1891	ASP	-	expression tag	UNP P0DTC2
B	1892	ILE	-	expression tag	UNP P0DTC2
B	1893	PHE	-	expression tag	UNP P0DTC2
B	1894	GLU	-	expression tag	UNP P0DTC2
B	1895	ALA	-	expression tag	UNP P0DTC2
B	1896	GLN	-	expression tag	UNP P0DTC2
B	1897	LYS	-	expression tag	UNP P0DTC2
B	1898	ILE	-	expression tag	UNP P0DTC2
B	1899	GLU	-	expression tag	UNP P0DTC2
B	1900	TRP	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1901	HIS	-	expression tag	UNP P0DTC2
B	1902	GLU	-	expression tag	UNP P0DTC2
B	1903	GLN	-	expression tag	UNP P0DTC2
B	1904	GLY	-	expression tag	UNP P0DTC2
B	1905	SER	-	expression tag	UNP P0DTC2
B	1906	HIS	-	expression tag	UNP P0DTC2
B	1907	HIS	-	expression tag	UNP P0DTC2
B	1908	HIS	-	expression tag	UNP P0DTC2
B	1909	HIS	-	expression tag	UNP P0DTC2
B	1910	HIS	-	expression tag	UNP P0DTC2
B	1911	HIS	-	expression tag	UNP P0DTC2
B	1912	HIS	-	expression tag	UNP P0DTC2
B	1913	HIS	-	expression tag	UNP P0DTC2
C	755	MET	-	initiating methionine	UNP Q12306
C	756	THR	-	expression tag	UNP Q12306
C	757	ARG	-	expression tag	UNP Q12306
C	758	LEU	-	expression tag	UNP Q12306
C	759	THR	-	expression tag	UNP Q12306
C	760	VAL	-	expression tag	UNP Q12306
C	761	LEU	-	expression tag	UNP Q12306
C	762	ALA	-	expression tag	UNP Q12306
C	763	LEU	-	expression tag	UNP Q12306
C	764	LEU	-	expression tag	UNP Q12306
C	765	ALA	-	expression tag	UNP Q12306
C	766	GLY	-	expression tag	UNP Q12306
C	767	LEU	-	expression tag	UNP Q12306
C	768	LEU	-	expression tag	UNP Q12306
C	769	ALA	-	expression tag	UNP Q12306
C	770	SER	-	expression tag	UNP Q12306
C	771	SER	-	expression tag	UNP Q12306
C	772	ARG	-	expression tag	UNP Q12306
C	773	ALA	-	expression tag	UNP Q12306
C	774	SER	-	expression tag	UNP Q12306
C	869	ASN	-	linker	UNP Q12306
C	870	ASP	-	linker	UNP Q12306
C	871	ASP	-	linker	UNP Q12306
C	872	ASP	-	linker	UNP Q12306
C	873	ASP	-	linker	UNP Q12306
C	874	LYS	-	linker	UNP Q12306
C	875	THR	-	linker	UNP Q12306
C	876	GLY	-	linker	UNP Q12306
C	877	THR	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	878	GLY	-	linker	UNP Q12306
C	879	SER	-	linker	UNP Q12306
C	880	GLN	-	linker	UNP Q12306
C	881	SER	-	linker	UNP Q12306
C	882	ASN	-	linker	UNP Q12306
C	883	ALA	-	linker	UNP Q12306
C	884	GLU	-	linker	UNP Q12306
C	885	SER	-	linker	UNP Q12306
C	886	VAL	-	linker	UNP Q12306
C	887	GLN	-	linker	UNP Q12306
C	888	ASN	-	linker	UNP Q12306
C	889	HIS	-	linker	UNP Q12306
C	890	THR	-	linker	UNP Q12306
C	891	PHE	-	linker	UNP Q12306
C	892	GLU	-	linker	UNP Q12306
C	893	VAL	-	linker	UNP Q12306
C	894	LEU	-	linker	UNP Q12306
C	895	ASN	-	linker	UNP Q12306
C	896	ASN	-	linker	UNP Q12306
C	897	THR	-	linker	UNP Q12306
C	898	ILE	-	linker	UNP Q12306
C	899	ARG	-	linker	UNP Q12306
C	900	ALA	-	linker	UNP Q12306
C	901	LEU	-	linker	UNP Q12306
C	902	GLU	-	linker	UNP Q12306
C	903	LEU	-	linker	UNP Q12306
C	904	ILE	-	linker	UNP Q12306
C	905	LEU	-	linker	UNP Q12306
C	906	ARG	-	linker	UNP Q12306
C	907	LYS	-	linker	UNP Q12306
C	908	LEU	-	linker	UNP Q12306
C	909	GLU	-	linker	UNP Q12306
C	910	ILE	-	linker	UNP Q12306
C	911	LEU	-	linker	UNP Q12306
C	912	TYR	-	linker	UNP Q12306
C	913	GLU	-	linker	UNP Q12306
C	914	MET	-	linker	UNP Q12306
C	915	ILE	-	linker	UNP Q12306
C	916	LEU	-	linker	UNP Q12306
C	917	GLN	-	linker	UNP Q12306
C	918	LEU	-	linker	UNP Q12306
C	919	HIS	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	920	GLU	-	linker	UNP Q12306
C	921	GLU	-	linker	UNP Q12306
C	922	VAL	-	linker	UNP Q12306
C	923	GLU	-	linker	UNP Q12306
C	924	ALA	-	linker	UNP Q12306
C	925	ILE	-	linker	UNP Q12306
C	926	GLN	-	linker	UNP Q12306
C	927	LYS	-	linker	UNP Q12306
C	928	ALA	-	linker	UNP Q12306
C	929	ILE	-	linker	UNP Q12306
C	1001	ALA	ASP	conflict	UNP P0DTC2
C	1702	THR	-	linker	UNP P0DTC2
C	1834	THR	-	expression tag	UNP P0DTC2
C	1835	ILE	-	expression tag	UNP P0DTC2
C	1836	ASP	-	expression tag	UNP P0DTC2
C	1837	LYS	-	expression tag	UNP P0DTC2
C	1838	GLU	-	expression tag	UNP P0DTC2
C	1839	LYS	-	expression tag	UNP P0DTC2
C	1840	TRP	-	expression tag	UNP P0DTC2
C	1841	LYS	-	expression tag	UNP P0DTC2
C	1842	GLU	-	expression tag	UNP P0DTC2
C	1843	TRP	-	expression tag	UNP P0DTC2
C	1844	ARG	-	expression tag	UNP P0DTC2
C	1845	LYS	-	expression tag	UNP P0DTC2
C	1846	GLU	-	expression tag	UNP P0DTC2
C	1847	MET	-	expression tag	UNP P0DTC2
C	1848	GLU	-	expression tag	UNP P0DTC2
C	1849	ASN	-	expression tag	UNP P0DTC2
C	1850	LEU	-	expression tag	UNP P0DTC2
C	1851	THR	-	expression tag	UNP P0DTC2
C	1852	LYS	-	expression tag	UNP P0DTC2
C	1853	GLU	-	expression tag	UNP P0DTC2
C	1854	ILE	-	expression tag	UNP P0DTC2
C	1855	LYS	-	expression tag	UNP P0DTC2
C	1856	GLU	-	expression tag	UNP P0DTC2
C	1857	THR	-	expression tag	UNP P0DTC2
C	1858	LEU	-	expression tag	UNP P0DTC2
C	1859	GLU	-	expression tag	UNP P0DTC2
C	1860	GLU	-	expression tag	UNP P0DTC2
C	1861	ALA	-	expression tag	UNP P0DTC2
C	1862	ARG	-	expression tag	UNP P0DTC2
C	1863	LYS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1864	THR	-	expression tag	UNP P0DTC2
C	1865	LEU	-	expression tag	UNP P0DTC2
C	1866	LYS	-	expression tag	UNP P0DTC2
C	1867	GLN	-	expression tag	UNP P0DTC2
C	1868	ALA	-	expression tag	UNP P0DTC2
C	1869	GLU	-	expression tag	UNP P0DTC2
C	1870	GLU	-	expression tag	UNP P0DTC2
C	1871	THR	-	expression tag	UNP P0DTC2
C	1872	PHE	-	expression tag	UNP P0DTC2
C	1873	LYS	-	expression tag	UNP P0DTC2
C	1874	THR	-	expression tag	UNP P0DTC2
C	1875	PRO	-	expression tag	UNP P0DTC2
C	1876	SER	-	expression tag	UNP P0DTC2
C	1877	SER	-	expression tag	UNP P0DTC2
C	1878	GLY	-	expression tag	UNP P0DTC2
C	1879	GLY	-	expression tag	UNP P0DTC2
C	1880	THR	-	expression tag	UNP P0DTC2
C	1881	ASP	-	expression tag	UNP P0DTC2
C	1882	ASP	-	expression tag	UNP P0DTC2
C	1883	ASP	-	expression tag	UNP P0DTC2
C	1884	ASP	-	expression tag	UNP P0DTC2
C	1885	LYS	-	expression tag	UNP P0DTC2
C	1886	THR	-	expression tag	UNP P0DTC2
C	1887	GLY	-	expression tag	UNP P0DTC2
C	1888	SER	-	expression tag	UNP P0DTC2
C	1889	LEU	-	expression tag	UNP P0DTC2
C	1890	ASN	-	expression tag	UNP P0DTC2
C	1891	ASP	-	expression tag	UNP P0DTC2
C	1892	ILE	-	expression tag	UNP P0DTC2
C	1893	PHE	-	expression tag	UNP P0DTC2
C	1894	GLU	-	expression tag	UNP P0DTC2
C	1895	ALA	-	expression tag	UNP P0DTC2
C	1896	GLN	-	expression tag	UNP P0DTC2
C	1897	LYS	-	expression tag	UNP P0DTC2
C	1898	ILE	-	expression tag	UNP P0DTC2
C	1899	GLU	-	expression tag	UNP P0DTC2
C	1900	TRP	-	expression tag	UNP P0DTC2
C	1901	HIS	-	expression tag	UNP P0DTC2
C	1902	GLU	-	expression tag	UNP P0DTC2
C	1903	GLN	-	expression tag	UNP P0DTC2
C	1904	GLY	-	expression tag	UNP P0DTC2
C	1905	SER	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1906	HIS	-	expression tag	UNP P0DTC2
C	1907	HIS	-	expression tag	UNP P0DTC2
C	1908	HIS	-	expression tag	UNP P0DTC2
C	1909	HIS	-	expression tag	UNP P0DTC2
C	1910	HIS	-	expression tag	UNP P0DTC2
C	1911	HIS	-	expression tag	UNP P0DTC2
C	1912	HIS	-	expression tag	UNP P0DTC2
C	1913	HIS	-	expression tag	UNP P0DTC2
A	755	MET	-	initiating methionine	UNP Q12306
A	756	THR	-	expression tag	UNP Q12306
A	757	ARG	-	expression tag	UNP Q12306
A	758	LEU	-	expression tag	UNP Q12306
A	759	THR	-	expression tag	UNP Q12306
A	760	VAL	-	expression tag	UNP Q12306
A	761	LEU	-	expression tag	UNP Q12306
A	762	ALA	-	expression tag	UNP Q12306
A	763	LEU	-	expression tag	UNP Q12306
A	764	LEU	-	expression tag	UNP Q12306
A	765	ALA	-	expression tag	UNP Q12306
A	766	GLY	-	expression tag	UNP Q12306
A	767	LEU	-	expression tag	UNP Q12306
A	768	LEU	-	expression tag	UNP Q12306
A	769	ALA	-	expression tag	UNP Q12306
A	770	SER	-	expression tag	UNP Q12306
A	771	SER	-	expression tag	UNP Q12306
A	772	ARG	-	expression tag	UNP Q12306
A	773	ALA	-	expression tag	UNP Q12306
A	774	SER	-	expression tag	UNP Q12306
A	869	ASN	-	linker	UNP Q12306
A	870	ASP	-	linker	UNP Q12306
A	871	ASP	-	linker	UNP Q12306
A	872	ASP	-	linker	UNP Q12306
A	873	ASP	-	linker	UNP Q12306
A	874	LYS	-	linker	UNP Q12306
A	875	THR	-	linker	UNP Q12306
A	876	GLY	-	linker	UNP Q12306
A	877	THR	-	linker	UNP Q12306
A	878	GLY	-	linker	UNP Q12306
A	879	SER	-	linker	UNP Q12306
A	880	GLN	-	linker	UNP Q12306
A	881	SER	-	linker	UNP Q12306
A	882	ASN	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	883	ALA	-	linker	UNP Q12306
A	884	GLU	-	linker	UNP Q12306
A	885	SER	-	linker	UNP Q12306
A	886	VAL	-	linker	UNP Q12306
A	887	GLN	-	linker	UNP Q12306
A	888	ASN	-	linker	UNP Q12306
A	889	HIS	-	linker	UNP Q12306
A	890	THR	-	linker	UNP Q12306
A	891	PHE	-	linker	UNP Q12306
A	892	GLU	-	linker	UNP Q12306
A	893	VAL	-	linker	UNP Q12306
A	894	LEU	-	linker	UNP Q12306
A	895	ASN	-	linker	UNP Q12306
A	896	ASN	-	linker	UNP Q12306
A	897	THR	-	linker	UNP Q12306
A	898	ILE	-	linker	UNP Q12306
A	899	ARG	-	linker	UNP Q12306
A	900	ALA	-	linker	UNP Q12306
A	901	LEU	-	linker	UNP Q12306
A	902	GLU	-	linker	UNP Q12306
A	903	LEU	-	linker	UNP Q12306
A	904	ILE	-	linker	UNP Q12306
A	905	LEU	-	linker	UNP Q12306
A	906	ARG	-	linker	UNP Q12306
A	907	LYS	-	linker	UNP Q12306
A	908	LEU	-	linker	UNP Q12306
A	909	GLU	-	linker	UNP Q12306
A	910	ILE	-	linker	UNP Q12306
A	911	LEU	-	linker	UNP Q12306
A	912	TYR	-	linker	UNP Q12306
A	913	GLU	-	linker	UNP Q12306
A	914	MET	-	linker	UNP Q12306
A	915	ILE	-	linker	UNP Q12306
A	916	LEU	-	linker	UNP Q12306
A	917	GLN	-	linker	UNP Q12306
A	918	LEU	-	linker	UNP Q12306
A	919	HIS	-	linker	UNP Q12306
A	920	GLU	-	linker	UNP Q12306
A	921	GLU	-	linker	UNP Q12306
A	922	VAL	-	linker	UNP Q12306
A	923	GLU	-	linker	UNP Q12306
A	924	ALA	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	925	ILE	-	linker	UNP Q12306
A	926	GLN	-	linker	UNP Q12306
A	927	LYS	-	linker	UNP Q12306
A	928	ALA	-	linker	UNP Q12306
A	929	ILE	-	linker	UNP Q12306
A	1001	ALA	ASP	conflict	UNP P0DTC2
A	1702	THR	-	linker	UNP P0DTC2
A	1834	THR	-	expression tag	UNP P0DTC2
A	1835	ILE	-	expression tag	UNP P0DTC2
A	1836	ASP	-	expression tag	UNP P0DTC2
A	1837	LYS	-	expression tag	UNP P0DTC2
A	1838	GLU	-	expression tag	UNP P0DTC2
A	1839	LYS	-	expression tag	UNP P0DTC2
A	1840	TRP	-	expression tag	UNP P0DTC2
A	1841	LYS	-	expression tag	UNP P0DTC2
A	1842	GLU	-	expression tag	UNP P0DTC2
A	1843	TRP	-	expression tag	UNP P0DTC2
A	1844	ARG	-	expression tag	UNP P0DTC2
A	1845	LYS	-	expression tag	UNP P0DTC2
A	1846	GLU	-	expression tag	UNP P0DTC2
A	1847	MET	-	expression tag	UNP P0DTC2
A	1848	GLU	-	expression tag	UNP P0DTC2
A	1849	ASN	-	expression tag	UNP P0DTC2
A	1850	LEU	-	expression tag	UNP P0DTC2
A	1851	THR	-	expression tag	UNP P0DTC2
A	1852	LYS	-	expression tag	UNP P0DTC2
A	1853	GLU	-	expression tag	UNP P0DTC2
A	1854	ILE	-	expression tag	UNP P0DTC2
A	1855	LYS	-	expression tag	UNP P0DTC2
A	1856	GLU	-	expression tag	UNP P0DTC2
A	1857	THR	-	expression tag	UNP P0DTC2
A	1858	LEU	-	expression tag	UNP P0DTC2
A	1859	GLU	-	expression tag	UNP P0DTC2
A	1860	GLU	-	expression tag	UNP P0DTC2
A	1861	ALA	-	expression tag	UNP P0DTC2
A	1862	ARG	-	expression tag	UNP P0DTC2
A	1863	LYS	-	expression tag	UNP P0DTC2
A	1864	THR	-	expression tag	UNP P0DTC2
A	1865	LEU	-	expression tag	UNP P0DTC2
A	1866	LYS	-	expression tag	UNP P0DTC2
A	1867	GLN	-	expression tag	UNP P0DTC2
A	1868	ALA	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

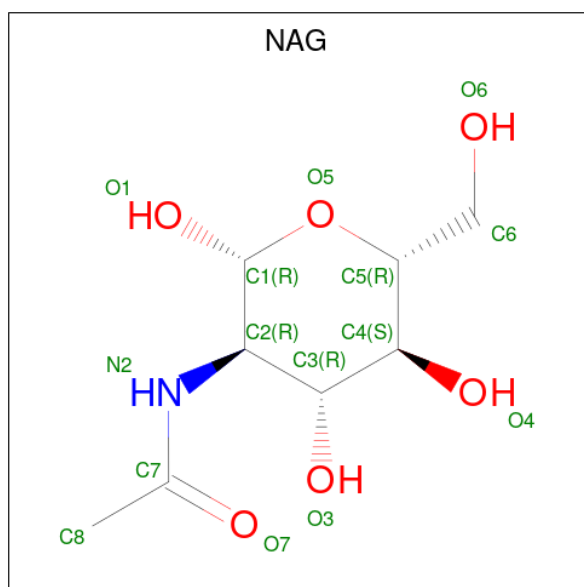
Chain	Residue	Modelled	Actual	Comment	Reference
A	1869	GLU	-	expression tag	UNP P0DTC2
A	1870	GLU	-	expression tag	UNP P0DTC2
A	1871	THR	-	expression tag	UNP P0DTC2
A	1872	PHE	-	expression tag	UNP P0DTC2
A	1873	LYS	-	expression tag	UNP P0DTC2
A	1874	THR	-	expression tag	UNP P0DTC2
A	1875	PRO	-	expression tag	UNP P0DTC2
A	1876	SER	-	expression tag	UNP P0DTC2
A	1877	SER	-	expression tag	UNP P0DTC2
A	1878	GLY	-	expression tag	UNP P0DTC2
A	1879	GLY	-	expression tag	UNP P0DTC2
A	1880	THR	-	expression tag	UNP P0DTC2
A	1881	ASP	-	expression tag	UNP P0DTC2
A	1882	ASP	-	expression tag	UNP P0DTC2
A	1883	ASP	-	expression tag	UNP P0DTC2
A	1884	ASP	-	expression tag	UNP P0DTC2
A	1885	LYS	-	expression tag	UNP P0DTC2
A	1886	THR	-	expression tag	UNP P0DTC2
A	1887	GLY	-	expression tag	UNP P0DTC2
A	1888	SER	-	expression tag	UNP P0DTC2
A	1889	LEU	-	expression tag	UNP P0DTC2
A	1890	ASN	-	expression tag	UNP P0DTC2
A	1891	ASP	-	expression tag	UNP P0DTC2
A	1892	ILE	-	expression tag	UNP P0DTC2
A	1893	PHE	-	expression tag	UNP P0DTC2
A	1894	GLU	-	expression tag	UNP P0DTC2
A	1895	ALA	-	expression tag	UNP P0DTC2
A	1896	GLN	-	expression tag	UNP P0DTC2
A	1897	LYS	-	expression tag	UNP P0DTC2
A	1898	ILE	-	expression tag	UNP P0DTC2
A	1899	GLU	-	expression tag	UNP P0DTC2
A	1900	TRP	-	expression tag	UNP P0DTC2
A	1901	HIS	-	expression tag	UNP P0DTC2
A	1902	GLU	-	expression tag	UNP P0DTC2
A	1903	GLN	-	expression tag	UNP P0DTC2
A	1904	GLY	-	expression tag	UNP P0DTC2
A	1905	SER	-	expression tag	UNP P0DTC2
A	1906	HIS	-	expression tag	UNP P0DTC2
A	1907	HIS	-	expression tag	UNP P0DTC2
A	1908	HIS	-	expression tag	UNP P0DTC2
A	1909	HIS	-	expression tag	UNP P0DTC2
A	1910	HIS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1911	HIS	-	expression tag	UNP P0DTC2
A	1912	HIS	-	expression tag	UNP P0DTC2
A	1913	HIS	-	expression tag	UNP P0DTC2

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



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

Continued on next page...

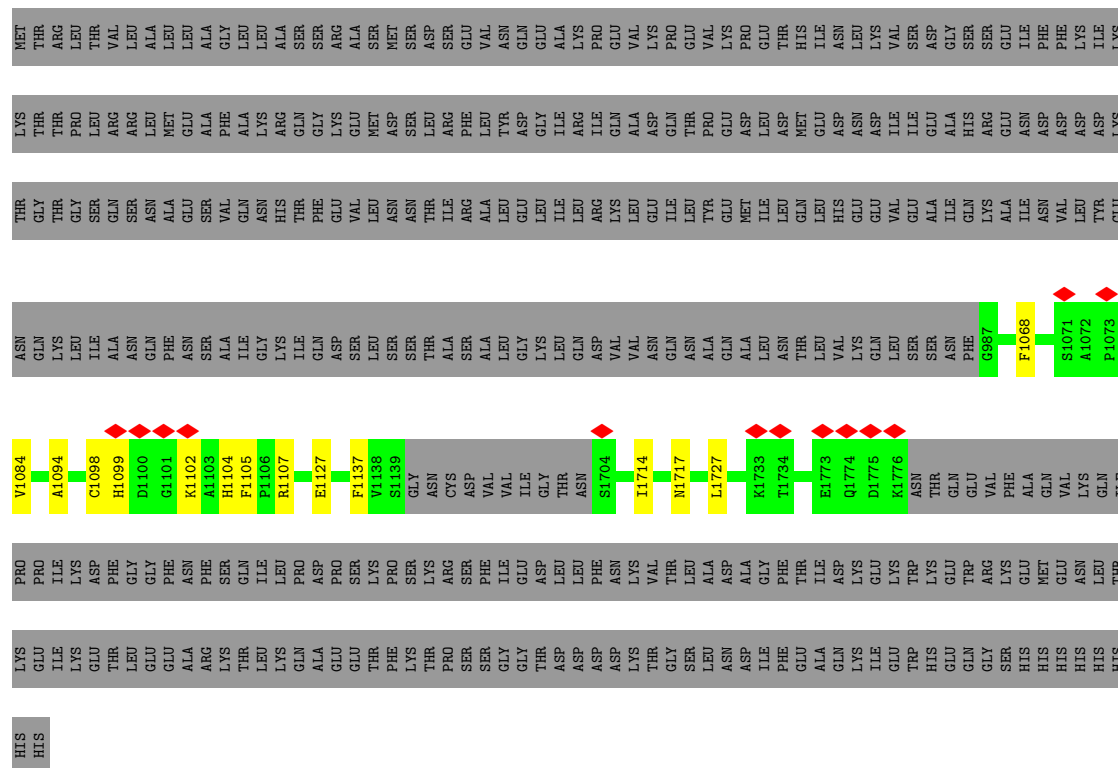
Continued from previous page...

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	B	21	Total	O	0
			21	21	
3	C	21	Total	O	0
			21	21	
3	A	21	Total	O	0
			21	21	

- Molecule 1: Spike protein S2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	225859	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.851	Depositor
Minimum map value	-3.536	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	1	Depositor
Map size (Å)	530.56, 530.56, 530.56	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	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	0.70	0/1680	0.88	14/2295 (0.6%)
1	B	0.70	0/1680	0.87	14/2295 (0.6%)
1	C	0.70	0/1680	0.88	14/2295 (0.6%)
All	All	0.70	0/5040	0.88	42/6885 (0.6%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1127	GLU	CA-C-N	7.70	127.69	119.76
1	B	1127	GLU	C-N-CA	7.70	127.69	119.76
1	A	1127	GLU	CA-C-N	7.67	127.67	119.76
1	A	1127	GLU	C-N-CA	7.67	127.67	119.76
1	C	1127	GLU	CA-C-N	7.66	127.65	119.76
1	C	1127	GLU	C-N-CA	7.66	127.65	119.76
1	C	1094	ALA	CA-C-N	6.45	126.38	119.28
1	C	1094	ALA	C-N-CA	6.45	126.38	119.28
1	A	1094	ALA	CA-C-N	6.45	126.37	119.28
1	A	1094	ALA	C-N-CA	6.45	126.37	119.28
1	B	1094	ALA	CA-C-N	6.43	126.36	119.28
1	B	1094	ALA	C-N-CA	6.43	126.36	119.28
1	B	1714	ILE	CA-C-N	6.42	126.45	119.90
1	B	1714	ILE	C-N-CA	6.42	126.45	119.90
1	A	1714	ILE	CA-C-N	6.41	126.44	119.90
1	A	1714	ILE	C-N-CA	6.41	126.44	119.90
1	C	1714	ILE	CA-C-N	6.40	126.43	119.90
1	C	1714	ILE	C-N-CA	6.40	126.43	119.90
1	A	1068	PHE	CA-C-N	6.24	126.76	120.14
1	A	1068	PHE	C-N-CA	6.24	126.76	120.14
1	C	1068	PHE	CA-C-N	6.23	126.75	120.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1068	PHE	C-N-CA	6.23	126.75	120.14
1	B	1068	PHE	CA-C-N	6.22	126.74	120.14
1	B	1068	PHE	C-N-CA	6.22	126.74	120.14
1	B	1727	LEU	CA-C-N	6.16	125.92	119.76
1	B	1727	LEU	C-N-CA	6.16	125.92	119.76
1	B	1105	PHE	CA-C-N	6.14	126.05	119.85
1	B	1105	PHE	C-N-CA	6.14	126.05	119.85
1	A	1105	PHE	CA-C-N	6.13	126.04	119.85
1	A	1105	PHE	C-N-CA	6.13	126.04	119.85
1	C	1105	PHE	CA-C-N	6.12	126.03	119.85
1	C	1105	PHE	C-N-CA	6.12	126.03	119.85
1	A	1727	LEU	CA-C-N	6.12	125.88	119.76
1	A	1727	LEU	C-N-CA	6.12	125.88	119.76
1	C	1727	LEU	CA-C-N	6.08	125.84	119.76
1	C	1727	LEU	C-N-CA	6.08	125.84	119.76
1	A	1084	VAL	CA-C-N	5.10	125.39	119.93
1	A	1084	VAL	C-N-CA	5.10	125.39	119.93
1	C	1084	VAL	CA-C-N	5.10	125.39	119.93
1	C	1084	VAL	C-N-CA	5.10	125.39	119.93
1	B	1084	VAL	CA-C-N	5.09	125.37	119.93
1	B	1084	VAL	C-N-CA	5.09	125.37	119.93

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	1649	0	1524	4	0
1	B	1649	0	1524	6	0
1	C	1649	0	1524	5	0
2	A	56	0	52	0	0
2	B	56	0	52	0	0
2	C	56	0	52	0	0
3	A	21	0	0	0	0
3	B	21	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	21	0	0	0	0
All	All	5178	0	4728	15	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 (15) 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:1107:ARG:HG2	1:A:1137:PHE:CE2	2.41	0.55
1:C:1107:ARG:HG2	1:C:1137:PHE:CE2	2.41	0.54
1:B:1107:ARG:HG2	1:B:1137:PHE:CE2	2.41	0.54
1:C:1098:CYS:HA	1:C:1102:LYS:O	2.10	0.52
1:A:1098:CYS:HA	1:A:1102:LYS:O	2.10	0.51
1:B:1098:CYS:HA	1:B:1102:LYS:O	2.10	0.51
1:B:1099:HIS:HB3	1:B:1104:HIS:CD2	2.54	0.43
1:B:1099:HIS:HB3	1:B:1104:HIS:CG	2.54	0.43
1:A:1099:HIS:HB3	1:A:1104:HIS:CD2	2.54	0.43
1:C:1099:HIS:HB3	1:C:1104:HIS:CD2	2.54	0.42
1:A:1099:HIS:HB3	1:A:1104:HIS:CG	2.54	0.42
1:C:1099:HIS:HB3	1:C:1104:HIS:CG	2.54	0.42
1:B:1105:PHE:CE1	1:B:1137:PHE:HB2	2.56	0.41
1:C:1105:PHE:CE1	1:C:1137:PHE:HB2	2.56	0.41
1:B:1084:VAL:HA	1:B:1085:PRO:HD3	1.95	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	222/605 (37%)	218 (98%)	4 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	222/605 (37%)	218 (98%)	4 (2%)	0	100	100
1	C	222/605 (37%)	218 (98%)	4 (2%)	0	100	100
All	All	666/1815 (37%)	654 (98%)	12 (2%)	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	155/533 (29%)	154 (99%)	1 (1%)	78	91
1	B	155/533 (29%)	154 (99%)	1 (1%)	78	91
1	C	155/533 (29%)	154 (99%)	1 (1%)	78	91
All	All	465/1599 (29%)	462 (99%)	3 (1%)	76	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1717	ASN
1	C	1717	ASN
1	A	1717	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1021	GLN
1	B	1027	GLN
1	B	1099	HIS
1	B	1104	HIS
1	C	1021	GLN
1	C	1027	GLN
1	C	1099	HIS
1	C	1104	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1021	GLN
1	A	1099	HIS
1	A	1104	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	A	1404	1	14,14,15	1.31	1 (7%)	17,19,21	1.12	2 (11%)
2	NAG	B	1404	1	14,14,15	1.29	1 (7%)	17,19,21	1.11	2 (11%)
2	NAG	A	1401	1	14,14,15	1.21	2 (14%)	17,19,21	1.24	2 (11%)
2	NAG	A	1402	1	14,14,15	1.32	1 (7%)	17,19,21	1.23	2 (11%)
2	NAG	C	1403	1	14,14,15	0.51	0	17,19,21	0.71	1 (5%)
2	NAG	B	1401	1	14,14,15	1.20	2 (14%)	17,19,21	1.23	2 (11%)
2	NAG	B	1402	1	14,14,15	1.32	1 (7%)	17,19,21	1.23	2 (11%)
2	NAG	C	1401	1	14,14,15	1.21	2 (14%)	17,19,21	1.24	2 (11%)
2	NAG	C	1402	1	14,14,15	1.32	1 (7%)	17,19,21	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1403	1	14,14,15	0.53	0	17,19,21	0.71	1 (5%)
2	NAG	C	1404	1	14,14,15	1.31	2 (14%)	17,19,21	1.12	2 (11%)
2	NAG	A	1403	1	14,14,15	0.52	0	17,19,21	0.71	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
2	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1403	1	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1402	NAG	C1-C2	3.95	1.57	1.52
2	A	1402	NAG	C1-C2	3.94	1.57	1.52
2	B	1402	NAG	C1-C2	3.91	1.57	1.52
2	A	1404	NAG	C1-C2	3.83	1.57	1.52
2	C	1404	NAG	C1-C2	3.81	1.57	1.52
2	B	1404	NAG	C1-C2	3.76	1.57	1.52
2	A	1401	NAG	C1-C2	3.62	1.57	1.52
2	C	1401	NAG	C1-C2	3.61	1.57	1.52
2	B	1401	NAG	C1-C2	3.59	1.57	1.52
2	A	1401	NAG	O5-C5	2.03	1.47	1.43
2	C	1401	NAG	O5-C5	2.03	1.47	1.43
2	B	1401	NAG	O5-C5	2.03	1.47	1.43
2	C	1404	NAG	O5-C5	2.00	1.47	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	NAG	C2-N2-C7	-2.88	119.04	122.90
2	C	1401	NAG	C2-N2-C7	-2.88	119.04	122.90
2	B	1401	NAG	C2-N2-C7	-2.87	119.05	122.90
2	B	1402	NAG	C2-N2-C7	-2.67	119.32	122.90
2	A	1402	NAG	C2-N2-C7	-2.66	119.33	122.90
2	C	1402	NAG	C2-N2-C7	-2.66	119.34	122.90
2	C	1402	NAG	C8-C7-N2	2.51	120.28	116.12
2	B	1402	NAG	C8-C7-N2	2.50	120.26	116.12
2	A	1402	NAG	C8-C7-N2	2.49	120.25	116.12
2	C	1404	NAG	C8-C7-N2	2.42	120.13	116.12
2	B	1404	NAG	C8-C7-N2	2.41	120.12	116.12
2	A	1404	NAG	C8-C7-N2	2.41	120.11	116.12
2	A	1401	NAG	C8-C7-N2	2.38	120.07	116.12
2	C	1401	NAG	C8-C7-N2	2.38	120.06	116.12
2	B	1401	NAG	C8-C7-N2	2.37	120.05	116.12
2	A	1404	NAG	C2-N2-C7	-2.35	119.75	122.90
2	C	1404	NAG	C2-N2-C7	-2.34	119.76	122.90
2	B	1404	NAG	C2-N2-C7	-2.34	119.77	122.90
2	C	1403	NAG	C2-N2-C7	-2.05	120.15	122.90
2	A	1403	NAG	C2-N2-C7	-2.03	120.18	122.90
2	B	1403	NAG	C2-N2-C7	-2.02	120.19	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

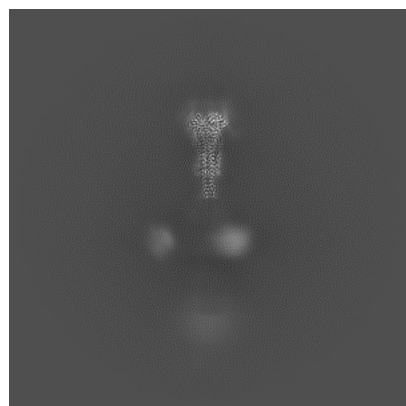
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75697. These allow visual inspection of the internal detail of the map and identification of artifacts.

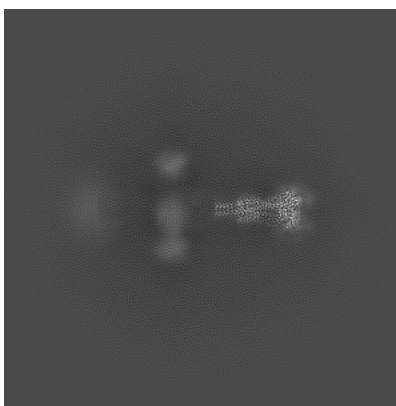
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

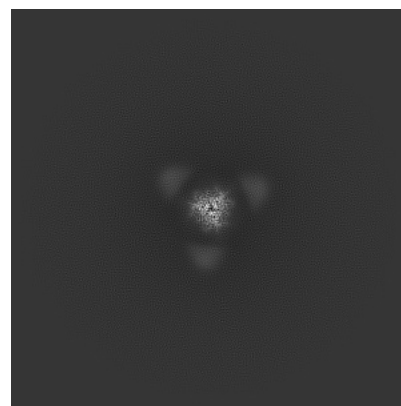
6.1.1 Primary map



X

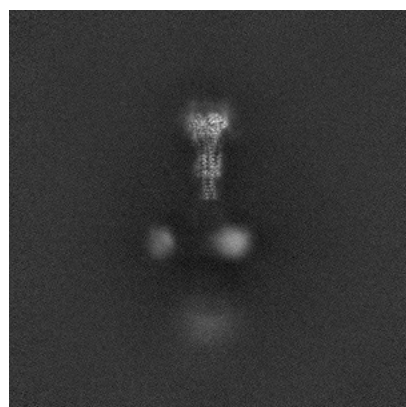


Y

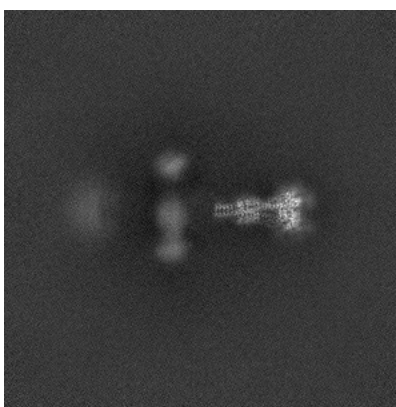


Z

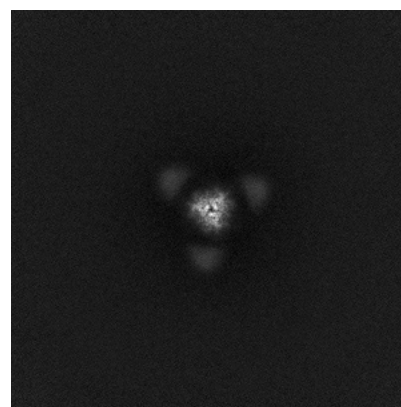
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

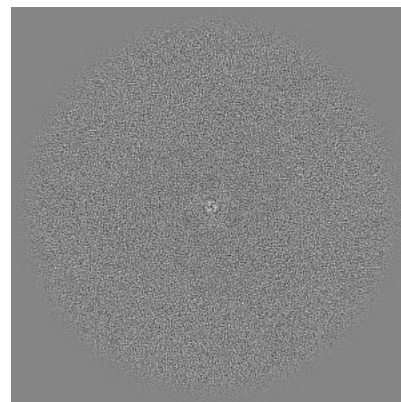
6.2.1 Primary map



X Index: 320



Y Index: 320



Z Index: 320

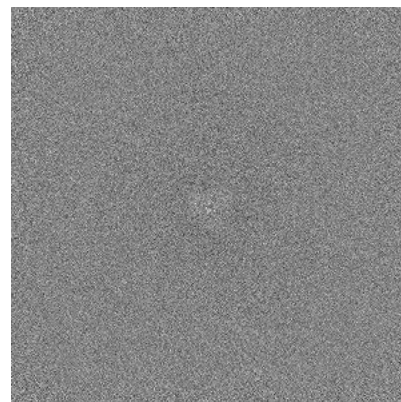
6.2.2 Raw map



X Index: 320



Y Index: 320

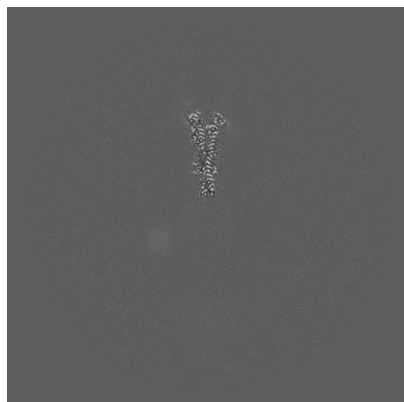


Z Index: 320

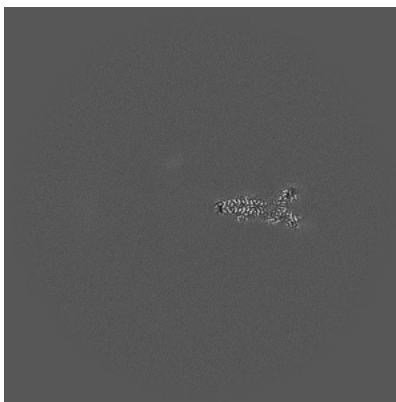
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

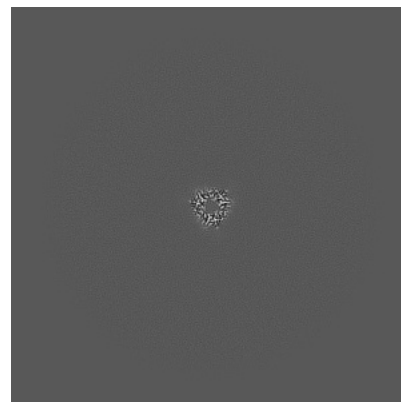
6.3.1 Primary map



X Index: 326



Y Index: 324



Z Index: 461

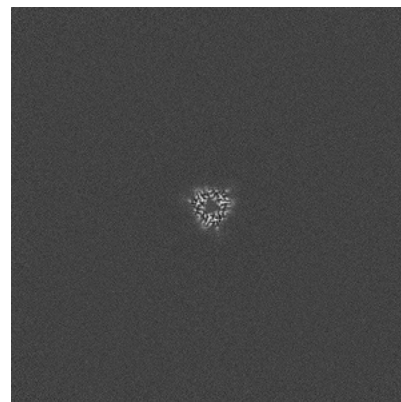
6.3.2 Raw map



X Index: 326



Y Index: 324

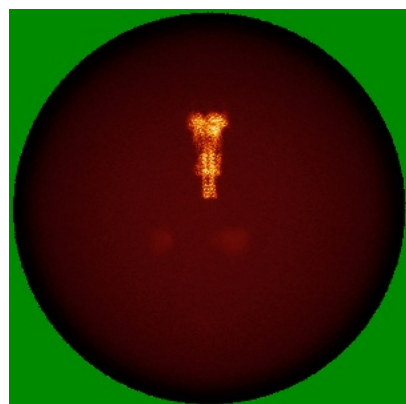


Z Index: 461

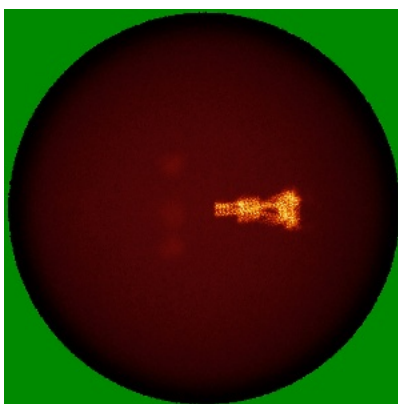
The images above show the largest variance slices of the map in three orthogonal directions.

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

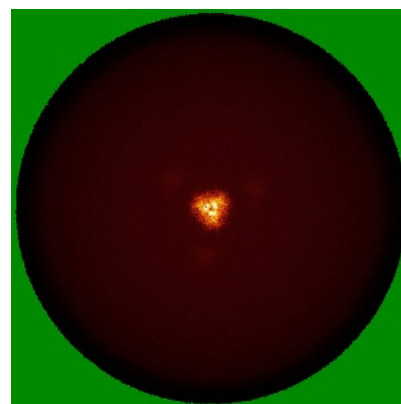
6.4.1 Primary map



X

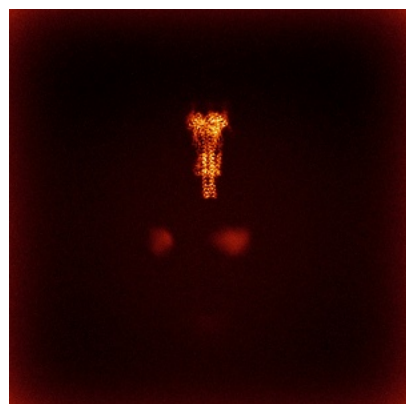


Y

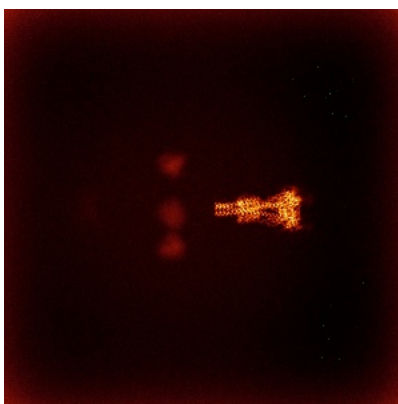


Z

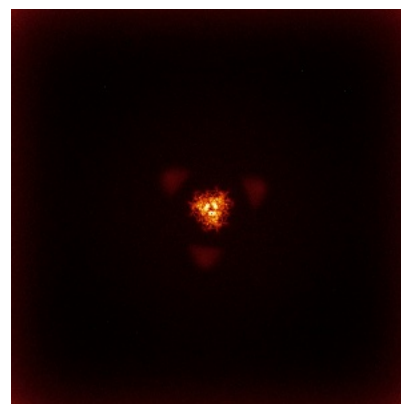
6.4.2 Raw map



X



Y

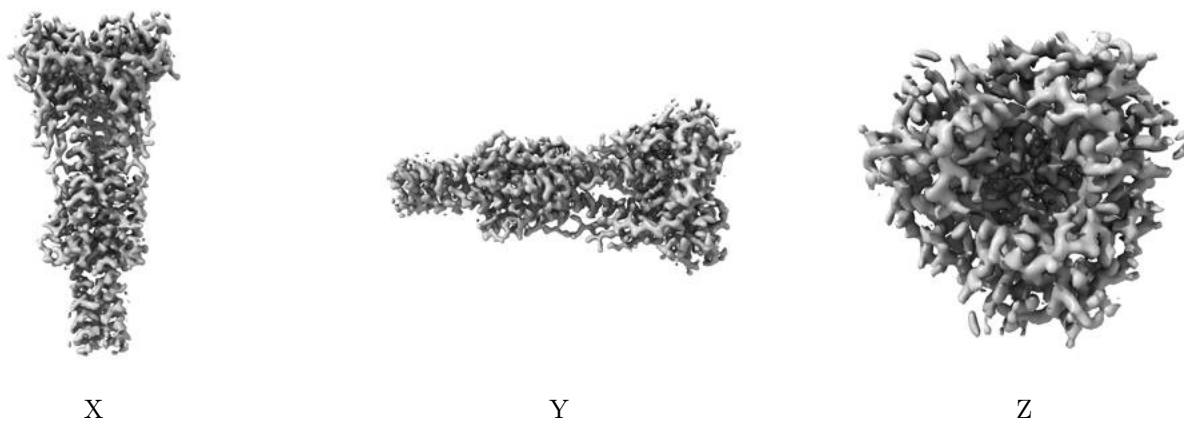


Z

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.

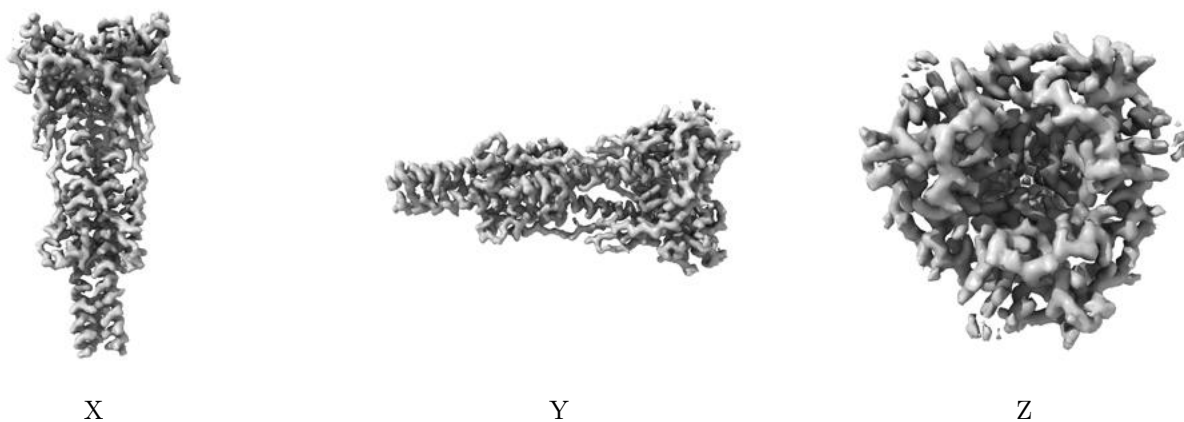
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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



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.

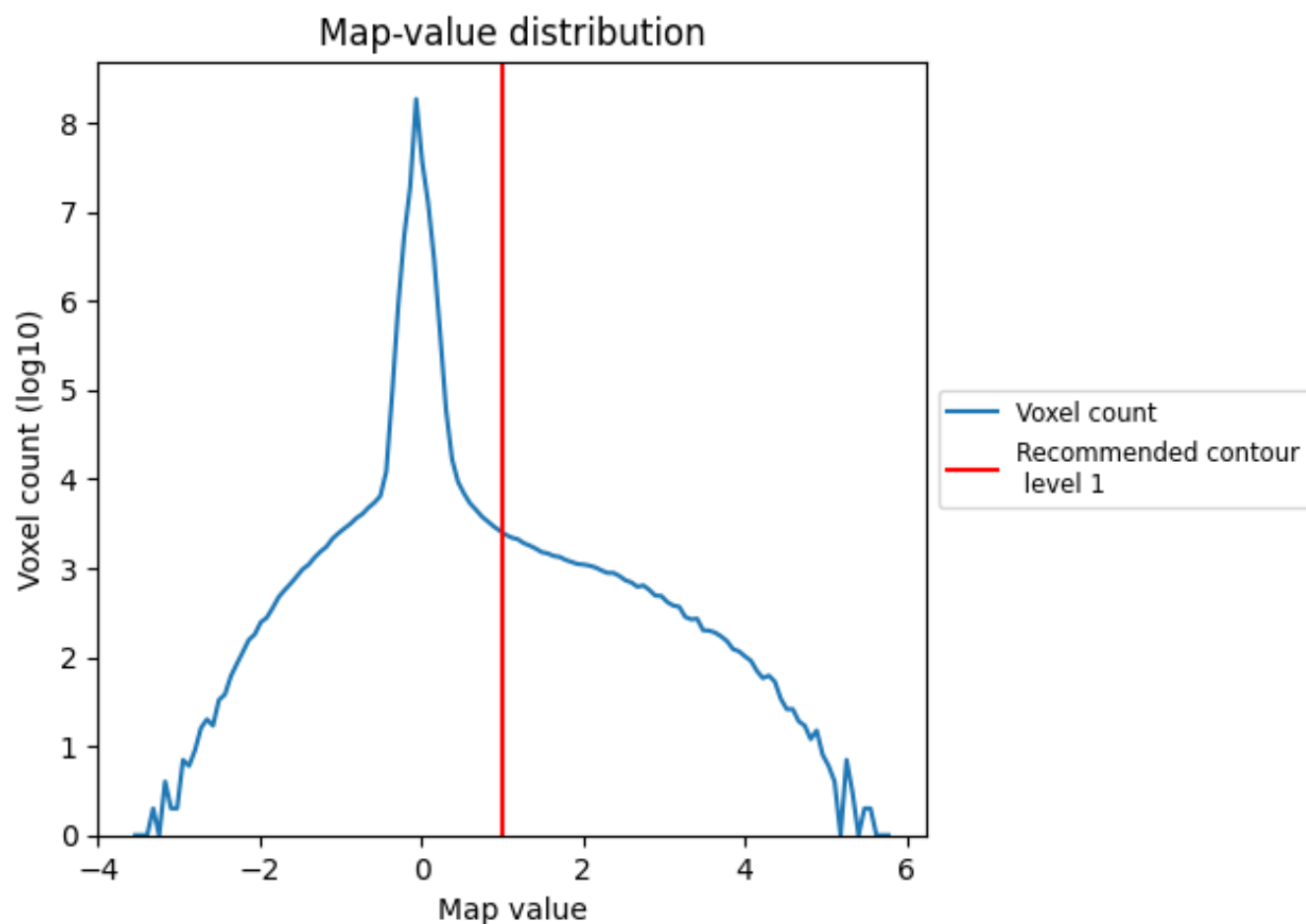
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

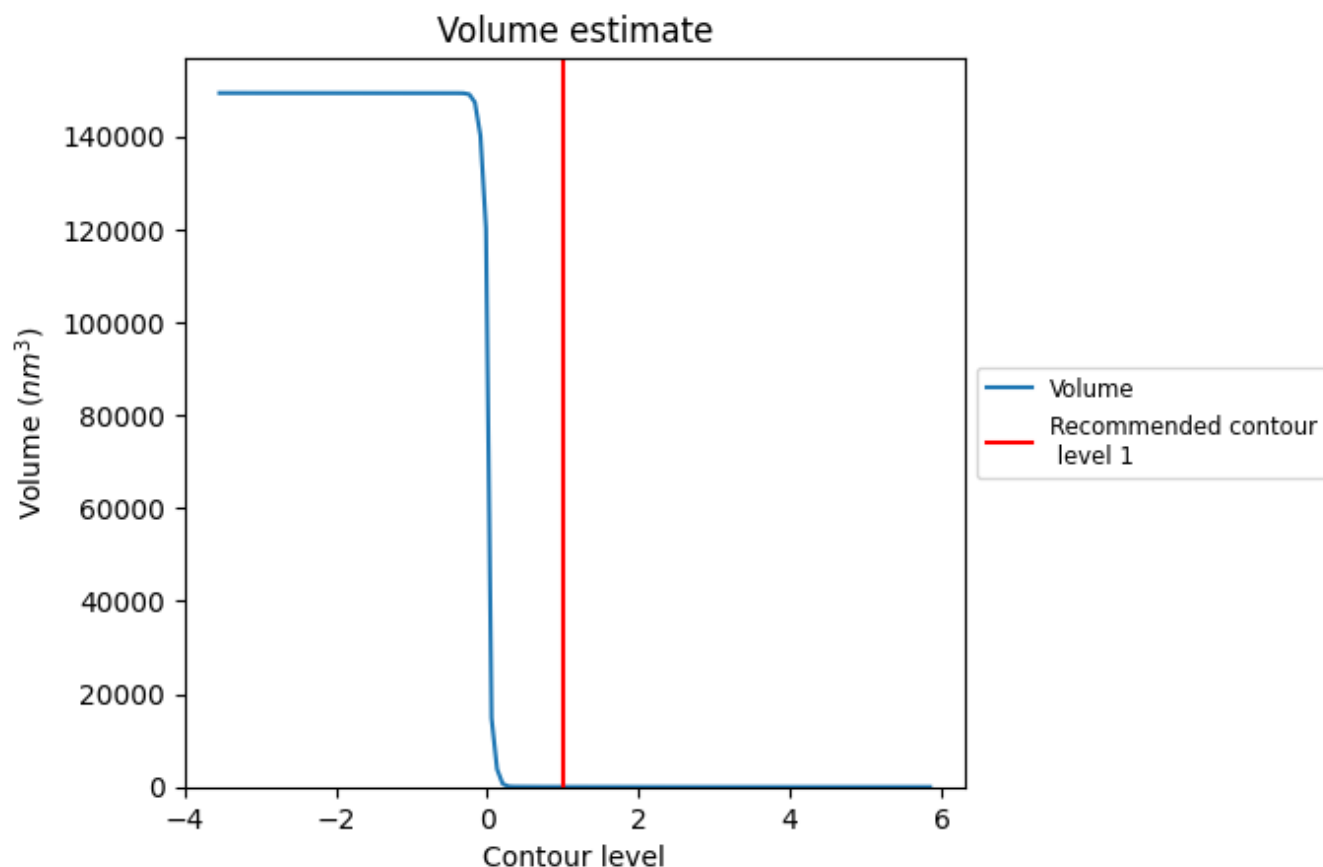
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

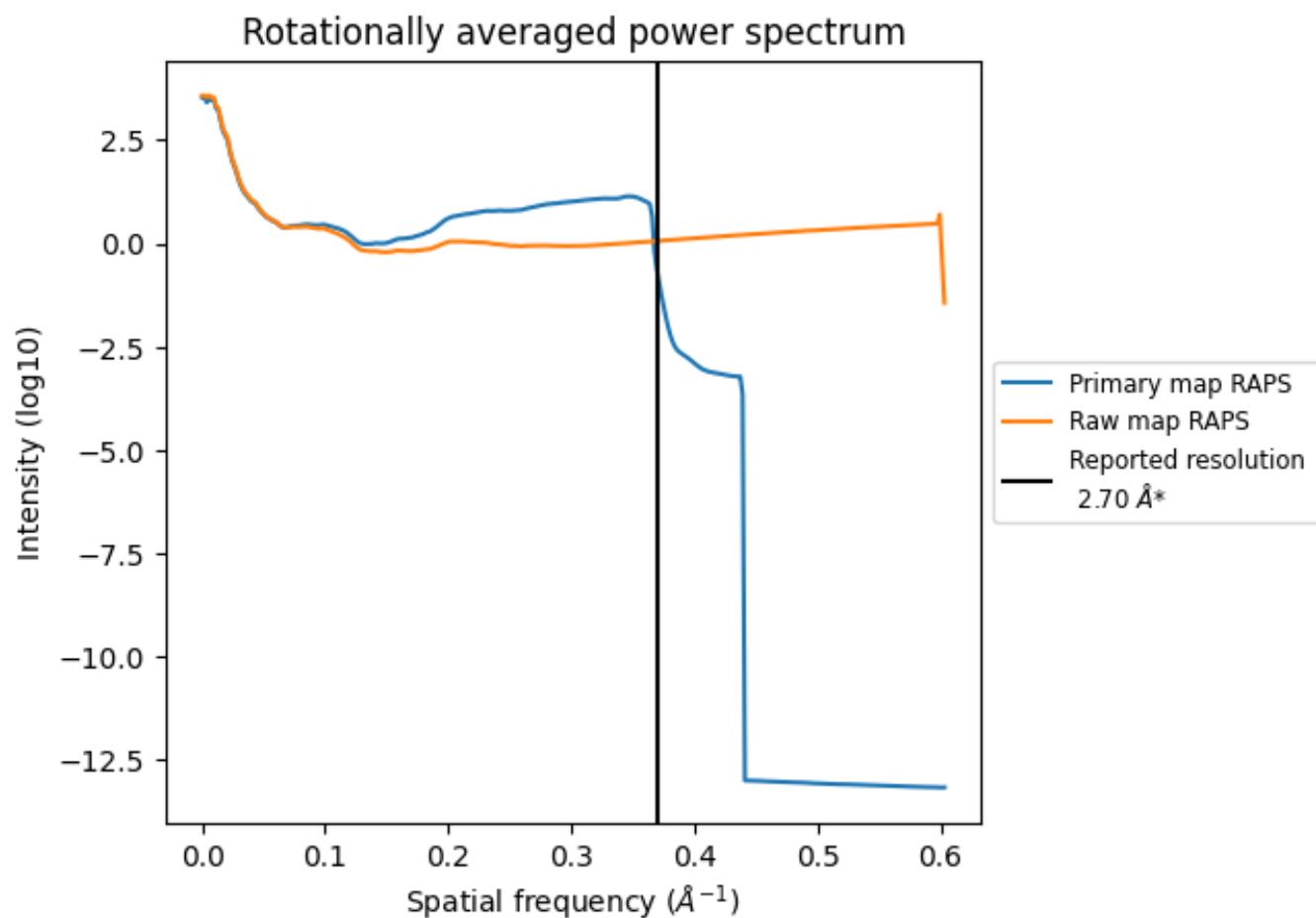
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 21 nm^3 ; this corresponds to an approximate mass of 19 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 ⓘ

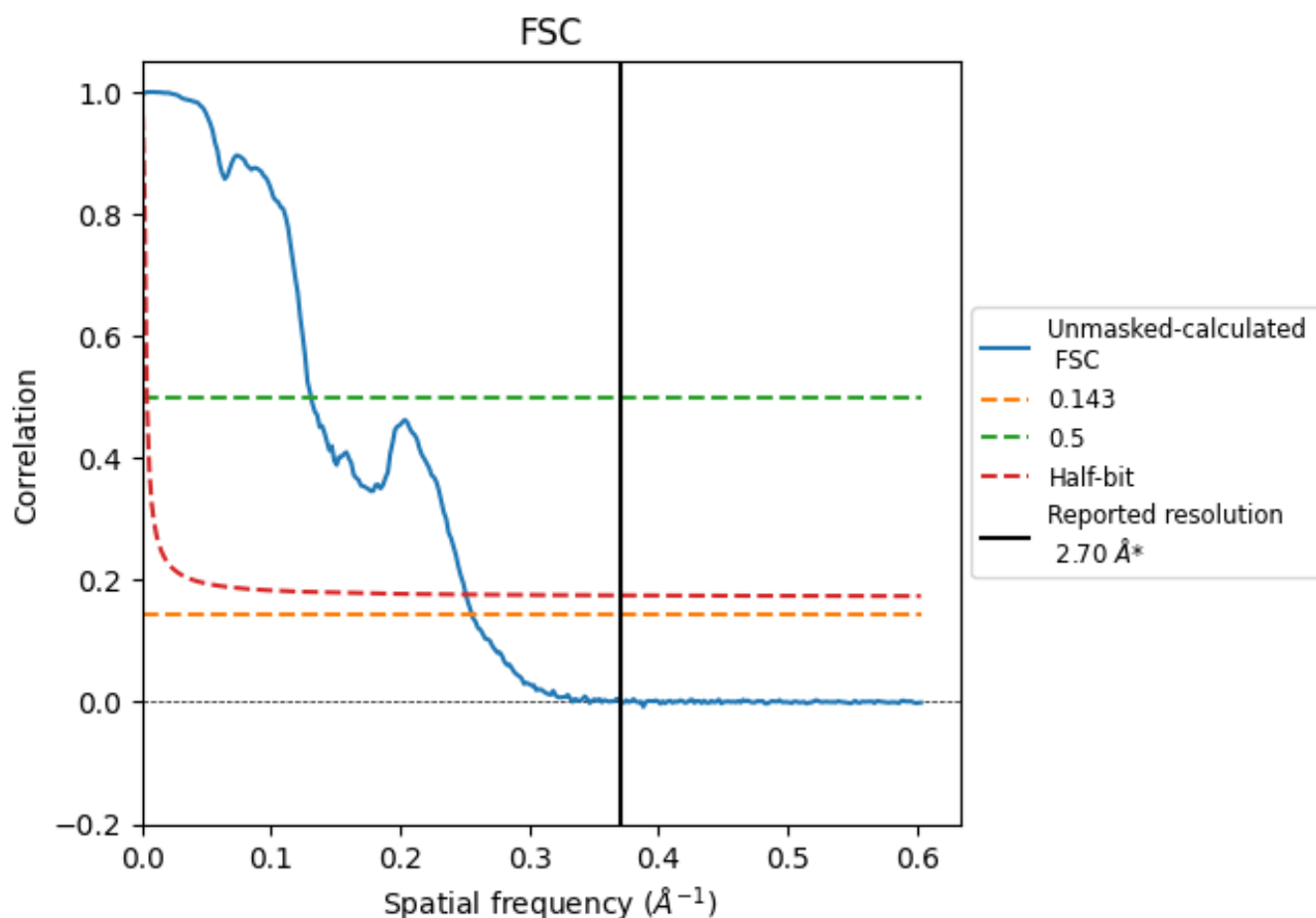


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

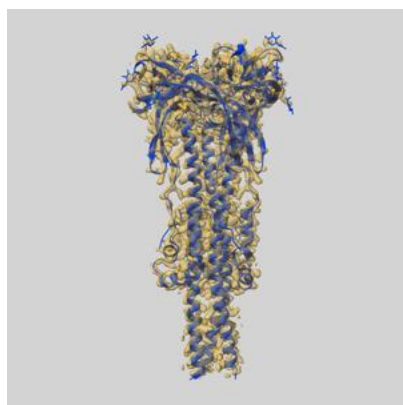
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	7.65	3.99

*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 3.91 differs from the reported value 2.7 by more than 10 %

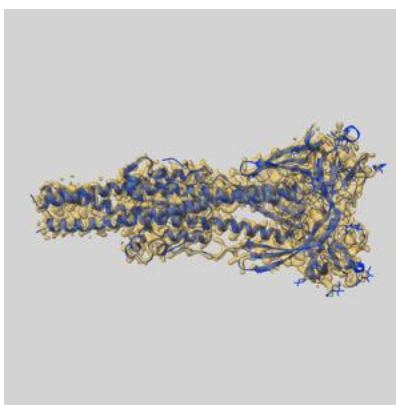
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75697 and PDB model 11HN. Per-residue inclusion information can be found in section [3](#) on page [17](#).

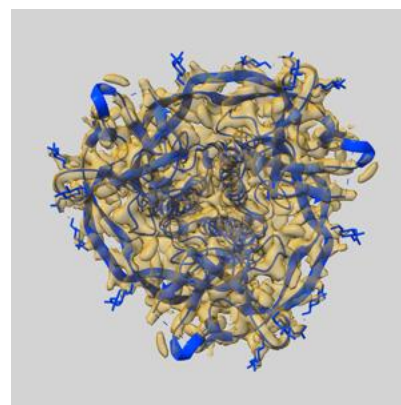
9.1 Map-model overlay [i](#)



X



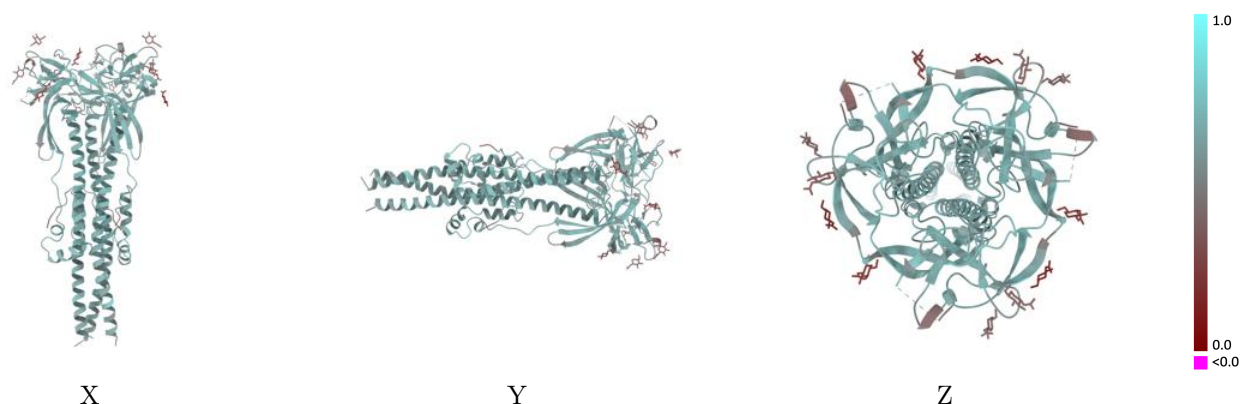
Y



Z

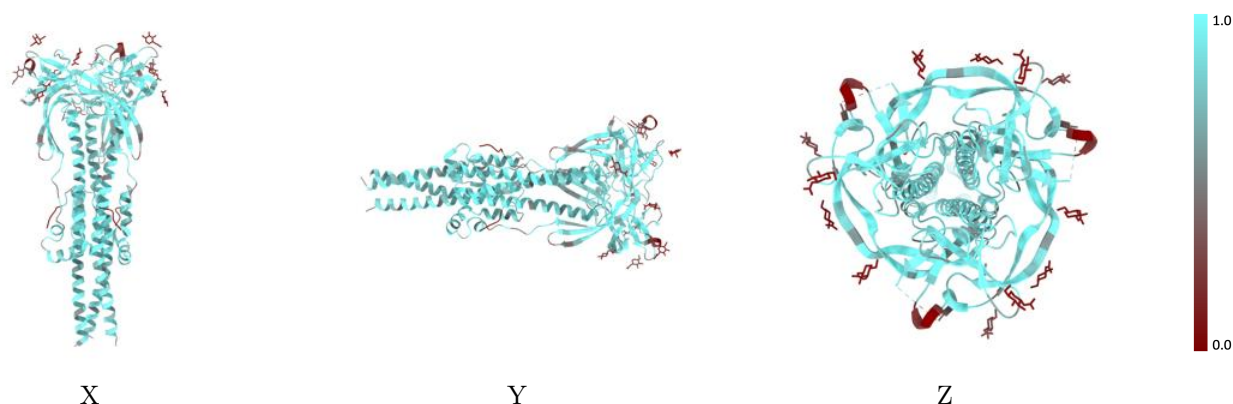
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



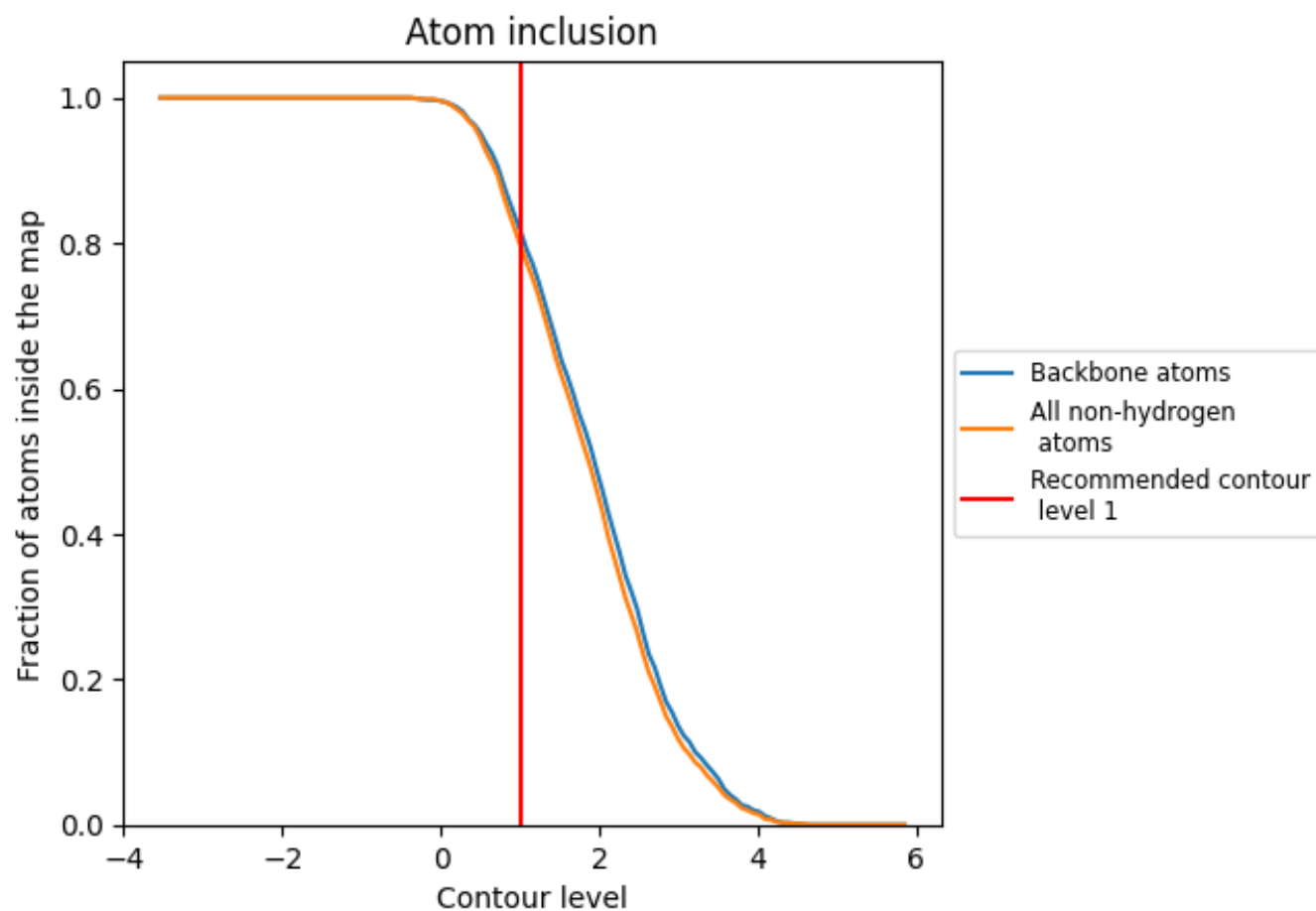
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.6060
A	0.7980	0.6060
B	0.8010	0.6050
C	0.8020	0.6070

