



Full wwPDB EM Validation Report ⓘ

May 21, 2026 – 12:49 AM EDT

PDB ID : 11HK / pdb_000011hk
EMDB ID : EMD-75694
Title : SARS-CoV-2 spike S2 trimer stabilized in the early fusion intermediate conformation (E-FICs-v3) bound to the VN01H1 Fab (Fab 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:

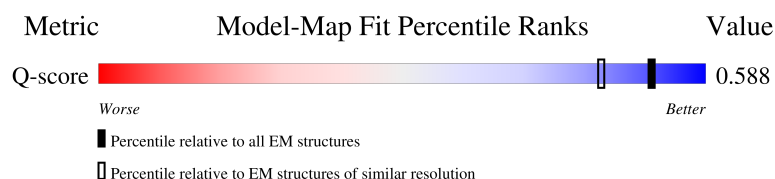
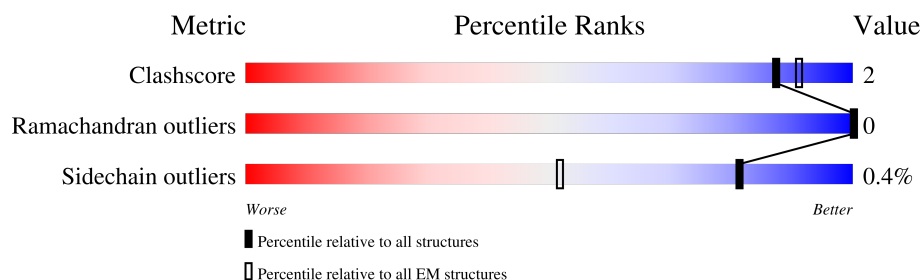
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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.





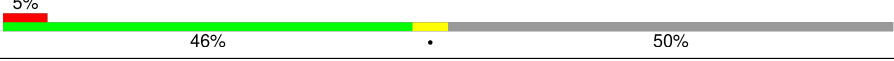

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	D	605	
1	G	605	
2	B	226	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	226	
2	H	226	
3	C	215	
3	F	215	
3	I	215	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9288 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 E-FICS-v3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	186	Total	C	N	O	S	0	0
			1389	893	241	253	2		
1	D	186	Total	C	N	O	S	0	0
			1389	893	241	253	2		
1	G	186	Total	C	N	O	S	0	0
			1389	893	241	253	2		

There are 489 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q12306
A	-18	THR	-	expression tag	UNP Q12306
A	-17	ARG	-	expression tag	UNP Q12306
A	-16	LEU	-	expression tag	UNP Q12306
A	-15	THR	-	expression tag	UNP Q12306
A	-14	VAL	-	expression tag	UNP Q12306
A	-13	LEU	-	expression tag	UNP Q12306
A	-12	ALA	-	expression tag	UNP Q12306
A	-11	LEU	-	expression tag	UNP Q12306
A	-10	LEU	-	expression tag	UNP Q12306
A	-9	ALA	-	expression tag	UNP Q12306
A	-8	GLY	-	expression tag	UNP Q12306
A	-7	LEU	-	expression tag	UNP Q12306
A	-6	LEU	-	expression tag	UNP Q12306
A	-5	ALA	-	expression tag	UNP Q12306
A	-4	SER	-	expression tag	UNP Q12306
A	-3	SER	-	expression tag	UNP Q12306
A	-2	ARG	-	expression tag	UNP Q12306
A	-1	ALA	-	expression tag	UNP Q12306
A	0	SER	-	expression tag	UNP Q12306
A	95	ASN	-	linker	UNP Q12306
A	96	ASP	-	linker	UNP Q12306
A	97	ASP	-	linker	UNP Q12306
A	98	ASP	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	ASP	-	linker	UNP Q12306
A	100	LYS	-	linker	UNP Q12306
A	101	THR	-	linker	UNP Q12306
A	102	GLY	-	linker	UNP Q12306
A	103	THR	-	linker	UNP Q12306
A	104	GLY	-	linker	UNP Q12306
A	105	SER	-	linker	UNP Q12306
A	106	GLN	-	linker	UNP Q12306
A	107	SER	-	linker	UNP Q12306
A	108	ASN	-	linker	UNP Q12306
A	109	ALA	-	linker	UNP Q12306
A	110	GLU	-	linker	UNP Q12306
A	111	SER	-	linker	UNP Q12306
A	112	VAL	-	linker	UNP Q12306
A	113	GLN	-	linker	UNP Q12306
A	114	ASN	-	linker	UNP Q12306
A	115	HIS	-	linker	UNP Q12306
A	116	THR	-	linker	UNP Q12306
A	117	PHE	-	linker	UNP Q12306
A	118	GLU	-	linker	UNP Q12306
A	119	VAL	-	linker	UNP Q12306
A	120	LEU	-	linker	UNP Q12306
A	121	ASN	-	linker	UNP Q12306
A	122	ASN	-	linker	UNP Q12306
A	123	THR	-	linker	UNP Q12306
A	124	ILE	-	linker	UNP Q12306
A	125	ARG	-	linker	UNP Q12306
A	126	ALA	-	linker	UNP Q12306
A	127	LEU	-	linker	UNP Q12306
A	128	GLU	-	linker	UNP Q12306
A	129	LEU	-	linker	UNP Q12306
A	130	ILE	-	linker	UNP Q12306
A	131	LEU	-	linker	UNP Q12306
A	132	ARG	-	linker	UNP Q12306
A	133	LYS	-	linker	UNP Q12306
A	134	LEU	-	linker	UNP Q12306
A	135	GLU	-	linker	UNP Q12306
A	136	ILE	-	linker	UNP Q12306
A	137	LEU	-	linker	UNP Q12306
A	138	TYR	-	linker	UNP Q12306
A	139	GLU	-	linker	UNP Q12306
A	140	MET	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ILE	-	linker	UNP Q12306
A	142	LEU	-	linker	UNP Q12306
A	143	GLN	-	linker	UNP Q12306
A	144	LEU	-	linker	UNP Q12306
A	145	HIS	-	linker	UNP Q12306
A	146	GLU	-	linker	UNP Q12306
A	147	GLU	-	linker	UNP Q12306
A	148	VAL	-	linker	UNP Q12306
A	149	GLU	-	linker	UNP Q12306
A	150	ALA	-	linker	UNP Q12306
A	151	ILE	-	linker	UNP Q12306
A	152	GLN	-	linker	UNP Q12306
A	153	LYS	-	linker	UNP Q12306
A	154	ALA	-	linker	UNP Q12306
A	155	ILE	-	linker	UNP Q12306
A	985	ALA	ASP	conflict	UNP P0DTC2
A	1132	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	1911	HIS	-	expression tag	UNP P0DTC2
A	1912	HIS	-	expression tag	UNP P0DTC2
A	1913	HIS	-	expression tag	UNP P0DTC2
D	-19	MET	-	initiating methionine	UNP Q12306
D	-18	THR	-	expression tag	UNP Q12306
D	-17	ARG	-	expression tag	UNP Q12306
D	-16	LEU	-	expression tag	UNP Q12306
D	-15	THR	-	expression tag	UNP Q12306
D	-14	VAL	-	expression tag	UNP Q12306
D	-13	LEU	-	expression tag	UNP Q12306
D	-12	ALA	-	expression tag	UNP Q12306
D	-11	LEU	-	expression tag	UNP Q12306
D	-10	LEU	-	expression tag	UNP Q12306
D	-9	ALA	-	expression tag	UNP Q12306
D	-8	GLY	-	expression tag	UNP Q12306
D	-7	LEU	-	expression tag	UNP Q12306
D	-6	LEU	-	expression tag	UNP Q12306
D	-5	ALA	-	expression tag	UNP Q12306
D	-4	SER	-	expression tag	UNP Q12306
D	-3	SER	-	expression tag	UNP Q12306
D	-2	ARG	-	expression tag	UNP Q12306
D	-1	ALA	-	expression tag	UNP Q12306
D	0	SER	-	expression tag	UNP Q12306
D	95	ASN	-	linker	UNP Q12306
D	96	ASP	-	linker	UNP Q12306
D	97	ASP	-	linker	UNP Q12306
D	98	ASP	-	linker	UNP Q12306
D	99	ASP	-	linker	UNP Q12306
D	100	LYS	-	linker	UNP Q12306
D	101	THR	-	linker	UNP Q12306
D	102	GLY	-	linker	UNP Q12306
D	103	THR	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	104	GLY	-	linker	UNP Q12306
D	105	SER	-	linker	UNP Q12306
D	106	GLN	-	linker	UNP Q12306
D	107	SER	-	linker	UNP Q12306
D	108	ASN	-	linker	UNP Q12306
D	109	ALA	-	linker	UNP Q12306
D	110	GLU	-	linker	UNP Q12306
D	111	SER	-	linker	UNP Q12306
D	112	VAL	-	linker	UNP Q12306
D	113	GLN	-	linker	UNP Q12306
D	114	ASN	-	linker	UNP Q12306
D	115	HIS	-	linker	UNP Q12306
D	116	THR	-	linker	UNP Q12306
D	117	PHE	-	linker	UNP Q12306
D	118	GLU	-	linker	UNP Q12306
D	119	VAL	-	linker	UNP Q12306
D	120	LEU	-	linker	UNP Q12306
D	121	ASN	-	linker	UNP Q12306
D	122	ASN	-	linker	UNP Q12306
D	123	THR	-	linker	UNP Q12306
D	124	ILE	-	linker	UNP Q12306
D	125	ARG	-	linker	UNP Q12306
D	126	ALA	-	linker	UNP Q12306
D	127	LEU	-	linker	UNP Q12306
D	128	GLU	-	linker	UNP Q12306
D	129	LEU	-	linker	UNP Q12306
D	130	ILE	-	linker	UNP Q12306
D	131	LEU	-	linker	UNP Q12306
D	132	ARG	-	linker	UNP Q12306
D	133	LYS	-	linker	UNP Q12306
D	134	LEU	-	linker	UNP Q12306
D	135	GLU	-	linker	UNP Q12306
D	136	ILE	-	linker	UNP Q12306
D	137	LEU	-	linker	UNP Q12306
D	138	TYR	-	linker	UNP Q12306
D	139	GLU	-	linker	UNP Q12306
D	140	MET	-	linker	UNP Q12306
D	141	ILE	-	linker	UNP Q12306
D	142	LEU	-	linker	UNP Q12306
D	143	GLN	-	linker	UNP Q12306
D	144	LEU	-	linker	UNP Q12306
D	145	HIS	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	146	GLU	-	linker	UNP Q12306
D	147	GLU	-	linker	UNP Q12306
D	148	VAL	-	linker	UNP Q12306
D	149	GLU	-	linker	UNP Q12306
D	150	ALA	-	linker	UNP Q12306
D	151	ILE	-	linker	UNP Q12306
D	152	GLN	-	linker	UNP Q12306
D	153	LYS	-	linker	UNP Q12306
D	154	ALA	-	linker	UNP Q12306
D	155	ILE	-	linker	UNP Q12306
D	985	ALA	ASP	conflict	UNP P0DTC2
D	1132	THR	-	linker	UNP P0DTC2
D	1834	THR	-	expression tag	UNP P0DTC2
D	1835	ILE	-	expression tag	UNP P0DTC2
D	1836	ASP	-	expression tag	UNP P0DTC2
D	1837	LYS	-	expression tag	UNP P0DTC2
D	1838	GLU	-	expression tag	UNP P0DTC2
D	1839	LYS	-	expression tag	UNP P0DTC2
D	1840	TRP	-	expression tag	UNP P0DTC2
D	1841	LYS	-	expression tag	UNP P0DTC2
D	1842	GLU	-	expression tag	UNP P0DTC2
D	1843	TRP	-	expression tag	UNP P0DTC2
D	1844	ARG	-	expression tag	UNP P0DTC2
D	1845	LYS	-	expression tag	UNP P0DTC2
D	1846	GLU	-	expression tag	UNP P0DTC2
D	1847	MET	-	expression tag	UNP P0DTC2
D	1848	GLU	-	expression tag	UNP P0DTC2
D	1849	ASN	-	expression tag	UNP P0DTC2
D	1850	LEU	-	expression tag	UNP P0DTC2
D	1851	THR	-	expression tag	UNP P0DTC2
D	1852	LYS	-	expression tag	UNP P0DTC2
D	1853	GLU	-	expression tag	UNP P0DTC2
D	1854	ILE	-	expression tag	UNP P0DTC2
D	1855	LYS	-	expression tag	UNP P0DTC2
D	1856	GLU	-	expression tag	UNP P0DTC2
D	1857	THR	-	expression tag	UNP P0DTC2
D	1858	LEU	-	expression tag	UNP P0DTC2
D	1859	GLU	-	expression tag	UNP P0DTC2
D	1860	GLU	-	expression tag	UNP P0DTC2
D	1861	ALA	-	expression tag	UNP P0DTC2
D	1862	ARG	-	expression tag	UNP P0DTC2
D	1863	LYS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1906	HIS	-	expression tag	UNP P0DTC2
D	1907	HIS	-	expression tag	UNP P0DTC2
D	1908	HIS	-	expression tag	UNP P0DTC2
D	1909	HIS	-	expression tag	UNP P0DTC2
D	1910	HIS	-	expression tag	UNP P0DTC2
D	1911	HIS	-	expression tag	UNP P0DTC2
D	1912	HIS	-	expression tag	UNP P0DTC2
D	1913	HIS	-	expression tag	UNP P0DTC2
G	-19	MET	-	initiating methionine	UNP Q12306
G	-18	THR	-	expression tag	UNP Q12306
G	-17	ARG	-	expression tag	UNP Q12306
G	-16	LEU	-	expression tag	UNP Q12306
G	-15	THR	-	expression tag	UNP Q12306
G	-14	VAL	-	expression tag	UNP Q12306
G	-13	LEU	-	expression tag	UNP Q12306
G	-12	ALA	-	expression tag	UNP Q12306
G	-11	LEU	-	expression tag	UNP Q12306
G	-10	LEU	-	expression tag	UNP Q12306
G	-9	ALA	-	expression tag	UNP Q12306
G	-8	GLY	-	expression tag	UNP Q12306
G	-7	LEU	-	expression tag	UNP Q12306
G	-6	LEU	-	expression tag	UNP Q12306
G	-5	ALA	-	expression tag	UNP Q12306
G	-4	SER	-	expression tag	UNP Q12306
G	-3	SER	-	expression tag	UNP Q12306
G	-2	ARG	-	expression tag	UNP Q12306
G	-1	ALA	-	expression tag	UNP Q12306
G	0	SER	-	expression tag	UNP Q12306
G	95	ASN	-	linker	UNP Q12306
G	96	ASP	-	linker	UNP Q12306
G	97	ASP	-	linker	UNP Q12306
G	98	ASP	-	linker	UNP Q12306
G	99	ASP	-	linker	UNP Q12306
G	100	LYS	-	linker	UNP Q12306
G	101	THR	-	linker	UNP Q12306
G	102	GLY	-	linker	UNP Q12306
G	103	THR	-	linker	UNP Q12306
G	104	GLY	-	linker	UNP Q12306
G	105	SER	-	linker	UNP Q12306
G	106	GLN	-	linker	UNP Q12306
G	107	SER	-	linker	UNP Q12306
G	108	ASN	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	109	ALA	-	linker	UNP Q12306
G	110	GLU	-	linker	UNP Q12306
G	111	SER	-	linker	UNP Q12306
G	112	VAL	-	linker	UNP Q12306
G	113	GLN	-	linker	UNP Q12306
G	114	ASN	-	linker	UNP Q12306
G	115	HIS	-	linker	UNP Q12306
G	116	THR	-	linker	UNP Q12306
G	117	PHE	-	linker	UNP Q12306
G	118	GLU	-	linker	UNP Q12306
G	119	VAL	-	linker	UNP Q12306
G	120	LEU	-	linker	UNP Q12306
G	121	ASN	-	linker	UNP Q12306
G	122	ASN	-	linker	UNP Q12306
G	123	THR	-	linker	UNP Q12306
G	124	ILE	-	linker	UNP Q12306
G	125	ARG	-	linker	UNP Q12306
G	126	ALA	-	linker	UNP Q12306
G	127	LEU	-	linker	UNP Q12306
G	128	GLU	-	linker	UNP Q12306
G	129	LEU	-	linker	UNP Q12306
G	130	ILE	-	linker	UNP Q12306
G	131	LEU	-	linker	UNP Q12306
G	132	ARG	-	linker	UNP Q12306
G	133	LYS	-	linker	UNP Q12306
G	134	LEU	-	linker	UNP Q12306
G	135	GLU	-	linker	UNP Q12306
G	136	ILE	-	linker	UNP Q12306
G	137	LEU	-	linker	UNP Q12306
G	138	TYR	-	linker	UNP Q12306
G	139	GLU	-	linker	UNP Q12306
G	140	MET	-	linker	UNP Q12306
G	141	ILE	-	linker	UNP Q12306
G	142	LEU	-	linker	UNP Q12306
G	143	GLN	-	linker	UNP Q12306
G	144	LEU	-	linker	UNP Q12306
G	145	HIS	-	linker	UNP Q12306
G	146	GLU	-	linker	UNP Q12306
G	147	GLU	-	linker	UNP Q12306
G	148	VAL	-	linker	UNP Q12306
G	149	GLU	-	linker	UNP Q12306
G	150	ALA	-	linker	UNP Q12306

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	151	ILE	-	linker	UNP Q12306
G	152	GLN	-	linker	UNP Q12306
G	153	LYS	-	linker	UNP Q12306
G	154	ALA	-	linker	UNP Q12306
G	155	ILE	-	linker	UNP Q12306
G	985	ALA	ASP	conflict	UNP P0DTC2
G	1132	THR	-	linker	UNP P0DTC2
G	1834	THR	-	expression tag	UNP P0DTC2
G	1835	ILE	-	expression tag	UNP P0DTC2
G	1836	ASP	-	expression tag	UNP P0DTC2
G	1837	LYS	-	expression tag	UNP P0DTC2
G	1838	GLU	-	expression tag	UNP P0DTC2
G	1839	LYS	-	expression tag	UNP P0DTC2
G	1840	TRP	-	expression tag	UNP P0DTC2
G	1841	LYS	-	expression tag	UNP P0DTC2
G	1842	GLU	-	expression tag	UNP P0DTC2
G	1843	TRP	-	expression tag	UNP P0DTC2
G	1844	ARG	-	expression tag	UNP P0DTC2
G	1845	LYS	-	expression tag	UNP P0DTC2
G	1846	GLU	-	expression tag	UNP P0DTC2
G	1847	MET	-	expression tag	UNP P0DTC2
G	1848	GLU	-	expression tag	UNP P0DTC2
G	1849	ASN	-	expression tag	UNP P0DTC2
G	1850	LEU	-	expression tag	UNP P0DTC2
G	1851	THR	-	expression tag	UNP P0DTC2
G	1852	LYS	-	expression tag	UNP P0DTC2
G	1853	GLU	-	expression tag	UNP P0DTC2
G	1854	ILE	-	expression tag	UNP P0DTC2
G	1855	LYS	-	expression tag	UNP P0DTC2
G	1856	GLU	-	expression tag	UNP P0DTC2
G	1857	THR	-	expression tag	UNP P0DTC2
G	1858	LEU	-	expression tag	UNP P0DTC2
G	1859	GLU	-	expression tag	UNP P0DTC2
G	1860	GLU	-	expression tag	UNP P0DTC2
G	1861	ALA	-	expression tag	UNP P0DTC2
G	1862	ARG	-	expression tag	UNP P0DTC2
G	1863	LYS	-	expression tag	UNP P0DTC2
G	1864	THR	-	expression tag	UNP P0DTC2
G	1865	LEU	-	expression tag	UNP P0DTC2
G	1866	LYS	-	expression tag	UNP P0DTC2
G	1867	GLN	-	expression tag	UNP P0DTC2
G	1868	ALA	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

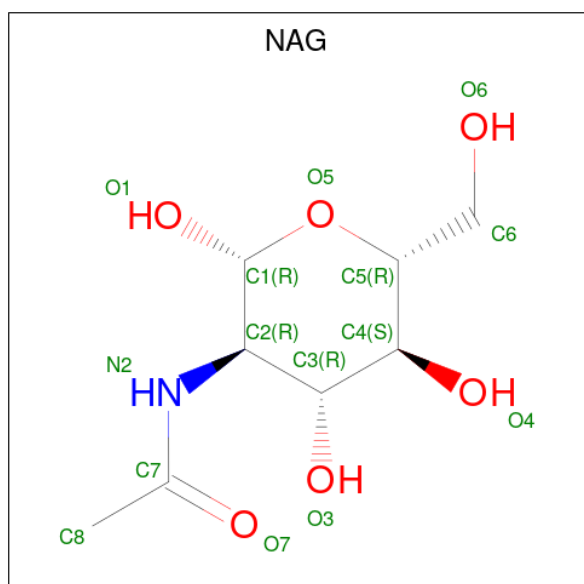
- Molecule 2 is a protein called Heavy chain of VN01H1 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	124	Total	C	N	O	S	0	0
			902	584	160	154	4		
2	E	124	Total	C	N	O	S	0	0
			902	584	160	154	4		
2	H	124	Total	C	N	O	S	0	0
			902	584	160	154	4		

- Molecule 3 is a protein called Light chain of VN01H1 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	108	Total	C	N	O	S	0	0
			749	479	134	133	3		
3	F	108	Total	C	N	O	S	0	0
			749	479	134	133	3		
3	I	108	Total	C	N	O	S	0	0
			749	479	134	133	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	

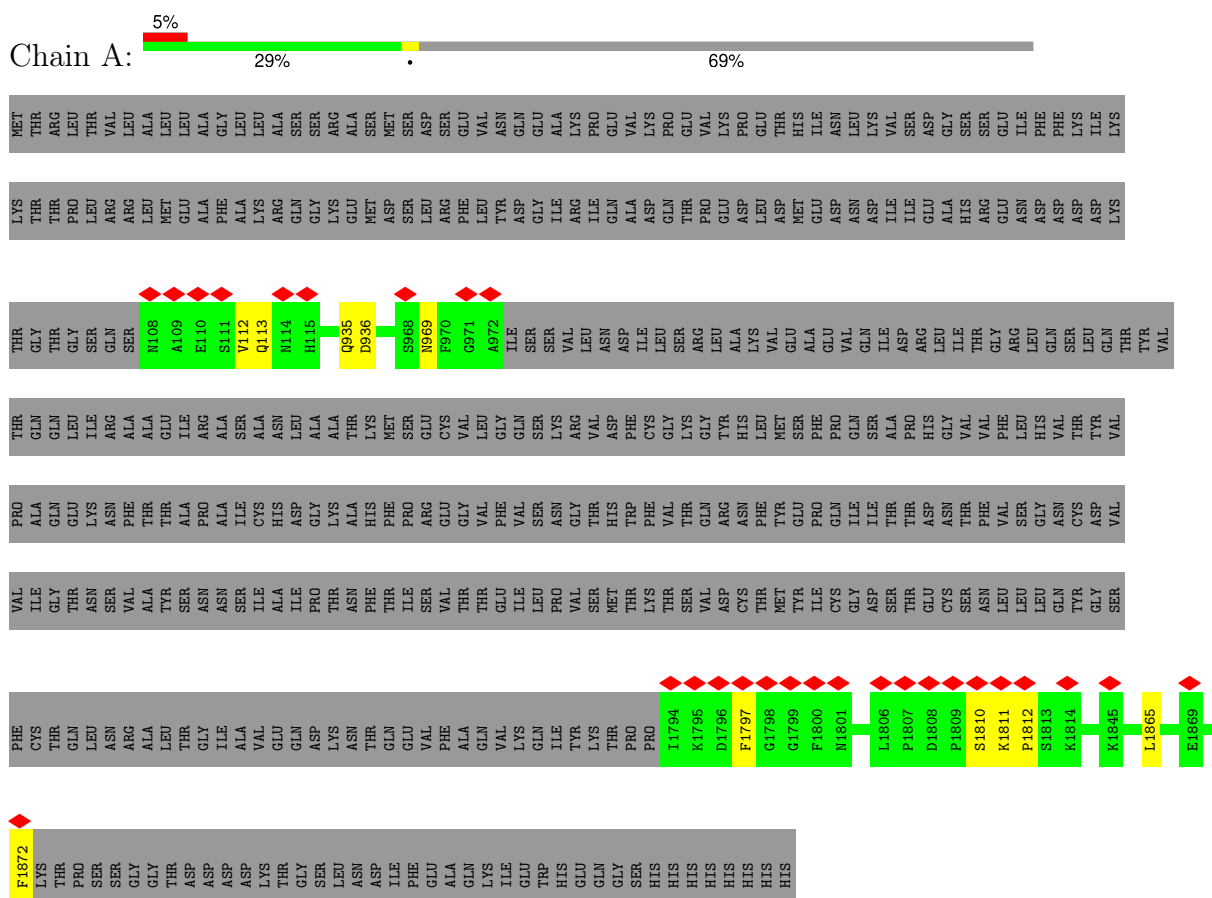
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	20	Total	O	0
			20	20	
5	B	3	Total	O	0
			3	3	
5	C	5	Total	O	0
			5	5	
5	D	20	Total	O	0
			20	20	
5	E	3	Total	O	0
			3	3	
5	F	5	Total	O	0
			5	5	
5	G	20	Total	O	0
			20	20	
5	H	3	Total	O	0
			3	3	
5	I	5	Total	O	0
			5	5	

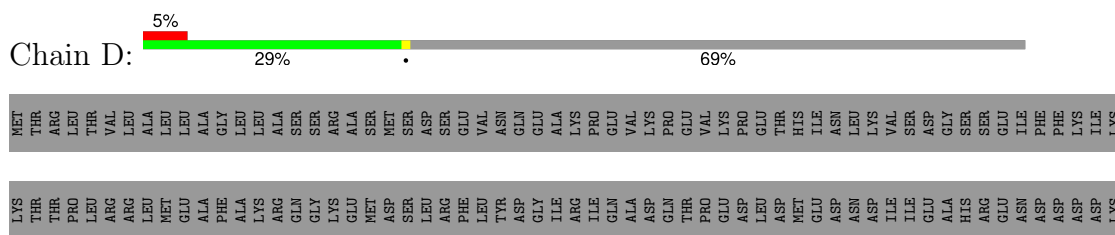
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

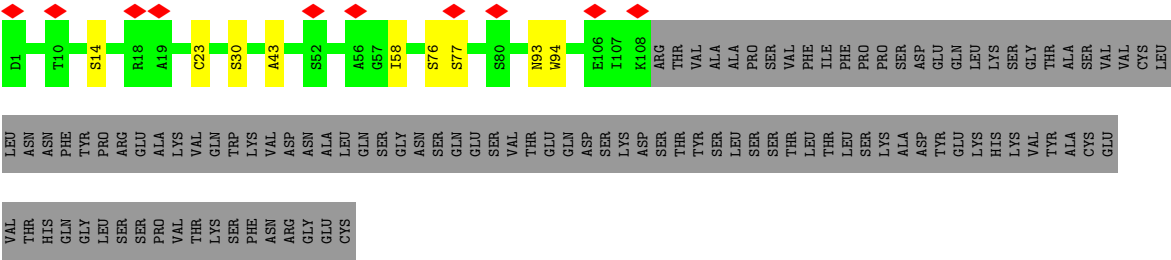
• Molecule 1: E-FICS-v3



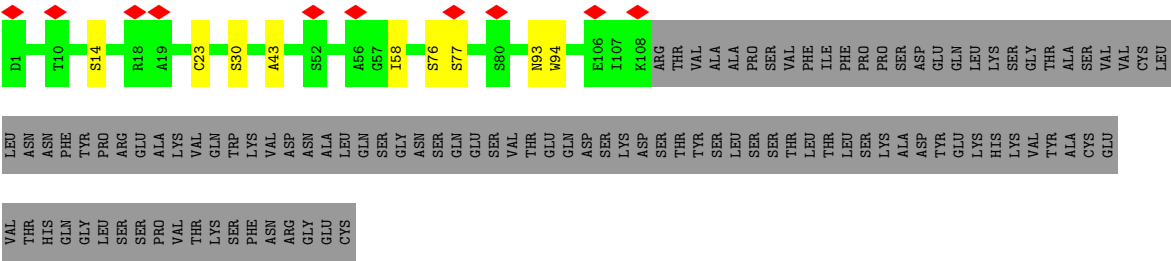
• Molecule 1: E-FICS-v3







● Molecule 3: Light chain of VN01H1 Fab



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121952	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	6.997	Depositor
Minimum map value	-4.384	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.090	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	0.76	0/1408	0.67	0/1912
1	D	0.76	0/1408	0.67	0/1912
1	G	0.76	0/1408	0.67	0/1912
2	B	0.89	2/926 (0.2%)	0.94	4/1264 (0.3%)
2	E	0.89	2/926 (0.2%)	0.93	4/1264 (0.3%)
2	H	0.89	2/926 (0.2%)	0.94	4/1264 (0.3%)
3	C	0.74	1/766 (0.1%)	0.95	7/1049 (0.7%)
3	F	0.74	1/766 (0.1%)	0.95	7/1049 (0.7%)
3	I	0.74	1/766 (0.1%)	0.95	7/1049 (0.7%)
All	All	0.79	9/9300 (0.1%)	0.83	33/12675 (0.3%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	22	CYS	C-O	9.70	1.35	1.24
2	B	22	CYS	C-O	9.68	1.35	1.24
2	E	22	CYS	C-O	9.65	1.35	1.24
3	I	23	CYS	C-O	-6.76	1.16	1.23
3	C	23	CYS	C-O	-6.74	1.16	1.23
3	F	23	CYS	C-O	-6.71	1.16	1.23
2	H	22	CYS	C-N	-5.41	1.25	1.33
2	B	22	CYS	C-N	-5.40	1.25	1.33
2	E	22	CYS	C-N	-5.37	1.25	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	58	ILE	CA-C-N	6.95	126.97	119.89
3	C	58	ILE	C-N-CA	6.95	126.97	119.89
3	I	58	ILE	CA-C-N	6.94	126.97	119.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	58	ILE	C-N-CA	6.94	126.97	119.89
3	F	58	ILE	CA-C-N	6.93	126.96	119.89
3	F	58	ILE	C-N-CA	6.93	126.96	119.89
2	B	60	TYR	CA-C-N	6.69	126.86	120.31
2	B	60	TYR	C-N-CA	6.69	126.86	120.31
2	H	60	TYR	CA-C-N	6.68	126.85	120.31
2	H	60	TYR	C-N-CA	6.68	126.85	120.31
2	E	60	TYR	CA-C-N	6.66	126.84	120.31
2	E	60	TYR	C-N-CA	6.66	126.84	120.31
2	B	13	LEU	CA-C-N	6.64	126.60	119.76
2	B	13	LEU	C-N-CA	6.64	126.60	119.76
2	H	13	LEU	CA-C-N	6.63	126.59	119.76
2	H	13	LEU	C-N-CA	6.63	126.59	119.76
2	E	13	LEU	CA-C-N	6.60	126.56	119.76
2	E	13	LEU	C-N-CA	6.60	126.56	119.76
3	I	43	ALA	CA-C-N	5.99	126.34	119.93
3	I	43	ALA	C-N-CA	5.99	126.34	119.93
3	I	30	SER	CB-CA-C	-5.96	109.72	116.63
3	C	43	ALA	CA-C-N	5.95	126.30	119.93
3	C	43	ALA	C-N-CA	5.95	126.30	119.93
3	F	43	ALA	CA-C-N	5.95	126.30	119.93
3	F	43	ALA	C-N-CA	5.95	126.30	119.93
3	F	30	SER	CB-CA-C	-5.94	109.74	116.63
3	C	30	SER	CB-CA-C	-5.93	109.75	116.63
3	C	14	SER	CA-C-N	5.46	125.77	119.93
3	C	14	SER	C-N-CA	5.46	125.77	119.93
3	F	14	SER	CA-C-N	5.45	125.76	119.93
3	F	14	SER	C-N-CA	5.45	125.76	119.93
3	I	14	SER	CA-C-N	5.44	125.75	119.93
3	I	14	SER	C-N-CA	5.44	125.75	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	1389	0	1311	7	0
1	D	1389	0	1311	6	0
1	G	1389	0	1311	6	0
2	B	902	0	789	4	0
2	E	902	0	789	3	0
2	H	902	0	789	3	0
3	C	749	0	640	2	0
3	F	749	0	640	2	0
3	I	749	0	640	2	0
4	A	28	0	26	1	0
4	D	28	0	26	1	0
4	G	28	0	26	1	0
5	A	20	0	0	0	0
5	B	3	0	0	0	0
5	C	5	0	0	0	0
5	D	20	0	0	0	0
5	E	3	0	0	0	0
5	F	5	0	0	0	0
5	G	20	0	0	0	0
5	H	3	0	0	0	0
5	I	5	0	0	0	0
All	All	9288	0	8298	35	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 (35) 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:D:1811:LYS:N	1:D:1812:PRO:HD2	2.23	0.54
1:A:1811:LYS:N	1:A:1812:PRO:HD2	2.23	0.53
1:G:1811:LYS:N	1:G:1812:PRO:HD2	2.23	0.52
1:A:112:VAL:HG21	1:A:1872:PHE:HB2	1.93	0.51
1:D:112:VAL:HG21	1:D:1872:PHE:HB2	1.93	0.50
3:I:93:ASN:O	3:I:94:TRP:C	2.54	0.50
3:F:93:ASN:O	3:F:94:TRP:C	2.54	0.50
1:G:112:VAL:HG21	1:G:1872:PHE:HB2	1.93	0.49
3:C:93:ASN:O	3:C:94:TRP:C	2.54	0.48
4:A:1402:NAG:H82	1:G:1865:LEU:HD23	1.96	0.47
2:H:111:ASP:OD1	2:H:112:VAL:N	2.47	0.47
2:E:111:ASP:OD1	2:E:112:VAL:N	2.48	0.47
2:H:84:GLY:O	2:H:85:SER:C	2.58	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:ASP:OD1	2:B:112:VAL:N	2.48	0.47
2:B:84:GLY:O	2:B:85:SER:C	2.58	0.47
2:E:84:GLY:O	2:E:85:SER:C	2.58	0.46
1:A:1865:LEU:HD23	4:D:1402:NAG:H82	1.96	0.46
1:D:1865:LEU:HD23	4:G:1402:NAG:H82	1.96	0.46
1:D:1811:LYS:N	1:D:1812:PRO:CD	2.80	0.45
1:G:1811:LYS:N	1:G:1812:PRO:CD	2.80	0.45
1:A:1811:LYS:N	1:A:1812:PRO:CD	2.80	0.45
3:I:76:SER:O	3:I:77:SER:C	2.60	0.45
3:C:76:SER:O	3:C:77:SER:C	2.60	0.44
3:F:76:SER:O	3:F:77:SER:C	2.60	0.44
2:E:73:ASP:OD1	2:E:73:ASP:C	2.62	0.42
1:D:1810:SER:O	1:D:1811:LYS:C	2.62	0.42
1:A:935:GLN:NE2	1:A:936:ASP:OD1	2.53	0.41
2:H:73:ASP:OD1	2:H:73:ASP:C	2.62	0.41
1:G:935:GLN:NE2	1:G:936:ASP:OD1	2.53	0.41
1:G:1810:SER:O	1:G:1811:LYS:C	2.62	0.41
2:B:73:ASP:OD1	2:B:73:ASP:C	2.62	0.41
1:D:935:GLN:NE2	1:D:936:ASP:OD1	2.53	0.41
2:B:104:ARG:O	2:B:105:PHE:C	2.64	0.41
1:A:1810:SER:O	1:A:1811:LYS:C	2.62	0.40
1:A:969:ASN:ND2	1:A:1797:PHE:CE1	2.90	0.40

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	182/605 (30%)	180 (99%)	2 (1%)	0	100	100
1	D	182/605 (30%)	180 (99%)	2 (1%)	0	100	100
1	G	182/605 (30%)	180 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	122/226 (54%)	122 (100%)	0	0	100	100
2	E	122/226 (54%)	122 (100%)	0	0	100	100
2	H	122/226 (54%)	122 (100%)	0	0	100	100
3	C	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
3	F	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
3	I	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
All	All	1230/3138 (39%)	1215 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	128/533 (24%)	127 (99%)	1 (1%)	73	88
1	D	128/533 (24%)	127 (99%)	1 (1%)	73	88
1	G	128/533 (24%)	127 (99%)	1 (1%)	73	88
2	B	75/196 (38%)	75 (100%)	0	100	100
2	E	75/196 (38%)	75 (100%)	0	100	100
2	H	75/196 (38%)	75 (100%)	0	100	100
3	C	56/185 (30%)	56 (100%)	0	100	100
3	F	56/185 (30%)	56 (100%)	0	100	100
3	I	56/185 (30%)	56 (100%)	0	100	100
All	All	777/2742 (28%)	774 (100%)	3 (0%)	81	93

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

Mol	Chain	Res	Type
1	A	113	GLN
1	D	113	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	113	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	920	GLN
2	B	39	GLN
3	C	38	GLN
1	D	122	ASN
1	D	920	GLN
2	E	39	GLN
3	F	32	ASN
3	F	38	GLN
1	G	122	ASN
1	G	920	GLN
2	H	39	GLN
3	I	38	GLN

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](#)

6 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	1402	1	14,14,15	0.49	0	17,19,21	0.94	1 (5%)
4	NAG	A	1401	1	14,14,15	0.46	0	17,19,21	0.67	0
4	NAG	D	1402	1	14,14,15	0.48	0	17,19,21	0.94	1 (5%)
4	NAG	D	1401	1	14,14,15	0.45	0	17,19,21	0.67	0
4	NAG	G	1402	1	14,14,15	0.49	0	17,19,21	0.94	1 (5%)
4	NAG	G	1401	1	14,14,15	0.46	0	17,19,21	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	G	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	G	1401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1402	NAG	C2-N2-C7	-2.79	119.16	122.90
4	D	1402	NAG	C2-N2-C7	-2.78	119.17	122.90
4	A	1402	NAG	C2-N2-C7	-2.78	119.18	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1402	NAG	1	0
4	D	1402	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1402	NAG	1	0

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.

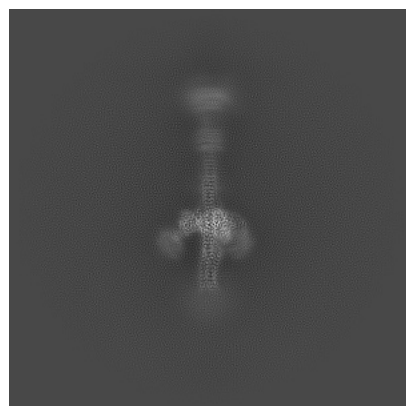
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75694. These allow visual inspection of the internal detail of the map and identification of artifacts.

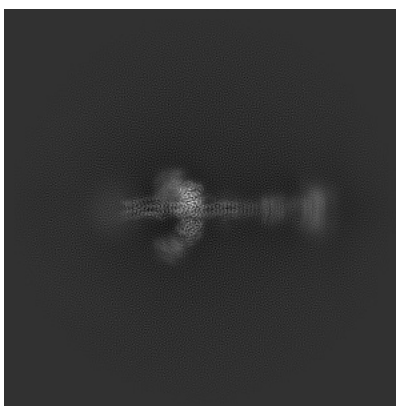
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

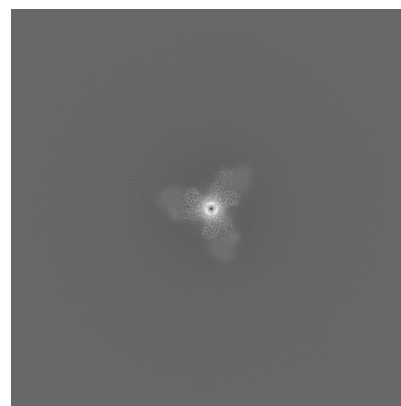
6.1.1 Primary map



X

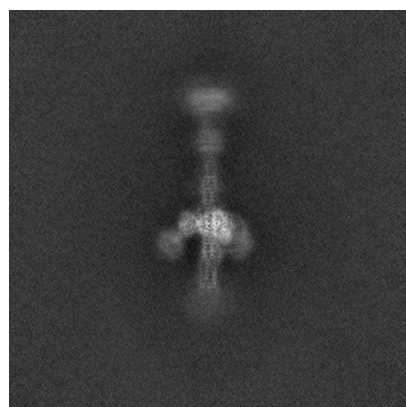


Y

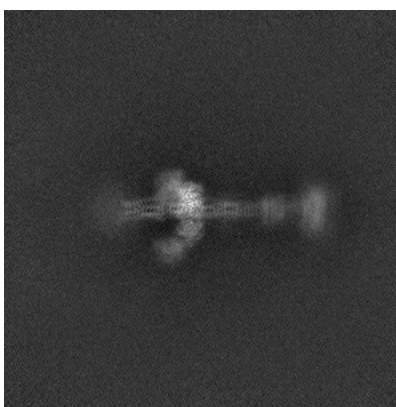


Z

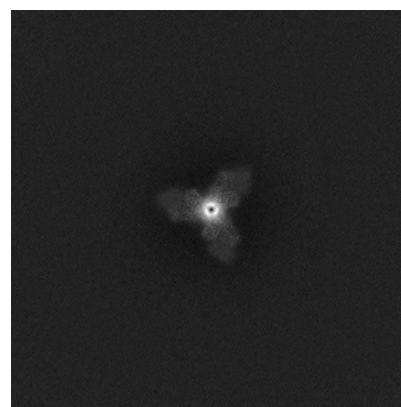
6.1.2 Raw map



X



Y



Z

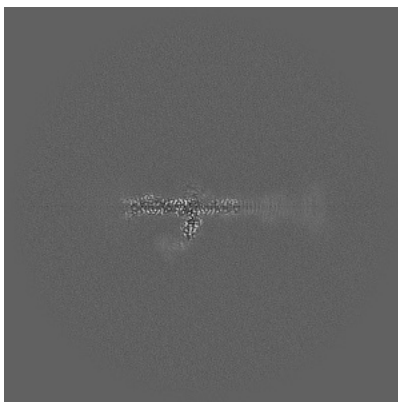
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

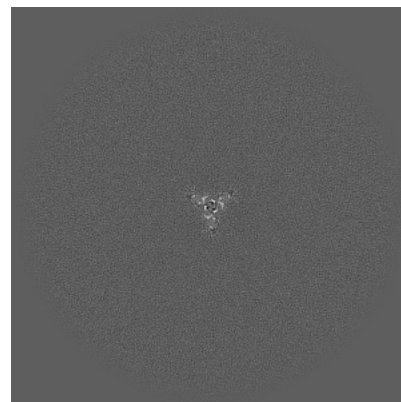
6.2.1 Primary map



X Index: 320



Y Index: 320

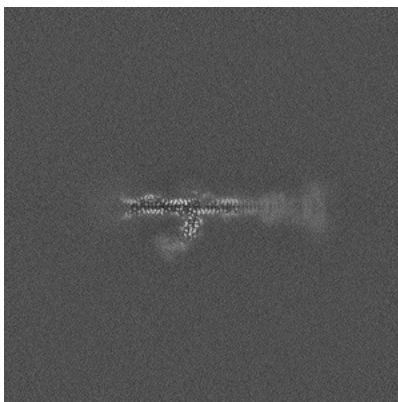


Z Index: 320

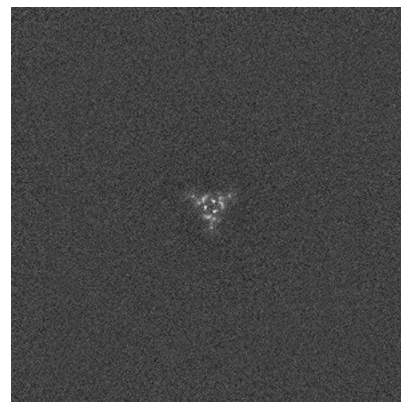
6.2.2 Raw map



X Index: 320



Y Index: 320



Z Index: 320

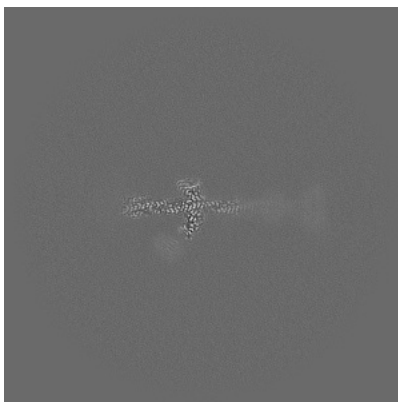
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

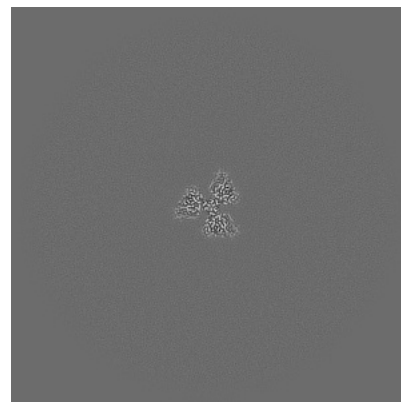
6.3.1 Primary map



X Index: 324



Y Index: 327

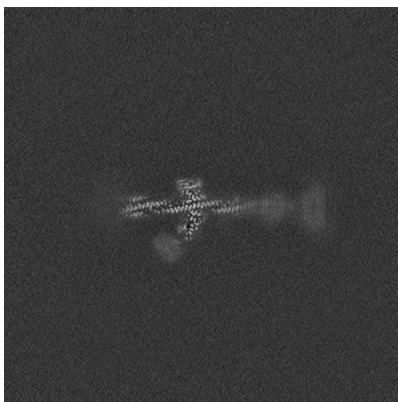


Z Index: 299

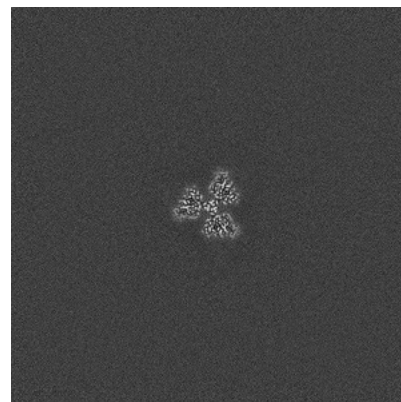
6.3.2 Raw map



X Index: 327



Y Index: 327

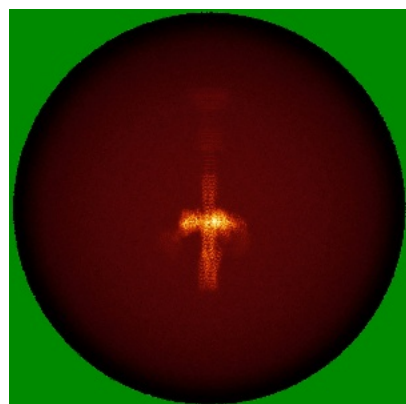


Z Index: 298

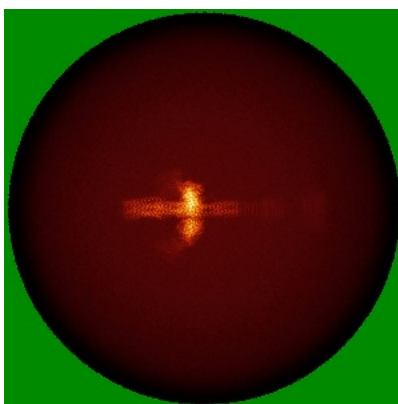
The images above show the largest variance slices of the map in three orthogonal directions.

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

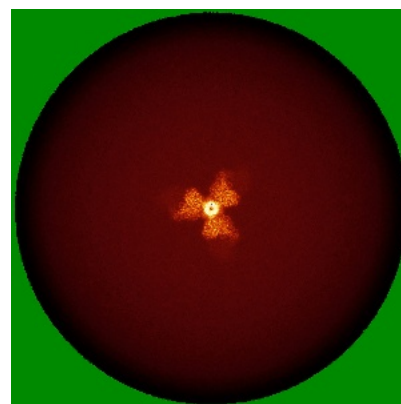
6.4.1 Primary map



X

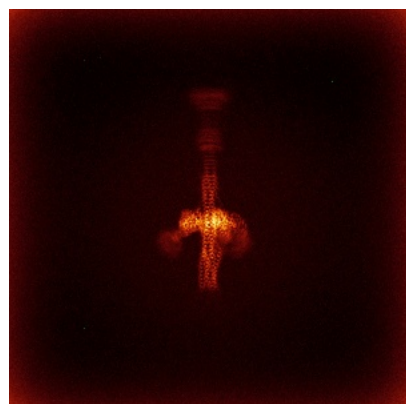


Y

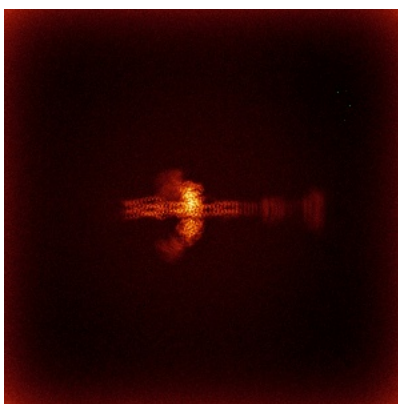


Z

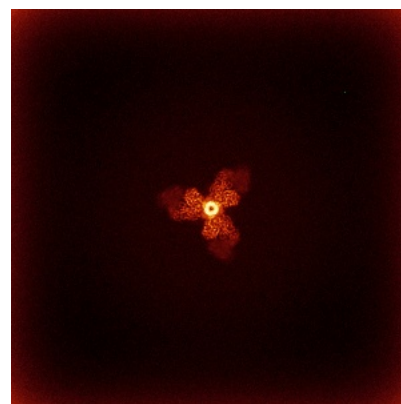
6.4.2 Raw map



X



Y

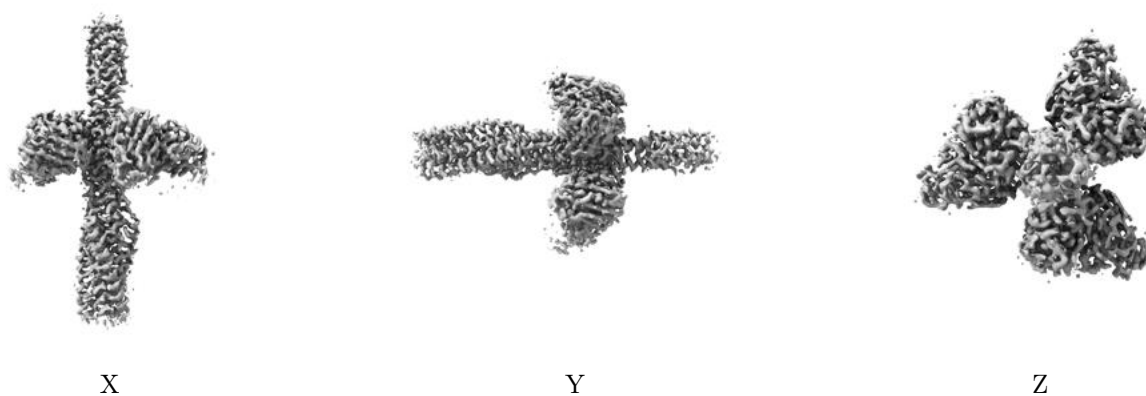


Z

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.

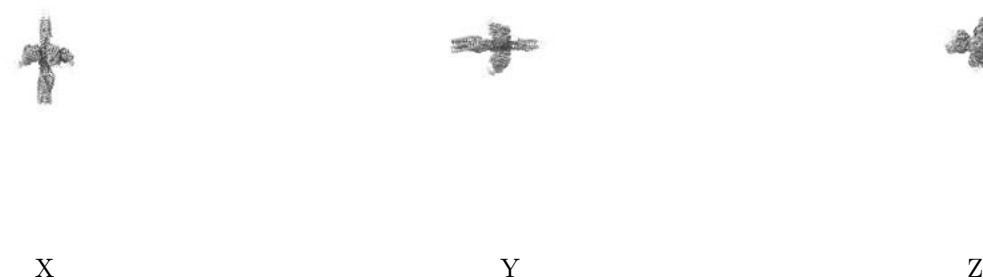
6.5 Orthogonal surface views [i](#)

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.

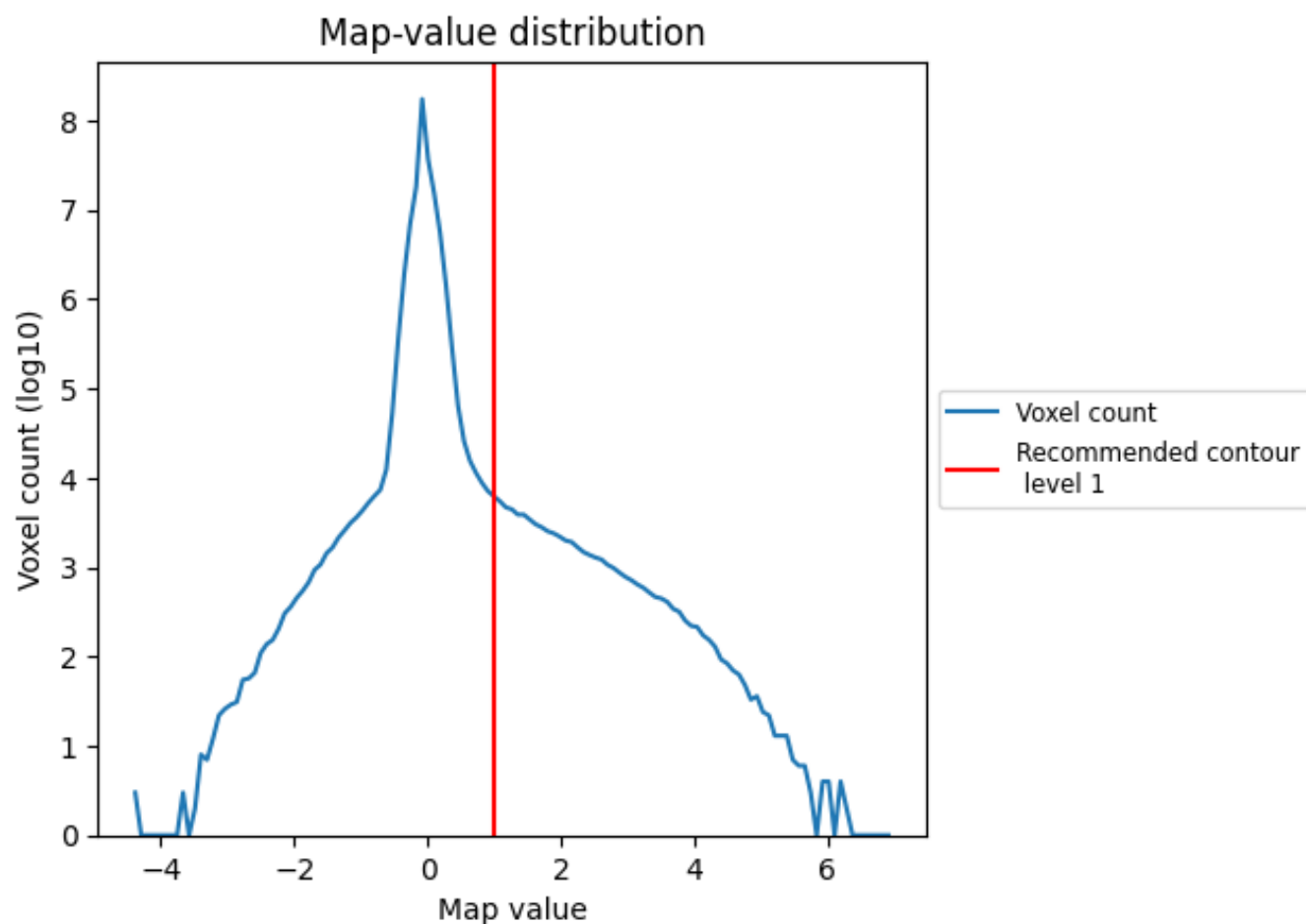
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

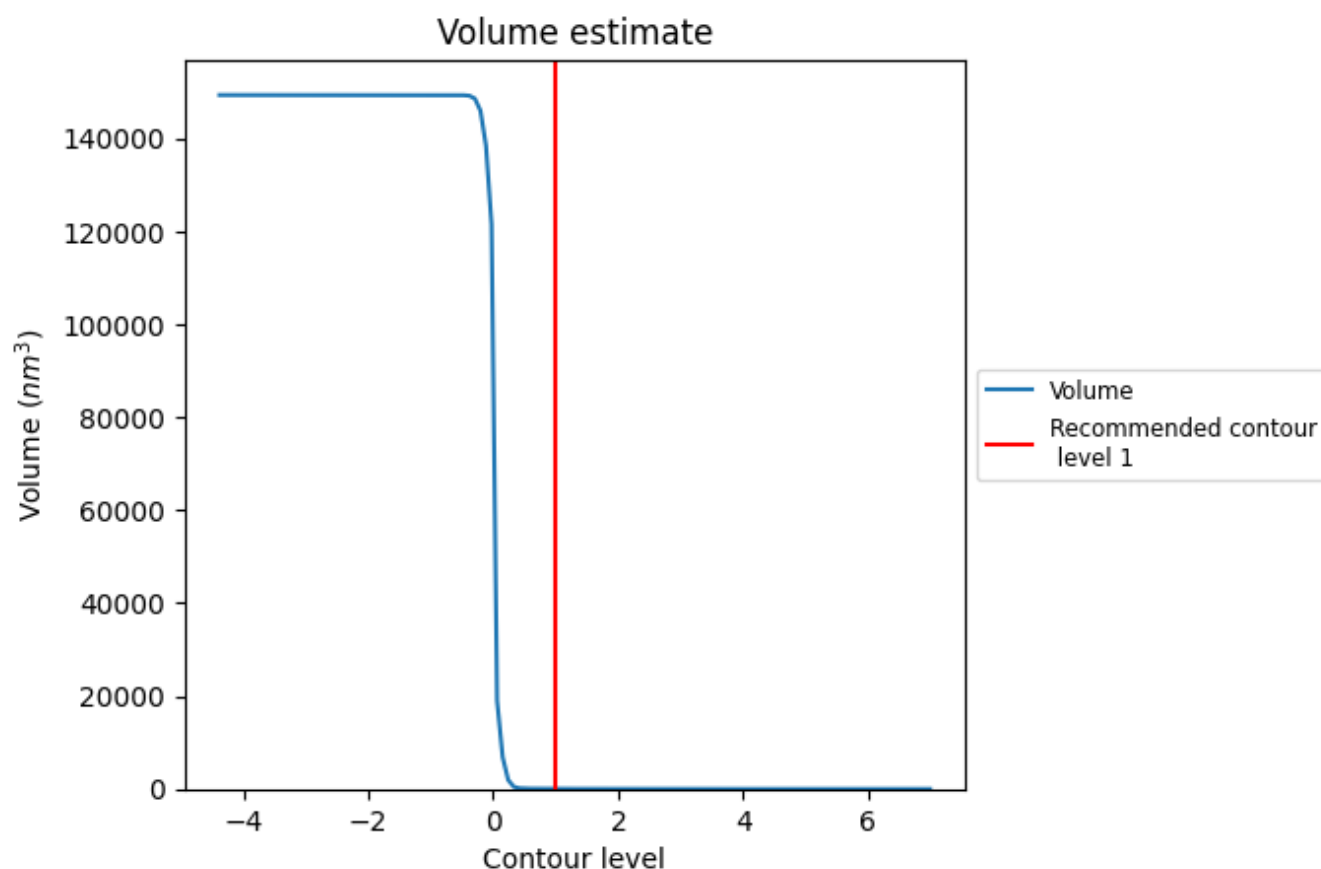
This section contains the results of statistical analysis of the map.

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.

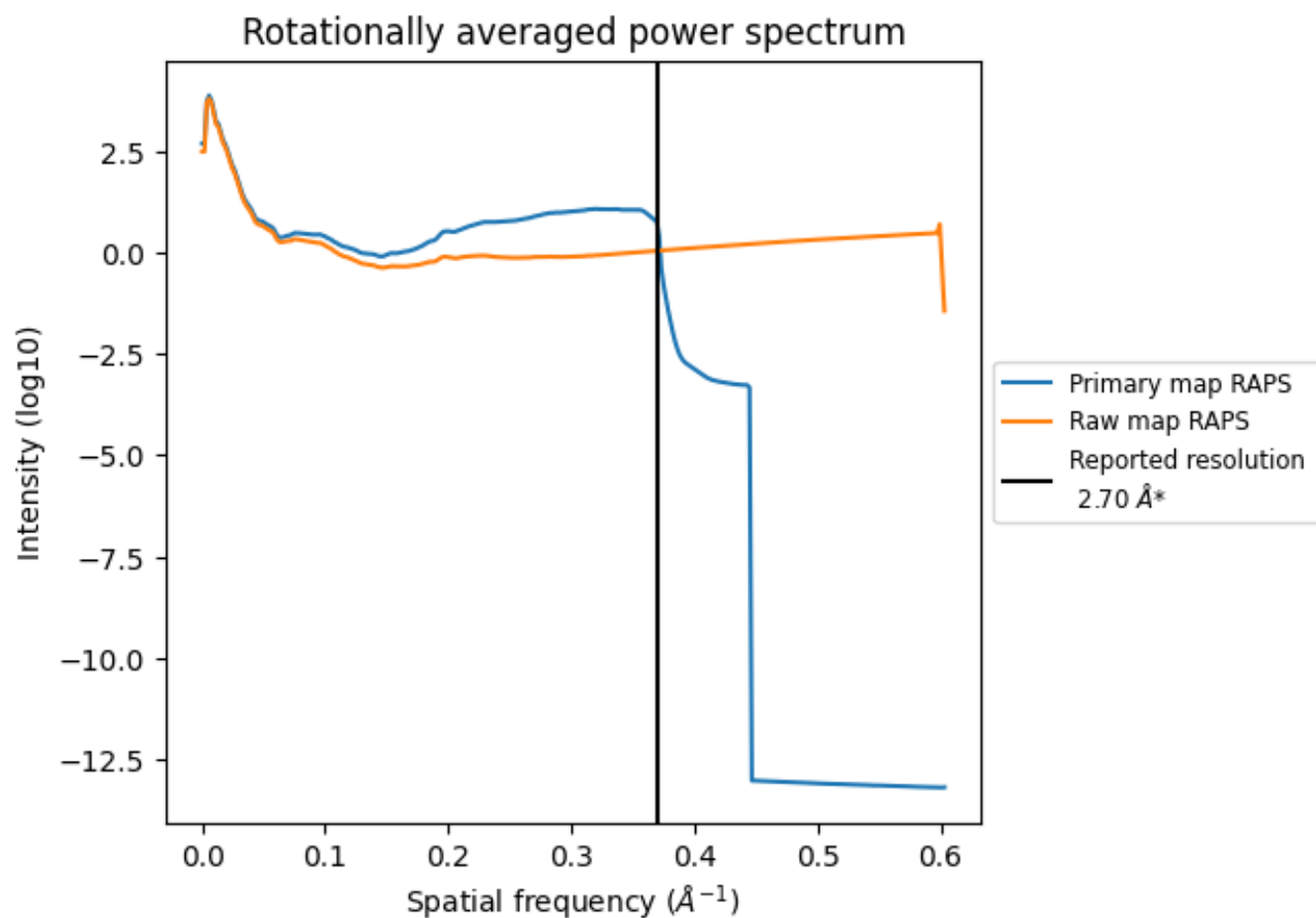
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 37 nm^3 ; this corresponds to an approximate mass of 34 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 ⓘ

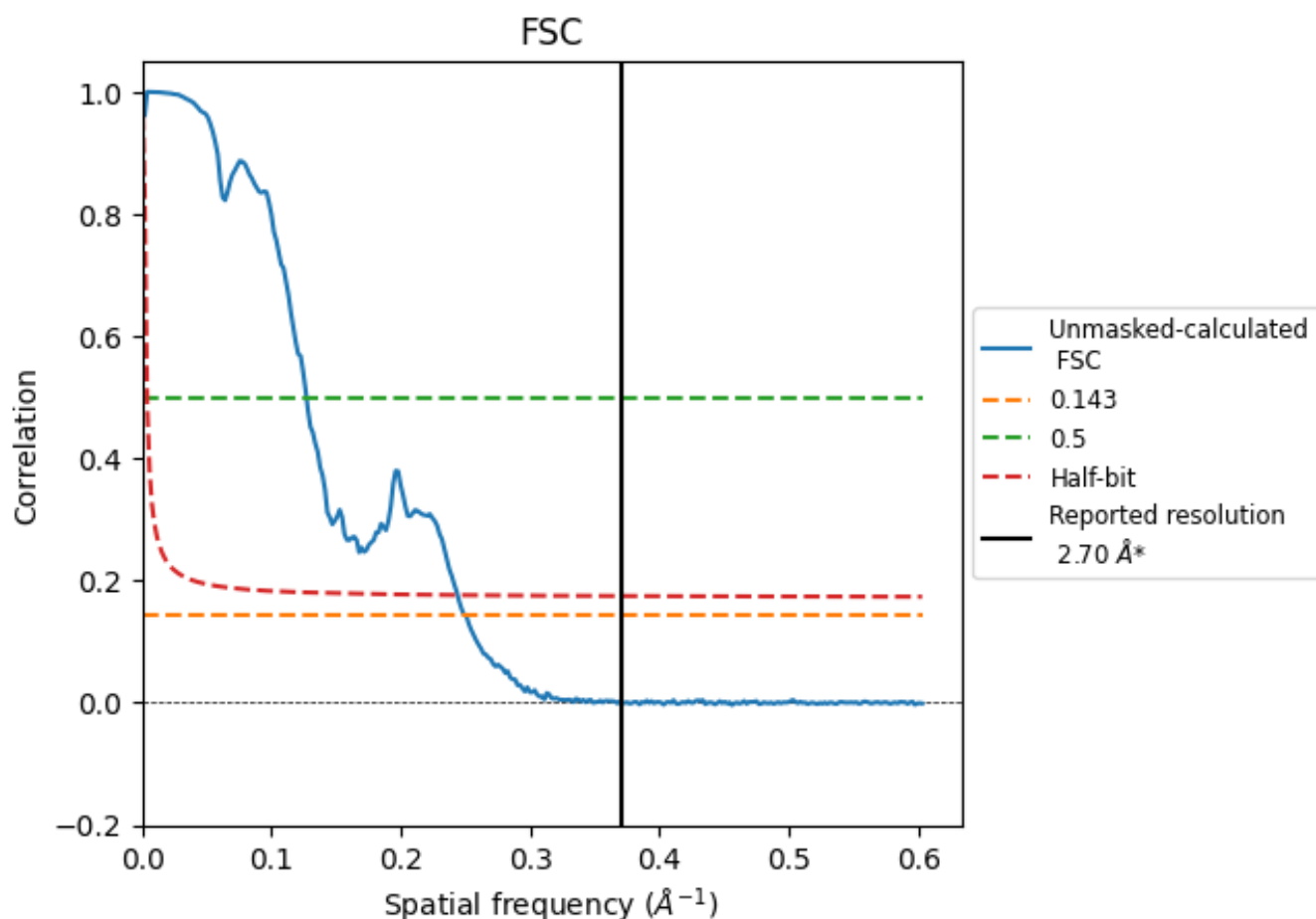


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

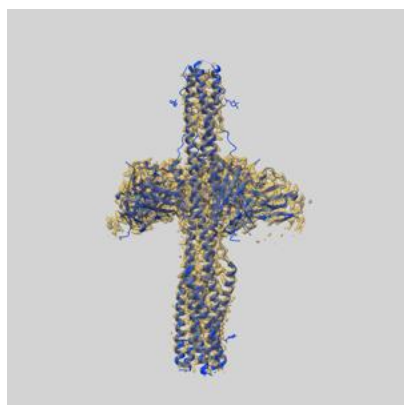
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.87	4.10

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

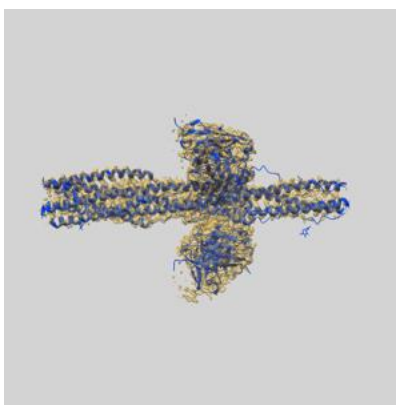
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75694 and PDB model 11HK. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

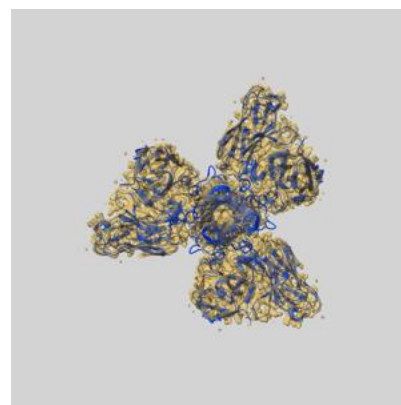
9.1 Map-model overlay [i](#)



X



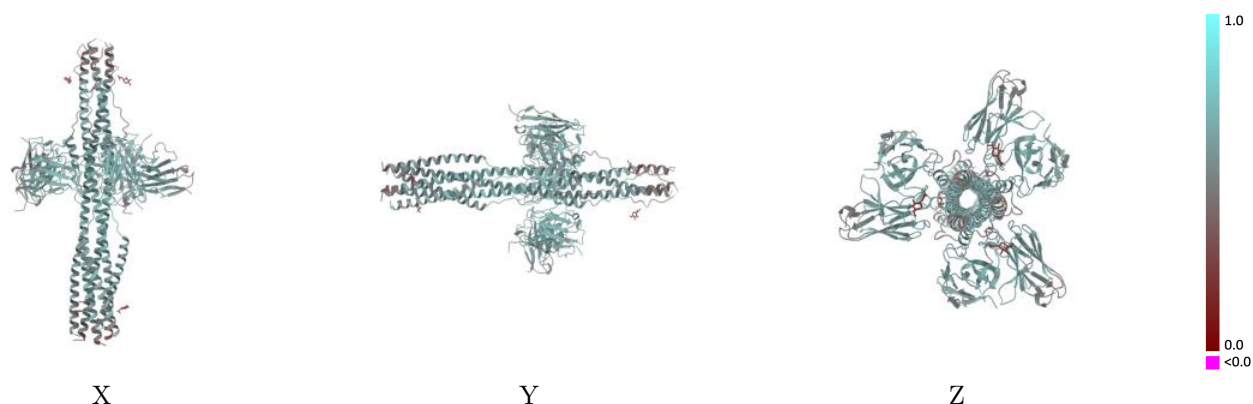
Y



Z

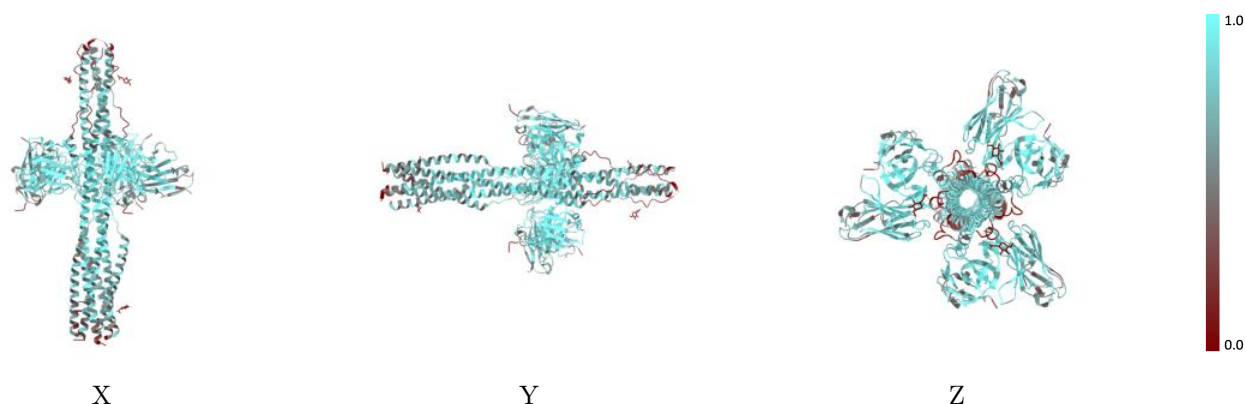
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



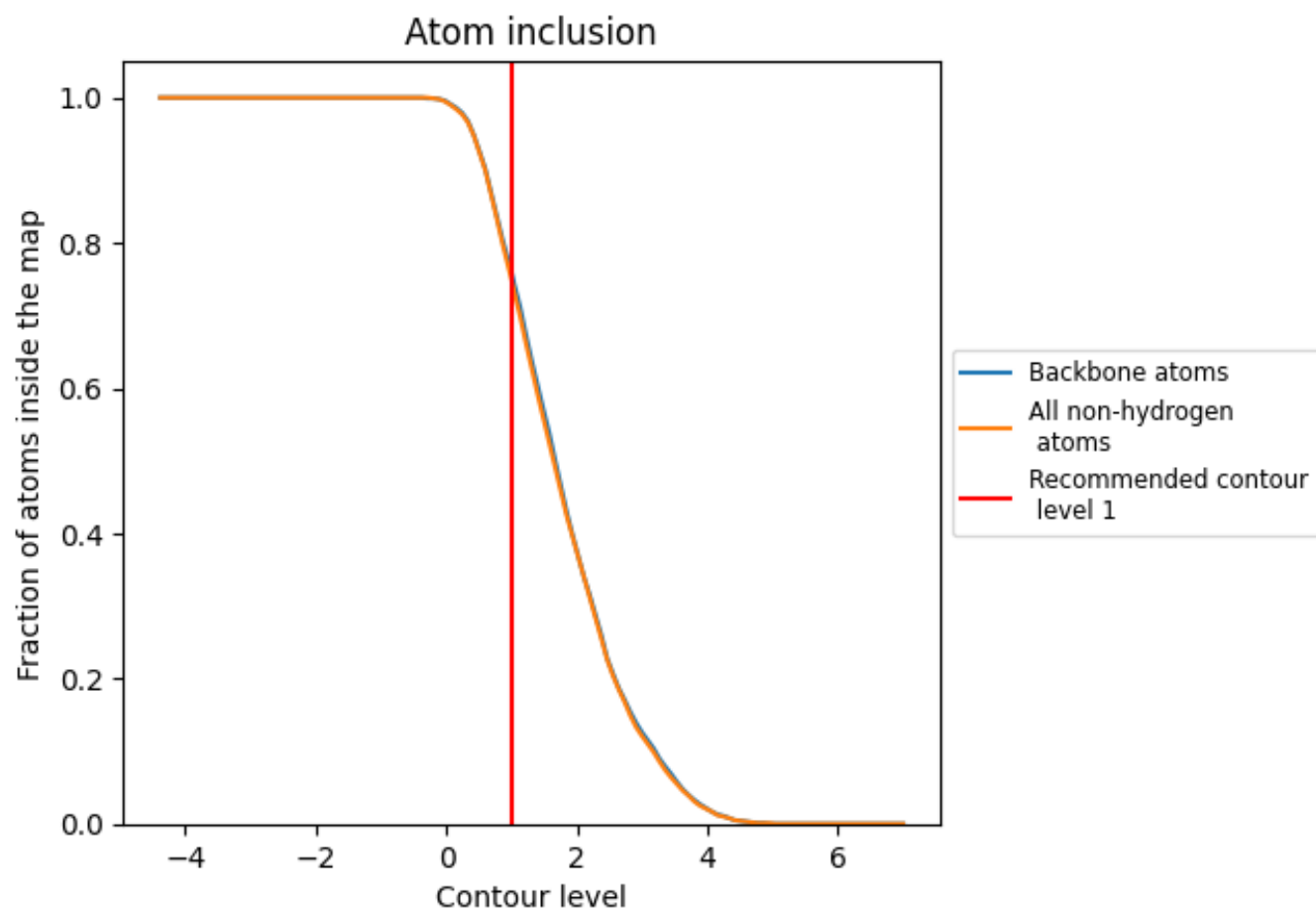
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 76% of all backbone atoms, 75% 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	<div><div></div></div> 0.7480	<div><div></div></div> 0.5880
A	<div><div></div></div> 0.6940	<div><div></div></div> 0.5720
B	<div><div></div></div> 0.8240	<div><div></div></div> 0.6110
C	<div><div></div></div> 0.7940	<div><div></div></div> 0.5920
D	<div><div></div></div> 0.6890	<div><div></div></div> 0.5720
E	<div><div></div></div> 0.8230	<div><div></div></div> 0.6100
F	<div><div></div></div> 0.7930	<div><div></div></div> 0.5920
G	<div><div></div></div> 0.6960	<div><div></div></div> 0.5700
H	<div><div></div></div> 0.8190	<div><div></div></div> 0.6100
I	<div><div></div></div> 0.7920	<div><div></div></div> 0.5920

1.0

0.0

<0.0