



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 12:24 AM EDT

PDB ID : 8FJP
EMDB ID : EMD-29245
Title : Cryo-EM structure of native mosquito salivary gland surface protein 1 (SGS1)
Authors : Liu, S.; Xia, X.; Calvo, E.; Zhou, Z.H.
Deposited on : 2022-12-20
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

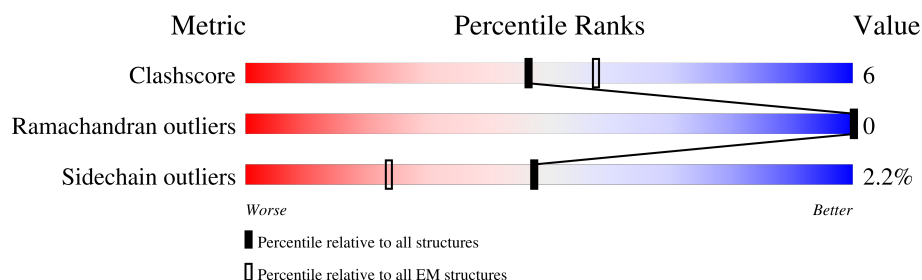
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	3364	
2	B	2	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23390 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 salivary gland surface protein 1.

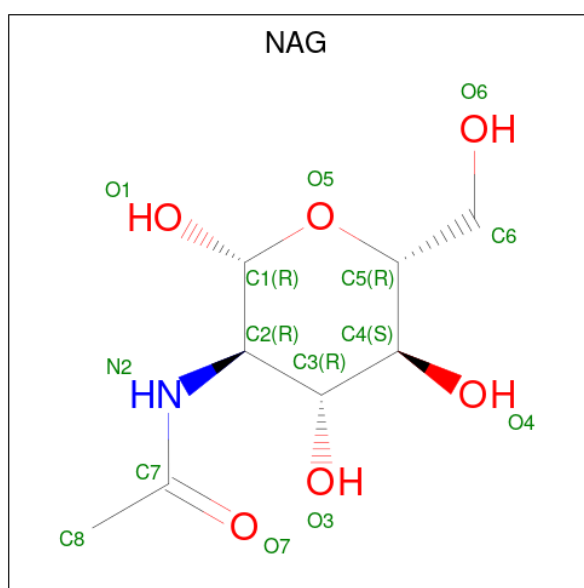
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2932	23348	14826	3974	4477	71	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	2	28	16	2	10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

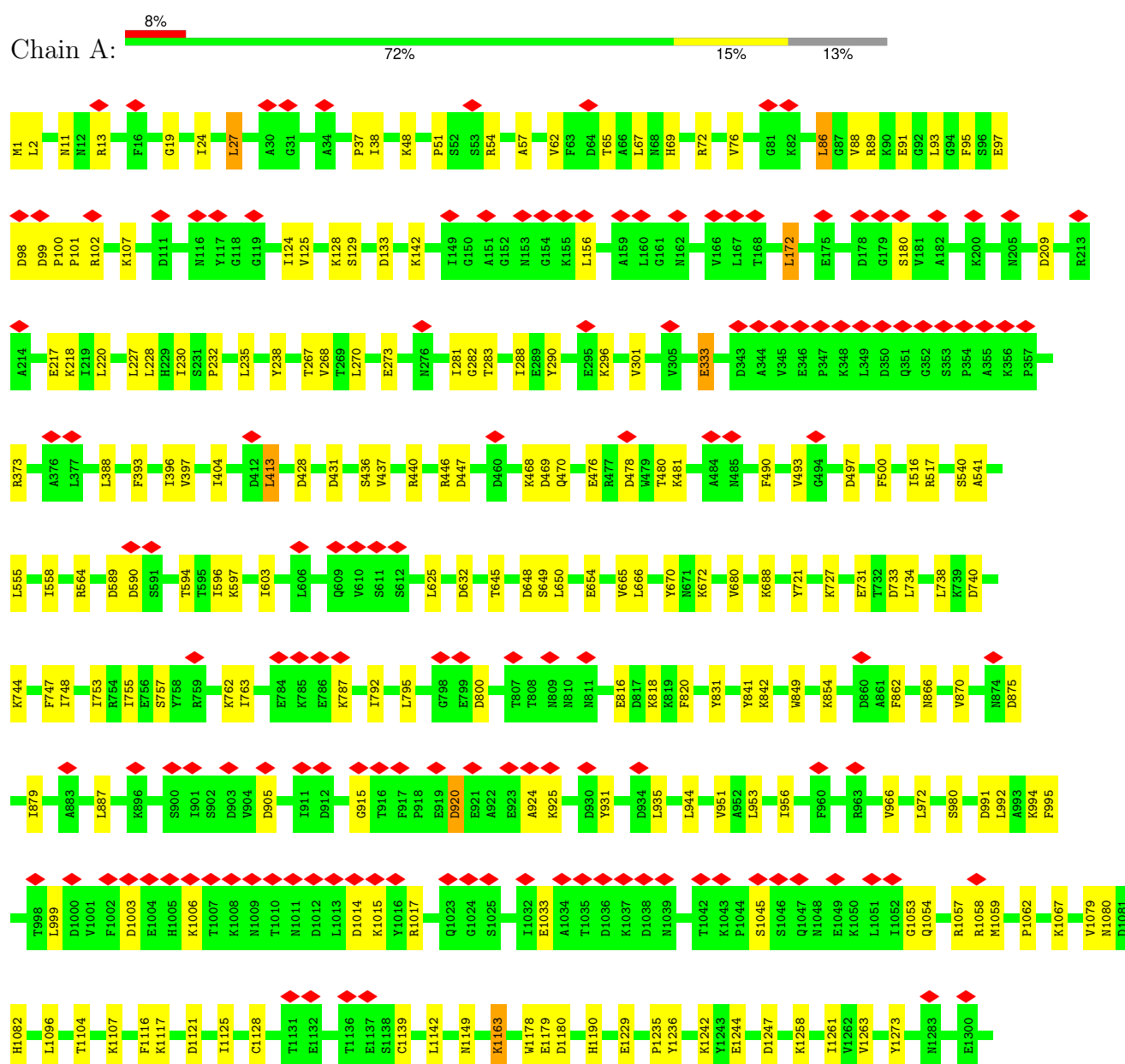


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	14	8	1	5	0

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: salivary gland surface protein 1



ALA	L2889	GLY	R2703	V2522	G2399	D2246	D2104	Y1983	S1819	V1578	T1517	E1311
PHE	L2890	ALA	R2704	R2529	K2400	F2247	R2105	Q1984	M1826	D1679	L1525	D1317
THR	F2891	ALA	F2705	L2538	G2401	G2402	S2107	I1985	P1827	L1682	V1536	G1318
PHE	Y2892	THR	S2723	S2548	D2403	E2251	L2122	I1996	L1828	I1683	E1538	A1319
SER	L2894	SER	Q2727	P2556	S2404	G2267	R2129	Y1997	R1831	I1684	I1321	Q1320
TVR	G2895	TVR	Q2727	R2556	S2405	G2267	R2137	Y1998	H1832	D1322	I1321	Q1320
PHE	G2896	PHE	D2731	R2561	I2406	S2405	R2137	F1999	H1836	A1323	I1542	A1343
THR	A2899	THR	Q2732	R2564	W2410	W2291	K2141	L2000	P1837	E1324	N1554	Q1325
ALA	Q2905	ALA	Q2733	R2567	D2414	L2299	T2142	N2002	H1836	V1698	N1555	A1344
GLY	I2906	GLY	I2734	K2567	D2415	Y2311	S2143	F2004	G1838	I1712	K1556	S1343
SER	D2910	SER	A2735	K2567	T2416	D2312	G2144	G2005	V1839	V1713	D1557	A1344
MET	W2911	MET	W2736	K2567	E2417	L2319	Q2145	R2006	M1840	D1716	K1559	N1366
ILE	S2912	ILE	L2737	N2571	E2418	L2319	Q2145	C2007	F1859	Q1720	K1560	K1367
ALA	S2913	ALA	L2738	D2575	E2418	A2321	T2149	C2008	F1859	Q1720	R1561	K1368
GLY	R2914	GLY	W2739	I2577	C2421	V2326	P2150	E2009	R1862	Q1720	Q1570	N1374
A2809	R2915	A2809	I2742	I2577	K2422	V2326	T2151	A2015	K1866	Y1723	M1571	N1374
L2810	M2920	L2810	I2743	V2583	R2423	K2339	D2155	P2017	K1876	Q1732	R1572	I1375
A2811	I2921	A2811	Q2744	R2584	R2423	K2339	K2164	T2018	S1877	L1735	K1574	R1376
V2814	V2814	V2814	V2747	Y2598	Q2426	A2343	N2168	Q2021	P1878	V1578	V1578	K1392
A2820	A2820	A2820	A2753	K2602	Q2427	N2344	N2168	Q2021	P1878	D1738	M1586	L1386
F2821	F2821	F2821	A2754	P2607	D2430	A2346	V2169	I2033	K1881	S1739	M1586	I1397
G2823	G2823	G2823	S2755	P2607	D2430	M2347	D2170	P2034	R1890	M1741	Q1591	A1398
A2824	A2824	A2824	A2756	I2615	L2432	K2348	S2172	N2035	R1897	Q1746	I1592	E1399
A2825	A2825	A2825	N2757	H2616	L2432	S2349	K2173	R2036	T1898	Q1746	T1596	F1400
A2826	A2826	A2826	N2757	H2616	Q2436	H2350	K2173	D2037	Q1899	R1754	A1596	T1403
A2827	A2827	A2827	S2759	L2621	L2441	E2351	V2179	Q2038	Q1899	R1754	V1597	A1404
S2828	S2828	S2828	P2762	L2634	L2442	R2354	V2180	D2043	K1901	D1768	V1598	V1405
N2829	N2829	N2829	W2765	L2635	E2443	F2355	K2182	R2059	D1902	G1769	E1599	F1409
Q2830	Q2830	Q2830	A2766	D2636	E2443	F2355	K2182	R2059	D1902	R1770	K1612	R1458
W2831	W2831	W2831	W2767	L2642	L2447	R2361	V2187	K2063	I1906	K1775	E1613	E1459
N2832	N2832	N2832	GLY	L2643	R2451	E2367	E2188	S2070	H1915	A1776	K1614	I1460
P2833	P2833	P2833	ASP	V2644	R2451	E2367	L2198	E2071	M1921	F1777	F1615	V1461
A2834	A2834	A2834	LYS	A2652	A2458	A2371	T2199	E2077	S1931	Q1778	I1622	V1462
S2835	S2835	S2835	THR	D2655	S2459	G2375	T2200	E2078	R1932	H1779	R1623	S1463
W2836	W2836	W2836	TRP	L2657	N2460	Q2376	T2201	K2084	G1934	H1780	I1638	E1464
D2837	D2837	D2837	ILE	Y2656	N2463	Q2375	E2202	I2087	V1949	M1789	K1653	S1465
N2845	N2845	N2845	GLY	L2657	S2464	Q2377	P2209	I2087	G1934	V1792	V1471	V1471
ALA	ALA	ALA	ALA	Q2661	P2465	Q2377	I2215	T2091	V1949	R1792	L1472	L1472
T2853	T2853	T2853	ALA	R2684	I2473	Q2378	T2218	T2092	F1959	Y1804	F1474	K1474
A2854	A2854	A2854	ALA	Y2692	D2474	L2379	T2218	E2093	F1959	V1805	I1475	I1475
V2855	V2855	V2855	ILE	Y2692	D2474	L2379	T2218	T2094	I1961	A1906	L1665	I1476
S2856	S2856	S2856	MET	Y2692	D2474	L2379	T2218	T2095	T1961	T1807	V1666	V1666
F2857	F2857	F2857	GLY	R2695	K2487	T2380	P2234	L2095	S1962	T1807	S1675	A1482
P2858	P2858	P2858	ALA	L2696	E2488	T2380	P2234	S2096	K1963	T1809	I1676	P1494
ALA	ALA	ALA	ALA	E2490	V2384	A2237	R2238	Q2101	R1970	Y1813	W1677	F1499
S2873	S2873	S2873	VAL	D2700	P2391	K2392	W2241	E2102	R1970	E1814	Q1516	Q1516
L2874	L2874	L2874	THR	T2500	L2393	L2393	W2241	E2102	R1970	E1814	Q1516	Q1516
N2884	N2884	N2884	GLY	K2508	L2396	L2397	W2241	E2102	R1970	E1814	Q1516	Q1516
F2888	F2888	F2888	GLY	H2516	L2396	L2397	W2241	E2102	R1970	E1814	Q1516	Q1516
ALA	K2971	ALA	R2967	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
PHE	D2972	PHE	W2967	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	T2973	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
ALA	I2974	ALA	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	L2975	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
ALA	L2976	ALA	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	L2976	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
ALA	K2980	ALA	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2986	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	K2987	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2988	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	L2989	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	L2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S2990	THR	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
VAL	S2990	VAL	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
LYS	S2990	LYS	R2968	L2968	ALA	L2968	ALA	ALA	ALA	ALA	ALA	ALA
THR	S											



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	161092	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.189	Depositor
Minimum map value	-0.100	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.30	0/23854	0.59	0/32262

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23348	0	23006	273	0
2	B	28	0	25	3	0
3	A	14	0	13	0	0
All	All	23390	0	23044	274	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 6.

The worst 5 of 274 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)
2:B:1:NAG:H62	2:B:2:NAG:HN2	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLU:HB2	1:A:102:ARG:HA	1.62	0.80
1:A:99:ASP:HB2	1:A:100:PRO:HD3	1.62	0.80
1:A:97:GLU:CB	1:A:102:ARG:HA	2.18	0.73
1:A:1586:MET:HG2	1:A:1592:ILE:HD11	1.77	0.67

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	2922/3364 (87%)	2756 (94%)	166 (6%)	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	2546/2935 (87%)	2490 (98%)	56 (2%)	47	69

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1516	GLN
1	A	3041	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1832	HIS
1	A	2943	TYR
1	A	2757	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1570	GLN
1	A	1720	GLN
1	A	1937	GLN
1	A	1763	GLN
1	A	1334	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	1,2	14,14,15	0.38	0	17,19,21	0.86	1 (5%)
2	NAG	B	2	2	14,14,15	0.27	0	17,19,21	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	2.48	115.51	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

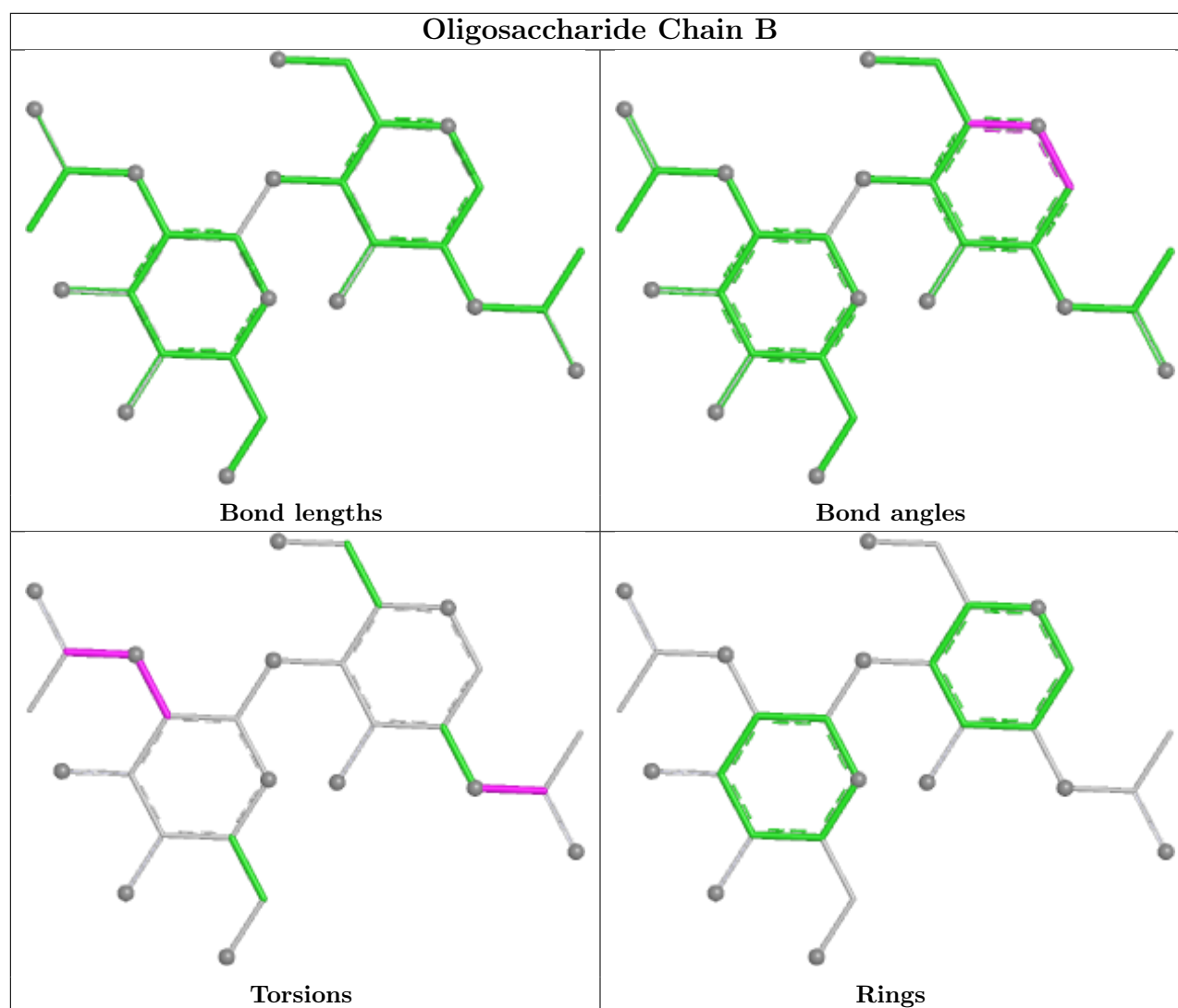
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C3-C2-N2-C7
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	2	0
2	B	2	NAG	2	0

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



5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	4001	1	14,14,15	0.29	0	17,19,21	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	4001	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

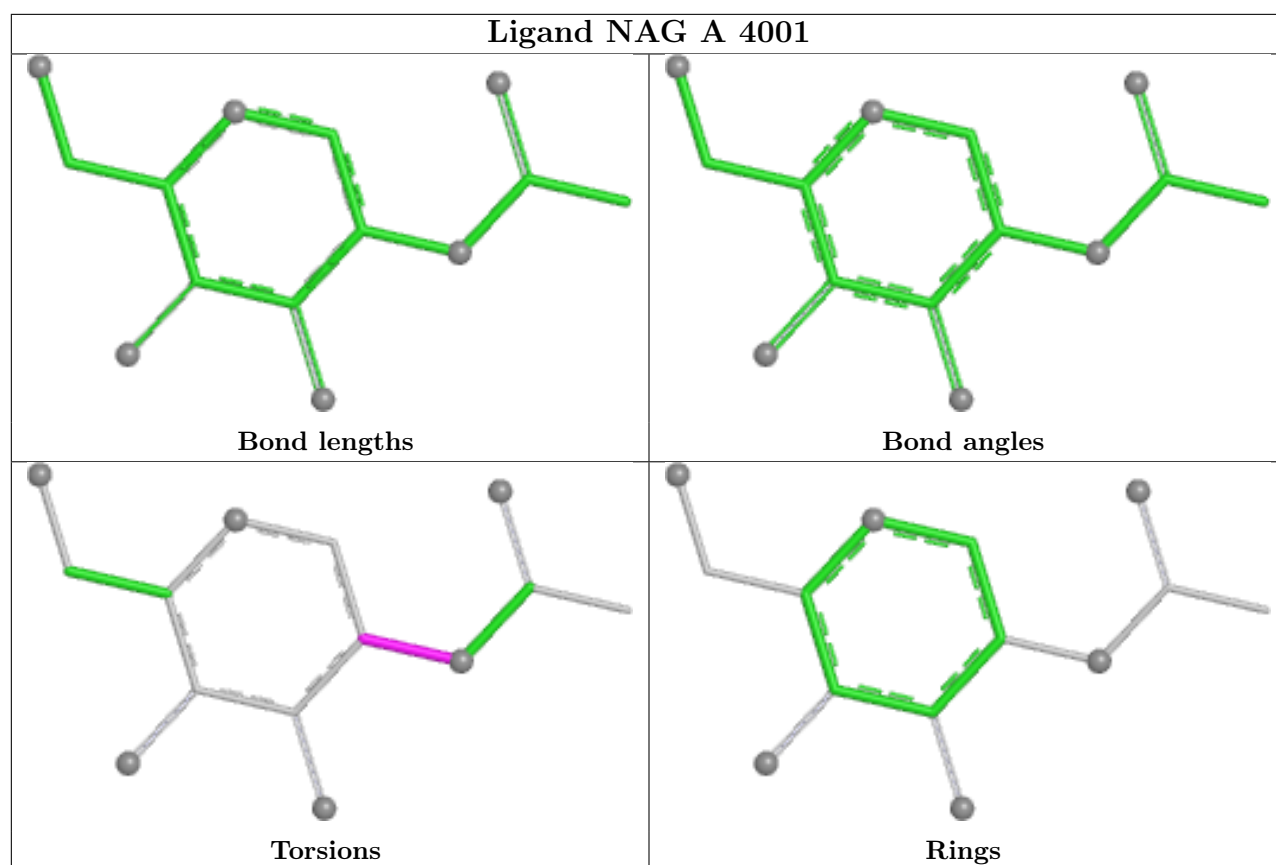
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4001	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

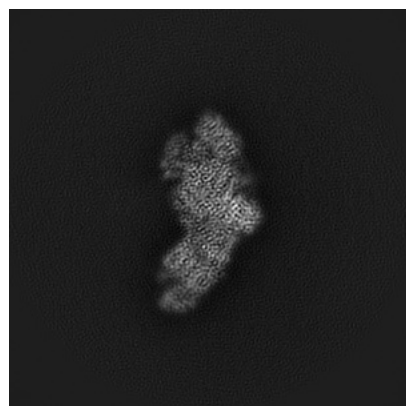
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29245. These allow visual inspection of the internal detail of the map and identification of artifacts.

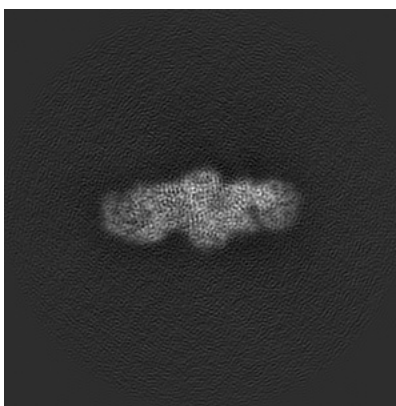
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

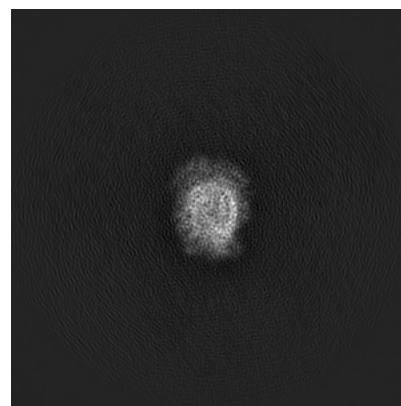
6.1.1 Primary map



X

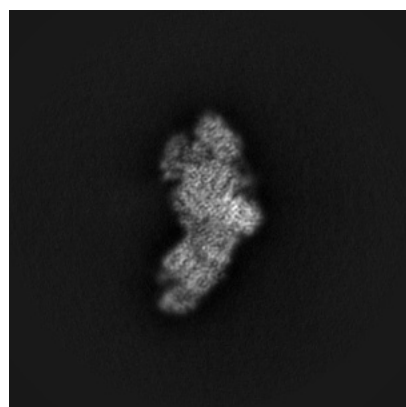


Y

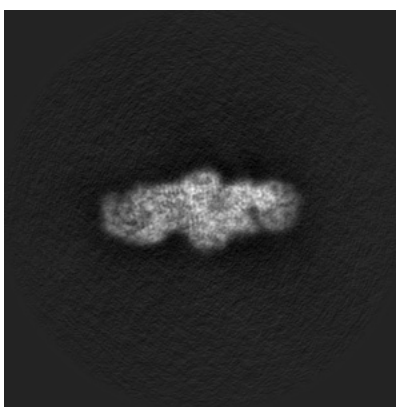


Z

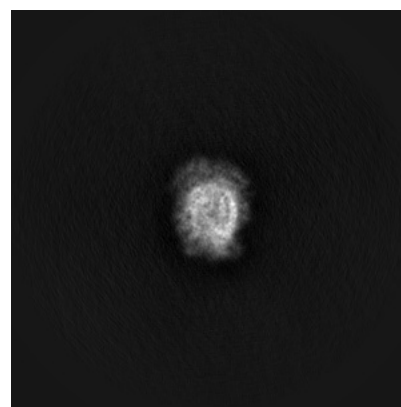
6.1.2 Raw map



X



Y

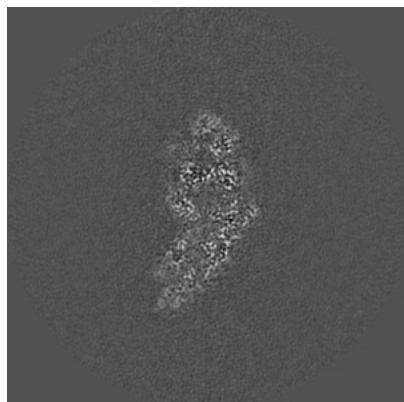


Z

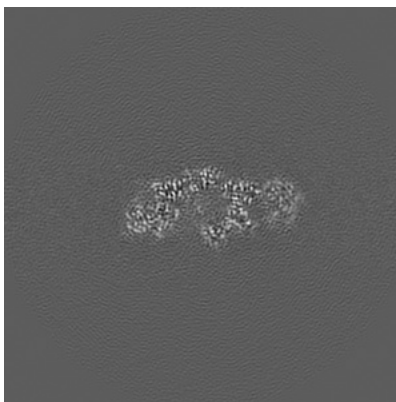
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

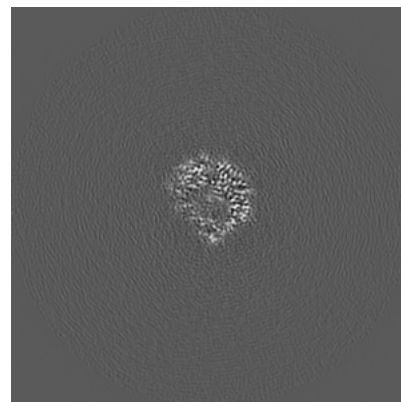
6.2.1 Primary map



X Index: 150

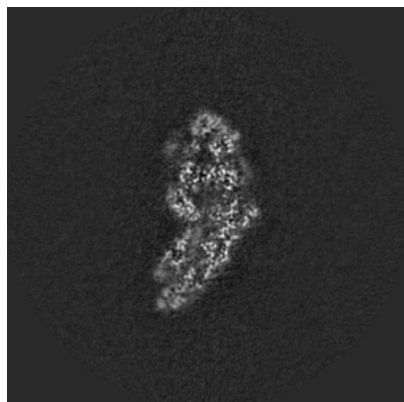


Y Index: 150

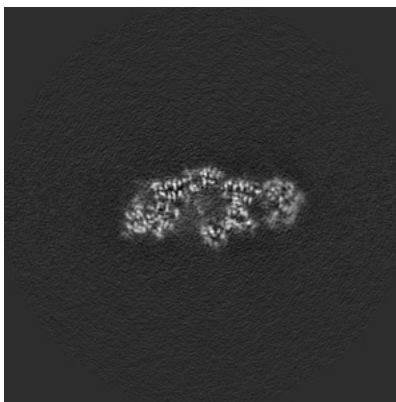


Z Index: 150

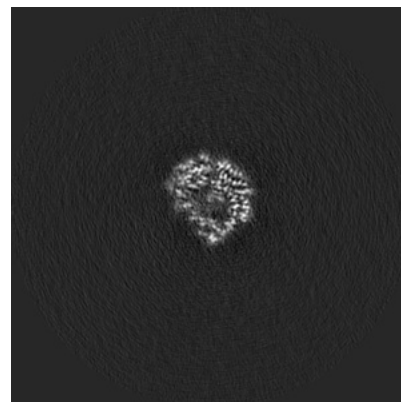
6.2.2 Raw map



X Index: 150



Y Index: 150

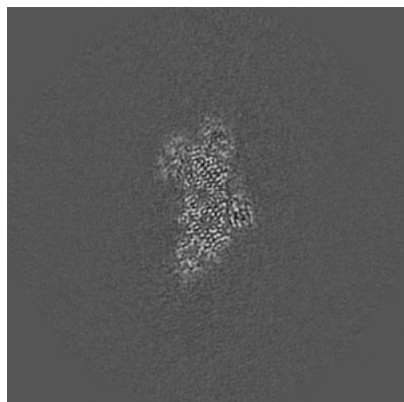


Z Index: 150

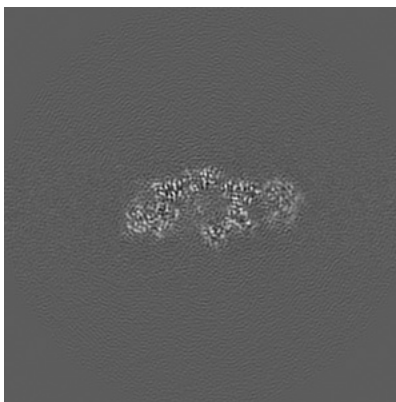
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

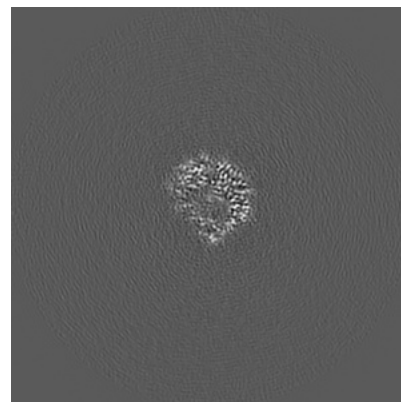
6.3.1 Primary map



X Index: 164

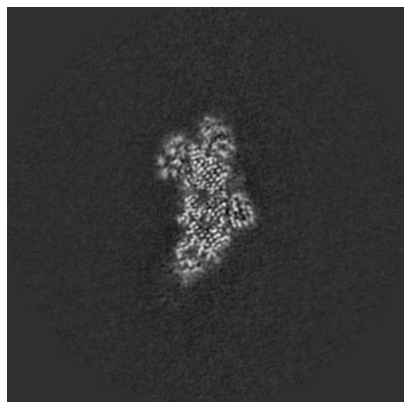


Y Index: 150

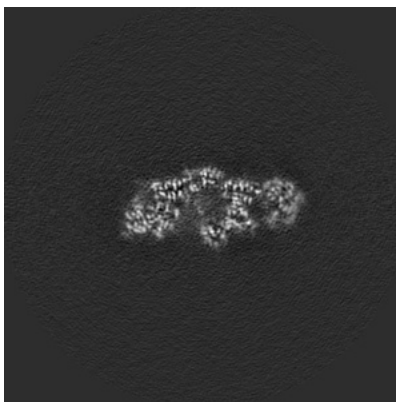


Z Index: 150

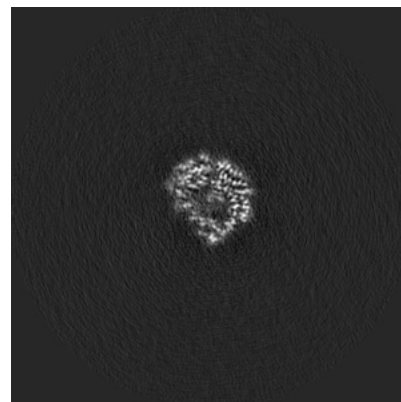
6.3.2 Raw map



X Index: 164



Y Index: 150

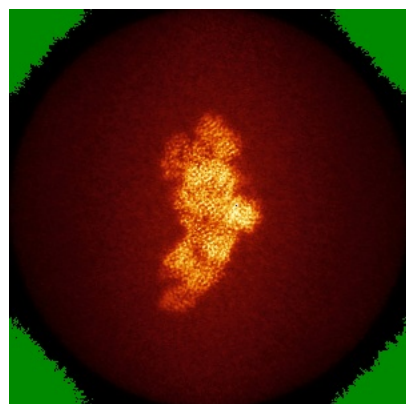


Z Index: 150

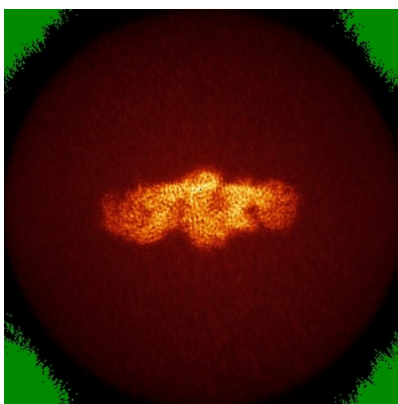
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

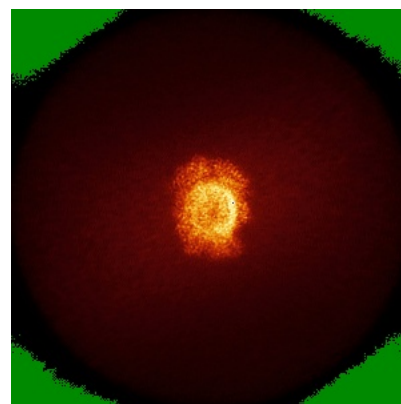
6.4.1 Primary map



X

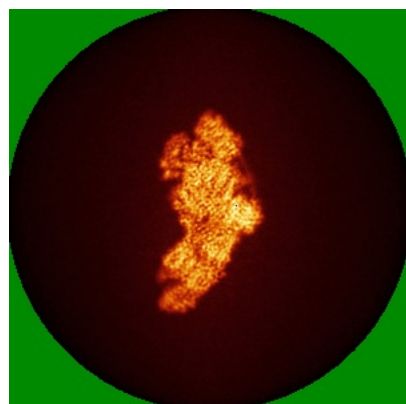


Y



Z

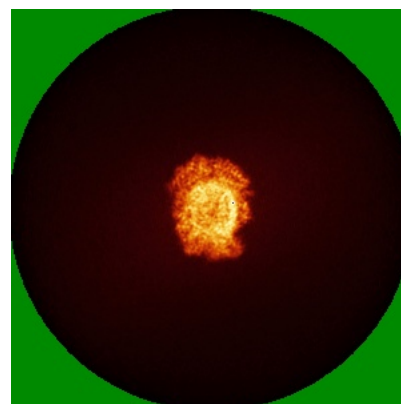
6.4.2 Raw map



X



Y

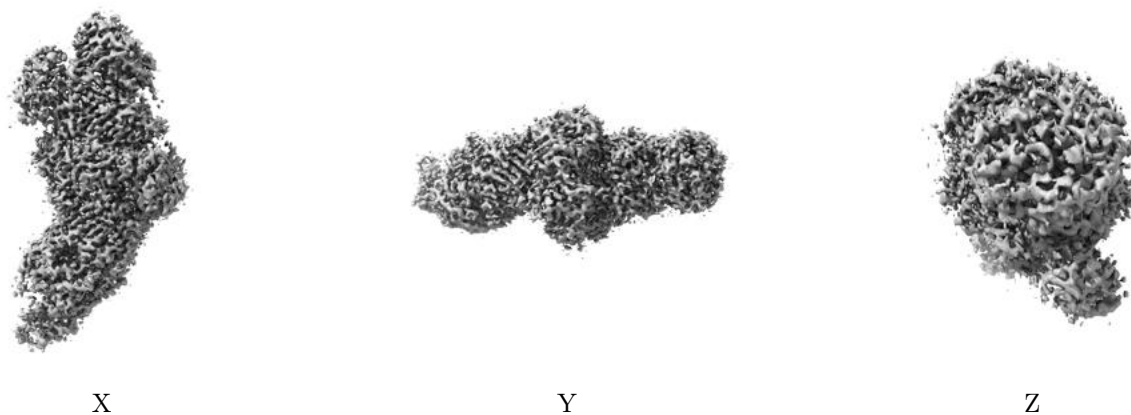


Z

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

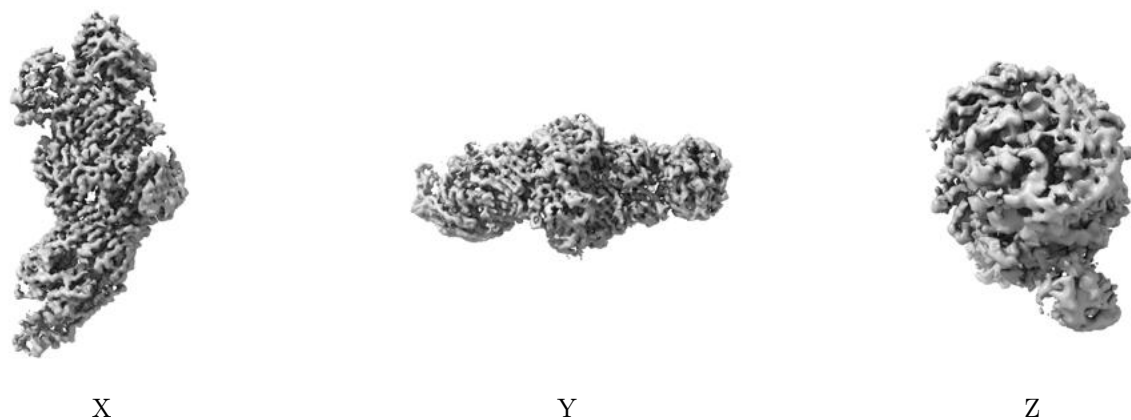
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

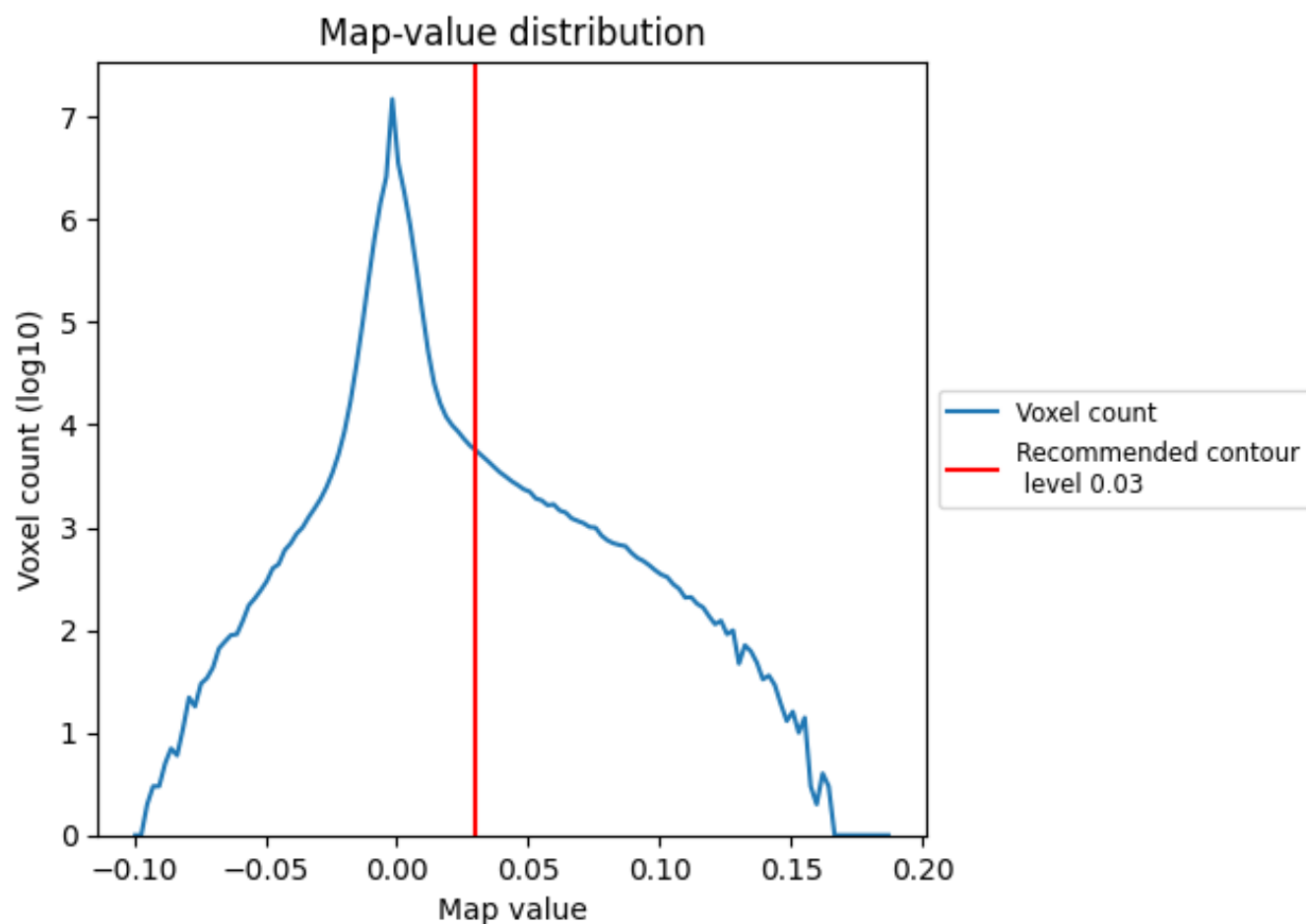
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

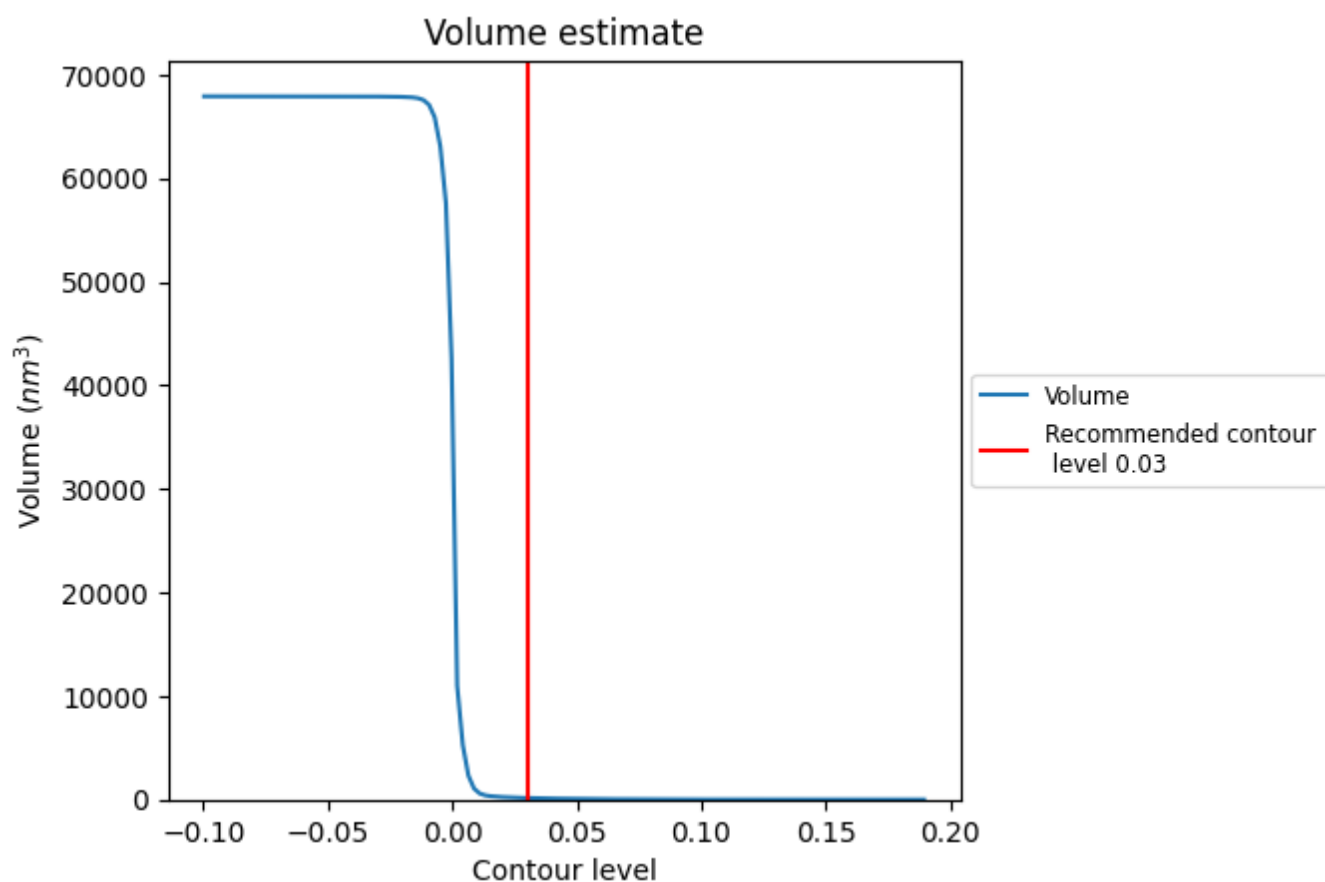
This section contains the results of statistical analysis of the map.

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.

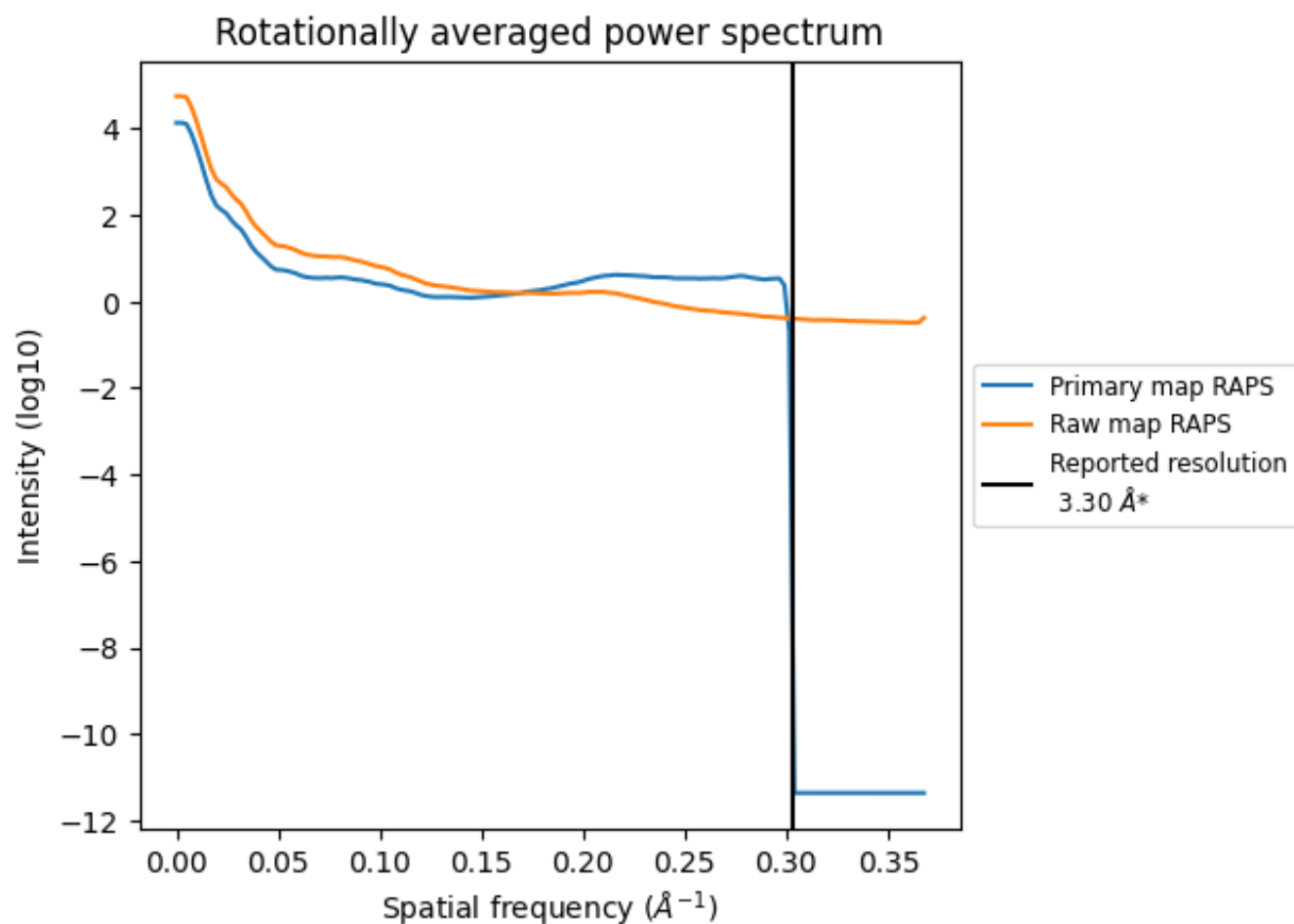
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 151 nm³; this corresponds to an approximate mass of 137 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 ⓘ

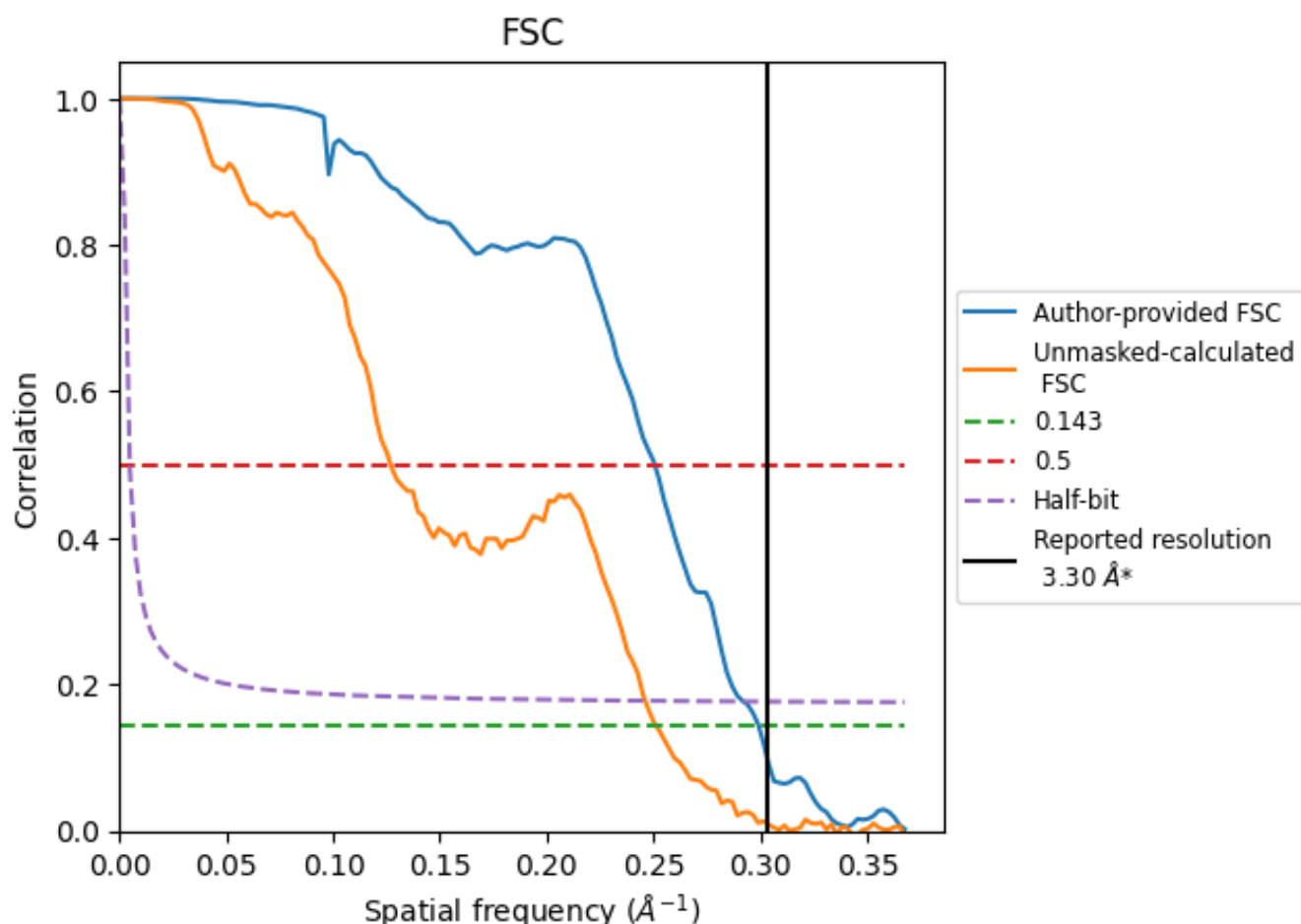


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

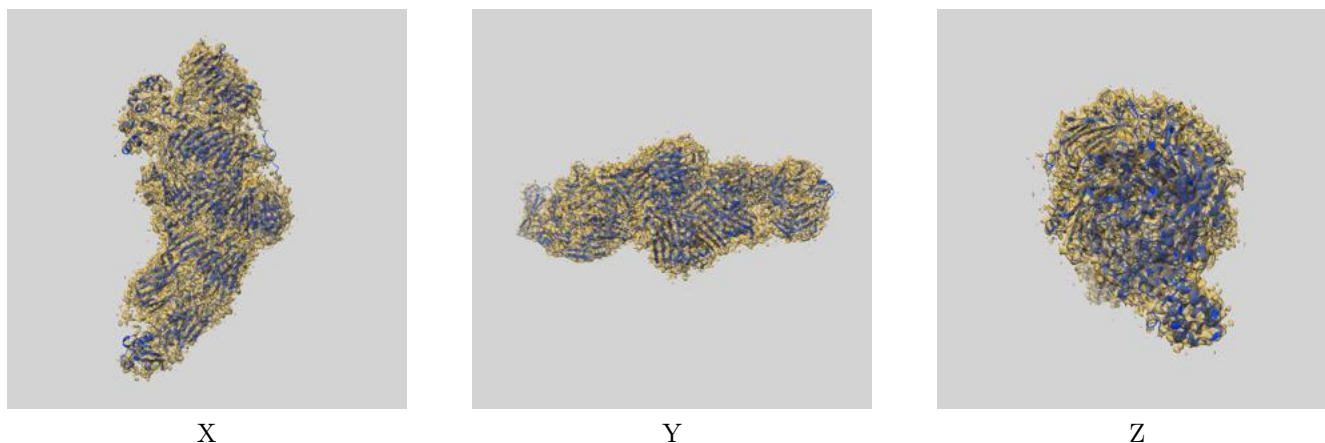
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.34	3.99	3.42
Unmasked-calculated*	3.98	7.88	4.06

*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 3.98 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

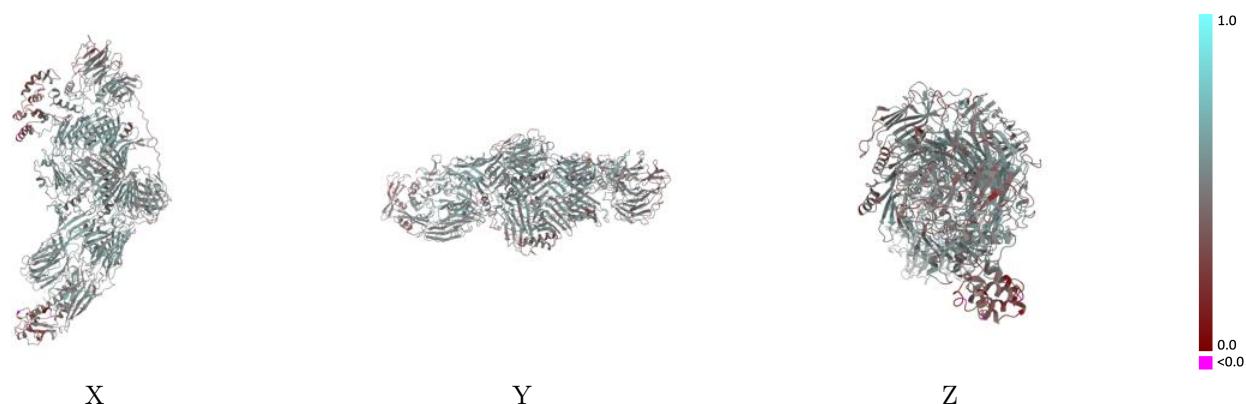
This section contains information regarding the fit between EMDB map EMD-29245 and PDB model 8FJP. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



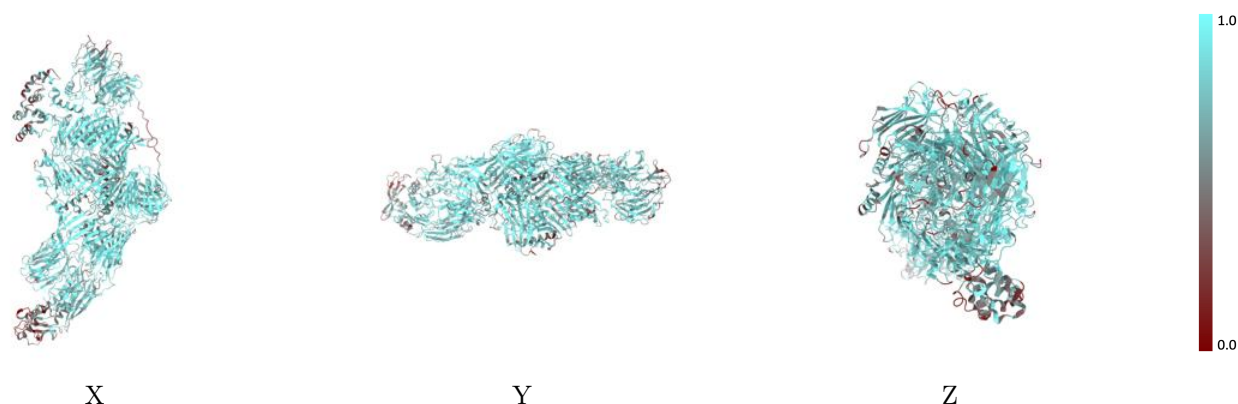
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



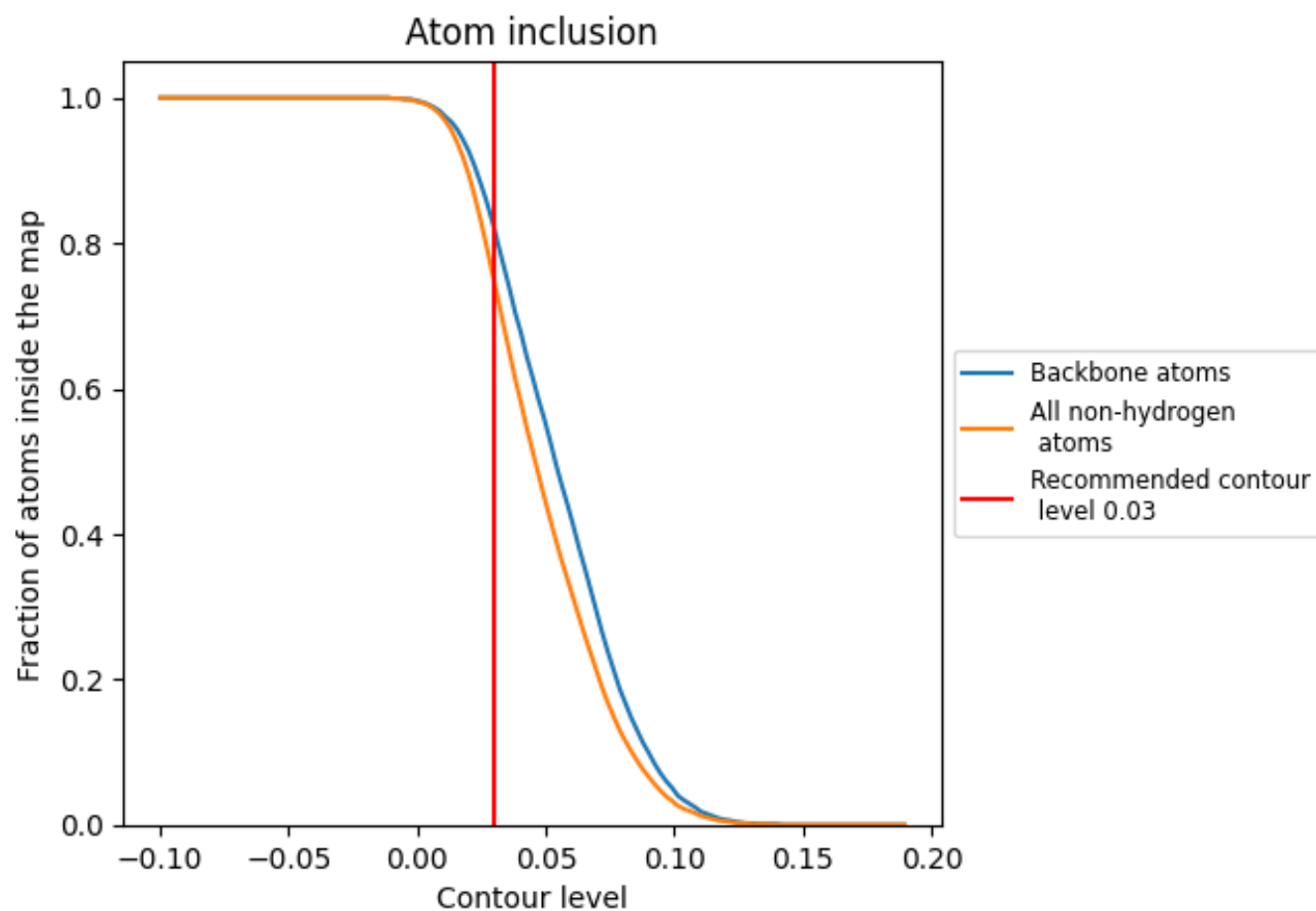
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7480	<div></div> 0.4870
A	<div></div> 0.7480	<div></div> 0.4870
B	<div></div> 0.7140	<div></div> 0.4780

