



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 12:57 PM UTC

PDB ID : 9BDT / pdb_00009bdt
EMDB ID : EMD-44469
Title : Apolipoprotein B 100 bound to LDL receptor and legobody
Authors : Dearborn, A.D.; Reimund, M.; Graziano, G.; Lei, H.; Kumar, A.; Neufeld, E.B.; Remaley, A.T.; Marcotrigiano, J.
Deposited on : 2024-04-12
Resolution : 5.40 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

<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:

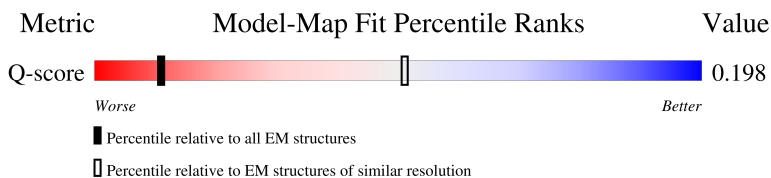
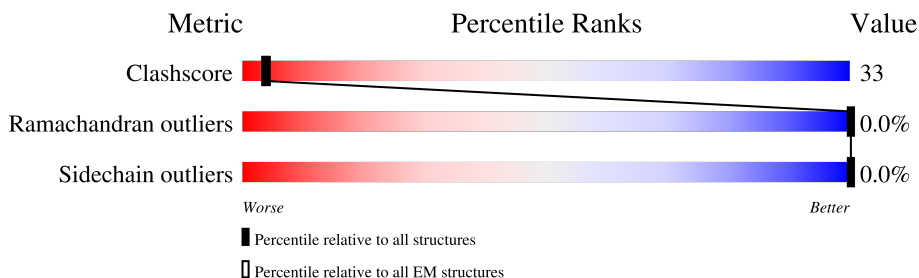
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

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

The reported resolution of this entry is 5.40 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.



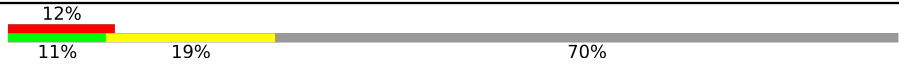


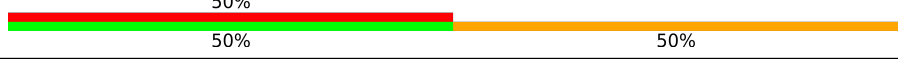
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	538 (4.90 - 5.90)

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	4563	<p>26% (Poor fit), 32% (0 outliers), 44% (1 outlier), 24% (2+ outliers)</p>
2	H	234	<p>6% (Poor fit), 34% (0 outliers), 53% (1 outlier), 13% (2+ outliers)</p>
3	L	219	<p>6% (Poor fit), 48% (0 outliers), 42% (1 outlier), 10% (2+ outliers)</p>
4	B	545	<p>8% (Poor fit), 39% (0 outliers), 55% (1 outlier), 6% (2+ outliers)</p>

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Mol	Chain	Length	Quality of chain
5	I	860	
5	R	860	
6	N	131	
7	G	2	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 38899 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 Apolipoprotein B-100.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3476	27163	17244	4563	5277	79	0	0

- Molecule 2 is a protein called Legobody 8D3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	203	1540	978	255	298	9	0	0

- Molecule 3 is a protein called Legobody 8D3 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	198	1410	887	232	286	5	0	0

- Molecule 4 is a protein called Maltodextrin-binding protein, Immunoglobulin G-binding protein A, Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	514	3948	2517	647	776	8	0	0

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	initiating methionine	UNP C3SHQ8
B	362	ALA	GLN	conflict	UNP P99134
B	363	LEU	ASN	conflict	UNP P99134
B	366	ALA	TYR	conflict	UNP P99134
B	368	ILE	VAL	conflict	UNP P99134
B	370	ILE	ASN	conflict	UNP P99134
B	375	THR	ASN	conflict	UNP P99134
B	376	GLU	ALA	conflict	UNP P99134

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Chain	Residue	Modelled	Actual	Comment	Reference
B	377	GLU	ASP	conflict	UNP P99134
B	392	VAL	GLN	conflict	UNP P99134
B	394	LYS	ALA	conflict	UNP P99134
B	395	GLU	ASN	conflict	UNP P99134
B	396	ILE	VAL	conflict	UNP P99134
B	398	ALA	GLY	conflict	UNP P99134
B	401	LYS	GLN	conflict	UNP P99134
B	405	GLU	ASP	conflict	UNP P99134
B	406	HIS	SER	conflict	UNP P99134
B	?	-	ALA	deletion	UNP P99134
B	411	GLY	ASP	conflict	UNP P99134
B	412	GLY	ALA	conflict	UNP P99134
B	413	SER	GLN	conflict	UNP P99134
B	414	GLY	GLN	conflict	UNP P99134
B	415	GLY	ASN	conflict	UNP P99134
B	416	ALA	ASN	conflict	UNP P99134
B	417	GLY	PHE	conflict	UNP P99134
B	418	SER	ASN	conflict	UNP P99134
B	419	GLY	LYS	conflict	UNP P99134
B	469	GLY	-	linker	UNP P99134
B	470	GLY	-	linker	UNP P99134
B	471	GLY	-	linker	UNP P99134
B	472	SER	-	linker	UNP P99134
B	473	GLY	-	linker	UNP P99134
B	474	GLY	-	linker	UNP P99134
B	475	GLY	-	linker	UNP P99134
B	476	SER	-	linker	UNP P99134
B	477	GLY	-	linker	UNP P99134
B	478	GLY	-	linker	UNP P99134
B	479	SER	-	linker	UNP P99134
B	538	GLY	-	expression tag	UNP P06654
B	539	SER	-	expression tag	UNP P06654
B	540	GLY	-	expression tag	UNP P06654
B	541	HIS	-	expression tag	UNP P06654
B	542	HIS	-	expression tag	UNP P06654
B	543	HIS	-	expression tag	UNP P06654
B	544	HIS	-	expression tag	UNP P06654
B	545	HIS	-	expression tag	UNP P06654
B	546	HIS	-	expression tag	UNP P06654

- Molecule 5 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	256	Total 1925	C 1230	N 317	O 373	S 5	0	0
5	R	273	Total 1910	C 1133	N 324	O 409	S 44	0	0

- Molecule 6 is a protein called ApoB100 nanobody 4.

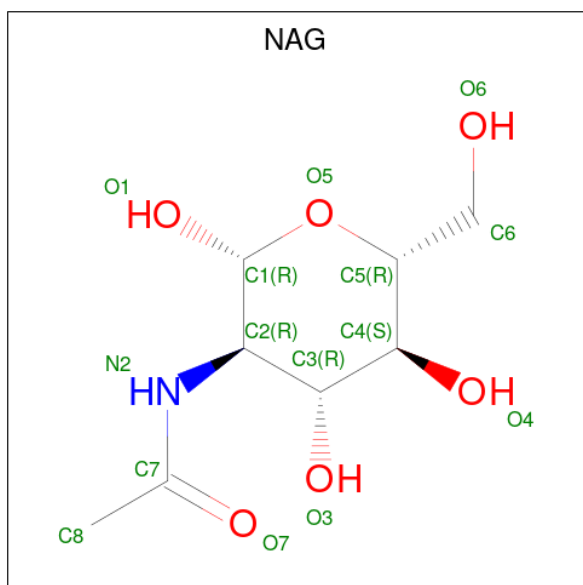
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	128	Total 912	C 572	N 162	O 174	S 4	0	0

- Molecule 7 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		
7	G	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



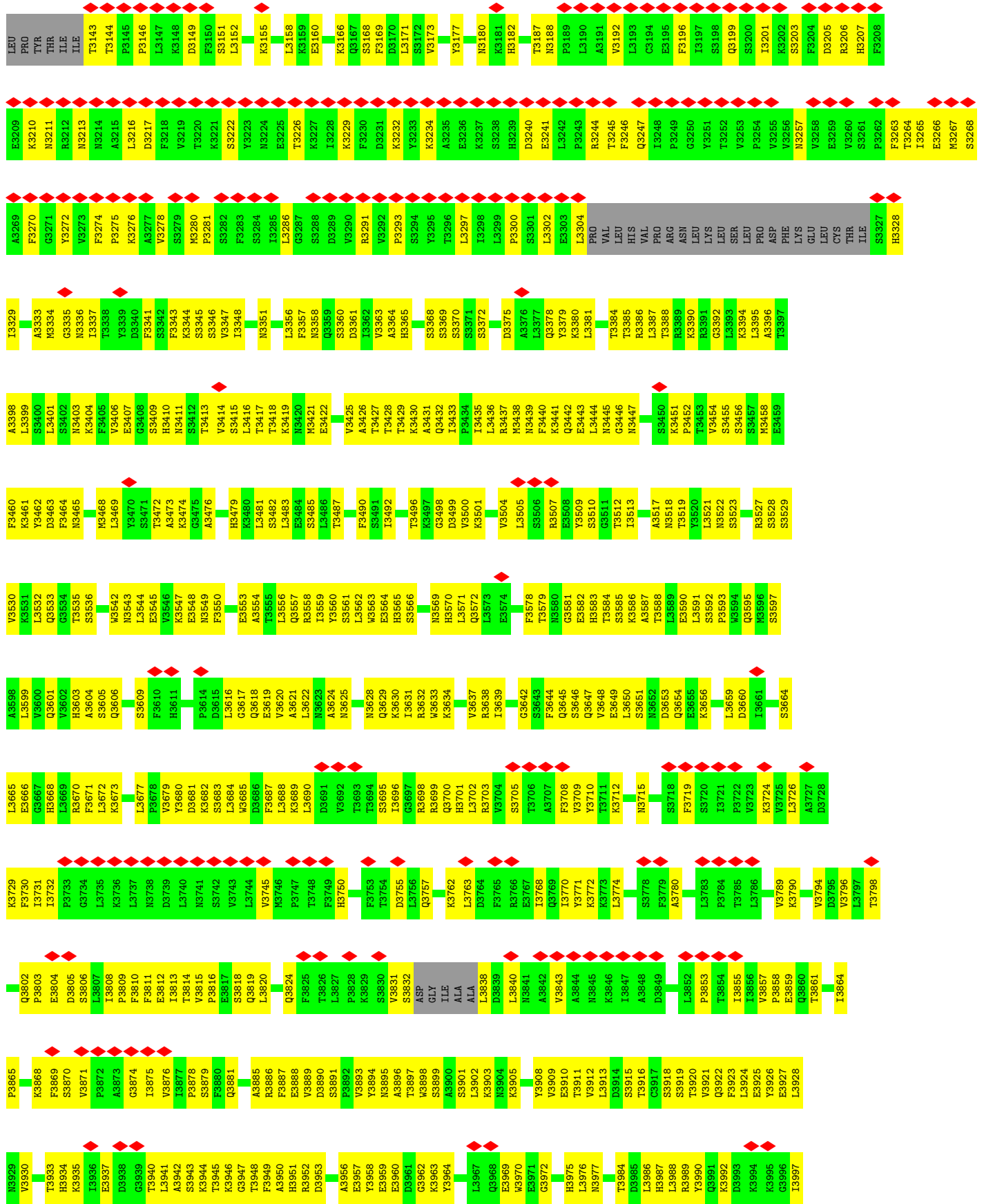
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	

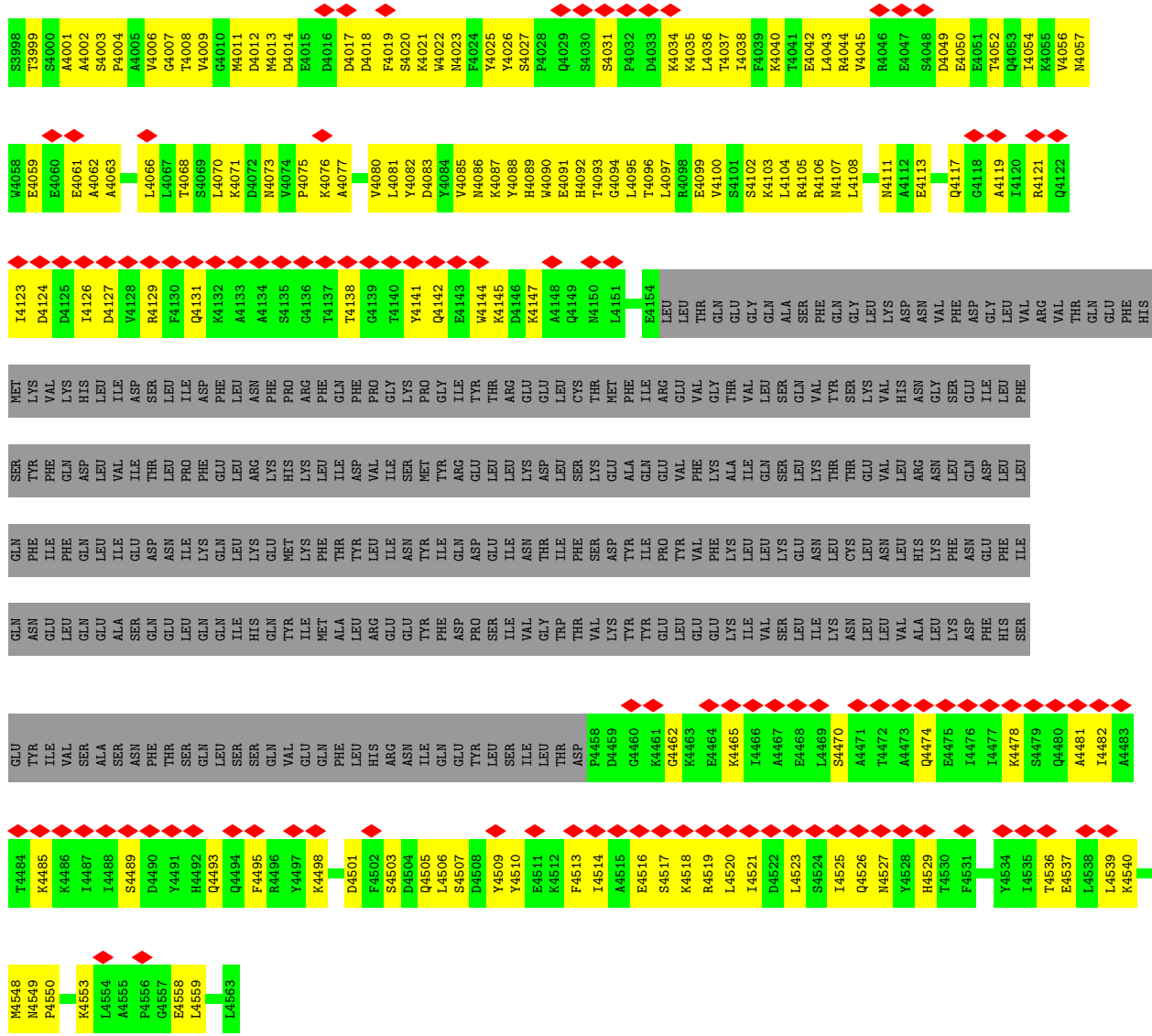
- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
9	R	7	Total	Ca	0
			7	7	

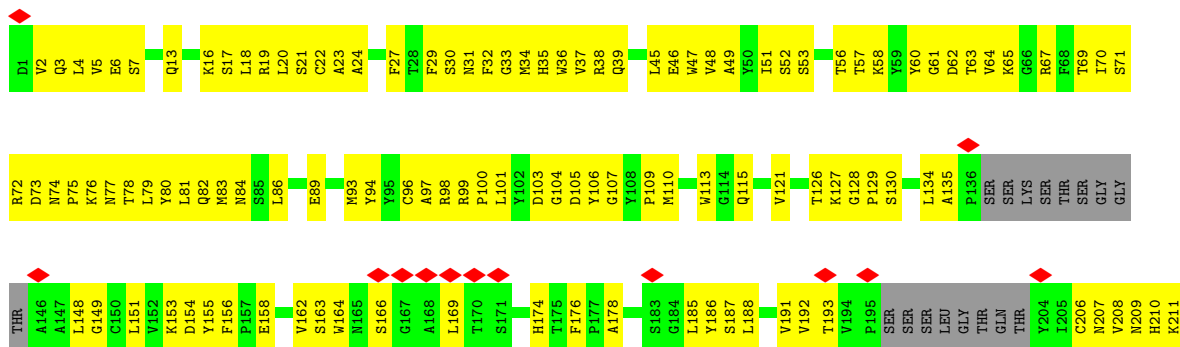
ALA	N2084	P2023	A1962	A1830	A1760	L1689	D1634	T1574	G1505	K1436	Y1373
LEU	R2085	ILE	A1963	Y1831	G1761	D1700	K1635	M1575	Q1506	F1437	S1374
THR	Q2086	LYS	L1964	Q1932	L1762	K1702	I1636	G1576	R1507	S1438	G1375
LYS	T2087	VAL	E1965	M1833	L1763	A1703	M1637	K1577	H1439	H1439	G1376
TRP	I2088	PRO	H1966	M1834	L1764	A1704	G1638	Y1578	D1508	V1440	M1377
ARG	I2089	LEU	K1967	E1835	D1765	A1705	G1639	K1579	P1509	E1441	T1378
ILE	V2090	LEU	V1968	H1838	F1766	L1706	A1640	M1580	M1510	K1442	S1379
THR	V2091	LEU	A1969	A1841	S1767	T1706	H1641	F1581	T1511	L1443	T1380
ASN	L2092	GLU	A1970	S1843	S1768	L1708	A1642	A1582	G1444	G1444	D1381
ASP	E2093	PRO	L1972	S1844	D1771	S1709	A1643	T1583	N1445	N1445	H1382
ILE	N2094	ILE	T1973	S1845	M1772	L1710	L1645	M1585	N1446	N1446	F1383
GLN	V2095	ASP	P1974	A1845	M1773	G1711	L1646	K1586	P1447	P1447	S1384
ALA	Q2096	LEU	A1975	S1848	S1775	S1712	R1647	M1587	V1448	V1448	L1385
ALA	Q2097	LEU	E1976	A1849	S1776	A1713	G1648	M1588	S1449	S1449	R1386
ASP	R2097	ASP	T1978	S1850	S1777	G1715	Q1649	T1590	K1450	K1450	A1387
ASP	N2098	A2039	G1979	A1851	D1777	A1716	Q1650	F1591	G1451	G1451	R1388
ALA	L2099	L2040	K1980	S1852	K1778	M1718	D1651	S1592	L1452	L1452	H1389
ILE	K2100	L2041	K1982	K1952	F1779	L1718	G1652	K1593	L1453	L1453	H1390
ASN	H2101	E2041	L1983	A1853	Y1780	L1719	S1653	Q1594	L1454	L1454	M1391
ASN	ASN	M2042	D1854	D1854	M1785	G1720	T1654	M1595	D1455	D1455	K1392
ASN	ASN	R2043	T1855	T1855	Q1787	M1721	S1655	A1596	A1457	A1457	A1393
GLU	ASP	D2044	V1856	V1856	L1788	D1722	L1656	A1597	S1458	S1458	D1394
LEU	PHE	A2045	A1857	A1857	Q1789	S1723	T1657	L1597	S1459	S1459	S1395
LEU	GLN	V2046	K1858	K1858	Q1789	M1725	T1658	L1598	Q1464	Q1464	V1396
SER	VAL	E2047	V1859	V1859	Q1790	G1726	T1659	R1599	M1465	M1465	V1397
GLN	ARG	K2048	Q1860	Q1860	Y1791	I1726	M1660	E1601	S1466	S1466	L1398
LEU	ARG	P2049	F1864	F1864	S1792	M1728	K1661	Q1602	A1467	A1467	L1399
THR	ARG	Q2050	S1865	S1865	L1793	K1729	S1662	Q1603	S1468	S1468	Y1402
TYR	ALA	E2051	H1866	H1866	L1736	A1604	S1663	Q1604	V1469	V1469	M1403
TYR	ALA	F2052	M1869	M1869	Q1733	D1730	L1664	D1605	H1470	H1470	M1404
ALA	LEU	T2053	T1870	T1870	E1734	K1730	L1665	Y1606	L1471	L1471	Q1405
GLY	LEU	L2054	I1872	I1872	G1735	S1732	L1666	E1607	D1472	D1472	G1406
GLY	LEU	V2055	L1796	L1796	L1736	Q1733	L1667	S1608	S1473	S1473	S1407
ASP	LEU	A2056	L1801	L1801	G1736	E1735	M1668	L1609	K1474	K1474	G1408
PRO	PRO	F2057	K1802	K1802	K1737	M1738	M1669	L1610	E1409	E1409	E1409
GLN	GLN	V2058	Y1803	Y1803	L1738	S1739	M1672	F1611	T1476	T1476	T1410
ILE	GLN	K2059	M1804	M1804	L1738	S1739	E1674	S1613	Q1477	Q1477	T1411
ALA	ALA	Y2060	A1805	A1805	L1738	S1739	L1675	L1614	H1478	H1478	Y1412
ASP	ASP	N2063	L1806	L1806	M1742	M1742	G1676	L1616	L1479	L1479	D1413
SER	TYR	Q2064	D1807	D1807	M1743	M1743	L1677	S1618	F1480	F1480	H1414
LEU	LEU	D2065	L1808	L1808	G1744	G1744	S1678	L1619	V1481	V1481	K1415
LEU	LEU	E2066	M1809	M1809	S1745	S1745	G1679	M1620	K1482	K1482	M1416
SER	SER	V2066	M1810	M1810	Y1746	Y1746	M1681	A1680	E1483	E1483	T1417
SER	PHE	H2067	Y1811	Y1811	E1748	E1748	M1682	A1559	V1484	V1484	F1418
ASN	ASN	S2068	G1812	G1812	M1749	M1749	K1683	A1559	K1485	K1485	T1419
TRP	TRP	I2069	K1813	K1813	F1750	F1750	T1686	H1622	G1488	G1488	L1420
ALA	GLU	N2070	L1814	L1814	F1751	F1751	E1625	G1624	Q1489	Q1489	S1421
ALA	GLN	L2071	R1815	R1815	D1752	D1752	M1687	L1626	F1490	F1490	S1422
ASN	VAL	P2072	L1816	L1816	H1753	H1753	G1688	M1627	G1423	G1423	D1423
SER	SER	F2073	E1817	E1817	T1754	T1754	R1689	A1628	G1424	G1424	G1424
ALA	ALA	F2074	L1819	L1819	S1756	S1756	M1693	A1628	A1487	A1487	S1425
LYS	LYS	E2075	K1820	K1820	F1896	F1896	M1694	D1629	K1498	K1498	H1428
GLY	GLY	T2076	L1827	L1827	R1997	R1997	M1694	L1630	T1500	T1500	K1429
LEU	LEU	L2077	K1828	K1828	S1998	S1998	F1697	G1632	Y1501	Y1501	H1428
THR	THR	Q2078	G1829	G1829	S1998	S1998	M1698	L1503	T1502	T1502	K1429
		E2079						L1503	G1502	G1502	H1428
		Y2080						L1503	L1503	L1503	H1428
		F2081						L1503	L1503	L1503	H1428
		E2082						L1503	L1503	L1503	H1428
		R2083						L1503	L1503	L1503	H1428

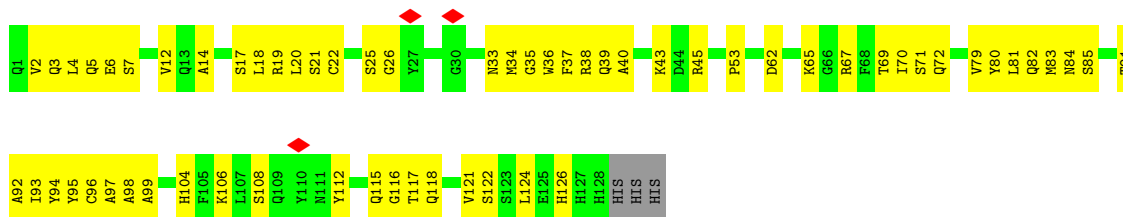
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T3093	A3004	K3005	A3008	L3009	F3010	G3011	E3012	G3013	G3014	A3015	E3016	F3017	G3018	H3019	G3020	H3021	K3028	G3031	K3034	N3035	S3036	L3037	F3038	F3039	S3040	A3041	Q3042	P3043	F3044	E3045	I3046	T3047	A3048	S3049	T3050	N3051	N3052	E3053	G3054	N3055	L3056	K3057	V3058	Q3059	F3060	F3061	R3062	L3064	T3065	S3066	K3067	I3068	D3069			
S2937	D2938	E2939	G2940	T2941	H2942	E2943	I2946	S2947	F2948	T2949	I2950	E2951	G2952	F2953	L2954	T2955	F2957	G2958	L2959	S2960	N2961	K2962	L2963	N2964	R2969	V2970	H2971	Q2972	N2973	L2974	V2975	Y2976	E2977	S2978	G2979	S2980	L2981	W2982	F2983	S2984	K2985	L2986	E2987	I2988	Q2989	Q2990	Q2991	V2992	D2993	S2994	G2998	H2999	S3000	V3001	L3002	
K2876	I2877	N2878	N2879	Q2880	L2881	T2882	F2883	D2884	S2885	N2886	K2888	T2887	F2889	Y2890	H2891	K2892	L2893	N2894	I2895	P2896	K2897	L2898	D2899	F2900	S2901	Q2902	Q2903	L2906	R2907	N2908	E2909	I2910	K2911	T2912	L2913	L2914	K2915	A2916	H2918	I2919	A2920	T2922	S2923	S2924	G2925	K2926	G2927	S2928	W2929	K2930	W2931	A2932	C2933	P2934	R2935	F2936
A2810	N2811	A2812	Q2813	L2814	S2815	N2816	F2817	K2818	L2819	W2820	F2821	L2822	L2823	L2824	K2825	E2826	S2827	V2828	K2829	F2830	S2831	Y2834	L2835	R2836	T2837	E2838	H2839	G2840	S2841	E2842	W2843	L2844	F2845	F2846	G2847	N2848	A2849	I2850	E2851	G2852	N2855	S2859	L2860	H2861	L2862	E2863	T2866	L2867	E2868	L2869	N2870	G2872	V2875			
I2746	S2747	H2748	T2749	S2750	E2751	V2752	P2753	T2754	F2755	G2756	K2757	L2758	Y2759	S2760	I2761	L2762	K2763	I2764	Q2765	S2766	P2767	L2768	F2769	T2770	A2773	N2774	A2775	D2776	I2777	G2778	N2779	G2780	THR	THR	ALA	ASN	GLU	A2787	G2788	I2789	A2790	I2793	T2794	A2795	K2796	G2797	E2798	S2799	K2800	L2801	F2806	D2807	F2808	Q2809		
LEU	GLN	TRP	PRO	VAL	ASP	TYR	LEU	ARG	ASP	LEU	ASP	LEU	VAL	ASP	LEU	ILE	PRO	ALA	ILE	THR	LEU	PRO	ASP	PHE	THR	PRO	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F2721	I2722	P2724	I2723	L2726	N2727	L2728	N2729	D2730	F2731	Q2732	V2733	A2734	D2735	L2736	H2737	I2738	P2739	E2740	F2741	Q2742	L2743		
LEU	ARG	ILE	PRO	SER	VAL	GLN	ILE	ASN	PHE	TRP	ASP	LEU	VAL	ASP	LEU	ILE	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	E2715	I2716	A2717	I2718	P2719	E2720	F																							





● Molecule 2: Legobody 8D3 Fab Heavy Chain





- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	527598	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 ($e^-/\text{\AA}^2$)	51.38	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.376	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	557.76, 557.76, 557.76	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6600001, 1.6600001, 1.6600001	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: CA, 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	0.12	0/27687	0.33	1/37490 (0.0%)
2	H	0.17	0/1581	0.41	0/2155
3	L	0.11	0/1438	0.33	0/1973
4	B	0.12	0/4032	0.33	1/5473 (0.0%)
5	I	0.15	0/1969	0.39	0/2700
5	R	0.19	1/1944 (0.1%)	0.43	0/2637
6	N	0.13	0/930	0.37	0/1258
All	All	0.13	1/39581 (0.0%)	0.34	2/53686 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	308	GLU	C-O	5.45	1.26	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	185	VAL	N-CA-C	-5.49	107.93	113.47
1	A	3101	ASN	N-CA-CB	5.29	119.57	110.68

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	27163	0	26925	1775	0
2	H	1540	0	1470	136	0
3	L	1410	0	1265	72	0
4	B	3948	0	3850	283	0
5	I	1925	0	1789	166	0
5	R	1910	0	1516	110	0
6	N	912	0	824	51	0
7	G	28	0	25	1	0
8	A	56	0	52	4	0
9	R	7	0	0	0	0
All	All	38899	0	37716	2548	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 33.

The worst 5 of 2548 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:H:83:MET:HB3	2:H:86:LEU:HD21	1.40	1.00
1:A:3549:ASN:HB3	1:A:3564:GLU:HB3	1.42	1.00
1:A:3590:GLU:HB2	1:A:3597:SER:HB2	1.48	0.95
5:I:534:THR:HB	5:I:565:GLY:HA2	1.50	0.94
4:B:456:VAL:HA	4:B:459:GLU:HB3	1.50	0.92

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	3450/4563 (76%)	3221 (93%)	229 (7%)	0	100 100
2	H	197/234 (84%)	182 (92%)	15 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	188/219 (86%)	179 (95%)	9 (5%)	0	100	100
4	B	508/545 (93%)	479 (94%)	29 (6%)	0	100	100
5	I	252/860 (29%)	212 (84%)	40 (16%)	0	100	100
5	R	263/860 (31%)	225 (86%)	37 (14%)	1 (0%)	30	67
6	N	126/131 (96%)	112 (89%)	14 (11%)	0	100	100
All	All	4984/7412 (67%)	4610 (92%)	373 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	R	298	MET

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	3013/4080 (74%)	3013 (100%)	0	100	100
2	H	169/199 (85%)	169 (100%)	0	100	100
3	L	145/192 (76%)	145 (100%)	0	100	100
4	B	408/433 (94%)	408 (100%)	0	100	100
5	I	201/755 (27%)	201 (100%)	0	100	100
5	R	204/755 (27%)	204 (100%)	0	100	100
6	N	80/103 (78%)	79 (99%)	1 (1%)	61	72
All	All	4220/6517 (65%)	4219 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	N	53	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2064	GLN
4	B	438	GLN
1	A	2989	GLN
4	B	407	GLN
6	N	115	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](#)

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$
7	NAG	G	1	7,1	14,14,15	1.25	2 (14%)	17,19,21	2.09	2 (11%)
7	NAG	G	2	7	14,14,15	0.41	0	17,19,21	0.55	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
7	NAG	G	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1	NAG	O5-C1	4.01	1.50	1.43
7	G	1	NAG	C1-C2	2.05	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1	NAG	C1-O5-C5	7.75	122.58	112.19
7	G	1	NAG	C1-C2-N2	2.41	114.23	110.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

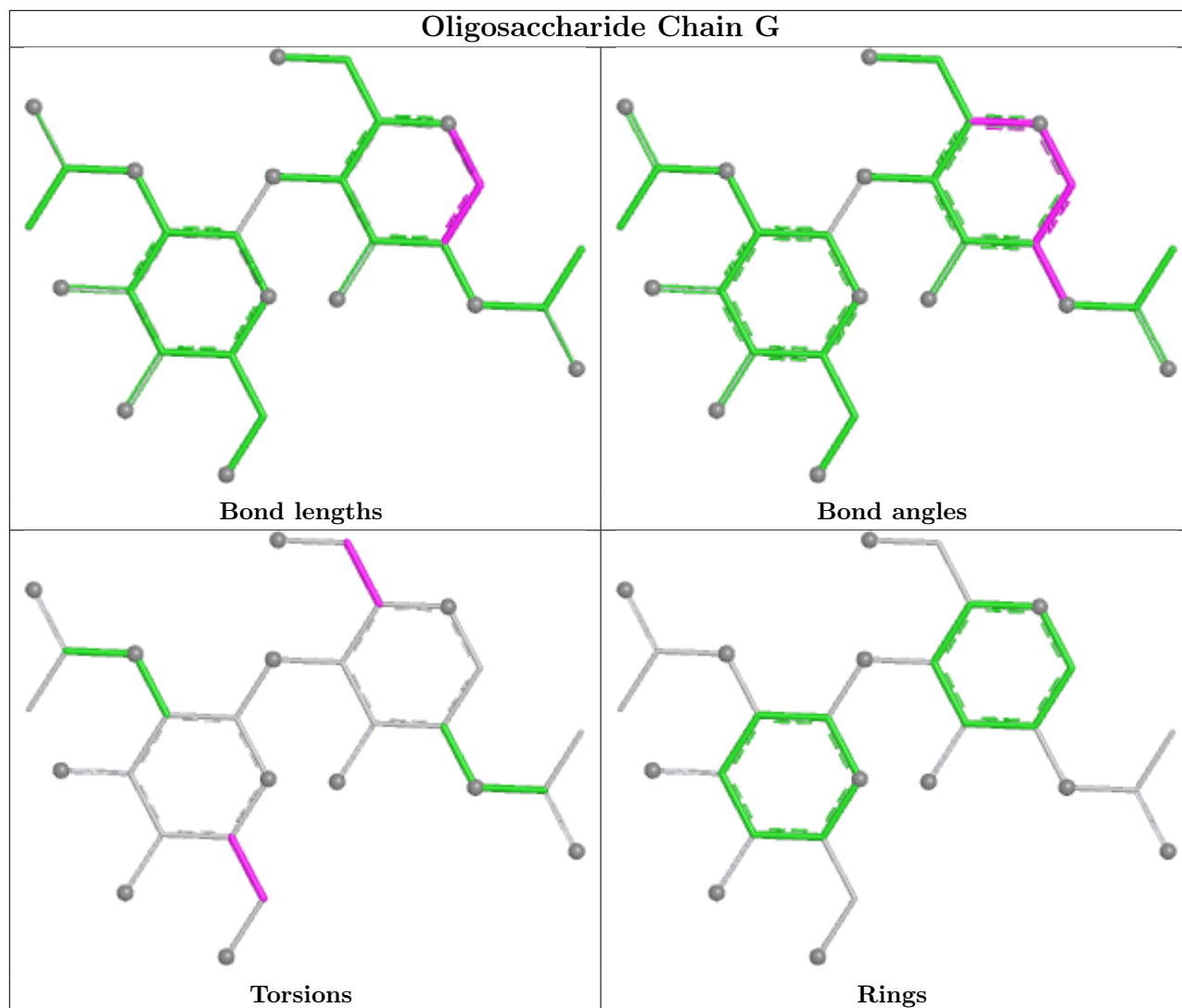
Mol	Chain	Res	Type	Atoms
7	G	2	NAG	C4-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
7	G	1	NAG	C4-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	1	NAG	1	0

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



5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
8	NAG	A	4601	1	14,14,15	0.27	0	17,19,21	0.46	0
8	NAG	A	4602	1	14,14,15	0.31	0	17,19,21	0.44	0
8	NAG	A	4604	1	14,14,15	0.37	0	17,19,21	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	4603	1	14,14,15	0.24	0	17,19,21	0.47	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
8	NAG	A	4601	1	-	2/6/23/26	0/1/1/1
8	NAG	A	4602	1	-	0/6/23/26	0/1/1/1
8	NAG	A	4604	1	-	5/6/23/26	0/1/1/1
8	NAG	A	4603	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	4604	NAG	C2-N2-C7	4.62	129.09	122.90
8	A	4604	NAG	C1-C2-N2	2.03	113.64	110.43

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	4603	NAG	C4-C5-C6-O6
8	A	4601	NAG	C4-C5-C6-O6
8	A	4603	NAG	O5-C5-C6-O6
8	A	4601	NAG	O5-C5-C6-O6
8	A	4603	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	4601	NAG	1	0
8	A	4602	NAG	2	0
8	A	4604	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.

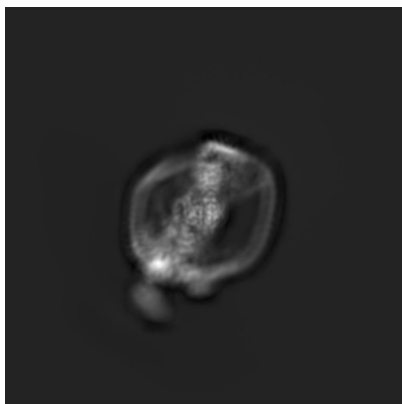
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44469. These allow visual inspection of the internal detail of the map and identification of artifacts.

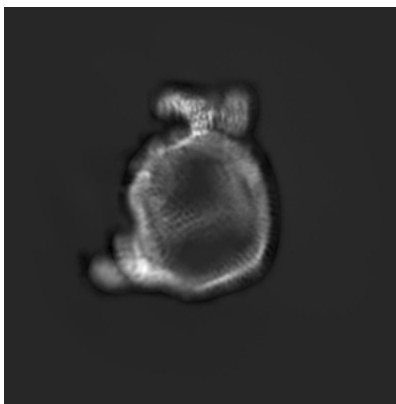
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

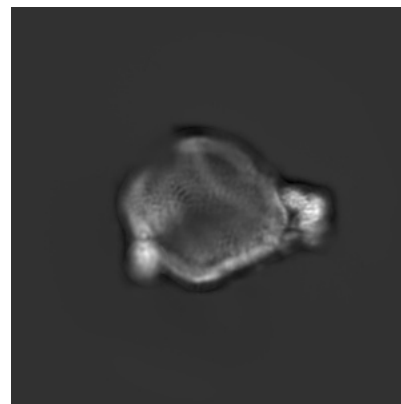
6.1.1 Primary map



X

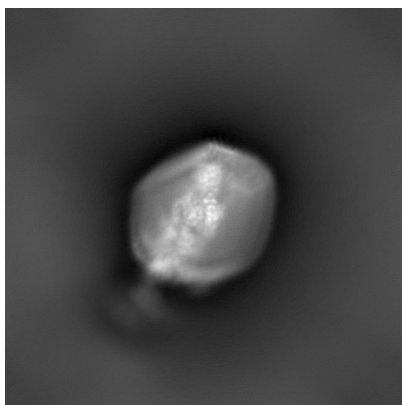


Y

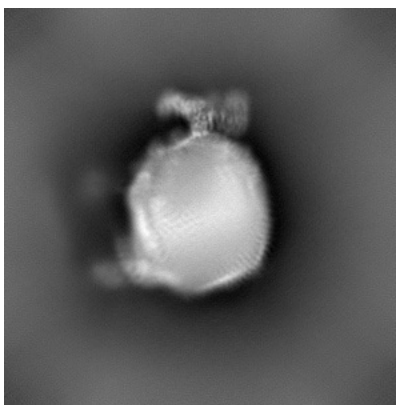


Z

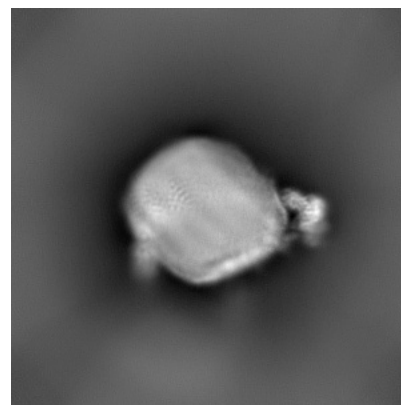
6.1.2 Raw map



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: 168

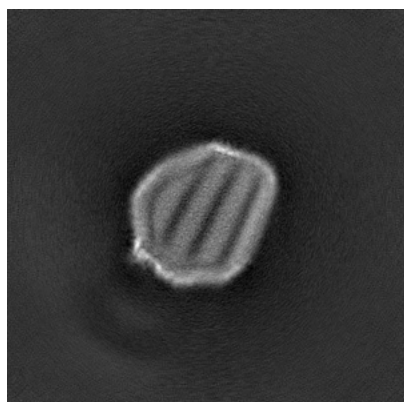


Y Index: 168

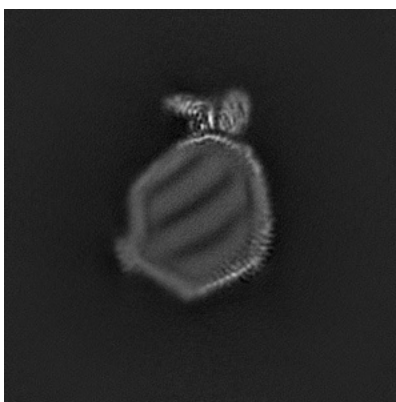


Z Index: 168

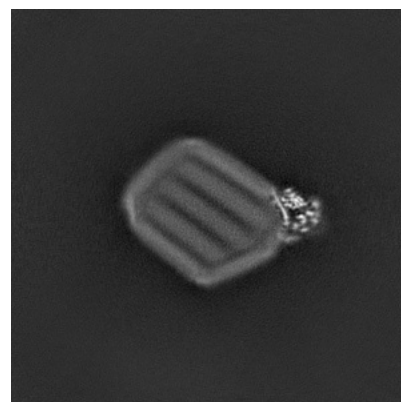
6.2.2 Raw map



X Index: 168



Y Index: 168

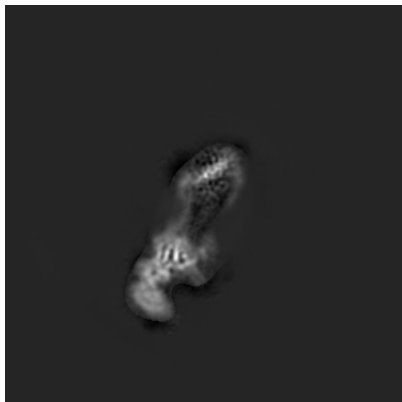


Z Index: 168

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

6.3 Largest variance slices [i](#)

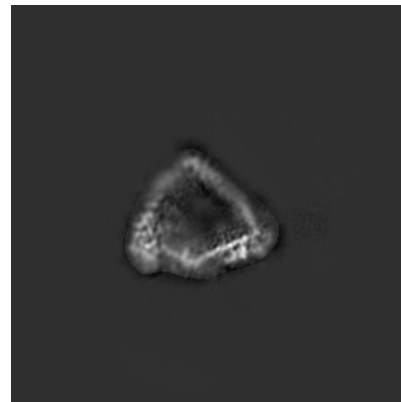
6.3.1 Primary map



X Index: 112

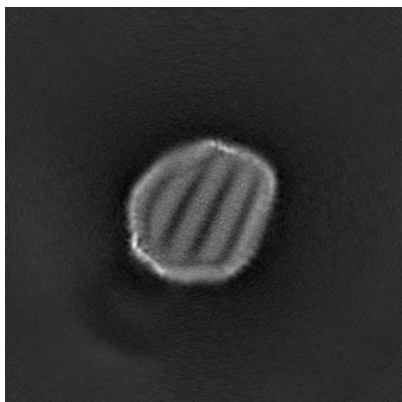


Y Index: 171

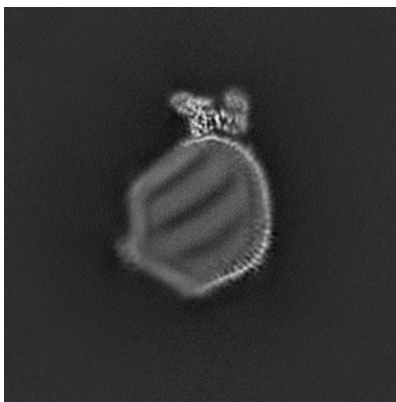


Z Index: 120

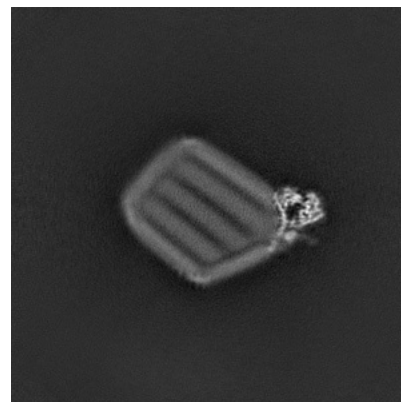
6.3.2 Raw map



X Index: 164



Y Index: 172

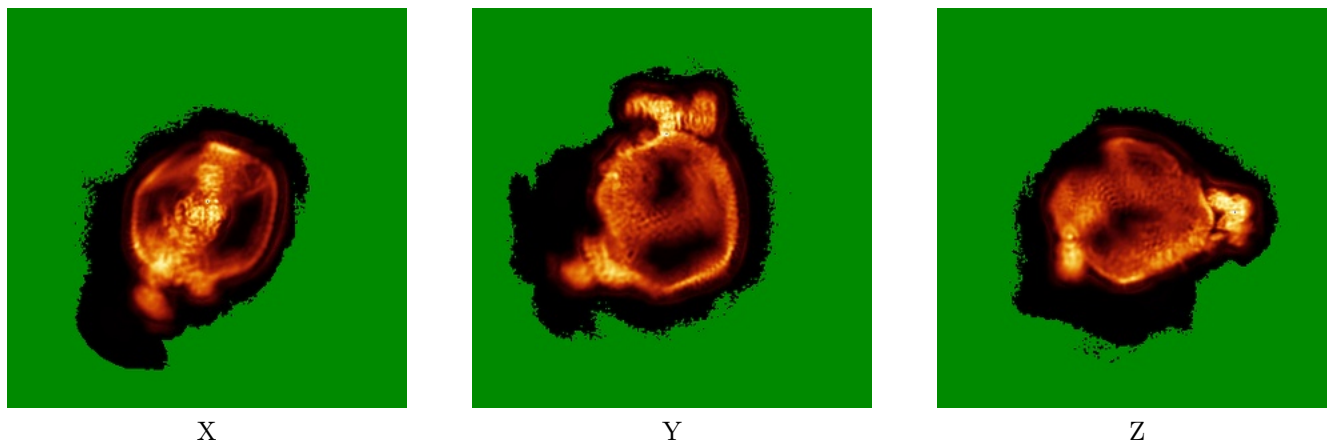


Z Index: 160

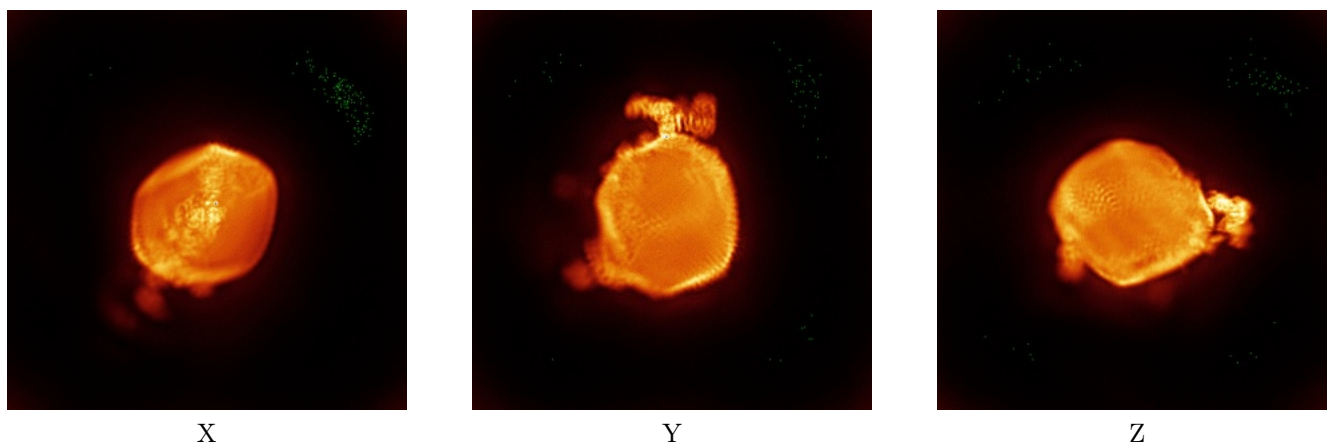
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

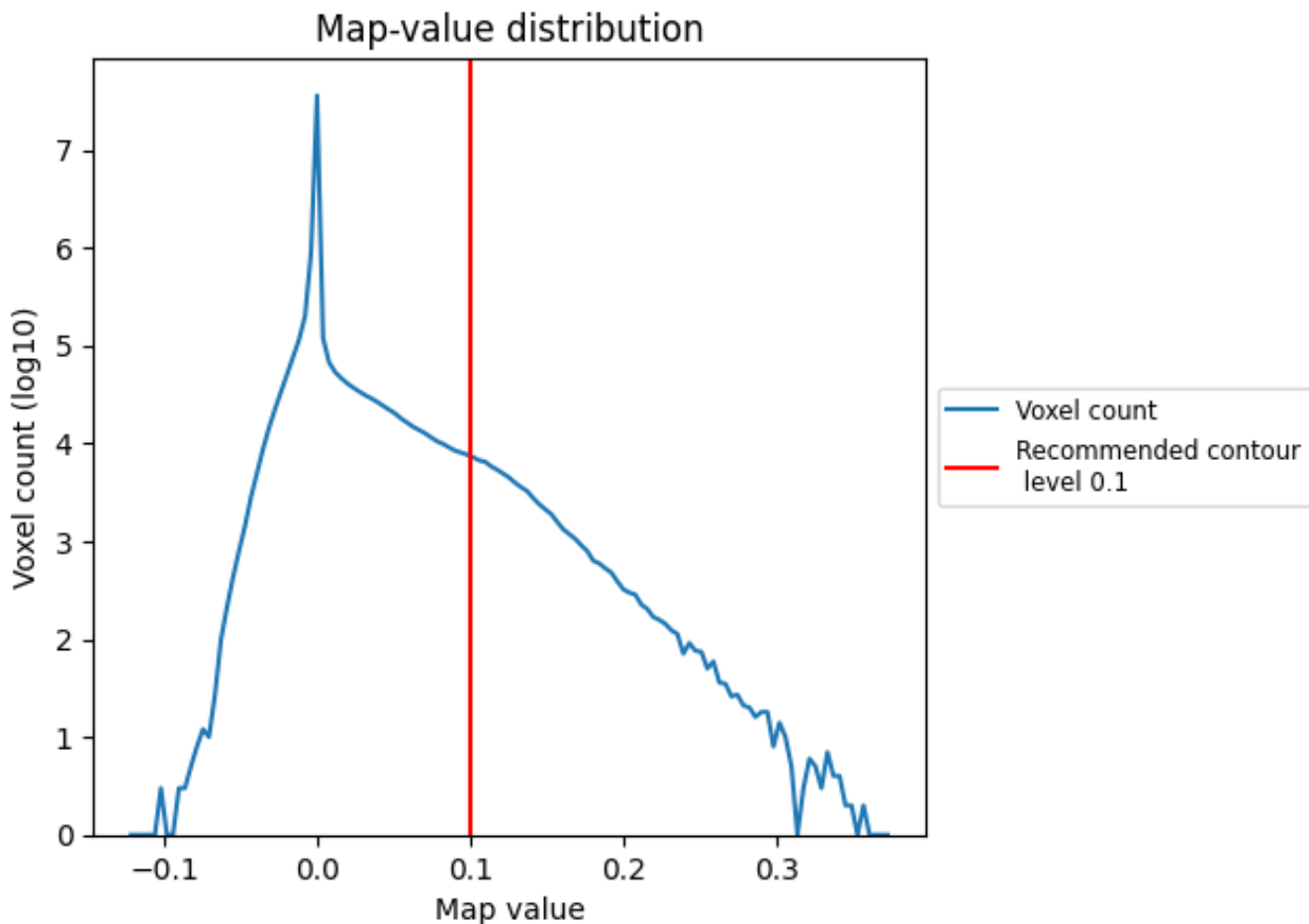
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

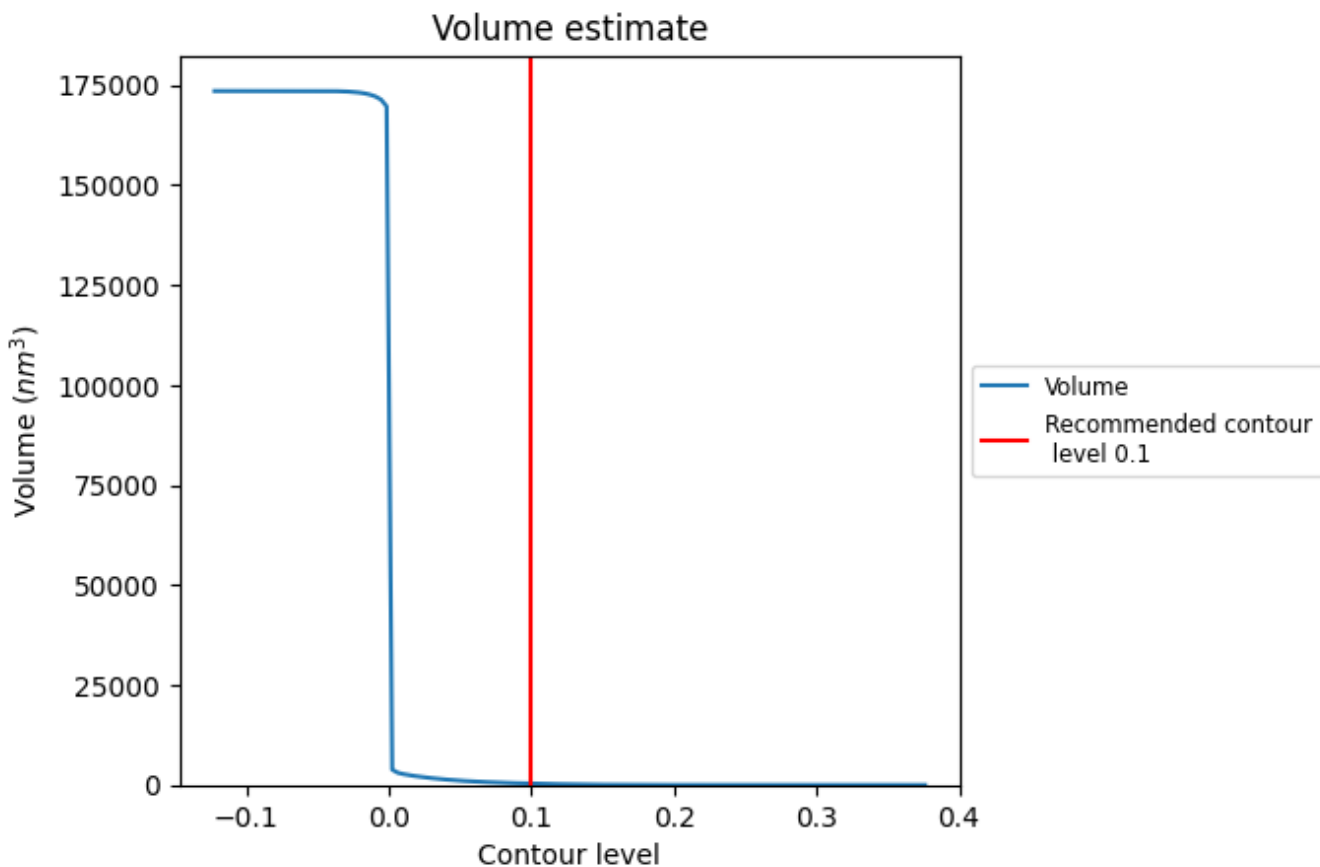
This section contains the results of statistical analysis of the map.

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.

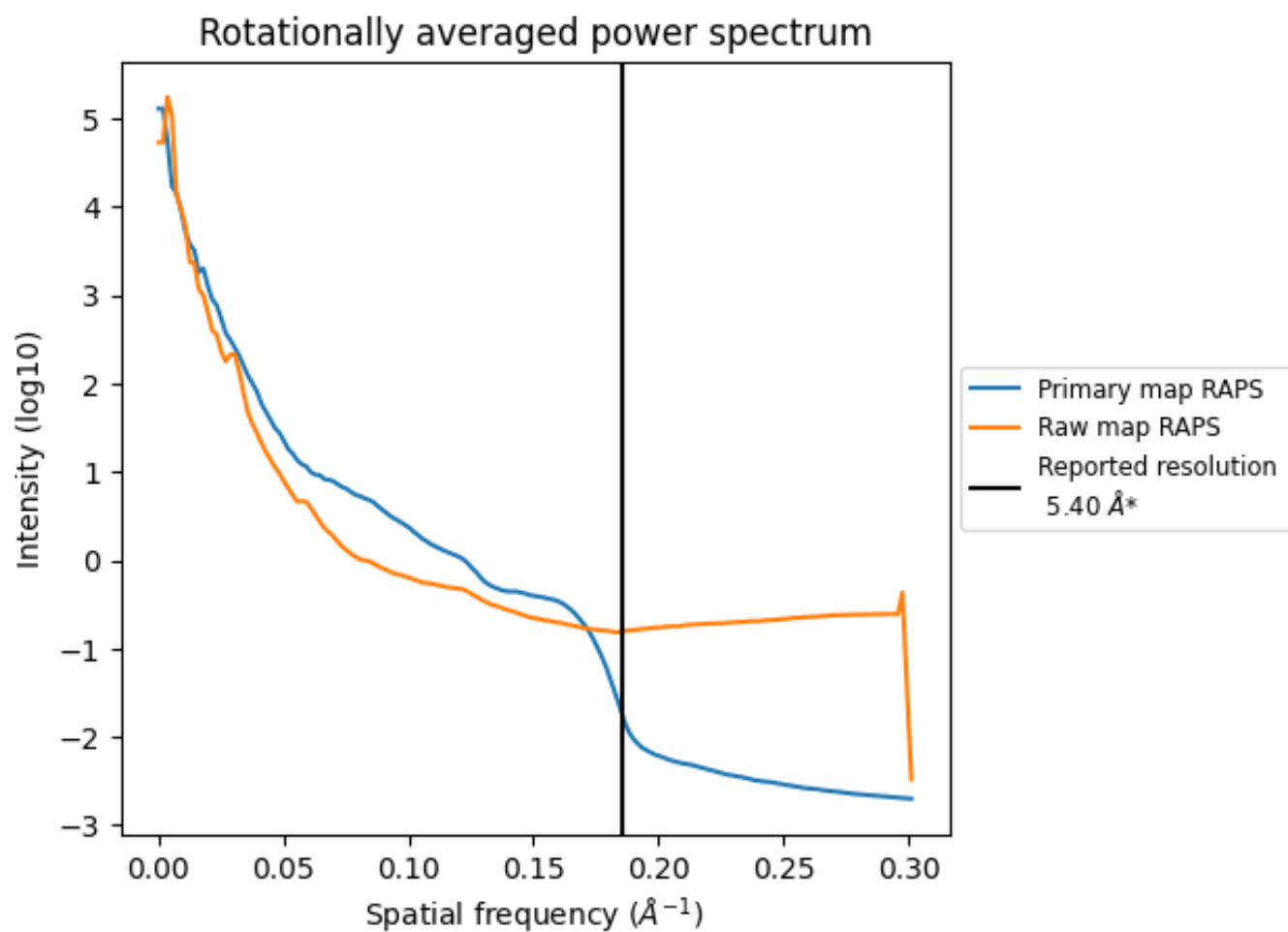
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 346 nm³; this corresponds to an approximate mass of 313 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

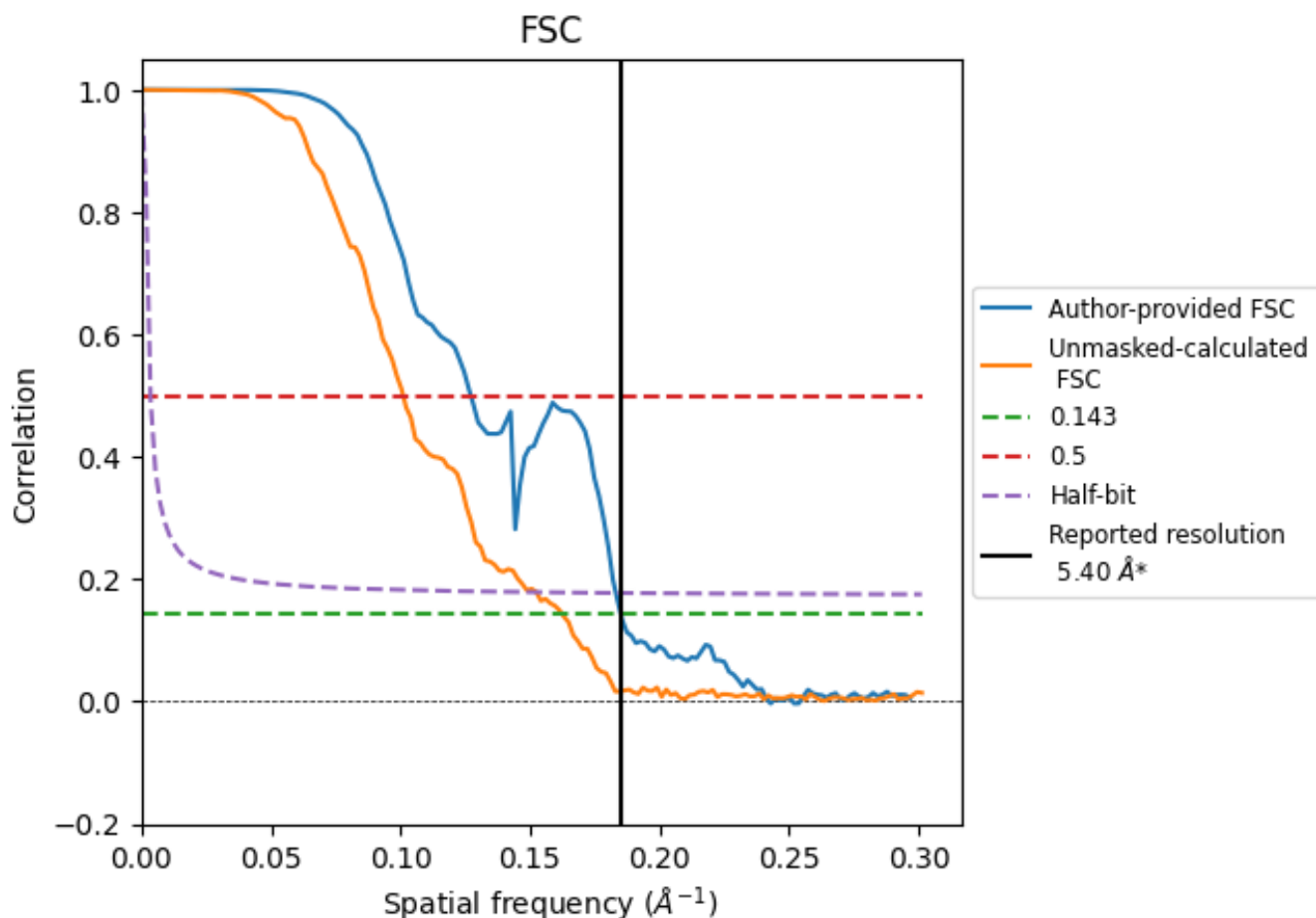


*Reported resolution corresponds to spatial frequency of 0.185 Å⁻¹

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 0.185 Å⁻¹

8.2 Resolution estimates [i](#)

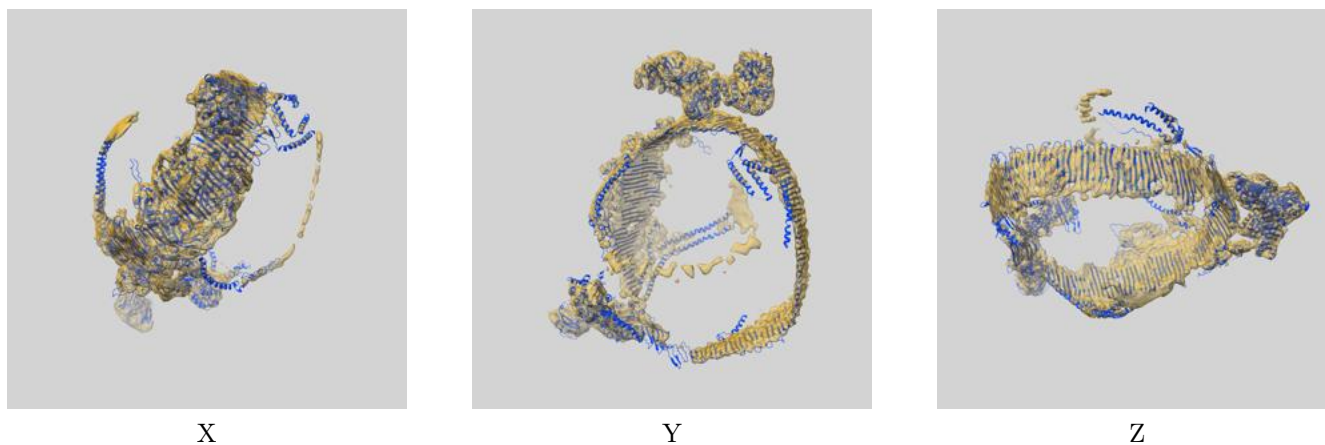
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	5.41	7.87	5.46
Unmasked-calculated*	6.16	9.90	6.56

*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 6.16 differs from the reported value 5.4 by more than 10 %

9 Map-model fit [i](#)

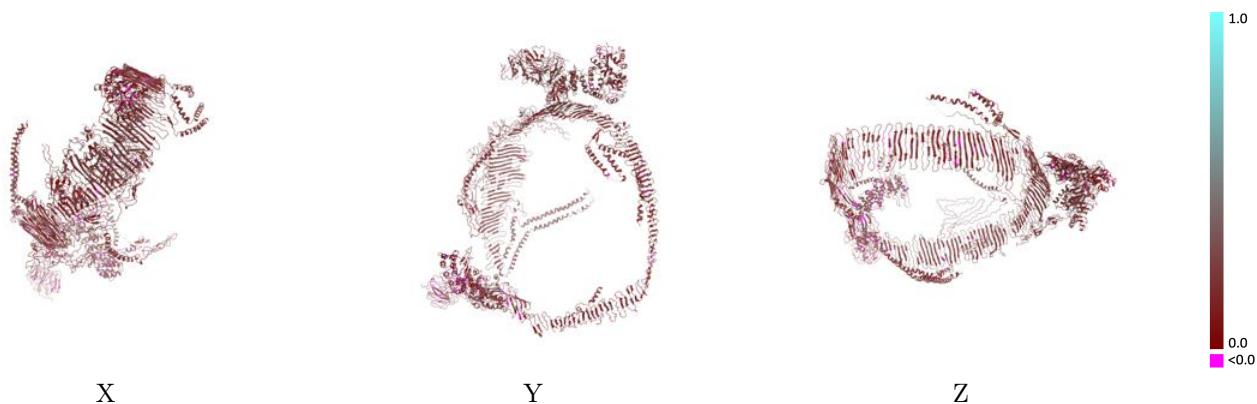
This section contains information regarding the fit between EMDB map EMD-44469 and PDB model 9BDT. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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 [\(i\)](#)

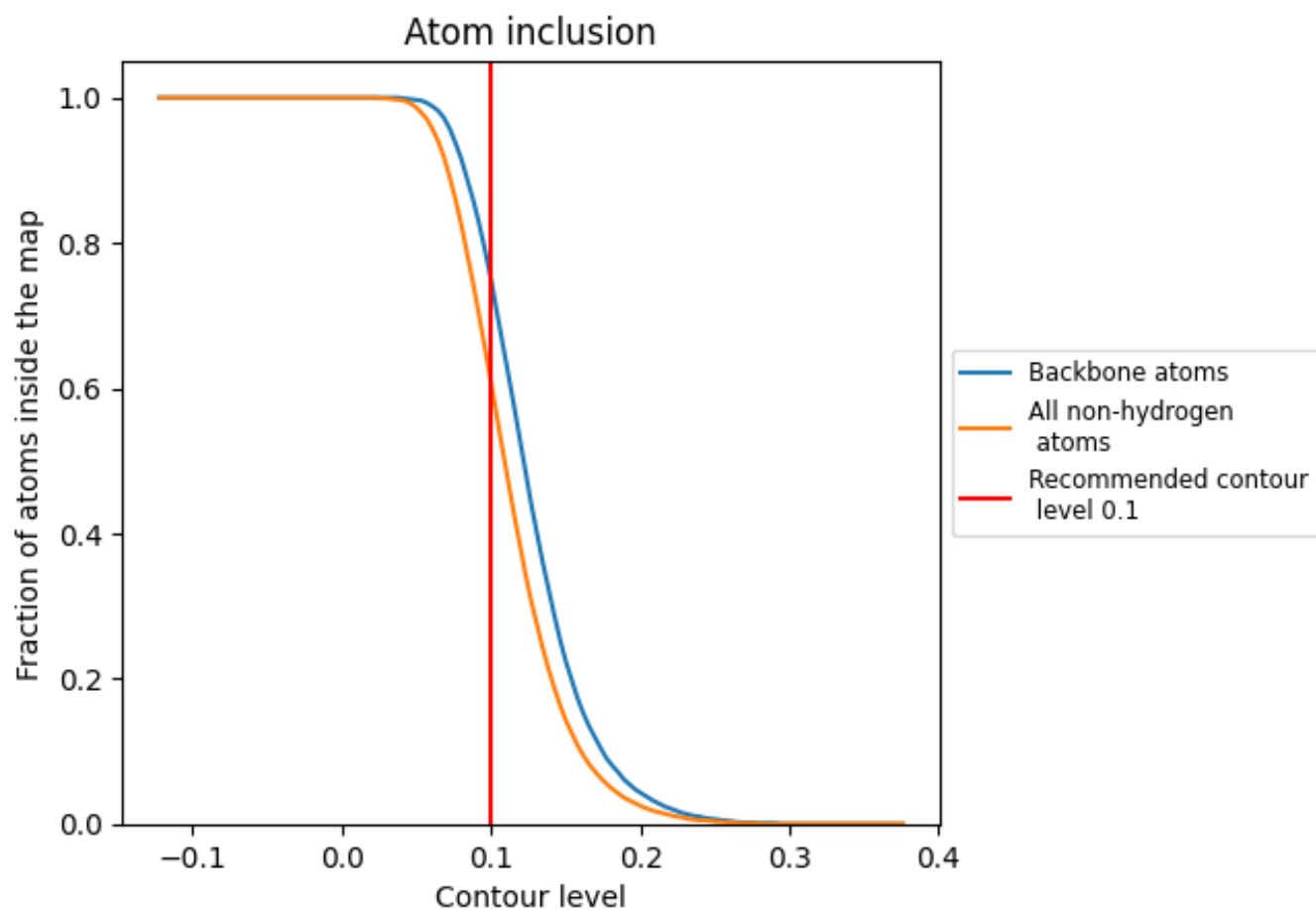


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.



















9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 61% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6080	 0.1980
A	 0.5500	 0.1950
B	 0.7640	 0.2050
G	 0.5000	 0.3120
H	 0.8240	 0.2450
I	 0.5950	 0.0930
L	 0.8130	 0.2580
N	 0.8820	 0.2910
R	 0.6770	 0.2090

