



wwPDB EM Validation Summary Report ⓘ

Feb 3, 2025 – 02:14 PM JST

PDB ID : 8Y1P
EMDB ID : EMD-38842
Title : Cryo-EM structure of human ABCA7 in DOPS-bound state
Authors : Fang, S.C.
Deposited on : 2024-01-25
Resolution : 3.45 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.40

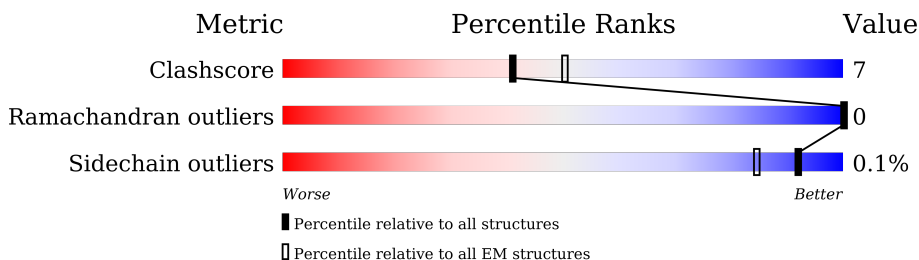
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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	2146	<div> <div>30%</div> <div>70%</div> <div>13%</div> <div>16%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	17F	A	2201	-	-	X	-

2 Entry composition [i](#)

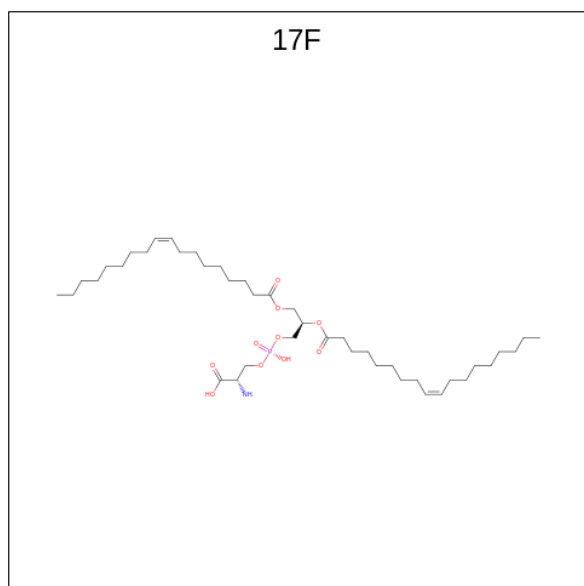
There are 2 unique types of molecules in this entry. The entry contains 14041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospholipid-transporting ATPase ABCA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1800	Total	C	N	O	S	1	0
			13933	8987	2449	2432	65		

- Molecule 2 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: C₄₂H₇₈NO₁₀P) (labeled as "Ligand of Interest" by depositor).

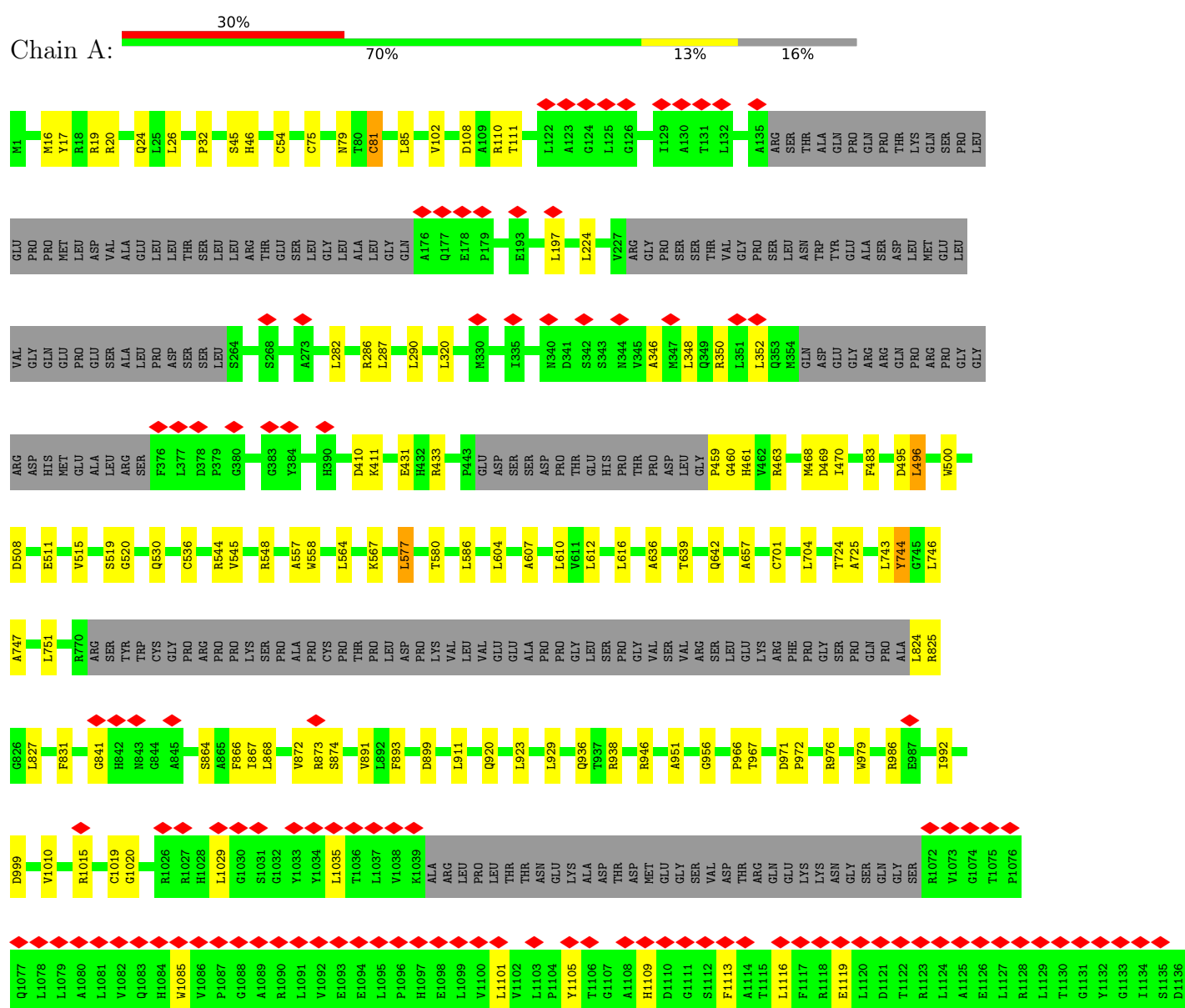


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			54	42	1	10	1	
2	A	1	Total	C	N	O	P	0
			54	42	1	10	1	

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: Phospholipid-transporting ATPase ABCA7



F2037	V2038	A2039	A2040	E2041	F2042	P2043	G2044	A2045	E2046	L2047	R2048	E2049	A2050	H2051	G2052	G2053	R2054	L2055	R2056	F2057	Q2058	L2059	P2060	P2061	G2062	G2063	R2064	C2065	A2066	L2067	A2068	R2069	V2070	F2071	G2072	E2073	L2074	A2075	V2076	H2077	G2078	A2079	E2080	H2081	G2082	V2083	E2084	D2085	F2086	S2087	V2088	T2091	P2092	L2093	E2094	E2095	V2096	F2097	
S1977	V1978	M1979	L1980	T1981	S1982	H1983	S1984	M1985	E1986	E1987	C1988	E1989	A1990	L1991	C1992	S1993	R1994	L1995	A1996	I1997	Q1998	V1999	N2000	G2001	R2002	F2003	R2004	C2005	L2006	G2007	S2008	R2009	Q2010	H2011	L2012	G2013	K2014	R2015	F2016	A2017	A2018	G2019	H2020	L2021	L2022	T2023	L2024	R2025	V2026	P2027	A2028	A2029	R2030	S2031	L2032	E2033	A2034	A2035	A2036
W1917	Y1918	A1919	D1920	R1921	P1922	A1923	G1924	T1925	Y1926	S1927	G1928	G1929	N1930	K1931	R1932	K1933	L1934	A1935	T1936	A1937	L1938	A1939	L1940	V1941	G1942	D1943	P1944	A1945	A1946	V1947	F1948	L1949	D1950	E1951	P1952	T1953	L1954	G1955	N1956	D1957	P1958	S1959	A1960	R1961	R1962	F1963	L1964	V1965	N1966	S1967	L1968	L1969	A1970	V1971	V1972	R1973	E1974	G1975	R1976
M1797	L1798	THR	LYS	VAL	TYR	ARG	GLY	GLN	ARG	MET	PRO	ALA	ASP	R1812	L1813	C1814	L1815	G1816	I1817	P1818	P1819	G1820	E1821	C1822	F1823	G1824	L1825	L1826	G1827	V1828	M1829	G1830	A1831	G1832	K1833	T1834	S1835	T1836	F1837	R1838	M1839	V1840	T1841	G1842	D1843	T1844	L1845	A1846	S1847	R1848	G1849	E1850	A1851	V1852	L1853	A1854	G1855	H1856	
S1857	V1858	A1859	R1860	E1861	P1862	S1863	A1864	A1865	H1866	L1867	S1868	M1869	G1870	Y1871	C1872	P1873	Q1874	S1875	D1876	I1877	L1878	F1879	E1880	L1881	L1882	T1883	G1884	R1885	E1886	H1887	L1888	E1889	L1890	L1891	A1892	R1893	L1894	R1895	G1896	V1897	P1898	E1899	A1900	Q1901	V1902	A1903	Q1904	T1905	A1906	G1907	S1908	G1909	L1910	A1911	R1912	L1913	G1914	L1915	S1916
M1737	V1738	I1739	Q1740	G1741	P1742	L1743	F1744	L1745	L1746	F1747	T1748	L1749	L1750	L1751	Q1752	H1753	R1754	S1755	Q1756	L1757	P1759	GLN	PRO	ARG	VAL	ARG	SER	LEU	PRO	LEU	LEU	GLY	GLU	ASP	GLU	ASP	VAL	ALA	ARG	GLU	ARG	GLU	VAL	GLN	ALA	THR	GLN	GLY	ASP	V1792	L1793	V1794	L1795	R1796					
S1673	D1674	Q1675	K1676	L1677	Q1678	E1679	V1680	S1681	R1682	I1683	L1684	K1685	Q1686	V1687	F1688	I1689	F1691	P1692	H1693	L1696	G1697	R1698	G1699	L1700	I1701	D1702	M1703	V1704	Q1707	A1708	M1709	A1710	D1711	A1712	F1713	E1714	R1715	L1716	G1717	D1718	R1719	Q1720	F1721	Q1722	S1723	P1724	L1725	W1727	E1728	V1729	M1733	L1734	L1735	A1736					
V1611	A1612	P1613	A1614	N1615	L1616	P1617	A1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	Y1626	G1627	W1628	S1629	I1630	L1633	M1634	Y1635	P1636	A1637	S1638	F1639	F1640	F1641	S1642	V1643	P1644	S1645	T1646	A1647	V1650	L1651	T1652	C1653	I1654	N1655	L1656	F1657	I1658	G1659	I1660	N1661	G1662	S1663	M1664	A1665	T1666	F1667	V1668	L1669	L1670	L1671	F1672		
A1551	S1552	F1553	T1554	L1555	V1556	L1557	I1558	E1559	E1560	R1561	T1562	T1563	R1564	A1565	K1566	H1567	L1568	S1569	L1570	M1571	G1572	G1573	L1574	S1575	P1576	T1577	L1578	Y1579	W1580	L1581	G1582	M1583	F1584	L1585	W1586	D1587	M1588	C1589	M1590	Y1591	L1592	V1593	P1594	A1595	C1596	I1597	V1598	V1599	L1600	I1601	F1602	L1603	A1604	F1605	Q1606	Q1607	R1608	A1609	Y1610
P1447	G1448	G1449	A1450	L1458	D1466	L1471	W1474	N1476	G1479	V1484	R1489	M1492	L1495	R1496	L1499	A1504	A1507	I1510	L1513	P1516	L1517	T1520	Q1523	L1524	A1531	S1532	S1533	V1534	D1535	V1536	L1537	V1542	V1543	F1544	A1545	M1546	S1547	F1548																					
P1267	L1271	T1274	M1275	Y1276	V1311	Q1312	V1327	L1331	W1336	C1347	S1348	A1362	A1363	G1364	Q1370	Q1380	W1381	L1382	R1385	F1390	L1391	V1392	T1394	G1402	K1406	V1409	M1410	E1411	A1241	Q1242	I1243	V1244	L1245	P1246	A1247	L1248	F1249	G1251	L1252	A1253	L1254	V1255	F1256	L1257	L1258	I1259	Y1260												
T1137	S1138	F1143	L1144	K1145	E1148	E1149	C1150	A1151	ALA	ASP	THR	ASP	GLU	ASP	GLY	SER	CYS	GLY	GLN	HIS	LEU	CYS	THR	GLY	TLE	ALA	GLY	LEU	ASP	R1233	VAL	R1234	S1235	R1236	R1237	LYS	MET	PRO	PRO	GLN	GLU	THR	ALA	LEU	GLU	ASN	GLY	GLU	PRO	ALA	SER	GLY	ALA	PRO	GLU	THR	ASP		

L2098	L2099	F2100	S2101	F2102	D2103	G2104	GLY	LYS	ASP	GLU	ASP	THR	GLU	GLN	LYS	GLU	ALA	GLY	VAL	GLY	VAL	ASP	PRO	ALA	PRO	GLY	LEU	GLN	HIS	PRO	LYS	ARG	VAL	SER	GLN	PHE	LEU	ASP	ASP	PRO	SER	THR	ALA	GLU	THR	VAL	LEU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	473349	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.547	Depositor
Minimum map value	-3.798	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.425	Depositor
Map size (Å)	299.6, 299.6, 299.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: 17F

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	0.64	8/14274 (0.1%)	0.77	33/19415 (0.2%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	CYS	CB-SG	-5.74	1.72	1.81
1	A	17	TYR	CD1-CE1	-5.51	1.31	1.39
1	A	701	CYS	CB-SG	-5.40	1.73	1.81
1	A	511	GLU	CG-CD	-5.36	1.44	1.51
1	A	1276	TYR	CE1-CZ	-5.24	1.31	1.38

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	CYS	CA-CB-SG	8.82	129.87	114.00
1	A	536	CYS	CA-CB-SG	8.10	128.58	114.00
1	A	604	LEU	CB-CG-CD1	-7.29	98.61	111.00
1	A	744	TYR	CA-CB-CG	7.18	127.05	113.40
1	A	992	ILE	CG1-CB-CG2	-7.06	95.86	111.40

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	13933	0	14149	177	0
2	A	108	0	152	39	0
All	All	14041	0	14301	191	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 7.

The worst 5 of 191 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ARG:HD2	2:A:2202:17F:N1	1.69	1.07
1:A:483:PHE:HB3	2:A:2202:17F:H1A	1.38	1.04
1:A:567:LYS:HD3	2:A:2201:17F:O1	1.58	1.03
1:A:567:LYS:CD	2:A:2201:17F:O1	2.11	0.98
2:A:2202:17F:H34	2:A:2202:17F:H18	1.51	0.93

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	1781/2146 (83%)	1577 (88%)	204 (12%)	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	1476/1764 (84%)	1475 (100%)	1 (0%)	92 97

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

Mol	Chain	Res	Type
1	A	1932	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	17F	A	2202	-	52,53,53	0.93	2 (3%)	56,60,60	1.07	4 (7%)
2	17F	A	2201	-	52,53,53	0.93	2 (3%)	56,60,60	1.08	4 (7%)

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	17F	A	2202	-	-	29/59/59/59	-
2	17F	A	2201	-	-	32/59/59/59	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2202	17F	O7-C7	4.29	1.45	1.33
2	A	2201	17F	O7-C7	4.27	1.45	1.33
2	A	2202	17F	O9-C17	4.10	1.45	1.34
2	A	2201	17F	O9-C17	4.08	1.45	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2201	17F	O9-C17-C18	4.06	120.24	111.50
2	A	2202	17F	O9-C17-C18	4.04	120.20	111.50
2	A	2202	17F	O7-C7-C8	2.64	120.19	111.91
2	A	2201	17F	O7-C7-C8	2.62	120.13	111.91
2	A	2201	17F	C5-O9-C17	-2.45	111.77	117.79

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

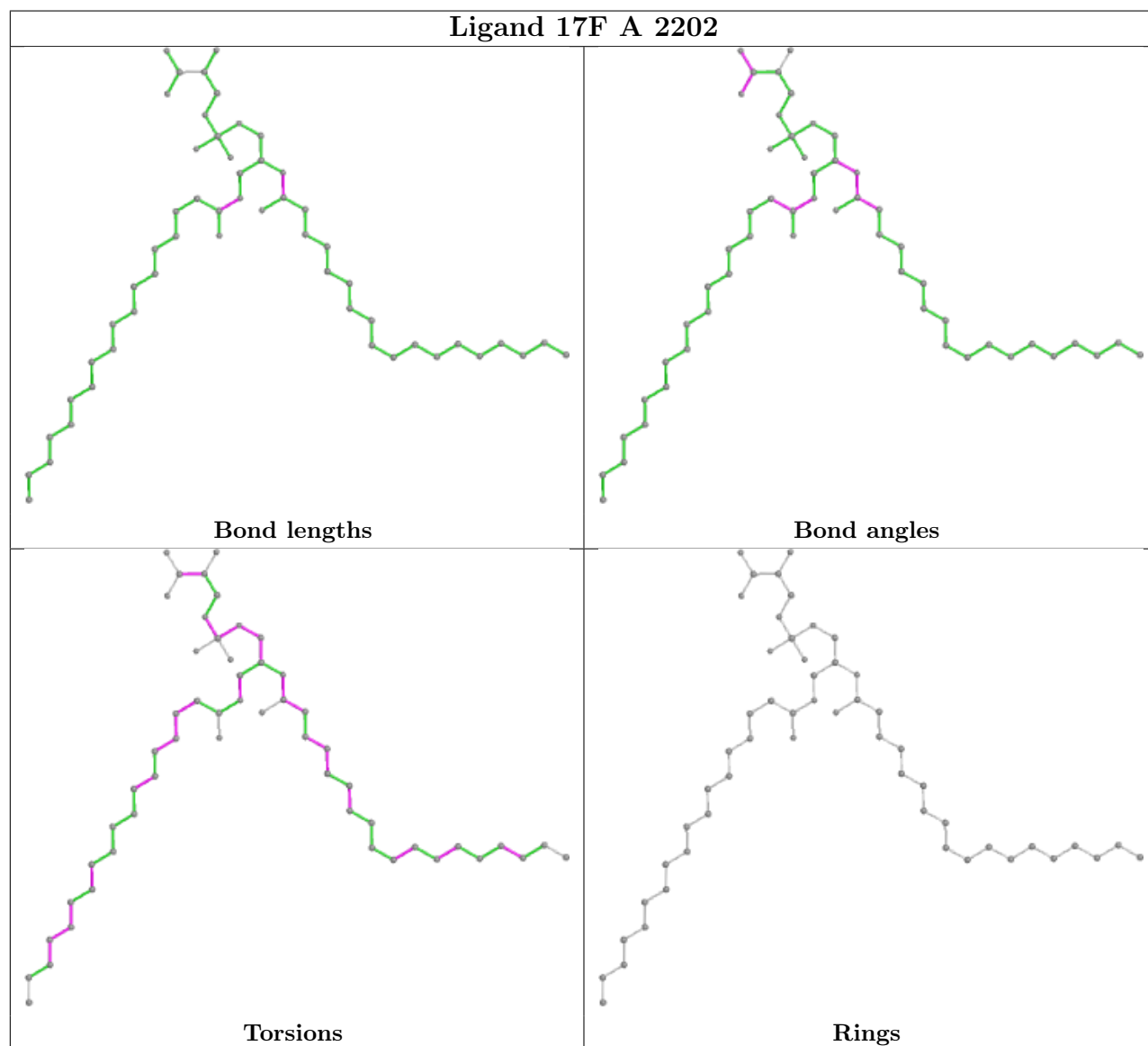
Mol	Chain	Res	Type	Atoms
2	A	2201	17F	O3-C1-C2-N1
2	A	2201	17F	O3-C1-C2-C3
2	A	2201	17F	C1-O3-P1-O1
2	A	2201	17F	N1-C2-C3-O4
2	A	2201	17F	O10-C17-O9-C5

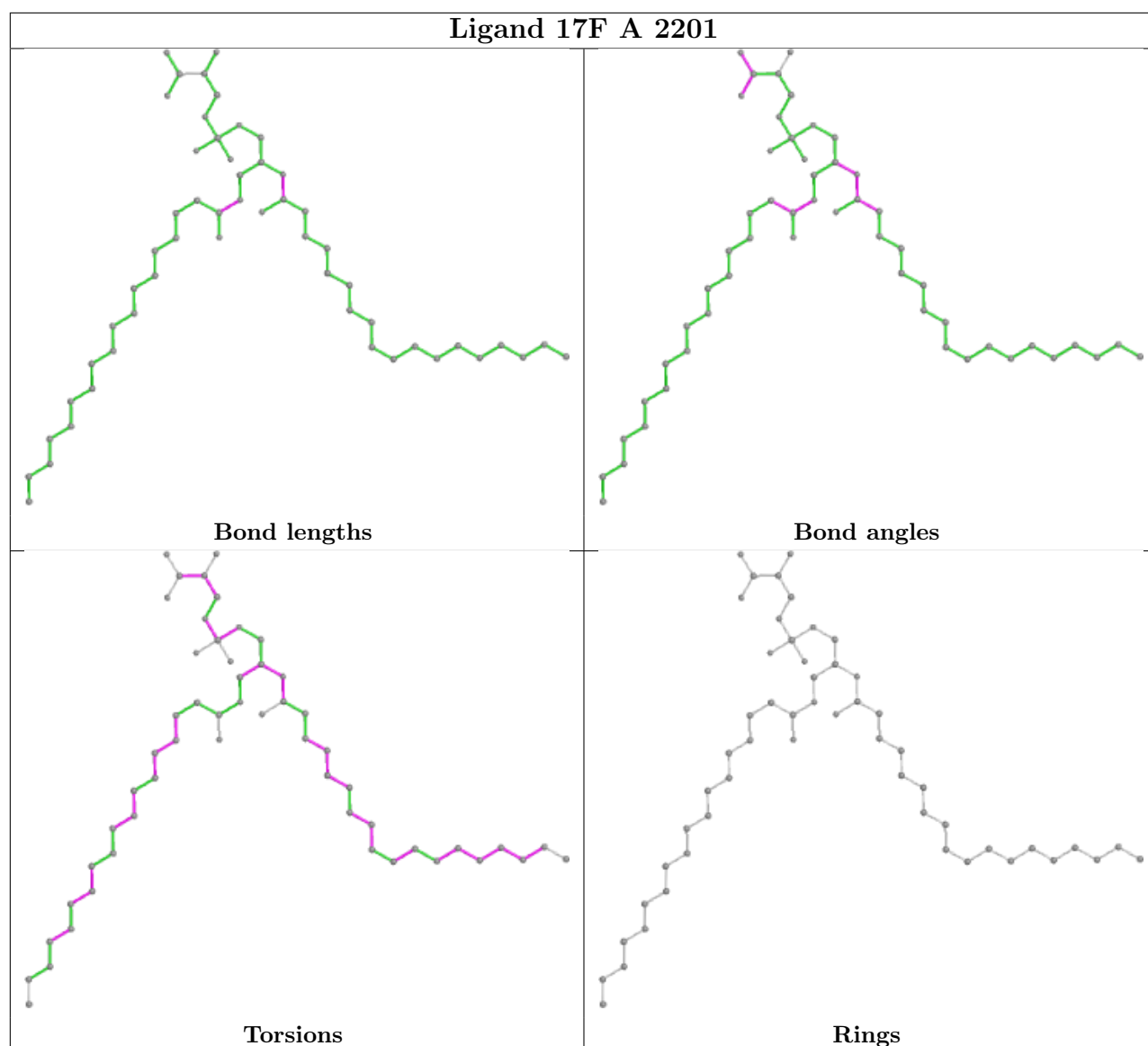
There are no ring outliers.

2 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2202	17F	17	0
2	A	2201	17F	22	0

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.

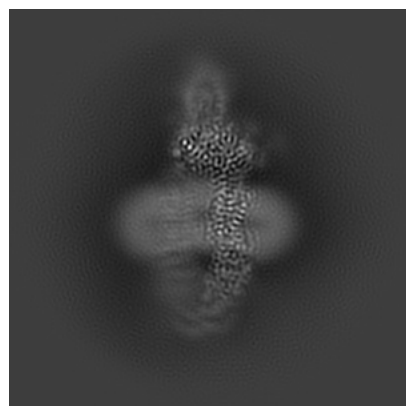
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38842. These allow visual inspection of the internal detail of the map and identification of artifacts.

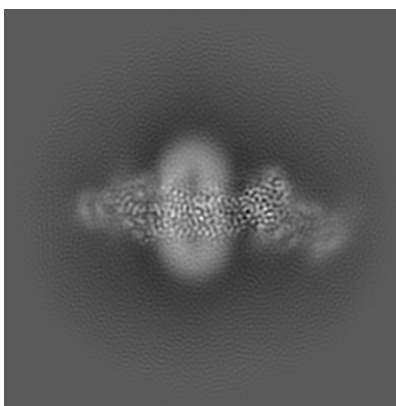
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

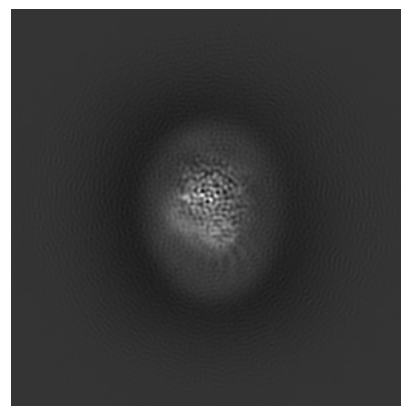
6.1.1 Primary map



X

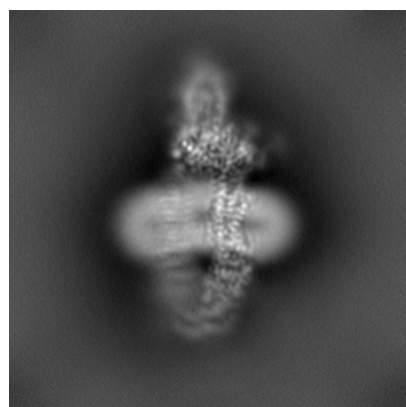


Y

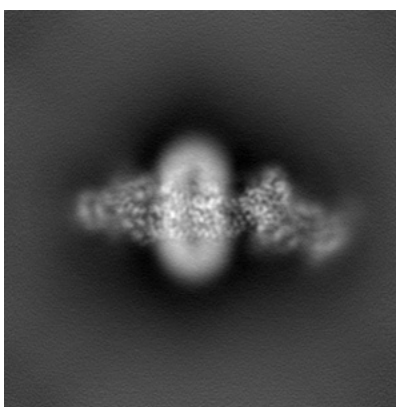


Z

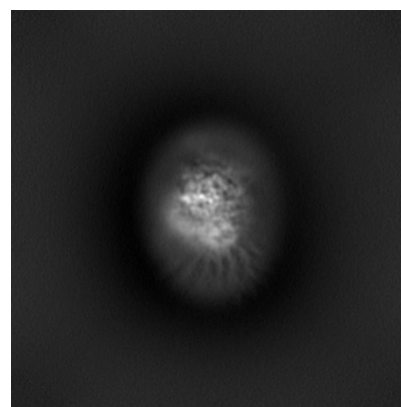
6.1.2 Raw map



X



Y

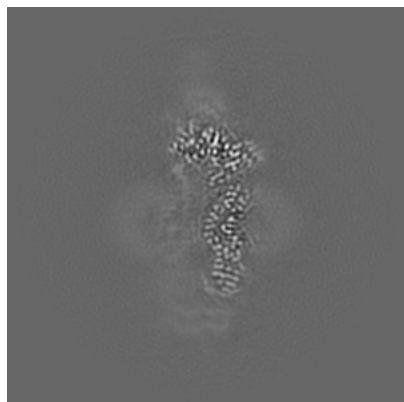


Z

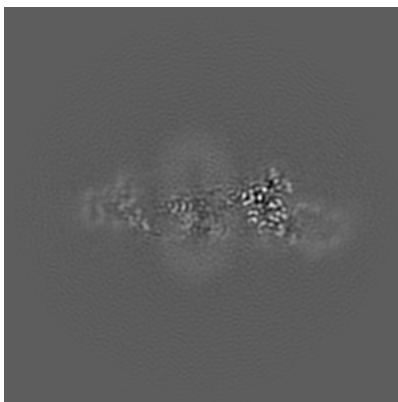
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

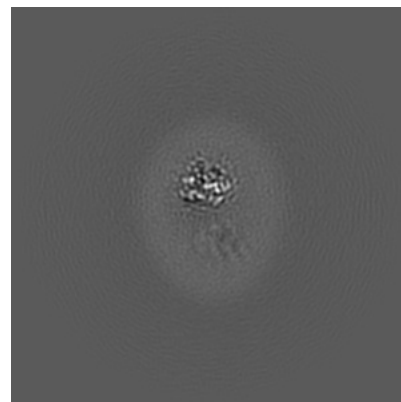
6.2.1 Primary map



X Index: 140

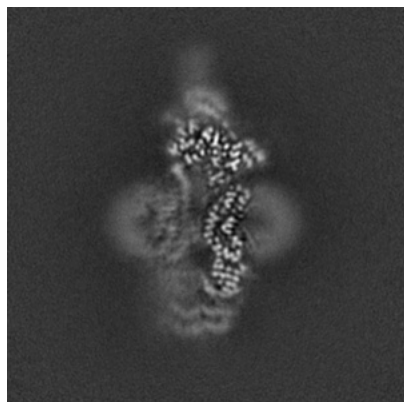


Y Index: 140

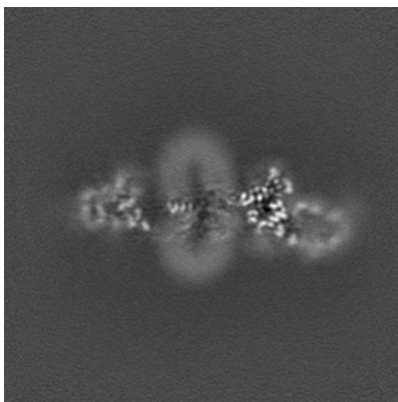


Z Index: 140

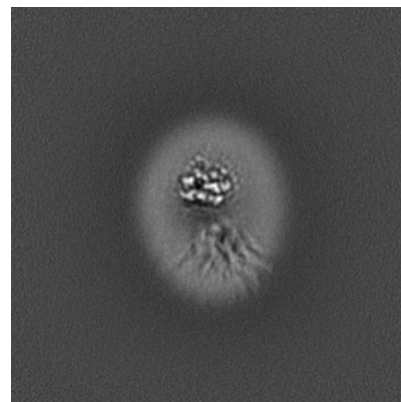
6.2.2 Raw map



X Index: 140



Y Index: 140

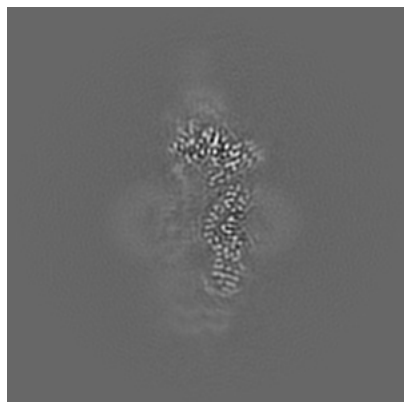


Z Index: 140

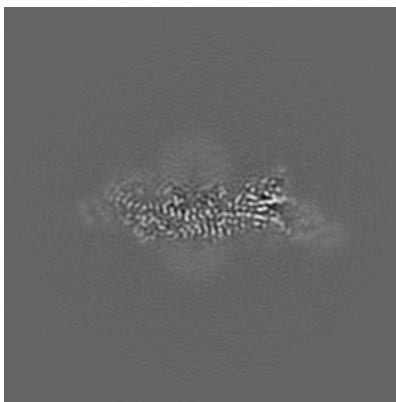
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

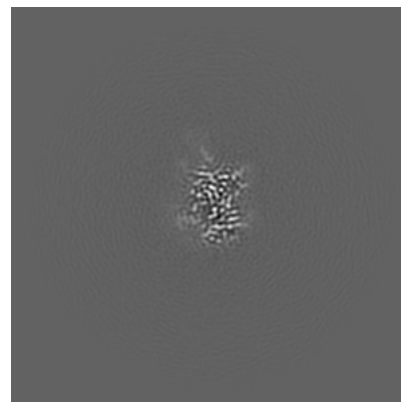
6.3.1 Primary map



X Index: 140

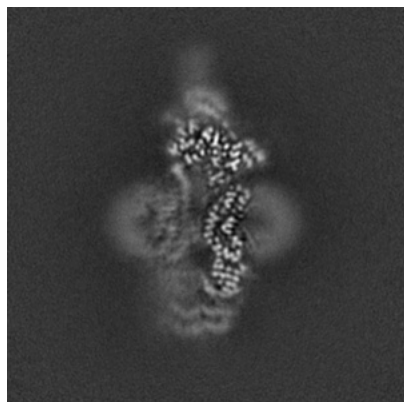


Y Index: 149

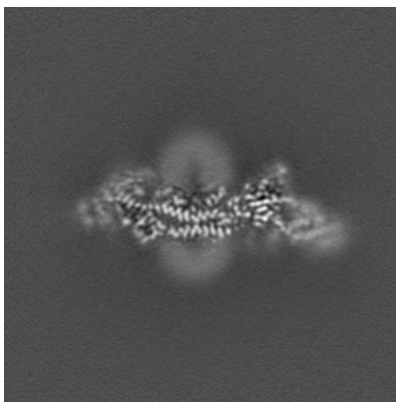


Z Index: 182

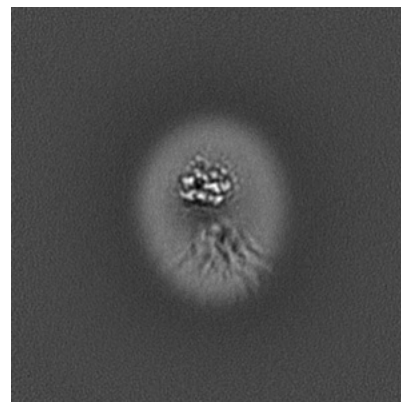
6.3.2 Raw map



X Index: 140



Y Index: 148

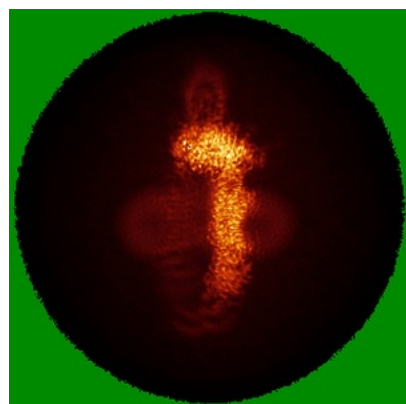


Z Index: 140

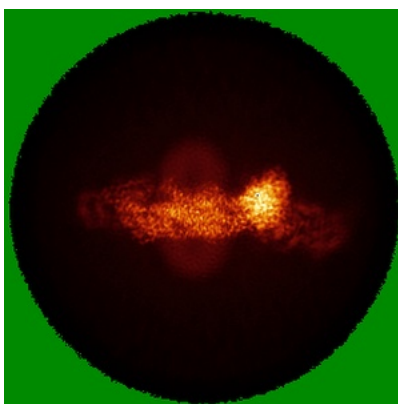
The images above show the largest variance slices of the map in three orthogonal directions.

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

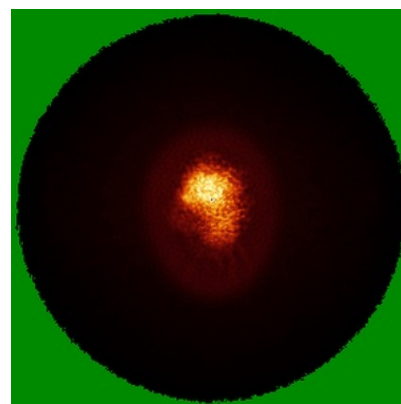
6.4.1 Primary map



X

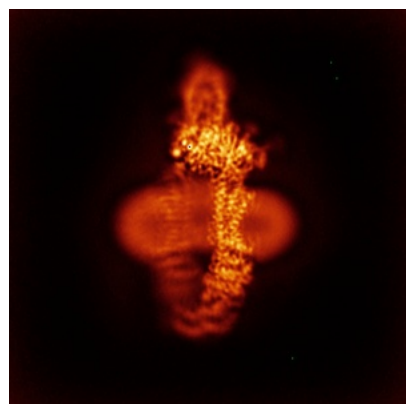


Y

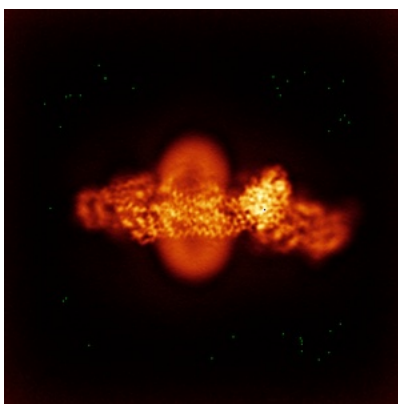


Z

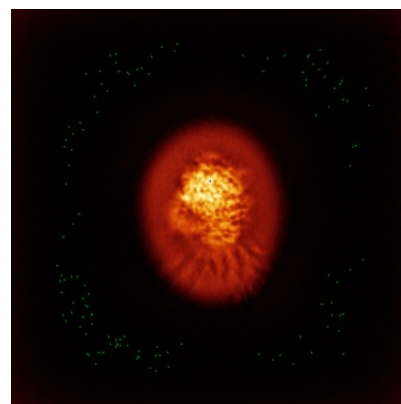
6.4.2 Raw map



X



Y

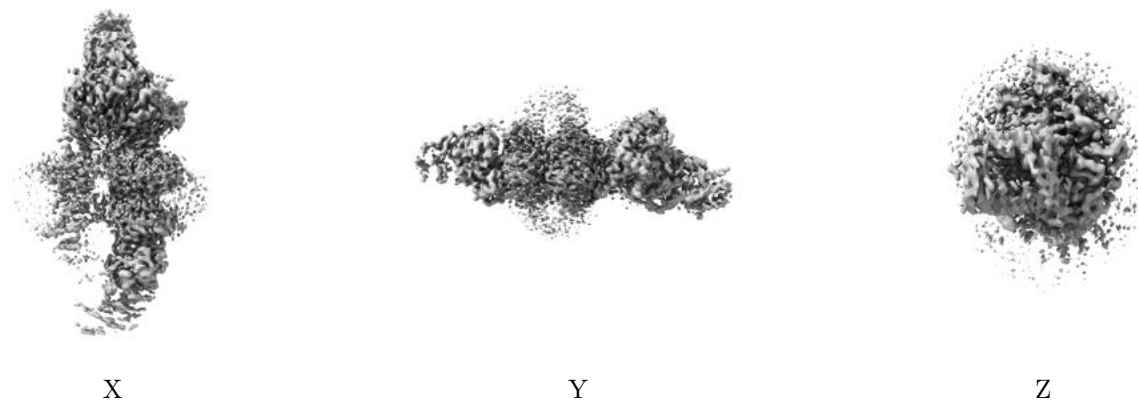


Z

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.

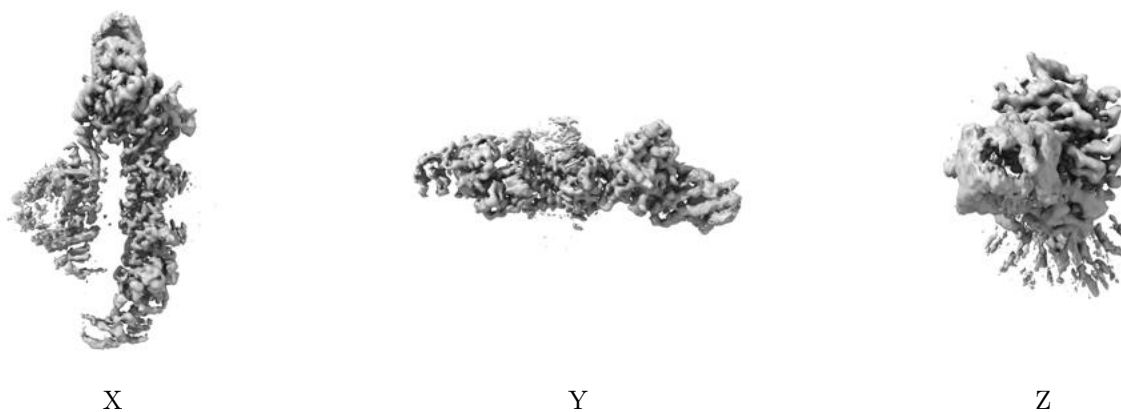
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.425. 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.

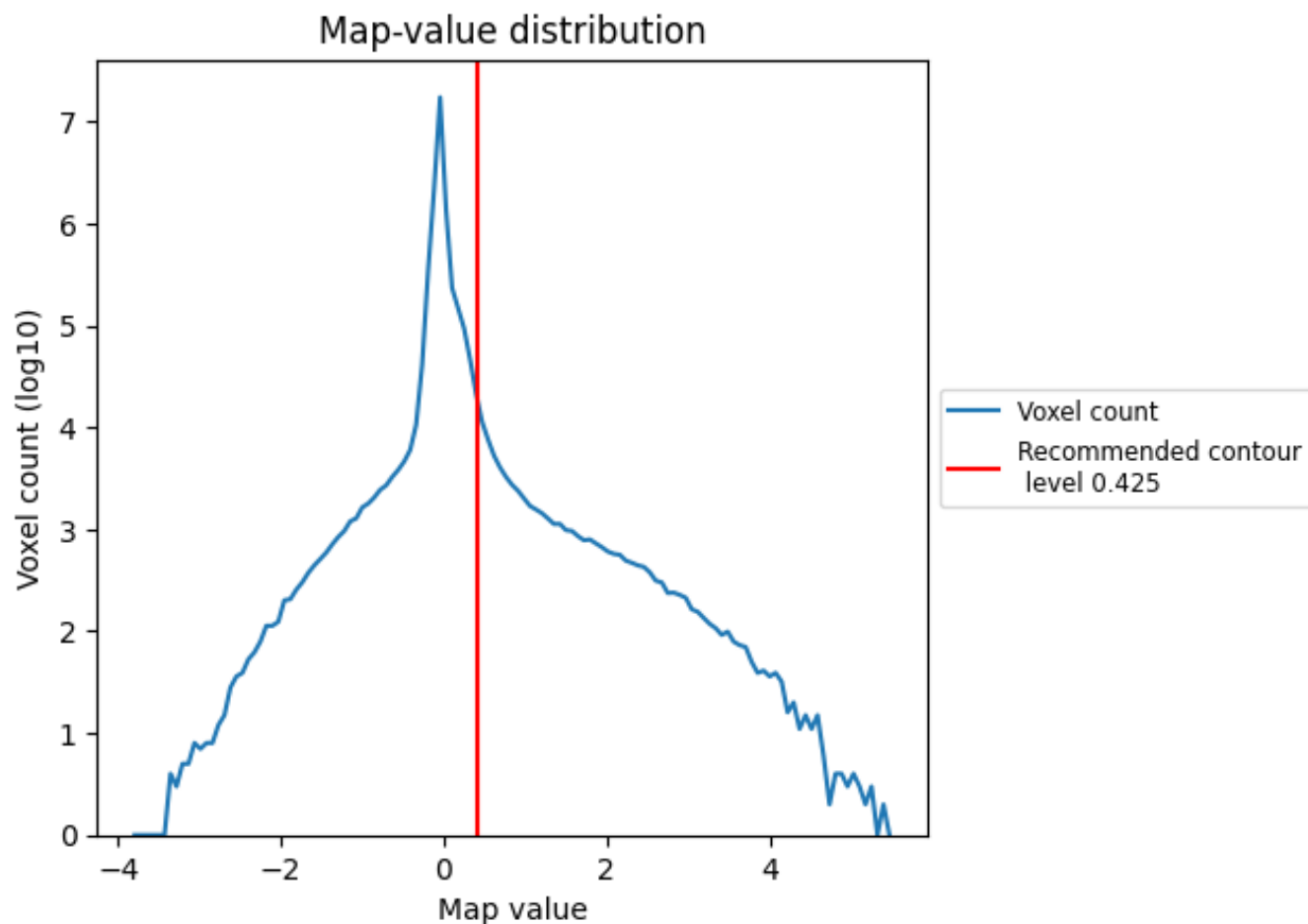
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

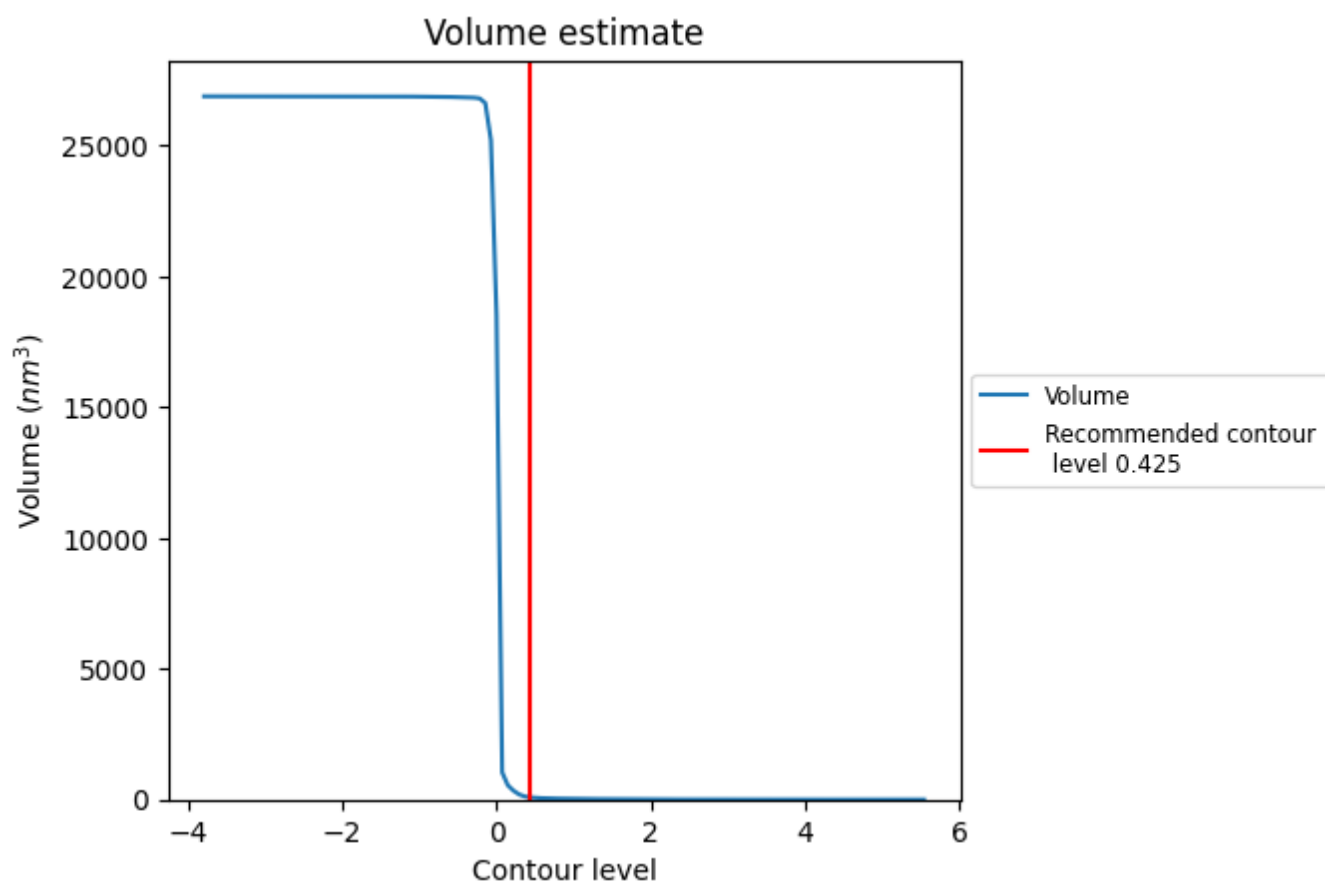
This section contains the results of statistical analysis of the map.

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.

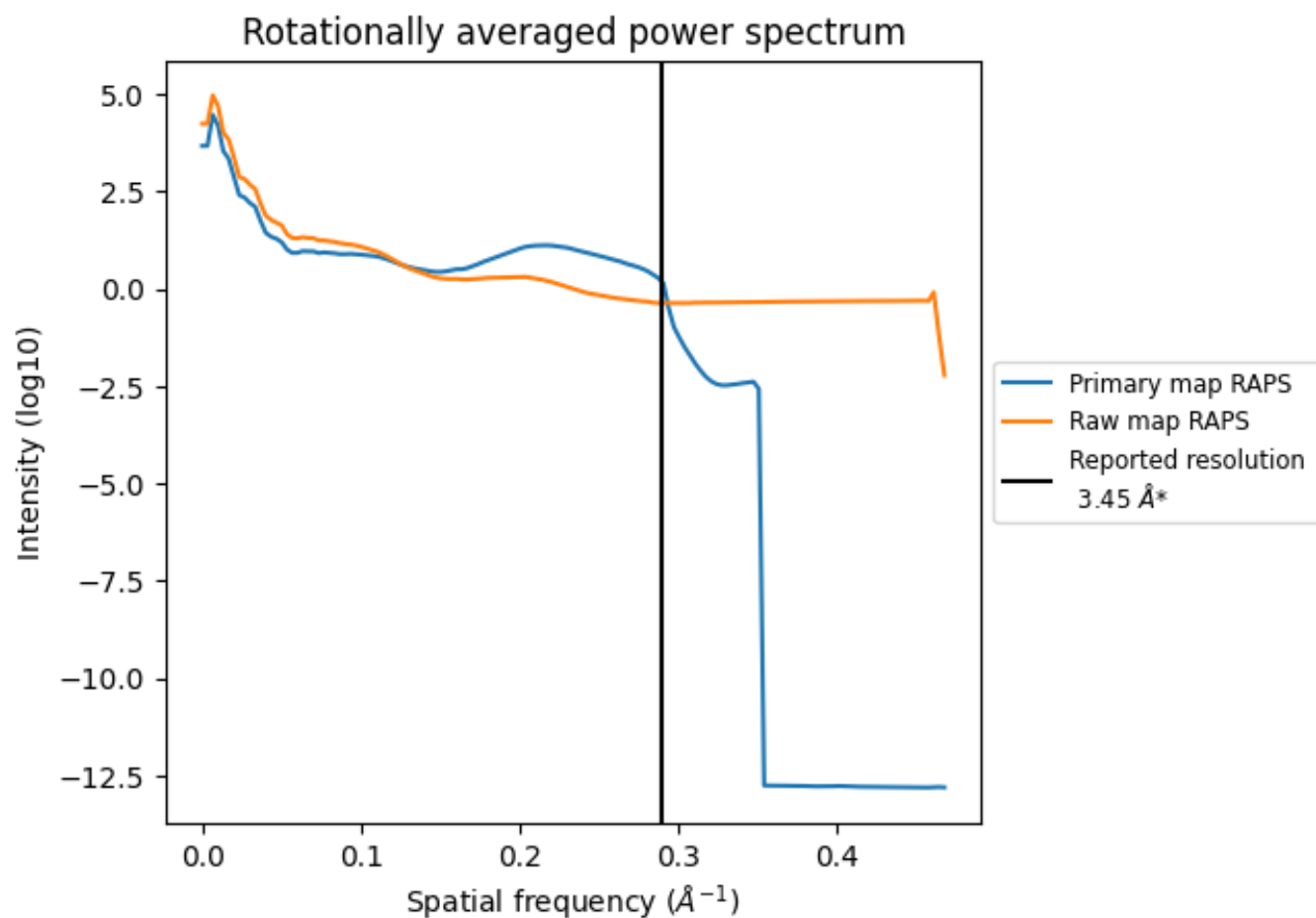
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 88 nm³; this corresponds to an approximate mass of 80 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 ⓘ

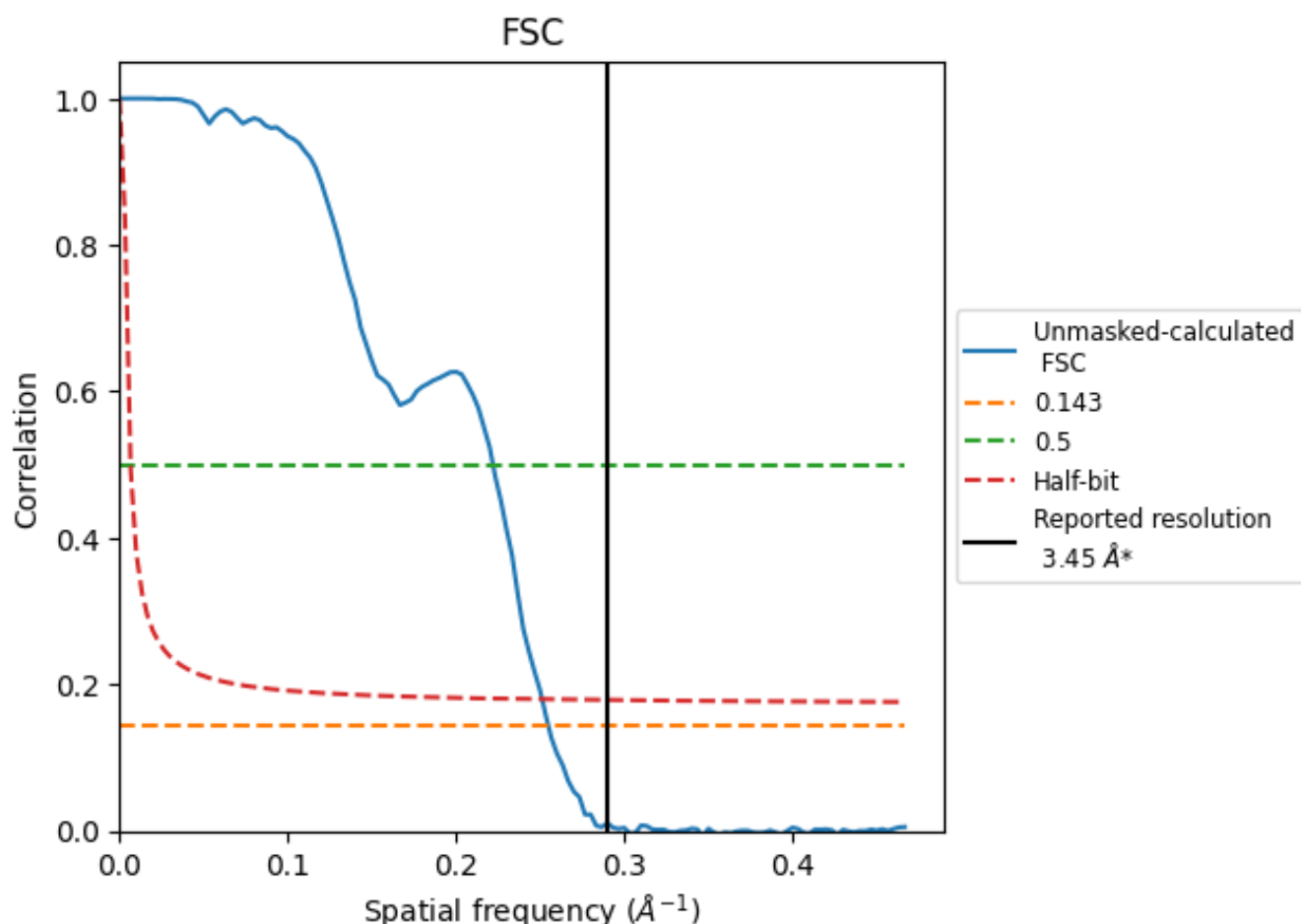


*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

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 0.290 \AA^{-1}

8.2 Resolution estimates [i](#)

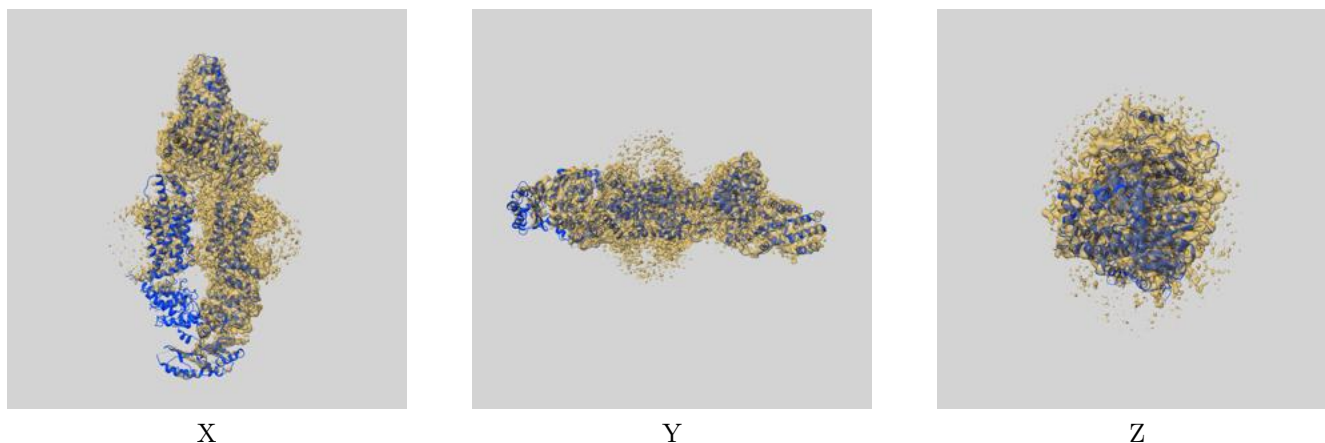
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	4.50	3.98

*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 3.92 differs from the reported value 3.45 by more than 10 %

9 Map-model fit [i](#)

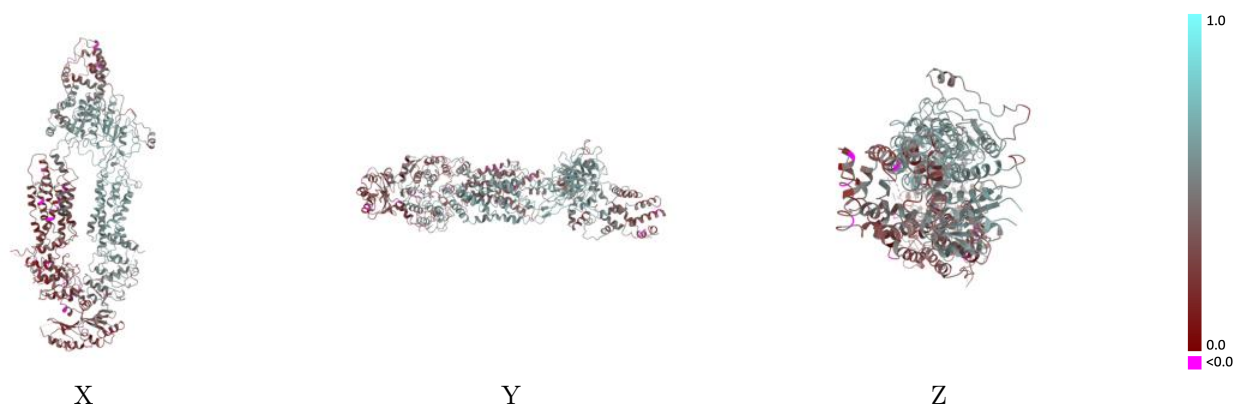
This section contains information regarding the fit between EMDB map EMD-38842 and PDB model 8Y1P. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



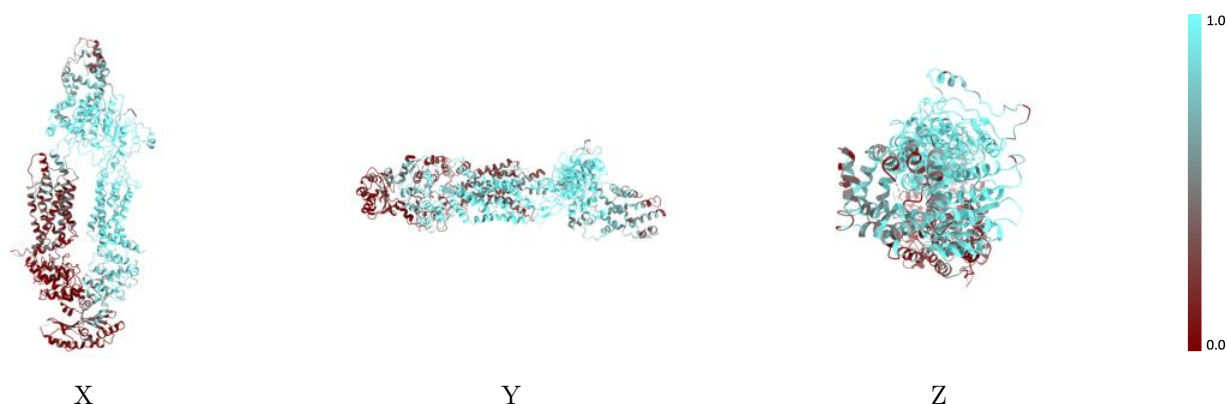
The images above show the 3D surface view of the map at the recommended contour level 0.425 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



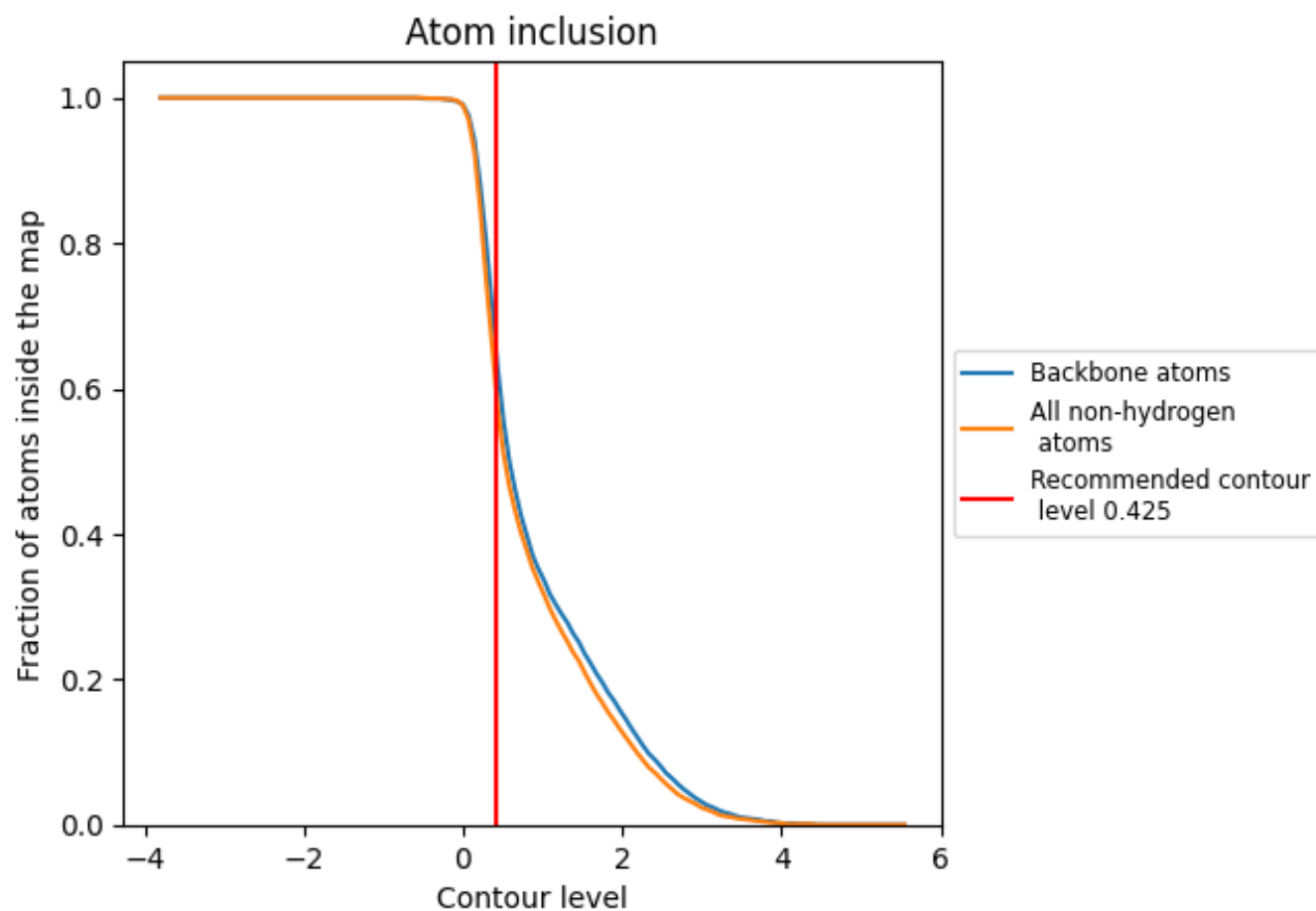
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.425).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 58% 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 (0.425) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5850	<div></div> 0.4180
A	<div></div> 0.5850	<div></div> 0.4180

