



## wwPDB EM Validation Summary Report ⓘ

Oct 20, 2024 – 09:27 PM EDT

PDB ID : 8EDW  
EMDB ID : EMD-28041  
Title : Cryo-EM Structure of human ABCA7 in BPL/Ch Nanodiscs  
Authors : Alam, A.; Le, L.T.M.; Thompson, J.R.  
Deposited on : 2022-09-06  
Resolution : 3.60 Å(reported)  
Based on initial model : 6JBJ

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : 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

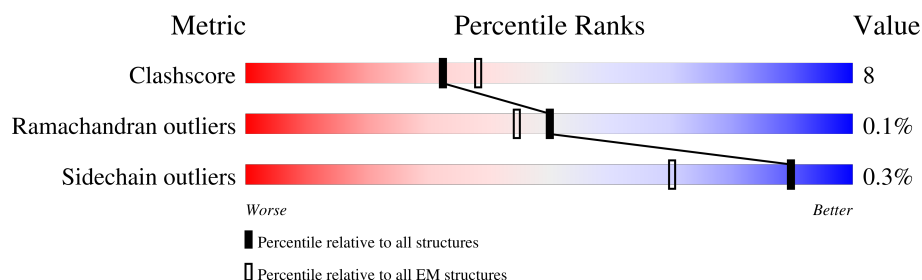
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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  $\geq 3$ , 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	
2	B	2	
2	D	2	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14321 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	1804	Total	C	N	O	S	0	0
			13931	8963	2452	2453	63		

- 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

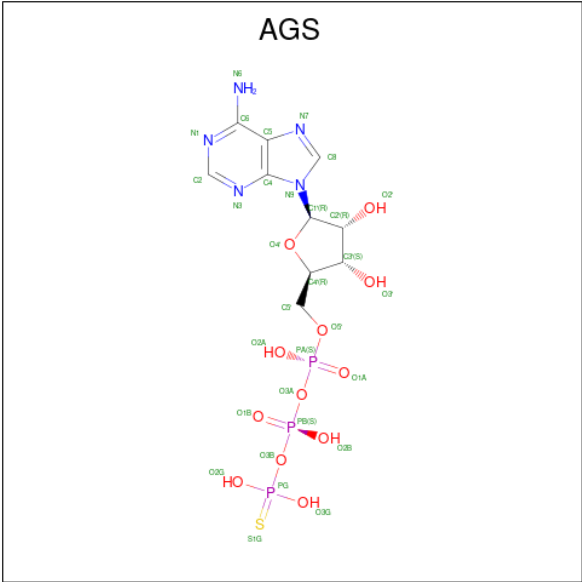


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	18	Total	C	0
			216	216	

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula:  $C_{10}H_{16}N_5O_{12}P_3S$ ).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	



GLU	S2031	S1908	M1907	V1729	L1651	A1545	L1443	K1329	I1243	LEU	R1090	R1015
ALA	Q2032	G1909	P1808	V1730	H1855	M1546	S1444	G1334	V1244	ASP	L1091	L1016
GLY	P2033	L1910	D1811	K1732	S1547	F1548	P1445	G1335	L1245	VAL	V1092	C1019
VAL	A2034	A1911	H1812	N1733	F1549	V1549	L1446	W1336	P1246	LEU	E1093	L1023
ASP	A2035	A1919	H1813	L1734	F1553	F1553	G1448	E1339	F1249	LEU	E1094	L1027
PRO	A2036	D1920	L1814	L1735	R1561	R1561	G1449	S1342	V1250	LYS	P1096	R1027
ALA	P2037	P1921	C1814	L1736	V1562	V1562	A1450	P1343	G1251	PRO	H1097	H1028
PRO	A2038	A1922	L1815	A1736	M1664	M1664	L1451	S1345	L1252	GLN	E1098	L1029
GLY	A2039	A1923	P1818	A1737	A1665	A1665	L1452	Q1346	A1253	GLN	A1099	G1030
LEU	A2040	G1924	E1821	I1739	T1666	T1666	L1453	C1347	L1254	THR	V1100	Y1034
GLN	G2044	Y1925	G1830	Q1740	F1667	H1567	R1454	S1348	L1101	ALA	L1101	A1040
HIS	A2045	Y1926	L1743	L1743	V1668	L1570	L1455	R1349	S1257	LEU	V1102	ARG
PRO	E2046	N1930	F1744	L1745	L1669	M1571	K1456	P1350	L1258	GLU	L1103	LEU
LYS	A2047	K1933	L1746	L1746	L1670	M1571	N1457	G1351	P1104	ASN	P1104	LEU
ARG	L2047	L1934	F1747	L1747	L1671	L1574	A1458	A1352	Y1105	GLY	Y1105	PRO
VAL	R2048	L1941	L1748	L1748	L1672	S1575	L1459	R1353	V1260	GLU	F1113	THR
SER	E2049	G1942	L1749	L1749	F1673	N1583	A1460	L1356	P1261	PRO	F1117	THR
GLN	G2052	A1946	Q1756	Q1756	D1674	D1587	W1461	P1357	G1264	GLY	Y1117	ASN
ASP	Q2058	G1949	LEU	LEU	Q1675	M1588	H1462	C1359	H1265	SER	D1121	GLU
PRO	L2059	E1850	PRO	PRO	L1676	C1589	H1463	P1360	Y1266	ALA	R1128	LYS
SER	P2060	L1853	GLN	GLN	L1677	M1590	S1464	P1366	P1267	PRO	L1129	ALA
THR	P2061	A1859	ARG	ARG	Q1678	Y1591	L1465	P1367	S1272	GLU	T1130	ASP
ALA	G2062	R1860	ARG	ARG	E1679	L1592	Q1468	P1368	M1275	THR	T1134	THR
THR	G2063	E1861	SER	SER	V1680	V1593	D1469	P1369	A1287	GLY	T1134	GLY
LEU	R2064	P1862	LEU	LEU	I1682	P1594	S1470	Q1370	S1135	GLY	S1135	SER
ASP	C2065	S1863	PRO	PRO	L1684	L1597	L1471	N1386	D1136	PRO	T1137	VAL
GLY	A2066	A1865	LEU	LEU	Q1686	L1600	P1500	L1387	G1292	ASP	S1138	ASP
ASP	L2067	H1866	LEU	LEU	I1688	L1601	L1499	K1403	R1293	ALA	E1139	THR
GLY	A2068	L1867	GLY	GLY	L1689	F1602	P1500	K1404	R1294	VAL	L1139	ARG
VAL	R2069	M1869	ASP	ASP	F1691	A1604	P1503	T1405	A1295	GLY	E1141	GLN
LEU	V2070	C1872	E1774	E1774	I1690	F1605	R1504	K1406	A1299	VAL	F1142	GLU
GLU	L2074	S1875	D1775	D1775	F1698	L1609	R1505	Q1302	Q1302	GLN	F1143	LYS
GLN	H2077	L1882	V1776	V1776	I1701	A1615	L1513	E1307	W1214	ASN	V1147	ASN
ARG	G2082	T1883	R1778	R1778	D1702	N1615	L1517	E1308	Q1220	SER	A1152	GLN
ASP	Q2090	G1884	E1779	E1779	R1705	G1627	T1520	P1309	L1224	GLN	D1153	GLY
THR	T2091	A1885	R1782	R1782	M1706	M1628	K1521	P1310	K1227	SER	T1154	SER
GLY	L2093	E1886	A1787	A1787	Q1707	S1629	E1522	Q1312	L1230	ASP	D1155	ARG
GLU	E2094	H1887	T1788	T1788	A1708	I1630	E1523	H1313	R1233	GLY	MET	V1073
LYS	L2096	L1888	Q1789	Q1789	M1709	T1631	Q1524	S1315	R1234	GLY	GLU	G1074
GLN	D2103	P1898	V1792	V1792	A1712	P1632	L1524	H1316	S1235	ASP	ASP	T1075
GLY	GLY	E1899	L1793	L1793	F1713	L1633	S1525	R1317	R1236	SER	GLY	P1076
LYS	LYS	A1900	V1794	V1794	L1716	P1636	G1526	F1318	R1237	CYS	GLY	Q1077
ASP	ASP	Q1901	L1795	L1795	GLY	V1643	E1528	S1319	G1238	GLY	HIS	L1078
GLU	GLU	A1903	L1798	L1798	ASP	P1644	M1530	A1320	L1239	HIS	LEU	H1084
THR	THR	A1906	Y1802	Y1802	ARG	P1645	E1531	P1321	F1240	CYS	CYS	P1087
GLY	GLY	G1907	Q1722	Q1722	GLN	T1646	S1532	E1322	GLY	THR	THR	G1088
GLN	GLN	LEU	R1726	R1726	PHE	A1647	V1534	P1324	ALA	GLY	ILE	A1089
LYS	LYS	LEU	E1728	E1728	LEU	F1544	D1536	V1327	GLY	GLY	ALA	GLY

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

Chain D:  100%

MAG1  
MAG2

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

Chain B:  100%

MAG1  
MAG2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	91381	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.188	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	343.68, 343.68, 343.68	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.895, 0.895, 0.895	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, UNL, AGS

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	0.25	0/14270	0.51	0/19416

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	13931	0	14109	238	0
2	B	28	0	25	0	0
2	D	28	0	25	0	0
3	A	56	0	52	1	0
4	A	216	0	0	0	0
5	A	62	0	24	3	0
All	All	14321	0	14235	238	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 8.

The worst 5 of 238 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:897:THR:HG22	1:A:898:VAL:H	1.22	1.03
1:A:310:GLN:HA	1:A:313:ARG:HE	1.40	0.86
1:A:897:THR:HG22	1:A:898:VAL:N	1.87	0.86
1:A:897:THR:HG21	1:A:936:GLN:HA	1.60	0.84
1:A:897:THR:CG2	1:A:898:VAL:H	1.94	0.79

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	1786/2146 (83%)	1711 (96%)	74 (4%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	876	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	1479/1764 (84%)	1475 (100%)	4 (0%)	91	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	477	ASN
1	A	1227	LYS
1	A	1295	ARG
1	A	1973	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1220	GLN
1	A	1346	GLN

### 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 ⓘ

4 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	0.29	0	17,19,21	0.65	0
2	NAG	B	2	2	14,14,15	0.34	0	17,19,21	0.69	0
2	NAG	D	1	1,2	14,14,15	0.28	0	17,19,21	0.88	1 (5%)
2	NAG	D	2	2	14,14,15	0.36	0	17,19,21	0.69	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	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(°)
2	D	1	NAG	C1-O5-C5	2.87	116.03	112.19
2	D	2	NAG	C1-O5-C5	2.21	115.15	112.19

There are no chirality outliers.

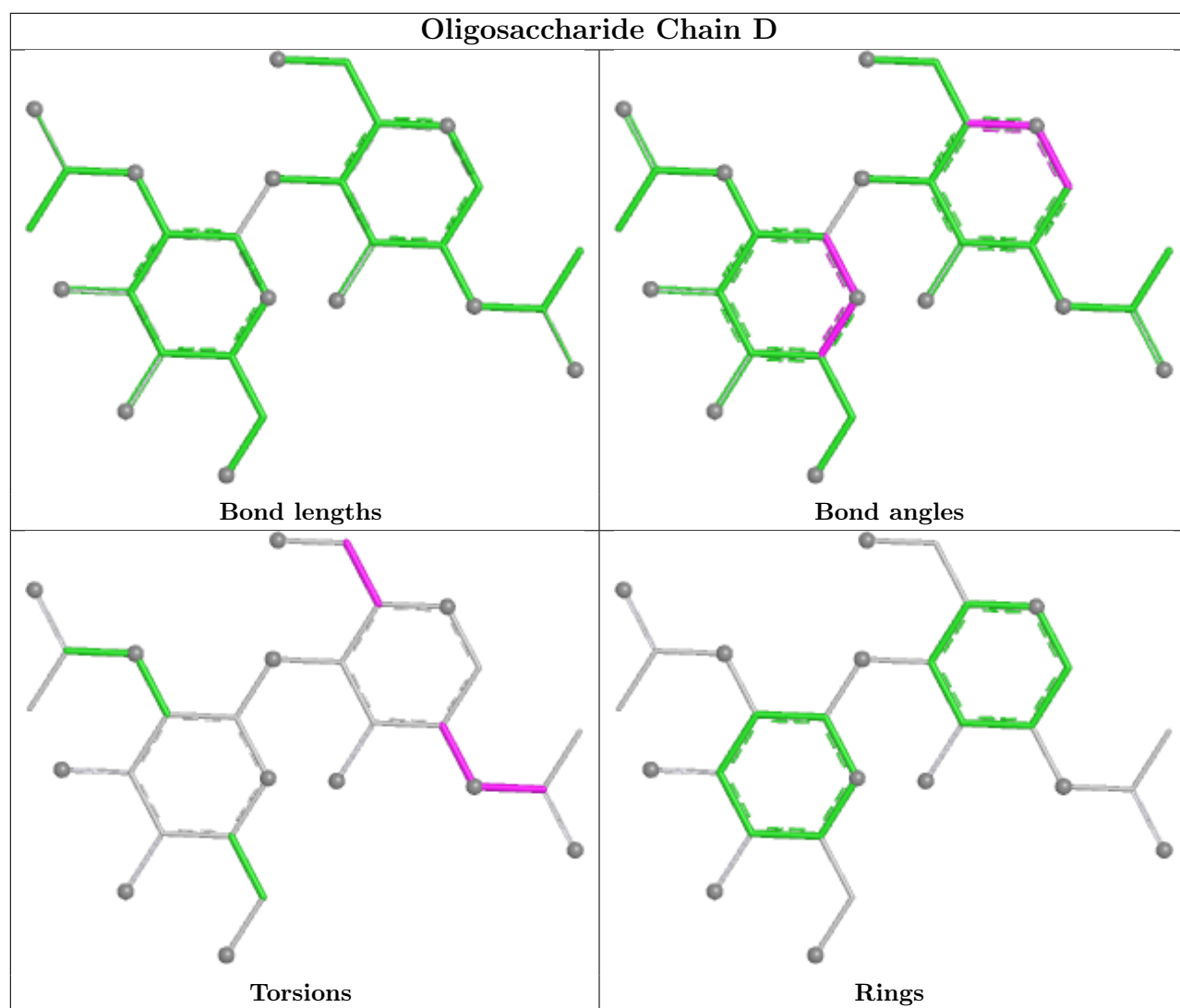
All (5) torsion outliers are listed below:

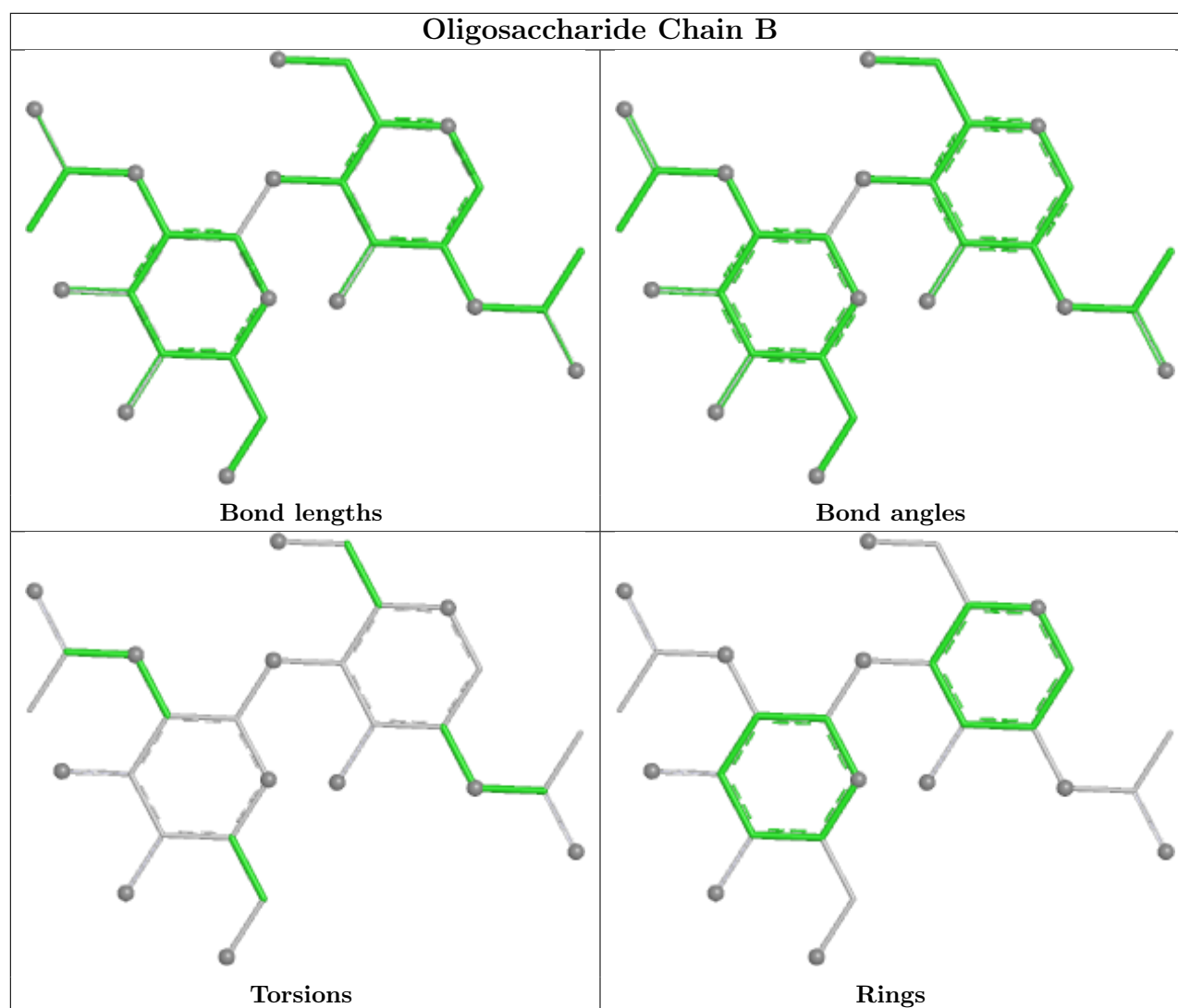
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

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 oligosaccharide.





## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 18 are unknown - leaving 6 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	$\# Z  > 2$
3	NAG	A	2203	1	14,14,15	0.35	0	17,19,21	1.32	2 (11%)
5	AGS	A	2223	-	28,33,33	0.88	1 (3%)	31,52,52	0.76	1 (3%)
5	AGS	A	2224	-	28,33,33	0.86	1 (3%)	31,52,52	0.81	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	2202	1	14,14,15	0.32	0	17,19,21	0.59	0
3	NAG	A	2204	1	14,14,15	0.30	0	17,19,21	0.58	0
3	NAG	A	2201	1	14,14,15	0.30	0	17,19,21	0.54	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	2203	1	-	4/6/23/26	0/1/1/1
5	AGS	A	2223	-	-	2/17/38/38	0/3/3/3
5	AGS	A	2224	-	-	2/17/38/38	0/3/3/3
3	NAG	A	2202	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2204	1	-	3/6/23/26	0/1/1/1
3	NAG	A	2201	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2224	AGS	PG-S1G	2.14	1.95	1.90
5	A	2223	AGS	PG-S1G	2.12	1.95	1.90

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2203	NAG	C1-O5-C5	-4.58	106.04	112.19
5	A	2224	AGS	C5-C6-N6	2.27	123.78	120.31
5	A	2223	AGS	C5-C6-N6	2.26	123.76	120.31
3	A	2203	NAG	O5-C5-C6	2.07	111.69	107.66

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2223	AGS	C5'-O5'-PA-O1A
5	A	2223	AGS	C4'-C5'-O5'-PA
5	A	2224	AGS	C4'-C5'-O5'-PA
3	A	2203	NAG	C8-C7-N2-C2
3	A	2203	NAG	O7-C7-N2-C2

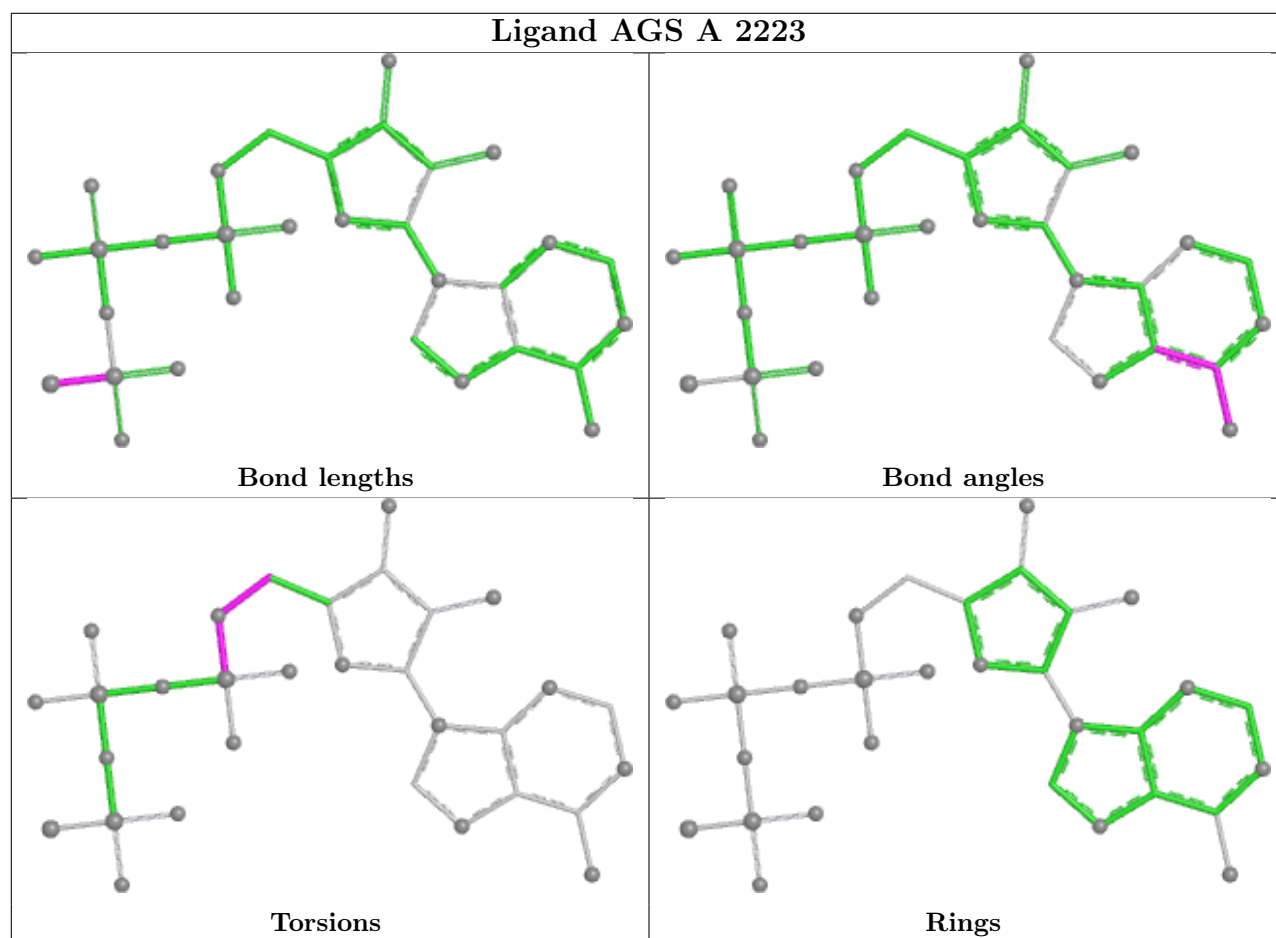


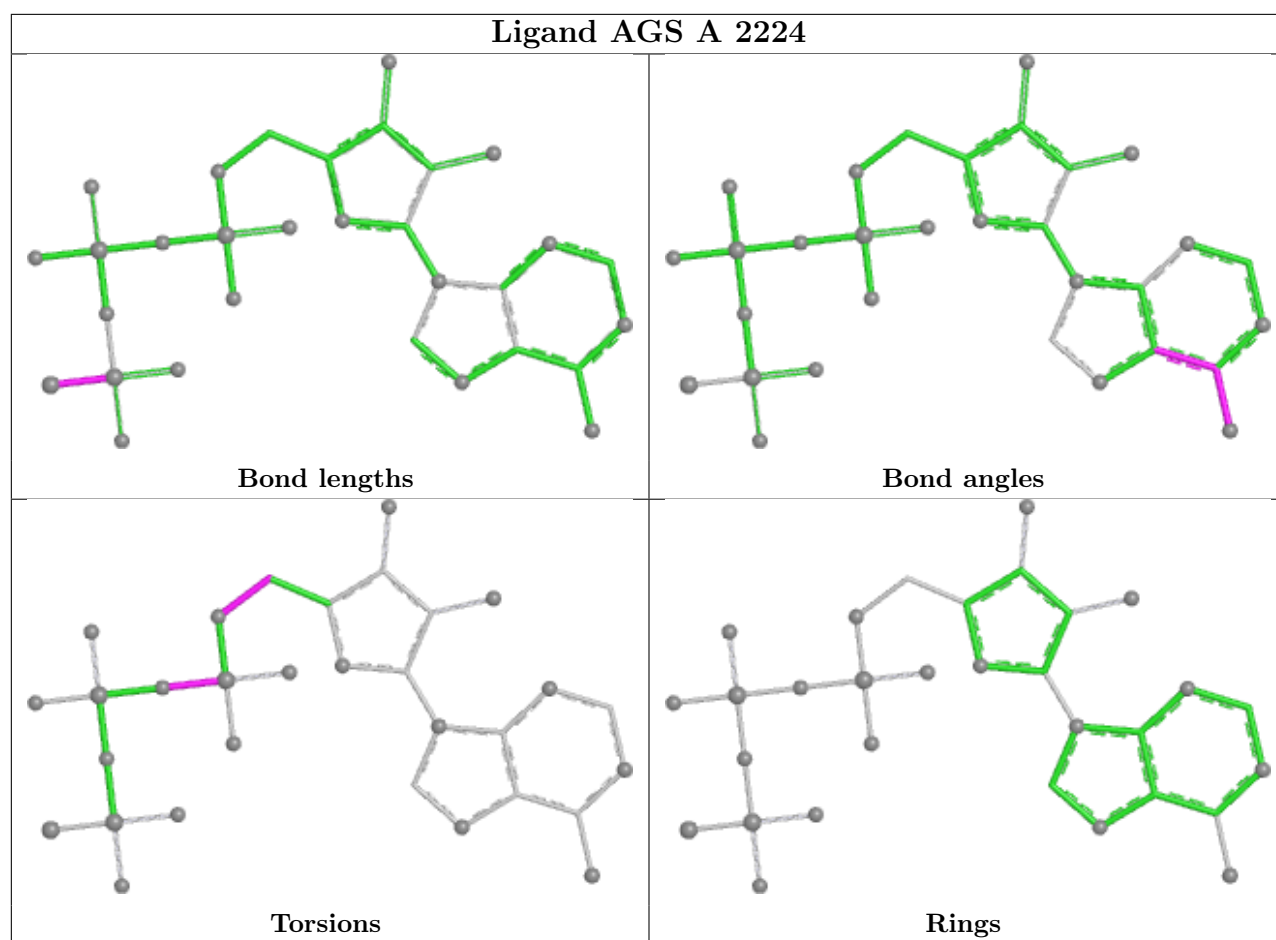
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2224	AGS	3	0
3	A	2202	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 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.

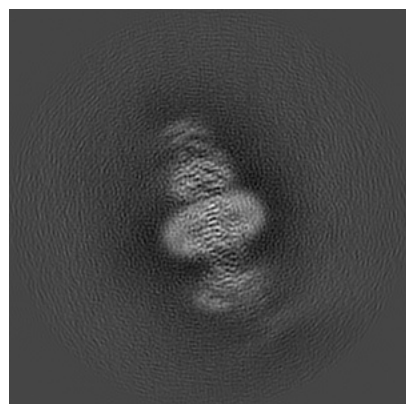
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28041. These allow visual inspection of the internal detail of the map and identification of artifacts.

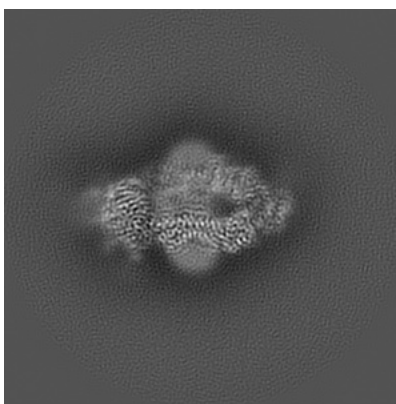
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

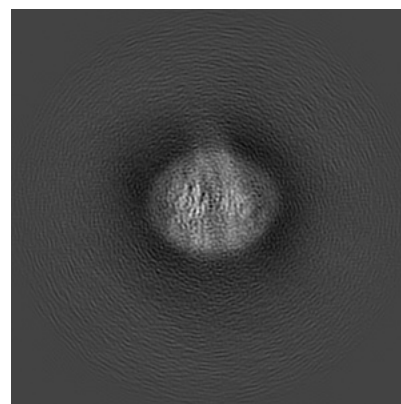
#### 6.1.1 Primary map



X

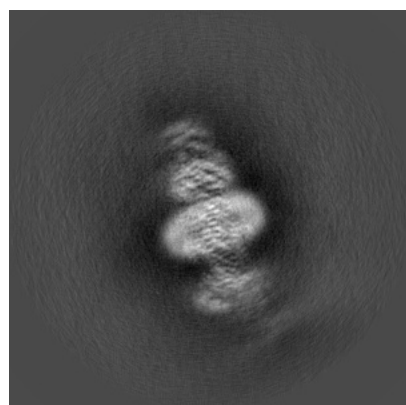


Y

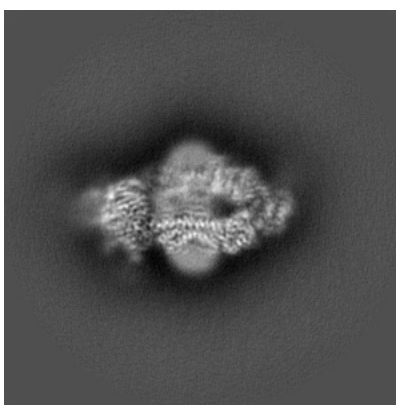


Z

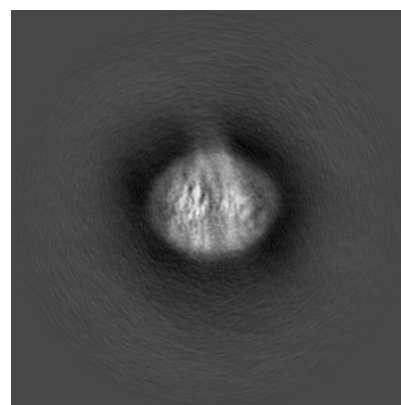
#### 6.1.2 Raw map



X



Y

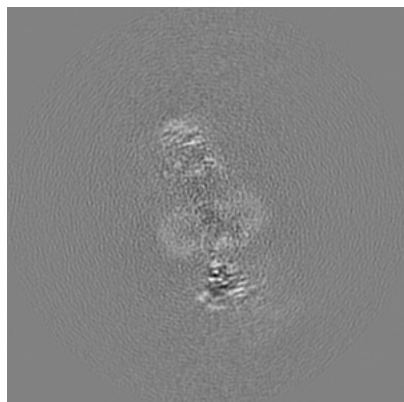


Z

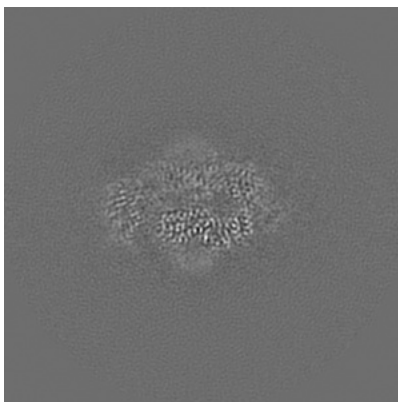
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

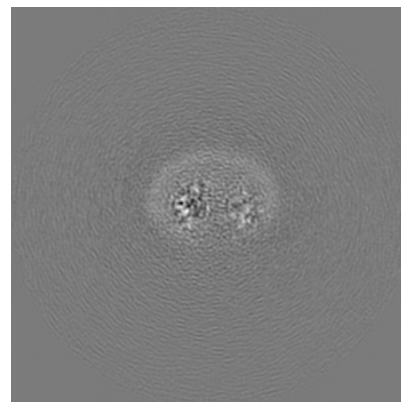
### 6.2.1 Primary map



X Index: 192

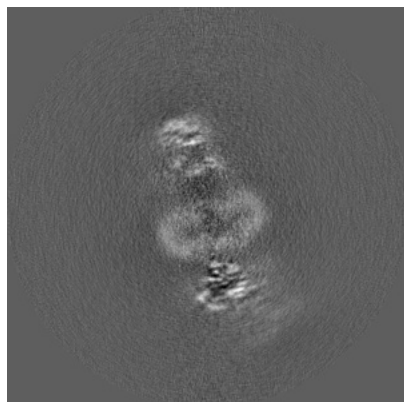


Y Index: 192

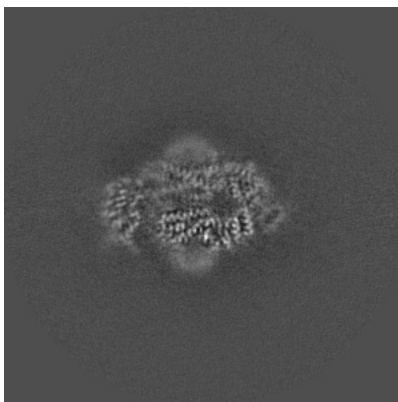


Z Index: 192

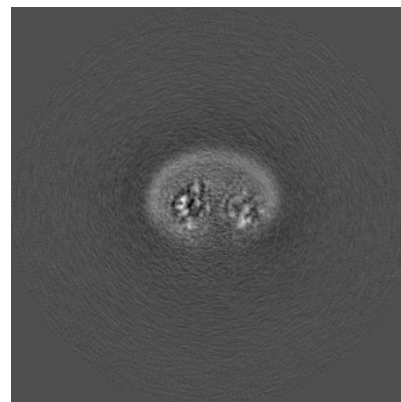
### 6.2.2 Raw map



X Index: 192



Y Index: 192

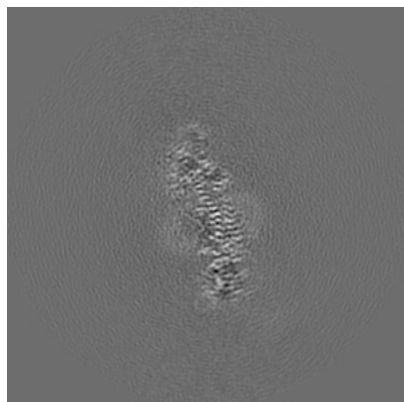


Z Index: 192

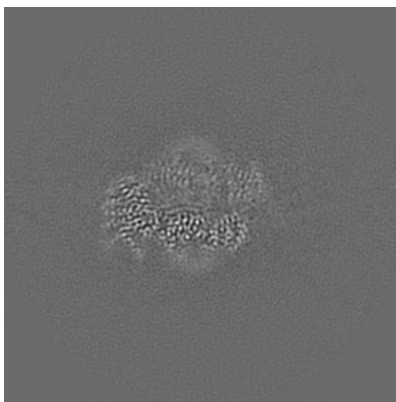
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

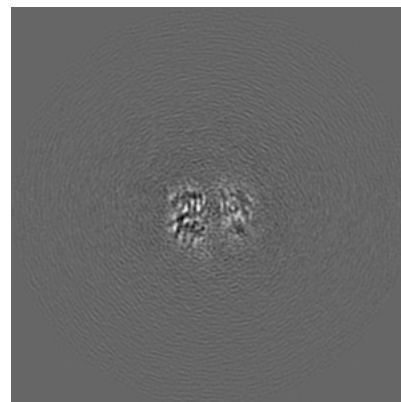
### 6.3.1 Primary map



X Index: 177

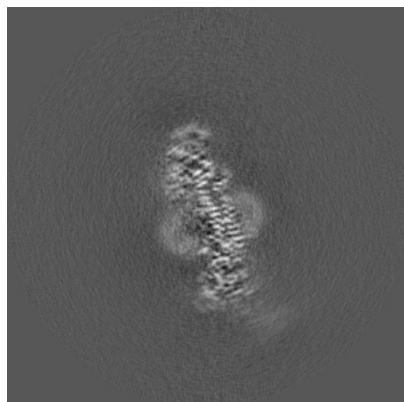


Y Index: 201

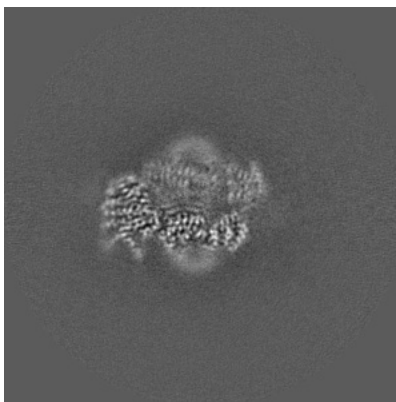


Z Index: 222

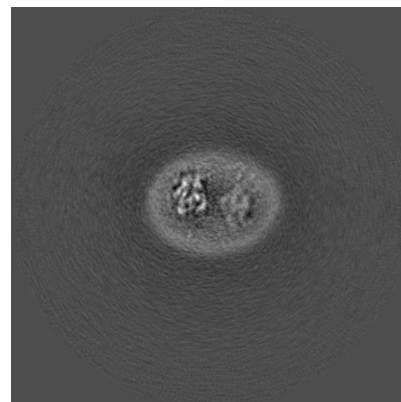
### 6.3.2 Raw map



X Index: 178



Y Index: 201



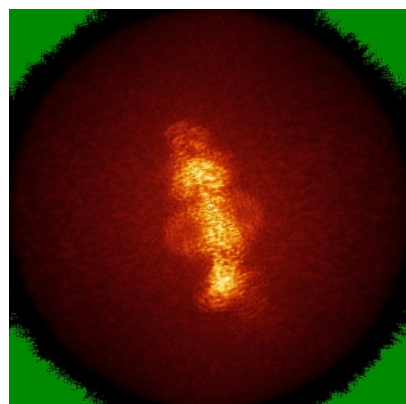
Z Index: 173

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

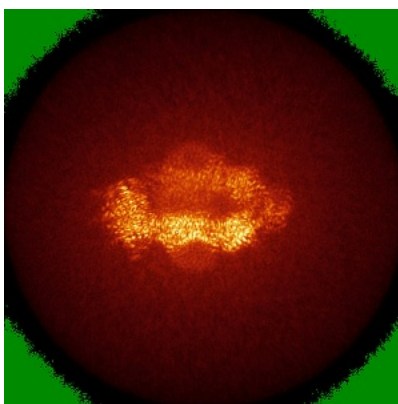


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

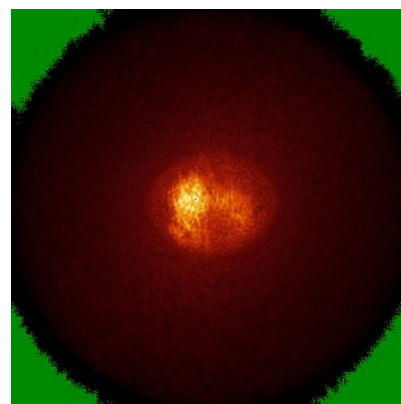
### 6.4.1 Primary map



X

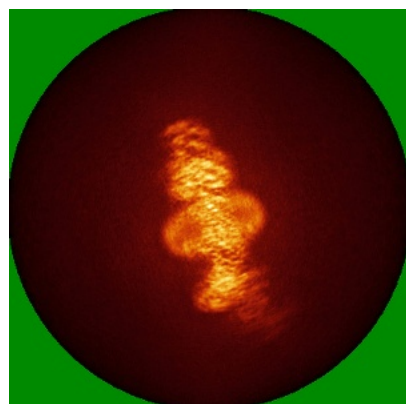


Y

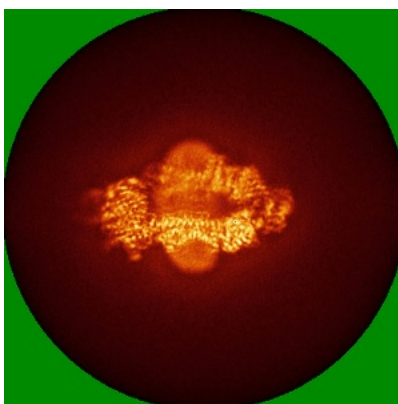


Z

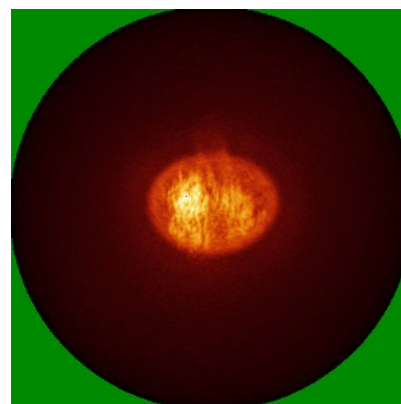
### 6.4.2 Raw map



X



Y

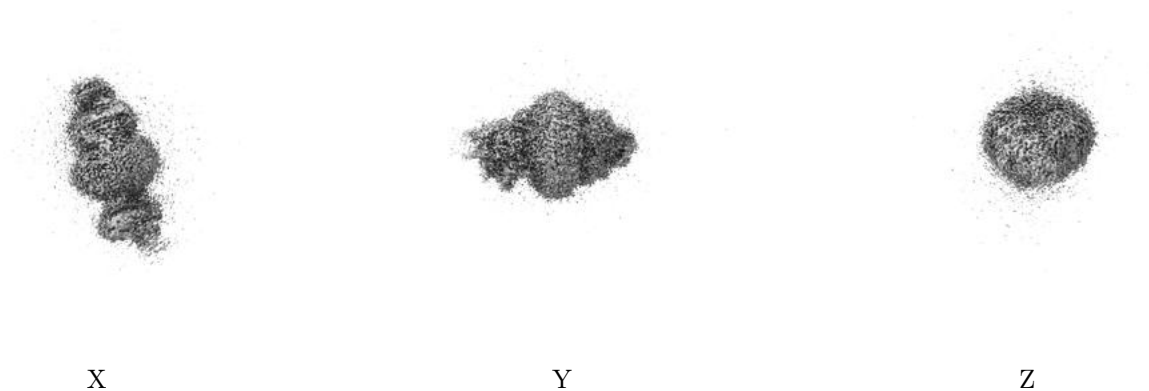


Z

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.

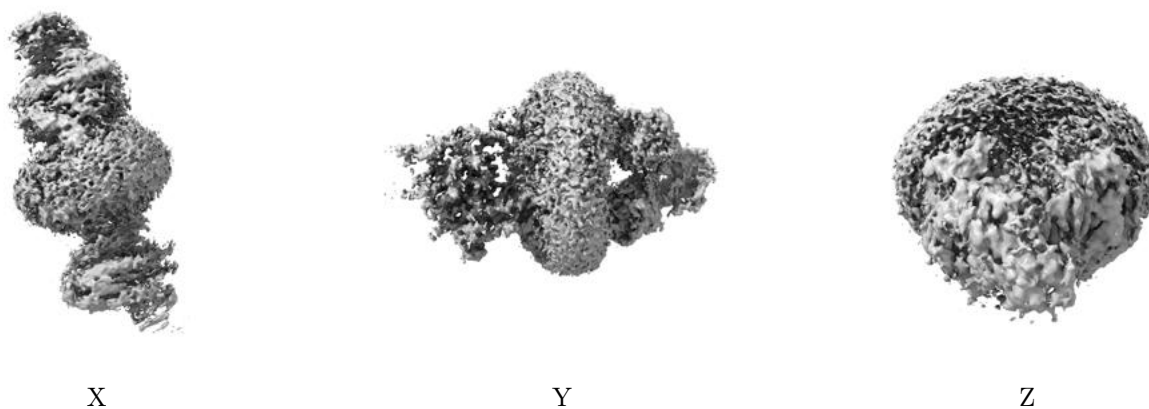
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

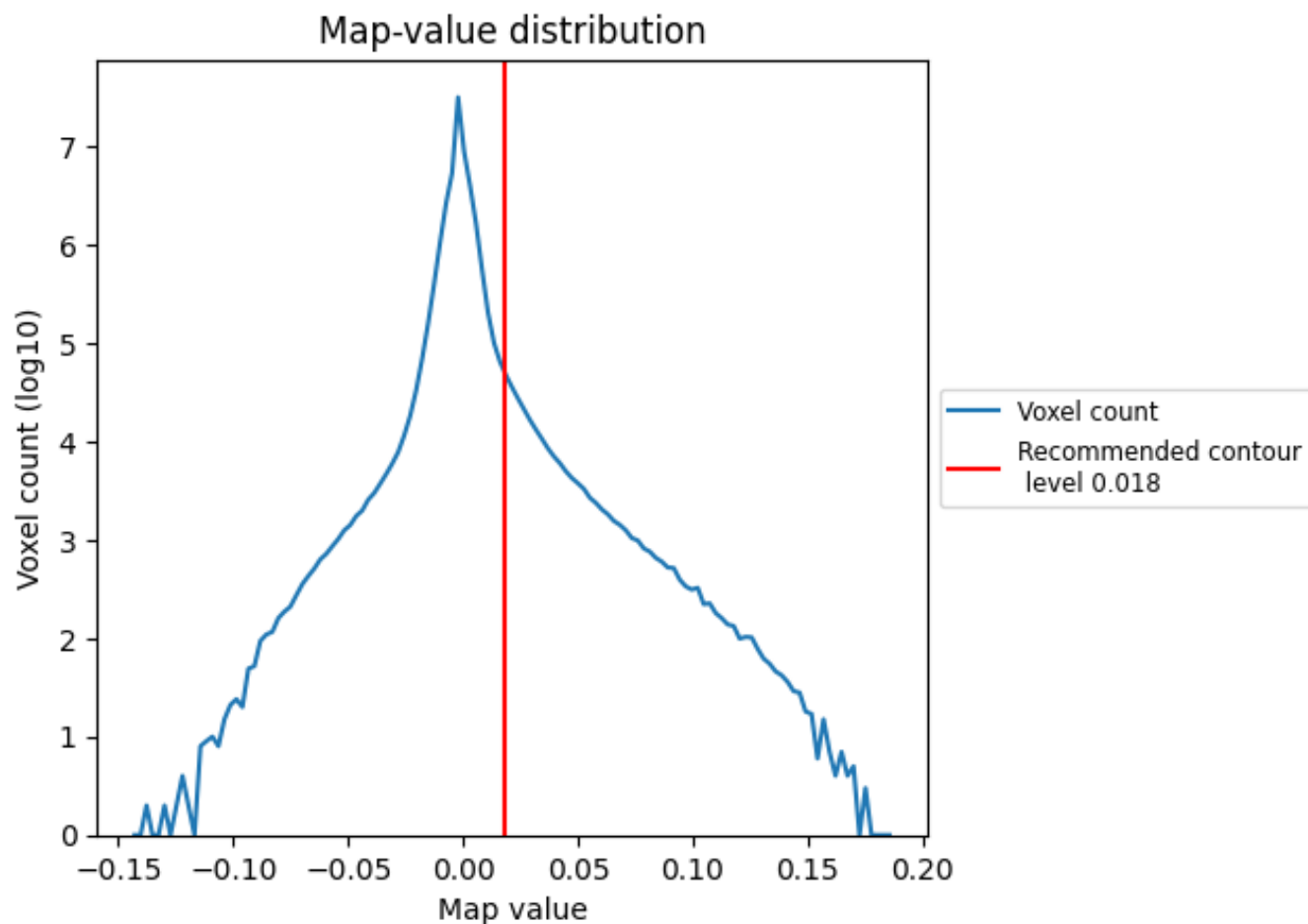
## 6.6 Mask visualisation [i](#)

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.

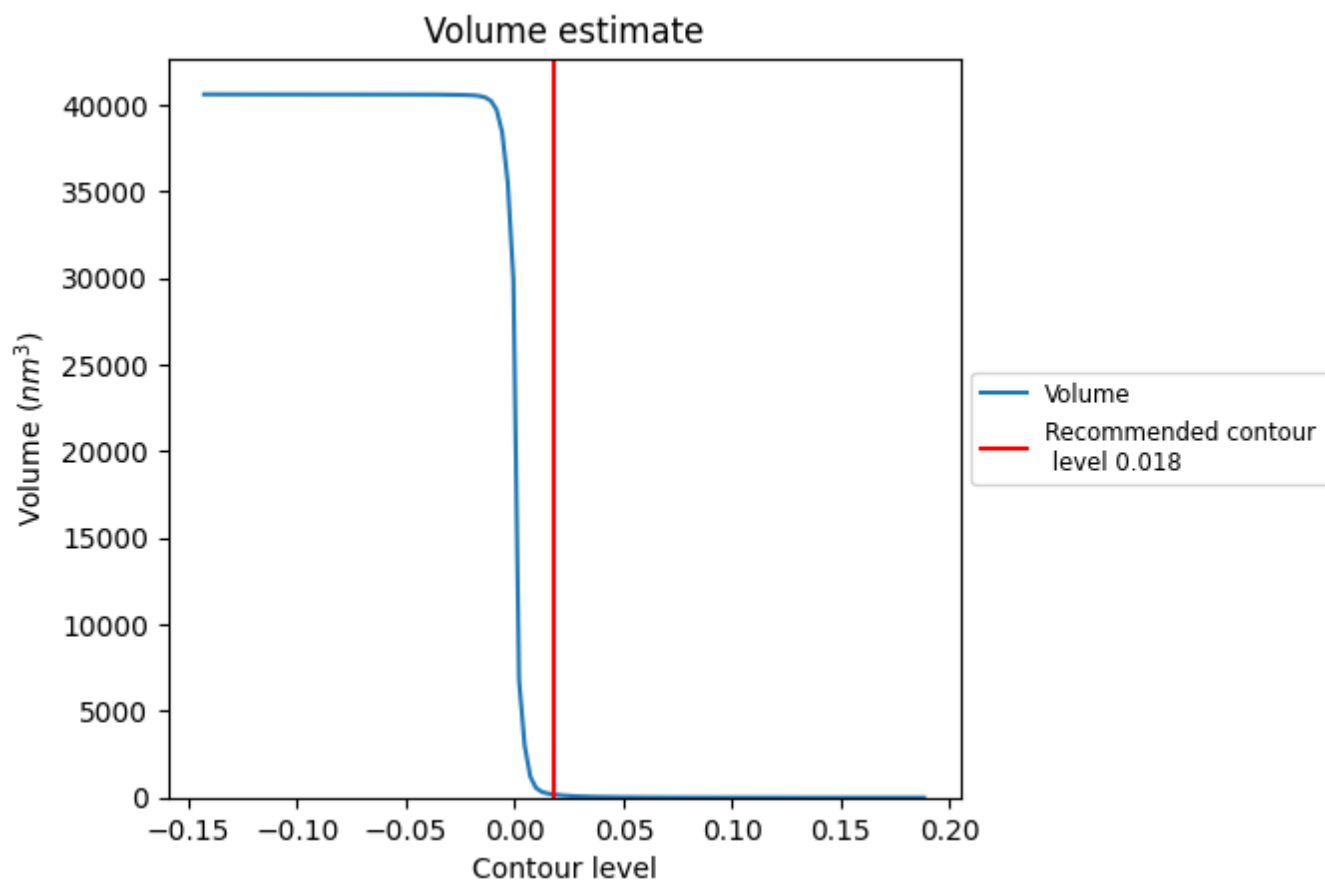
### 7.1 Map-value distribution [i](#)



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.



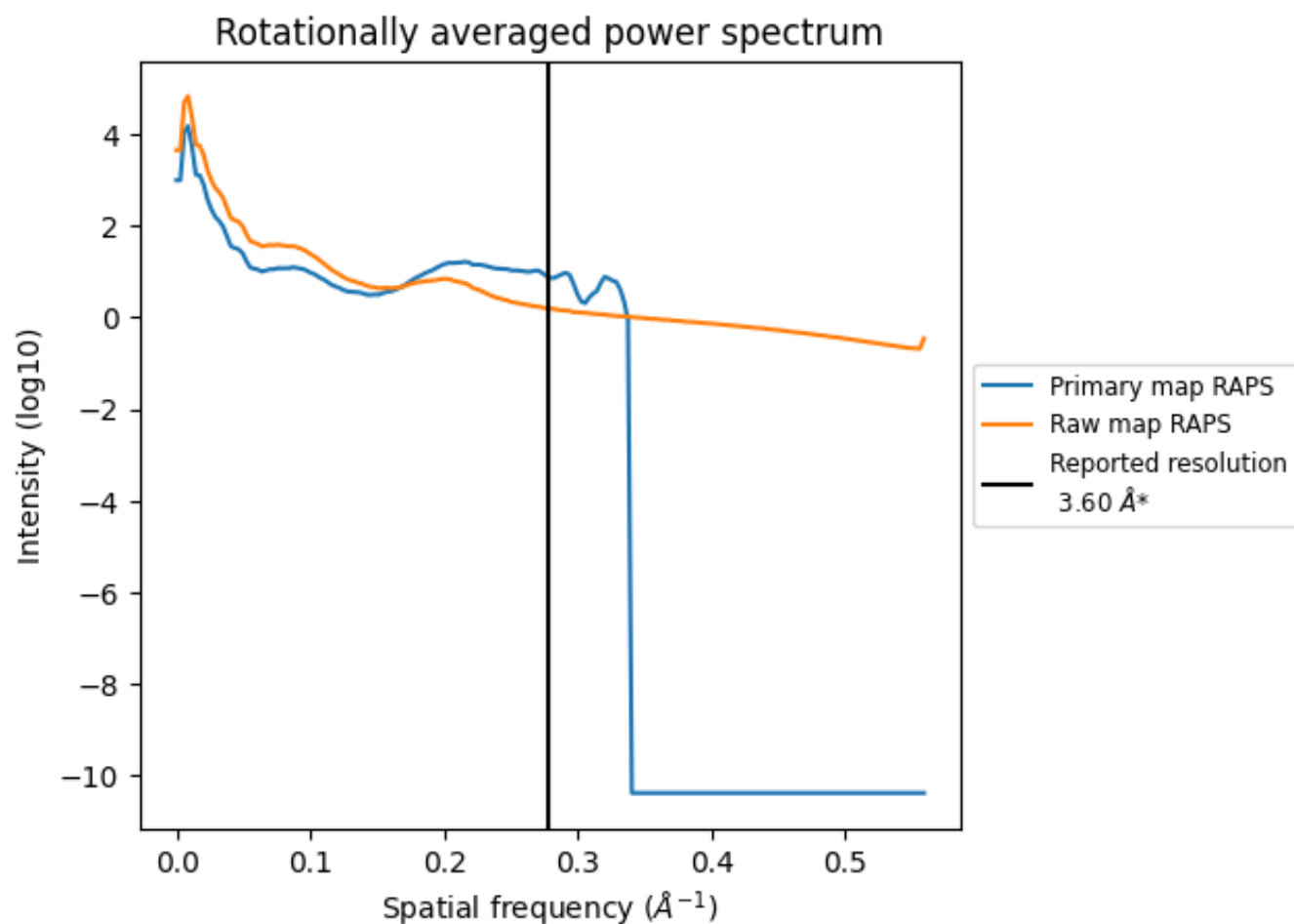
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 178  $\text{nm}^3$ ; this corresponds to an approximate mass of 161 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 ⓘ

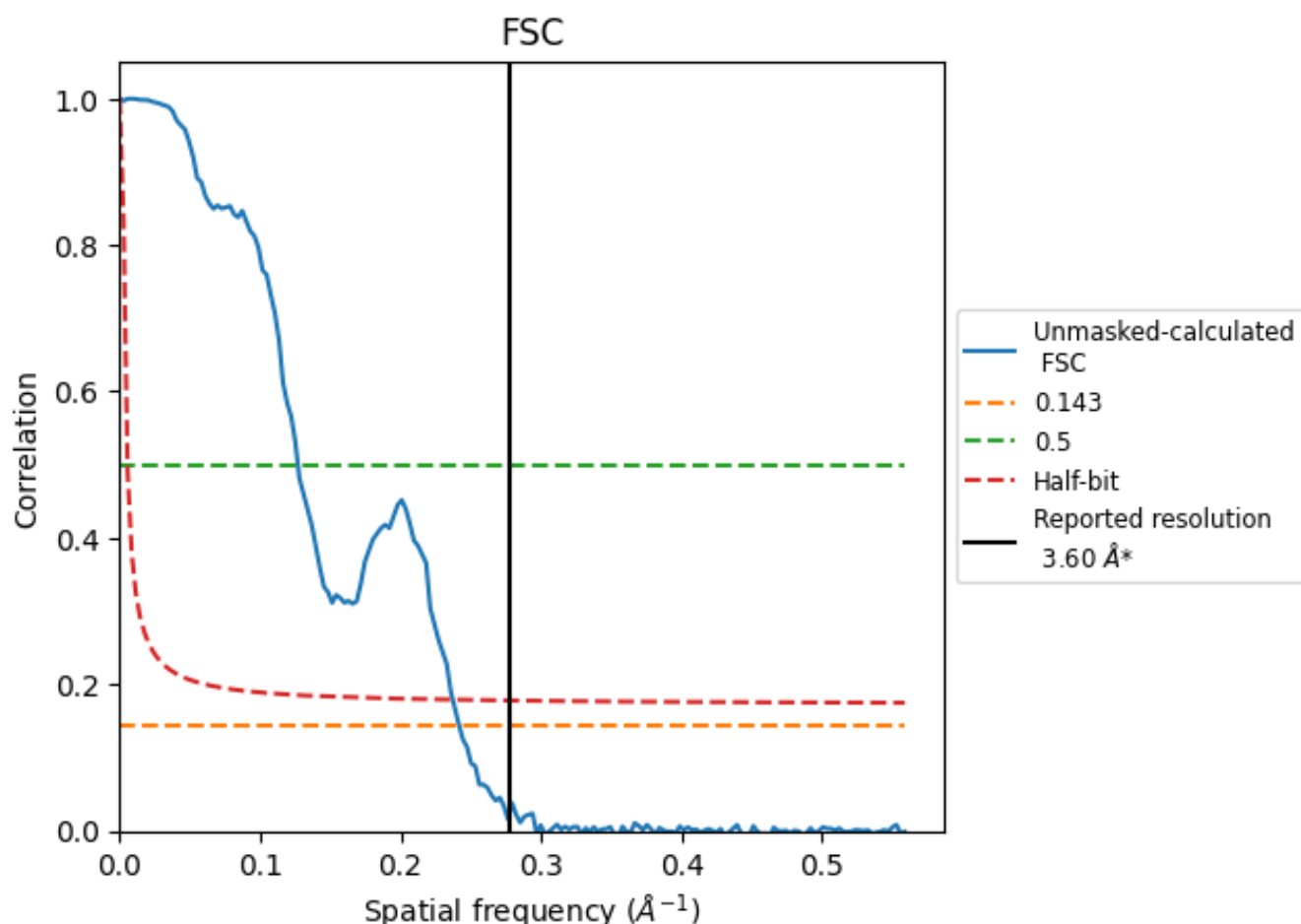


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

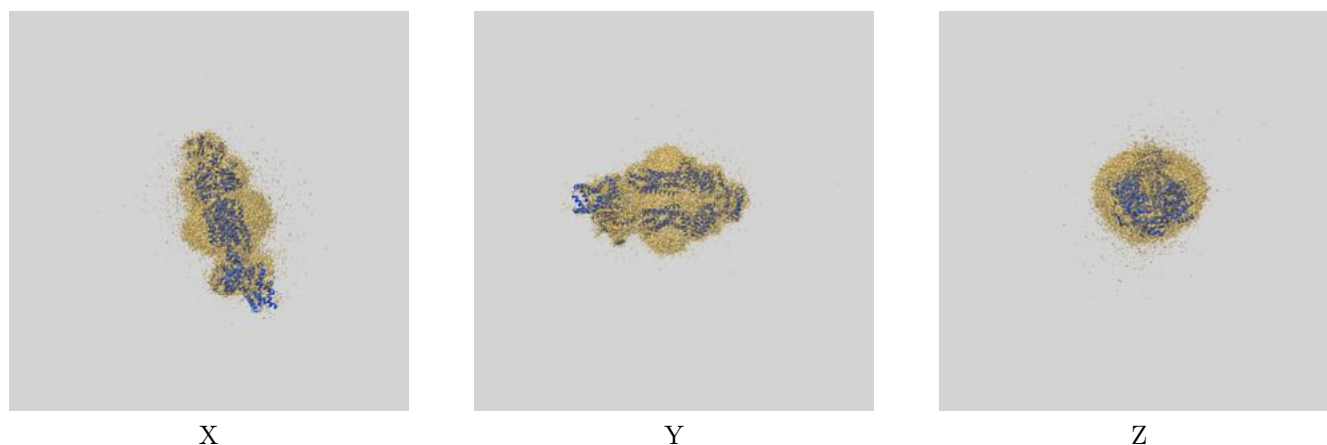
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	7.88	4.22

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.6 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28041 and PDB model 8EDW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

### 9.1 Map-model overlay [i](#)



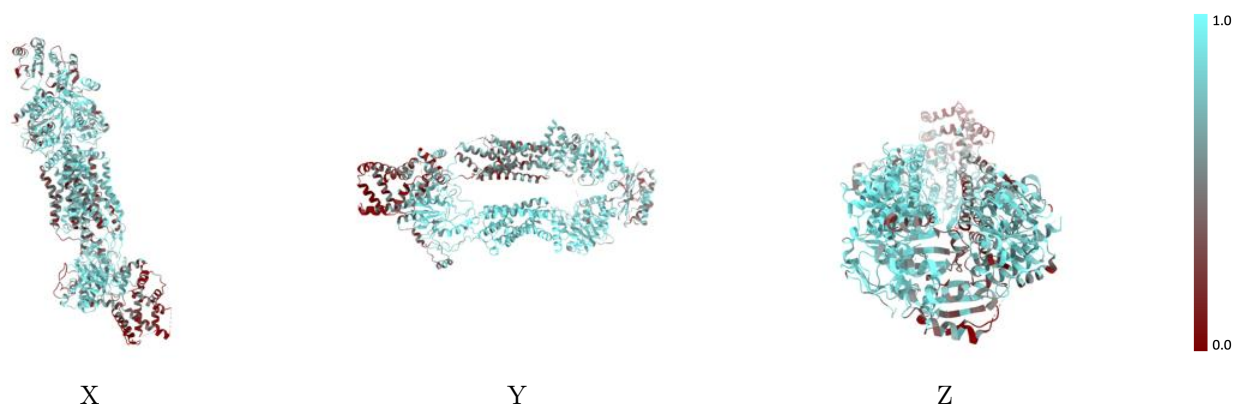
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



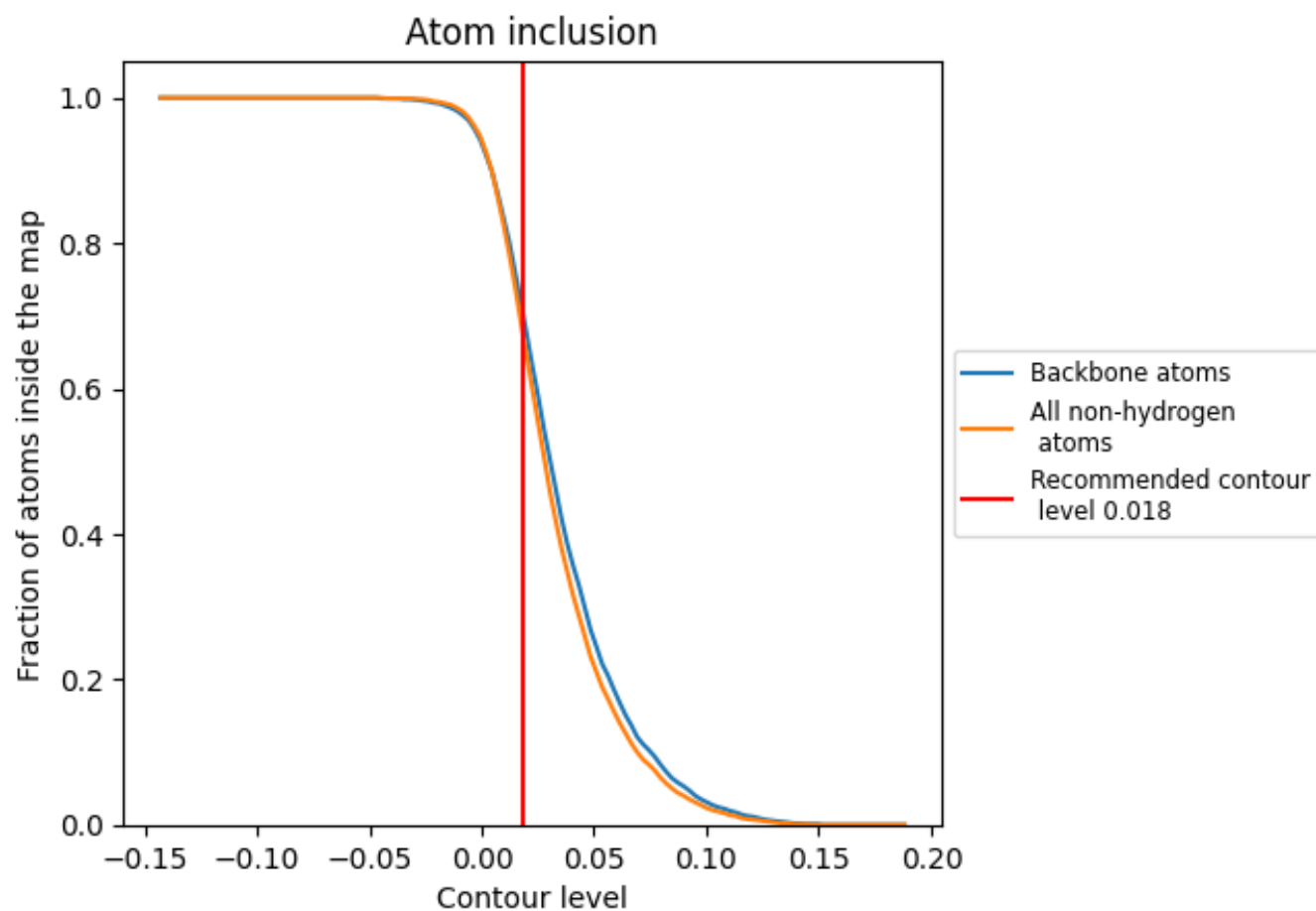
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 68% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6810	<div></div> 0.3400
A	<div></div> 0.6810	<div></div> 0.3400
B	<div></div> 0.6790	<div></div> 0.4150
D	<div></div> 0.7140	<div></div> 0.3710

