



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:39 PM UTC

PDB ID : 8EE6 / pdb_00008ee6
EMDB ID : EMD-28047
Title : Cryo-EM Structure of human ABCA7 in PE/Ch nanodiscs
Authors : Alam, A.; Le, L.T.M.; Thompson, J.R.
Deposited on : 2022-09-06
Resolution : 4.00 Å(reported)
Based on initial model : 6JBj

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

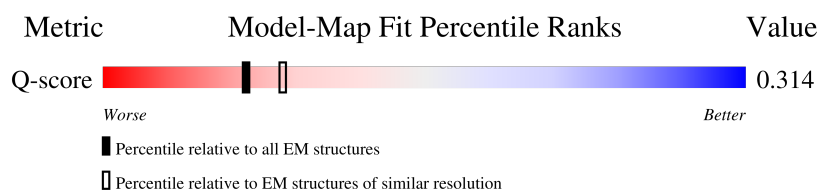
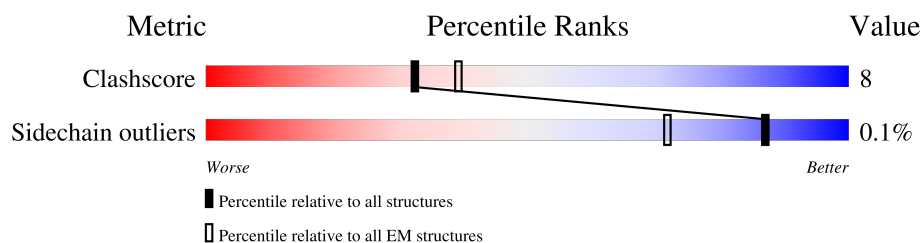
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	15% 67% 17% 16%
2	C	3	67% 33%
2	D	3	33% 100%
3	B	4	50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14475 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	1808	Total	C	N	O	S	0	0
			13975	8993	2460	2459	63		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	3	Total	C	N	O	0	0
			39	22	2	15		
2	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

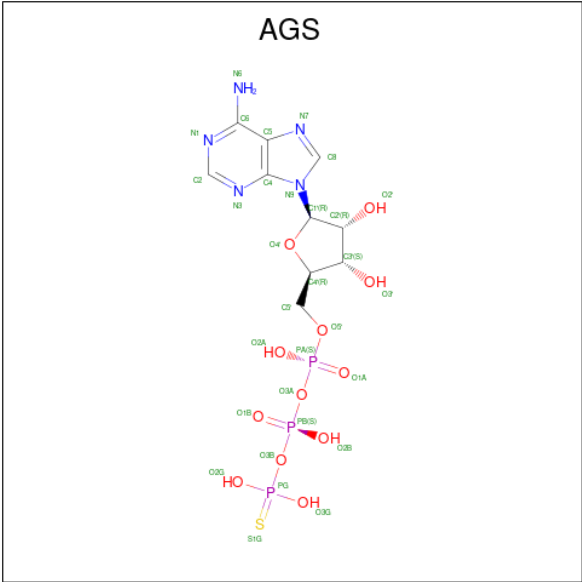


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	20	Total	C	0
			240	240	

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



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

S2087	E1987	P1898	E1779	D1711	S1829	T1554	M1457	A1352	F1256	THR	A1108	LEU
V2088	C1988	P1899	R1782	D1711	T1630	L1555	L1458	R1353	S1257	ALA	G1111	PRO
Q2089	E1989	A1900	A1787	R1715	L1633	V1556	T1459	L1356	L1258	LEU	L1116	THR
T2091	A1990	Q1901	T1787	L1716	M1634	L1557	A1460	D1358	I1259	ASN	F1117	THR
M2092	C1992	V1902	Q1788	L1716	P1635	R1560	H1463	C1359	V1260	GLY	L1124	ASN
L2093	S1993	A1903	Q1789	ASP	P1636	R1561	S1464	A1363	P1261	GLU	A1125	GLU
E2094	R1994	A1906	K1800	ARG	F1641	V1562	Q1468	P1366	P1262	PRO	R1128	LYS
D2103	L1995	G1907	V1801	PHE	P1644	T1563	K1472	P1367	H1265	ALA	L1129	ALA
GLN	I1997	S1908	Y1802	Q1722	S1645	H1567	M1477	F1368	Y1266	GLY	R1128	THR
LYS	F2003	A1911	M1807	S1723	Y1648	Q1568	Y1484	Q1370	P1267	ALA	L1129	ASP
ASP	C2005	G1914	D1811	R1726	L1651	L1570	M1492	L1387	S1272	PRO	G1133	GLU
GLU	L2006	Y1918	R1812	Y1727	L1655	M1571	R1496	L1391	M1275	GLY	I1134	GLY
THR	G2019	Y1919	L1813	E1728	L1656	Y1579	P1500	R1400	S1281	VAL	S1136	SER
GLU	T2023	A1921	E1821	G1731	F1657	L1578	F1504	W1408	F1282	GLN	D1136	ASP
GLN	R2030	G1922	L1826	L1734	I1658	M1583	R1505	W1408	A1287	GLY	T1137	THR
ALA	R2030	A1923	G1830	L1735	I1659	F1584	T1511	R1413	R1293	LYS	T1142	LYS
GLY	V2037	G1924	A1831	L1736	G1659	W1586	R1505	G1416	E1298	ASN	F1143	ASN
VAL	V2038	T1925	K1833	Y1738	I1660	W1586	T1511	P1424	E1307	GLY	K1144	GLY
VAL	A2039	Y1926	T1834	Q1739	M1661	D1587	L1513	G1426	E1308	SER	V1146	SER
ASP	A2040	Y1927	S1835	I1740	G1662	M1588	L1513	P1427	P1310	GLN	C1150	GLY
PRO	E2041	G1928	T1836	G1741	M1664	Y1591	T1520	Q1430	P1310	GLY	T1154	ARG
ALA	G2044	G1928	P1742	P1742	A1665	L1592	T1520	Q1430	D1155	ARG	D1155	ARG
PRO	A2044	G1929	L1743	L1743	T1666	Y1593	Q1523	E1431	Q1220	GLU	Q1220	GLU
GLY	A2045	N1930	F1744	L1745	F1667	P1594	L1524	H1313	A1223	ASP	A1223	ASP
LEU	E2046	K1933	L1746	L1746	V1668	A1595	S1626	L1432	Q1228	GLY	Q1228	GLY
GLN	L2047	L1934	F1747	F1747	L1669	C1596	E1526	G1433	R1236	CYS	C1150	CYS
HIS	R2048	L1934	T1748	T1748	E1670	V1599	G1627	R1434	R1237	GLY	C1150	GLY
PRO	E2049	L1938	L1749	L1749	L1671	V1599	L1528	S1435	R1233	GLN	C1150	GLN
ARG	H2051	V1941	Q1752	Q1752	F1672	A1604	M1530	V1436	R1234	HIS	C1150	HIS
VAL	R2056	P1944	Q1756	Q1756	Q1675	F1606	A1531	E1437	S1235	LEU	C1150	LEU
SER	P2057	A1945	LEU	LEU	K1676	F1606	S1532	E1438	S1319	CYS	C1150	CYS
PHE	Q2058	L1946	PRO	PRO	L1677	R1608	S1533	L1439	A1320	THR	C1150	THR
LEU	L2059	Y1946	GLN	GLN	Q1678	A1609	V1534	W1440	P1321	GLY	C1150	GLY
ASP	P2060	L1949	PRO	PRO	E1679	Y1610	D1535	A1441	V1327	ILE	C1150	ILE
PRO	P2061	Y1949	ARG	ARG	V1680	S1681	V1536	L1442	A1328	ALA	C1150	ALA
SER	G2062	L1952	L1881	L1881	S1681	P1613	L1537	L1443	F1240	GLY	C1150	GLY
THR	G2063	T1953	T1882	T1882	R1682	A1614	V1538	L1443	A1241	LEU	C1150	LEU
GLU	R2064	M1956	G1884	G1884	I1683	L1615	S1539	P1445	Q1242	ASP	C1150	ASP
VAL	A2068	D1957	R1885	R1885	L1684	L1616	I1540	P1446	I1243	VAL	C1150	VAL
LEU	G2072	P1958	E1886	E1886	K1685	L1617	F1544	P1447	V1244	THR	C1150	THR
LEU	E2073	R1961	L1888	L1888	V1686	A1618	L1619	G1448	L1245	LEU	C1150	LEU
LEU	L2074	R1961	E1889	E1889	Q1687	L1619	M1545	P1449	P1246	ARG	C1150	ARG
LEU	G2077	W1965	L1890	L1890	F1688	L1620	M1546	A1450	A1247	LYS	C1150	LYS
LEU	H2077	L1968	L1891	L1891	L1689	L1621	S1547	L1451	L1248	MET	C1150	MET
LEU	G2078	L1969	A1892	A1892	I1690	L1625	F1548	D1452	F1249	PRO	C1150	PRO
LEU	A2079	M1978	D1775	D1775	I1701	Y1626	F1548	R1453	L1254	GLN	C1150	GLN
LEU	E2080	M1979	V1776	V1776	T1702	G1627	A1551	V1454	V1255	GLU	C1150	GLU
LEU	F2086				W1703	W1628	S1552	L1455				
					R1704		F1553	K1456				
					R1705							
					Q1707							

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



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



- Molecule 3: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-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	50704	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	0.139	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	341.376, 341.376, 341.376	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.889, 0.889, 0.889	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: BMA, UNL, NAG, 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	0.17	0/14317	0.34	0/19480

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	13975	0	14147	243	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	B	50	0	43	2	0
4	A	70	0	65	1	0
5	A	240	0	0	0	0
6	A	62	0	24	3	0
All	All	14475	0	14347	244	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.

All (244) 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:1499:LEU:HD12	1:A:1500:PRO:HD2	1.69	0.74
1:A:1634:MET:HE3	1:A:1651:LEU:HD13	1.69	0.74
1:A:2089:SER:HA	1:A:2092:MET:HE2	1.71	0.72
1:A:327:VAL:HA	1:A:330:MET:HE2	1.72	0.70
1:A:1331:LEU:HD21	1:A:1366:PRO:HG2	1.76	0.68
1:A:1836:THR:HA	1:A:1839:MET:HE2	1.74	0.68
1:A:58:ASN:O	1:A:76:ASN:ND2	2.28	0.67
1:A:1298:GLU:HG2	1:A:1310:PRO:HB3	1.76	0.66
1:A:1520:THR:O	1:A:1524:LEU:N	2.26	0.66
1:A:1220:GLN:HE21	1:A:1574:LEU:HA	1.60	0.66
1:A:892:LEU:HD23	1:A:938:ARG:HD2	1.77	0.65
1:A:1853:LEU:HD11	1:A:1946:VAL:HG11	1.79	0.64
1:A:1555:LEU:HD21	1:A:1648:TYR:HB2	1.80	0.64
1:A:1036:THR:HA	1:A:1100:VAL:HA	1.79	0.63
1:A:584:MET:HE2	1:A:908:LEU:HD22	1.81	0.62
1:A:1037:LEU:HB2	1:A:1099:LEU:HB3	1.81	0.61
1:A:298:ALA:HB2	1:A:421:LEU:HD22	1.83	0.61
1:A:453:PRO:O	1:A:463:ARG:NH1	2.34	0.61
1:A:496:LEU:O	1:A:500:TRP:NE1	2.33	0.61
1:A:1584:PHE:O	1:A:1588:MET:HG2	2.00	0.61
1:A:20:ARG:HH22	1:A:897:THR:HG23	1.66	0.60
1:A:1949:LEU:HD23	1:A:1952:PRO:HB3	1.84	0.60
1:A:1830:GLY:HA2	6:A:2227:AGS:H5'1	1.84	0.59
1:A:1293:ARG:NH2	1:A:1468:GLN:O	2.36	0.59
1:A:1615:ASN:ND2	1:A:1707:GLN:OE1	2.36	0.59
1:A:1800:LYS:HB2	1:A:1839:MET:SD	2.43	0.58
1:A:1636:PRO:HG3	1:A:1748:THR:HB	1.83	0.58
1:A:897:THR:O	1:A:938:ARG:NH2	2.25	0.58
1:A:1320:ALA:HB2	1:A:1370:GLN:HG3	1.84	0.58
1:A:1223:ALA:HB2	1:A:1893:ARG:HD2	1.85	0.58
1:A:1690:ILE:O	1:A:1740:GLN:NE2	2.36	0.57
1:A:667:LEU:HB3	1:A:692:LEU:HD23	1.86	0.57
1:A:540:ASP:O	1:A:544:ARG:NH2	2.37	0.57
1:A:1220:GLN:NE2	1:A:1574:LEU:HA	2.19	0.57
1:A:1349:ARG:HD3	1:A:1351:GLY:H	1.68	0.57
1:A:1034:TYR:HB2	1:A:1135:SER:HB3	1.87	0.57
1:A:1499:LEU:HD23	1:A:1505:ARG:HD3	1.86	0.57
1:A:1883:THR:O	1:A:1887:HIS:ND1	2.36	0.57
1:A:927:VAL:HG23	1:A:929:LEU:HG	1.86	0.57
1:A:492:PRO:HA	1:A:496:LEU:HB2	1.88	0.56
1:A:1560:GLU:OE1	1:A:1579:TYR:OH	2.21	0.56
1:A:1280:VAL:HB	1:A:1413:ARG:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ARG:HG3	1:A:1408:TRP:HE1	1.69	0.56
1:A:1336:TRP:CD1	1:A:1342:SER:HB3	2.41	0.56
1:A:2046:GLU:HB2	1:A:2058:GLN:HB3	1.87	0.56
1:A:39:LEU:HD13	1:A:553:PHE:HE2	1.71	0.56
1:A:1136:ASP:OD2	1:A:2087:SER:OG	2.23	0.56
1:A:28:GLU:OE2	1:A:561:SER:OG	2.23	0.56
1:A:1888:LEU:HD22	1:A:1906:ALA:HA	1.87	0.56
1:A:482:ARG:HA	1:A:1408:TRP:HE1	1.70	0.55
1:A:650:PHE:HB2	1:A:656:ALA:HB2	1.88	0.55
3:B:1:NAG:H62	3:B:2:NAG:H83	1.87	0.55
1:A:1833:LYS:NZ	6:A:2227:AGS:O2B	2.38	0.55
1:A:1779:GLU:OE2	1:A:1782:ARG:NH1	2.40	0.55
1:A:1895:ARG:HH21	1:A:1944:PRO:HG3	1.71	0.55
1:A:339:MET:SD	1:A:340:ASN:N	2.80	0.55
1:A:1117:PHE:HB2	1:A:2068:ALA:HB2	1.88	0.55
1:A:1535:ASP:CG	1:A:1704:VAL:HG11	2.32	0.54
1:A:1143:PHE:HD1	1:A:1144:LEU:HD22	1.73	0.54
1:A:1090:ARG:HB3	1:A:1102:VAL:HB	1.88	0.54
1:A:901:HIS:HB2	1:A:938:ARG:NH2	2.22	0.54
1:A:1093:GLU:HB2	1:A:1100:VAL:HB	1.89	0.54
1:A:1577:THR:HG22	1:A:1749:LEU:HD22	1.89	0.54
1:A:1321:PRO:HD2	1:A:1368:PRO:HB2	1.90	0.54
1:A:1009:ALA:HB1	1:A:1016:LEU:HD11	1.90	0.54
1:A:1591:TYR:CE2	1:A:1627:GLY:HA3	2.43	0.54
1:A:1826:LEU:HB2	1:A:1997:ILE:HG22	1.89	0.54
1:A:1496:ARG:HH11	1:A:1505:ARG:HG3	1.72	0.54
1:A:293:GLY:HA3	1:A:435:TRP:HB2	1.89	0.53
1:A:308:MET:HB3	1:A:412:LEU:HD11	1.90	0.53
1:A:1033:TYR:HB3	1:A:1103:LEU:HB2	1.89	0.53
1:A:1878:ILE:HD12	1:A:1923:ALA:HB1	1.90	0.53
1:A:1357:PRO:HG2	1:A:1400:ARG:HH21	1.73	0.53
1:A:1800:LYS:HZ1	1:A:1802:TYR:HD1	1.57	0.53
1:A:812:LEU:HD21	1:A:853:ILE:HG21	1.90	0.53
1:A:1535:ASP:OD2	1:A:1704:VAL:HG11	2.07	0.53
1:A:2050:ALA:O	1:A:2051:HIS:ND1	2.42	0.53
1:A:1239:LEU:HD12	1:A:1242:GLN:HE21	1.73	0.52
1:A:1309:PRO:HB2	1:A:1312:GLN:HG2	1.92	0.52
1:A:678:ARG:NH1	1:A:702:GLU:OE1	2.42	0.52
1:A:1965:TRP:HZ2	1:A:1987:GLU:HG2	1.74	0.52
1:A:299:PRO:HB2	1:A:304:THR:HG21	1.91	0.51
1:A:482:ARG:HA	1:A:1408:TRP:NE1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ILE:HD11	1:A:986:ARG:HB2	1.92	0.51
1:A:849:THR:O	1:A:853:ILE:HG12	2.10	0.51
1:A:1228:ARG:NH1	1:A:1583:ASN:OD1	2.44	0.51
1:A:1587:ASP:OD2	1:A:1635:TYR:OH	2.22	0.51
1:A:1628:TRP:HZ3	1:A:1741:GLY:HA3	1.76	0.50
1:A:1958:PRO:HA	1:A:1961:ARG:HG2	1.93	0.50
1:A:847:LYS:HE2	1:A:994:SER:OG	2.12	0.50
1:A:313:ARG:HH21	1:A:516:ARG:HH11	1.58	0.50
1:A:1535:ASP:OD2	1:A:1704:VAL:CG1	2.59	0.50
1:A:1835:SER:O	1:A:1839:MET:HG3	2.10	0.50
1:A:407:LEU:HG	1:A:409:LEU:H	1.77	0.50
1:A:883:LEU:HD13	1:A:960:VAL:HG23	1.94	0.49
1:A:1625:LEU:HB3	1:A:1737:MET:SD	2.52	0.49
1:A:1776:VAL:HA	1:A:2006:LEU:HD23	1.94	0.49
1:A:1337:THR:OG1	1:A:1340:SER:HB3	2.12	0.49
1:A:1821:GLU:OE1	1:A:1993:SER:OG	2.29	0.49
1:A:2077:HIS:HA	1:A:2080:GLU:HB2	1.94	0.49
1:A:290:LEU:O	1:A:411:LYS:NZ	2.39	0.49
1:A:500:TRP:H	1:A:500:TRP:CD1	2.30	0.49
1:A:1341:PRO:HG3	3:B:1:NAG:H4	1.95	0.49
1:A:323:ASP:O	1:A:327:VAL:HG13	2.12	0.49
1:A:979:TRP:NE1	1:A:1000:GLU:OE2	2.46	0.49
1:A:873:ARG:HH21	1:A:874:SER:HG	1.57	0.49
1:A:678:ARG:NH2	1:A:702:GLU:OE2	2.46	0.49
1:A:1440:TRP:HB2	1:A:1455:LEU:HD13	1.94	0.49
1:A:1857:SER:HB3	1:A:1860:ARG:HB3	1.95	0.49
1:A:1492:ASN:O	1:A:1496:ARG:HG2	2.13	0.48
1:A:1312:GLN:O	1:A:1316:HIS:ND1	2.41	0.48
1:A:1243:ILE:HG23	1:A:1594:PRO:HG3	1.94	0.48
1:A:1574:LEU:HD21	1:A:1579:TYR:HB2	1.96	0.48
1:A:456:ASP:HB2	1:A:461:HIS:CE1	2.48	0.48
1:A:1961:ARG:O	1:A:1965:TRP:HD1	1.96	0.48
1:A:446:SER:HB2	1:A:453:PRO:HB3	1.95	0.48
1:A:1591:TYR:O	1:A:1594:PRO:HD2	2.13	0.48
1:A:886:CYS:HB2	1:A:953:ALA:HB2	1.95	0.48
1:A:1085:TRP:CD1	1:A:1116:LEU:HA	2.49	0.47
1:A:1968:LEU:HD22	1:A:1978:VAL:HG21	1.96	0.47
1:A:2048:ARG:HD3	1:A:2058:GLN:HB2	1.96	0.47
1:A:88:GLY:O	1:A:1472:LYS:NZ	2.47	0.47
1:A:105:LEU:HD23	1:A:199:SER:HB3	1.96	0.47
1:A:1930:ASN:HA	1:A:1933:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:HIS:CD2	1:A:279:LEU:HB2	2.50	0.47
1:A:1037:LEU:N	1:A:1099:LEU:O	2.46	0.47
1:A:1569:GLN:HB3	1:A:1574:LEU:HD23	1.97	0.47
1:A:1356:LEU:HB3	1:A:1357:PRO:HD3	1.96	0.47
1:A:542:PHE:CE2	1:A:546:LEU:HD11	2.50	0.47
1:A:954:PHE:CE1	1:A:961:VAL:HG21	2.50	0.47
1:A:1036:THR:N	1:A:1133:GLY:O	2.45	0.47
1:A:1625:LEU:HD12	1:A:1734:LEU:HG	1.97	0.47
1:A:758:GLN:OE1	6:A:2226:AGS:N6	2.47	0.46
1:A:1029:LEU:HD22	1:A:1137:THR:HG21	1.96	0.46
1:A:1239:LEU:HA	1:A:1242:GLN:HE21	1.80	0.46
1:A:1496:ARG:NH1	1:A:1505:ARG:HG3	2.31	0.46
1:A:57:PRO:HG3	1:A:82:PHE:HE2	1.81	0.46
1:A:499:VAL:HG23	1:A:500:TRP:HD1	1.80	0.46
1:A:2005:CYS:SG	1:A:2006:LEU:N	2.89	0.46
1:A:965:GLU:HB3	1:A:968:ALA:HB2	1.98	0.46
1:A:287:LEU:O	1:A:290:LEU:HG	2.16	0.46
1:A:325:ARG:HG3	1:A:397:VAL:HG13	1.97	0.46
1:A:324:VAL:O	1:A:327:VAL:HG22	2.16	0.46
1:A:428:LEU:O	1:A:432:HIS:N	2.49	0.46
1:A:310:GLN:CD	1:A:313:ARG:HH12	2.24	0.46
1:A:1265:HIS:O	1:A:1267:PRO:HD3	2.16	0.45
1:A:20:ARG:NH1	1:A:895:MET:O	2.49	0.45
1:A:1142:ILE:O	1:A:1146:VAL:HG12	2.17	0.45
1:A:1727:TRP:HA	1:A:1731:GLY:HA3	1.99	0.45
1:A:1032:GLY:O	1:A:1137:THR:OG1	2.35	0.45
1:A:1139:LEU:HD23	1:A:1139:LEU:H	1.81	0.45
1:A:1921:ARG:HB3	1:A:1926:TYR:HE1	1.81	0.45
1:A:686:ARG:HG3	1:A:699:PHE:CE2	2.51	0.45
1:A:967:THR:HB	1:A:975:ARG:HD3	1.99	0.45
1:A:2023:THR:HG22	1:A:2056:ARG:HG2	1.98	0.45
1:A:2044:GLY:HA3	1:A:2060:PRO:HD3	1.98	0.45
1:A:298:ALA:HB3	1:A:299:PRO:HD3	1.99	0.45
1:A:840:LEU:HD13	1:A:1001:ALA:HB2	1.97	0.45
1:A:1567:HIS:O	1:A:1571:MET:HG2	2.16	0.45
1:A:1499:LEU:HD23	1:A:1505:ARG:HA	1.98	0.45
1:A:1625:LEU:O	1:A:1737:MET:HE1	2.17	0.45
1:A:2074:LEU:HD13	1:A:2086:PHE:CD1	2.52	0.45
1:A:574:GLU:HG3	1:A:575:THR:HG23	1.98	0.45
1:A:53:GLU:N	1:A:536:CYS:SG	2.90	0.44
1:A:465:LYS:HE2	1:A:1513:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:SER:OG	1:A:810:ARG:NH1	2.49	0.44
1:A:1347:CYS:SG	1:A:1359:CYS:N	2.70	0.44
1:A:1366:PRO:HB2	1:A:1367:PRO:HD3	1.98	0.44
1:A:1898:PRO:O	1:A:1902:VAL:HG23	2.18	0.44
1:A:323:ASP:O	1:A:326:GLU:HG3	2.16	0.44
1:A:1282:PHE:HD2	1:A:1416:GLY:HA3	1.81	0.44
1:A:489:ALA:O	1:A:1477:ASN:ND2	2.50	0.44
1:A:1090:ARG:HA	1:A:1090:ARG:HD2	1.90	0.44
1:A:2058:GLN:OE1	1:A:2058:GLN:HA	2.17	0.44
1:A:560:TYR:O	1:A:563:THR:OG1	2.29	0.44
1:A:1883:THR:OG1	1:A:1886:GLU:HG2	2.17	0.44
1:A:1035:LEU:O	1:A:1101:LEU:N	2.36	0.43
1:A:1588:MET:O	1:A:1592:LEU:HG	2.18	0.43
1:A:1890:LEU:O	1:A:1894:LEU:HG	2.17	0.43
1:A:1918:TYR:O	1:A:1926:TYR:OH	2.25	0.43
1:A:16:MET:HE1	1:A:19:ARG:CZ	2.48	0.43
1:A:2060:PRO:HA	1:A:2061:PRO:HD3	1.83	0.43
1:A:328:TRP:CD1	1:A:397:VAL:HG21	2.53	0.43
1:A:335:ILE:O	1:A:339:MET:HG3	2.18	0.43
1:A:1037:LEU:HD12	1:A:1129:LEU:HD13	2.00	0.43
1:A:1961:ARG:O	1:A:1965:TRP:CD1	2.71	0.43
1:A:281:ARG:HB3	1:A:285:ARG:HH21	1.84	0.43
1:A:743:LEU:HD23	1:A:743:LEU:HA	1.83	0.43
1:A:1610:TYR:HD1	1:A:1619:LEU:HD22	1.84	0.43
1:A:304:THR:O	1:A:308:MET:HG2	2.19	0.43
1:A:1666:THR:HG23	1:A:1685:LYS:HE2	2.00	0.43
1:A:313:ARG:HH21	1:A:516:ARG:NH1	2.16	0.43
1:A:891:VAL:C	1:A:892:LEU:HD12	2.43	0.43
1:A:1821:GLU:HB2	1:A:1993:SER:OG	2.19	0.43
1:A:1953:THR:HA	1:A:1956:MET:HE3	2.00	0.43
1:A:998:LEU:HD11	1:A:1143:PHE:CG	2.54	0.43
1:A:1813:LEU:HD11	1:A:2003:PHE:CZ	2.54	0.43
1:A:209:ARG:HA	1:A:209:ARG:HD3	1.86	0.42
1:A:1679:GLU:HG3	1:A:1682:ARG:HH21	1.84	0.42
1:A:1938:LEU:HD23	1:A:1938:LEU:HA	1.88	0.42
1:A:1681:SER:O	1:A:1685:LYS:HG3	2.19	0.42
1:A:1349:ARG:CZ	1:A:1351:GLY:HA2	2.50	0.42
1:A:1387:LEU:O	1:A:1391:LEU:HG	2.19	0.42
1:A:1035:LEU:HD13	1:A:1134:ILE:HD13	2.02	0.42
1:A:1272:SER:O	1:A:1275:MET:HG2	2.18	0.42
1:A:1979:MET:HE3	1:A:1979:MET:HB2	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.89	0.42
1:A:507:GLN:OE1	1:A:1484:VAL:HG13	2.19	0.42
1:A:2047:LEU:C	1:A:2048:ARG:HD2	2.44	0.42
1:A:1327:VAL:HG13	1:A:1363:ALA:HB2	2.02	0.42
1:A:1991:LEU:HD12	1:A:1992:CYS:N	2.34	0.42
1:A:16:MET:HE2	1:A:16:MET:HA	2.01	0.41
1:A:1104:PRO:O	1:A:1108:ALA:HB2	2.20	0.41
1:A:1436:VAL:HG13	1:A:1455:LEU:HD22	2.02	0.41
1:A:566:VAL:HG23	1:A:647:SER:OG	2.20	0.41
1:A:814:LYS:HD2	1:A:853:ILE:HD11	2.02	0.41
1:A:1082:VAL:HG21	1:A:1101:LEU:HD13	2.02	0.41
1:A:1242:GLN:HG3	1:A:1243:ILE:HG12	2.03	0.41
1:A:1997:ILE:HG12	1:A:2005:CYS:SG	2.60	0.41
1:A:711:GLY:HA3	1:A:1353:ARG:HD2	2.02	0.41
1:A:1260:VAL:HA	1:A:1261:PRO:HD3	1.91	0.41
1:A:1811:ASP:HB2	1:A:1812:ARG:NH1	2.34	0.41
1:A:1929:GLY:O	1:A:1933:LYS:HG2	2.20	0.41
1:A:98:ASN:HD22	4:A:2202:NAG:H62	1.84	0.41
1:A:751:LEU:O	1:A:754:VAL:HG12	2.20	0.41
1:A:851:LEU:HD22	1:A:962:ILE:HG23	2.02	0.41
1:A:1630:ILE:HA	1:A:1633:LEU:HD23	2.01	0.41
1:A:1702:ASP:HB3	1:A:1705:ARG:HH21	1.85	0.41
1:A:609:LEU:HD23	1:A:609:LEU:HA	1.85	0.41
1:A:987:GLU:OE1	1:A:987:GLU:HA	2.20	0.41
1:A:1686:GLN:HA	1:A:1689:LEU:HD23	2.03	0.41
1:A:1628:TRP:CZ3	1:A:1741:GLY:HA3	2.56	0.41
1:A:1891:LEU:HD13	1:A:1894:LEU:HD12	2.01	0.41
1:A:1885:ARG:HG2	1:A:1919:ALA:O	2.21	0.41
1:A:197:LEU:HD23	1:A:197:LEU:HA	1.94	0.41
1:A:463:ARG:HG2	1:A:1511:THR:HB	2.03	0.41
1:A:1094:GLU:N	1:A:1094:GLU:OE1	2.54	0.41
1:A:1037:LEU:O	1:A:1099:LEU:N	2.51	0.41
1:A:1536:VAL:HG21	1:A:1667:PHE:CE2	2.56	0.40
1:A:1988:CYS:HB3	1:A:1995:LEU:HD11	2.03	0.40
1:A:278:PRO:HA	1:A:281:ARG:HB2	2.02	0.40
1:A:1563:THR:HG22	1:A:1564:ARG:H	1.86	0.40
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.91	0.40
1:A:1726:ARG:HB3	1:A:1728:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	1484/1764 (84%)	1483 (100%)	1 (0%)	88 89

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

Mol	Chain	Res	Type
1	A	923	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	A	432	HIS
1	A	461	HIS
1	A	842	HIS
1	A	882	HIS
1	A	920	GLN
1	A	1028	HIS
1	A	1220	GLN
1	A	1242	GLN
1	A	1477	ASN
1	A	1481	HIS
1	A	1567	HIS
1	A	1607	GLN
1	A	1733	ASN
1	A	1740	GLN
1	A	2020	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 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	$\# Z > 2$
3	NAG	B	1	3,1	14,14,15	0.32	0	17,19,21	0.69	0
3	NAG	B	2	3	14,14,15	0.31	0	17,19,21	0.80	0
3	BMA	B	3	3	11,11,12	0.49	0	15,15,17	0.73	0
3	BMA	B	4	3	11,11,12	0.55	0	15,15,17	0.78	0
2	NAG	C	1	1,2	14,14,15	0.29	0	17,19,21	0.72	1 (5%)
2	NAG	C	2	2	14,14,15	0.32	0	17,19,21	0.60	0
2	BMA	C	3	2	11,11,12	0.57	0	15,15,17	0.72	0
2	NAG	D	1	1,2	14,14,15	0.29	0	17,19,21	0.55	0
2	NAG	D	2	2	14,14,15	0.33	0	17,19,21	0.61	0
2	BMA	D	3	2	11,11,12	0.55	0	15,15,17	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	B	2	3	-	3/6/23/26	0/1/1/1
3	BMA	B	3	3	-	2/2/19/22	0/1/1/1
3	BMA	B	4	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

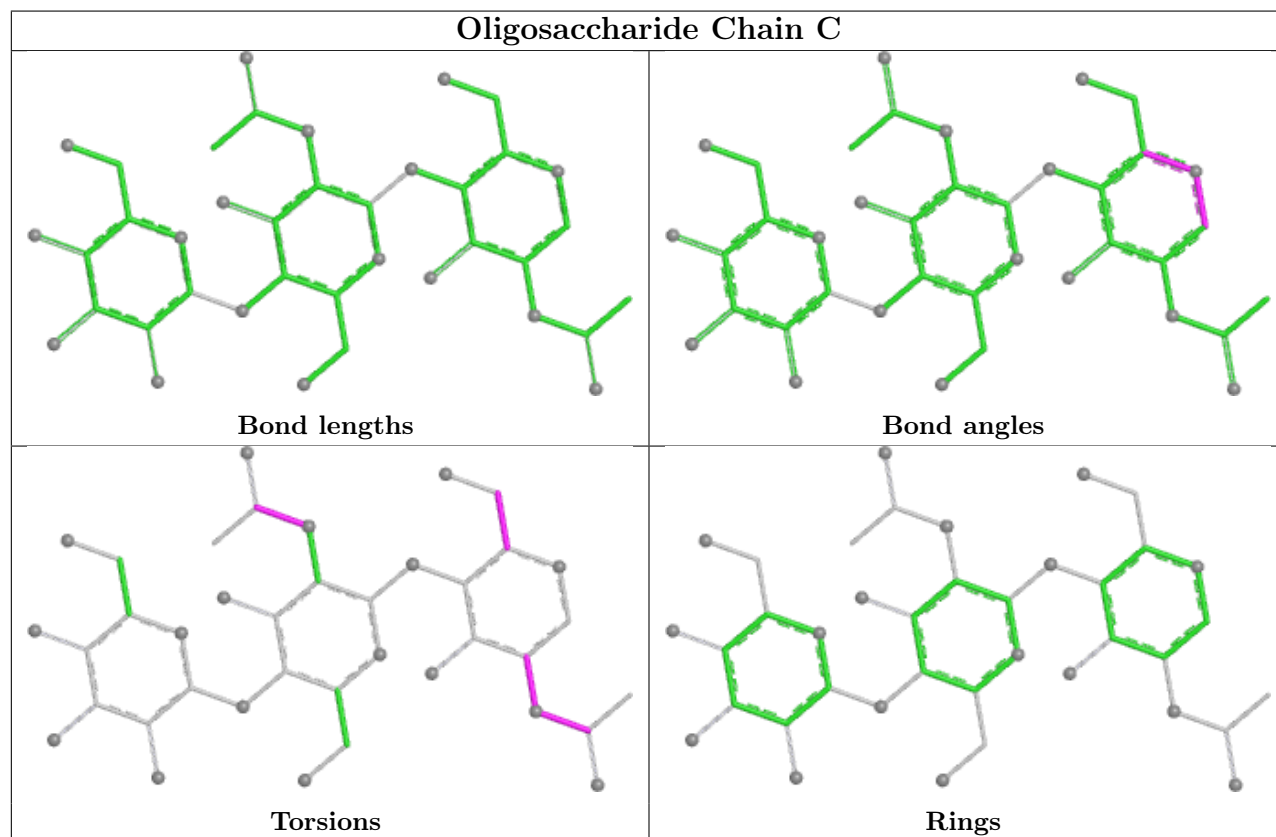
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
3	B	1	NAG	C3-C2-N2-C7
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
3	B	2	NAG	C1-C2-N2-C7
3	B	2	NAG	C8-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
3	B	3	BMA	O5-C5-C6-O6
3	B	4	BMA	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
3	B	4	BMA	C4-C5-C6-O6
3	B	3	BMA	C4-C5-C6-O6
2	D	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7

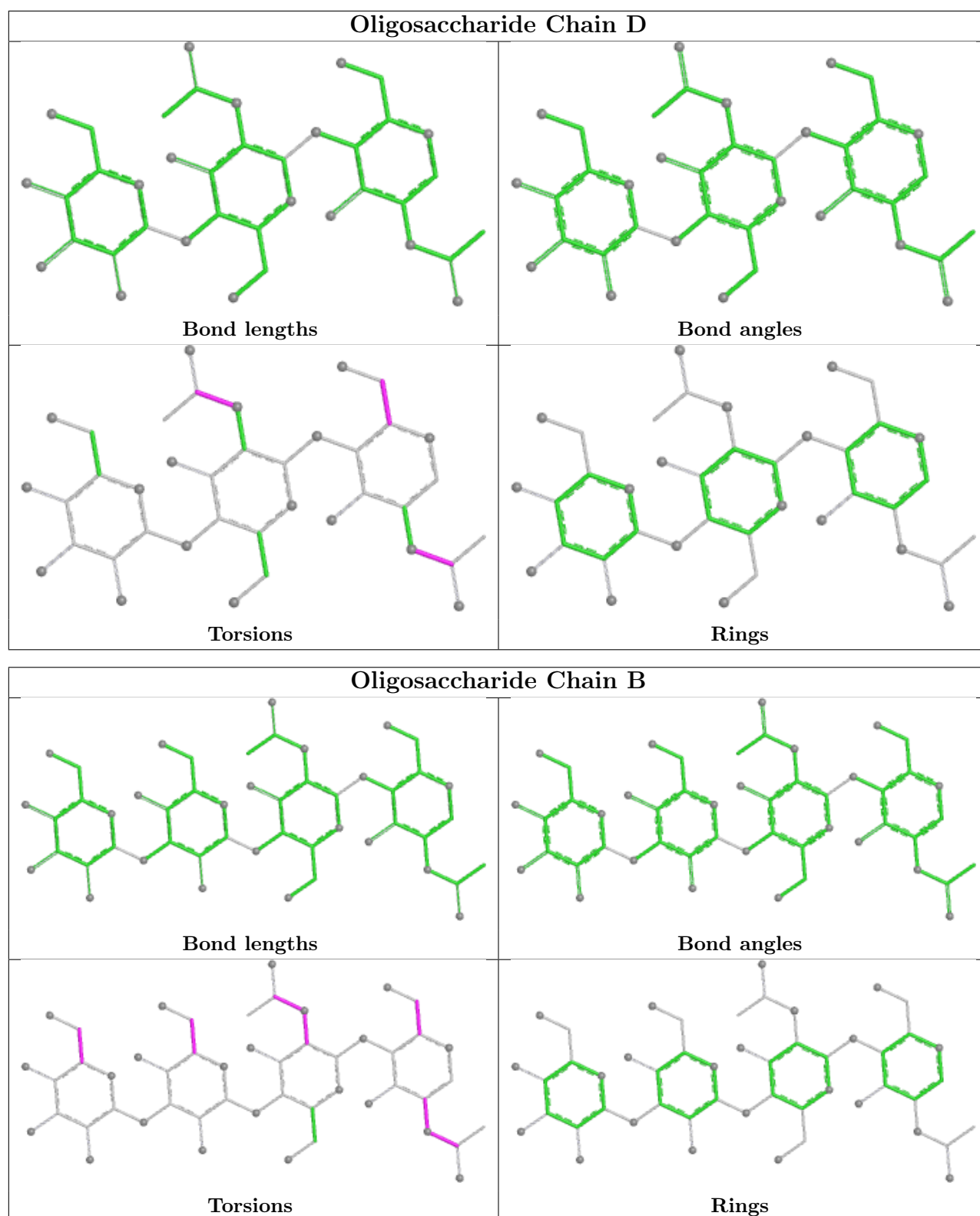
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	NAG	2	0
3	B	2	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 27 ligands modelled in this entry, 20 are unknown - leaving 7 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	$\# Z > 2$
4	NAG	A	2203	1	14,14,15	0.30	0	17,19,21	0.59	0
6	AGS	A	2226	-	32,33,33	0.66	1 (3%)	45,52,52	0.55	0
4	NAG	A	2204	1	14,14,15	0.31	0	17,19,21	0.56	0
4	NAG	A	2202	1	14,14,15	0.37	0	17,19,21	1.54	2 (11%)
4	NAG	A	2201	1	14,14,15	0.37	0	17,19,21	0.68	0
6	AGS	A	2227	-	32,33,33	0.67	1 (3%)	45,52,52	0.60	0
4	NAG	A	2205	1	14,14,15	0.37	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
4	NAG	A	2203	1	-	1/6/23/26	0/1/1/1
6	AGS	A	2226	-	-	6/21/38/38	0/3/3/3
4	NAG	A	2204	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2202	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2201	1	-	1/6/23/26	0/1/1/1
6	AGS	A	2227	-	-	4/21/38/38	0/3/3/3
4	NAG	A	2205	1	-	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)
6	A	2227	AGS	PG-S1G	2.17	1.95	1.90
6	A	2226	AGS	PG-S1G	2.09	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2202	NAG	C1-O5-C5	5.29	119.28	112.19
4	A	2202	NAG	C4-C3-C2	-2.21	107.78	111.02

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2202	NAG	C8-C7-N2-C2
4	A	2202	NAG	O7-C7-N2-C2
4	A	2204	NAG	C8-C7-N2-C2
4	A	2204	NAG	O7-C7-N2-C2
6	A	2226	AGS	C5'-O5'-PA-O1A
6	A	2226	AGS	C5'-O5'-PA-O3A
6	A	2226	AGS	C4'-C5'-O5'-PA
6	A	2227	AGS	C4'-C5'-O5'-PA
4	A	2205	NAG	C8-C7-N2-C2
4	A	2205	NAG	O7-C7-N2-C2
4	A	2202	NAG	O5-C5-C6-O6
4	A	2202	NAG	C4-C5-C6-O6
6	A	2226	AGS	C2'-C1'-N9-C8
6	A	2227	AGS	C2'-C1'-N9-C8
6	A	2227	AGS	O4'-C1'-N9-C8
6	A	2227	AGS	O4'-C1'-N9-C4
6	A	2226	AGS	C2'-C1'-N9-C4
4	A	2203	NAG	C1-C2-N2-C7
4	A	2201	NAG	C8-C7-N2-C2
6	A	2226	AGS	O4'-C1'-N9-C8

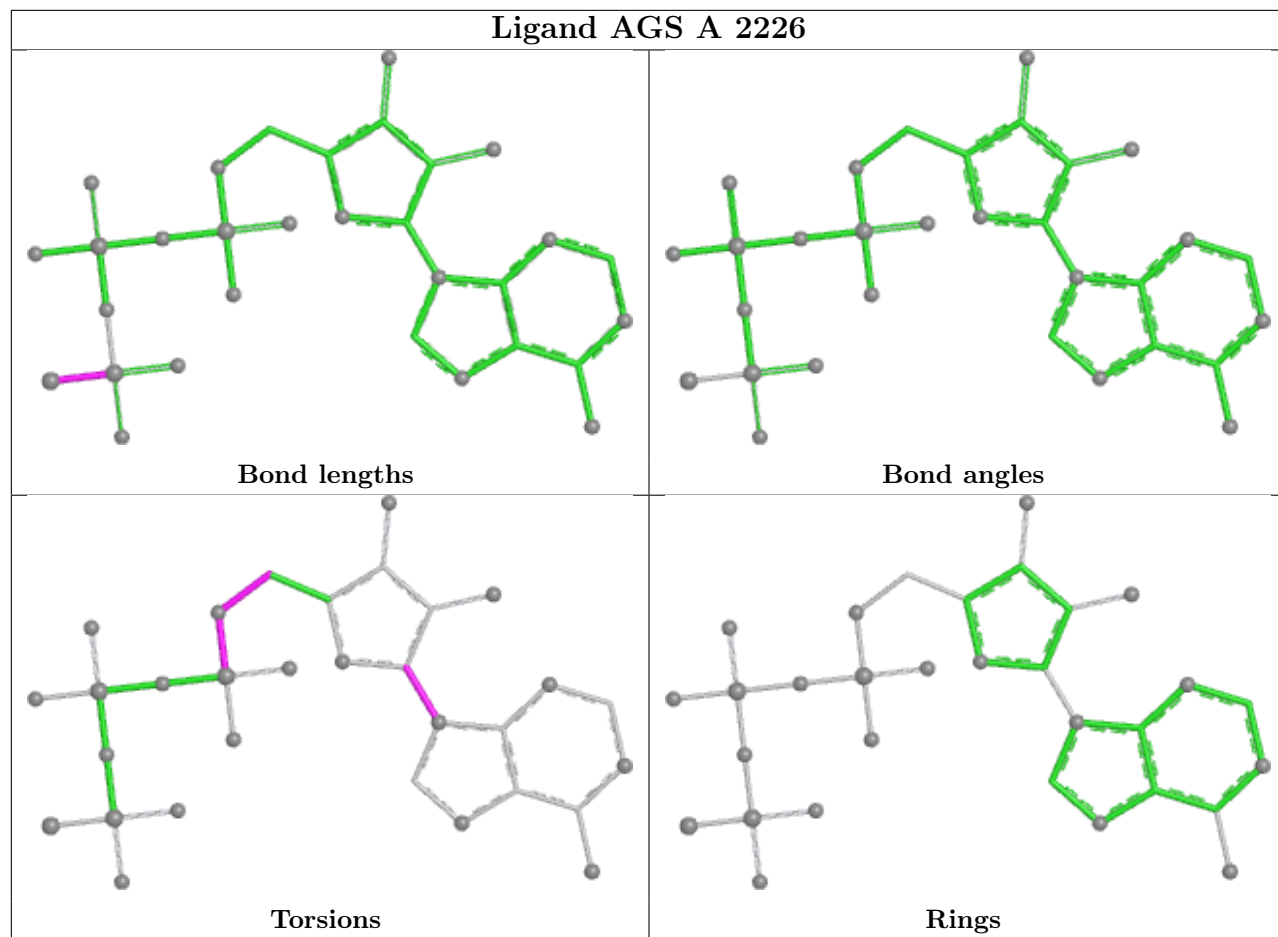
There are no ring outliers.

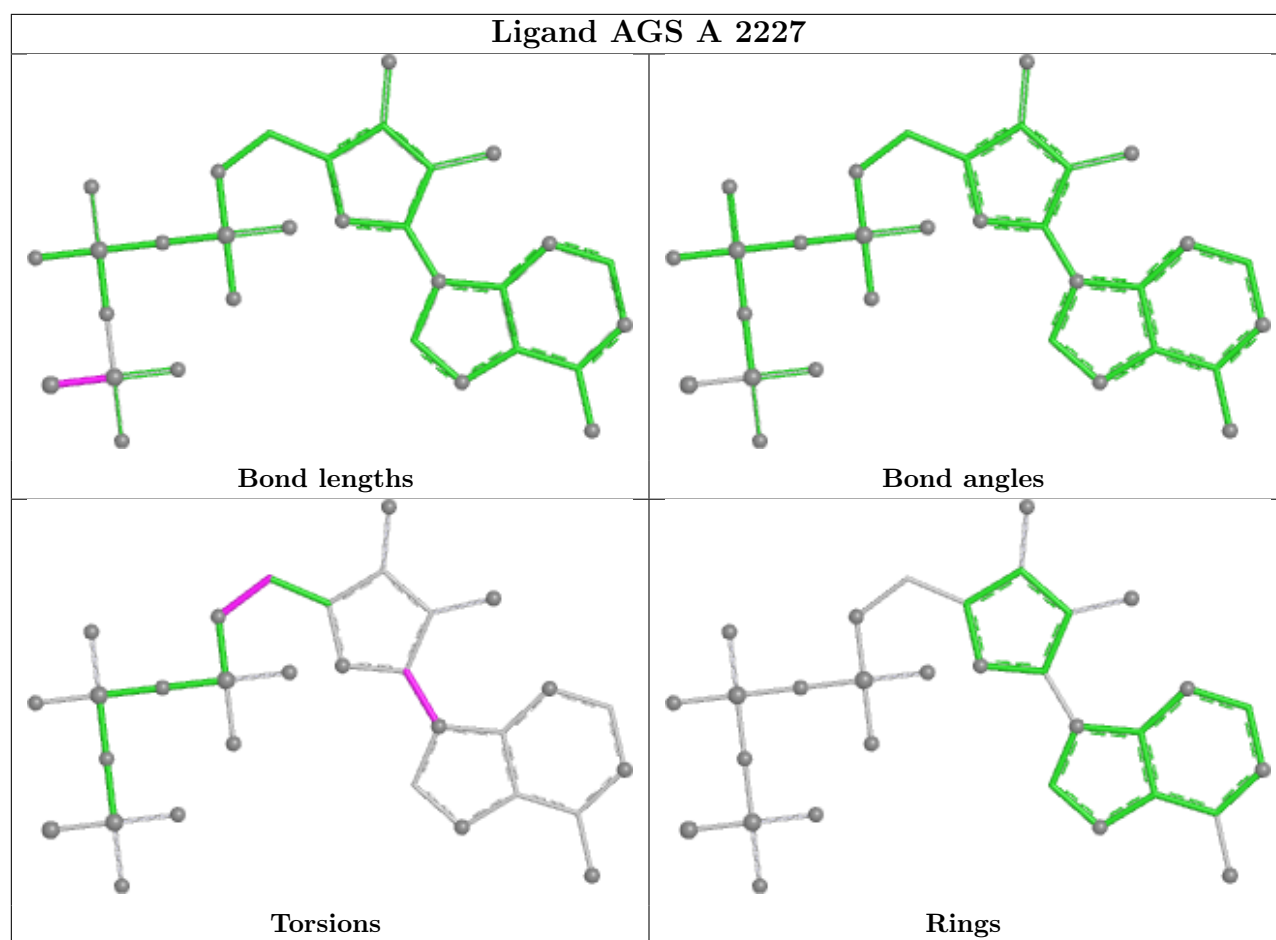
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2226	AGS	1	0
4	A	2202	NAG	1	0
6	A	2227	AGS	2	0

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

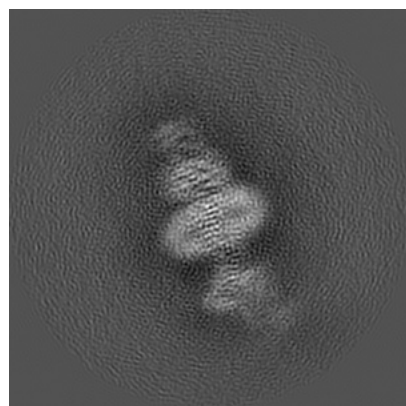
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28047. These allow visual inspection of the internal detail of the map and identification of artifacts.

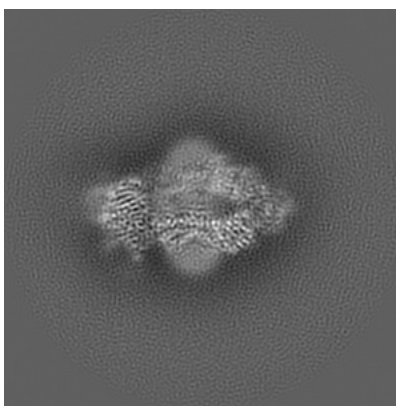
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

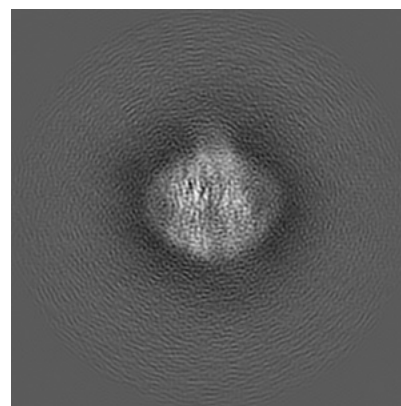
6.1.1 Primary map



X

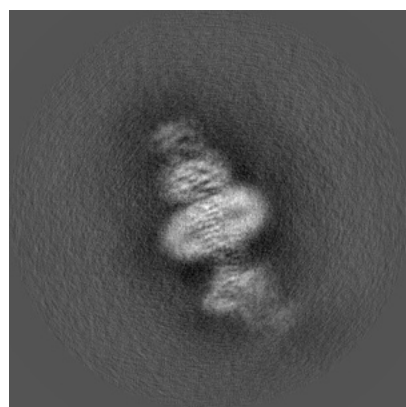


Y

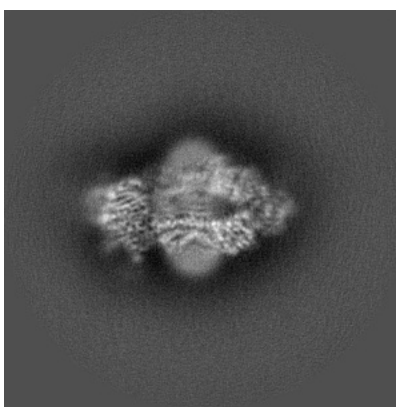


Z

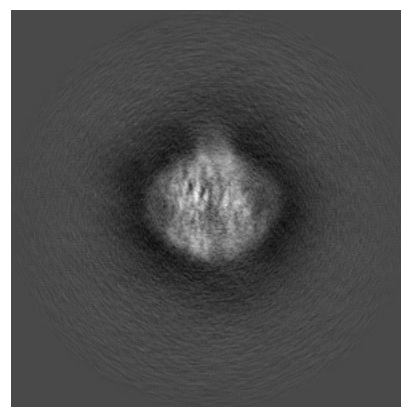
6.1.2 Raw map



X



Y

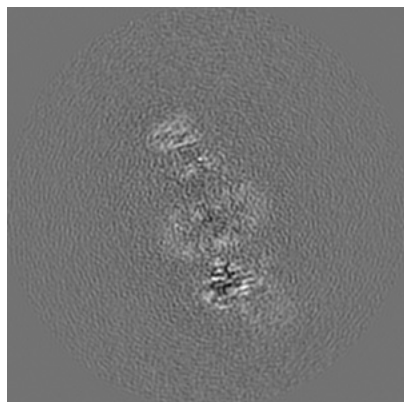


Z

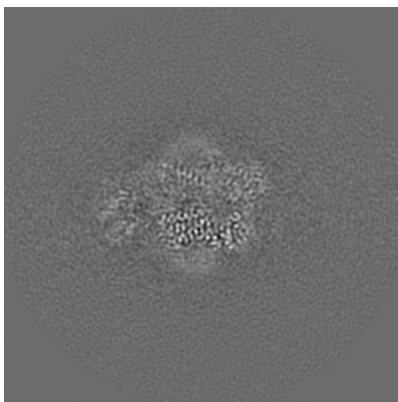
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

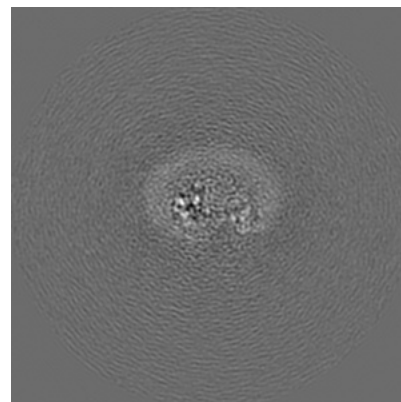
6.2.1 Primary map



X Index: 192



Y Index: 192

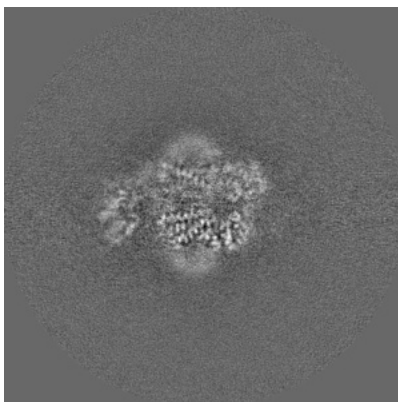


Z Index: 192

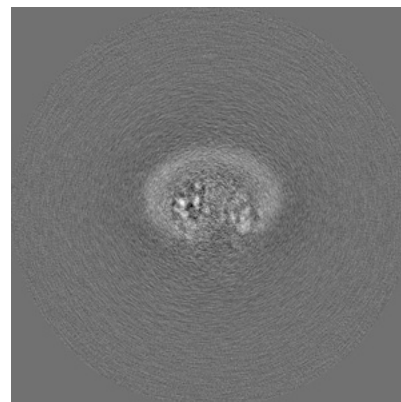
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

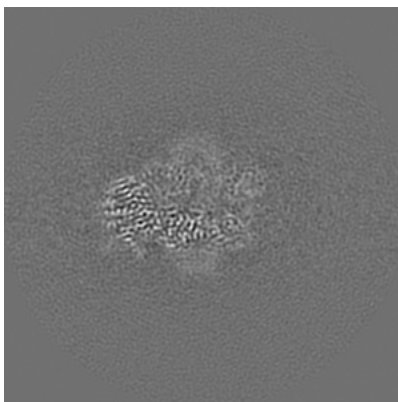
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

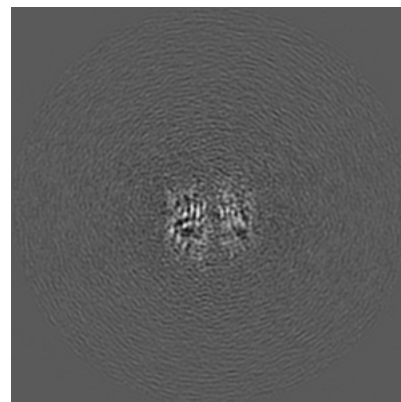
6.3.1 Primary map



X Index: 177

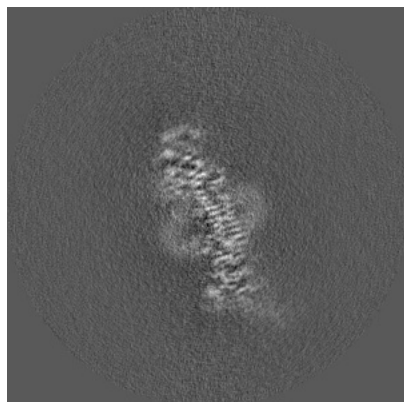


Y Index: 203

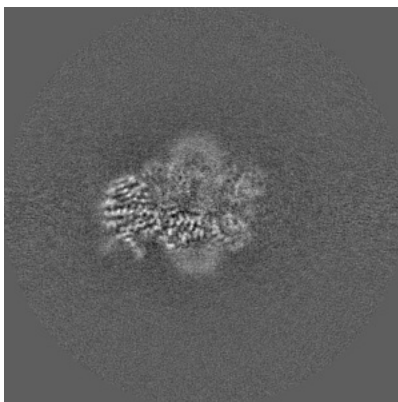


Z Index: 222

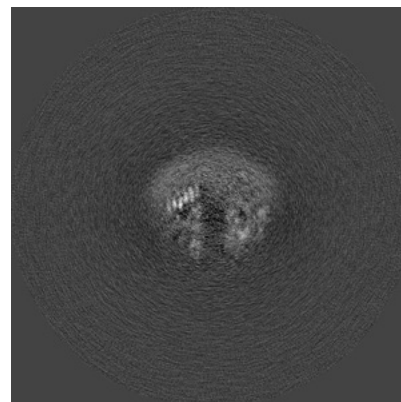
6.3.2 Raw map



X Index: 178



Y Index: 203

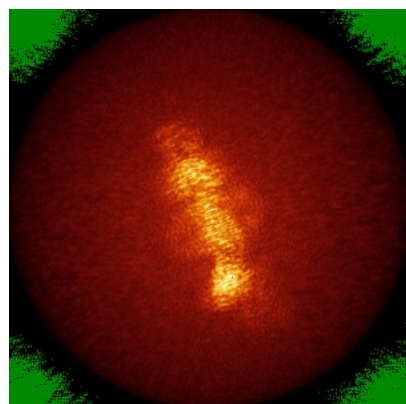


Z Index: 202

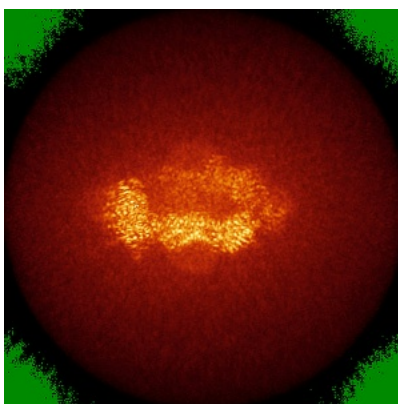
The images above show the largest variance slices of the map in three orthogonal directions.

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

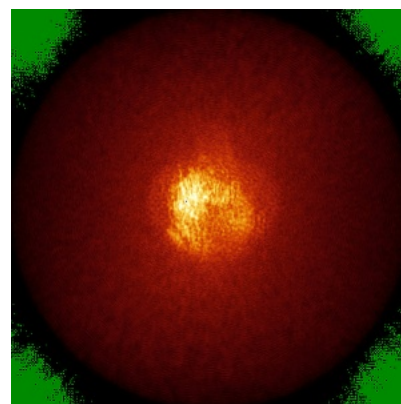
6.4.1 Primary map



X

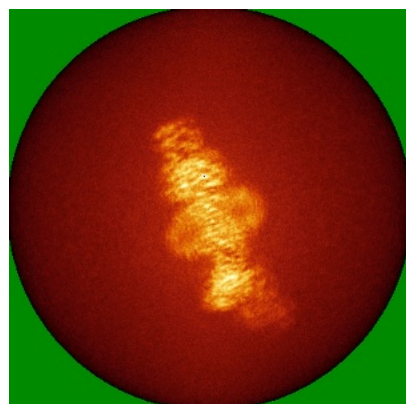


Y

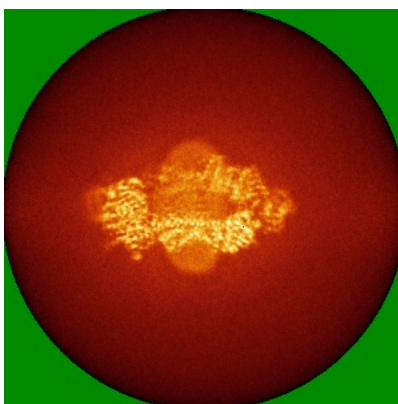


Z

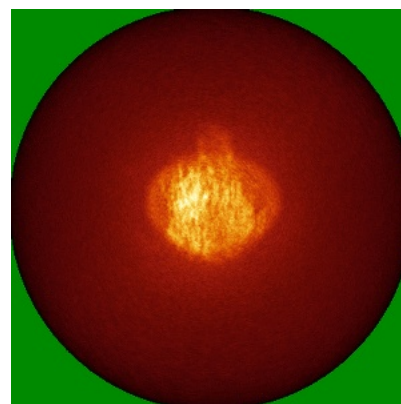
6.4.2 Raw map



X



Y

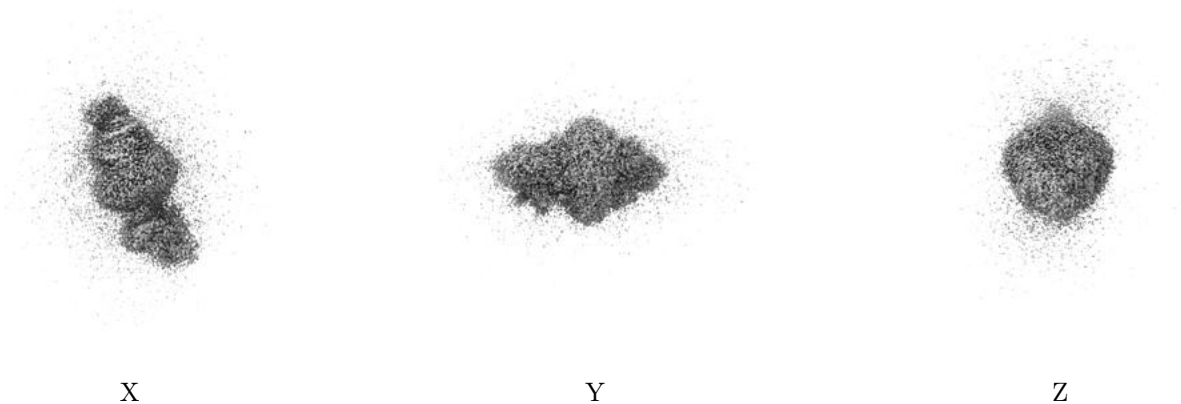


Z

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.

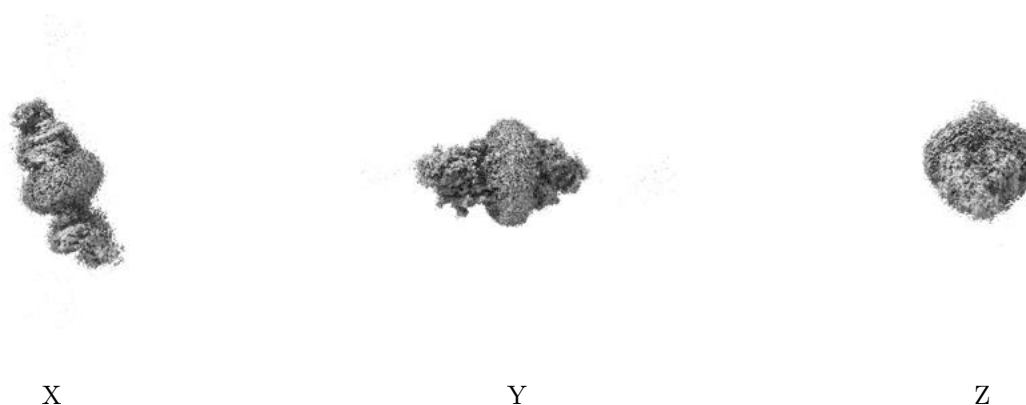
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

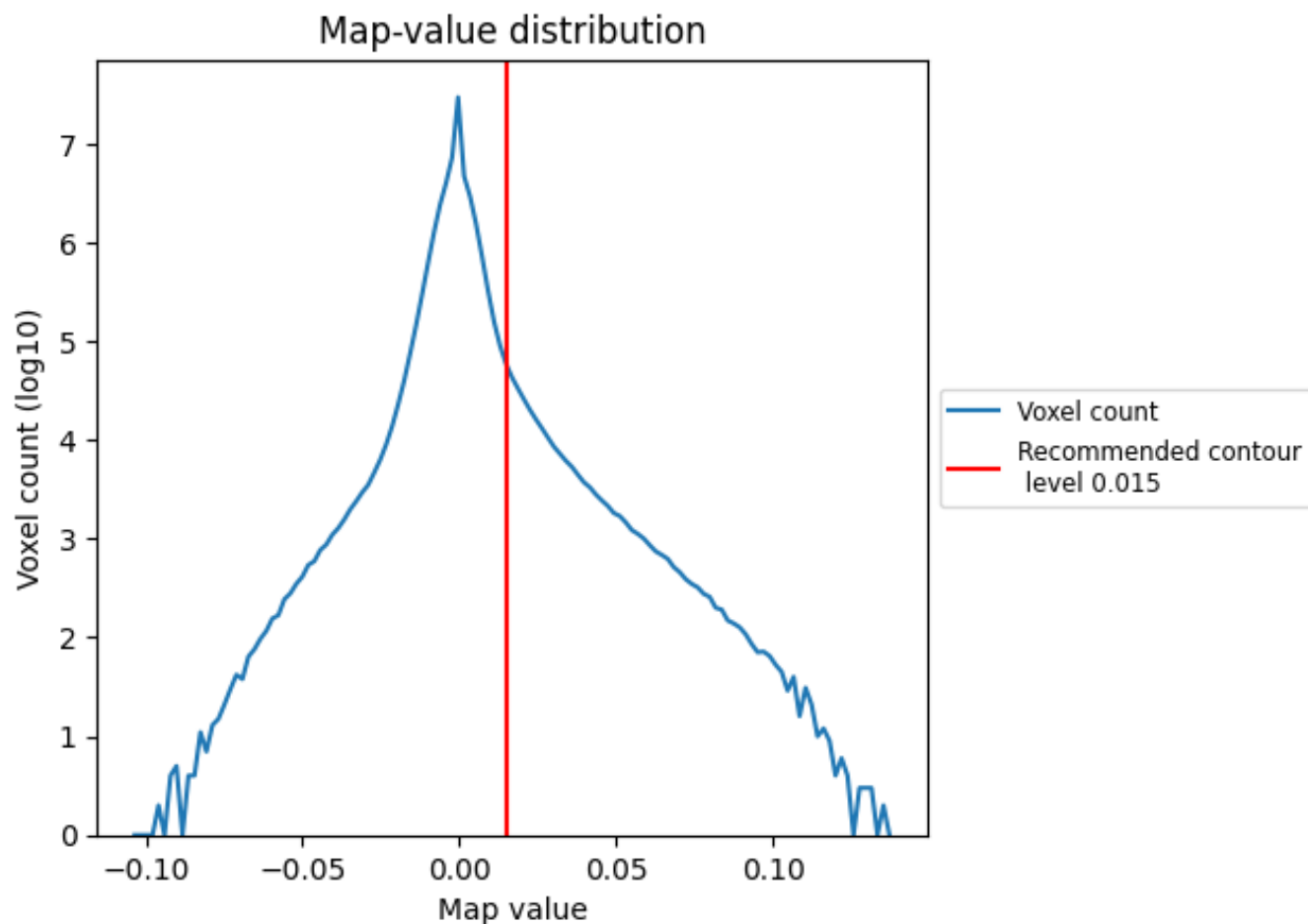
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

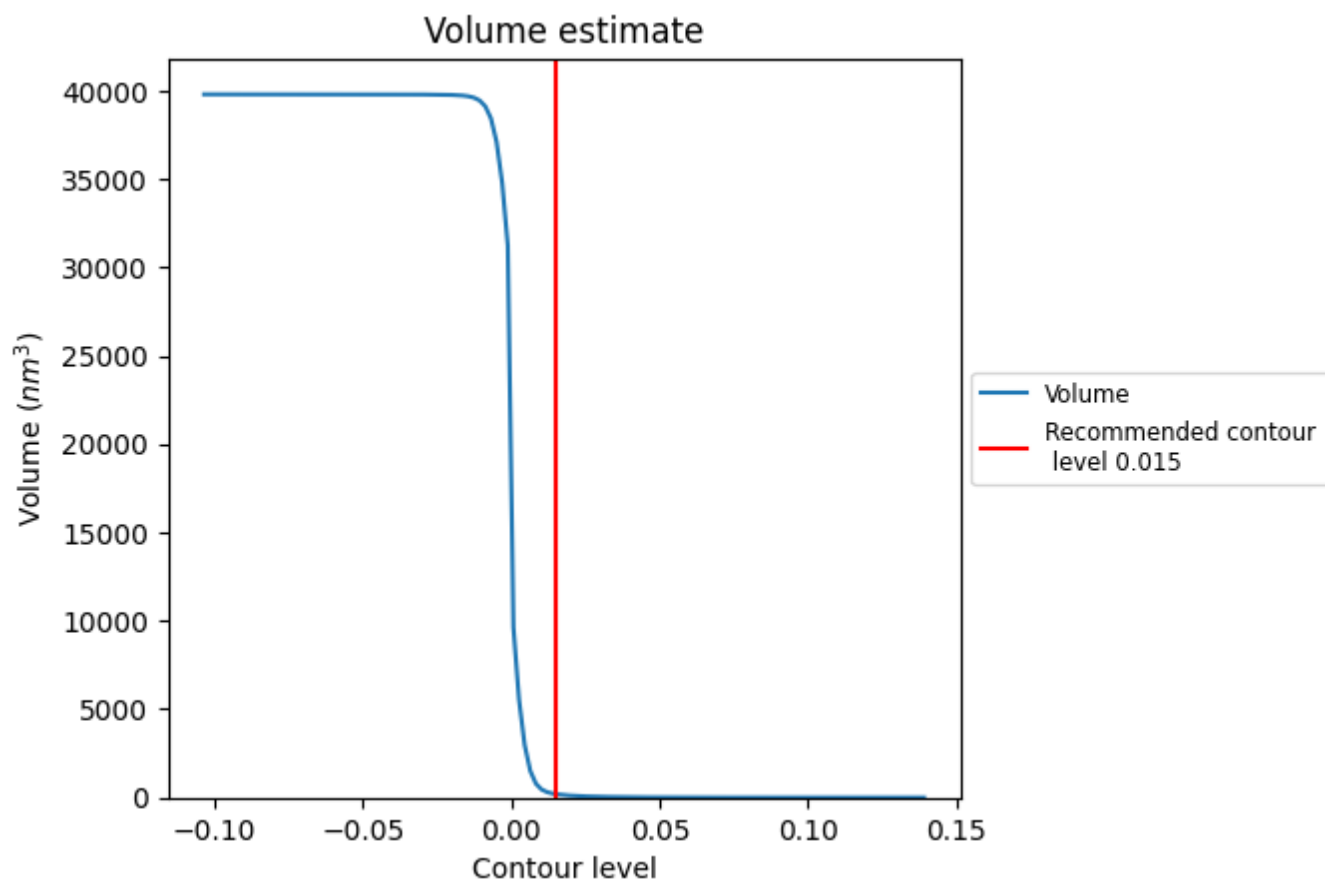
This section contains the results of statistical analysis of the map.

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.

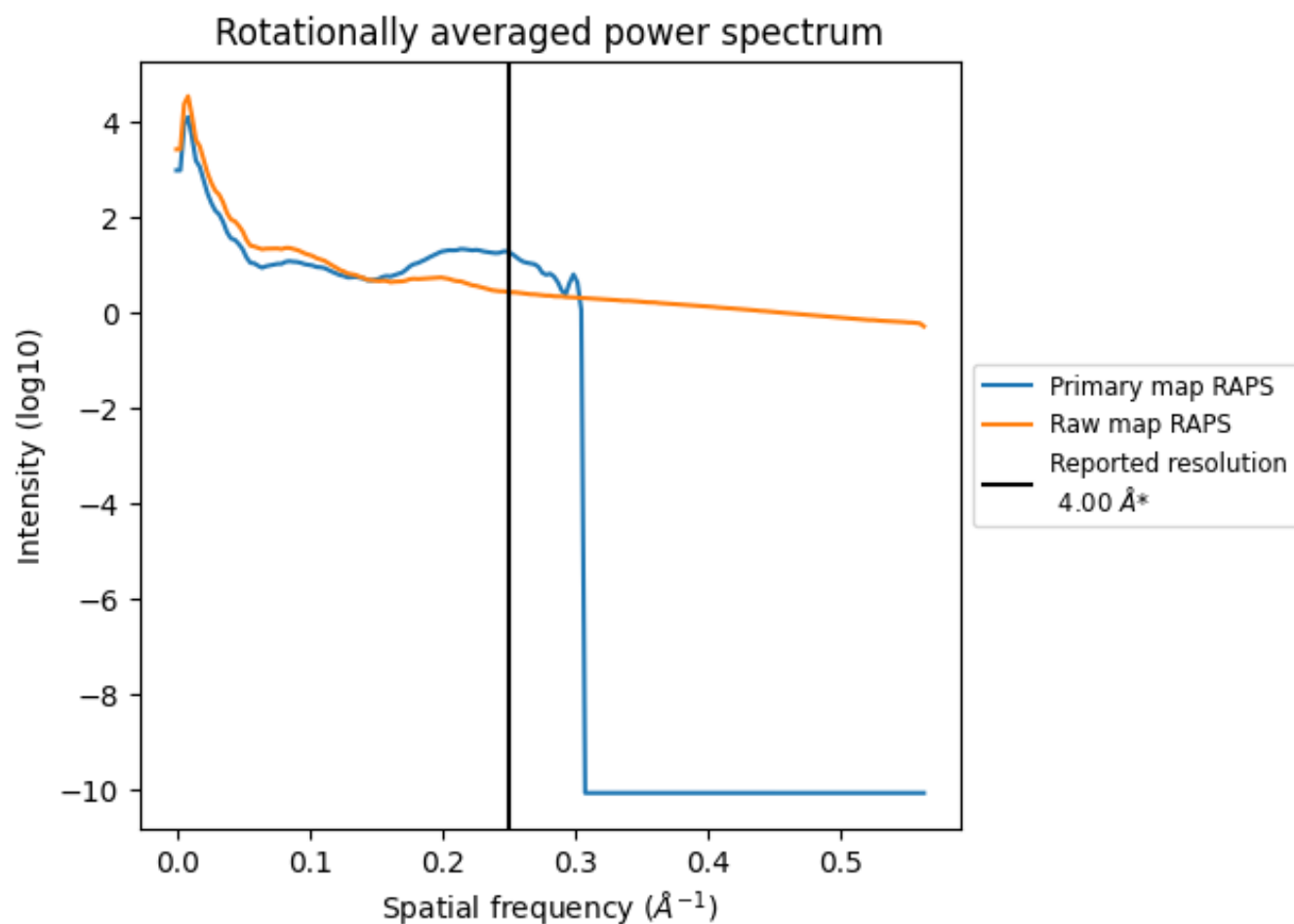
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm³; this corresponds to an approximate mass of 180 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 ⓘ

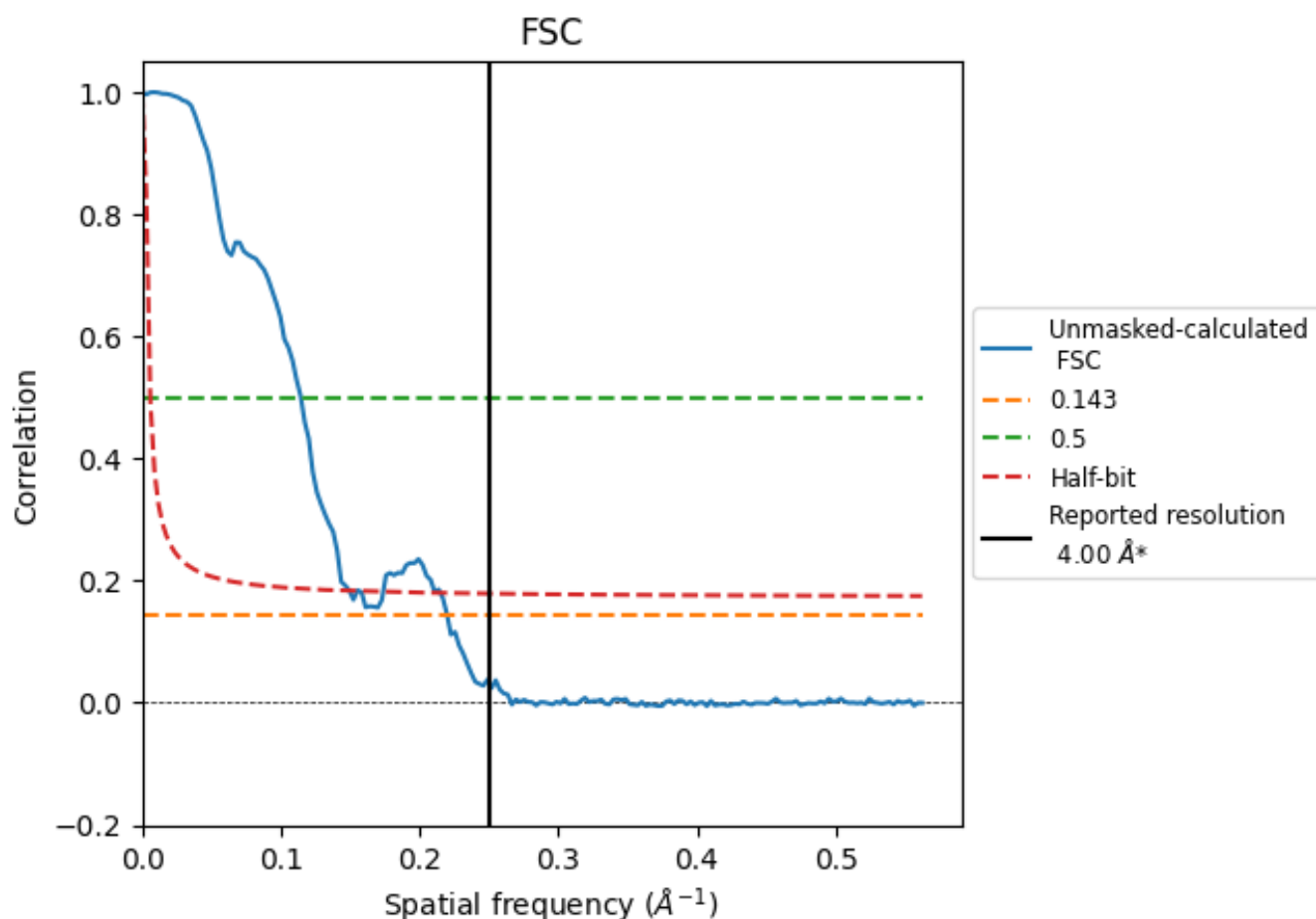


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.55	8.74	6.69

*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 4.55 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-28047 and PDB model 8EE6. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

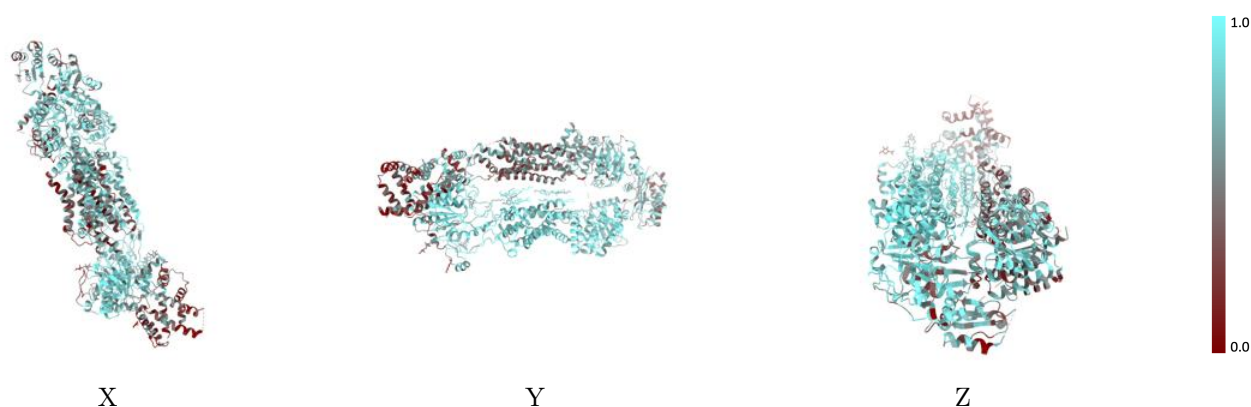
This section was not generated.

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



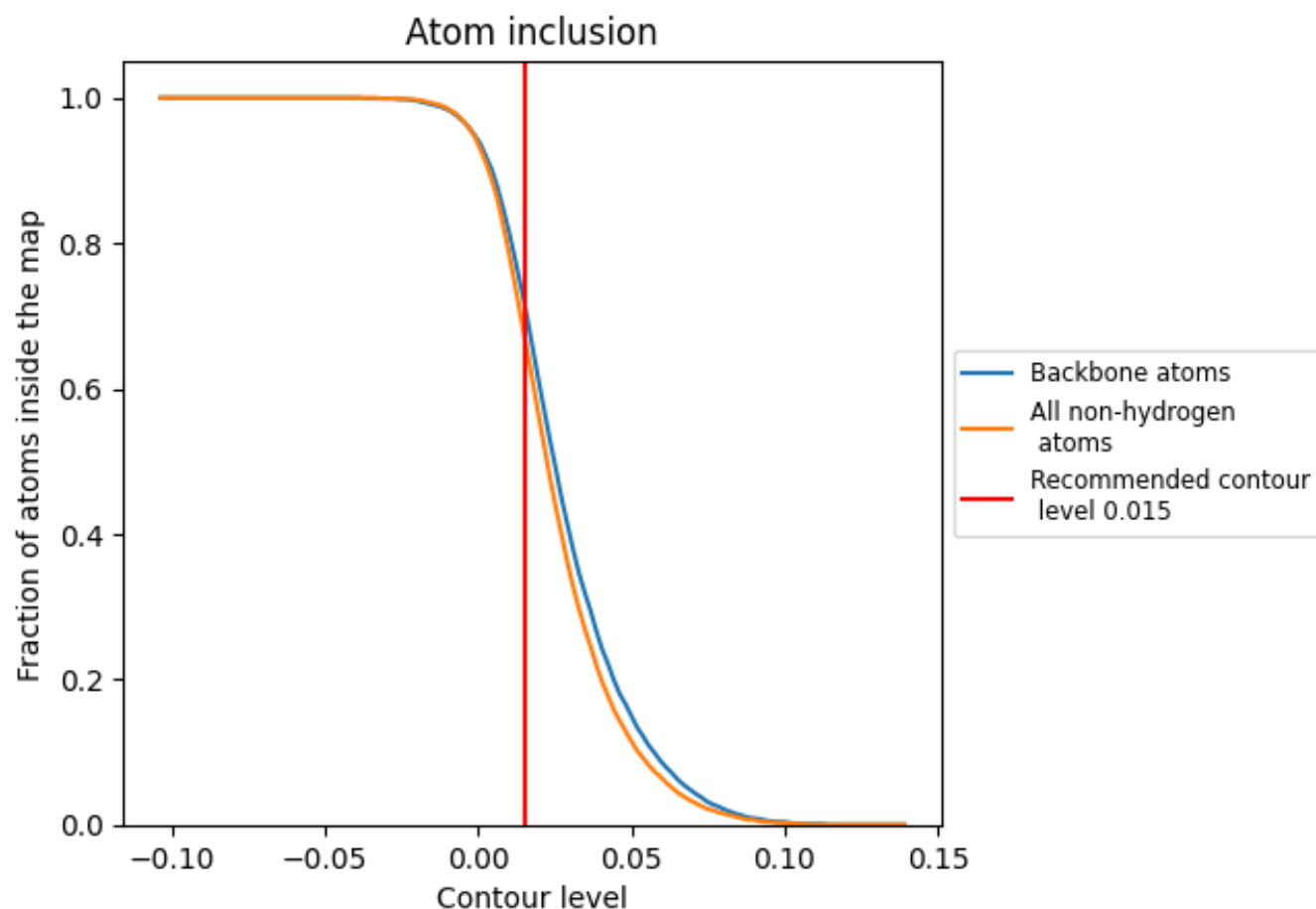
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6750	0.3140
A	0.6760	0.3140
B	0.6600	0.2780
C	0.5380	0.1840
D	0.5380	0.2520

