wwPDB EM Validation Summary Report

Dec 31, 2024 – 11:46 PM EST

PDB ID	:	8RF0
EMDB ID	:	EMD-19114
Title	:	WT-CGS sample in nanodisc
Authors	:	Sedzicki, J.; Ni, D.; Lehmann, F.; Stahlberg, H.; Dehio, C.
Deposited on	:	2023-12-12
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

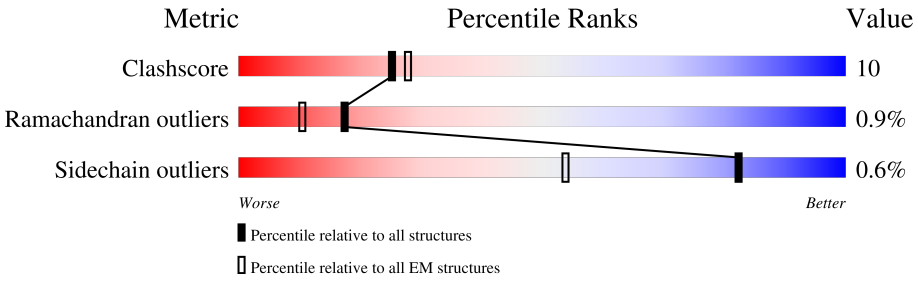
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 <=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	2818	11% 74% 24% ··
2	B	9	11% 22% 67%
3	C	9	67% 44% 44% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21922 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.

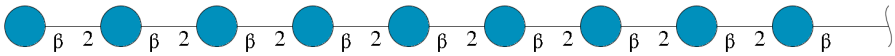
- Molecule 1 is a protein called Cyclic beta-(1,2)-glucan synthase NdvB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2780	21699	13698	3879	4052	70	2	0

There are 2 discrepancies between the modelled and reference sequences:

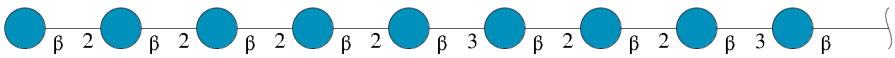
Chain	Residue	Modelled	Actual	Comment	Reference
A	610	SER	ALA	conflict	UNP A0A6V6ZZ23
A	866	PHE	HIS	conflict	UNP A0A6V6ZZ23

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



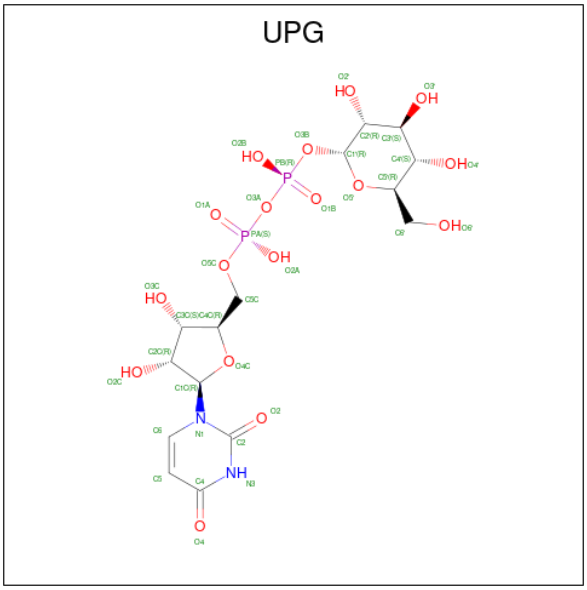
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
2	B	9	99	54	45	0	0

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
3	C	9	Total	C	O	0	0
			99	54	45		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



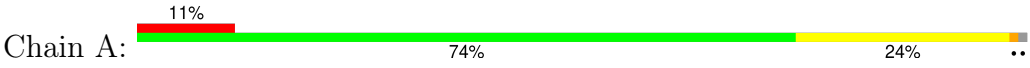
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			25	9	2	12	2	

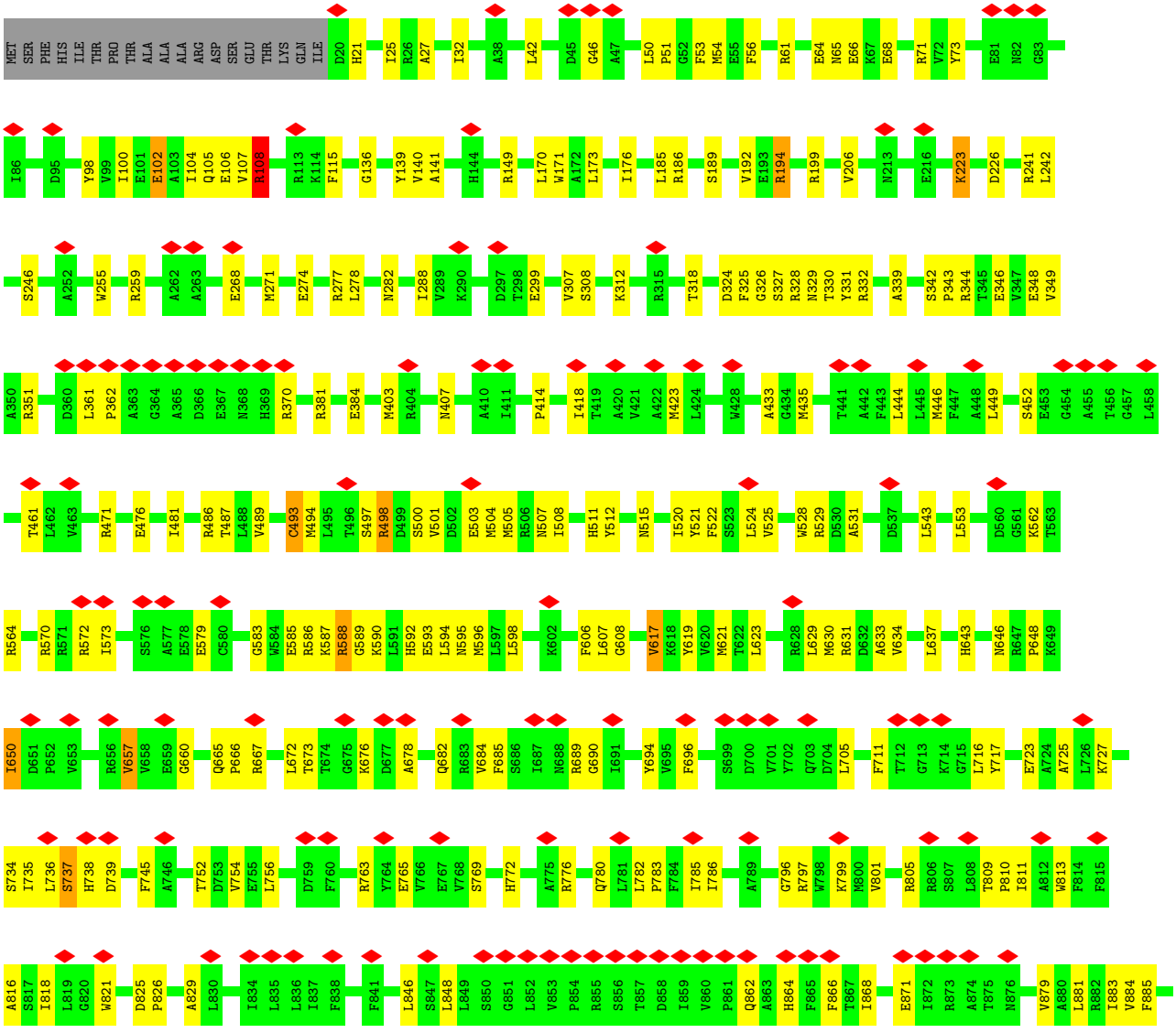
3 Residue-property plots (i)

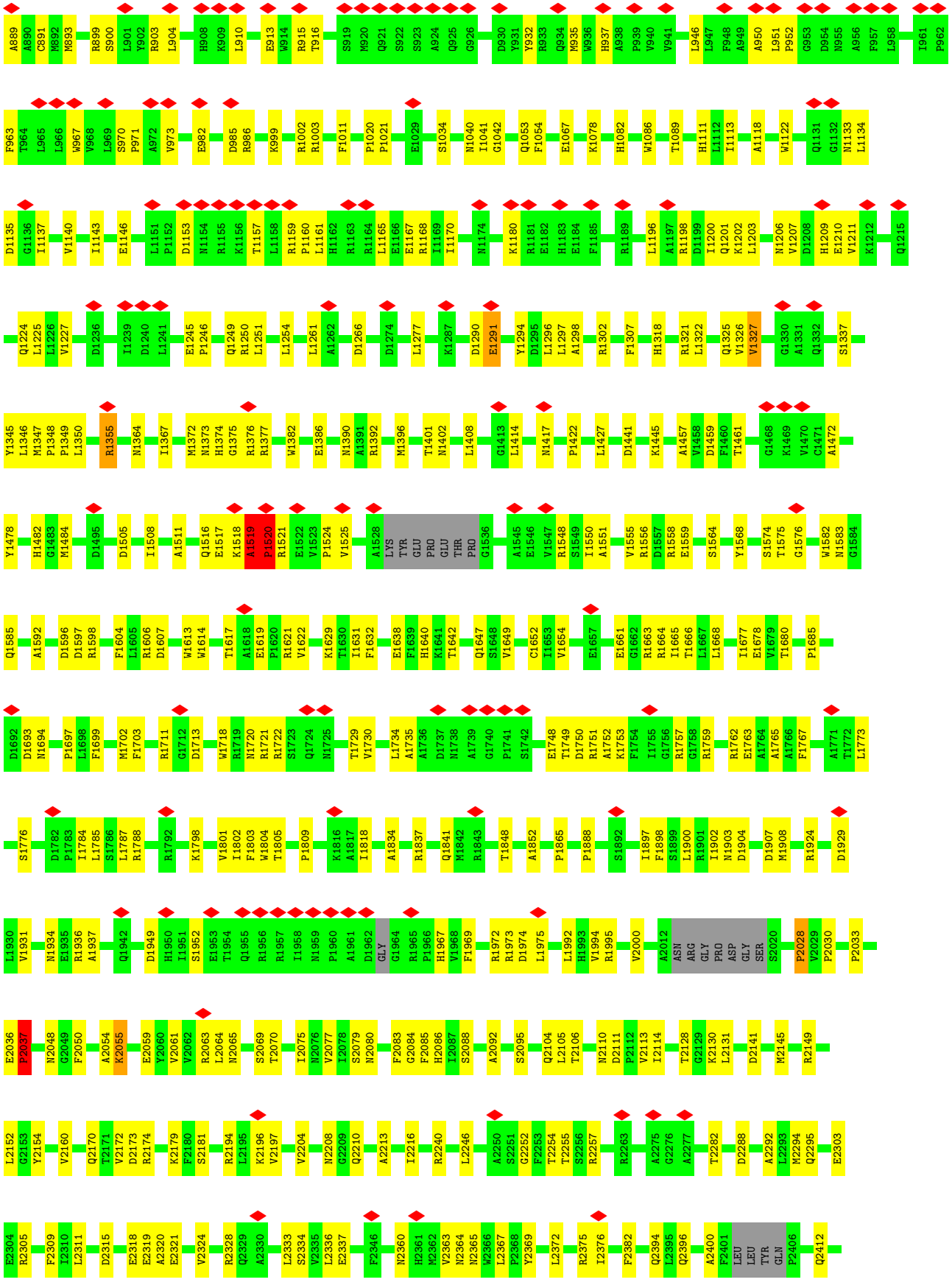
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

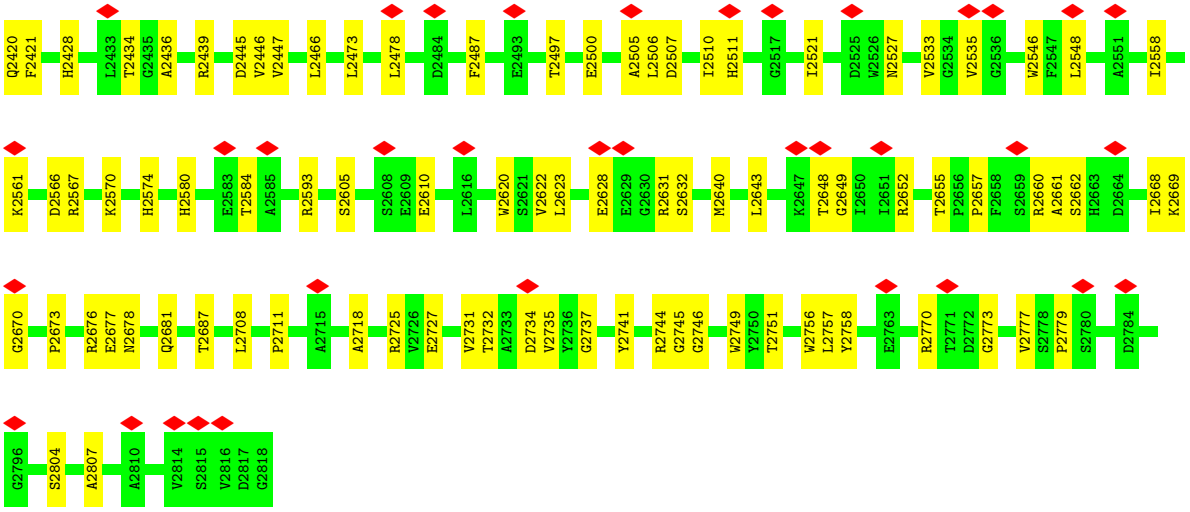
- Molecule 1: Cyclic beta-(1,2)-glucan synthase NdvB

Chain A:






A889 A890 C891 M892 M893 R899 S900 L901 Y902 R903 L904 H908 K909 L910 E913 W914 R915 T916 S919 M920 Q921 S922 S923 A924 Q925 G926 D930 Y931 Y932 R933 Q934 M935 W936 H937 A938 P939 V940 V941 L946 L947 F948 A949 A950 L951 P952 G953 D954 N955 A956 F957 L958 I961 P962
F963 T964 L965 L966 W967 V968 L969 S970 P971 A972 V973 E982 D985 R986 K999 R1002 R1003 F1011 P1020 P1021 E1029 S1034 N1040 I1041 G1042 Q1053 F1054 E1067 K1078 H1082 W1086 T1089 H1111 L1112 I1113 A1118 W1122 Q1131 G1132 N1133 L1134
D1135 G1136 I1137 V1140 I1143 E1146 L1151 P1152 D1153 N1154 R1155 K1156 T1157 L1158 R1159 P1160 L1161 H1162 R1163 R1164 L1165 E1166 E1167 R1168 I1169 I1170 N1174 K1180 R1181 E1182 H1183 E1184 F1185 R1189 L1196 A1197 R1198 D1199 I1200 Q1201 K1202 L1203 N1206 V1207 D1208 H1209 E1210 V1211 K1212 Q1215
Q1224 L1225 L1226 V1227 D1236 I1239 D1240 L1241 E1245 P1246 Q1249 R1250 L1251 L1254 L1261 A1262 D1266 D1274 L1277 K1287 D1290 E1291 Y1294 D1295 L1296 L1297 A1298 R1302 F1307 H1318 R1321 L1322 Q1325 V1326 V1327 G1330 A1331 Q1332 S1337
Y1345 L1346 M1347 P1348 P1349 L1350 R1355 N1364 I1367 M1372 N1373 H1374 G1375 R1376 R1377 W1382 E1386 N1390 A1391 R1392 M1396 T1401 N1402 L1408 G1413 L1414 N1417 P1422 L1427 D1441 K1445 A1457 Y1458 D1459 F1460 T1461 G1468 K1469 V1470 C1471 A1472
Y1478 H1482 G1483 M1484 D1495 D1505 I1508 A1511 Q1516 E1517 K1518 A1519 P1520 R1521 E1522 V1523 P1524 V1525 A1528 LYS TYR GLU PRO GLU THR PRO G1536 A1545 E1546 V1547 R1548 S1549 I1550 A1551 V1555 R1556 D1557 R1558 E1559 S1564 Y1568 S1574 T1575 G1576 W1582 N1583 G1584
Q1585 A1592 D1596 D1597 R1598 F1604 L1605 R1606 D1607 W1613 W1614 T1617 A1618 E1619 P1620 R1621 V1622 K1629 T1630 I1631 F1632 E1638 F1639 H1640 K1641 T1642 Q1647 S1648 V1649 C1652 I1653 V1654 E1657 E1661 G1662 R1663 R1664 I1665 T1666 L1667 L1668 I1677 E1678 V1679 T1680 P1685
D1692 D1693 N1694 P1697 L1698 F1699 M1702 F1703 R1711 G1712 D1713 W1718 R1719 N1720 R1721 R1722 S1723 Q1724 N1725 T1729 V1730 L1734 A1735 A1736 D1737 N1738 A1739 G1740 P1741 S1742 E1748 T1749 D1750 R1751 A1752 K1753 F1754 I1755 G1756 R1757 G1758 R1759 R1762 E1763 A1764 A1765 A1766 F1767 A1771 T1772 L1773
S1776 D1782 P1783 I1784 L1785 S1786 L1787 R1788 R1792 K1798 V1801 I1802 F1803 W1804 T1805 P1809 K1816 A1817 I1818 A1834 R1837 Q1841 M1842 R1843 T1848 A1852 P1865 P1888 S1892 I1897 F1898 S1899 L1900 R1901 I1902 N1903 D1904 D1907 M1908 R1924 D1929
L1930 V1931 N1934 E1935 R1936 A1937 Q1942 D1949 H1950 I1951 S1952 E1953 T1954 Q1955 R1956 R1957 I1958 N1959 P1960 A1961 D1962 GLY G1964 R1965 P1966 H1967 V1968 F1969 R1972 R1973 D1974 L1975 L1992 H1993 V1994 R1995 V2000 A2012 ASN ARG GLY PRO ASP GLY SER S2020 P2028 V2029 P2030 P2033
E2036 P2037 N2048 G2049 F2050 A2054 K2055 E2059 Y2060 V2061 V2062 R2063 L2064 N2065 S2069 T2070 I2075 N2076 V2077 I2078 S2079 N2080 F2083 G2084 F2085 H2086 I2087 S2088 A2092 S2095 Q2104 L2105 T2106 N2110 D2111 P2112 V2113 I2114 T2128 G2129 K2130 L2131 D2141 M2145 R2149
L2152 G2153 Y2154 V2160 Q2170 T2171 V2172 D2173 R2174 K2179 F2180 S2181 R2194 L2195 K2196 V2197 V2204 N2208 G2209 Q2210 A2213 I2216 R2240 L2246 A2250 S2251 G2252 F2253 T2254 T2255 S2256 R2257 R2263 A2275 G2276 A2277 T2282 D2288 A2292 L2293 M2294 Q2295 E2303
E2304 R2305 F2309 I2310 L2311 D2315 E2318 E2319 A2320 E2321 V2324 R2328 Q2329 A2330 L2333 S2334 V2335 L2336 E2337 F2346 N2360 H2361 M2362 V2363 N2364 N2365 W2366 L2367 P2368 Y2369 L2372 R2375 I2376 F2382 Q2394 L2395 Q2396 A2400 F2401 LEU LEU TYR GLN P2406 Q2412

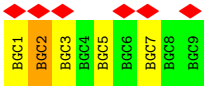


• Molecule 2: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose

Chain B:

• Molecule 3: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-2)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.637	Depositor
Minimum map value	-0.305	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	394.8, 394.8, 394.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.316, 1.316, 1.316	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, UPG

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	0.26	1/22196 (0.0%)	0.55	8/30155 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1519	ALA	C-N	7.03	1.47	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1519	ALA	O-C-N	-20.42	82.30	121.10
1	A	2037	PRO	N-CA-CB	6.24	110.79	103.30
1	A	2028	PRO	N-CA-CB	6.22	110.77	103.30
1	A	2033	PRO	N-CA-CB	6.09	110.61	103.30
1	A	1520	PRO	CA-C-N	6.03	130.47	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	139	TYR	Peptide
1	A	1519	ALA	Mainchain

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	21699	0	20972	436	0
2	B	99	0	82	8	0
3	C	99	0	82	2	0
4	A	25	0	11	0	0
All	All	21922	0	21147	437	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 10.

The worst 5 of 437 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:115:PHE:CD1	2:B:9:BGC:O2	2.30	0.83
1:A:619:TYR:HB3	1:A:716:LEU:HD11	1.63	0.81
1:A:682:GLN:HB3	1:A:689:ARG:HH22	1.46	0.79
1:A:423:MET:HG2	1:A:444:LEU:HD22	1.65	0.79
1:A:1748:GLU:HB2	1:A:1773:LEU:HG	1.65	0.76

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	2772/2818 (98%)	2502 (90%)	245 (9%)	25 (1%)	14 41

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	TYR
1	A	246	SER
1	A	407	ASN
1	A	498	ARG
1	A	737	SER

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	2222/2333 (95%)	2207 (99%)	15 (1%)	81 88

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	586	ARG
1	A	2194	ARG
1	A	915	ARG
1	A	2527	ASN
1	A	1355[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	515	ASN
1	A	1111	HIS
1	A	1516	GLN
1	A	2412	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

18 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	BGC	B	1	2	11,11,12	0.72	0	15,15,17	1.49	2 (13%)
2	BGC	B	2	2	11,11,12	0.41	0	15,15,17	1.43	3 (20%)
2	BGC	B	3	2	11,11,12	0.61	0	15,15,17	1.92	2 (13%)
2	BGC	B	4	2	11,11,12	0.49	0	15,15,17	1.20	2 (13%)
2	BGC	B	5	2	11,11,12	0.52	0	15,15,17	1.12	2 (13%)
2	BGC	B	6	2	11,11,12	0.49	0	15,15,17	0.99	1 (6%)
2	BGC	B	7	2	11,11,12	0.59	0	15,15,17	1.79	3 (20%)
2	BGC	B	8	2	11,11,12	0.26	0	15,15,17	0.73	0
2	BGC	B	9	2	11,11,12	0.47	0	15,15,17	1.42	2 (13%)
3	BGC	C	1	3	11,11,12	0.21	0	15,15,17	0.37	0
3	BGC	C	2	3	11,11,12	0.73	1 (9%)	15,15,17	1.08	1 (6%)
3	BGC	C	3	3	11,11,12	0.33	0	15,15,17	0.68	0
3	BGC	C	4	3	11,11,12	0.33	0	15,15,17	0.45	0
3	BGC	C	5	3	11,11,12	0.70	1 (9%)	15,15,17	0.87	1 (6%)
3	BGC	C	6	3	11,11,12	0.21	0	15,15,17	0.40	0
3	BGC	C	7	3	11,11,12	0.67	0	15,15,17	0.87	1 (6%)
3	BGC	C	8	3	11,11,12	0.18	0	15,15,17	0.43	0
3	BGC	C	9	3	11,11,12	0.18	0	15,15,17	0.37	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	B	1	2	-	0/2/19/22	0/1/1/1
2	BGC	B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	B	4	2	-	1/2/19/22	0/1/1/1
2	BGC	B	5	2	-	2/2/19/22	0/1/1/1
2	BGC	B	6	2	-	2/2/19/22	0/1/1/1
2	BGC	B	7	2	-	0/2/19/22	0/1/1/1
2	BGC	B	8	2	-	2/2/19/22	0/1/1/1
2	BGC	B	9	2	-	2/2/19/22	0/1/1/1
3	BGC	C	1	3	-	2/2/19/22	0/1/1/1
3	BGC	C	2	3	-	2/2/19/22	0/1/1/1
3	BGC	C	3	3	-	0/2/19/22	0/1/1/1
3	BGC	C	4	3	-	2/2/19/22	0/1/1/1
3	BGC	C	5	3	-	2/2/19/22	0/1/1/1
3	BGC	C	6	3	-	2/2/19/22	0/1/1/1
3	BGC	C	7	3	-	2/2/19/22	0/1/1/1
3	BGC	C	8	3	-	0/2/19/22	0/1/1/1
3	BGC	C	9	3	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	BGC	O5-C1	2.22	1.47	1.43
3	C	5	BGC	O5-C1	2.06	1.47	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	BGC	C1-C2-C3	6.02	118.40	109.64
2	B	7	BGC	C1-C2-C3	5.09	117.05	109.64
3	C	2	BGC	C1-O5-C5	3.84	117.33	112.19
2	B	9	BGC	C1-C2-C3	3.83	115.22	109.64
2	B	1	BGC	C1-C2-C3	3.19	114.29	109.64

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

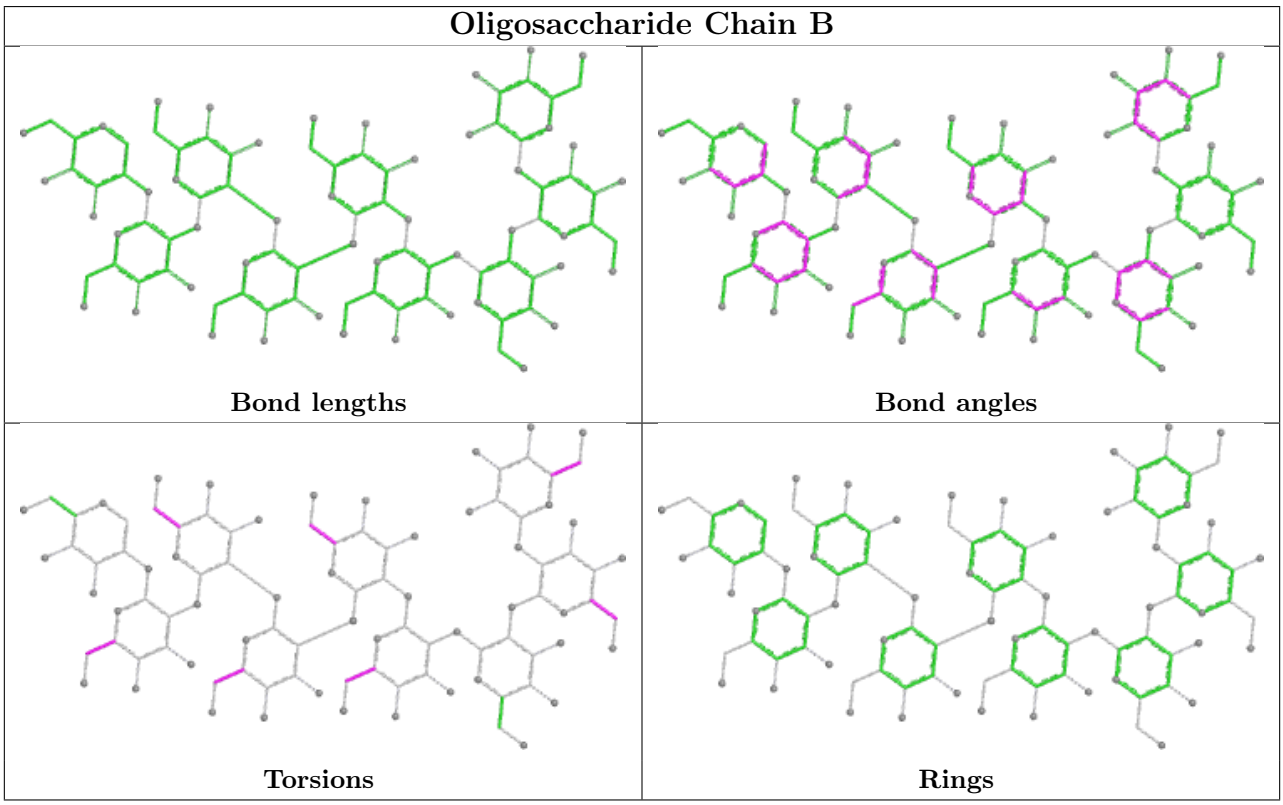
Mol	Chain	Res	Type	Atoms
3	C	7	BGC	O5-C5-C6-O6
2	B	5	BGC	O5-C5-C6-O6
2	B	2	BGC	O5-C5-C6-O6
2	B	9	BGC	O5-C5-C6-O6
3	C	7	BGC	C4-C5-C6-O6

There are no ring outliers.

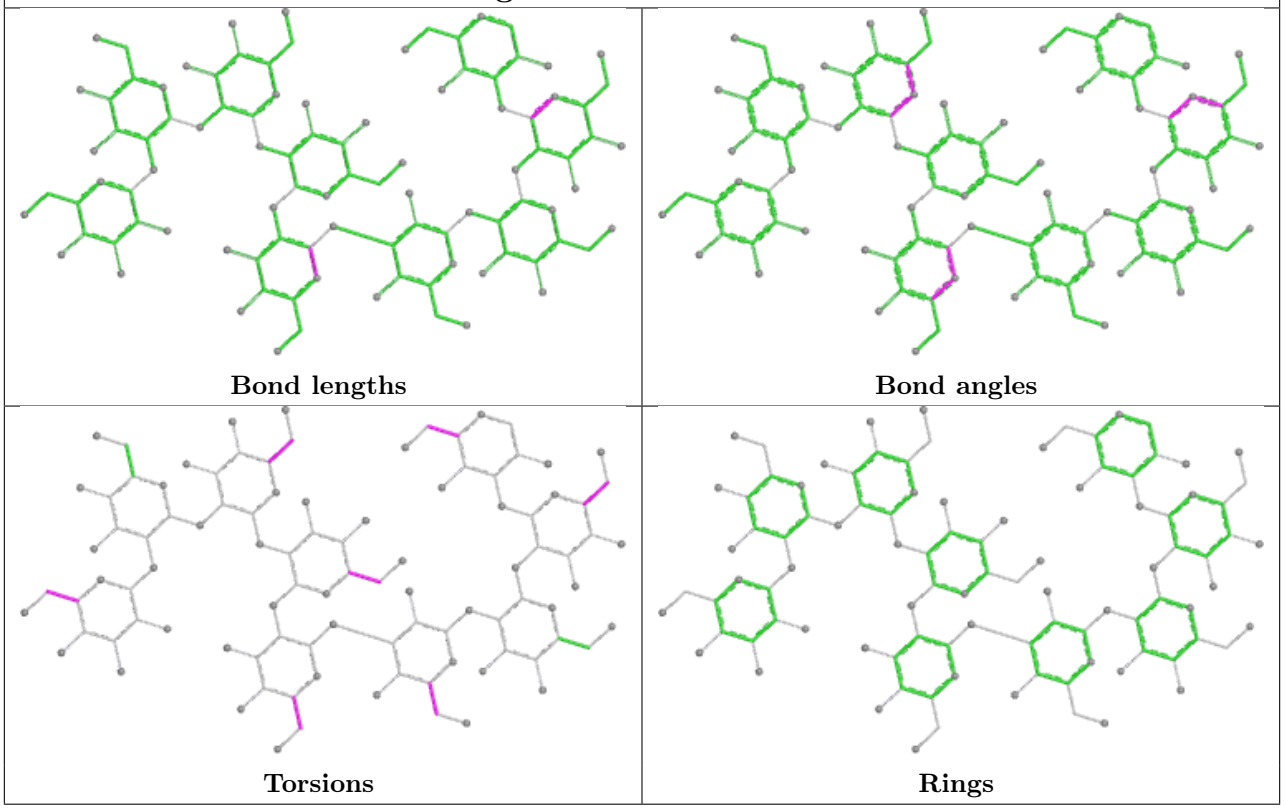
9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	BGC	1	0
2	B	1	BGC	1	0
3	C	3	BGC	1	0
2	B	4	BGC	1	0
2	B	6	BGC	1	0
2	B	9	BGC	3	0
3	C	1	BGC	1	0
2	B	7	BGC	1	0
2	B	5	BGC	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.



Oligosaccharide Chain C



5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	UPG	A	2901	-	25,26,38	0.84	1 (4%)	38,40,58	0.75	1 (2%)

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	UPG	A	2901	-	-	3/16/32/59	0/2/2/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2901	UPG	PB-O1B	3.20	1.60	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2901	UPG	O3B-PB-O2B	2.69	117.90	107.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

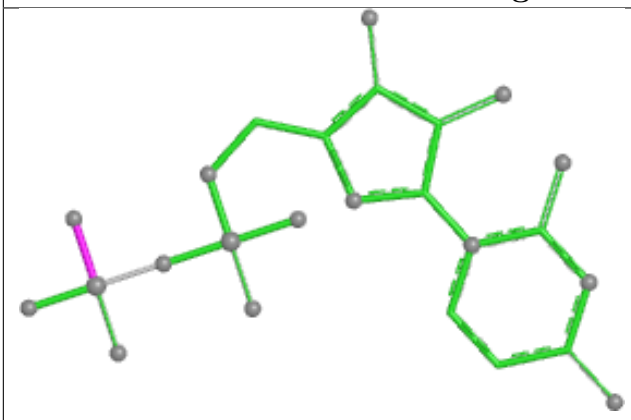
Mol	Chain	Res	Type	Atoms
4	A	2901	UPG	C5C-O5C-PA-O1A
4	A	2901	UPG	C5C-O5C-PA-O2A
4	A	2901	UPG	C5C-O5C-PA-O3A

There are no ring outliers.

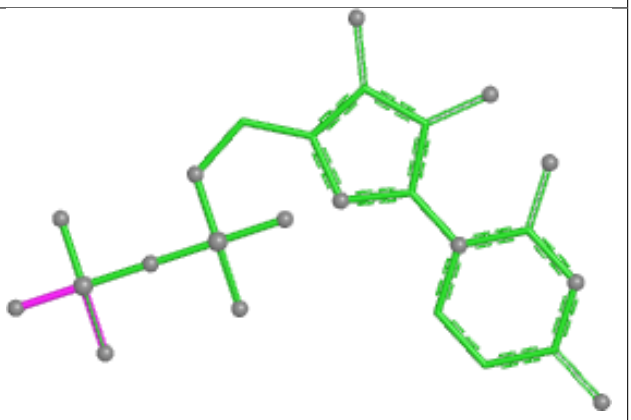
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

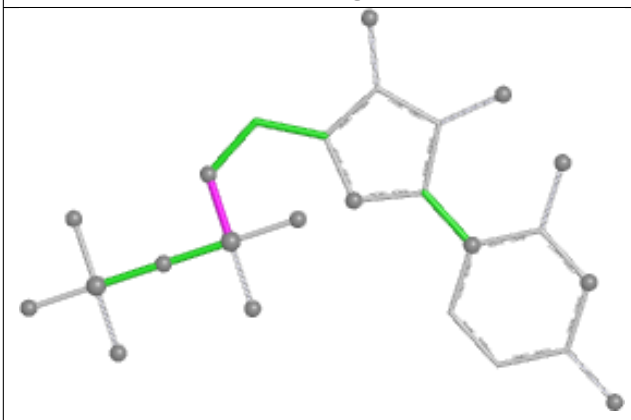
Ligand UPG A 2901



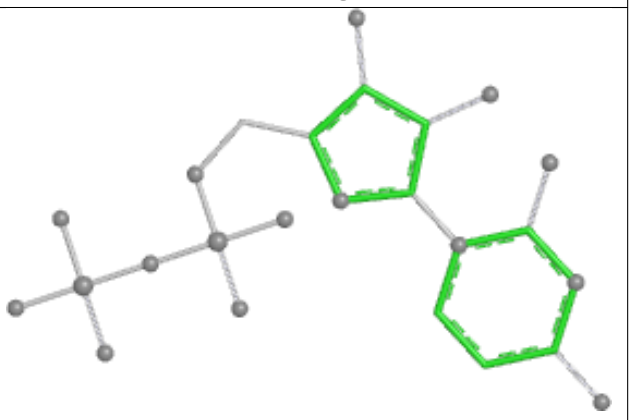
Bond lengths



Bond angles



Torsions



Rings

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.

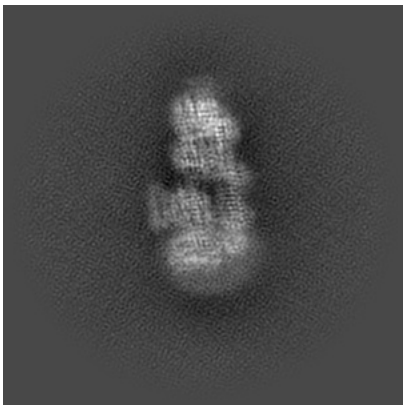
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19114. These allow visual inspection of the internal detail of the map and identification of artifacts.

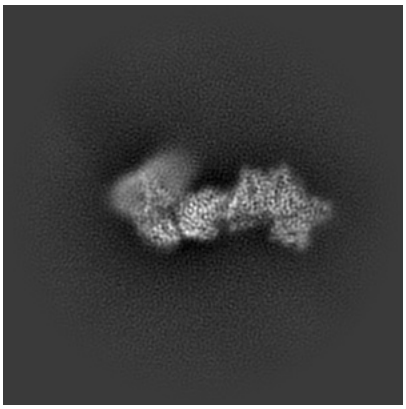
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

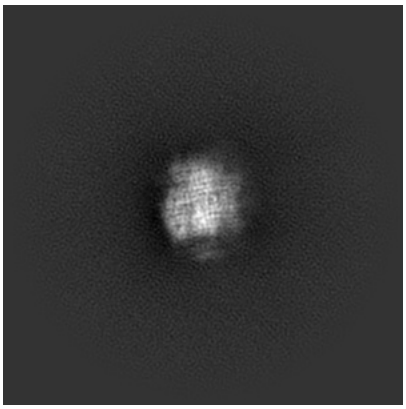
6.1.1 Primary map



X

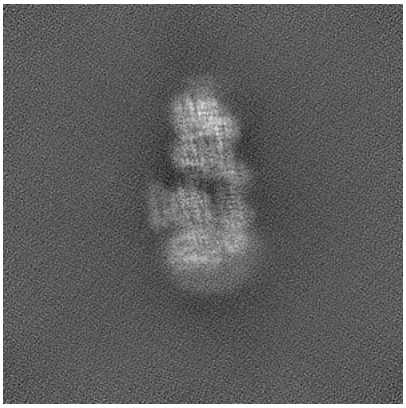


Y

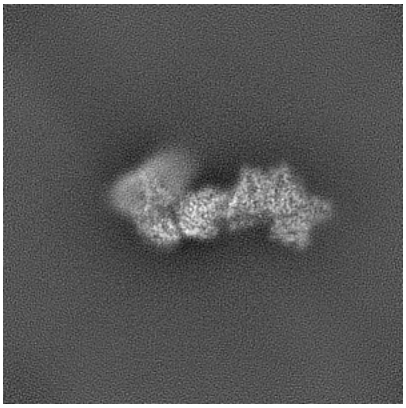


Z

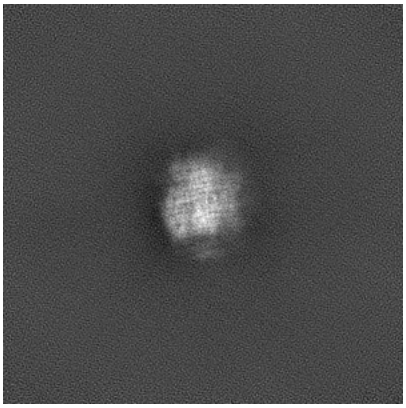
6.1.2 Raw map



X



Y



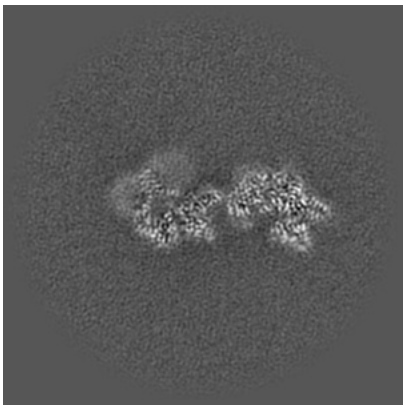
Z

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

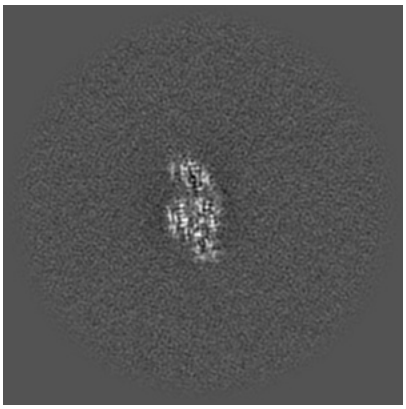
6.2 Central slices (i)

6.2.1 Primary map

X Index: 150

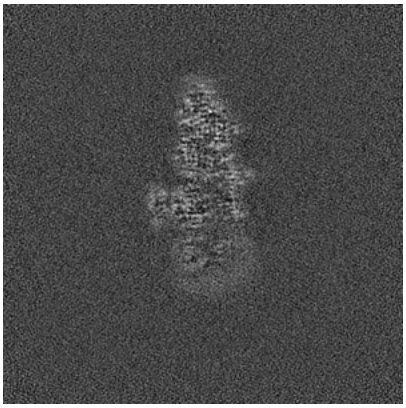


Y Index: 150

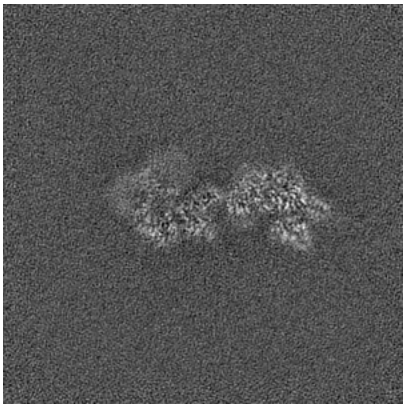


Z Index: 150

6.2.2 Raw map



X Index: 150



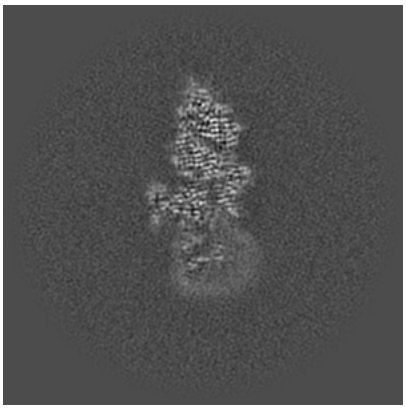
Y Index: 150

Z Index: 150

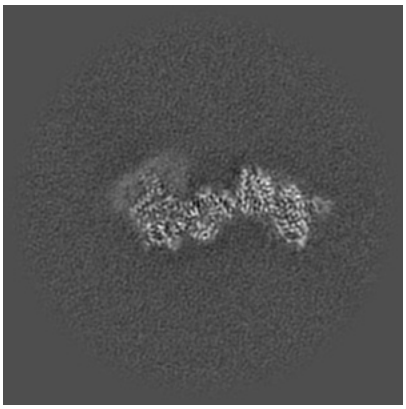
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

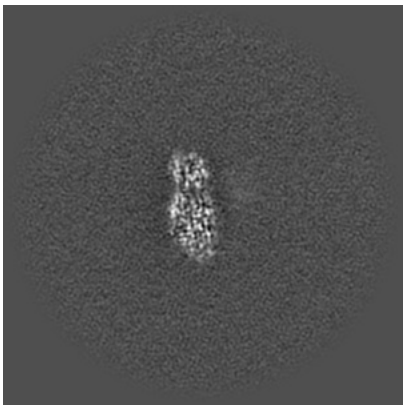
6.3.1 Primary map



X Index: 152

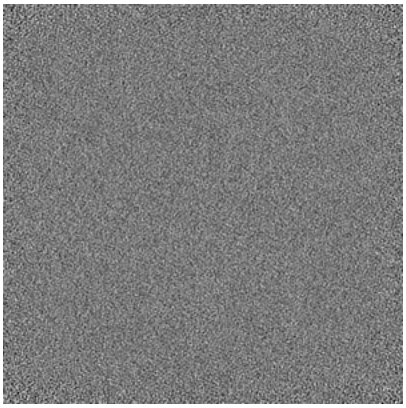


Y Index: 141

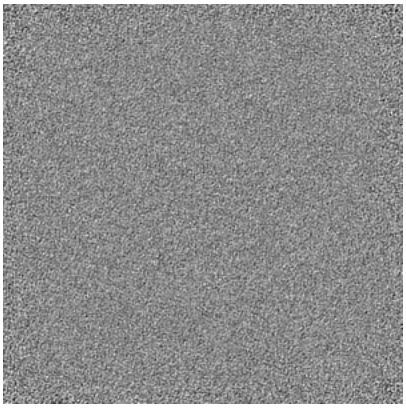


Z Index: 144

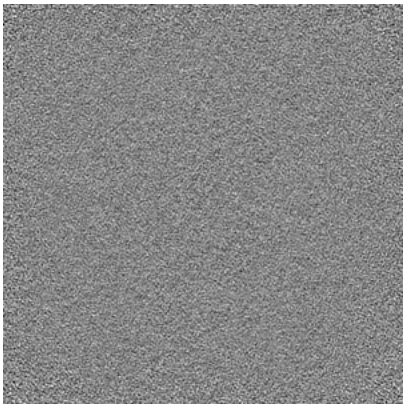
6.3.2 Raw map



X Index: 0



Y Index: 0

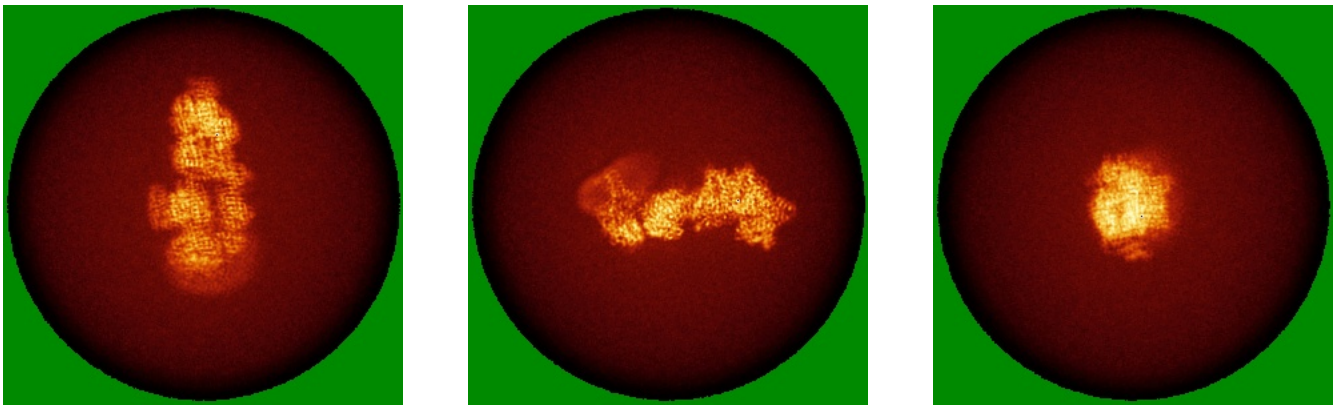


Z Index: 0

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

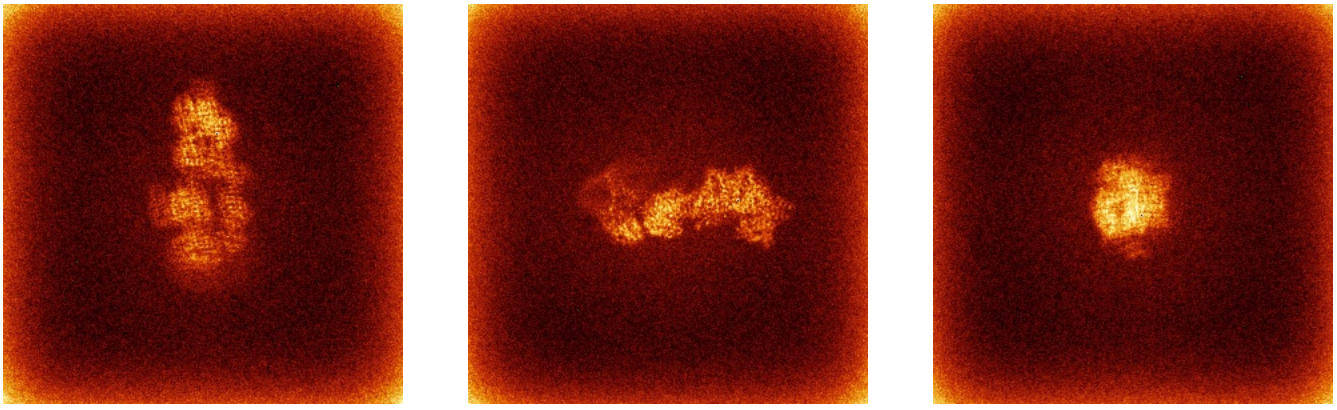
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

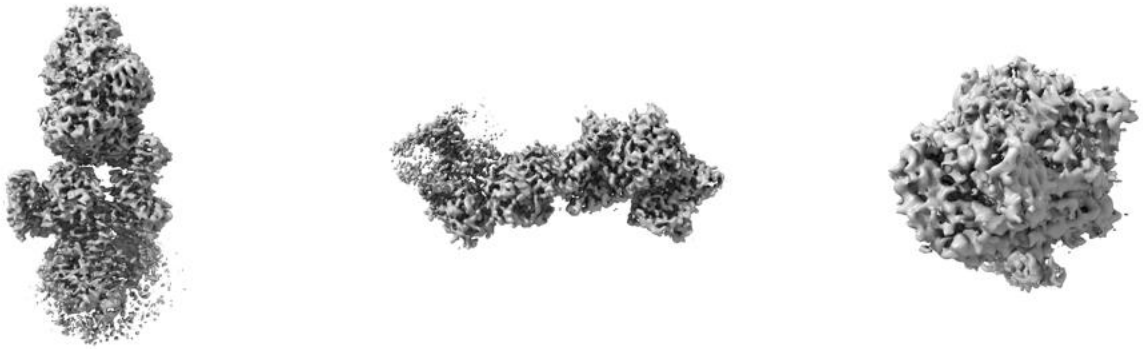


X Y Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. 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

X Y Z

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.

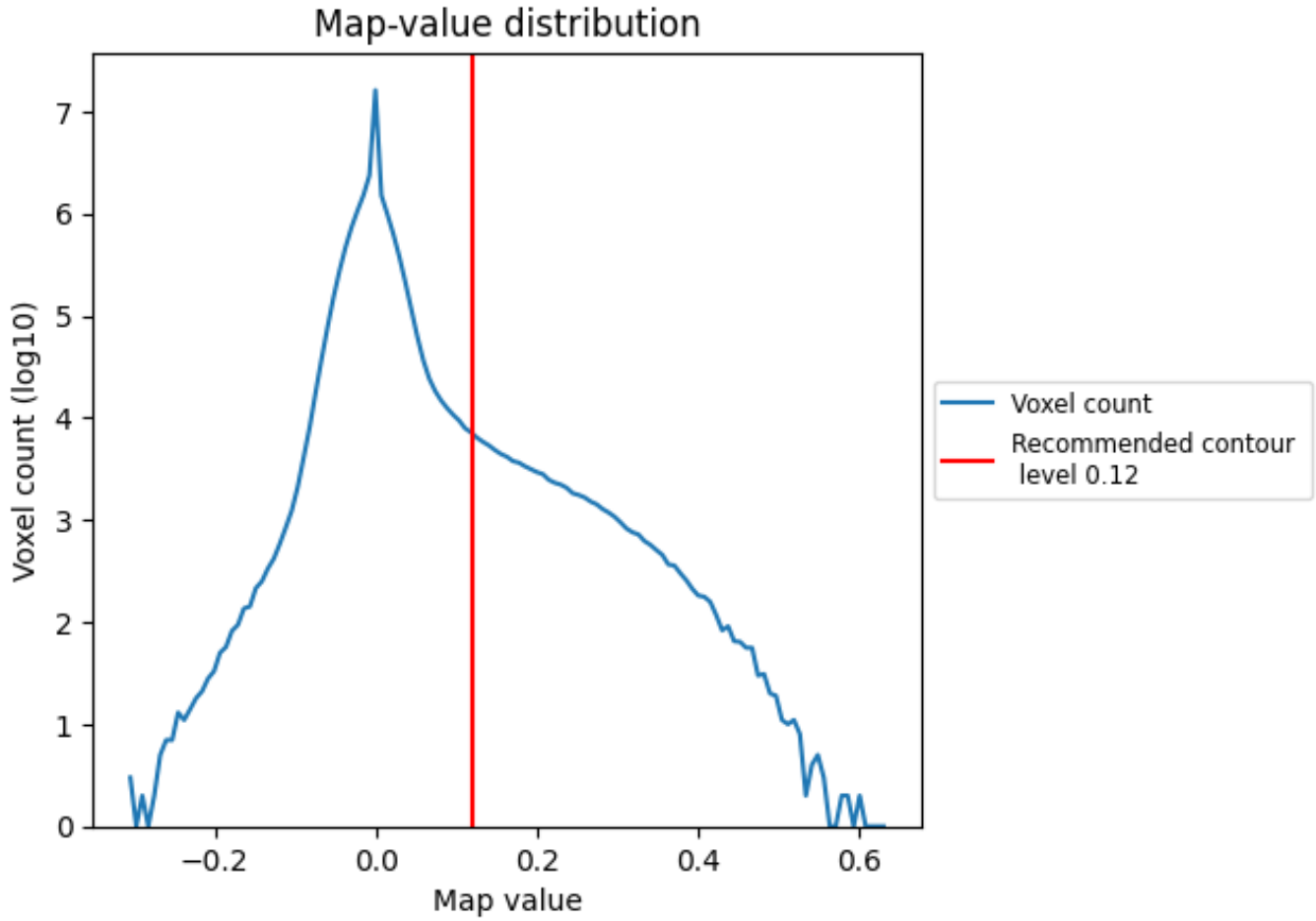
6.6 Mask visualisation (i)

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

7 Map analysis

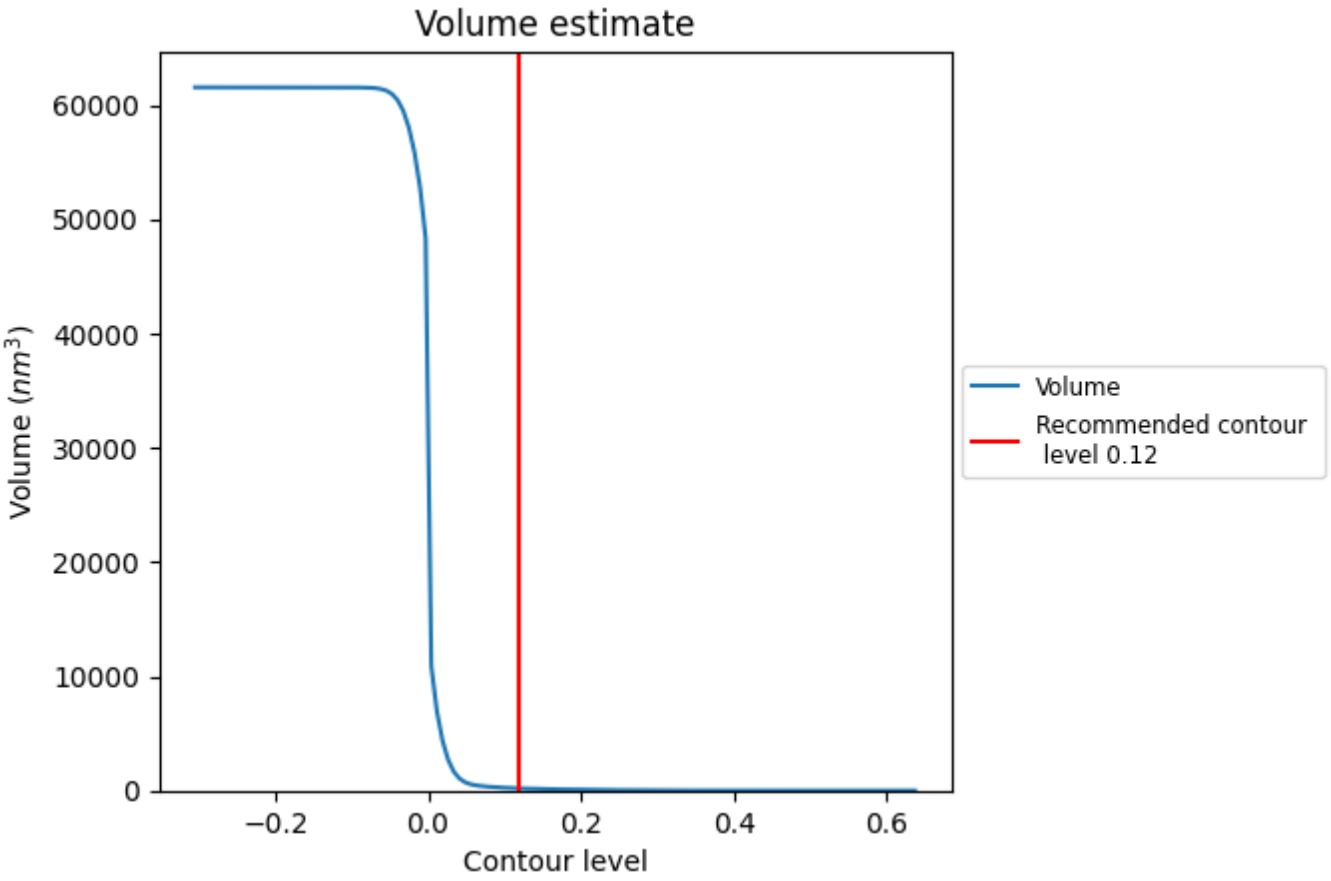
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

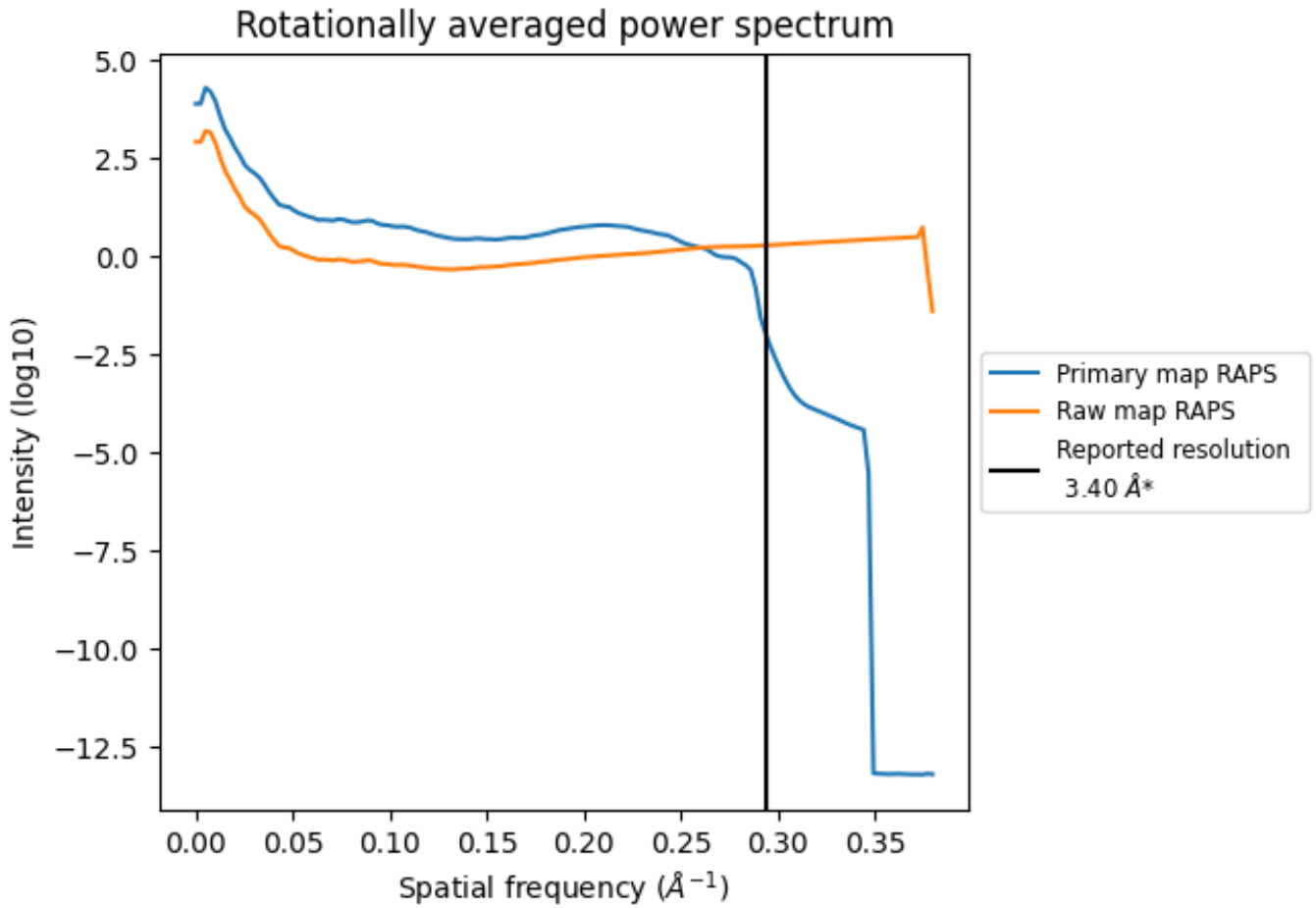
7.2 Volume estimate (i)



The volume at the recommended contour level is 193 nm^3; this corresponds to an approximate mass of 174 kDa.

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

7.3 Rotationally averaged power spectrum (i)

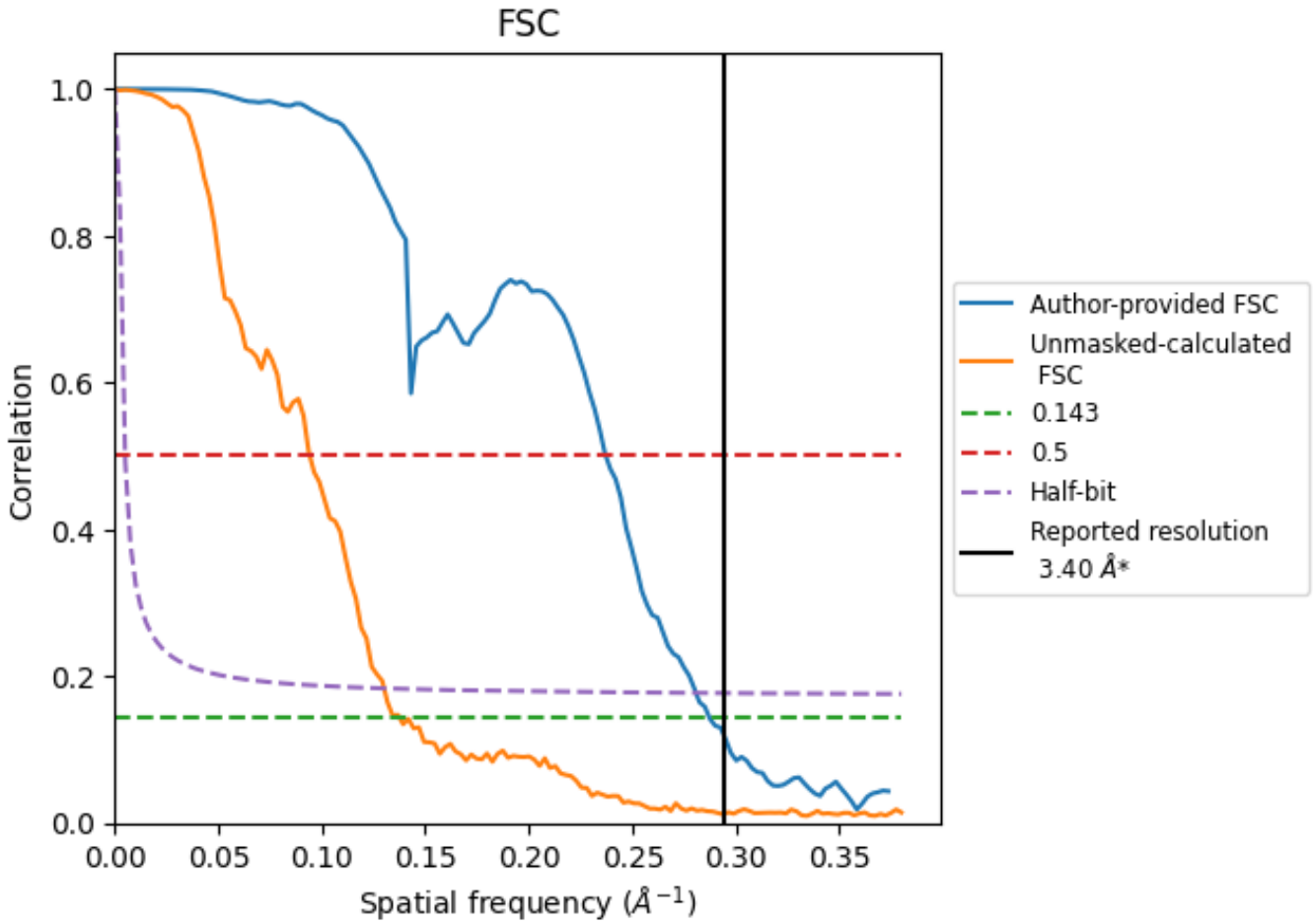


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

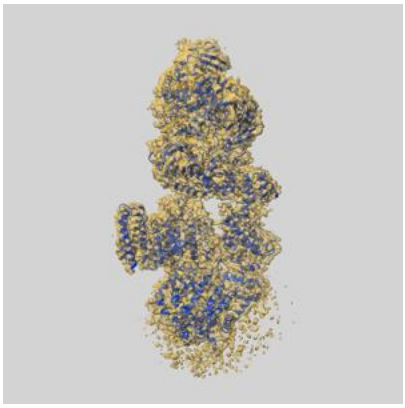
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.48	4.22	3.56
Unmasked-calculated*	7.27	10.62	7.69

*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 7.27 differs from the reported value 3.4 by more than 10 %

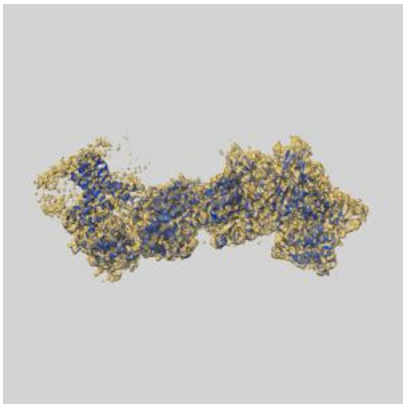
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19114 and PDB model 8RF0. Per-residue inclusion information can be found in section 3 on page 5.

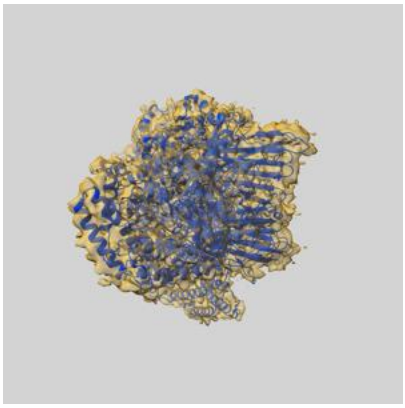
9.1 Map-model overlay



X



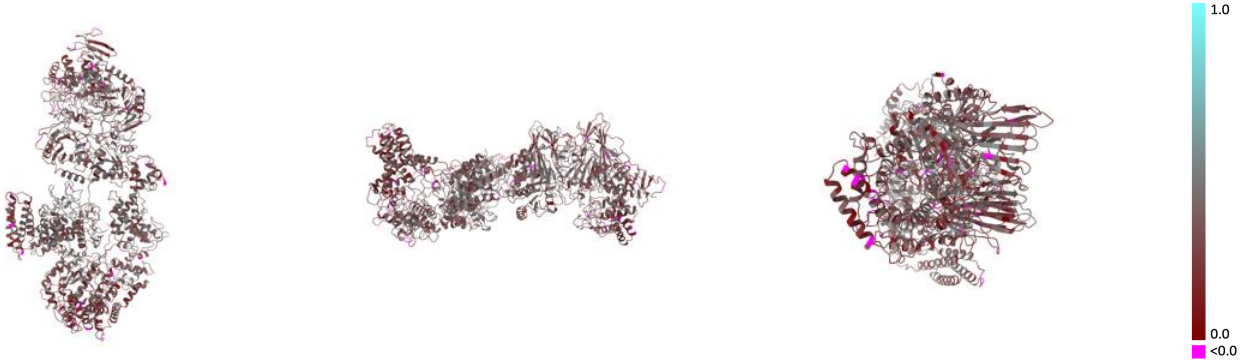
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

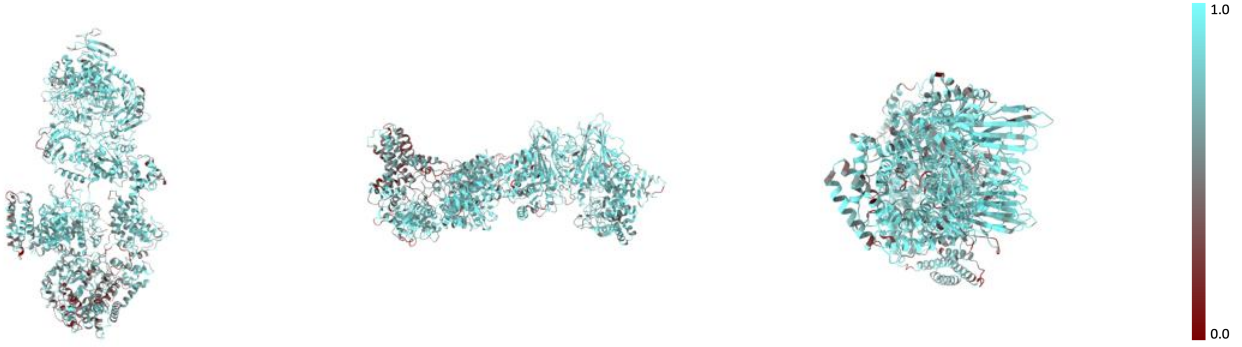
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

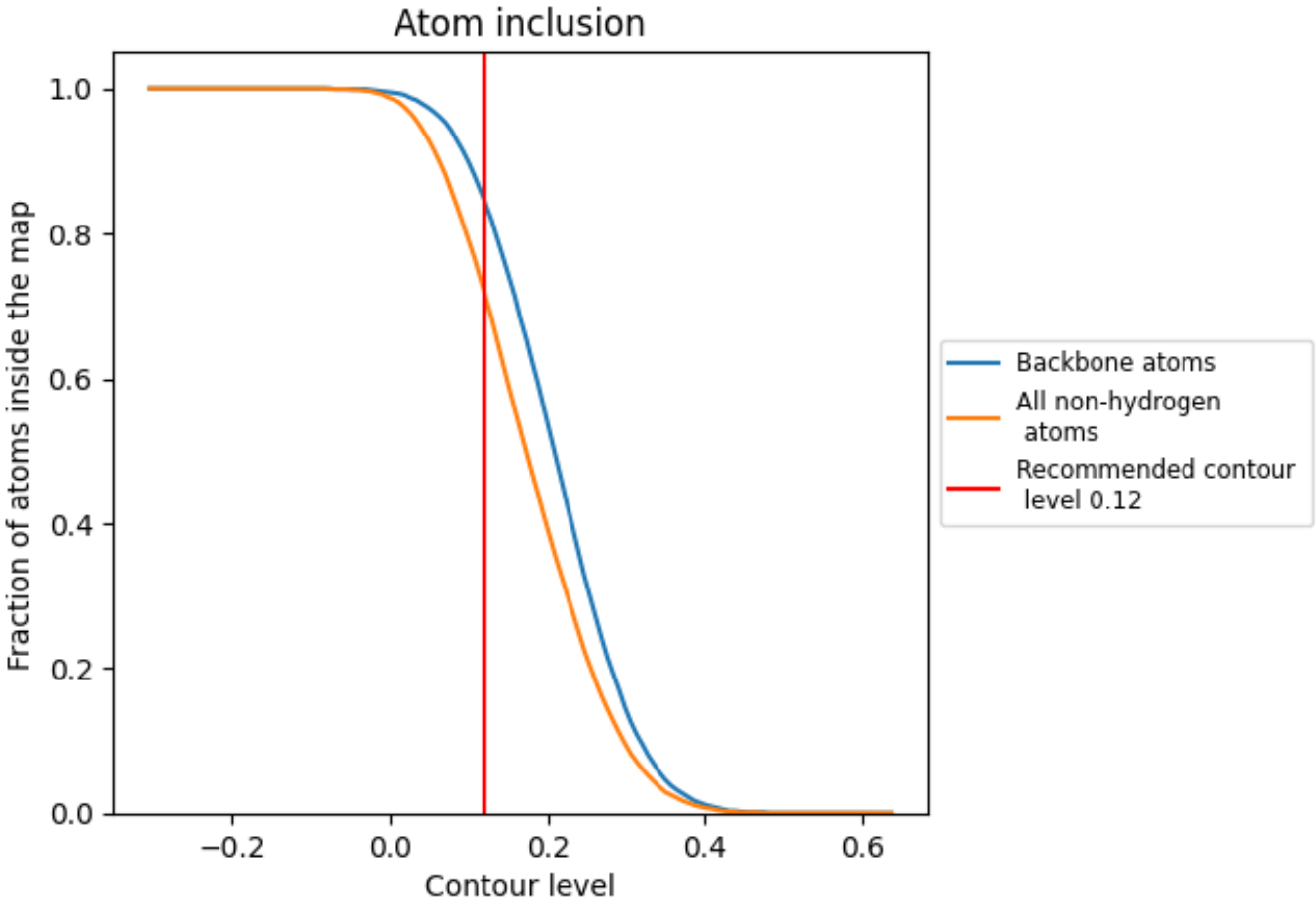
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 72% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7190	0.3220
A	0.7210	0.3210
B	0.8280	0.4980
C	0.2930	0.2020