wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 02:53 PM JST

PDB ID	:	5XJY
EMDB ID	:	EMD-6724
Title	:	Cryo-EM structure of human ABCA1
Authors	:	Qian, H.W.; Yan, N.; Gong, X.
Deposited on	:	2017-05-04
Resolution	:	4.10 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 (i) 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 (i)) were used in the production of this report:

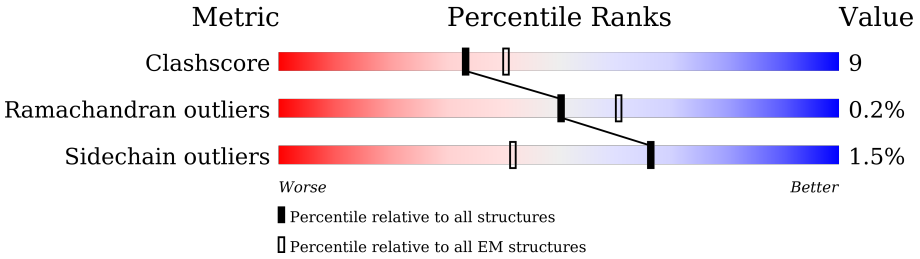
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2305	19% 67% 15% • 18%
2	B	5	40% 60%
3	C	2	50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12785 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 ATP-binding cassette sub-family A member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1901	12626	8005	2236	2328	57	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP O95477
A	-19	ALA	-	expression tag	UNP O95477
A	-18	ASP	-	expression tag	UNP O95477
A	-17	TYR	-	expression tag	UNP O95477
A	-16	LYS	-	expression tag	UNP O95477
A	-15	ASP	-	expression tag	UNP O95477
A	-14	ASP	-	expression tag	UNP O95477
A	-13	ASP	-	expression tag	UNP O95477
A	-12	ASP	-	expression tag	UNP O95477
A	-11	LYS	-	expression tag	UNP O95477
A	-10	SER	-	expression tag	UNP O95477
A	-9	GLY	-	expression tag	UNP O95477
A	-8	PRO	-	expression tag	UNP O95477
A	-7	ASP	-	expression tag	UNP O95477
A	-6	GLU	-	expression tag	UNP O95477
A	-5	VAL	-	expression tag	UNP O95477
A	-4	ASP	-	expression tag	UNP O95477
A	-3	ALA	-	expression tag	UNP O95477
A	-2	SER	-	expression tag	UNP O95477
A	-1	GLY	-	expression tag	UNP O95477
A	0	ARG	-	expression tag	UNP O95477
A	2262	LEU	-	expression tag	UNP O95477
A	2263	GLU	-	expression tag	UNP O95477
A	2264	GLY	-	expression tag	UNP O95477
A	2265	SER	-	expression tag	UNP O95477
A	2266	ASP	-	expression tag	UNP O95477
A	2267	GLU	-	expression tag	UNP O95477
A	2268	VAL	-	expression tag	UNP O95477

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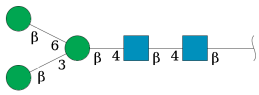
Chain	Residue	Modelled	Actual	Comment	Reference
A	2269	ASP	-	expression tag	UNP O95477
A	2270	ALA	-	expression tag	UNP O95477
A	2271	VAL	-	expression tag	UNP O95477
A	2272	GLU	-	expression tag	UNP O95477
A	2273	GLY	-	expression tag	UNP O95477
A	2274	SER	-	expression tag	UNP O95477
A	2275	HIS	-	expression tag	UNP O95477
A	2276	HIS	-	expression tag	UNP O95477
A	2277	HIS	-	expression tag	UNP O95477
A	2278	HIS	-	expression tag	UNP O95477
A	2279	HIS	-	expression tag	UNP O95477
A	2280	HIS	-	expression tag	UNP O95477
A	2281	HIS	-	expression tag	UNP O95477
A	2282	HIS	-	expression tag	UNP O95477
A	2283	HIS	-	expression tag	UNP O95477
A	2284	HIS	-	expression tag	UNP O95477

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

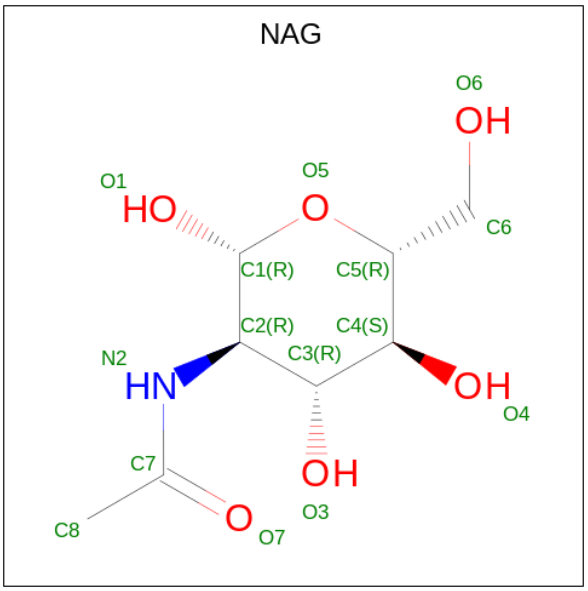


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	5	61	34	2	25	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	2	28	16	2	10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



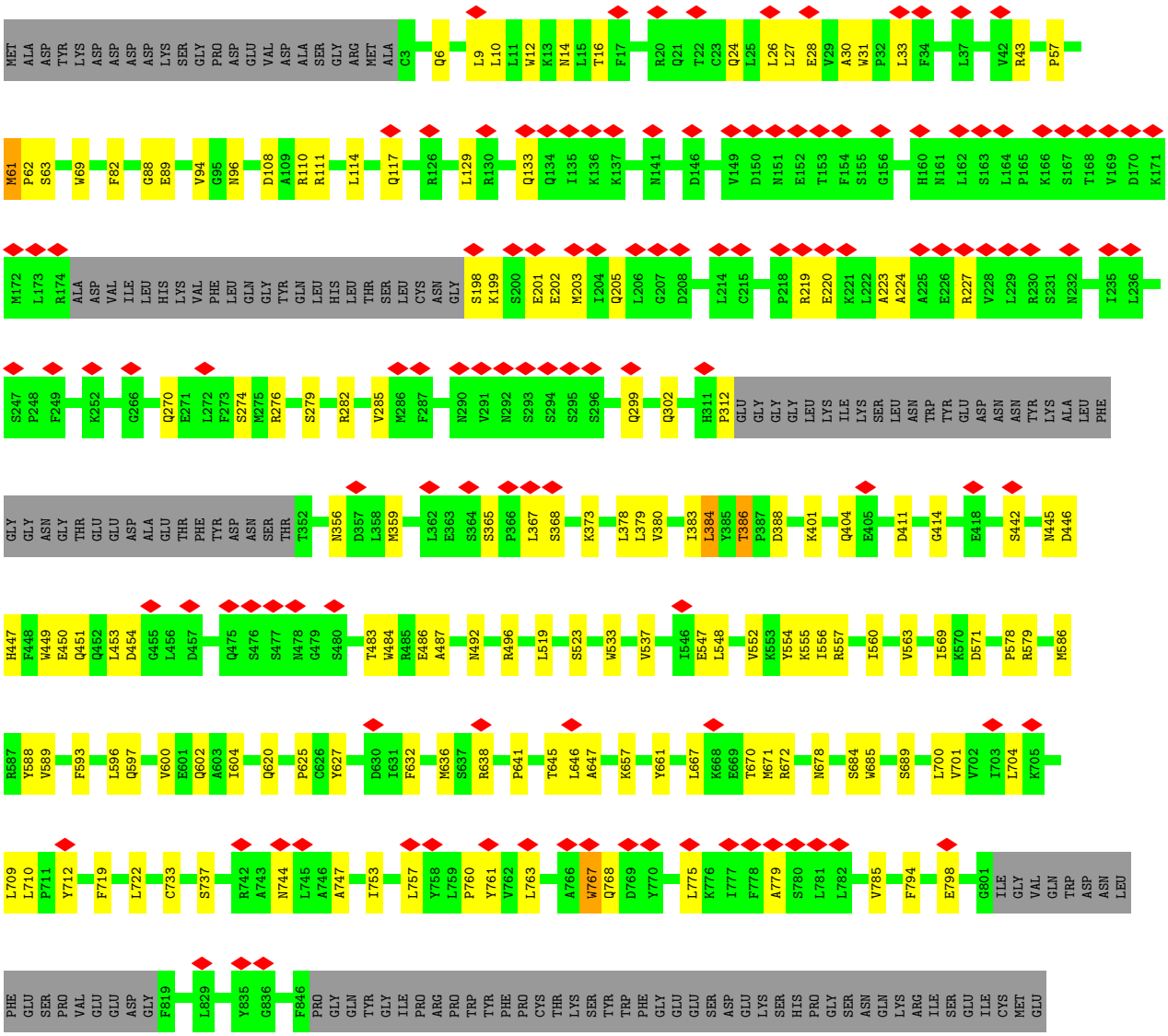
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	70	40	5	25	0
			Total	C	N	O	
4	A	1	70	40	5	25	0
			Total	C	N	O	
4	A	1	70	40	5	25	0
			Total	C	N	O	
4	A	1	70	40	5	25	0
			Total	C	N	O	
4	A	1	70	40	5	25	0

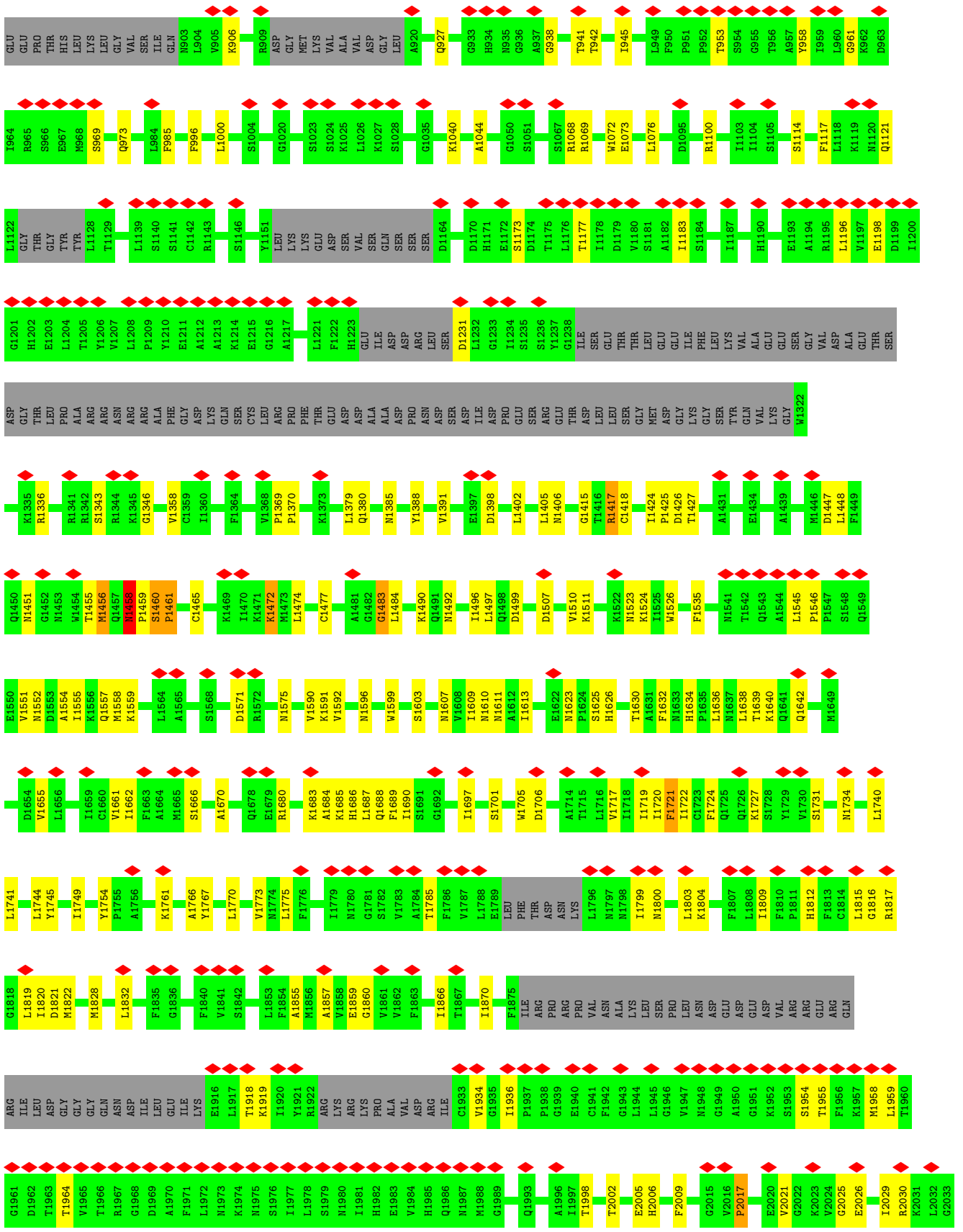
3 Residue-property plots (i)

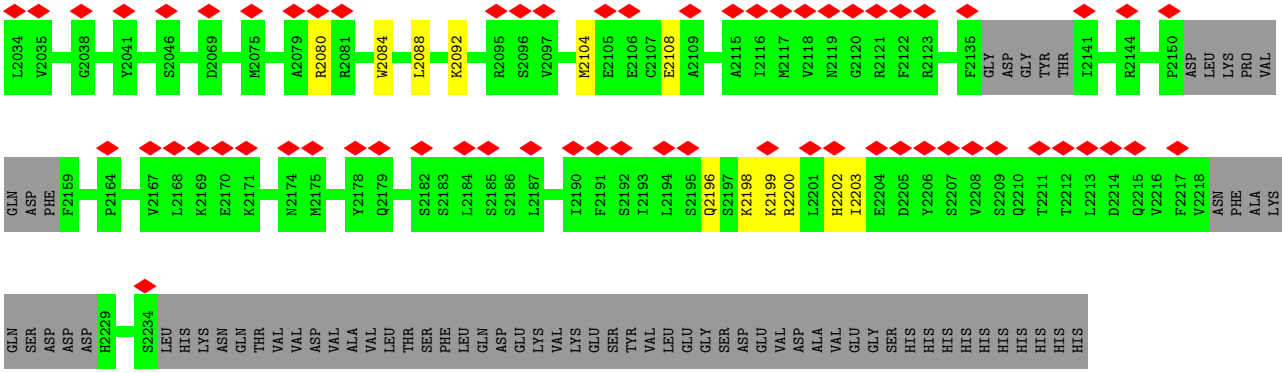
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ATP-binding cassette sub-family A member 1

Chain A:

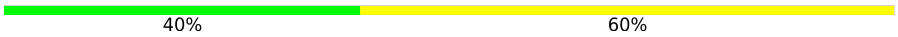



GLU GLU PRO THR HIS LEU LYS LEU GLY VAL SER ILE GLN N903 L904 V905 K906 R909 ASP GLY MET LYS VAL ALA VAL ASP GLY LEU A920 Q927 G933 H934 N935 G936 A937 G938 T941 T942 I945 L949 F950 P951 P952 T953 S954 G955 T956 A957 Y958 I959 L960 G961 K962 D963
I964 R965 S966 E967 M968 S969 Q973 L984 F985 F996 L1000 S1004 G1020 S1023 S1024 K1025 L1026 K1027 S1028 G1035 K1040 A1044 G1050 S1051 S1067 R1068 R1069 W1072 E1073 L1076 D1095 R1100 I1103 I1104 S1105 S1114 F1117 L1118 K1119 N1120 Q1121
L1122 GLY THR GLY TYR TYR L1128 T1129 L1139 S1140 S1141 C1142 R1143 S1146 Y1151 LEU LYS LYS GLU ASP SER VAL SER GLN SER SER SER D1164 D1170 H1171 E1172 S1173 D1174 T1175 L1176 T1177 I1178 D1179 V1180 S1181 A1182 I1183 S1184 I1187 H1190 E1193 A1194 R1195 L1196 V1197 E1198 D1199 I1200
G1201 H1202 E1203 L1204 T1205 Y1206 V1207 L1208 P1209 Y1210 E1211 A1212 A1213 K1214 E1215 G1216 A1217 L1221 F1222 H1223 GLU ILE ASP ASP ARG LEU SER D1231 L1232 G1233 I1234 S1235 S1236 Y1237 G1238 ILE SER GLU THR THR LEU GLU GLU ILE PHE LEU LYS VAL ALA GLU GLU SER GLY VAL ASP ALA GLU THR SER
ASP GLY THR LEU PRO ALA ARG ARG ASN ARG ARG ALA PHE GLY ASP LYS GLN SER CYS LEU ARG PRO PHE THR GLU ASP ASP ALA ALA ASP PRO ASN ASP SER ASP ILE ASP PRO GLU SER ARG GLU THR ASP LEU LEU SER GLY MET ASP GLY LYS GLY SER TYR GLN VAL LYS GLY W1322
K1335 R1336 R1341 R1342 S1343 R1344 K1345 G1346 V1358 C1359 I1360 F1364 V1368 P1369 P1370 K1373 L1379 Q1380 N1385 Y1388 V1391 E1397 D1398 L1402 L1405 N1406 G1415 T1416 R1417 C1418 I1424 P1425 D1426 T1427 A1431 E1434 A1439 M1446 D1447 L1448 F1449
Q1450 N1451 G1452 N1453 W1454 T1455 M1456 Q1457 N1458 P1459 S1460 P1461 C1465 K1469 I1470 K1471 K1472 M1473 L1474 C1477 A1481 G1482 G1483 L1484 K1490 Q1491 N1492 I1496 L1497 Q1498 D1499 D1507 V1510 K1511 K1522 N1523 K1524 I1525 W1526 F1535 N1541 T1542 Q1543 A1544 L1545 P1546 P1547 S1548 Q1549
E1550 V1551 N1552 D1553 A1554 I1555 K1556 Q1557 M1558 K1559 L1564 A1565 S1568 D1571 R1572 N1575 V1590 K1591 V1592 N1596 W1599 S1603 N1607 V1608 I1609 N1610 N1611 A1612 I1613 E1622 N1623 P1624 S1625 H1626 T1630 A1631 F1632 N1633 H1634 P1635 L1636 N1637 L1638 T1639 K1640 Q1641 Q1642 M1649
D1654 V1655 L1656 I1659 C1660 V1661 I1662 F1663 A1664 M1665 S1666 A1670 Q1678 E1679 R1680 K1683 A1684 K1685 H1686 L1687 Q1688 F1689 I1690 S1691 G1692 I1697 S1701 W1705 D1706 A1714 T1715 L1716 V1717 I1718 I1719 I1720 F1721 I1722 C1723 F1724 Q1725 Q1726 K1727 S1728 Y1729 V1730 S1731 N1734 L1740
L1741 L1744 Y1745 I1749 Y1754 P1755 A1756 K1761 A1766 Y1767 L1770 V1773 N1774 L1775 F1776 I1779 N1780 G1781 S1782 V1783 A1784 T1785 F1786 V1787 L1788 E1789 LEU PHE THR ASP ASN LYS L1796 N1797 N1798 I1799 N1800 L1803 K1804 F1807 L1808 I1809 F1810 P1811 H1812 F1813 C1814 L1815 G1816 R1817
G1818 L1819 I1820 D1821 M1822 M1828 L1832 F1835 G1836 F1840 V1841 S1842 L1853 F1854 A1855 M1856 A1857 V1858 E1859 G1860 V1861 V1862 F1863 I1866 T1867 I1870 F1875 ILE ARG PRO ARG PRO VAL ASN ALA LYS LEU SER PRO LEU ASN ASP GLU ASP GLU ASP VAL ARG ARG GLU ARG GLN
ARG ILE LEU ASP GLY GLY GLY GLN ASN ASP ILE LEU GLU ILE LYS E1916 L1917 T1918 K1919 I1920 Y1921 R1922 ARG LYS ARG LYS PRO ALA VAL ASP ARG ILE C1933 V1934 G1935 I1936 P1937 P1938 G1939 E1940 C1941 F1942 G1943 L1944 L1945 G1946 V1947 N1948 G1949 A1950 G1951 K1952 S1953 S1954 T1955 F1956 K1957 M1958 L1959 T1960
G1961 D1962 T1963 T1964 V1965 T1966 R1967 G1968 D1969 A1970 F1971 L1972 N1973 K1974 N1975 S1976 I1977 L1978 S1979 N1980 I1981 H1982 E1983 V1984 H1985 Q1986 N1987 M1988 G1989 Q1993 A1996 T1997 T1998 T2002 E2005 H2006 F2009 G2015 V2016 P2017 E2020 V2021 G2022 K2023 V2024 G2025 E2026 I2029 R2030 K2031 L2032 G2033



• Molecule 2: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-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	790156	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.485	Depositor
Minimum map value	-0.354	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	261.308, 261.308, 261.308	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	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, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.49	0/12840	0.69	9/17577 (0.1%)

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	15

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1636	LEU	CA-CB-CG	8.43	134.69	115.30
1	A	367	LEU	CA-CB-CG	6.60	130.48	115.30
1	A	1497	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	569	ILE	CG1-CB-CG2	-5.88	98.46	111.40
1	A	1815	LEU	CA-CB-CG	5.63	128.25	115.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	384	LEU	Peptide
1	A	386	THR	Peptide
1	A	586	MET	Peptide
1	A	589	VAL	Peptide
1	A	94	VAL	Peptide

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	12626	0	10430	213	0
2	B	61	0	52	0	0
3	C	28	0	25	0	0
4	A	70	0	65	0	0
All	All	12785	0	10572	213	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 9.

The worst 5 of 213 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:1817:ARG:O	1:A:1821:ASP:HB2	1.80	0.81
1:A:1816:GLY:O	1:A:1820:ILE:HB	1.83	0.79
1:A:1402:LEU:O	1:A:1406:ASN:HB2	1.86	0.76
1:A:1685:LYS:O	1:A:1689:PHE:HB2	1.86	0.75
1:A:1461:PRO:HB3	1:A:1483:GLY:H	1.53	0.73

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	1869/2305 (81%)	1603 (86%)	263 (14%)	3 (0%)	47 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2017	PRO
1	A	1461	PRO
1	A	1459	PRO

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	943/2027 (46%)	929 (98%)	14 (2%)	65 79

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	767	TRP
1	A	1417	ARG
1	A	1552	ASN
1	A	1472	LYS
1	A	1523	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1523	ASN
1	A	1552	ASN
1	A	1734	ASN
1	A	1610	ASN
1	A	1623	ASN

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)

7 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	2,1	14,14,15	0.83	1 (7%)	17,19,21	0.65	0
2	NAG	B	2	2	14,14,15	0.73	1 (7%)	17,19,21	1.16	2 (11%)
2	BMA	B	3	2	11,11,12	0.62	0	15,15,17	0.88	1 (6%)
2	BMA	B	4	2	11,11,12	0.71	0	15,15,17	0.90	0
2	BMA	B	5	2	11,11,12	0.91	0	15,15,17	0.95	0
3	NAG	C	1	3,1	14,14,15	0.36	0	17,19,21	0.77	0
3	NAG	C	2	3	14,14,15	0.65	0	17,19,21	1.20	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	2,1	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	BMA	B	4	2	-	0/2/19/22	0/1/1/1
2	BMA	B	5	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O5-C1	-2.97	1.39	1.43
2	B	2	NAG	O5-C1	-2.45	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	NAG	C2-N2-C7	3.23	127.51	122.90
2	B	2	NAG	C2-N2-C7	2.98	127.14	122.90
2	B	2	NAG	C1-O5-C5	2.91	116.13	112.19
2	B	3	BMA	O2-C2-C3	-2.12	105.89	110.14

There are no chirality outliers.

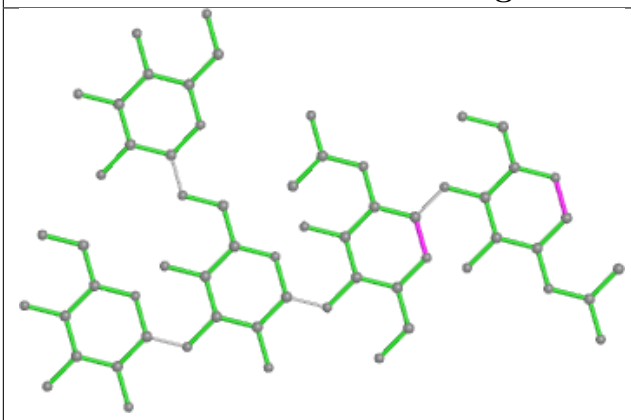
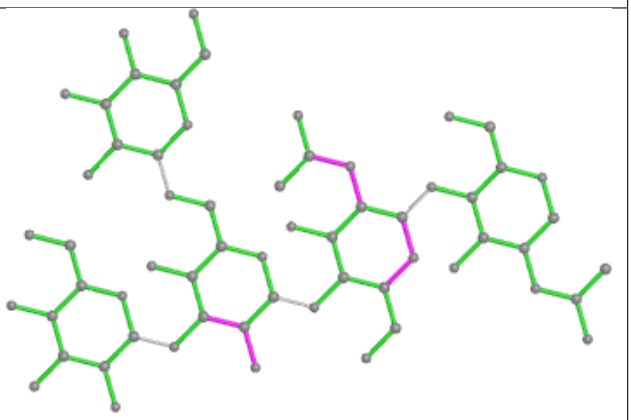
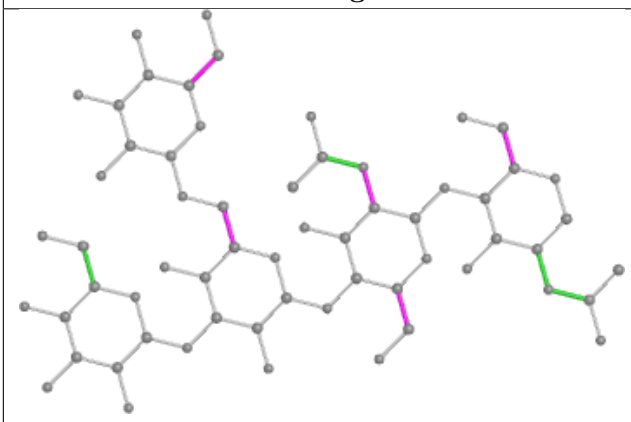
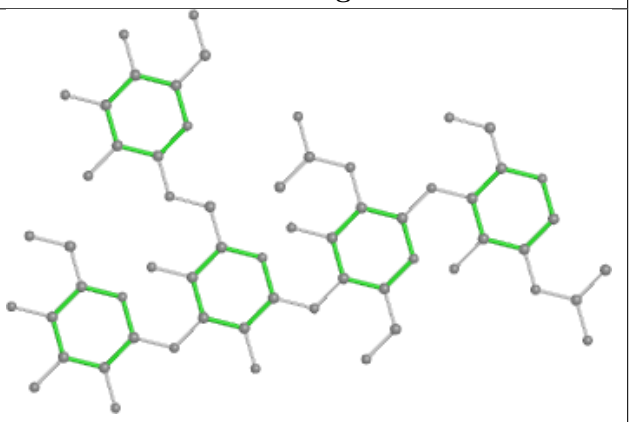
5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	BMA	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	5	BMA	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

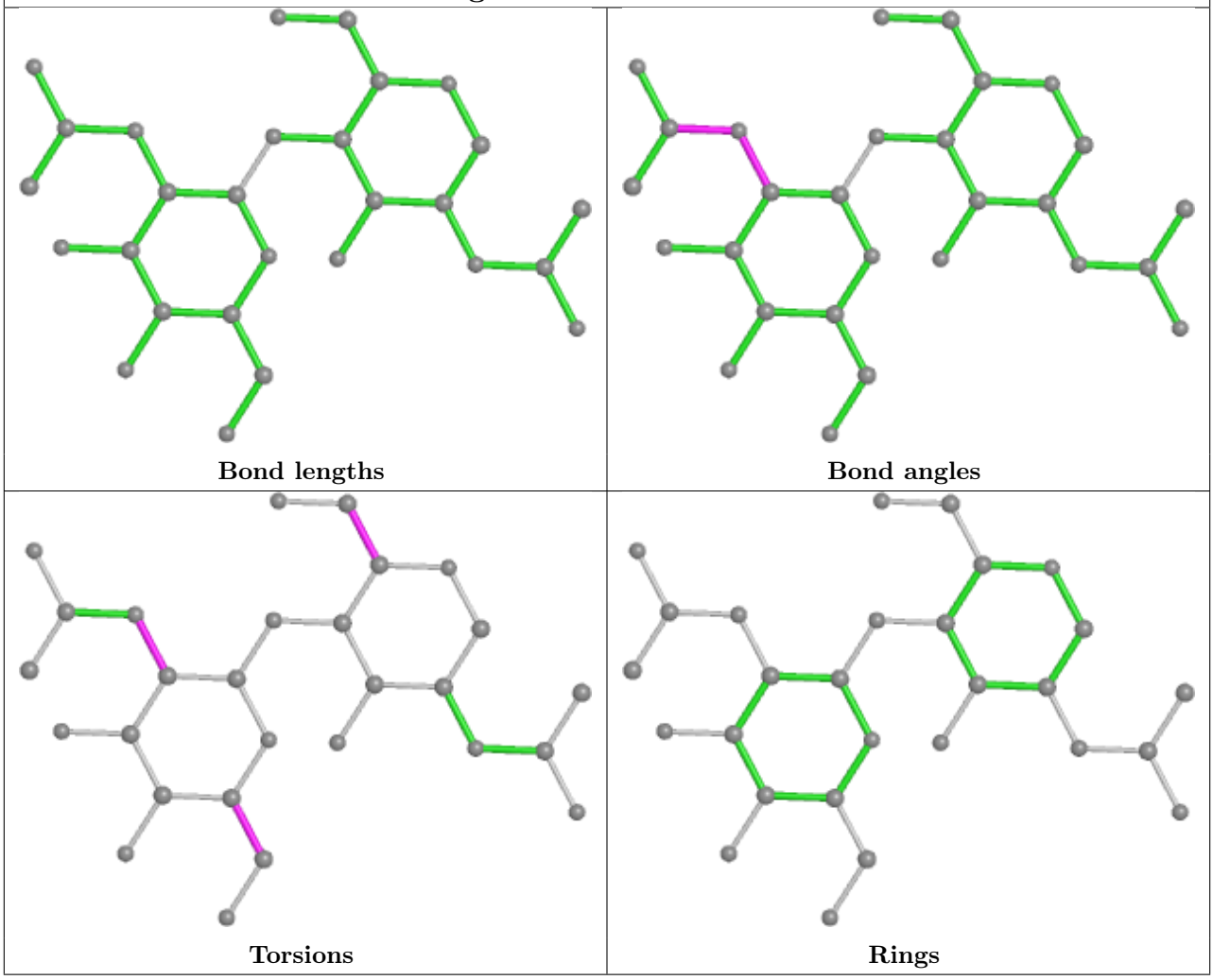
There are no ring outliers.

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.

Oligosaccharide Chain B	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain C



5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	2305	1	14,14,15	0.82	2 (14%)	17,19,21	0.85	1 (5%)
4	NAG	A	2301	1	14,14,15	0.48	0	17,19,21	0.74	1 (5%)
4	NAG	A	2303	1	14,14,15	0.25	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	2302	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	A	2304	1	14,14,15	0.30	0	17,19,21	0.45	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	2305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2302	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2304	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)
4	A	2305	NAG	O5-C1	2.21	1.47	1.43
4	A	2305	NAG	C1-C2	2.03	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2305	NAG	C1-O5-C5	2.79	115.97	112.19
4	A	2301	NAG	C1-O5-C5	2.67	115.81	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2301	NAG	O5-C5-C6-O6
4	A	2305	NAG	C8-C7-N2-C2
4	A	2305	NAG	O7-C7-N2-C2
4	A	2301	NAG	C4-C5-C6-O6
4	A	2303	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

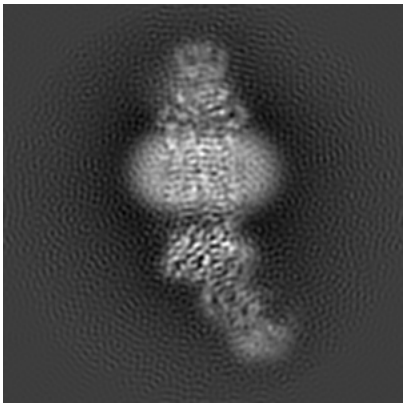
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6724. These allow visual inspection of the internal detail of the map and identification of artifacts.

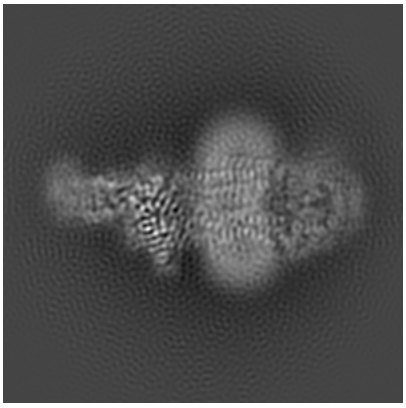
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

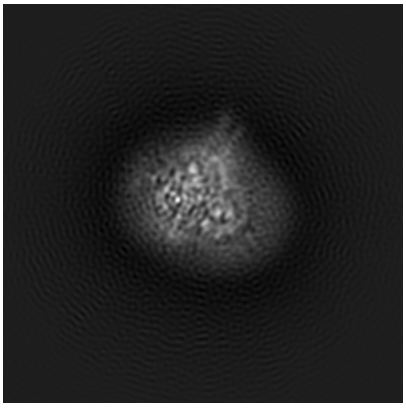
6.1.1 Primary map



X



Y

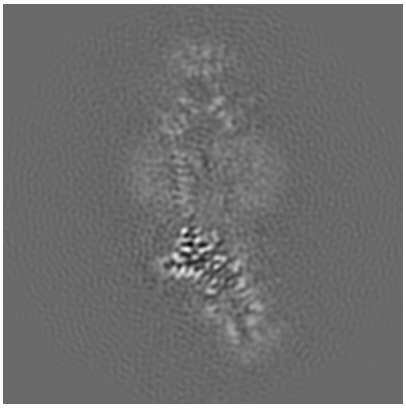


Z

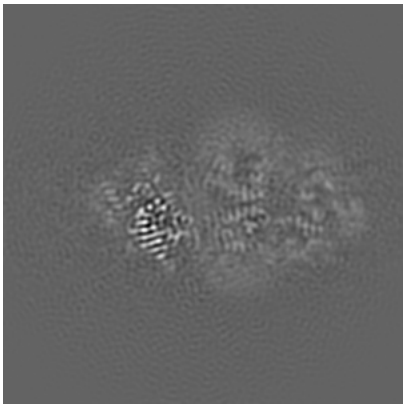
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

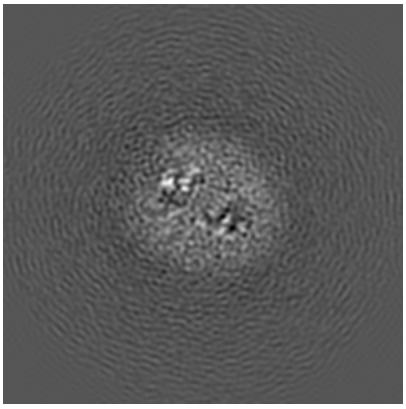
6.2.1 Primary map



X Index: 100



Y Index: 100

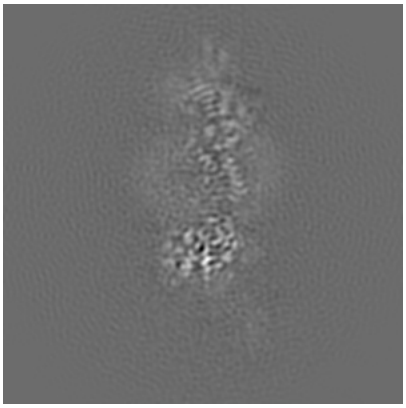


Z Index: 100

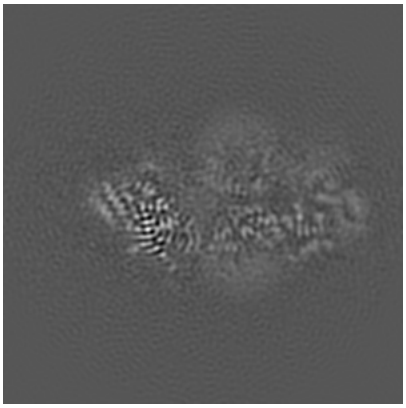
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

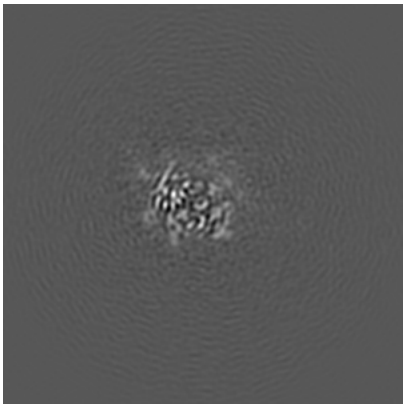
6.3.1 Primary map



X Index: 87



Y Index: 102



Z Index: 76

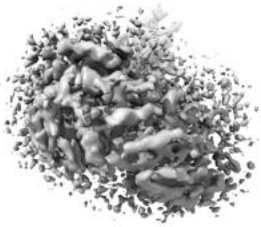
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

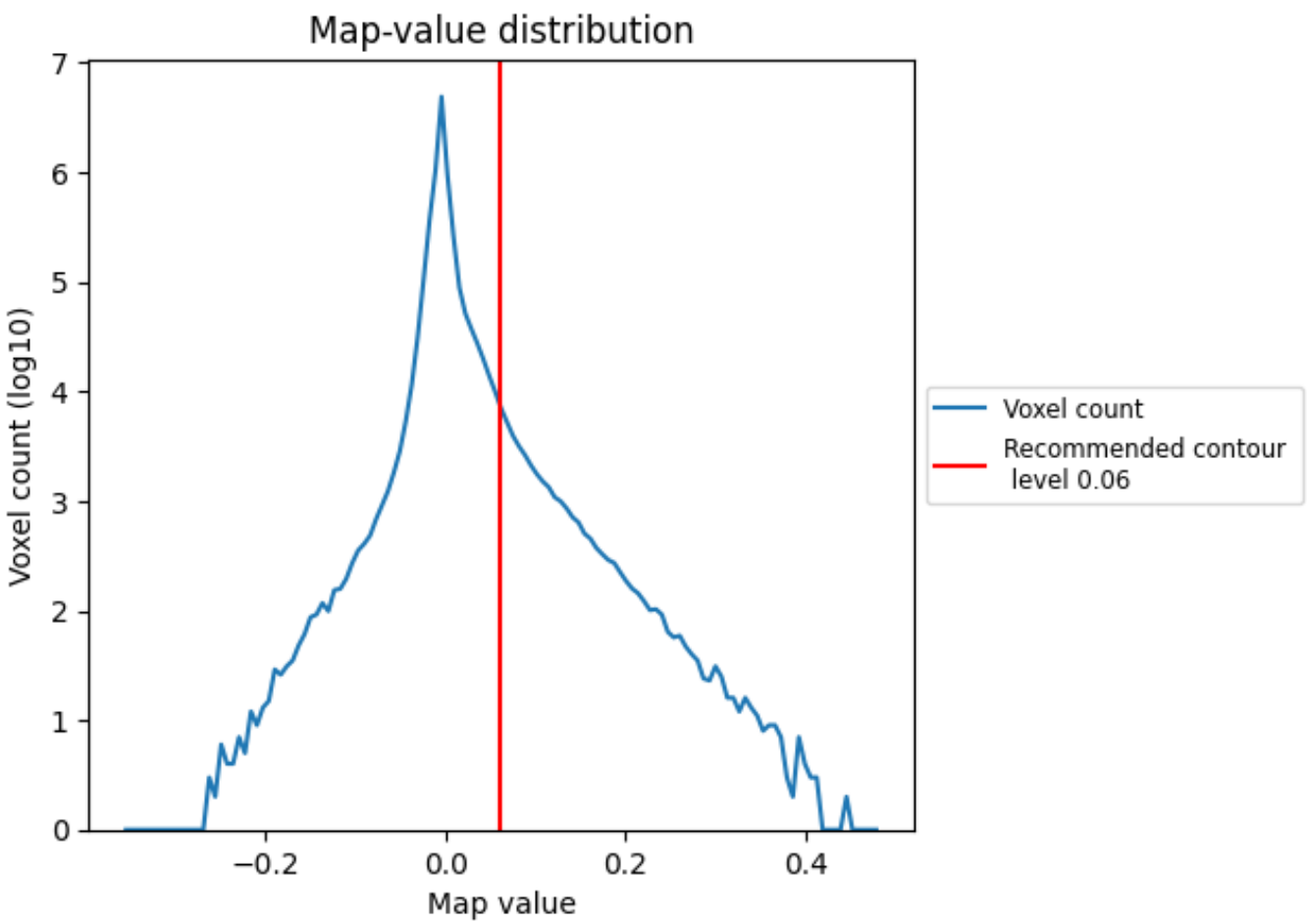
6.5 Mask visualisation (i)

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

7 Map analysis (i)

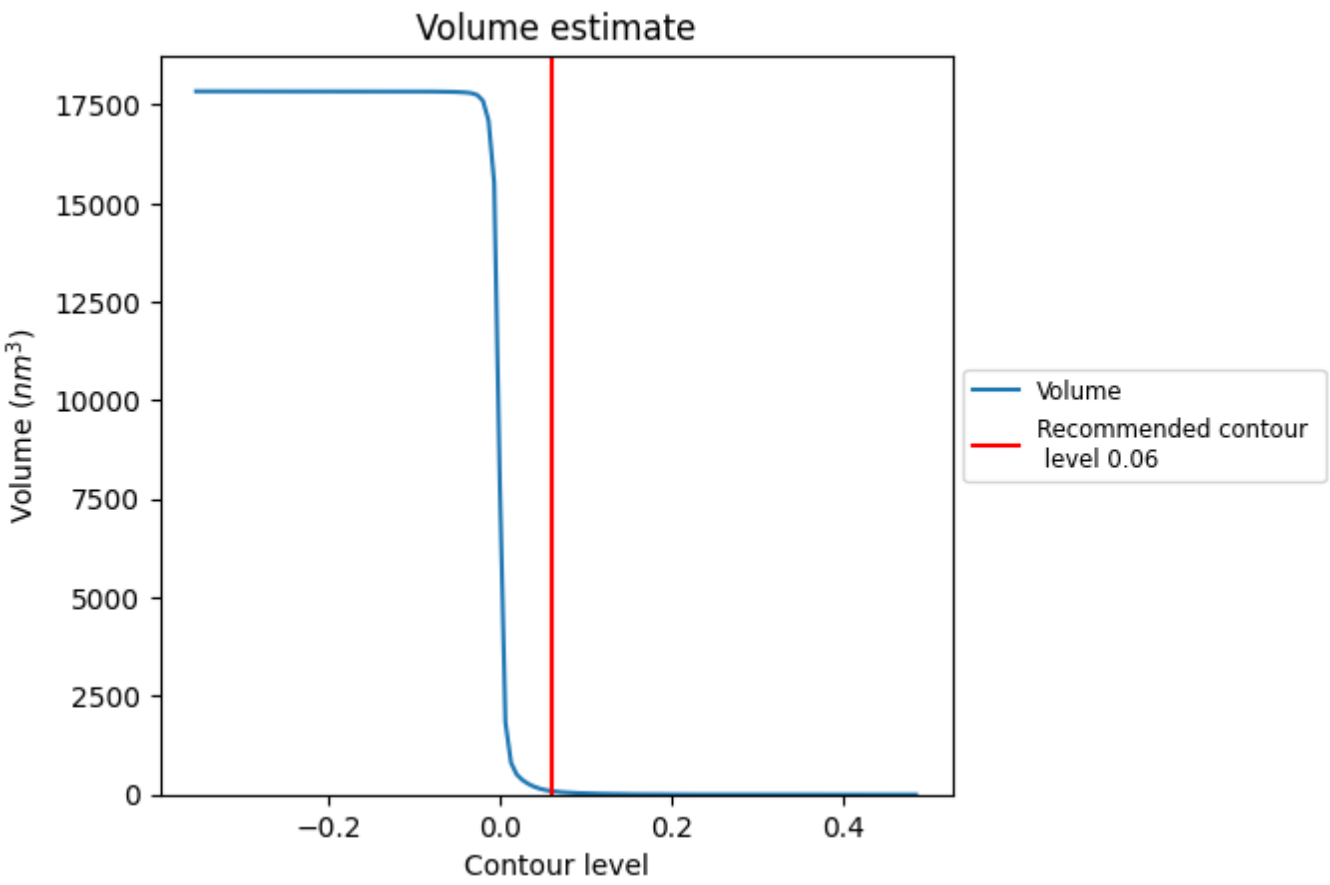
This section contains the results of statistical analysis of the map.

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.

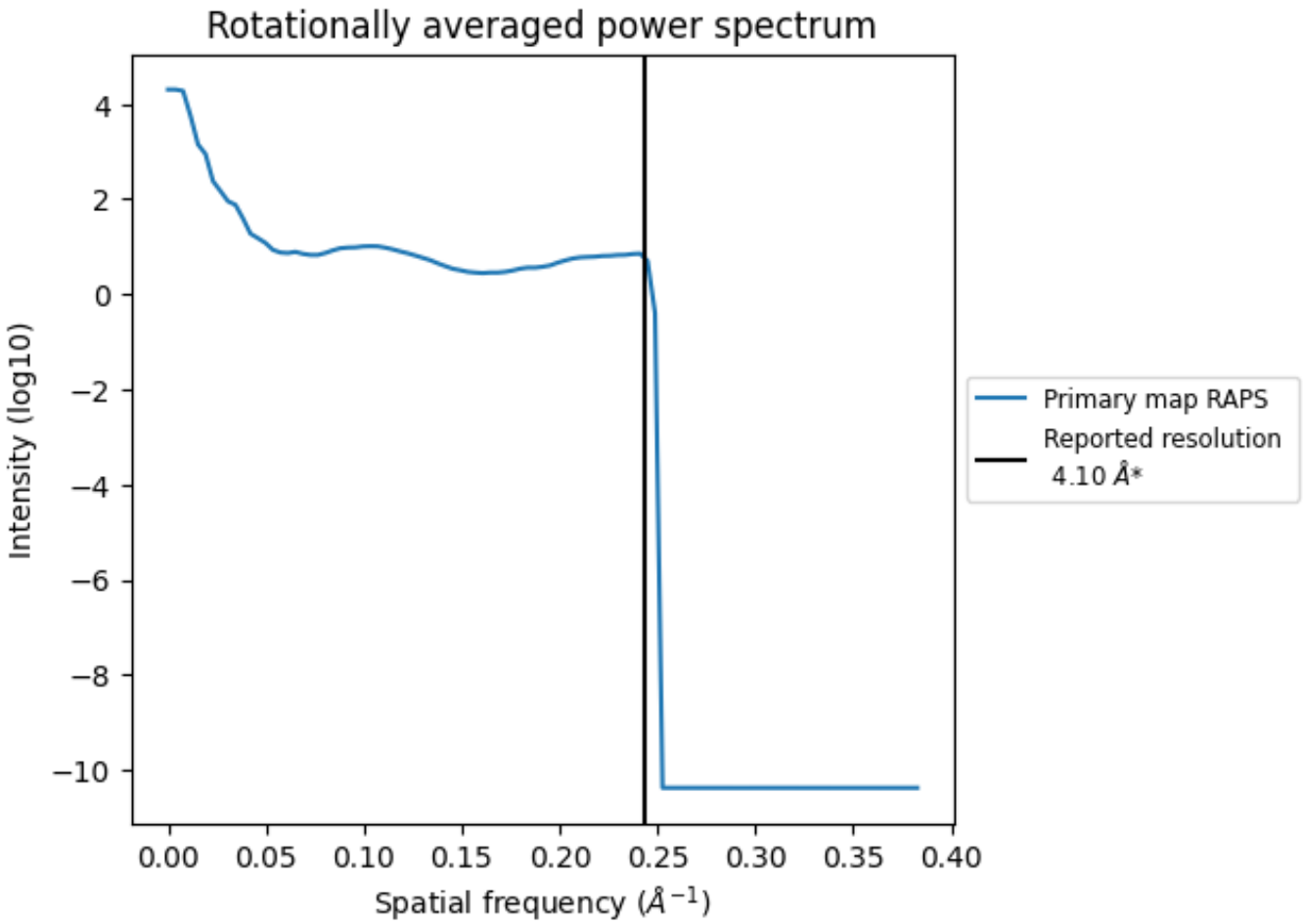
7.2 Volume estimate (i)



The volume at the recommended contour level is 89 nm^3; this corresponds to an approximate mass of 81 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 0.244 Å^{-1}

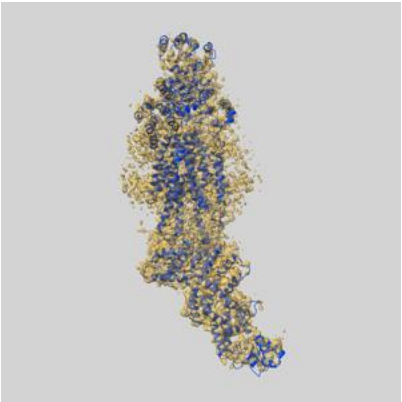
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

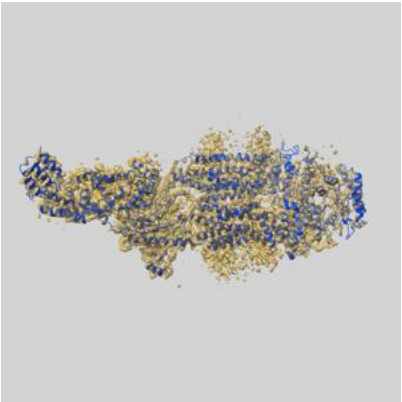
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6724 and PDB model 5XJY. Per-residue inclusion information can be found in section 3 on page 6.

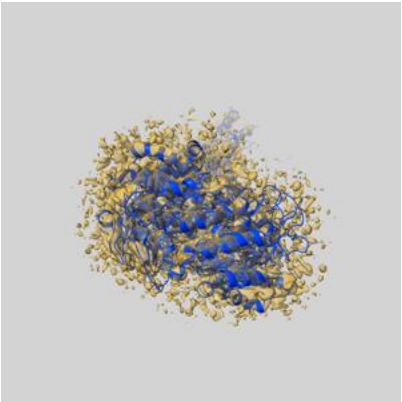
9.1 Map-model overlay (i)



X



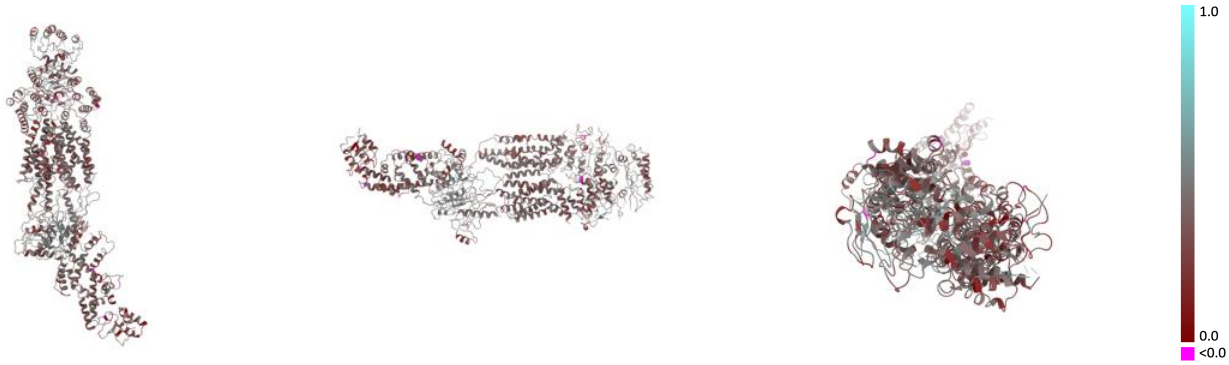
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

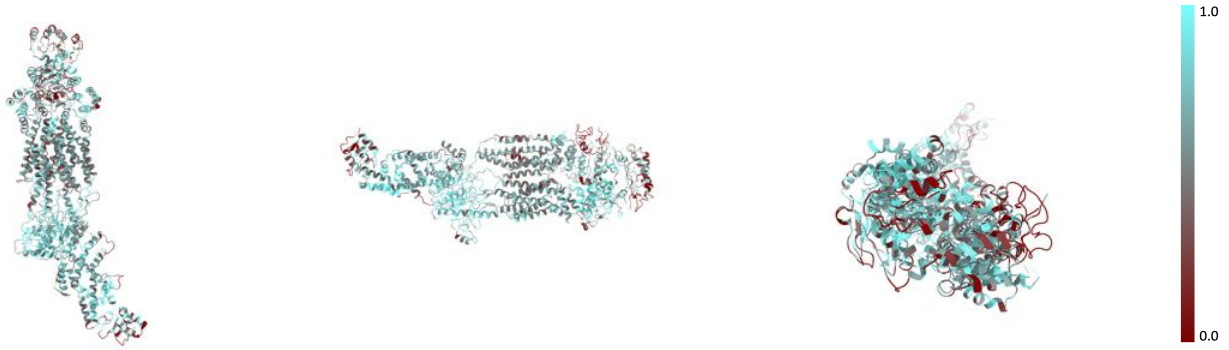
9.2 Q-score mapped to coordinate model (i)



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.

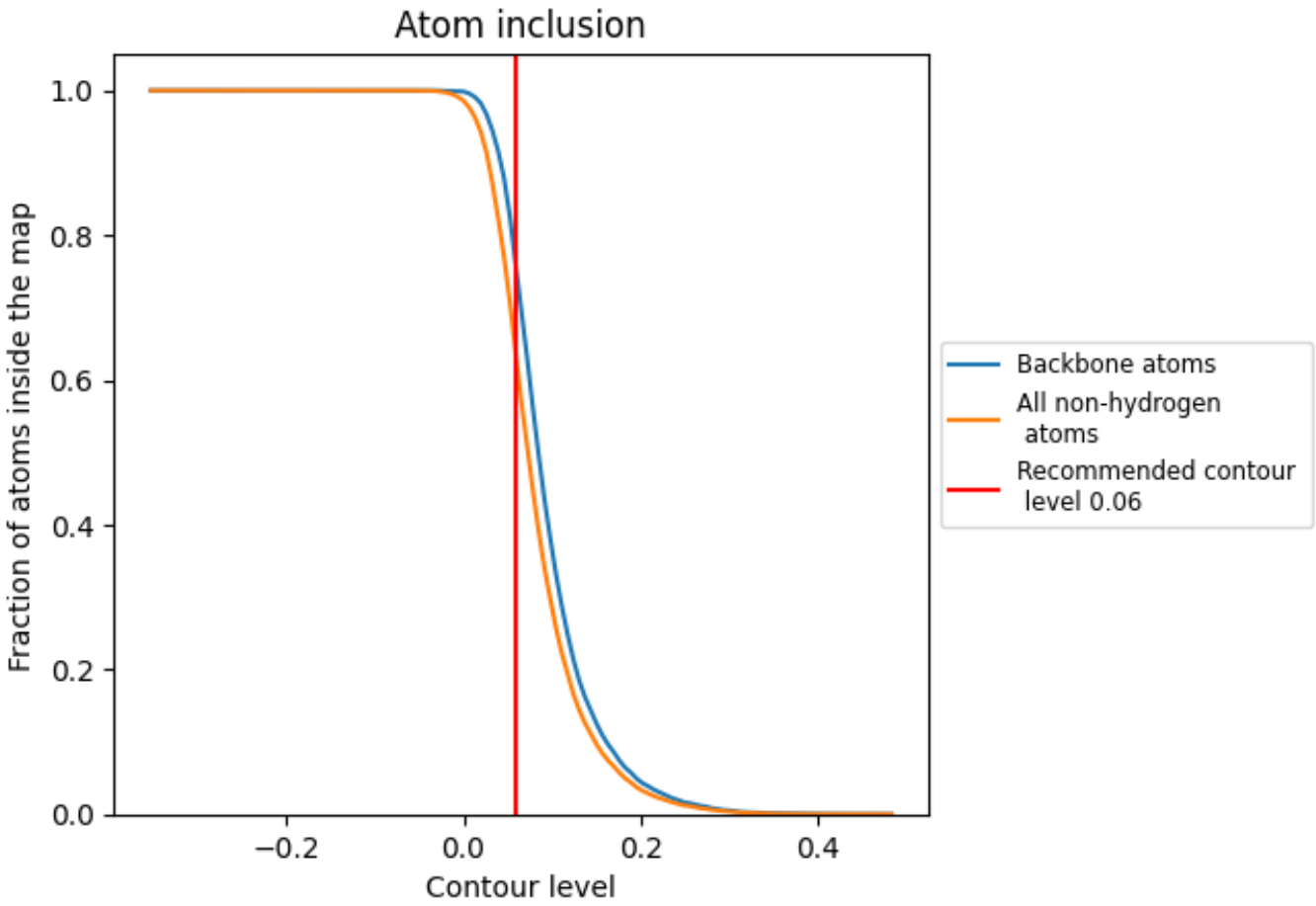
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6276	0.3870
A	0.6268	0.3860
B	0.7705	0.5080
C	0.6786	0.4410