Full wwPDB EM Validation Report (i)

Nov 6, 2022 – 09:18 AM EST

PDB ID	:	6CMX
EMDB ID	:	EMD-7526
Title	:	Human Teneurin 2 extra-cellular region
Authors	:	Shalev-Benami, M.; Li, J.; Sudhof, T.; Skiniotis, G.; Arac, D.
Deposited on	:	2018-03-06
Resolution	:	3.10 Å(reported)

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 (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:

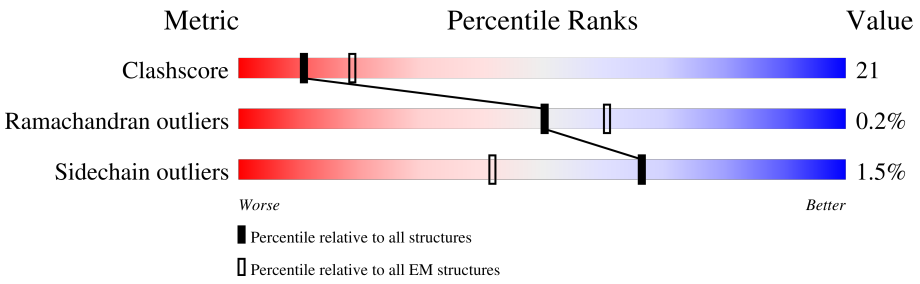
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 3.10 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	1999	40% 24% 35%
2	B	3	33% 100%
3	C	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1	X	-	-	-
4	NAG	A	2704	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	2708	X	-	-	-

2 Entry composition (i)

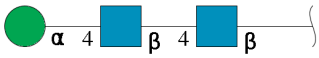
There are 5 unique types of molecules in this entry. The entry contains 10139 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Teneurin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1300	9919	6354	1729	1803	33	0	0

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

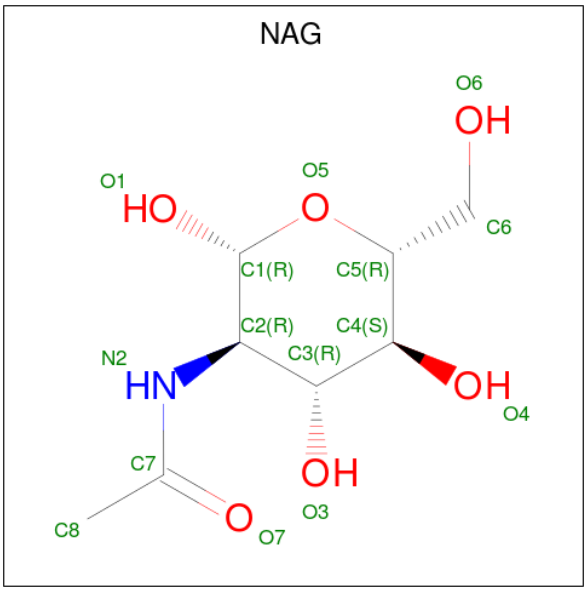


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	3	39	22	2	15	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran ose.

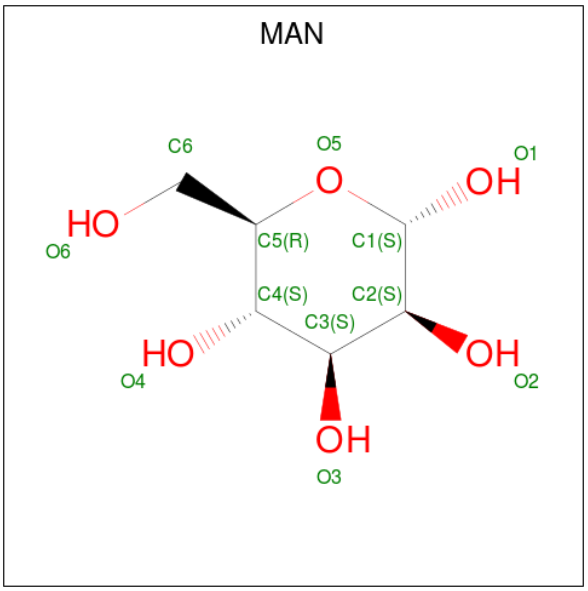
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	C	2	22	12	10	0	0

- 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	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



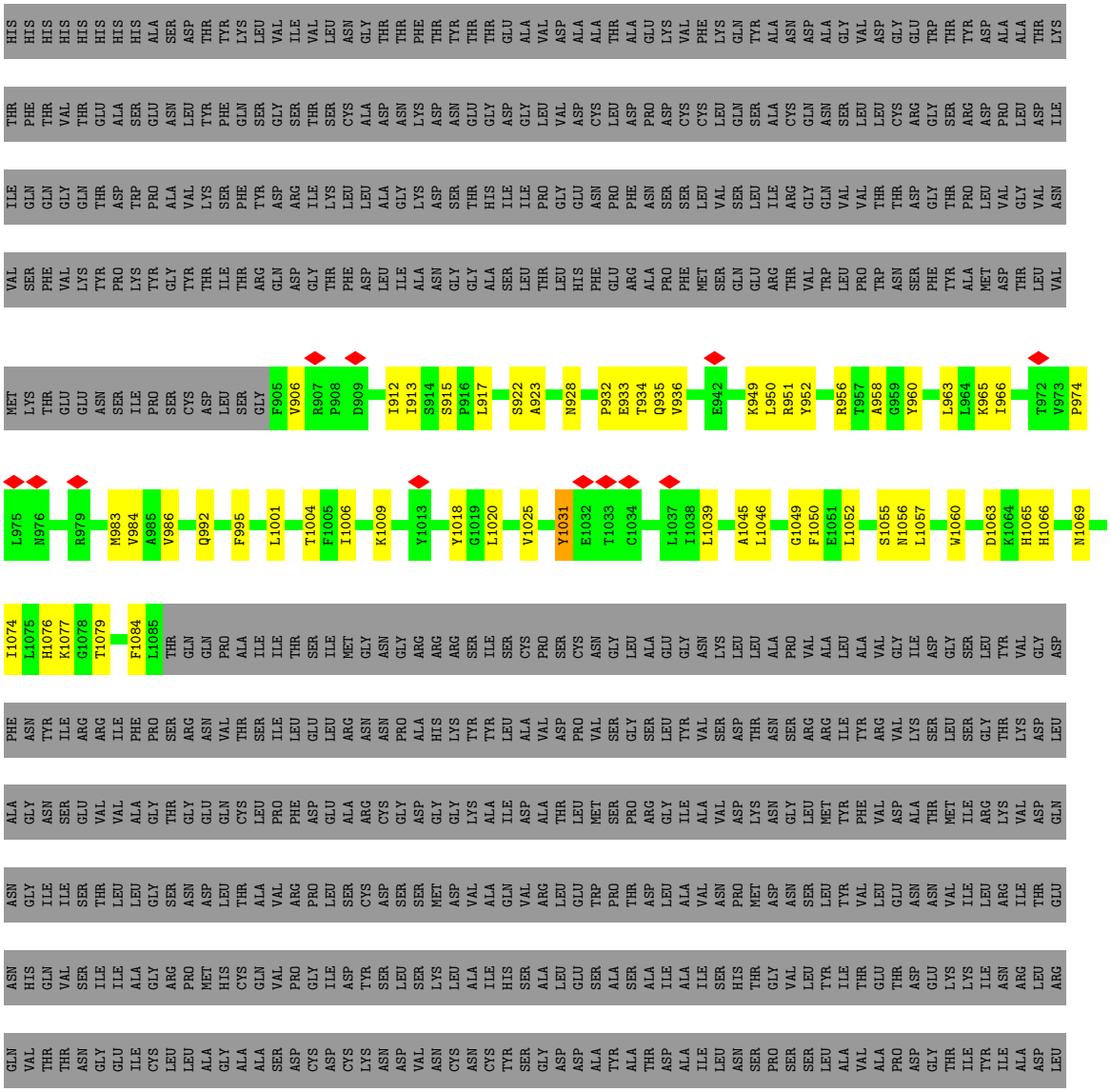
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	A	1	33	18	15	0
			Total	C	O	
5	A	1	33	18	15	0
			Total	C	O	
5	A	1	33	18	15	0

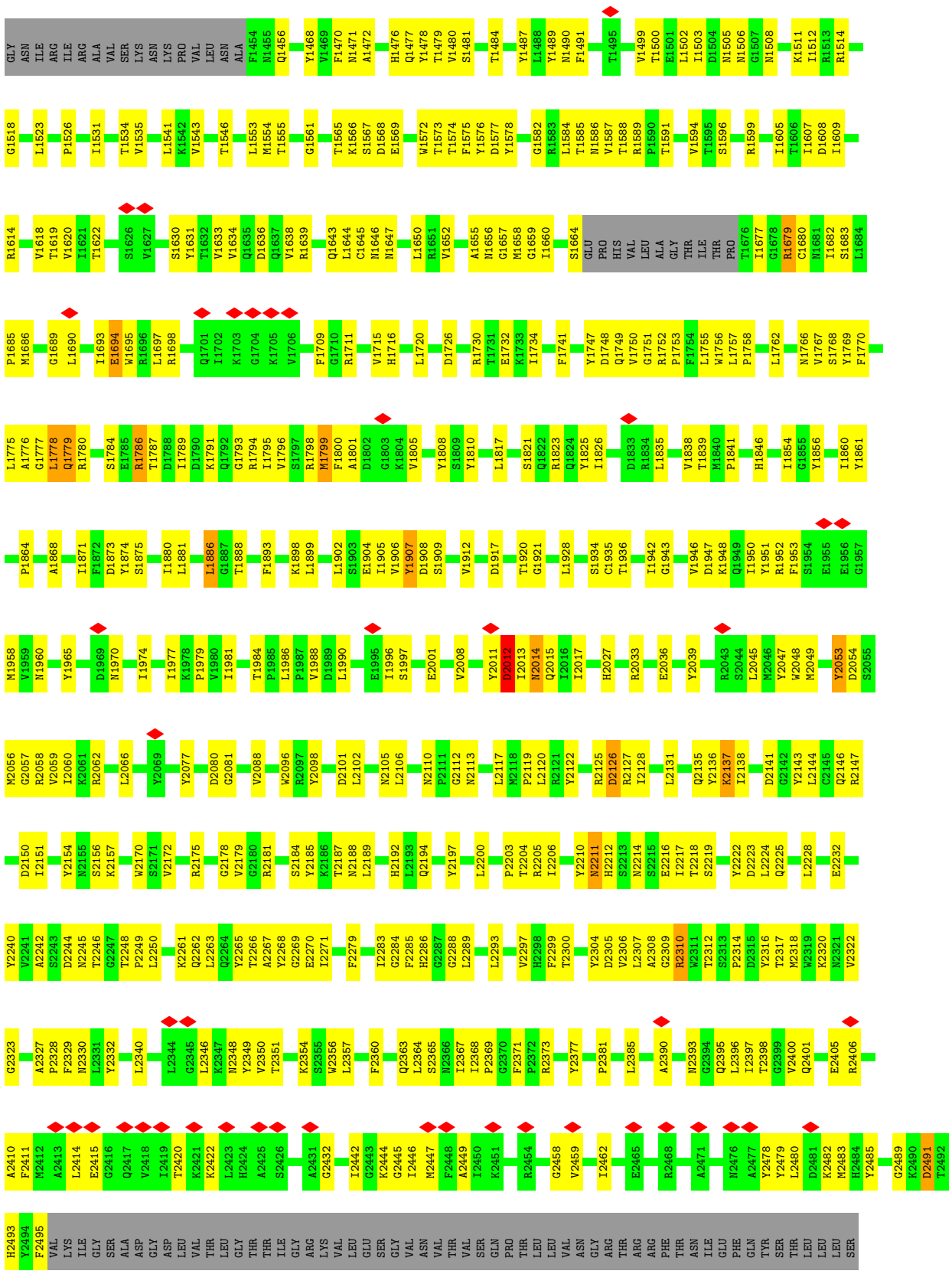
3 Residue-property plots (i)

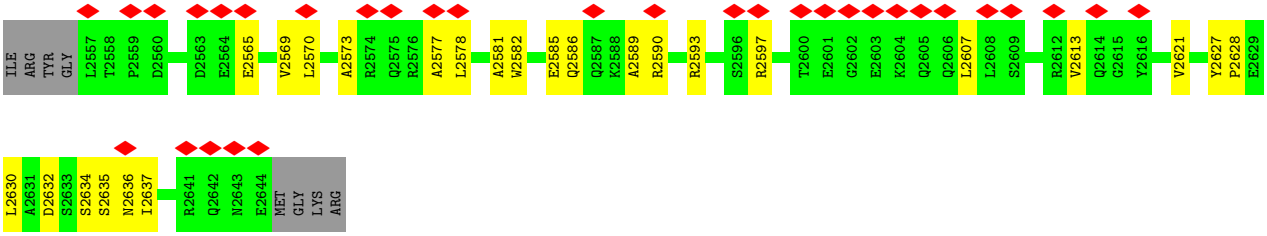
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Teneurin-2

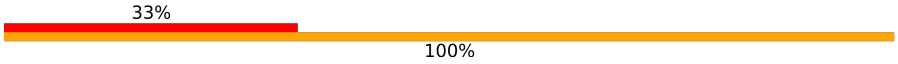
Chain A: 40% 24% • 35%




GLY ASN ILE ARG ILE ARG ALA VAL SER LYS ASN LYS PRO VAL LEU ASN ALA F1454 N1455 Q1456 Y1468 V1469 F1470 N1471 A1472 H1476 Q1477 Y1478 T1479 V1480 S1481 T1484 Y1487 L1488 Y1489 N1490 F1491 T1495 V1499 T1500 E1501 L1502 I1503 D1504 N1505 N1506 G1507 N1508 K1511 I1512 R1513 R1514
G1518 L1523 P1526 I1531 T1534 V1535 L1541 K1542 V1543 T1546 L1553 M1554 T1555 G1561 T1565 K1566 S1567 D1568 E1569 W1572 T1573 T1574 F1575 Y1576 D1577 Y1578 G1582 R1583 L1584 T1585 N1586 V1587 T1588 R1589 P1590 T1591 V1594 T1595 S1596 R1599 T1605 T1606 I1607 D1608 I1609
R1614 V1618 T1619 V1620 I1621 T1622 S1626 V1627 S1630 Y1631 T1632 V1633 V1634 Q1635 D1636 Q1637 V1638 R1639 Q1643 L1644 C1645 N1646 N1647 L1650 R1651 V1652 A1655 N1656 N1657 G1658 G1659 I1660 S1664 GLU PRO HIS VAL LEU ALA GLY THR ILE THR PRO T1676 I1677 G1678 R1679 C1680 N1681 I1682 S1683 L1684
P1685 M1686 G1689 L1690 I1693 E1694 W1695 R1696 L1697 R1698 Q1701 I1702 K1703 G1704 K1705 V1706 F1709 G1710 R1711 V1715 H1716 L1720 D1726 R1730 T1731 E1732 K1733 I1734 F1741 Y1747 D1748 Q1749 V1750 G1751 R1752 P1753 F1754 L1755 W1756 L1757 P1758 L1762 N1766 V1767 S1768 Y1769 F1770
L1775 A1776 G1777 L1778 Q1779 R1780 S1784 E1785 R1786 T1787 D1788 I1789 D1790 K1791 Q1792 G1793 R1794 I1795 V1796 S1797 R1798 M1799 F1800 A1801 D1802 G1803 K1804 V1805 Y1808 S1809 Y1810 L1817 S1821 Q1822 R1823 Q1824 Y1825 I1826 D1833 R1834 L1835 V1838 T1839 M1840 P1841 H1846 I1854 G1855 Y1856 I1860 Y1861
P1864 A1868 I1871 F1872 D1873 Y1874 S1875 I1880 L1881 L1886 G1887 T1888 F1893 K1898 L1899 L1902 S1903 E1904 I1905 V1906 Y1907 D1908 S1909 V1912 D1917 T1920 G1921 L1928 S1934 C1935 T1936 I1942 G1943 V1946 D1947 K1948 Q1949 I1950 Y1951 R1952 F1953 S1954 E1955 E1956 G1957
M1958 V1959 N1960 Y1965 D1969 N1970 I1974 I1977 K1978 P1979 V1980 I1981 T1984 P1985 L1986 P1987 V1988 D1989 L1990 E1995 I1996 S1997 E2001 V2008 Y2011 D2012 I2013 N2014 Q2015 I2016 I2017 H2027 R2033 E2036 Y2039 R2043 S2044 L2045 M2046 Y2047 W2048 M2049 Y2053 D2054 S2055
M2056 G2057 R2058 V2059 I2060 K2061 R2062 L2066 Y2069 Y2077 D2080 G2081 V2088 W2096 R2097 Y2098 D2101 L2102 N2105 L2106 N2110 P2111 G2112 N2113 L2117 M2118 P2119 L2120 R2121 Y2122 R2125 D2126 R2127 I2128 L2131 Q2135 Y2136 K2137 I2138 D2141 G2142 Y2143 L2144 C2145 Q2146 R2147
D2150 I2151 Y2154 N2155 S2156 K2157 W2170 S2171 V2172 R2175 G2178 V2179 G2180 R2181 S2184 Y2185 K2186 T2187 N2188 L2189 H2192 L2193 Q2194 Y2197 L2200 P2203 T2204 R2205 I2206 Y2210 N2211 H2212 S2213 N2214 S2215 E2216 I2217 T2218 S2219 Y2222 D2223 L2224 Q2225 L2228 E2232
Y2240 V2241 A2242 S2243 D2244 N2245 T2246 G2247 T2248 P2249 L2250 K2261 Q2262 L2263 Q2264 Y2265 T2266 A2267 Y2268 G2269 E2270 I2271 F2279 I2283 G2284 F2285 H2286 G2287 G2288 L2289 L2293 V2297 H2298 F2299 T2300 Y2304 D2305 V2306 L2307 A2308 G2309 R2310 W2311 T2312 S2313 P2314 D2315 Y2316 T2317 M2318 W2319 K2320 N2321 V2322
G2323 A2327 P2328 F2329 N2330 L2331 Y2332 L2340 L2344 G2345 L2346 K2347 N2348 Y2349 V2350 T2351 K2354 S2355 W2356 L2357 F2360 Q2363 G2364 S2365 N2366 I2367 I2368 P2369 G2370 F2371 P2372 R2373 Y2377 P2381 L2385 A2390 N2393 G2394 Q2395 L2396 I2397 T2398 G2399 V2400 Q2401 E2405 R2406
A2410 F2411 M2412 A2413 L2414 E2415 G2416 Q2417 V2418 I2419 T2420 K2421 K2422 L2423 H2424 A2425 S2426 A2431 G2432 I2442 G2443 K2444 G2445 I2446 M2447 F2448 A2449 I2450 K2451 R2454 G2458 V2459 I2462 E2465 R2468 A2471 N2476 A2477 Y2478 Y2479 L2480 D2481 K2482 M2483 H2484 Y2485 G2489 K2490 D2491 T2492
H2493 Y2494 F2495 VAL LYS ILE GLY SER ALA ASP GLY ASP LEU VAL THR LEU GLY THR THR ILE GLY ARG LYS VAL LEU GLU SER GLY VAL ASN VAL THR VAL SER GLN PRO THR LEU LEU VAL ASN GLY ARG THR ARG ARG PHE THR ASN ILE GLU PHE GLN TYR SER THR LEU LEU LEU SER



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

Chain B: 

• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose

Chain C:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	426107	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 ($e^-/Å^2$)	44	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	0.373	Depositor
Minimum map value	-0.250	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	260.0, 260.0, 260.0	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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: MAN, 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	0.38	0/10159	0.55	2/13820 (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	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	986	VAL	CG1-CB-CG2	7.40	122.75	110.90
1	A	2053	TYR	CA-CB-CG	5.10	123.09	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1907	TYR	Peptide
1	A	2012	ASP	Peptide
1	A	2137	LYS	Peptide
1	A	2432	GLY	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	9919	0	9403	400	0
2	B	39	0	34	2	0
3	C	22	0	19	1	0
4	A	126	0	115	14	0
5	A	33	0	30	2	0
All	All	10139	0	9601	410	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 21.

All (410) 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:1646:ASN:O	4:A:2705:NAG:C1	1.97	1.11
1:A:2128:ILE:HD11	1:A:2310:ARG:HD2	1.50	0.91
1:A:1888:THR:OG1	1:A:2141:ASP:OD2	1.89	0.88
1:A:1577:ASP:HB2	1:A:1586:ASN:OD1	1.74	0.88
1:A:933:GLU:HG2	1:A:1620:VAL:HG11	1.57	0.85
1:A:1573:THR:OG1	1:A:2444:LYS:O	1.94	0.84
1:A:960:TYR:O	1:A:1009:LYS:NZ	2.11	0.83
4:A:2706:NAG:H3	4:A:2706:NAG:H82	1.61	0.83
1:A:2126:ASP:O	1:A:2310:ARG:NH2	2.11	0.82
1:A:1732:GLU:OE2	1:A:1747:TYR:OH	1.98	0.81
1:A:1917:ASP:OD2	1:A:1920:THR:OG1	1.98	0.81
1:A:2012:ASP:O	1:A:2014:ASN:N	2.12	0.79
1:A:2284:GLY:N	1:A:2288:GLY:O	2.16	0.78
1:A:1835:LEU:HD11	1:A:2323:GLY:HA3	1.68	0.76
1:A:1491:PHE:CE1	1:A:1502:LEU:HD13	2.21	0.76
1:A:933:GLU:OE2	1:A:2400:VAL:HG12	1.86	0.75
1:A:2349:TYR:O	1:A:2422:LYS:NZ	2.20	0.75
1:A:1555:THR:OG1	1:A:1565:THR:OG1	2.03	0.75
1:A:1886:LEU:N	1:A:1886:LEU:HD23	2.01	0.74
1:A:1756:TRP:NE1	1:A:2351:THR:O	2.22	0.73
1:A:1904:GLU:OE1	1:A:2627:TYR:OH	2.07	0.73
1:A:1585:THR:HB	4:A:2704:NAG:H82	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:TYR:OH	1:A:1561:GLY:O	2.07	0.71
1:A:2573:ALA:HB1	1:A:2632:ASP:CB	2.20	0.71
1:A:1476:HIS:NE2	1:A:1479:THR:OG1	2.24	0.70
1:A:2245:ASN:ND2	1:A:2340:LEU:O	2.24	0.70
1:A:1799:MET:HB3	1:A:1805:VAL:HG23	1.72	0.70
4:A:2705:NAG:O7	4:A:2705:NAG:O3	2.05	0.69
1:A:2062:ARG:HH22	1:A:2340:LEU:HD22	1.58	0.69
1:A:2172:VAL:HG22	1:A:2187:THR:HG22	1.74	0.69
1:A:2261:LYS:NZ	1:A:2279:PHE:O	2.24	0.69
1:A:1596:SER:HB2	4:A:2704:NAG:H83	1.75	0.68
1:A:2223:ASP:OD1	1:A:2224:LEU:N	2.26	0.68
5:A:2717:MAN:H3	3:C:2:MAN:O3	1.94	0.68
2:B:1:NAG:O3	2:B:1:NAG:H82	1.93	0.68
1:A:2228:LEU:HD22	1:A:2283:ILE:HD12	1.76	0.68
1:A:2310:ARG:NH2	1:A:2332:TYR:CD2	2.62	0.67
1:A:1568:ASP:OD1	1:A:1569:GLU:N	2.26	0.67
1:A:1645:CYS:SG	1:A:1646:ASN:N	2.67	0.67
1:A:934:THR:O	1:A:936:VAL:N	2.27	0.67
1:A:2248:THR:HB	1:A:2285:PHE:O	1.94	0.66
1:A:1775:LEU:HD21	1:A:2422:LYS:HA	1.77	0.66
1:A:1856:TYR:HB3	1:A:1881:LEU:HD12	1.77	0.66
1:A:1481:SER:HG	1:A:1484:THR:HG1	1.40	0.66
1:A:2128:ILE:HD11	1:A:2310:ARG:CD	2.25	0.65
1:A:1762:LEU:HD11	1:A:2360:PHE:HE1	1.59	0.65
1:A:1531:ILE:HG12	1:A:1546:THR:HG22	1.78	0.65
1:A:2001:GLU:HA	1:A:2008:VAL:HG22	1.79	0.65
1:A:1614:ARG:HH12	1:A:1881:LEU:HD21	1.62	0.64
1:A:1846:HIS:ND1	1:A:1861:TYR:OH	2.28	0.64
4:A:2706:NAG:H82	4:A:2706:NAG:C3	2.24	0.64
1:A:2565:GLU:O	1:A:2569:VAL:N	2.30	0.63
1:A:1646:ASN:O	1:A:1647:ASN:HB2	1.99	0.63
1:A:1780:ARG:NH2	1:A:2348:ASN:O	2.32	0.62
1:A:1886:LEU:CD1	1:A:2489:GLY:HA2	2.29	0.62
1:A:2304:TYR:CE1	1:A:2309:GLY:O	2.52	0.62
1:A:2077:TYR:HD1	1:A:2088:VAL:HG22	1.64	0.62
1:A:1693:ILE:HG22	1:A:1715:VAL:HG13	1.81	0.62
1:A:1505:ASN:OD1	1:A:1506:ASN:N	2.32	0.62
1:A:932:PRO:O	1:A:1607:ILE:HD13	2.00	0.61
1:A:1953:PHE:N	1:A:1960:ASN:OD1	2.31	0.61
1:A:1734:ILE:HG22	1:A:1741:PHE:HE2	1.65	0.61
1:A:2011:TYR:O	1:A:2012:ASP:O	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1553:LEU:O	1:A:1567:SER:N	2.32	0.61
1:A:1679:ARG:NH1	1:A:1679:ARG:HG2	2.15	0.61
1:A:1020:LEU:HG	1:A:1046:LEU:HD11	1.82	0.60
1:A:1787:THR:HB	1:A:1795:ILE:HD11	1.83	0.60
1:A:949:LYS:O	1:A:1063:ASP:N	2.32	0.60
1:A:1609:ILE:O	1:A:1609:ILE:HG22	2.00	0.60
1:A:1776:ALA:HB1	1:A:1787:THR:OG1	2.02	0.60
1:A:1020:LEU:HB2	1:A:1074:ILE:HD11	1.84	0.60
1:A:1679:ARG:HH11	1:A:1679:ARG:CG	2.14	0.60
1:A:965:LYS:HD2	1:A:1004:THR:HG22	1.82	0.60
1:A:1471:ASN:O	1:A:1472:ALA:HB3	2.02	0.60
1:A:1784:SER:OG	1:A:1801:ALA:HB2	2.02	0.60
1:A:1948:LYS:HE2	1:A:1950:ILE:HD11	1.84	0.60
1:A:2105:ASN:O	1:A:2122:TYR:OH	2.16	0.60
1:A:1535:VAL:HA	1:A:1541:LEU:HA	1.84	0.59
1:A:1756:TRP:HZ3	1:A:1767:VAL:CG2	2.15	0.59
1:A:1906:VAL:HG12	1:A:2630:LEU:HD21	1.85	0.59
1:A:2244:ASP:OD1	1:A:2246:THR:OG1	2.15	0.59
1:A:2080:ASP:OD1	1:A:2081:GLY:N	2.34	0.58
1:A:1074:ILE:HG21	1:A:1076:HIS:CE1	2.39	0.58
1:A:1555:THR:O	1:A:1565:THR:OG1	2.21	0.58
1:A:1756:TRP:CZ3	1:A:1767:VAL:CG2	2.87	0.58
1:A:2203:PRO:O	1:A:2204:THR:OG1	2.15	0.58
1:A:2206:ILE:HD13	1:A:2289:LEU:HD21	1.85	0.58
1:A:1846:HIS:HD1	1:A:1861:TYR:HH	1.47	0.58
1:A:1958:MET:SD	1:A:2194:GLN:OE1	2.62	0.58
1:A:2015:GLN:OE1	1:A:2225:GLN:NE2	2.37	0.58
1:A:923:ALA:HB2	1:A:2406:ARG:HH21	1.69	0.58
1:A:1958:MET:SD	1:A:2184:SER:OG	2.62	0.57
1:A:1720:LEU:HD21	1:A:2367:ILE:HG21	1.84	0.57
1:A:2634:SER:O	1:A:2637:ILE:HG22	2.04	0.57
1:A:2011:TYR:O	1:A:2014:ASN:ND2	2.37	0.57
1:A:2245:ASN:OD1	1:A:2246:THR:N	2.37	0.57
1:A:2014:ASN:HD22	1:A:2014:ASN:C	2.08	0.56
1:A:2066:LEU:HD13	1:A:2262:GLN:OE1	2.05	0.56
1:A:1480:VAL:HG22	1:A:1487:TYR:CD1	2.40	0.56
1:A:2088:VAL:HB	1:A:2096:TRP:HB2	1.87	0.56
1:A:1575:PHE:HE2	1:A:2459:VAL:H	1.53	0.56
1:A:1638:VAL:HG21	1:A:1899:LEU:HD21	1.86	0.56
1:A:2390:ALA:O	1:A:2393:ASN:ND2	2.39	0.56
1:A:2485:TYR:OH	1:A:2628:PRO:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:LYS:CD	1:A:1004:THR:HG22	2.36	0.56
1:A:1679:ARG:HD3	1:A:1679:ARG:H	1.70	0.56
1:A:1756:TRP:CZ3	1:A:1767:VAL:HG21	2.40	0.56
1:A:2101:ASP:OD1	1:A:2102:LEU:N	2.38	0.56
1:A:2491:ASP:OD1	1:A:2491:ASP:N	2.27	0.56
1:A:1899:LEU:O	1:A:2395:GLN:NE2	2.38	0.55
1:A:917:LEU:HD13	1:A:1084:PHE:CE2	2.41	0.55
1:A:2304:TYR:CZ	1:A:2309:GLY:O	2.59	0.55
1:A:2364:LEU:O	1:A:2368:ILE:N	2.38	0.55
1:A:1730:ARG:NH2	1:A:1748:ASP:O	2.40	0.55
1:A:2179:VAL:HG12	1:A:2179:VAL:O	2.06	0.55
1:A:1996:ILE:O	1:A:1997:SER:OG	2.17	0.55
1:A:1039:LEU:HG	1:A:1039:LEU:O	2.07	0.54
1:A:1906:VAL:HG21	1:A:2627:TYR:CE1	2.43	0.54
1:A:1664:SER:OG	1:A:1677:ILE:O	2.26	0.54
1:A:1679:ARG:HG2	1:A:1679:ARG:HH11	1.72	0.54
1:A:2266:THR:OG1	1:A:2269:GLY:O	2.17	0.54
1:A:1893:PHE:CE2	1:A:2630:LEU:HD23	2.42	0.54
1:A:2077:TYR:CD1	1:A:2088:VAL:HG22	2.42	0.54
1:A:1770:PHE:CE2	1:A:1789:ILE:HD12	2.42	0.54
1:A:2014:ASN:ND2	1:A:2014:ASN:O	2.26	0.54
1:A:2119:PRO:C	1:A:2120:LEU:HD12	2.28	0.54
1:A:1854:ILE:HD12	1:A:2493:HIS:CB	2.38	0.54
1:A:2222:TYR:OH	1:A:2283:ILE:HD11	2.07	0.53
1:A:1787:THR:CB	1:A:1795:ILE:HD11	2.38	0.53
1:A:1487:TYR:HB3	1:A:1490:ASN:HD21	1.73	0.53
1:A:1588:THR:HG22	1:A:1594:VAL:HG13	1.91	0.53
1:A:1789:ILE:HG22	1:A:1791:LYS:H	1.74	0.53
1:A:1912:VAL:HG22	1:A:1928:LEU:HD12	1.91	0.53
1:A:1690:LEU:HD12	1:A:1970:ASN:OD1	2.08	0.53
1:A:1584:LEU:HD11	1:A:1587:VAL:HG22	1.90	0.53
1:A:1679:ARG:HA	1:A:1694:GLU:HB3	1.91	0.53
1:A:1755:LEU:CD1	1:A:1757:LEU:HB2	2.39	0.53
1:A:2120:LEU:HG	1:A:2131:LEU:HD12	1.90	0.52
1:A:2138:ILE:HG23	1:A:2143:TYR:O	2.09	0.52
1:A:1875:SER:HB3	1:A:1881:LEU:HD21	1.91	0.52
1:A:1936:THR:O	1:A:1951:TYR:HA	2.09	0.52
1:A:1838:VAL:HG11	1:A:2329:PHE:HZ	1.74	0.52
1:A:2582:TRP:CH2	1:A:2613:VAL:HG12	2.44	0.52
1:A:952:TYR:HB2	1:A:1060:TRP:CD2	2.44	0.52
1:A:1886:LEU:N	1:A:1886:LEU:CD2	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1476:HIS:HD2	1:A:1491:PHE:CE2	2.27	0.52
1:A:1491:PHE:CZ	1:A:1502:LEU:HD13	2.44	0.52
1:A:2630:LEU:HB3	1:A:2636:ASN:HD22	1.75	0.52
1:A:1565:THR:HA	1:A:1575:PHE:CD1	2.45	0.51
1:A:2135:GLN:OE1	1:A:2136:TYR:O	2.26	0.51
1:A:2154:TYR:OH	1:A:2312:THR:HG21	2.10	0.51
1:A:1711:ARG:NH1	1:A:2415:GLU:O	2.37	0.51
1:A:1720:LEU:HD11	1:A:2367:ILE:HG21	1.90	0.51
1:A:984:VAL:HG22	1:A:1025:VAL:HG22	1.93	0.51
1:A:2346:LEU:HB3	1:A:2422:LYS:HD3	1.92	0.51
1:A:2483:MET:SD	1:A:2570:LEU:HD11	2.51	0.51
4:A:2702:NAG:O4	5:A:2703:MAN:O5	2.29	0.51
1:A:1534:THR:HB	1:A:1543:VAL:HB	1.93	0.51
1:A:1006:ILE:HG13	1:A:1006:ILE:O	2.11	0.51
1:A:1775:LEU:HD12	1:A:1776:ALA:N	2.26	0.51
1:A:1979:PRO:HG2	1:A:1986:LEU:HB2	1.93	0.51
1:A:906:VAL:N	1:A:1031:TYR:OH	2.38	0.51
1:A:2194:GLN:HG2	1:A:2212:HIS:NE2	2.25	0.51
1:A:1775:LEU:HD12	1:A:1776:ALA:H	1.75	0.51
1:A:1977:ILE:HG22	1:A:1979:PRO:HD3	1.92	0.51
1:A:2049:MET:SD	1:A:2244:ASP:HA	2.51	0.51
1:A:2211:ASN:N	1:A:2216:GLU:O	2.44	0.50
1:A:2197:TYR:CE1	1:A:2206:ILE:HG12	2.47	0.50
1:A:2462:ILE:HG22	1:A:2462:ILE:O	2.12	0.50
1:A:1576:TYR:HD1	1:A:1587:VAL:HG22	1.77	0.50
1:A:1935:CYS:SG	1:A:1936:THR:N	2.85	0.50
1:A:1566:LYS:O	1:A:1573:THR:O	2.30	0.50
1:A:2054:ASP:HB3	1:A:2060:ILE:HD12	1.94	0.50
1:A:1468:TYR:HD1	1:A:1479:THR:HG1	1.60	0.49
1:A:1756:TRP:HZ3	1:A:1767:VAL:HG23	1.77	0.49
1:A:2136:TYR:CE1	1:A:2147:ARG:HG3	2.47	0.49
1:A:1778:LEU:HD12	1:A:1778:LEU:H	1.77	0.49
1:A:2210:TYR:HD1	1:A:2217:ILE:HD13	1.77	0.49
1:A:1069:ASN:OD1	1:A:1076:HIS:NE2	2.44	0.49
1:A:2105:ASN:ND2	1:A:2126:ASP:OD1	2.44	0.49
1:A:1756:TRP:CZ3	1:A:1767:VAL:HG23	2.48	0.49
1:A:2045:LEU:HD11	1:A:2048:TRP:HB2	1.94	0.49
1:A:2214:ASN:O	1:A:2216:GLU:N	2.43	0.49
1:A:1787:THR:HG22	1:A:1798:ARG:HG3	1.95	0.49
1:A:1730:ARG:HH22	1:A:1749:GLN:HA	1.77	0.49
1:A:1578:TYR:HB3	1:A:1582:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2014:ASN:HB2	1:A:2027:HIS:HA	1.95	0.49
1:A:1686:MET:HB3	1:A:1942:ILE:HD11	1.95	0.48
1:A:2410:ALA:HA	1:A:2414:LEU:HD12	1.94	0.48
1:A:1652:VAL:N	1:A:1660:ILE:O	2.42	0.48
1:A:958:ALA:HB2	1:A:1050:PHE:HE1	1.78	0.48
1:A:1594:VAL:CG2	1:A:2449:ALA:HB1	2.43	0.48
1:A:1630:SER:HA	1:A:1643:GLN:HA	1.94	0.48
1:A:1826:ILE:HB	1:A:1839:THR:HB	1.96	0.48
4:A:2706:NAG:C3	4:A:2706:NAG:C8	2.90	0.48
1:A:2175:ARG:HB2	1:A:2184:SER:HB2	1.95	0.48
1:A:2586:GLN:HE21	1:A:2590:ARG:HE	1.61	0.48
1:A:1503:ILE:HG21	4:A:2701:NAG:H83	1.94	0.48
1:A:1799:MET:O	1:A:1799:MET:HG2	2.13	0.48
1:A:1908:ASP:CB	1:A:2635:SER:HB3	2.43	0.48
1:A:2151:ILE:HG23	1:A:2593:ARG:NH2	2.28	0.48
1:A:922:SER:OG	1:A:928:ASN:O	2.26	0.48
1:A:906:VAL:CB	1:A:974:PRO:HG2	2.44	0.48
1:A:2047:TYR:CD2	1:A:2242:ALA:HB1	2.49	0.48
1:A:1456:GLN:HB2	1:A:1470:PHE:O	2.14	0.48
1:A:1808:TYR:CE1	1:A:1817:LEU:HD13	2.49	0.48
1:A:2480:LEU:N	1:A:2480:LEU:HD23	2.29	0.48
1:A:2630:LEU:O	1:A:2636:ASN:ND2	2.47	0.48
1:A:1695:TRP:HD1	1:A:2411:PHE:CE1	2.32	0.48
1:A:1716:HIS:O	1:A:1716:HIS:ND1	2.47	0.48
1:A:1591:THR:O	1:A:1854:ILE:O	2.31	0.47
1:A:912:ILE:HG22	1:A:966:ILE:HG12	1.96	0.47
1:A:2395:GLN:O	1:A:2401:GLN:HB3	2.14	0.47
1:A:2110:ASN:HB3	1:A:2117:LEU:HD23	1.95	0.47
1:A:2297:VAL:HG23	1:A:2306:VAL:HG23	1.97	0.47
1:A:1066:HIS:ND1	1:A:1077:LYS:HA	2.30	0.47
1:A:1756:TRP:O	1:A:1758:PRO:HD3	2.14	0.47
1:A:1770:PHE:CE2	1:A:1776:ALA:CB	2.97	0.47
1:A:2585:GLU:O	1:A:2589:ALA:N	2.45	0.47
1:A:1608:ASP:OD1	1:A:1619:THR:HG23	2.13	0.47
1:A:1750:VAL:HG12	1:A:1751:GLY:N	2.30	0.47
1:A:1789:ILE:HG23	1:A:1793:GLY:O	2.14	0.47
1:A:1720:LEU:HD11	1:A:2367:ILE:CG2	2.45	0.47
1:A:1777:GLY:HA2	1:A:1786:ARG:HA	1.96	0.47
1:A:1928:LEU:HD13	1:A:2178:GLY:HA2	1.96	0.47
1:A:2127:ARG:HB3	1:A:2138:ILE:HB	1.96	0.47
1:A:1514:ARG:NH2	1:A:1518:GLY:O	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1553:LEU:HB3	1:A:1567:SER:HB3	1.96	0.47
1:A:2350:VAL:HG12	1:A:2356:TRP:CD1	2.49	0.47
4:A:2706:NAG:H3	4:A:2706:NAG:C8	2.32	0.46
1:A:1906:VAL:CG1	1:A:2630:LEU:HD11	2.46	0.46
1:A:2112:GLY:O	1:A:2113:ASN:OD1	2.32	0.46
1:A:1585:THR:HB	4:A:2704:NAG:C8	2.44	0.46
1:A:2098:TYR:HD1	1:A:2106:LEU:HD11	1.81	0.46
1:A:1905:ILE:HB	1:A:1912:VAL:HB	1.97	0.46
1:A:1907:TYR:HB2	1:A:2156:SER:HB2	1.98	0.46
1:A:2265:TYR:CE1	1:A:2271:ILE:HG22	2.50	0.46
1:A:1057:LEU:O	1:A:1541:LEU:HD23	2.16	0.46
1:A:1796:VAL:O	1:A:1808:TYR:N	2.42	0.46
1:A:1066:HIS:CD2	1:A:1468:TYR:CE1	3.02	0.46
1:A:1575:PHE:CZ	1:A:2445:GLY:O	2.68	0.46
4:A:2701:NAG:O4	4:A:2702:NAG:C1	2.64	0.46
1:A:1800:PHE:HB3	1:A:2056:MET:SD	2.56	0.46
1:A:1864:PRO:CG	1:A:2125:ARG:HG2	2.46	0.46
1:A:2585:GLU:HB3	1:A:2607:LEU:HD21	1.97	0.46
1:A:1508:ASN:OD1	1:A:1526:PRO:CB	2.64	0.46
1:A:2033:ARG:HH21	1:A:2057:GLY:HA2	1.81	0.46
1:A:2286:HIS:HB3	1:A:2299:PHE:CZ	2.51	0.46
1:A:1576:TYR:CE1	1:A:1587:VAL:HG13	2.51	0.45
1:A:2181:ARG:HE	1:A:2197:TYR:HD2	1.64	0.45
1:A:1874:TYR:CE1	1:A:1880:ILE:HG12	2.52	0.45
1:A:2181:ARG:NH1	1:A:2385:LEU:HD13	2.32	0.45
1:A:2261:LYS:CE	1:A:2279:PHE:O	2.65	0.45
1:A:1655:ALA:HB1	1:A:1920:THR:HA	1.99	0.45
1:A:1986:LEU:HD11	1:A:2217:ILE:HG21	1.97	0.45
1:A:2249:PRO:HD3	1:A:2283:ILE:HG22	1.98	0.45
1:A:2297:VAL:HG23	1:A:2306:VAL:CG2	2.46	0.45
1:A:2059:VAL:O	1:A:2077:TYR:HB2	2.15	0.45
1:A:2270:GLU:H	1:A:2306:VAL:CG1	2.30	0.45
1:A:1060:TRP:NE1	1:A:1554:MET:SD	2.82	0.45
1:A:1605:ILE:HG22	1:A:1607:ILE:HG13	1.99	0.45
1:A:1633:VAL:HG11	1:A:2401:GLN:NE2	2.31	0.45
1:A:1657:GLY:HA3	1:A:1685:PRO:HG3	1.98	0.45
1:A:1680:CYS:HB2	1:A:2411:PHE:CZ	2.51	0.45
1:A:1950:ILE:HG22	1:A:1952:ARG:HG2	1.97	0.45
1:A:2184:SER:OG	1:A:2194:GLN:OE1	2.32	0.45
1:A:1065:HIS:CE1	1:A:1499:VAL:HG21	2.52	0.45
1:A:1871:ILE:HD12	1:A:1886:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:VAL:CB	1:A:974:PRO:CG	2.95	0.45
1:A:1468:TYR:HB3	1:A:1476:HIS:CE1	2.52	0.45
1:A:1471:ASN:O	1:A:1472:ALA:CB	2.65	0.45
1:A:1543:VAL:HG22	1:A:1553:LEU:HD13	1.97	0.45
1:A:1886:LEU:HD13	1:A:2489:GLY:HA2	1.99	0.45
1:A:2096:TRP:HA	1:A:2110:ASN:HD21	1.82	0.45
1:A:2377:TYR:CD2	1:A:2381:PRO:HD3	2.52	0.45
1:A:2181:ARG:HB3	1:A:2197:TYR:HE2	1.82	0.44
1:A:2205:ARG:HG3	1:A:2222:TYR:CE2	2.52	0.44
1:A:2482:LYS:O	1:A:2482:LYS:HG3	2.16	0.44
2:B:2:NAG:H4	2:B:3:MAN:H2	1.43	0.44
1:A:1574:THR:O	1:A:1574:THR:HG23	2.17	0.44
1:A:1902:LEU:HD21	1:A:1905:ILE:HD11	1.98	0.44
1:A:1946:VAL:HB	1:A:2200:LEU:HD11	1.99	0.44
1:A:1620:VAL:CG2	1:A:2398:THR:HG21	2.47	0.44
1:A:1656:ASN:HB3	1:A:1943:GLY:HA2	2.00	0.44
1:A:1697:LEU:HD11	1:A:1709:PHE:CE1	2.53	0.44
1:A:1864:PRO:HG2	1:A:2125:ARG:HG2	1.99	0.44
1:A:2581:ALA:HB2	1:A:2637:ILE:HG21	1.99	0.44
1:A:1683:SER:HA	1:A:1689:GLY:O	2.17	0.44
1:A:1928:LEU:O	1:A:1934:SER:HA	2.18	0.44
1:A:1018:TYR:CG	1:A:1052:LEU:HD21	2.53	0.44
1:A:1594:VAL:HG21	1:A:2449:ALA:HB1	1.99	0.44
1:A:1766:ASN:HB2	1:A:1779:GLN:HG2	2.00	0.44
1:A:2211:ASN:OD1	4:A:2712:NAG:H2	2.18	0.44
1:A:2263:LEU:HD22	1:A:2265:TYR:HE1	1.82	0.44
1:A:983:MET:H	1:A:992:GLN:HA	1.83	0.44
1:A:2261:LYS:HD3	1:A:2263:LEU:HG	1.99	0.44
1:A:912:ILE:HG13	1:A:912:ILE:O	2.18	0.44
1:A:1965:TYR:CD1	1:A:1977:ILE:HG12	2.53	0.44
1:A:2192:HIS:ND1	1:A:2212:HIS:CD2	2.86	0.44
1:A:2447:MET:H	1:A:2458:GLY:HA3	1.83	0.44
1:A:1658:MET:HA	1:A:1683:SER:O	2.18	0.44
1:A:917:LEU:HD13	1:A:1084:PHE:HE2	1.83	0.43
1:A:950:LEU:HG	1:A:1060:TRP:HB3	2.00	0.43
1:A:2219:SER:N	1:A:2232:GLU:O	2.50	0.43
1:A:1489:TYR:HA	1:A:1503:ILE:O	2.18	0.43
1:A:1856:TYR:HB2	1:A:1874:TYR:O	2.18	0.43
1:A:1981:ILE:O	1:A:1984:THR:OG1	2.17	0.43
1:A:1787:THR:HG22	1:A:1798:ARG:CB	2.49	0.43
1:A:2105:ASN:OD1	1:A:2126:ASP:OD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2314:PRO:HG3	1:A:2332:TYR:CE1	2.54	0.43
1:A:1056:ASN:O	1:A:1514:ARG:NH2	2.38	0.43
1:A:1682:ILE:HD12	1:A:2369:PRO:CG	2.49	0.43
1:A:1726:ASP:O	1:A:1730:ARG:N	2.49	0.43
1:A:1909:SER:HB2	1:A:2621:VAL:HG11	2.01	0.43
1:A:2217:ILE:O	1:A:2218:THR:OG1	2.24	0.43
1:A:2314:PRO:HG2	1:A:2316:TYR:CZ	2.53	0.43
1:A:2442:ILE:O	1:A:2446:ILE:HG12	2.18	0.43
1:A:915:SER:N	1:A:963:LEU:O	2.48	0.43
1:A:2248:THR:HG23	1:A:2250:LEU:CD1	2.48	0.43
1:A:1596:SER:HB2	4:A:2704:NAG:C8	2.47	0.43
1:A:1599:ARG:HG2	1:A:1607:ILE:HG12	2.00	0.43
1:A:2146:GLN:O	1:A:2146:GLN:HG2	2.18	0.43
1:A:2318:MET:O	1:A:2322:VAL:HG13	2.18	0.43
1:A:1825:TYR:CE1	1:A:1841:PRO:HD3	2.54	0.43
1:A:2008:VAL:HG12	1:A:2017:ILE:HG12	1.99	0.43
1:A:2478:TYR:O	1:A:2495:PHE:CD2	2.72	0.43
1:A:1747:TYR:CE1	1:A:1753:PRO:HB3	2.54	0.43
1:A:1817:LEU:HB3	1:A:1825:TYR:HB2	2.00	0.43
1:A:2170:TRP:HB2	1:A:2293:LEU:HD21	2.01	0.43
1:A:913:ILE:HG13	1:A:913:ILE:O	2.18	0.43
1:A:1009:LYS:HD2	1:A:1049:GLY:HA2	2.01	0.43
1:A:1860:ILE:HG12	1:A:1871:ILE:HG12	2.00	0.43
1:A:2147:ARG:O	1:A:2150:ASP:N	2.48	0.43
1:A:2270:GLU:OE1	1:A:2307:LEU:HD23	2.18	0.43
1:A:2578:LEU:HD12	1:A:2582:TRP:HE1	1.83	0.43
1:A:1659:GLY:O	1:A:1682:ILE:HA	2.19	0.42
1:A:956:ARG:NH2	1:A:1077:LYS:O	2.42	0.42
1:A:1618:VAL:HG21	1:A:2397:ILE:HD13	2.01	0.42
1:A:1974:ILE:HD11	1:A:2200:LEU:HD23	2.00	0.42
1:A:2365:SER:HA	1:A:2371:PHE:HB3	2.01	0.42
1:A:1942:ILE:HB	1:A:1947:ASP:OD2	2.18	0.42
1:A:1477:GLN:O	1:A:1478:TYR:HB3	2.19	0.42
1:A:2105:ASN:O	1:A:2122:TYR:CZ	2.73	0.42
1:A:995:PHE:HE1	1:A:1001:LEU:HD21	1.84	0.42
1:A:1620:VAL:HG12	1:A:1620:VAL:O	2.19	0.42
1:A:1622:THR:HB	1:A:1631:TYR:CD1	2.54	0.42
1:A:1794:ARG:HG2	1:A:1810:TYR:CE1	2.54	0.42
1:A:2144:LEU:HD21	1:A:2147:ARG:HB2	2.01	0.42
1:A:2179:VAL:HG11	1:A:2385:LEU:HD13	2.01	0.42
1:A:2317:THR:O	1:A:2320:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:ARG:NH2	1:A:1079:THR:HG22	2.34	0.42
1:A:1020:LEU:CG	1:A:1046:LEU:HD11	2.49	0.42
1:A:1697:LEU:HD12	1:A:1698:ARG:N	2.35	0.42
1:A:1768:SER:OG	1:A:1768:SER:O	2.30	0.42
1:A:2157:LYS:O	1:A:2157:LYS:HG2	2.19	0.42
1:A:1577:ASP:CB	1:A:1586:ASN:OD1	2.57	0.42
1:A:1499:VAL:O	1:A:1514:ARG:NE	2.47	0.42
1:A:1644:LEU:HD23	1:A:1650:LEU:HA	2.01	0.42
1:A:1873:ASP:O	1:A:1881:LEU:N	2.38	0.42
1:A:2188:ASN:OD1	1:A:2189:LEU:HD12	2.20	0.42
1:A:2286:HIS:O	1:A:2286:HIS:CD2	2.73	0.42
1:A:2396:LEU:HD21	1:A:2405:GLU:HG2	2.01	0.42
1:A:2577:ALA:O	1:A:2581:ALA:N	2.50	0.42
1:A:1508:ASN:OD1	1:A:1526:PRO:HG3	2.20	0.42
1:A:1584:LEU:HD11	1:A:1587:VAL:CG2	2.50	0.42
1:A:2053:TYR:HD2	1:A:2057:GLY:C	2.22	0.42
1:A:2131:LEU:HD22	1:A:2136:TYR:OH	2.19	0.42
1:A:1636:ASP:CB	1:A:1898:LYS:HD2	2.49	0.42
1:A:2185:TYR:O	1:A:2192:HIS:HA	2.19	0.42
1:A:2267:ALA:O	1:A:2268:TYR:HB2	2.20	0.42
1:A:1988:VAL:HG12	1:A:1990:LEU:HG	2.01	0.41
1:A:2286:HIS:O	1:A:2286:HIS:CG	2.73	0.41
1:A:995:PHE:CE1	1:A:1001:LEU:HD21	2.55	0.41
1:A:1769:TYR:HA	1:A:1775:LEU:HA	2.02	0.41
1:A:1835:LEU:HD12	1:A:1835:LEU:H	1.85	0.41
1:A:2304:TYR:OH	1:A:2309:GLY:O	2.38	0.41
1:A:1500:THR:O	1:A:1511:LYS:HA	2.21	0.41
1:A:1512:ILE:HG12	1:A:1523:LEU:HD13	2.02	0.41
1:A:1846:HIS:HB3	1:A:1861:TYR:HE1	1.86	0.41
1:A:2036:GLU:OE2	1:A:2048:TRP:NE1	2.50	0.41
1:A:2363:GLN:OE1	1:A:2373:ARG:NH1	2.53	0.41
1:A:2479:TYR:HE1	1:A:2493:HIS:HB3	1.86	0.41
1:A:935:GLN:NE2	1:A:1599:ARG:HG3	2.35	0.41
1:A:1574:THR:HA	1:A:1589:ARG:HA	2.02	0.41
1:A:1756:TRP:HH2	1:A:2420:THR:HG21	1.86	0.41
1:A:2204:THR:HG22	1:A:2300:THR:HG21	2.03	0.41
1:A:1020:LEU:HD21	1:A:1046:LEU:HD21	2.03	0.41
1:A:1770:PHE:CE2	1:A:1776:ALA:HB2	2.55	0.41
1:A:2039:TYR:OH	1:A:2240:TYR:HB3	2.21	0.41
1:A:2636:ASN:OD1	1:A:2636:ASN:C	2.59	0.41
1:A:1917:ASP:OD1	1:A:1921:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1951:TYR:O	1:A:1952:ARG:C	2.59	0.41
1:A:2017:ILE:HD11	1:A:2223:ASP:OD1	2.20	0.41
1:A:2137:LYS:HB2	1:A:2138:ILE:HA	2.03	0.41
1:A:912:ILE:HD12	1:A:1045:ALA:HB2	2.02	0.40
1:A:1055:SER:HB3	1:A:1065:HIS:ND1	2.36	0.40
1:A:1750:VAL:HG12	1:A:1751:GLY:H	1.86	0.40
1:A:1779:GLN:HB2	1:A:1784:SER:HB3	2.03	0.40
1:A:1800:PHE:CB	1:A:2056:MET:SD	3.10	0.40
1:A:1821:SER:O	1:A:1823:ARG:N	2.54	0.40
1:A:2305:ASP:O	1:A:2308:ALA:O	2.38	0.40
1:A:2327:ALA:HB1	1:A:2328:PRO:HD2	2.03	0.40
1:A:2062:ARG:NH2	1:A:2340:LEU:HD13	2.36	0.40
1:A:2126:ASP:OD2	1:A:2330:ASN:CG	2.60	0.40
1:A:1634:VAL:HG13	1:A:1639:ARG:NH1	2.37	0.40
1:A:2058:ARG:O	1:A:2059:VAL:C	2.60	0.40
1:A:2128:ILE:CD1	1:A:2310:ARG:HD2	2.36	0.40
1:A:1568:ASP:HB3	1:A:1572:TRP:HB3	2.03	0.40
1:A:1575:PHE:CD2	1:A:2447:MET:CB	3.04	0.40
1:A:2354:LYS:HA	1:A:2357:LEU:HD12	2.04	0.40

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	1292/1999 (65%)	1165 (90%)	124 (10%)	3 (0%)	47 79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2012	ASP
1	A	2013	ILE

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Mol	Chain	Res	Type
1	A	1868	ALA

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	991/1735 (57%)	976 (98%)	15 (2%)	65 85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1031	TYR
1	A	1679	ARG
1	A	1694	GLU
1	A	1752	ARG
1	A	1778	LEU
1	A	1779	GLN
1	A	1786	ARG
1	A	1799	MET
1	A	1886	LEU
1	A	2014	ASN
1	A	2126	ASP
1	A	2211	ASN
1	A	2310	ARG
1	A	2491	ASP
1	A	2597	ARG

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

Mol	Chain	Res	Type
1	A	935	GLN
1	A	2586	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)

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	1	1,2	14,14,15	2.26	1 (7%)	17,19,21	2.13	5 (29%)
2	NAG	B	2	2	14,14,15	0.91	1 (7%)	17,19,21	2.08	5 (29%)
2	MAN	B	3	2	11,11,12	2.06	3 (27%)	15,15,17	1.11	1 (6%)
3	MAN	C	1	3	11,11,12	1.92	3 (27%)	15,15,17	1.66	3 (20%)
3	MAN	C	2	3	11,11,12	1.78	3 (27%)	15,15,17	0.92	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	MAN	B	3	2	-	2/2/19/22	0/1/1/1
3	MAN	C	1	3	-	2/2/19/22	0/1/1/1
3	MAN	C	2	3	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	8.12	1.64	1.52
2	B	3	MAN	O5-C1	4.63	1.51	1.43
3	C	1	MAN	O5-C1	4.39	1.50	1.43
3	C	2	MAN	O5-C1	3.93	1.50	1.43
2	B	3	MAN	C2-C3	-3.42	1.47	1.52
3	C	1	MAN	C2-C3	-3.02	1.48	1.52
3	C	2	MAN	C2-C3	-3.00	1.48	1.52
2	B	3	MAN	O5-C5	2.65	1.48	1.43
2	B	2	NAG	O4-C4	2.48	1.48	1.43
3	C	1	MAN	O5-C5	2.42	1.48	1.43
3	C	2	MAN	O5-C5	2.12	1.47	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C4-C3-C2	6.12	119.98	111.02
2	B	1	NAG	O5-C1-C2	-5.49	102.62	111.29
2	B	1	NAG	C1-O5-C5	4.03	117.65	112.19
2	B	1	NAG	C4-C3-C2	-3.28	106.21	111.02
3	C	1	MAN	C3-C4-C5	3.20	115.95	110.24
2	B	2	NAG	C2-N2-C7	-3.00	118.63	122.90
3	C	1	MAN	C2-C3-C4	2.97	116.04	110.89
2	B	2	NAG	O5-C1-C2	-2.79	106.89	111.29
2	B	2	NAG	O4-C4-C3	2.43	115.97	110.35
2	B	1	NAG	O4-C4-C5	2.38	115.21	109.30
3	C	1	MAN	C1-C2-C3	2.36	112.56	109.67
2	B	1	NAG	O5-C5-C4	2.18	116.13	110.83
2	B	2	NAG	O3-C3-C2	-2.10	105.11	109.47
3	C	2	MAN	C1-O5-C5	-2.09	109.37	112.19
2	B	3	MAN	C1-O5-C5	2.08	115.02	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2
3	C	1	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O7-C7-N2-C2
2	B	3	MAN	O5-C5-C6-O6
3	C	1	MAN	O5-C5-C6-O6
2	B	3	MAN	C4-C5-C6-O6

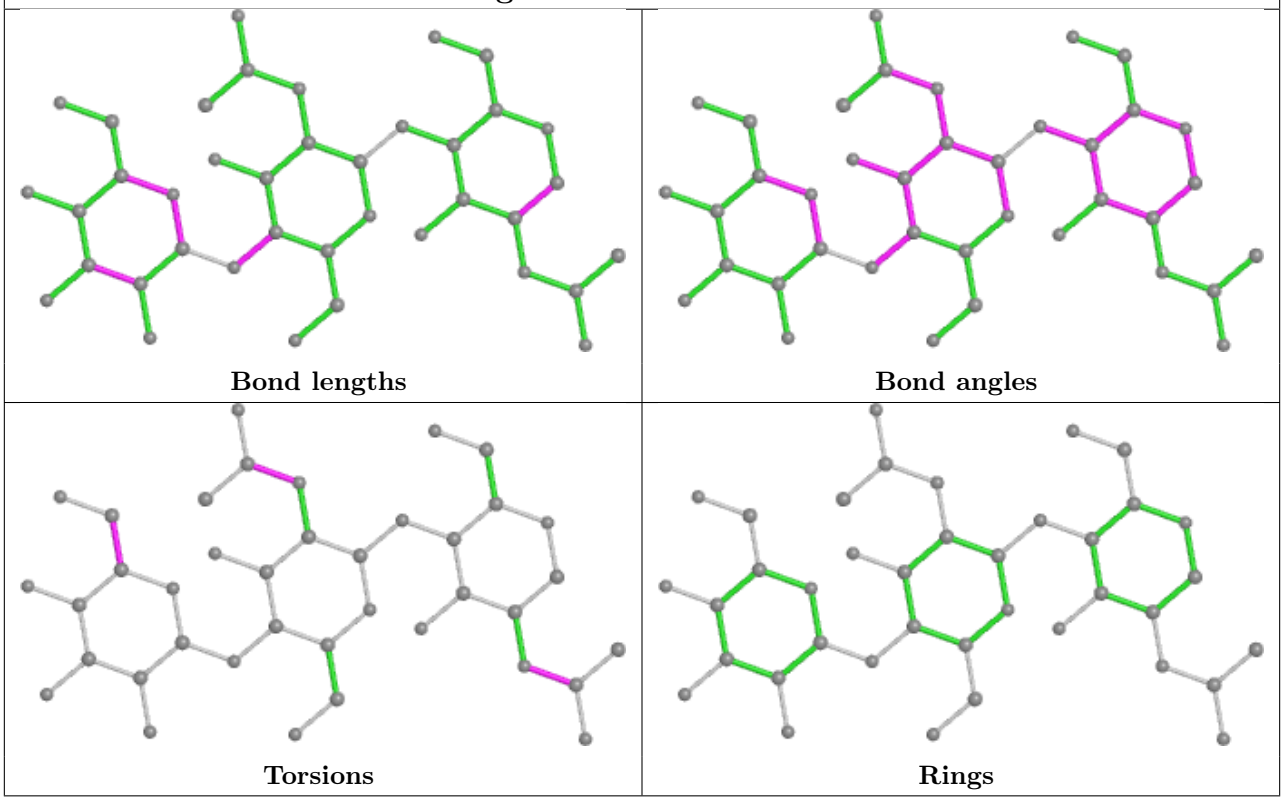
There are no ring outliers.

4 monomers are involved in 3 short contacts:

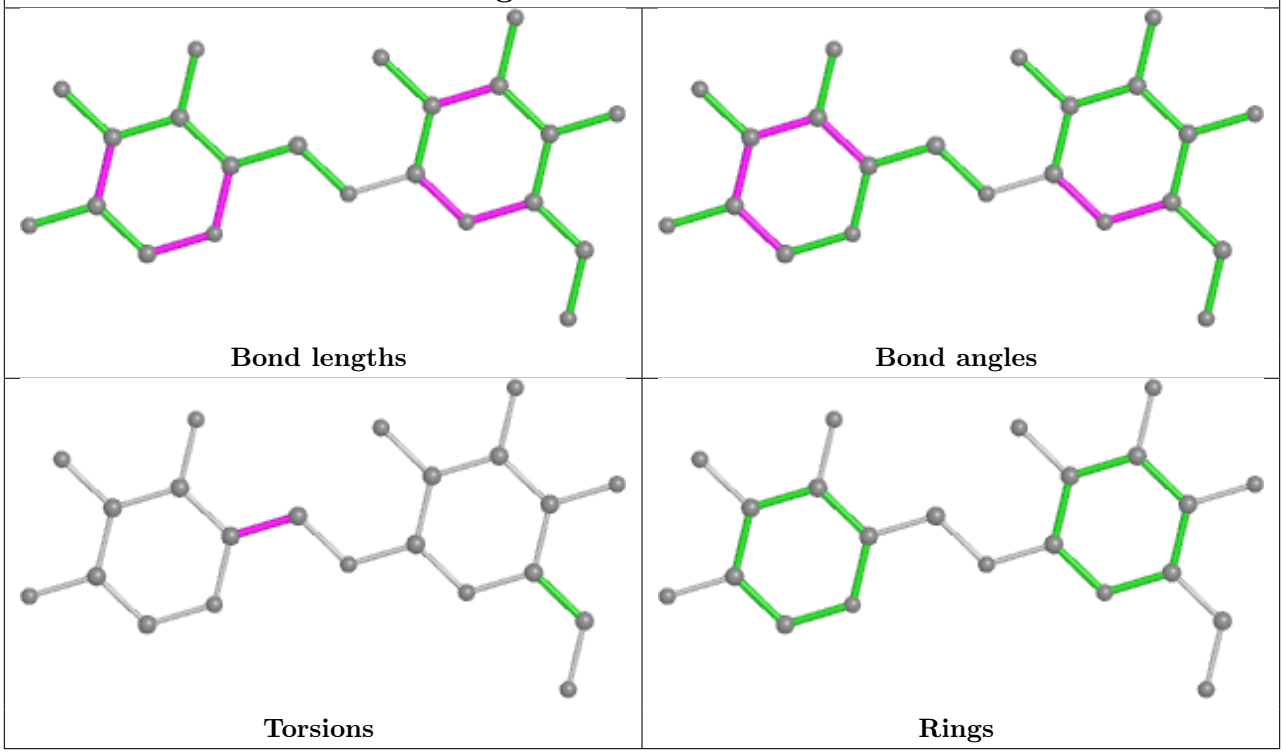
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
2	B	3	MAN	1	0
2	B	1	NAG	1	0
3	C	2	MAN	1	0

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 B



Oligosaccharide Chain C



5.6 Ligand geometry (i)

12 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	2705	-	14,14,15	0.35	0	17,19,21	0.73	1 (5%)
4	NAG	A	2701	1	14,14,15	1.90	4 (28%)	17,19,21	1.82	3 (17%)
4	NAG	A	2702	-	14,14,15	1.82	3 (21%)	17,19,21	1.54	3 (17%)
4	NAG	A	2713	-	14,14,15	1.78	3 (21%)	17,19,21	1.55	3 (17%)
4	NAG	A	2708	1	14,14,15	2.09	1 (7%)	17,19,21	2.02	2 (11%)
5	MAN	A	2716	-	11,11,12	1.99	3 (27%)	15,15,17	1.12	1 (6%)
4	NAG	A	2707	-	14,14,15	0.33	0	17,19,21	0.90	2 (11%)
4	NAG	A	2704	1	14,14,15	1.97	1 (7%)	17,19,21	2.95	3 (17%)
5	MAN	A	2717	-	11,11,12	0.25	0	15,15,17	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	2712	-	14,14,15	1.97	5 (35%)	17,19,21	1.86	5 (29%)
4	NAG	A	2706	-	14,14,15	0.41	0	17,19,21	1.02	1 (5%)
5	MAN	A	2703	-	11,11,12	2.03	3 (27%)	15,15,17	1.25	3 (20%)

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	2701	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2702	-	-	0/6/23/26	0/1/1/1
4	NAG	A	2713	-	-	2/6/23/26	0/1/1/1
4	NAG	A	2708	1	1/1/5/7	5/6/23/26	0/1/1/1
5	MAN	A	2716	-	-	2/2/19/22	1/1/1/1
4	NAG	A	2707	-	-	4/6/23/26	0/1/1/1
4	NAG	A	2704	1	1/1/5/7	2/6/23/26	0/1/1/1
5	MAN	A	2717	-	-	0/2/19/22	1/1/1/1
4	NAG	A	2706	-	-	6/6/23/26	0/1/1/1
4	NAG	A	2712	-	-	1/6/23/26	0/1/1/1
4	NAG	A	2705	-	-	4/6/23/26	0/1/1/1
5	MAN	A	2703	-	-	0/2/19/22	1/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2708	NAG	C1-C2	7.73	1.63	1.52
4	A	2704	NAG	C1-C2	7.06	1.62	1.52
5	A	2703	MAN	O5-C1	4.80	1.51	1.43
5	A	2716	MAN	O5-C1	4.51	1.50	1.43
4	A	2712	NAG	O5-C1	4.18	1.50	1.43
4	A	2701	NAG	O5-C1	4.14	1.50	1.43
4	A	2702	NAG	O5-C1	4.02	1.50	1.43
4	A	2713	NAG	O5-C1	3.84	1.49	1.43
4	A	2702	NAG	C7-N2	3.34	1.45	1.34
4	A	2701	NAG	C7-N2	3.32	1.45	1.34
4	A	2712	NAG	C7-N2	3.28	1.45	1.34
5	A	2716	MAN	C2-C3	-3.25	1.47	1.52
4	A	2713	NAG	C7-N2	3.22	1.45	1.34
5	A	2703	MAN	C2-C3	-3.00	1.48	1.52

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2712	NAG	O5-C5	2.67	1.48	1.43
5	A	2703	MAN	O5-C5	2.51	1.48	1.43
4	A	2701	NAG	O5-C5	2.51	1.48	1.43
5	A	2716	MAN	O5-C5	2.49	1.48	1.43
4	A	2712	NAG	C3-C2	-2.38	1.47	1.52
4	A	2702	NAG	C2-N2	2.13	1.49	1.46
4	A	2712	NAG	C2-N2	2.12	1.49	1.46
4	A	2701	NAG	C2-N2	2.09	1.49	1.46
4	A	2713	NAG	O5-C5	2.02	1.47	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2704	NAG	O5-C1-C2	-10.88	94.10	111.29
4	A	2708	NAG	O5-C1-C2	-7.60	99.29	111.29
4	A	2701	NAG	C1-O5-C5	-4.52	106.07	112.19
4	A	2704	NAG	C1-O5-C5	-4.41	106.21	112.19
4	A	2712	NAG	C3-C4-C5	4.04	117.44	110.24
4	A	2701	NAG	C3-C4-C5	3.45	116.40	110.24
4	A	2702	NAG	C2-N2-C7	-2.96	118.69	122.90
4	A	2713	NAG	C3-C4-C5	2.95	115.50	110.24
4	A	2712	NAG	C1-O5-C5	2.88	116.09	112.19
4	A	2702	NAG	C8-C7-N2	2.85	120.93	116.10
4	A	2702	NAG	C3-C4-C5	2.76	115.17	110.24
4	A	2712	NAG	O5-C5-C4	2.76	117.55	110.83
4	A	2701	NAG	C8-C7-N2	2.72	120.70	116.10
4	A	2712	NAG	C2-N2-C7	-2.62	119.17	122.90
4	A	2712	NAG	C8-C7-N2	2.61	120.52	116.10
4	A	2704	NAG	C2-N2-C7	-2.57	119.25	122.90
4	A	2706	NAG	C4-C3-C2	2.45	114.61	111.02
4	A	2707	NAG	C2-N2-C7	-2.37	119.53	122.90
4	A	2713	NAG	C2-N2-C7	-2.34	119.56	122.90
4	A	2707	NAG	O5-C5-C6	2.33	110.85	107.20
5	A	2703	MAN	C1-C2-C3	2.31	112.51	109.67
4	A	2708	NAG	O5-C5-C6	2.22	110.69	107.20
5	A	2703	MAN	O5-C1-C2	2.22	114.20	110.77
4	A	2713	NAG	C8-C7-N2	2.18	119.79	116.10
4	A	2705	NAG	O5-C5-C6	2.13	110.54	107.20
5	A	2716	MAN	C6-C5-C4	-2.10	108.08	113.00
5	A	2703	MAN	O5-C5-C6	2.03	110.39	107.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2704	NAG	C1
4	A	2708	NAG	C1

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2704	NAG	C8-C7-N2-C2
4	A	2704	NAG	O7-C7-N2-C2
4	A	2705	NAG	C3-C2-N2-C7
4	A	2706	NAG	C8-C7-N2-C2
4	A	2708	NAG	C1-C2-N2-C7
4	A	2708	NAG	C8-C7-N2-C2
4	A	2708	NAG	O7-C7-N2-C2
4	A	2713	NAG	O5-C5-C6-O6
4	A	2706	NAG	C1-C2-N2-C7
4	A	2706	NAG	O7-C7-N2-C2
4	A	2708	NAG	O5-C5-C6-O6
4	A	2713	NAG	C4-C5-C6-O6
4	A	2701	NAG	C4-C5-C6-O6
5	A	2716	MAN	O5-C5-C6-O6
4	A	2706	NAG	C4-C5-C6-O6
4	A	2701	NAG	C8-C7-N2-C2
4	A	2701	NAG	O7-C7-N2-C2
4	A	2705	NAG	C8-C7-N2-C2
4	A	2708	NAG	C4-C5-C6-O6
4	A	2701	NAG	O5-C5-C6-O6
4	A	2706	NAG	O5-C5-C6-O6
4	A	2705	NAG	O5-C5-C6-O6
4	A	2705	NAG	O7-C7-N2-C2
5	A	2716	MAN	C4-C5-C6-O6
4	A	2707	NAG	C1-C2-N2-C7
4	A	2707	NAG	C4-C5-C6-O6
4	A	2712	NAG	C4-C5-C6-O6
4	A	2707	NAG	O5-C5-C6-O6
4	A	2706	NAG	C3-C2-N2-C7
4	A	2707	NAG	C3-C2-N2-C7

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2716	MAN	C1-C2-C3-C4-C5-O5
5	A	2717	MAN	C1-C2-C3-C4-C5-O5
5	A	2703	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2705	NAG	2	0
4	A	2701	NAG	2	0
4	A	2702	NAG	2	0
4	A	2704	NAG	4	0
5	A	2717	MAN	1	0
4	A	2712	NAG	1	0
4	A	2706	NAG	4	0
5	A	2703	MAN	1	0

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.

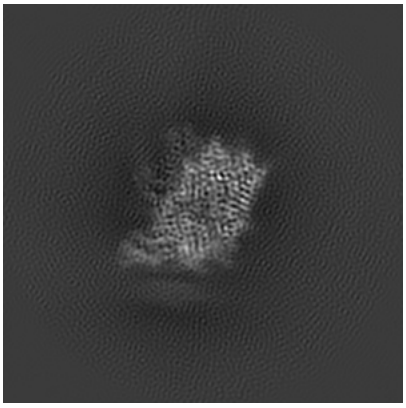
6 Map visualisation (i)

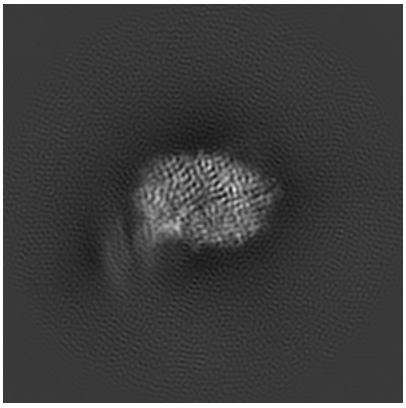
This section contains visualisations of the EMDB entry EMD-7526. These allow visual inspection of the internal detail of the map and identification of artifacts.

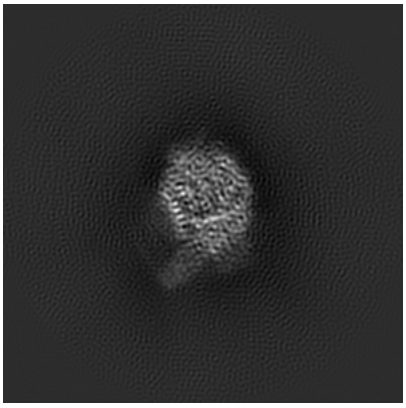
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

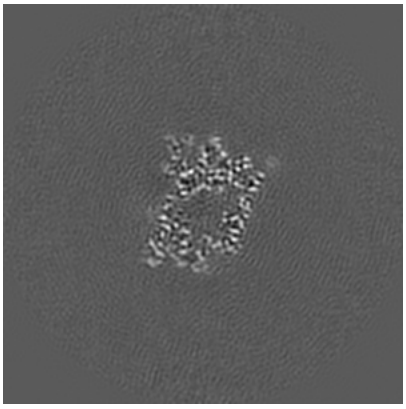

Y

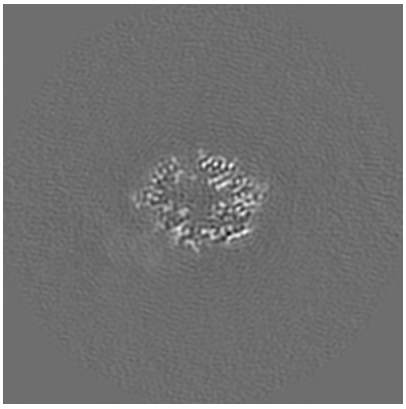

Z

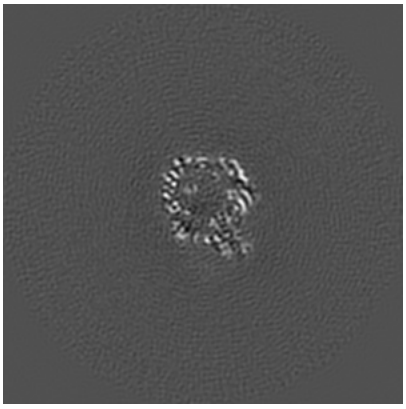
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 130

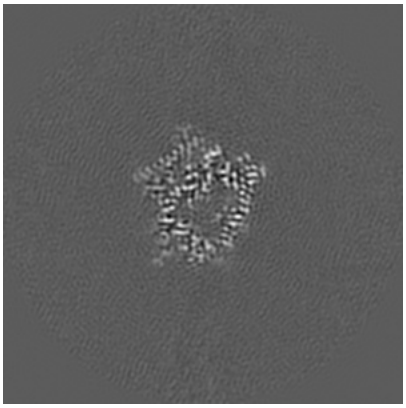

Y Index: 130


Z Index: 130

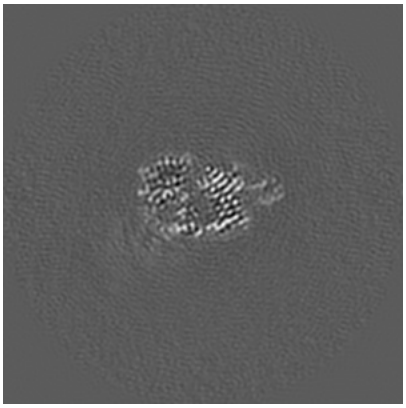
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

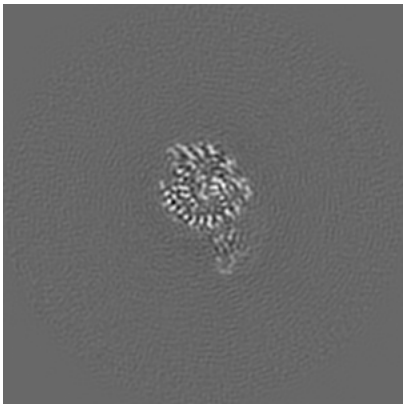
6.3.1 Primary map



X Index: 141



Y Index: 121

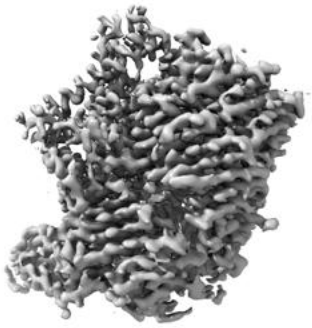


Z Index: 146

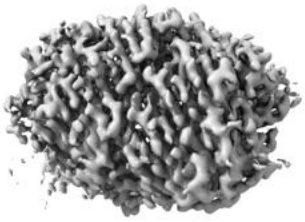
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

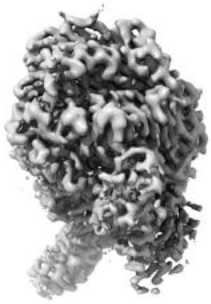
6.4.1 Primary map



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.

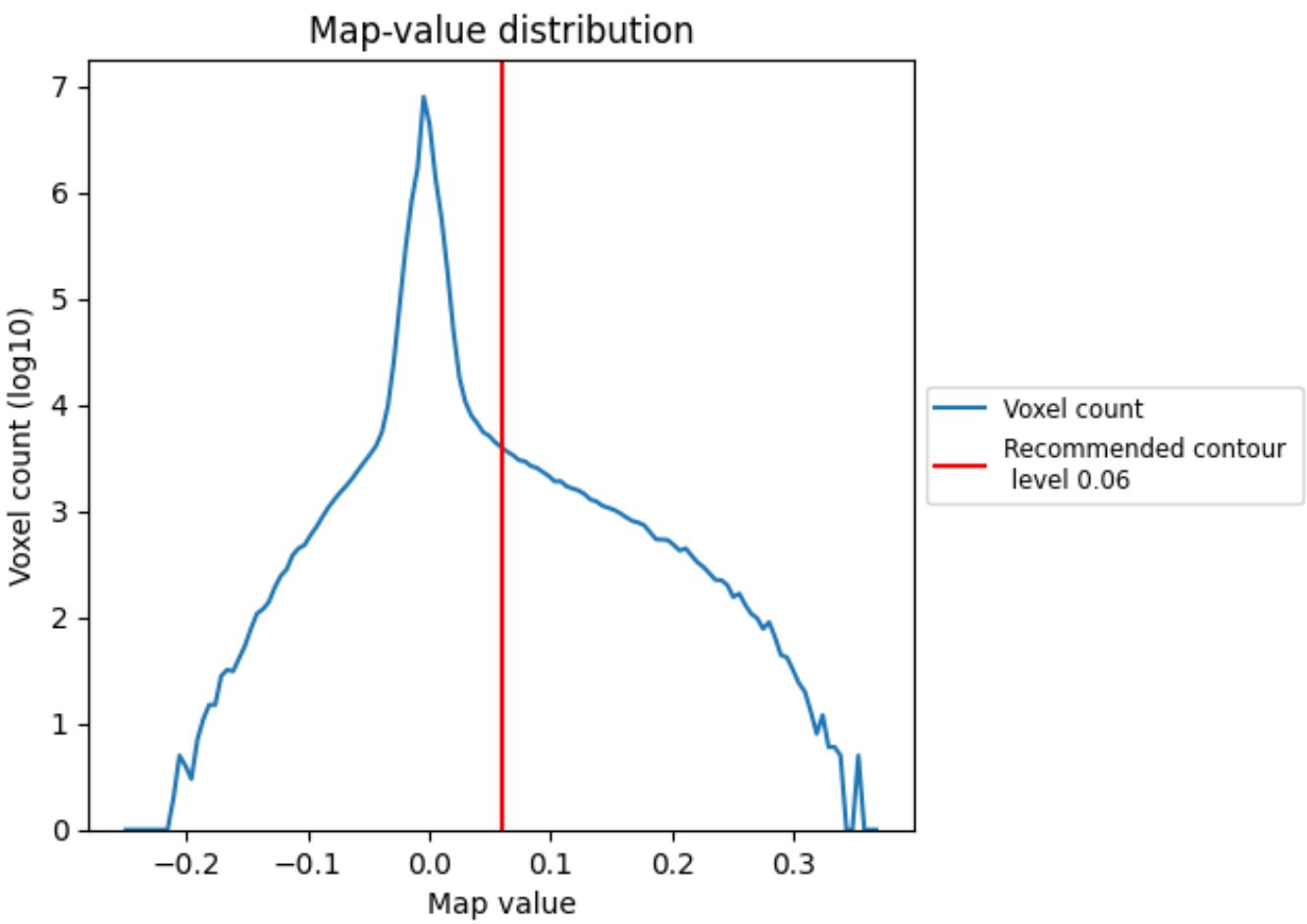
6.5 Mask visualisation (i)

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

7 Map analysis (i)

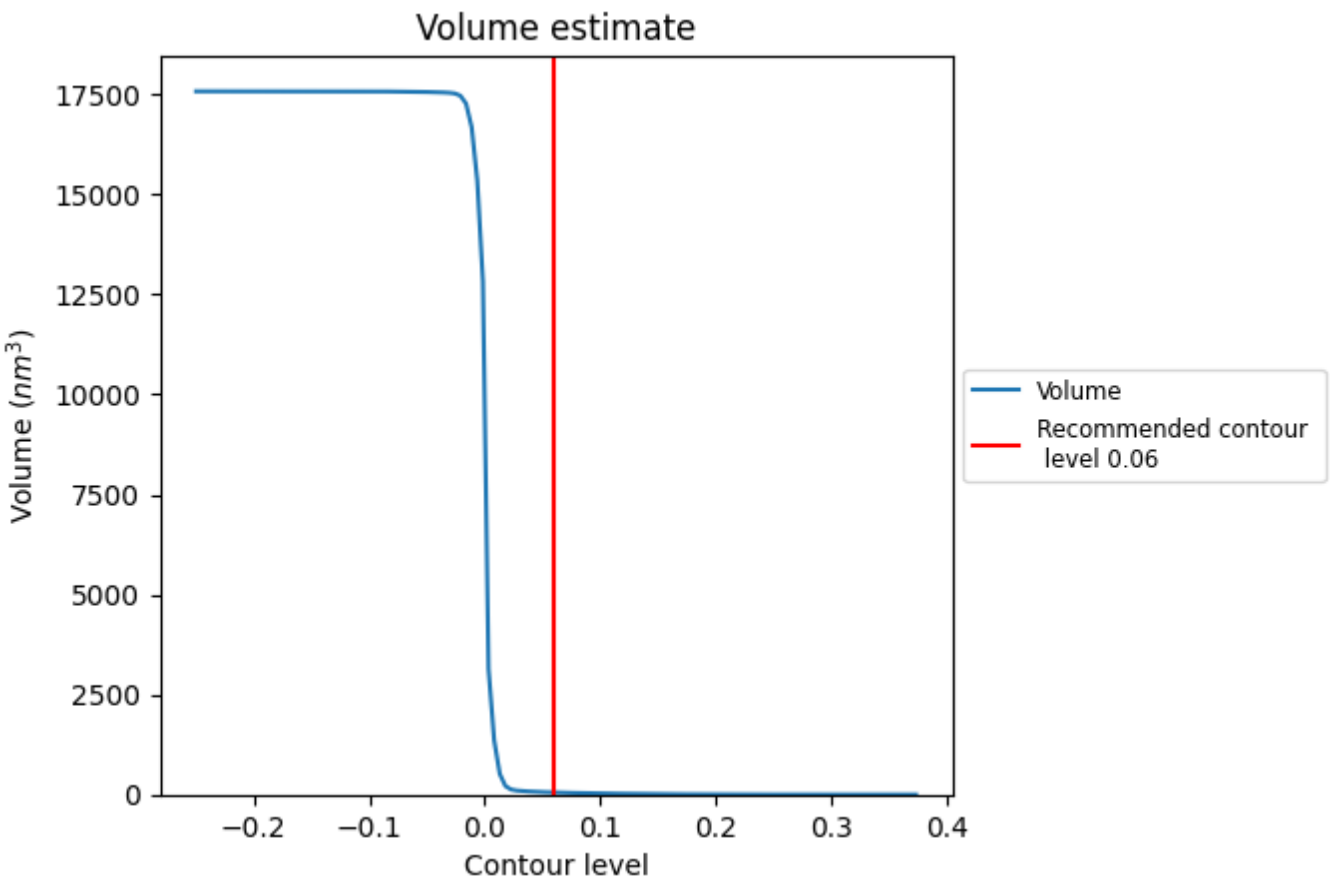
This section contains the results of statistical analysis of the map.

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.

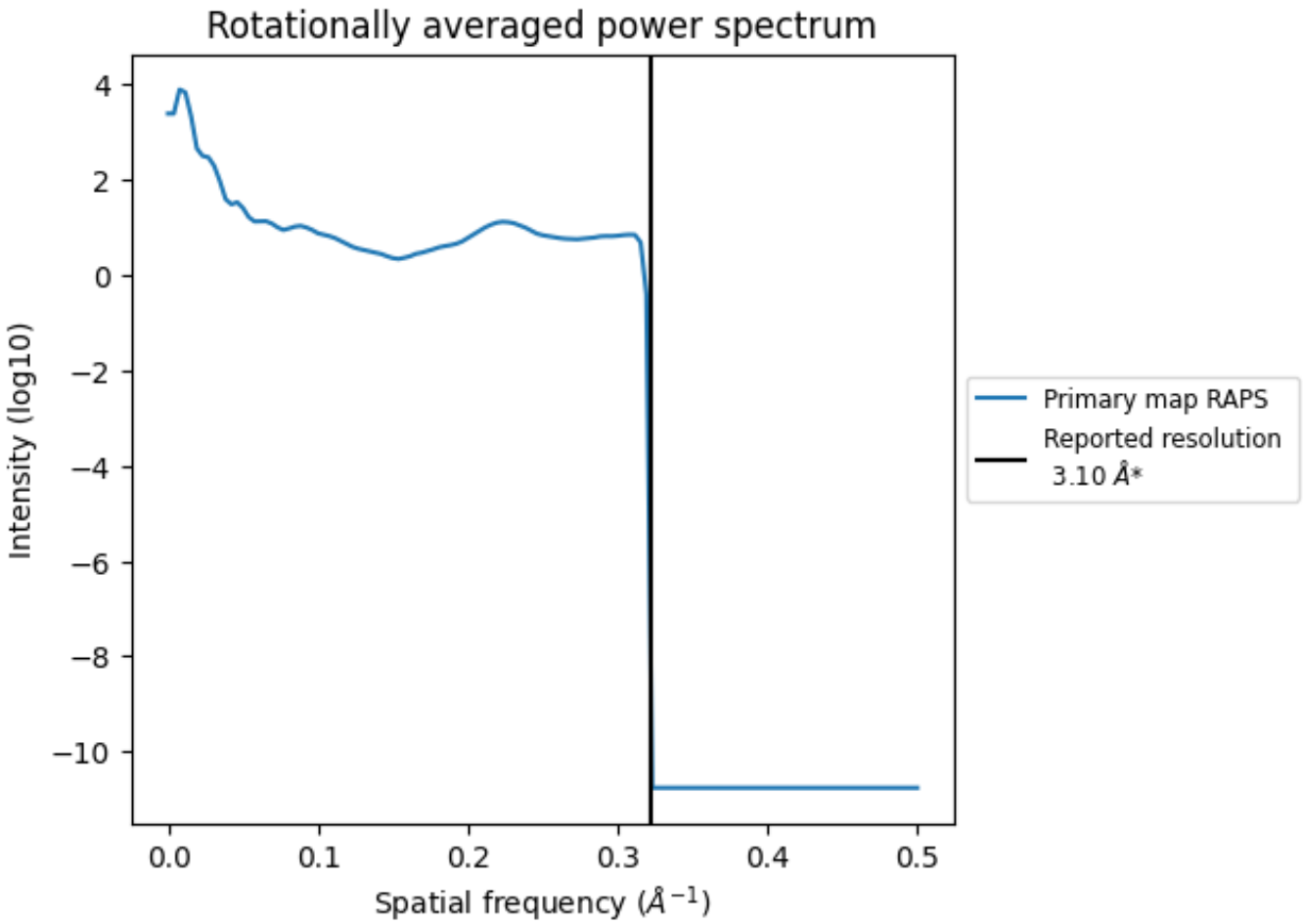
7.2 Volume estimate (i)



The volume at the recommended contour level is 53 nm^3; this corresponds to an approximate mass of 48 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 0.323 Å^{-1}

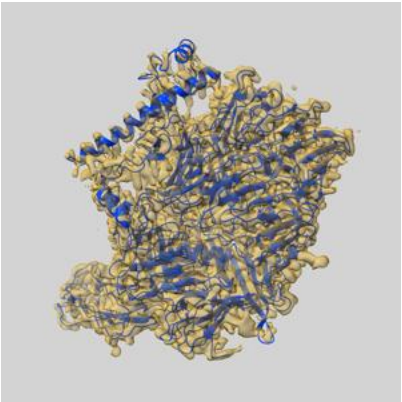
8 Fourier-Shell correlation (i)

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

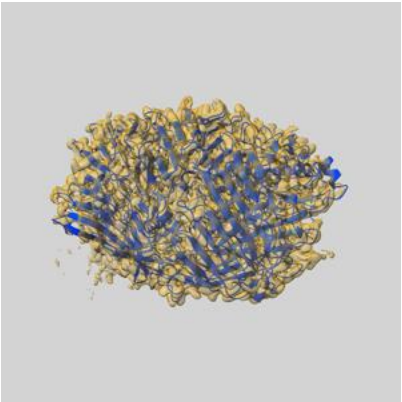
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7526 and PDB model 6CMX. Per-residue inclusion information can be found in section 3 on page 7.

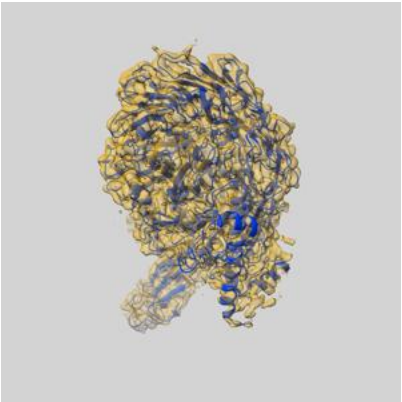
9.1 Map-model overlay (i)



X



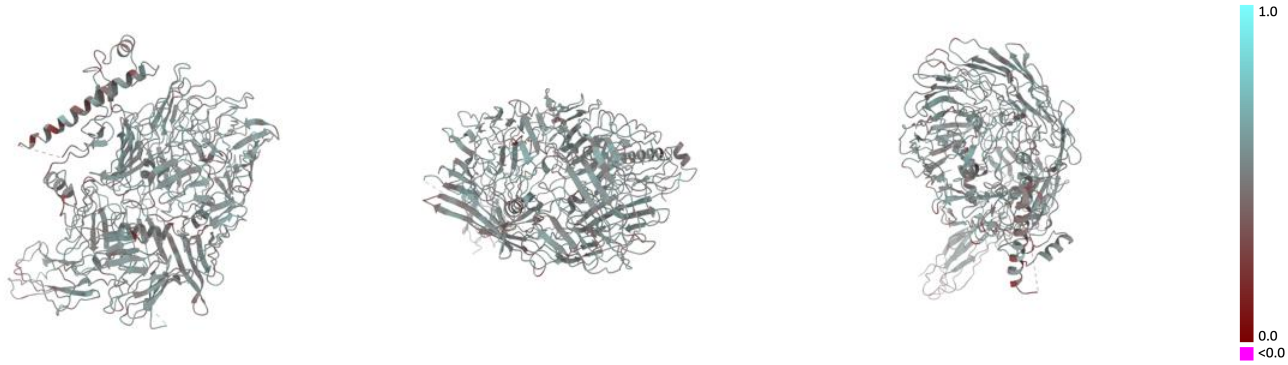
Y



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.

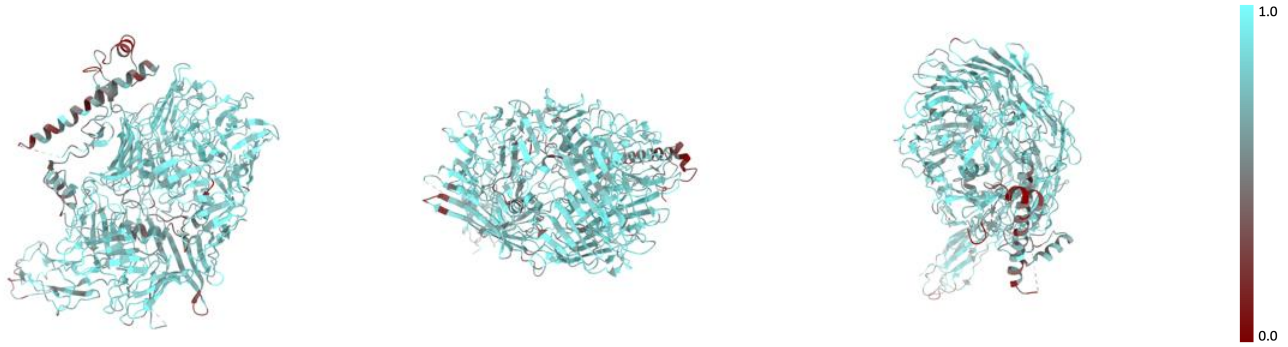
9.2 Q-score mapped to coordinate model (i)



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.

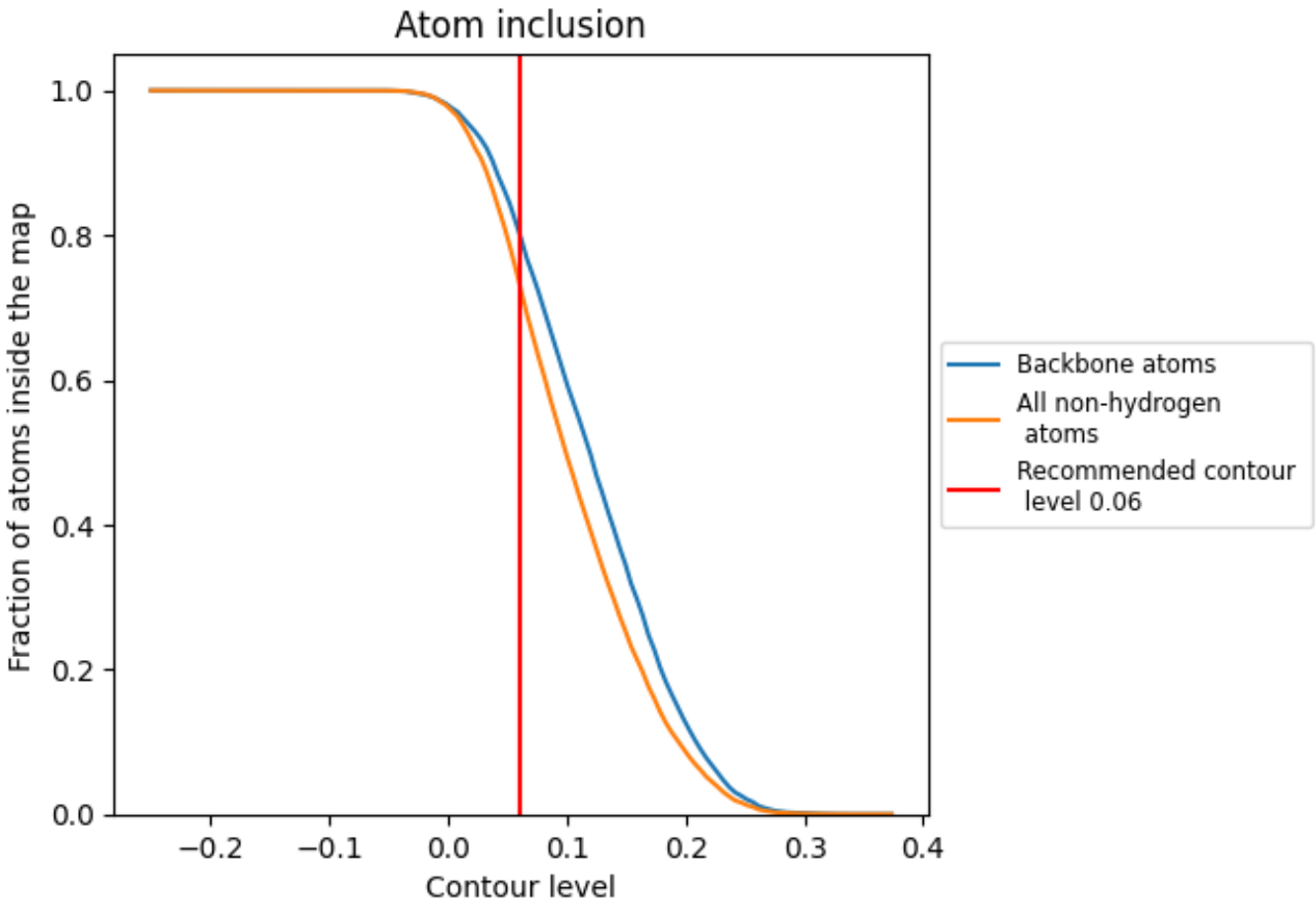
9.3 Atom inclusion mapped to coordinate model (i)



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, 80% of all backbone atoms, 73% 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	0.7345	0.4970
A	0.7362	0.4980
B	0.4359	0.4000
C	0.5000	0.3700