Full wwPDB EM Validation Report ⓘ

Oct 15, 2024 – 12:46 PM JST

PDB ID	:	8XL0
EMDB ID	:	EMD-38433
Title	:	Citrate-induced filament of human acetyl-coenzyme A carboxylase 1 (ACC1-citrate)
Authors	:	Zhou, F.Y.; Zhang, Y.Y.; Zhou, Q.; Hu, Q.
Deposited on	:	2023-12-25
Resolution	:	4.14 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 ⓘ 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:

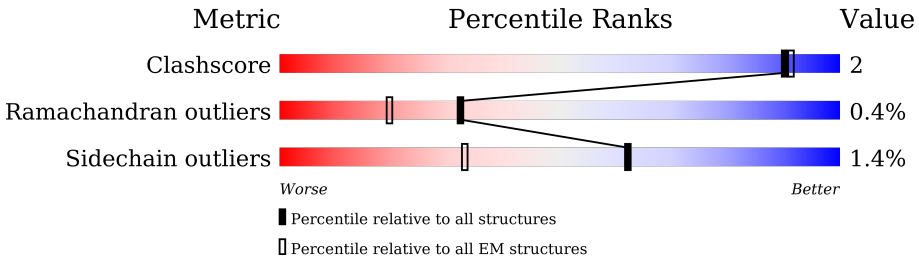
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.14 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	2346	11% 88% • 9%
1	B	2346	5% 88% • • 9%
1	C	2346	88% • • 9%
1	D	2346	88% • • 9%
1	E	2346	38% 74% • • 22%
1	F	2346	38% 53% • 45%

2 Entry composition (i)

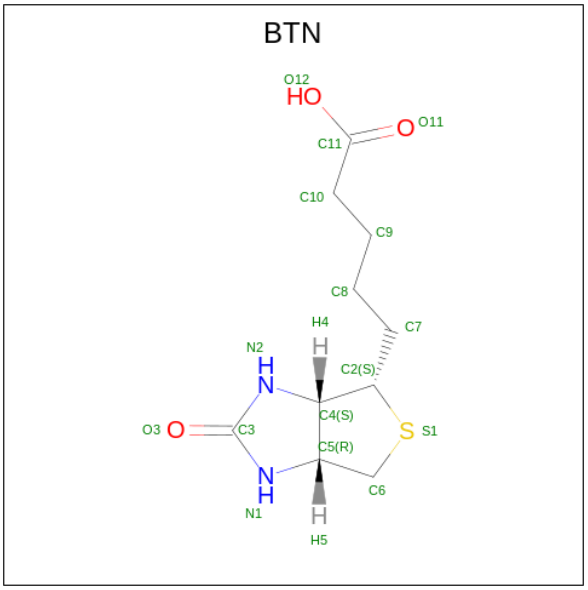
There are 2 unique types of molecules in this entry. The entry contains 93175 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetyl-CoA carboxylase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2146	Total	C	N	O	S	0	0
			17120	10879	2976	3166	99		
1	B	2146	Total	C	N	O	S	0	0
			17120	10879	2976	3166	99		
1	C	2146	Total	C	N	O	S	0	0
			17120	10879	2976	3166	99		
1	D	2146	Total	C	N	O	S	0	0
			17120	10879	2976	3166	99		
1	E	1819	Total	C	N	O	S	0	0
			14435	9170	2503	2676	86		
1	F	1289	Total	C	N	O	S	0	0
			10185	6478	1764	1890	53		

- Molecule 2 is BIOTIN (three-letter code: BTN) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



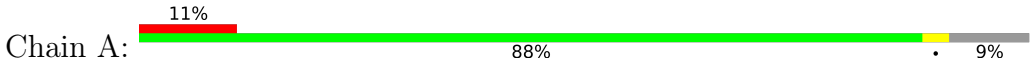
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			15	10	2	2	1	
2	B	1	Total	C	N	O	S	0
			15	10	2	2	1	
2	C	1	Total	C	N	O	S	0
			15	10	2	2	1	
2	D	1	Total	C	N	O	S	0
			15	10	2	2	1	
2	E	1	Total	C	N	O	S	0
			15	10	2	2	1	

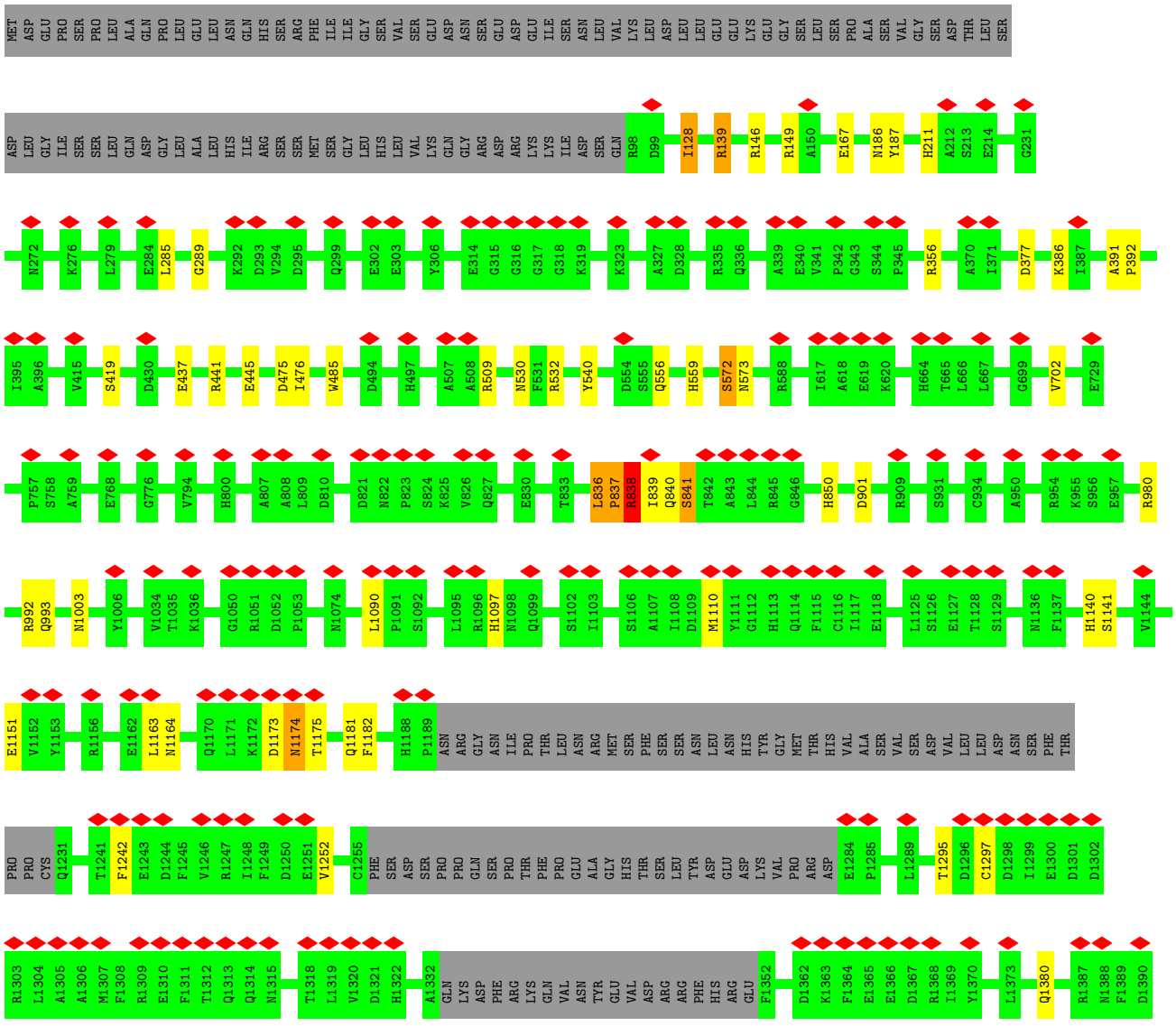
3 Residue-property plots (i)

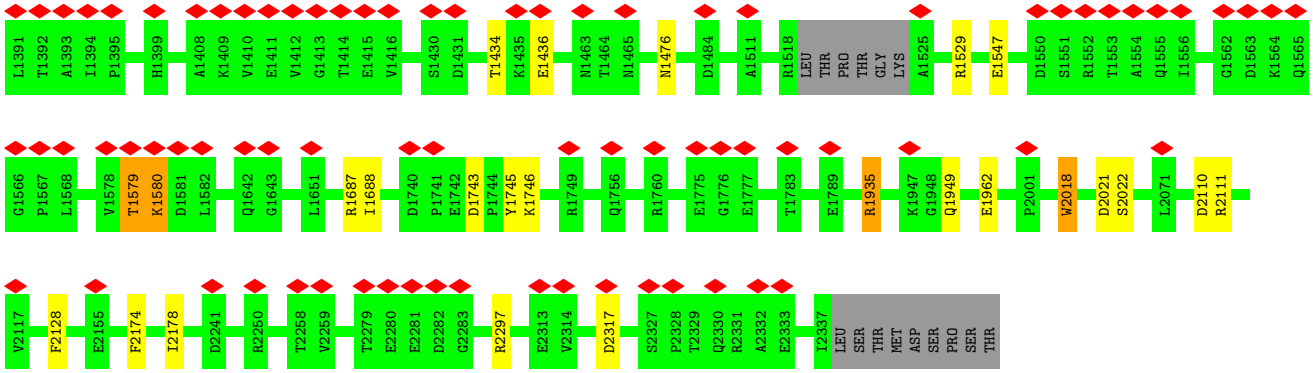
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:

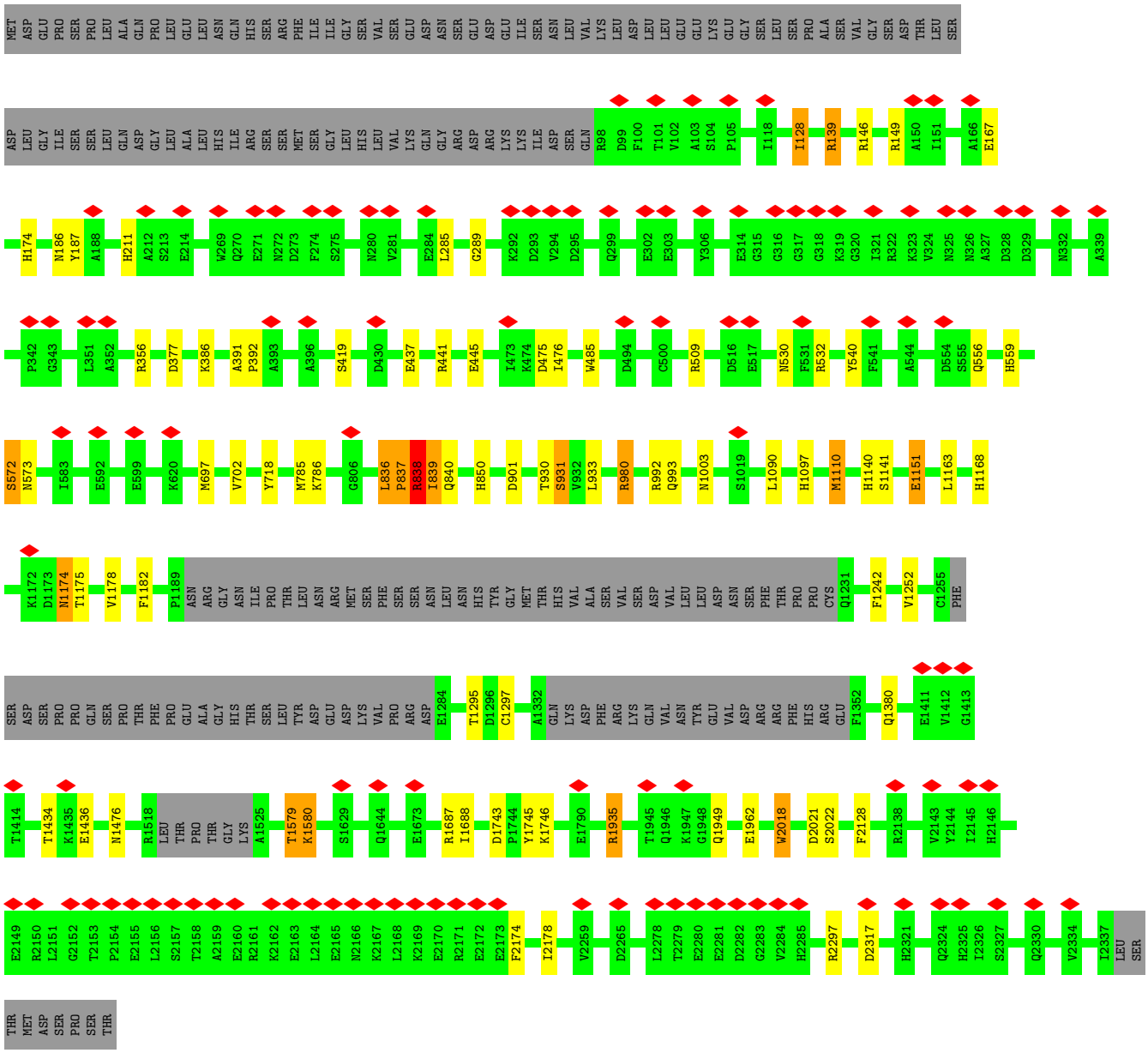






• Molecule 1: Acetyl-CoA carboxylase 1

Chain B:

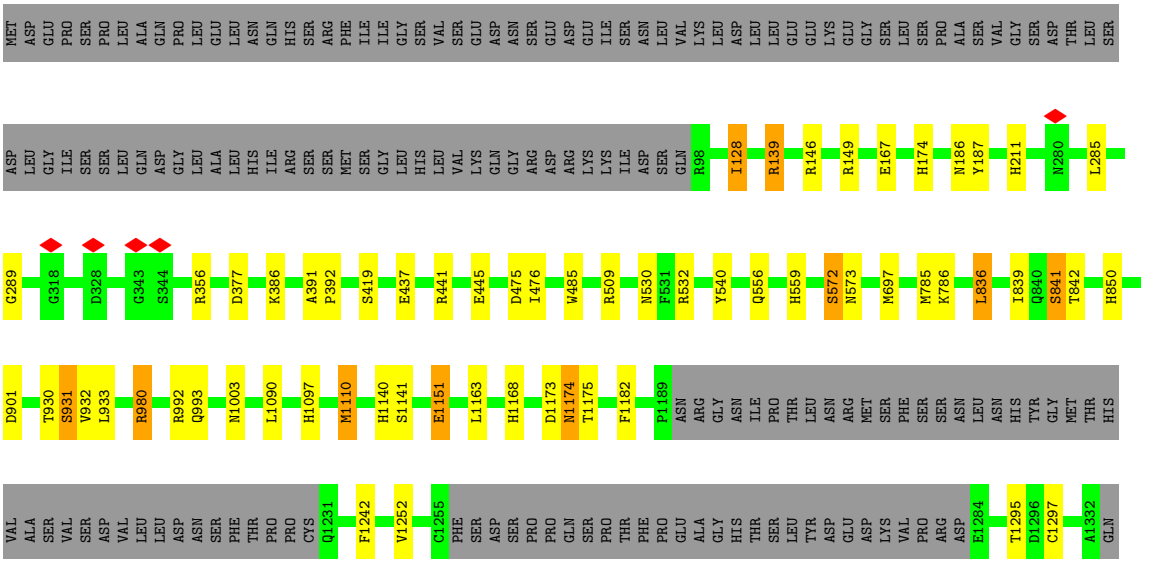


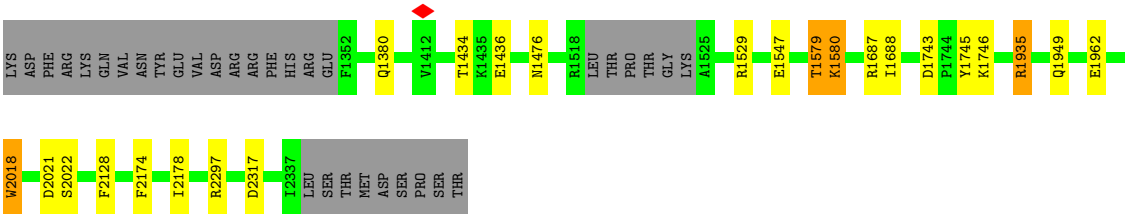
• Molecule 1: Acetyl-CoA carboxylase 1

Chain C:

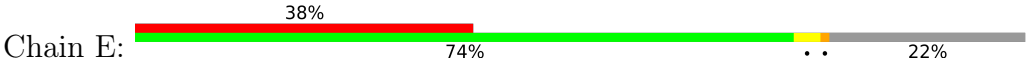
• Molecule 1: Acetyl-CoA carboxylase 1

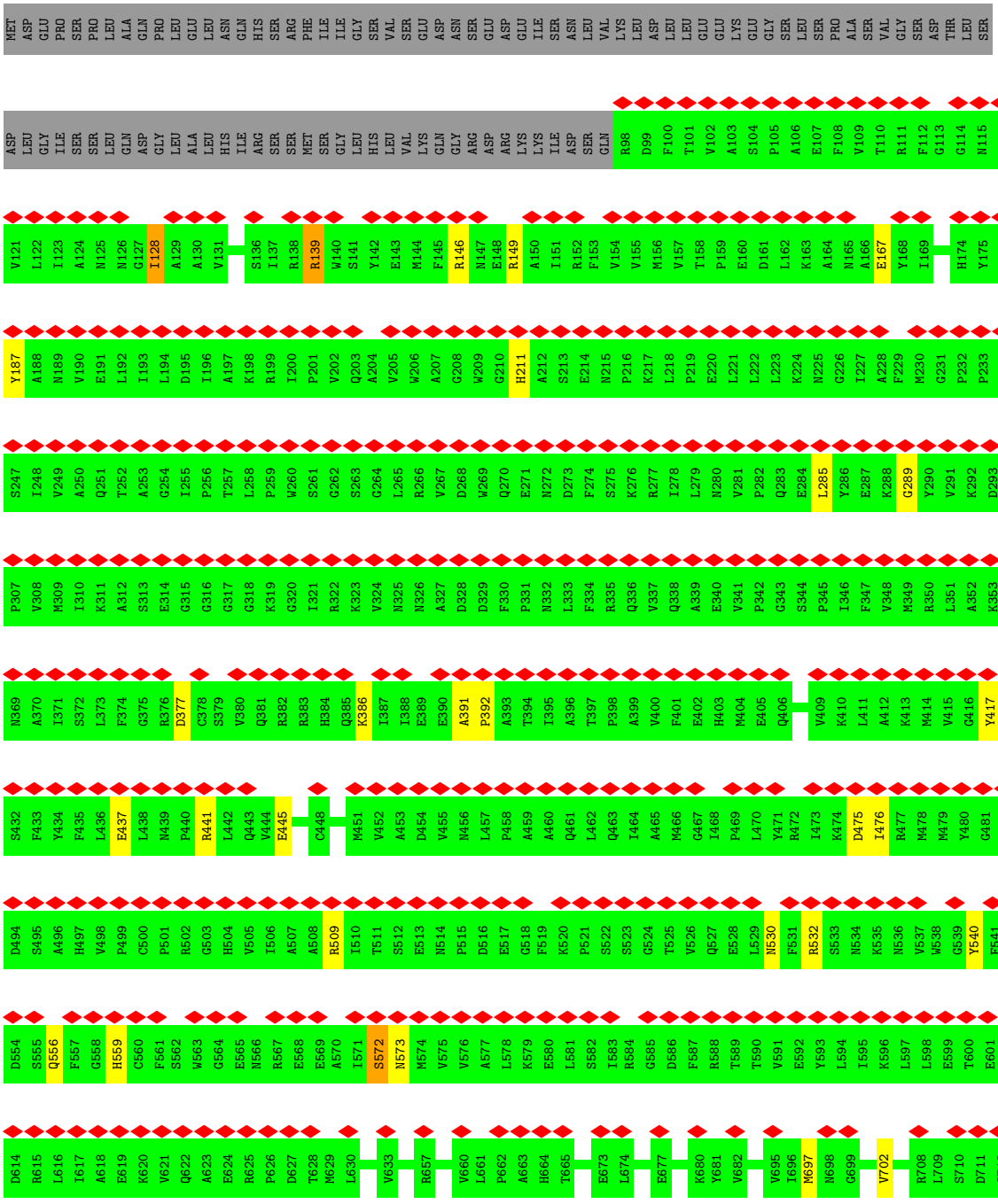
Chain D:

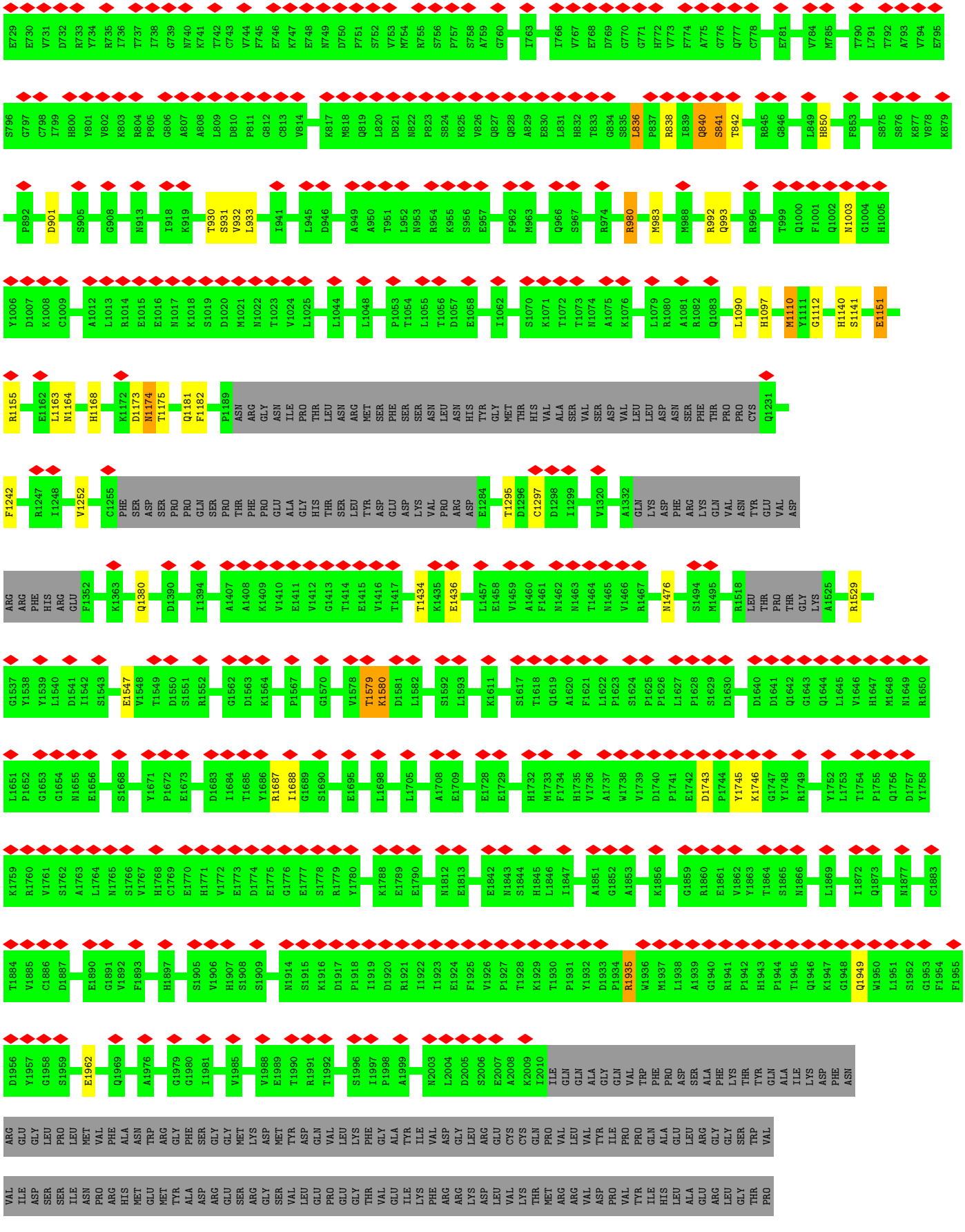




• Molecule 1: Acetyl-CoA carboxylase 1



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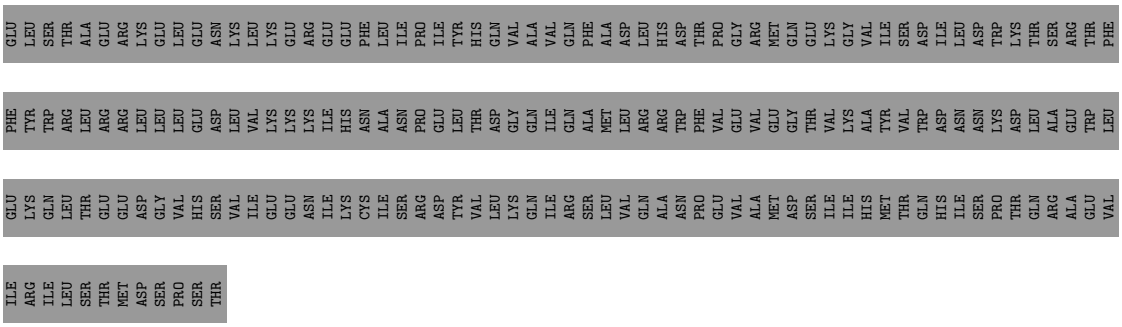
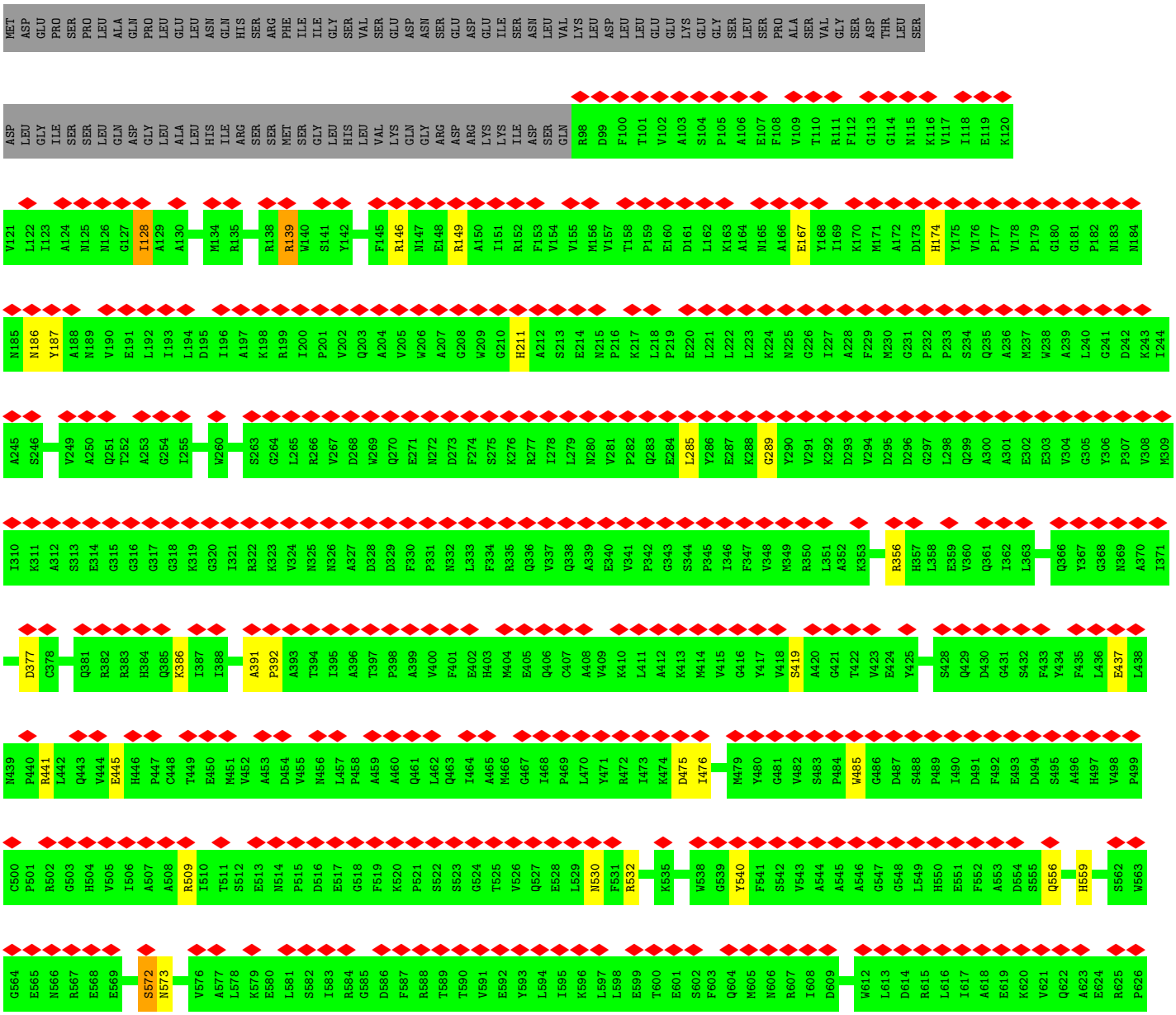
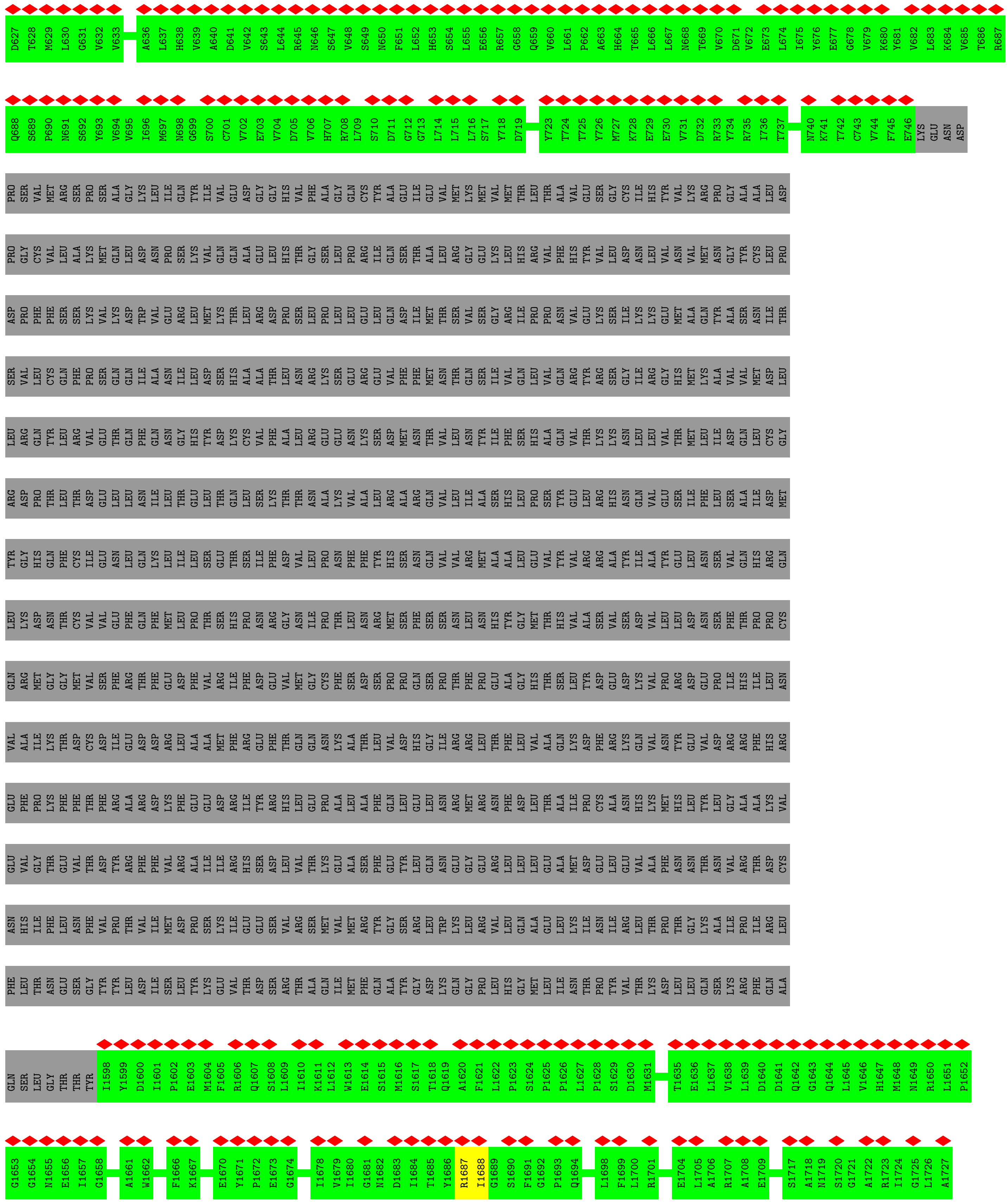
S796 G797 C798 T799 H800 Y801 V802 K803 R804 P805 G806 A807 A808 L809 D810 P811 G812 C813 V814 K817 H818 Q819 L820 D821 N822 P823 S824 K825 V826 Q827 Q828 A829 E830 L831 H832 T833 G834 S835 L836 P837 R838 I839 Q840 S841 T842 R845 G846 L849 H850 F853 S875 S876 K877 V878 K879
P892 D901 S905 G908 N913 I918 K919 T930 S931 V932 L933 I941 L945 D946 A949 A950 T951 L952 N953 R954 K955 S956 E957 F962 M963 Q966 S967 R974 R980 M983 M988 R992 Q993 R996 T999 Q1000 F1001 Q1002 N1003 G1004 H1005
Y1006 D1007 K1008 C1009 A1012 L1013 R1014 E1015 E1016 N1017 K1018 S1019 D1020 M1021 N1022 T1023 V1024 L1025 L1044 L1048 P1053 T1054 L1055 T1056 D1057 E1058 I1062 S1070 K1071 T1072 T1073 N1074 A1075 K1076 L1079 R1080 A1081 R1082 Q1083 L1090 H1097 M1110 Y1111 G1112 H1140 S1141 E1151
R1155 E1162 L1163 N1164 H1168 K1172 D1173 N1174 T1175 Q1181 F1182 P1189 ASN ARG GLY ASN ILE PRO THR LEU ASN ARG MET SER PHE SER SER ASN LEU ASN HIS TYR GLY MET THR HIS VAL ALA SER VAL SER ASP VAL LEU LEU ASP ASN SER PHE THR PRO PRO CYS Q1231
F1242 R1247 I1248 V1252 C1255 PHE SER ASP SER PRO PRO GLN SER PRO THR PHE PRO GLU ALA GLY HIS THR SER LEU TYR ASP GLU ASP LYS VAL PRO ARG ASP E1284 T1295 D1296 C1297 D1298 I1299 V1320 A1332 GLN LYS ASP PHE ARG LYS GLN VAL ASN TYR GLU VAL ASP
ARG ARG PHE HIS ARG GLU F1352 K1363 Q1380 D1390 T1394 A1407 A1408 K1409 V1410 E1411 V1412 G1413 T1414 E1415 V1416 T1417 T1434 K1435 E1436 L1457 E1458 V1459 A1460 F1461 N1462 N1463 T1464 N1465 V1466 R1467 N1476 S1494 M1495 R1518 LEU THR PRO THR GLY LYS A1525 R1529
G1537 Y1538 Y1539 L1540 D1541 I1542 S1543 E1547 V1548 T1549 D1550 S1551 R1552 G1562 D1563 K1564 P1567 G1570 V1578 T1579 K1580 D1581 L1582 S1592 L1593 K1611 S1617 T1618 Q1619 A1620 F1621 L1622 P1623 S1624 P1625 P1626 L1627 P1628 S1629 D1630 D1640 D1641 Q1642 G1643 Q1644 L1645 V1646 H1647 M1648 N1649 R1650
L1651 P1652 G1653 G1654 N1655 E1656 S1668 Y1671 P1672 E1673 D1683 I1684 T1685 Y1686 R1687 I1688 G1689 S1690 E1695 L1698 L1705 A1708 E1709 E1728 E1729 H1732 M1733 F1734 H1735 V1736 A1737 W1738 V1739 D1740 P1741 E1742 D1743 P1744 Y1745 K1746 G1747 Y1748 R1749 Y1752 L1753 T1754 P1755 Q1756 D1757 Y1758
K1759 R1760 V1761 S1762 A1763 L1764 N1765 S1766 V1767 H1768 C1769 E1770 H1771 V1772 E1773 D1774 E1775 G1776 E1777 S1778 R1779 Y1780 K1788 E1789 E1790 N1812 E1813 E1842 N1843 S1844 H1845 L1846 I1847 A1851 G1852 A1853 K1856 G1859 R1860 E1861 V1862 Y1863 T1864 S1865 N1866 L1869 I1872 Q1873 N1877 C1883
T1884 V1885 C1886 D1887 E1890 G1891 V1892 F1893 H1897 S1905 V1906 H1907 S1908 S1909 N1914 S1915 K1916 D1917 P1918 I1919 D1920 R1921 I1922 I1923 E1924 F1925 V1926 P1927 T1928 K1929 T1930 P1931 Y1932 D1933 P1934 R1935 W1936 M1937 L1938 A1939 G1940 R1941 P1942 H1943 P1944 T1945 Q1946 K1947 G1948 Q1949 W1950 L1951 S1962 G1963 F1964 F1965
D1956 Y1957 G1958 S1959 E1962 Q1969 A1976 G1979 G1980 I1981 V1985 V1988 E1989 T1990 R1991 T1992 S1996 I1997 P1998 A1999 N2003 L2004 D2005 S2006 E2007 A2008 K2009 I2010 ILE GLN GLN ALA GLY GLN VAL TRP PHE PRO ASP SER ALA PHE LYS THR TYR GLN ALA ILE LYS ASP PHE ASN
ARG GLU GLY LEU PRO LEU MET VAL PHE ALA ASN TRP ARG GLY PHE SER GLY GLY MET LYS ASP MET TYR ASP GLN VAL LEU LYS PHE GLY ALA TYR ILE PRO PRO GLN ALA GLU LEU ARG GLY GLY SER TRP VAL
VAL ILE ASP SER SER ILE ASN PRO ARG HIS MET GLU MET TYR ALA ASP ARG GLU SER ARG GLY SER VAL LEU GLU PRO GLU GLY THR VAL GLU ILE LYS PHE ARG ARG LYS ASP LEU VAL LYS THR MET ARG ARG VAL ASP PRO VAL TYR ILE HIS LEU GLU ALA GLU ARG LEU GLY THR PRO



• Molecule 1: Acetyl-CoA carboxylase 1

Chain F: 38% 53% • 45%

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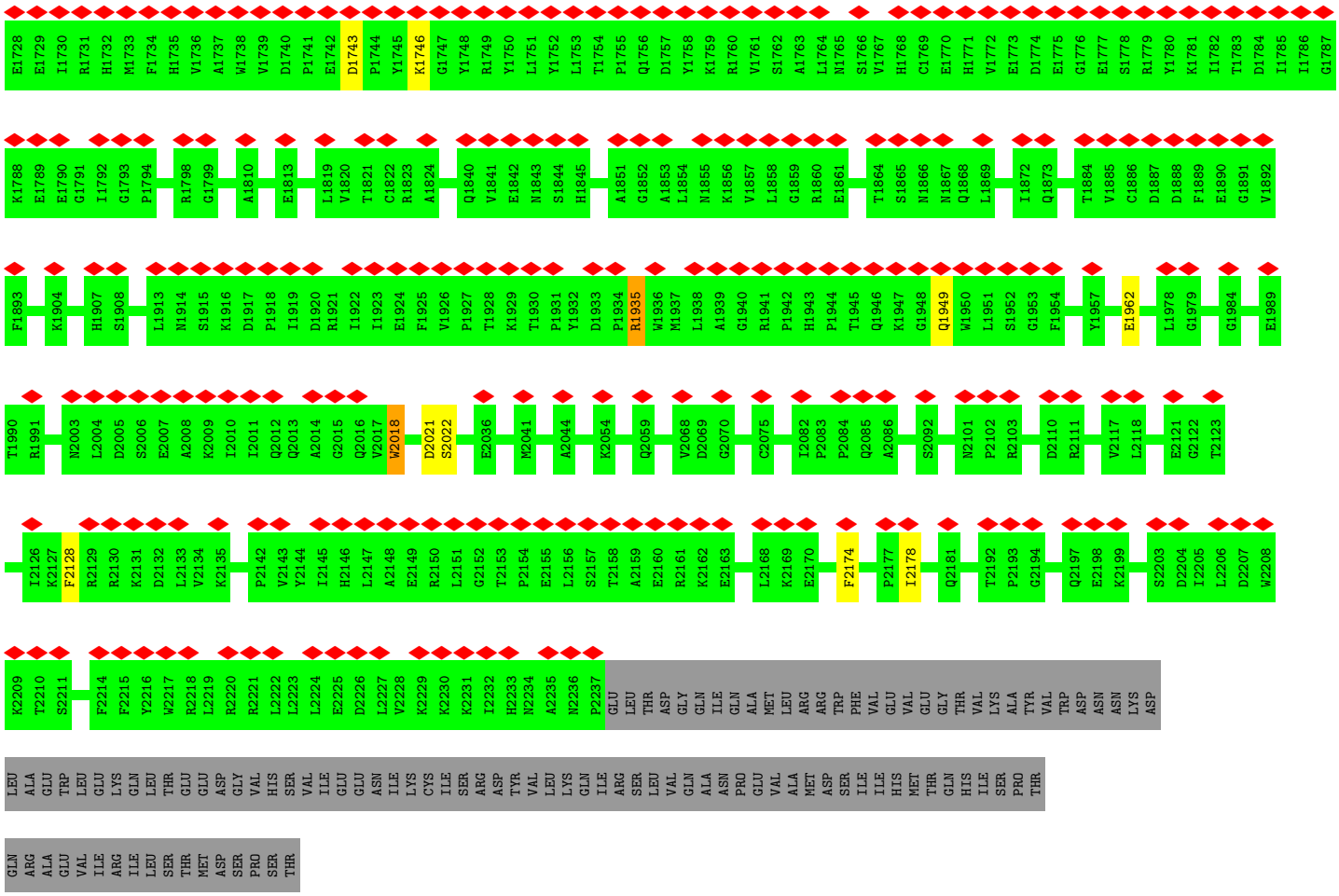
Q688 S689 P690 N691 S692 Y693 V694 V695 I696 M697 N698 G699 S700 C701 V702 E703 V704 D705 V706 H707 R708 L709 S710 D711 G712 G713 L714 L715 L716 S717 Y718 D719 Y723 T724 T725 Y726 M727 K728 E729 E730 V731 D732 R733 Y734 R735 I736 T737 N740 K741 T742 C743 V744 F745 E746 LYS GLU ASN ASP
PRO SER VAL MET ARG SER PRO SER ALA GLY LYS LEU ILE GLN TYR ILE VAL GLU ASP GLY GLY HIS VAL PHE ALA GLY GLN CYS TYR ALA GLU ILE GLU VAL MET LYS MET VAL MET THR LEU THR ALA VAL GLU SER GLY CYS ILE HIS TYR VAL LYS ARG PRO GLY ALA ALA LEU ASP
PRO GLY CYS VAL LEU ALA LYS MET GLN LEU ASP ASN PRO SER LYS VAL GLN GLN ALA GLU LEU HIS THR GLY SER LEU PRO ARG ILE GLN SER THR ALA LEU ARG GLY GLU LYS LEU HIS ARG VAL PHE HIS TYR VAL LEU ASP ASN LEU VAL ASN VAL MET ASN GLY TYR CYS LEU PRO
ASP PRO PHE PHE SER SER LYS VAL LYS ASP TRP VAL GLU ARG LEU MET LYS THR LEU ARG ASP PRO SER LEU PRO LEU LEU GLU LEU GLN ASP ILE MET THR SER VAL SER GLY ARG ILE PRO PRO ASN VAL GLU LYS SER ILE LYS LYS GLU MET ALA GLN TYR ALA SER ASN ILE THR
SER VAL LEU CYS GLN PHE PRO SER GLN GLN ILE ALA ASN ILE LEU ASP SER HIS ALA ALA THR LEU ASN ARG LYS SER GLU ARG GLU VAL PHE PHE MET ASN THR GLN SER ILE VAL GLN LEU VAL GLN ARG TYR ARG SER GLY ILE ARG GLY HIS MET LYS ALA VAL VAL MET ASP LEU
LEU ARG GLN TYR LEU ARG VAL GLU THR GLN PHE GLN ASN GLY HIS TYR ASP LYS CYS VAL PHE ALA LEU ARG GLU GLU ASN LYS SER ASP MET ASN THR VAL LEU ASN TYR ILE PHE SER HIS ALA GLN VAL THR LYS LYS ASN LEU LEU VAL THR MET LEU ILE ASP GLN LEU CYS GLY
ARG ASP PRO THR LEU THR ASP GLU LEU LEU ASN ILE LEU THR GLU LEU THR GLN LEU SER LYS THR THR ASN ALA LYS VAL ALA LEU ARG ALA ARG GLN VAL LEU ILE ALA SER HIS LEU PRO SER TYR GLU LEU ARG HIS ASN GLN VAL GLU SER ILE PHE LEU SER ALA ILE ASP MET
TYR GLY HIS GLN PHE CYS ILE GLU ASN LEU GLN LYS LEU ILE LEU SER GLU THR SER ILE PHE ASP VAL LEU PRO ASN PHE PHE TYR HIS SER ASN GLN VAL VAL ARG MET ALA ALA LEU GLU VAL TYR VAL ARG ARG ALA TYR ILE ALA TYR GLU LEU ASN SER VAL GLN HIS ARG GLN
LEU LYS ASP ASN THR CYS VAL VAL GLU PHE GLN PHE MET LEU PRO THR SER HIS PRO ASN ARG GLY ASN ILE PRO THR LEU ASN ARG MET SER PHE SER SER ASN LEU ASN HIS TYR GLY MET THR HIS VAL ALA SER VAL SER ASP VAL LEU LEU ASP ASN SER PHE THR PRO PRO CYS
GLN ARG MET GLY GLY MET VAL SER PHE ARG THR PHE GLU ASP PHE VAL ARG ILE PHE ASP GLU VAL MET GLY CYS PHE SER ASP SER PRO PRO GLN SER PRO THR PHE PRO GLU ALA GLY HIS THR SER LEU TYR ASP GLU ASP LYS VAL PRO ARG ASP GLU PRO ILE HIS ILE LEU ASN
VAL ALA ILE LYS THR ASP CYS ASP ILE GLU ASP ASP ARG LEU ALA ALA MET PHE ARG GLU PHE THR GLN GLN ASN LYS ALA THR LEU VAL ASP HIS GLY ILE ARG ARG LEU THR PHE LEU VAL ALA GLN LYS ASP PHE ARG LYS GLN VAL ASN TYR GLU VAL ASP ARG ARG PHE HIS ARG
GLU PHE PRO LYS PHE PHE THR PHE ARG ALA ARG ASP LYS PHE GLU GLU ASP ARG ILE TYR ARG HIS LEU GLU PRO ALA LEU ALA PHE GLN LEU GLU LEU ASN ARG MET ARG ASN PHE ASP LEU THR ALA ILE PRO CYS ALA ASN HIS LYS MET HIS LEU TYR LEU GLY ALA ALA LYS VAL
GLU VAL GLY THR GLU VAL THR ASP TYR ARG PHE PHE VAL ARG ALA ILE ILE ARG HIS SER ASP LEU VAL THR LYS GLU ALA SER PHE GLU TYR LEU GLU ASN GLU GLY GLU ARG LEU LEU LEU GLU ALA MET ASP GLU LEU GLU VAL ALA PHE ASN ASN THR ASN VAL ARG THR ASP CYS
ASN HIS ILE PHE LEU ASN PHE VAL PRO THR VAL ILE MET ASP PRO SER LYS ILE GLU GLU SER VAL ARG SER MET VAL MET ARG TYR GLY SER ARG LEU TRP LYS LEU ARG VAL LEU GLN ALA GLU LEU LYS ILE ASN ILE ARG LEU THR PRO THR GLY LYS ALA ILE PRO ILE ARG LEU
PHE LEU THR ASN GLU SER GLY TYR TYR LEU ASP ILE SER LEU TYR LYS GLU VAL THR ASP SER ARG THR ALA GLN ILE MET PHE GLN ALA TYR GLY ASP LYS GLN GLY PRO LEU HIS GLY MET LEU ILE ASN THR PRO TYR VAL THR LYS ASP LEU LEU GLN SER LYS ARG PHE GLN ALA
GLN SER LEU GLY THR THR TYR I1598 Y1599 D1600 I1601 P1602 E1603 M1604 F1605 R1606 Q1607 S1608 L1609 I1610 K1611 L1612 W1613 E1614 S1615 M1616 S1617 T1618 Q1619 A1620 F1621 L1622 P1623 S1624 P1625 P1626 L1627 P1628 S1629 D1630 M1631 T1635 E1636 L1637 V1638 L1639 D1640 D1641 Q1642 G1643 Q1644 L1645 V1646 H1647 M1648 N1649 R1650 L1651 P1652
G1653 G1654 N1655 E1656 I1657 G1658 A1661 W1662 F1666 K1667 E1670 Y1671 P1672 E1673 G1674 I1678 V1679 I1680 G1681 N1682 D1683 I1684 T1685 Y1686 R1687 I1688 G1689 S1690 F1691 G1692 P1693 Q1694 L1698 F1699 L1700 R1701 E1704 L1705 A1706 R1707 A1708 E1709 S1717 A1718 N1719 S1720 G1721 A1722 R1723 I1724 G1725 L1726 A1727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K1788 E1789 E1790 G1791 I1792 G1793 P1794 R1798 G1799 A1810 E1813 L1819 V1820 T1821 C1822 R1823 A1824 Q1840 V1841 E1842 N1843 S1844 H1845 A1851 G1852 A1853 L1854 N1855 K1856 V1857 L1858 G1859 R1860 E1861 T1864 S1865 N1866 N1867 Q1868 L1869 I1872 Q1873 T1884 V1885 C1886 D1887 D1888 F1889 E1890 G1891 V1892
F1893 K1904 H1907 S1908 L1913 N1914 S1915 K1916 D1917 P1918 I1919 D1920 R1921 I1922 I1923 E1924 F1925 V1926 P1927 T1928 K1929 T1930 P1931 Y1932 D1933 P1934 R1935 W1936 M1937 L1938 A1939 G1940 R1941 P1942 H1943 P1944 T1945 Q1946 K1947 G1948 Q1949 W1950 L1951 S1952 G1953 F1954 Y1957 E1962 L1978 G1979 G1984 E1989
T1990 R1991 N2003 L2004 D2005 S2006 E2007 A2008 K2009 I2010 I2011 Q2012 Q2013 A2014 G2015 Q2016 V2017 W2018 D2021 S2022 E2036 M2041 A2044 K2054 Q2059 V2068 D2069 G2070 C2075 I2082 P2083 P2084 Q2085 A2086 S2092 N2101 P2102 R2103 D2110 R2111 V2117 L2118 E2121 G2122 T2123
I2126 K2127 F2128 R2129 R2130 K2131 D2132 L2133 V2134 K2135 P2142 V2143 Y2144 I2145 H2146 L2147 A2148 E2149 R2150 L2151 G2152 T2153 P2154 E2155 L2156 S2157 T2158 A2159 E2160 R2161 K2162 E2163 L2168 K2169 E2170 F2174 P2177 I2178 Q2181 T2192 P2193 G2194 Q2197 E2198 K2199 S2203 D2204 I2205 L2206 D2207 W2208
K2209 T2210 S2211 F2214 F2215 Y2216 W2217 R2218 L2219 R2220 R2221 L2222 L2223 L2224 E2225 D2226 L2227 V2228 K2229 K2230 K2231 I2232 H2233 N2234 A2235 N2236 P2237 GLU LEU THR ASP GLY GLN ILE GLN ALA MET LEU ARG ARG TRP PHE VAL GLU VAL GLU GLY THR VAL LYS ALA TYR VAL TRP ASP ASN ASN LYS ASP
LEU ALA GLU TRP LEU GLU LYS GLN LEU THR GLU GLU ASP GLY VAL HIS SER VAL ILE GLU GLU ASN ILE LYS CYS ILE SER ARG ASP TYR VAL LEU LYS GLN ILE ARG SER LEU VAL GLN ALA ASN PRO GLU VAL ALA MET ASP SER ILE ILE HIS MET THR GLN HIS ILE SER PRO THR
GLN ARG ALA GLU VAL ILE ARG ILE LEU SER THR MET ASP SER PRO SER THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36041	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.719	Depositor
Minimum map value	-0.669	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	525.72235, 525.72235, 525.72235	wwPDB
Map dimensions	488, 488, 488	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0773, 1.0773, 1.0773	Depositor

5 Model quality

5.1 Standard geometry

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

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	1/17490 (0.0%)	0.59	0/23691
1	B	0.49	1/17490 (0.0%)	0.58	0/23691
1	C	0.49	1/17490 (0.0%)	0.59	0/23691
1	D	0.49	1/17490 (0.0%)	0.58	0/23691
1	E	0.49	0/14745	0.59	0/19979
1	F	0.55	1/10423 (0.0%)	0.60	0/14139
All	All	0.50	5/95128 (0.0%)	0.59	0/128882

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
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	2
All	All	0	22

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2018	TRP	C-N	-5.87	1.20	1.34
1	F	2018	TRP	C-N	-5.87	1.20	1.34
1	B	2018	TRP	C-N	-5.83	1.20	1.34
1	A	2018	TRP	C-N	-5.42	1.21	1.34
1	C	2018	TRP	C-N	-5.41	1.21	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1140	HIS	Peptide
1	A	1579	THR	Mainchain
1	A	1687	ARG	Peptide
1	A	419	SER	Mainchain
1	B	1140	HIS	Peptide
1	B	1579	THR	Mainchain
1	B	1687	ARG	Peptide
1	B	419	SER	Mainchain
1	C	1140	HIS	Peptide
1	C	1579	THR	Mainchain
1	C	1687	ARG	Peptide
1	C	419	SER	Mainchain
1	D	1140	HIS	Peptide
1	D	1579	THR	Mainchain
1	D	1687	ARG	Peptide
1	D	419	SER	Mainchain
1	E	1140	HIS	Peptide
1	E	1579	THR	Mainchain
1	E	1687	ARG	Peptide
1	E	419	SER	Mainchain
1	F	1687	ARG	Peptide
1	F	419	SER	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	17120	0	17047	48	0
1	B	17120	0	17046	83	0
1	C	17120	0	17047	71	0
1	D	17120	0	17046	73	0
1	E	14435	0	14365	79	0
1	F	10185	0	10085	20	0
2	A	15	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	15	1	0
2	C	15	0	15	0	0
2	D	15	0	15	0	0
2	E	15	0	15	0	0
All	All	93175	0	92711	290	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 2.

All (290) 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:D:930:THR:HG22	1:E:1168:HIS:HB2	1.23	1.10
1:D:1168:HIS:HB2	1:E:930:THR:HG22	1.44	0.99
1:B:1168:HIS:HB2	1:C:930:THR:HG22	1.51	0.92
1:B:930:THR:HG22	1:C:1168:HIS:HB2	1.49	0.92
1:B:933:LEU:HG	1:C:1151:GLU:OE1	1.72	0.89
1:B:1110:MET:HG2	1:C:980:ARG:HH22	1.40	0.84
1:E:840:GLN:O	1:E:841:SER:HB3	1.78	0.83
1:B:1168:HIS:HD2	1:B:1178:VAL:HG22	1.43	0.83
1:B:931:SER:HA	1:C:1168:HIS:ND1	1.96	0.80
1:B:1110:MET:HB3	1:C:980:ARG:NH2	1.97	0.80
1:D:980:ARG:HD2	1:E:1112:GLY:O	1.83	0.79
1:B:931:SER:HA	1:C:1168:HIS:CE1	2.20	0.77
1:D:933:LEU:HG	1:E:1151:GLU:OE1	1.88	0.74
1:A:702:VAL:HB	1:A:836:LEU:HD12	1.70	0.74
1:B:697:MET:HB3	1:B:836:LEU:CD2	2.18	0.73
1:B:836:LEU:N	1:B:836:LEU:HD23	2.03	0.73
1:D:980:ARG:NH2	1:E:1110:MET:HB3	2.04	0.73
1:E:836:LEU:HD23	1:E:836:LEU:N	2.03	0.73
1:B:930:THR:O	1:C:1168:HIS:ND1	2.20	0.73
1:B:838:ARG:HG2	1:B:838:ARG:O	1.89	0.72
1:B:1168:HIS:HD2	1:B:1178:VAL:CG2	2.02	0.72
1:C:139:ARG:NH1	1:D:573:ASN:OD1	2.23	0.71
1:E:139:ARG:NH1	1:F:573:ASN:OD1	2.23	0.71
1:A:139:ARG:NH1	1:B:573:ASN:OD1	2.23	0.71
1:B:931:SER:HA	1:C:1168:HIS:HD1	1.52	0.71
1:E:573:ASN:OD1	1:F:139:ARG:NH1	2.24	0.71
1:B:1110:MET:CG	1:C:980:ARG:HH22	2.04	0.70
1:C:573:ASN:OD1	1:D:139:ARG:NH1	2.24	0.70
1:A:573:ASN:OD1	1:B:139:ARG:NH1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1110:MET:HG2	1:E:980:ARG:NH2	2.06	0.70
1:B:697:MET:HB3	1:B:836:LEU:HD21	1.74	0.70
1:E:838:ARG:O	1:E:838:ARG:HG3	1.90	0.70
1:E:1743:ASP:OD2	1:E:1746:LYS:NZ	2.25	0.69
1:C:1743:ASP:OD2	1:C:1746:LYS:NZ	2.25	0.69
1:D:930:THR:CG2	1:E:1168:HIS:HB2	2.15	0.68
1:B:930:THR:O	1:C:1168:HIS:HB2	1.93	0.68
1:D:1743:ASP:OD2	1:D:1746:LYS:NZ	2.26	0.68
1:F:1743:ASP:OD2	1:F:1746:LYS:NZ	2.26	0.68
1:A:1743:ASP:OD2	1:A:1746:LYS:NZ	2.25	0.68
1:B:1743:ASP:OD2	1:B:1746:LYS:NZ	2.26	0.67
1:D:931:SER:HA	1:E:1168:HIS:ND1	2.09	0.67
1:D:931:SER:HA	1:E:1168:HIS:HD1	1.58	0.67
1:B:1151:GLU:OE1	1:C:933:LEU:HG	1.93	0.67
1:D:1935:ARG:NH1	1:D:1962:GLU:OE1	2.28	0.67
1:D:697:MET:HB3	1:D:836:LEU:CD2	2.25	0.67
1:B:1935:ARG:NH1	1:B:1962:GLU:OE1	2.28	0.67
1:E:836:LEU:HD23	1:E:836:LEU:H	1.58	0.67
1:F:1935:ARG:NH1	1:F:1962:GLU:OE1	2.28	0.67
1:D:980:ARG:HH22	1:E:1110:MET:HG2	1.62	0.65
1:B:1110:MET:HB3	1:C:980:ARG:HH22	1.59	0.65
1:C:837:PRO:O	1:C:838:ARG:HB3	1.97	0.65
1:D:391:ALA:HB3	1:D:392:PRO:HD3	1.79	0.65
1:E:980:ARG:HH11	1:E:983:MET:CE	2.10	0.64
1:F:391:ALA:HB3	1:F:392:PRO:HD3	1.79	0.64
1:B:391:ALA:HB3	1:B:392:PRO:HD3	1.79	0.64
1:E:697:MET:HB3	1:E:836:LEU:CD2	2.26	0.64
1:A:391:ALA:HB3	1:A:392:PRO:HD3	1.80	0.64
1:B:836:LEU:HD23	1:B:836:LEU:H	1.61	0.64
1:E:391:ALA:HB3	1:E:392:PRO:HD3	1.80	0.64
1:A:1935:ARG:NH1	1:A:1962:GLU:OE1	2.31	0.64
1:D:980:ARG:CD	1:E:1112:GLY:O	2.46	0.64
1:D:931:SER:HA	1:E:1168:HIS:CE1	2.32	0.63
1:D:980:ARG:HH22	1:E:1110:MET:HB3	1.61	0.63
1:D:1151:GLU:OE1	1:E:933:LEU:HG	1.99	0.63
1:D:697:MET:HB3	1:D:836:LEU:HD21	1.81	0.63
1:E:1935:ARG:NH1	1:E:1962:GLU:OE1	2.31	0.63
1:C:1935:ARG:NH1	1:C:1962:GLU:OE1	2.31	0.62
1:C:391:ALA:HB3	1:C:392:PRO:HD3	1.80	0.62
1:B:1151:GLU:OE2	1:C:931:SER:HB2	2.01	0.61
1:D:930:THR:HG21	1:E:1168:HIS:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:ARG:N	1:A:838:ARG:HD3	2.16	0.60
1:B:836:LEU:O	1:B:837:PRO:O	2.19	0.60
1:D:1168:HIS:HD1	1:E:931:SER:HA	1.66	0.60
1:B:933:LEU:CG	1:C:1151:GLU:OE1	2.49	0.60
1:F:128:ILE:HD11	1:F:556:GLN:O	2.02	0.60
1:B:1110:MET:CB	1:C:980:ARG:HH22	2.15	0.60
1:D:933:LEU:HD12	1:E:1155:ARG:NE	2.17	0.60
1:B:1168:HIS:CD2	1:B:1178:VAL:HG22	2.32	0.59
1:D:128:ILE:HD11	1:D:556:GLN:O	2.02	0.59
1:D:1110:MET:HG2	1:E:980:ARG:HH22	1.67	0.59
1:D:186:ASN:OD1	1:D:187:TYR:N	2.36	0.59
1:A:838:ARG:HH21	1:A:838:ARG:HG3	1.67	0.58
1:B:128:ILE:HD11	1:B:556:GLN:O	2.02	0.58
1:F:186:ASN:OD1	1:F:187:TYR:N	2.36	0.58
1:B:186:ASN:OD1	1:B:187:TYR:N	2.36	0.58
1:C:186:ASN:OD1	1:C:187:TYR:N	2.37	0.58
1:A:186:ASN:OD1	1:A:187:TYR:N	2.37	0.57
1:D:836:LEU:HD23	1:D:836:LEU:H	1.69	0.57
1:E:186:ASN:OD1	1:E:187:TYR:N	2.37	0.57
1:A:128:ILE:HD11	1:A:556:GLN:O	2.05	0.57
1:A:356:ARG:NH1	1:A:377:ASP:OD2	2.38	0.57
1:E:1579:THR:O	1:E:1579:THR:OG1	2.21	0.57
1:D:1168:HIS:ND1	1:E:931:SER:HA	2.20	0.56
1:D:932:VAL:CG2	1:E:1151:GLU:OE1	2.53	0.56
1:E:356:ARG:NH1	1:E:377:ASP:OD2	2.38	0.56
1:E:386:LYS:NZ	1:E:445:GLU:OE2	2.38	0.56
1:C:356:ARG:NH1	1:C:377:ASP:OD2	2.38	0.56
1:C:128:ILE:HD11	1:C:556:GLN:O	2.05	0.56
1:E:285:LEU:O	1:E:289:GLY:N	2.38	0.56
1:A:386:LYS:NZ	1:A:445:GLU:OE2	2.38	0.56
1:A:702:VAL:HB	1:A:836:LEU:CD1	2.36	0.56
1:C:386:LYS:NZ	1:C:445:GLU:OE2	2.38	0.56
1:D:930:THR:O	1:E:1168:HIS:ND1	2.37	0.56
1:E:128:ILE:HD11	1:E:556:GLN:O	2.05	0.55
1:D:932:VAL:HG22	1:E:1151:GLU:OE1	2.06	0.55
1:A:837:PRO:O	1:A:838:ARG:HB3	2.06	0.55
1:A:167:GLU:OE2	1:B:532:ARG:NH1	2.40	0.55
1:C:167:GLU:OE2	1:D:532:ARG:NH1	2.40	0.55
1:E:167:GLU:OE2	1:F:532:ARG:NH1	2.40	0.55
1:E:980:ARG:HH11	1:E:983:MET:HE1	1.70	0.55
1:A:285:LEU:O	1:A:289:GLY:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:980:ARG:HH21	1:B:980:ARG:CG	2.19	0.55
1:B:285:LEU:O	1:B:289:GLY:N	2.40	0.54
1:E:697:MET:HB3	1:E:836:LEU:HD21	1.89	0.54
1:C:285:LEU:O	1:C:289:GLY:N	2.38	0.54
1:C:836:LEU:O	1:C:837:PRO:O	2.26	0.54
1:E:980:ARG:NH1	1:E:983:MET:CE	2.70	0.54
1:B:837:PRO:O	1:B:838:ARG:HB3	2.07	0.53
1:B:980:ARG:NH2	1:C:1110:MET:HB3	2.23	0.53
1:B:931:SER:CA	1:C:1168:HIS:HD1	2.21	0.53
1:D:785:MET:O	1:D:786:LYS:HB2	2.09	0.53
1:A:1174:ASN:OD1	1:A:1174:ASN:N	2.42	0.53
1:B:838:ARG:C	1:B:839:ILE:HG13	2.29	0.53
1:F:285:LEU:O	1:F:289:GLY:N	2.40	0.53
1:C:1174:ASN:N	1:C:1174:ASN:OD1	2.42	0.52
1:D:1110:MET:HG2	1:E:980:ARG:CZ	2.39	0.52
1:E:1174:ASN:N	1:E:1174:ASN:OD1	2.42	0.52
1:D:285:LEU:O	1:D:289:GLY:N	2.40	0.52
1:D:980:ARG:HH22	1:E:1110:MET:CG	2.23	0.51
1:A:702:VAL:HG12	1:A:836:LEU:HD13	1.92	0.51
1:B:785:MET:O	1:B:786:LYS:HB2	2.09	0.51
1:D:1168:HIS:CE1	1:E:931:SER:HA	2.46	0.51
1:F:386:LYS:NZ	1:F:445:GLU:OE2	2.43	0.51
1:A:850:HIS:NE2	1:A:901:ASP:OD2	2.43	0.51
1:E:850:HIS:NE2	1:E:901:ASP:OD2	2.42	0.51
1:B:1174:ASN:OD1	1:B:1174:ASN:N	2.44	0.51
1:B:930:THR:O	1:C:1168:HIS:CB	2.59	0.51
1:D:386:LYS:NZ	1:D:445:GLU:OE2	2.43	0.51
1:D:1174:ASN:OD1	1:D:1174:ASN:N	2.44	0.51
1:B:850:HIS:NE2	1:B:901:ASP:OD2	2.44	0.51
1:B:386:LYS:NZ	1:B:445:GLU:OE2	2.43	0.50
1:B:475:ASP:OD1	1:B:476:ILE:N	2.45	0.50
1:F:2021:ASP:OD1	1:F:2022:SER:N	2.44	0.50
1:A:128:ILE:HD11	1:A:556:GLN:HG3	1.93	0.50
1:A:702:VAL:CG1	1:A:836:LEU:HD13	2.42	0.50
1:D:2021:ASP:OD1	1:D:2022:SER:N	2.44	0.50
1:E:128:ILE:HD11	1:E:556:GLN:HG3	1.94	0.50
1:F:475:ASP:OD1	1:F:476:ILE:N	2.45	0.49
1:B:2021:ASP:OD1	1:B:2022:SER:N	2.44	0.49
1:B:1579:THR:O	1:B:1579:THR:OG1	2.21	0.49
1:C:532:ARG:NH1	1:D:167:GLU:OE2	2.45	0.49
1:F:128:ILE:HD11	1:F:556:GLN:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:ASP:OD1	1:D:476:ILE:N	2.45	0.49
1:D:980:ARG:HH22	1:E:1110:MET:CB	2.24	0.49
1:C:128:ILE:HD11	1:C:556:GLN:HG3	1.94	0.49
1:B:718:TYR:OH	1:B:837:PRO:HG2	2.13	0.49
1:E:532:ARG:NH1	1:F:167:GLU:OE2	2.45	0.49
1:A:702:VAL:HG12	1:A:836:LEU:CD1	2.43	0.49
1:B:128:ILE:HD11	1:B:556:GLN:HG3	1.95	0.49
1:A:532:ARG:NH1	1:B:167:GLU:OE2	2.45	0.49
1:D:850:HIS:NE2	1:D:901:ASP:OD2	2.44	0.48
1:E:1380:GLN:O	1:E:1476:ASN:ND2	2.46	0.48
1:B:356:ARG:NH1	1:B:377:ASP:OD2	2.46	0.48
1:C:1380:GLN:O	1:C:1476:ASN:ND2	2.46	0.48
1:C:2317:ASP:OD2	1:D:2297:ARG:NH2	2.46	0.48
1:A:1003:ASN:O	1:A:1003:ASN:ND2	2.46	0.48
1:B:702:VAL:HG12	1:B:836:LEU:HD12	1.94	0.48
1:D:128:ILE:HD11	1:D:556:GLN:HG3	1.95	0.48
1:B:930:THR:CG2	1:C:1168:HIS:HB2	2.33	0.48
1:C:1295:THR:O	1:C:1297:CYS:N	2.47	0.48
1:D:836:LEU:HD23	1:D:836:LEU:N	2.27	0.48
1:A:2317:ASP:OD2	1:B:2297:ARG:NH2	2.46	0.48
1:D:356:ARG:NH1	1:D:377:ASP:OD2	2.47	0.48
1:E:1745:TYR:OH	1:F:2174:PHE:O	2.30	0.48
1:A:702:VAL:CG1	1:A:836:LEU:CD1	2.92	0.48
1:A:139:ARG:NH2	1:B:572:SER:OG	2.47	0.48
1:A:2174:PHE:O	1:B:1745:TYR:OH	2.31	0.48
1:C:139:ARG:NH2	1:D:572:SER:OG	2.47	0.48
1:D:1175:THR:HG21	1:D:1252:VAL:HG12	1.96	0.48
1:E:697:MET:HB3	1:E:836:LEU:HD22	1.95	0.48
1:A:1579:THR:O	1:A:1579:THR:OG1	2.21	0.47
1:F:356:ARG:NH1	1:F:377:ASP:OD2	2.47	0.47
1:A:1745:TYR:OH	1:B:2174:PHE:O	2.30	0.47
1:D:509:ARG:HB2	1:D:556:GLN:OE1	2.15	0.47
1:E:139:ARG:NH2	1:F:572:SER:OG	2.47	0.47
1:D:980:ARG:CG	1:D:980:ARG:HH21	2.26	0.47
1:C:1003:ASN:O	1:C:1003:ASN:ND2	2.46	0.47
1:C:1579:THR:O	1:C:1579:THR:OG1	2.21	0.47
1:C:2021:ASP:OD1	1:C:2022:SER:N	2.47	0.47
1:D:930:THR:HG22	1:E:1168:HIS:CB	2.17	0.47
1:B:509:ARG:HB2	1:B:556:GLN:OE1	2.15	0.47
1:B:980:ARG:CG	1:B:980:ARG:NH2	2.76	0.47
1:B:838:ARG:O	1:B:839:ILE:CG1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1295:THR:O	1:A:1297:CYS:N	2.47	0.47
1:C:850:HIS:NE2	1:C:901:ASP:OD2	2.43	0.47
1:F:509:ARG:HB2	1:F:556:GLN:OE1	2.15	0.47
1:B:1175:THR:HG21	1:B:1252:VAL:HG12	1.96	0.46
1:A:2021:ASP:OD1	1:A:2022:SER:N	2.47	0.46
1:B:697:MET:HB3	1:B:836:LEU:HD22	1.94	0.46
1:B:1003:ASN:O	1:B:1003:ASN:ND2	2.48	0.46
1:E:841:SER:O	1:E:842:THR:OG1	2.30	0.46
1:C:2297:ARG:NH2	1:D:2317:ASP:OD2	2.47	0.46
1:D:932:VAL:HG22	1:E:1151:GLU:CD	2.35	0.46
1:E:836:LEU:H	1:E:836:LEU:CD2	2.22	0.46
1:A:475:ASP:OD1	1:A:476:ILE:N	2.49	0.46
1:A:2297:ARG:NH2	1:B:2317:ASP:OD2	2.47	0.46
1:C:1745:TYR:OH	1:D:2174:PHE:O	2.30	0.46
1:B:1168:HIS:HB2	1:C:930:THR:CG2	2.34	0.45
1:E:1434:THR:HG22	1:E:1436:GLU:H	1.81	0.45
1:D:1380:GLN:O	1:D:1476:ASN:ND2	2.48	0.45
1:D:1579:THR:O	1:D:1579:THR:OG1	2.21	0.45
1:E:417:TYR:OH	1:E:420:ALA:O	2.23	0.45
1:E:1003:ASN:O	1:E:1003:ASN:ND2	2.46	0.45
1:A:1434:THR:HG22	1:A:1436:GLU:H	1.81	0.45
1:C:475:ASP:OD1	1:C:476:ILE:N	2.49	0.45
1:E:475:ASP:OD1	1:E:476:ILE:N	2.49	0.45
1:D:1003:ASN:ND2	1:D:1003:ASN:O	2.49	0.45
1:B:930:THR:HG22	1:C:1168:HIS:CB	2.34	0.45
1:D:1168:HIS:O	1:E:930:THR:HG21	2.16	0.45
1:A:1380:GLN:O	1:A:1476:ASN:ND2	2.46	0.45
1:C:2174:PHE:O	1:D:1745:TYR:OH	2.31	0.45
1:C:128:ILE:HG22	1:C:540:TYR:CE2	2.52	0.44
1:E:1175:THR:HG21	1:E:1252:VAL:HG12	1.99	0.44
1:A:128:ILE:HG22	1:A:540:TYR:CE2	2.52	0.44
1:C:391:ALA:HB3	1:C:392:PRO:CD	2.47	0.44
1:E:128:ILE:HG22	1:E:540:TYR:CE2	2.52	0.44
1:B:1380:GLN:O	1:B:1476:ASN:ND2	2.48	0.44
1:E:1295:THR:O	1:E:1297:CYS:N	2.47	0.44
1:B:930:THR:O	1:C:1168:HIS:CG	2.71	0.44
1:B:980:ARG:HH22	1:C:1110:MET:HB3	1.83	0.44
1:A:391:ALA:HB3	1:A:392:PRO:CD	2.47	0.44
1:B:1168:HIS:CD2	1:B:1178:VAL:CG2	2.91	0.44
1:C:836:LEU:H	1:C:836:LEU:HG	1.55	0.44
1:A:1175:THR:HG21	1:A:1252:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1175:THR:HG21	1:C:1252:VAL:HG12	1.99	0.44
1:A:2110:ASP:OD1	1:A:2111:ARG:N	2.46	0.43
1:C:1434:THR:HG22	1:C:1436:GLU:H	1.81	0.43
1:A:1579:THR:O	1:A:1580:LYS:O	2.37	0.43
1:C:1163:LEU:HD23	1:C:1182:PHE:HB3	2.00	0.43
1:C:1579:THR:O	1:C:1580:LYS:O	2.36	0.43
1:E:391:ALA:HB3	1:E:392:PRO:CD	2.47	0.43
1:A:1163:LEU:HD23	1:A:1182:PHE:HB3	2.00	0.43
1:B:838:ARG:O	1:B:839:ILE:HG13	2.18	0.43
1:B:838:ARG:HH21	1:B:838:ARG:HG3	1.82	0.43
1:B:980:ARG:HD2	1:C:1112:GLY:O	2.18	0.43
1:D:1295:THR:O	1:D:1297:CYS:N	2.48	0.43
1:E:1579:THR:O	1:E:1580:LYS:O	2.36	0.43
1:A:509:ARG:HB2	1:A:556:GLN:OE1	2.19	0.42
1:A:1173:ASP:N	1:A:1173:ASP:OD1	2.53	0.42
1:B:1579:THR:O	1:B:1580:LYS:O	2.36	0.42
1:E:509:ARG:HB2	1:E:556:GLN:OE1	2.19	0.42
1:D:1579:THR:O	1:D:1580:LYS:O	2.36	0.42
1:E:572:SER:OG	1:F:139:ARG:NH2	2.53	0.42
1:E:1163:LEU:HD23	1:E:1182:PHE:HB3	2.00	0.42
1:B:1163:LEU:HD23	1:B:1182:PHE:HB3	2.01	0.42
1:B:1434:THR:HG22	1:B:1436:GLU:H	1.84	0.42
1:C:2110:ASP:OD1	1:C:2111:ARG:N	2.46	0.42
1:D:1163:LEU:HD23	1:D:1182:PHE:HB3	2.01	0.42
1:A:572:SER:OG	1:B:139:ARG:NH2	2.53	0.42
1:D:1434:THR:HG22	1:D:1436:GLU:H	1.84	0.42
1:B:836:LEU:O	1:B:837:PRO:C	2.58	0.42
1:C:572:SER:OG	1:D:139:ARG:NH2	2.53	0.41
1:C:702:VAL:CG1	1:C:836:LEU:HD13	2.49	0.41
1:C:509:ARG:HB2	1:C:556:GLN:OE1	2.19	0.41
1:E:980:ARG:NH1	1:E:983:MET:HE2	2.35	0.41
1:C:1173:ASP:N	1:C:1173:ASP:OD1	2.52	0.41
1:B:1295:THR:O	1:B:1297:CYS:N	2.48	0.41
1:C:980:ARG:HE	1:C:984:LYS:HE3	1.84	0.41
1:E:1164:ASN:ND2	1:E:1181:GLN:O	2.53	0.41
1:E:1173:ASP:N	1:E:1173:ASP:OD1	2.53	0.41
1:A:1164:ASN:ND2	1:A:1181:GLN:O	2.53	0.41
1:C:697:MET:HB3	1:C:836:LEU:HD23	2.02	0.41
1:D:128:ILE:HG22	1:D:540:TYR:CE2	2.56	0.41
1:E:702:VAL:HG12	1:E:836:LEU:HD12	2.01	0.41
1:A:1529:ARG:NH1	1:A:1547:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:980:ARG:HH21	1:B:980:ARG:HG3	1.85	0.41
1:C:1529:ARG:NH1	1:C:1547:GLU:OE2	2.54	0.41
1:F:128:ILE:HG22	1:F:540:TYR:CE2	2.56	0.41
1:B:128:ILE:HG22	1:B:540:TYR:CE2	2.56	0.41
1:A:838:ARG:HH21	1:A:838:ARG:CG	2.33	0.41
1:C:1164:ASN:ND2	1:C:1181:GLN:O	2.53	0.41
1:E:1529:ARG:NH1	1:E:1547:GLU:OE2	2.54	0.41
2:B:2401:BTN:H92	2:B:2401:BTN:H2	1.93	0.41
1:D:841:SER:O	1:D:842:THR:OG1	2.31	0.41
1:D:1173:ASP:N	1:D:1173:ASP:OD1	2.54	0.40
1:B:933:LEU:CD1	1:C:1151:GLU:OE1	2.69	0.40
1:D:1110:MET:HG2	1:E:980:ARG:NH1	2.36	0.40
1:D:1151:GLU:OE1	1:E:932:VAL:CG2	2.69	0.40
1:B:1168:HIS:ND1	1:C:931:SER:HA	2.37	0.40
1:D:1529:ARG:NH1	1:D:1547:GLU:OE2	2.55	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	2136/2346 (91%)	2005 (94%)	122 (6%)	9 (0%)	30	67
1	B	2136/2346 (91%)	1998 (94%)	130 (6%)	8 (0%)	30	67
1	C	2136/2346 (91%)	2004 (94%)	123 (6%)	9 (0%)	30	67
1	D	2136/2346 (91%)	2000 (94%)	129 (6%)	7 (0%)	37	71
1	E	1809/2346 (77%)	1691 (94%)	110 (6%)	8 (0%)	30	67
1	F	1285/2346 (55%)	1226 (95%)	57 (4%)	2 (0%)	44	77
All	All	11638/14076 (83%)	10924 (94%)	671 (6%)	43 (0%)	32	67

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	841	SER
1	A	1580	LYS
1	B	837	PRO
1	B	1580	LYS
1	C	837	PRO
1	C	841	SER
1	C	1580	LYS
1	D	1580	LYS
1	E	840	GLN
1	E	841	SER
1	E	1580	LYS
1	A	1242	PHE
1	A	1688	ILE
1	B	839	ILE
1	B	1242	PHE
1	B	1688	ILE
1	C	838	ARG
1	C	1242	PHE
1	C	1688	ILE
1	D	841	SER
1	D	1242	PHE
1	D	1688	ILE
1	E	1242	PHE
1	E	1688	ILE
1	F	1688	ILE
1	A	838	ARG
1	A	1141	SER
1	B	838	ARG
1	B	1141	SER
1	C	1141	SER
1	D	839	ILE
1	D	1141	SER
1	E	1141	SER
1	A	837	PRO
1	A	1949	GLN
1	B	1949	GLN
1	C	1949	GLN
1	D	1949	GLN
1	E	1949	GLN
1	F	1949	GLN
1	E	420	ALA
1	C	839	ILE
1	A	839	ILE

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	1873/2057 (91%)	1846 (99%)	27 (1%)	62	75
1	B	1873/2057 (91%)	1845 (98%)	28 (2%)	60	75
1	C	1873/2057 (91%)	1847 (99%)	26 (1%)	62	75
1	D	1873/2057 (91%)	1847 (99%)	26 (1%)	62	75
1	E	1581/2057 (77%)	1560 (99%)	21 (1%)	65	77
1	F	1101/2057 (54%)	1085 (98%)	16 (2%)	60	75
All	All	10174/12342 (82%)	10030 (99%)	144 (1%)	62	75

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ILE
1	A	139	ARG
1	A	146	ARG
1	A	149	ARG
1	A	211	HIS
1	A	437	GLU
1	A	441	ARG
1	A	485	TRP
1	A	530	ASN
1	A	559	HIS
1	A	572	SER
1	A	836	LEU
1	A	838	ARG
1	A	840	GLN
1	A	841	SER
1	A	980	ARG
1	A	992	ARG
1	A	993	GLN
1	A	1090	LEU
1	A	1097	HIS
1	A	1110	MET
1	A	1151	GLU

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Mol	Chain	Res	Type
1	A	1174	ASN
1	A	1935	ARG
1	A	2018	TRP
1	A	2128	PHE
1	A	2178	ILE
1	B	128	ILE
1	B	139	ARG
1	B	146	ARG
1	B	149	ARG
1	B	174	HIS
1	B	211	HIS
1	B	437	GLU
1	B	441	ARG
1	B	485	TRP
1	B	530	ASN
1	B	559	HIS
1	B	572	SER
1	B	836	LEU
1	B	838	ARG
1	B	840	GLN
1	B	931	SER
1	B	980	ARG
1	B	992	ARG
1	B	993	GLN
1	B	1090	LEU
1	B	1097	HIS
1	B	1110	MET
1	B	1151	GLU
1	B	1174	ASN
1	B	1935	ARG
1	B	2018	TRP
1	B	2128	PHE
1	B	2178	ILE
1	C	128	ILE
1	C	139	ARG
1	C	146	ARG
1	C	149	ARG
1	C	211	HIS
1	C	437	GLU
1	C	441	ARG
1	C	485	TRP
1	C	530	ASN

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Mol	Chain	Res	Type
1	C	559	HIS
1	C	572	SER
1	C	836	LEU
1	C	838	ARG
1	C	840	GLN
1	C	980	ARG
1	C	992	ARG
1	C	993	GLN
1	C	1090	LEU
1	C	1097	HIS
1	C	1110	MET
1	C	1151	GLU
1	C	1174	ASN
1	C	1935	ARG
1	C	2018	TRP
1	C	2128	PHE
1	C	2178	ILE
1	D	128	ILE
1	D	139	ARG
1	D	146	ARG
1	D	149	ARG
1	D	174	HIS
1	D	211	HIS
1	D	437	GLU
1	D	441	ARG
1	D	485	TRP
1	D	530	ASN
1	D	559	HIS
1	D	572	SER
1	D	836	LEU
1	D	931	SER
1	D	980	ARG
1	D	992	ARG
1	D	993	GLN
1	D	1090	LEU
1	D	1097	HIS
1	D	1110	MET
1	D	1151	GLU
1	D	1174	ASN
1	D	1935	ARG
1	D	2018	TRP
1	D	2128	PHE

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Mol	Chain	Res	Type
1	D	2178	ILE
1	E	128	ILE
1	E	139	ARG
1	E	146	ARG
1	E	149	ARG
1	E	211	HIS
1	E	437	GLU
1	E	441	ARG
1	E	485	TRP
1	E	530	ASN
1	E	559	HIS
1	E	572	SER
1	E	836	LEU
1	E	980	ARG
1	E	992	ARG
1	E	993	GLN
1	E	1090	LEU
1	E	1097	HIS
1	E	1110	MET
1	E	1151	GLU
1	E	1174	ASN
1	E	1935	ARG
1	F	128	ILE
1	F	139	ARG
1	F	146	ARG
1	F	149	ARG
1	F	174	HIS
1	F	211	HIS
1	F	437	GLU
1	F	441	ARG
1	F	485	TRP
1	F	530	ASN
1	F	559	HIS
1	F	572	SER
1	F	1935	ARG
1	F	2018	TRP
1	F	2128	PHE
1	F	2178	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1164	ASN
1	A	1398	ASN
1	B	1168	HIS
1	B	1398	ASN
1	B	2285	HIS
1	C	1164	ASN
1	C	1398	ASN
1	D	1398	ASN
1	D	2285	HIS
1	E	1164	ASN
1	E	1398	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)

There are no oligosaccharides in this entry.

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	$\#\|Z\| > 2$
2	BTN	C	2401	1	16,16,17	1.16	1 (6%)	21,21,23	1.78	4 (19%)
2	BTN	B	2401	1	16,16,17	1.15	1 (6%)	21,21,23	1.77	5 (23%)
2	BTN	E	2401	1	16,16,17	1.17	1 (6%)	21,21,23	1.78	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BTN	D	2401	1	16,16,17	1.16	1 (6%)	21,21,23	1.77	5 (23%)
2	BTN	A	2401	1	16,16,17	1.16	1 (6%)	21,21,23	1.78	4 (19%)

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	BTN	C	2401	1	-	0/5/27/28	0/2/2/2
2	BTN	B	2401	1	-	0/5/27/28	0/2/2/2
2	BTN	E	2401	1	-	0/5/27/28	0/2/2/2
2	BTN	D	2401	1	-	0/5/27/28	0/2/2/2
2	BTN	A	2401	1	-	0/5/27/28	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2401	BTN	C2-S1	-3.61	1.76	1.82
2	A	2401	BTN	C2-S1	-3.60	1.76	1.82
2	C	2401	BTN	C2-S1	-3.56	1.76	1.82
2	B	2401	BTN	C2-S1	-3.53	1.77	1.82
2	D	2401	BTN	C2-S1	-3.53	1.77	1.82

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2401	BTN	C4-C2-S1	3.64	108.67	105.20
2	C	2401	BTN	C4-C2-S1	3.64	108.67	105.20
2	E	2401	BTN	C4-C2-S1	3.63	108.66	105.20
2	B	2401	BTN	C4-C2-S1	3.55	108.58	105.20
2	D	2401	BTN	C4-C2-S1	3.54	108.58	105.20
2	C	2401	BTN	C6-C5-C4	3.38	111.59	108.66
2	A	2401	BTN	C6-C5-C4	3.37	111.58	108.66
2	E	2401	BTN	C6-C5-C4	3.32	111.54	108.66
2	A	2401	BTN	C6-S1-C2	3.29	96.65	89.89
2	E	2401	BTN	C6-S1-C2	3.29	96.65	89.89
2	C	2401	BTN	C6-S1-C2	3.28	96.63	89.89
2	D	2401	BTN	C6-S1-C2	3.27	96.60	89.89
2	B	2401	BTN	C6-S1-C2	3.27	96.60	89.89
2	D	2401	BTN	C6-C5-C4	3.23	111.46	108.66
2	B	2401	BTN	C5-C6-S1	3.23	109.07	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2401	BTN	C6-C5-C4	3.21	111.44	108.66
2	D	2401	BTN	C5-C6-S1	3.20	109.05	106.31
2	A	2401	BTN	C5-C6-S1	3.17	109.02	106.31
2	E	2401	BTN	C5-C6-S1	3.15	109.01	106.31
2	C	2401	BTN	C5-C6-S1	3.15	109.00	106.31
2	B	2401	BTN	N2-C3-N1	2.00	110.64	108.76
2	D	2401	BTN	N2-C3-N1	2.00	110.64	108.76

There are no chirality outliers.

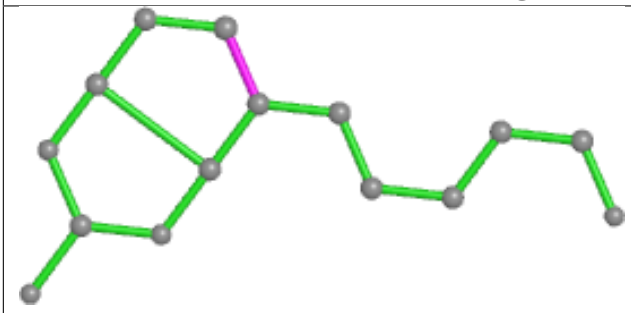
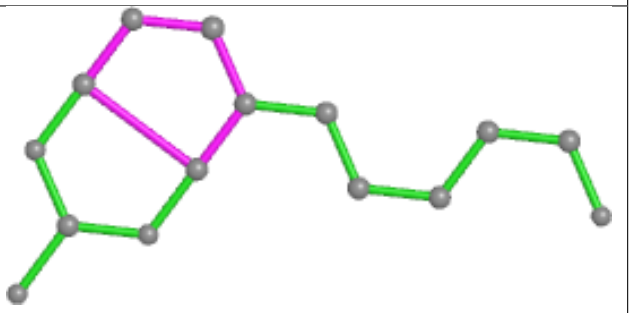
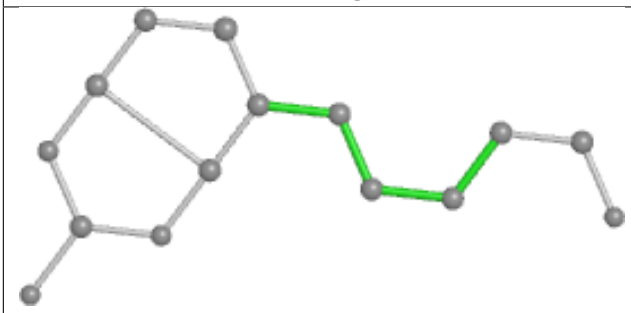
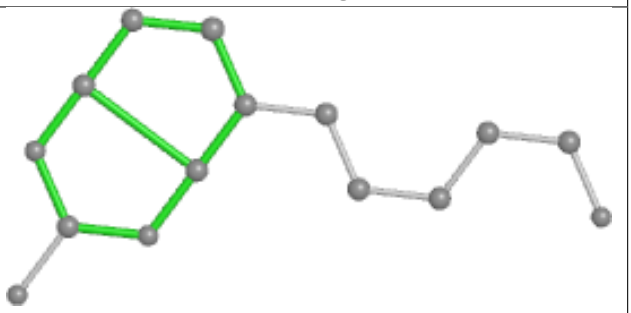
There are no torsion outliers.

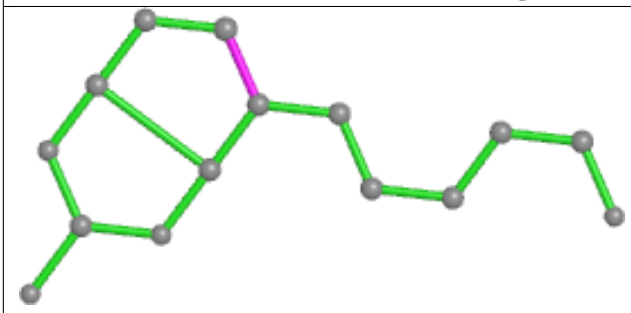
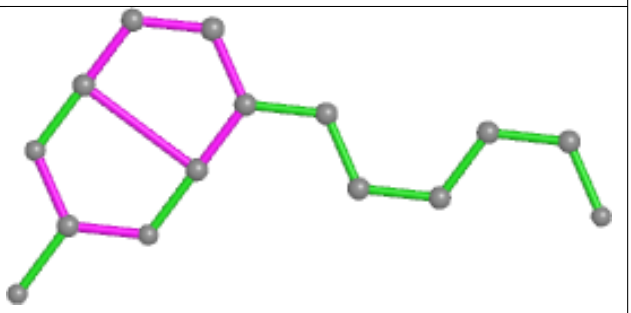
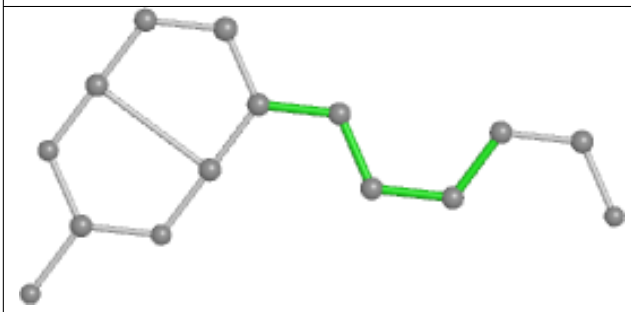
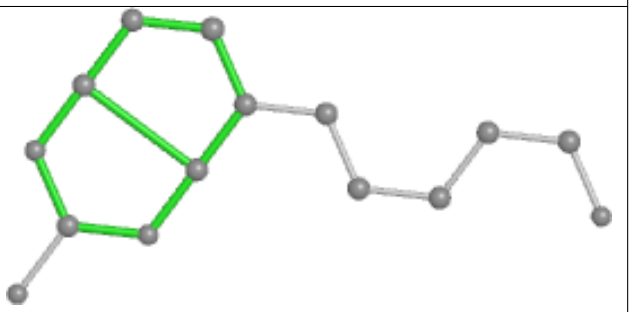
There are no ring outliers.

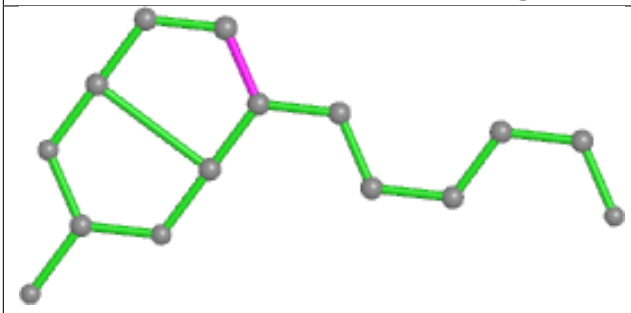
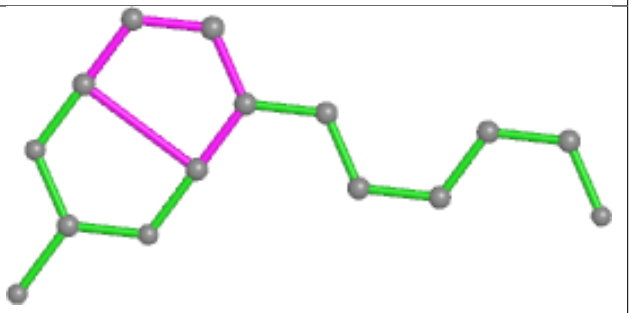
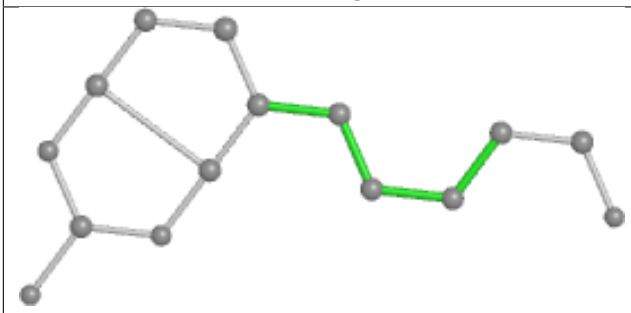
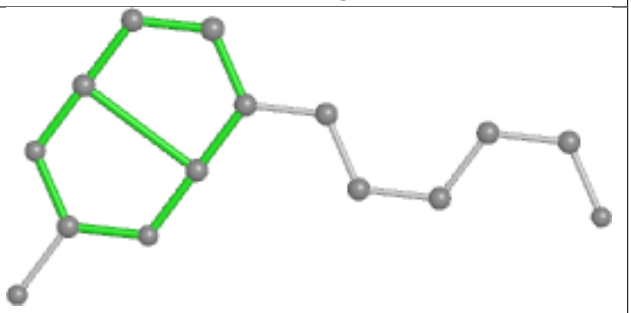
1 monomer is involved in 1 short contact:

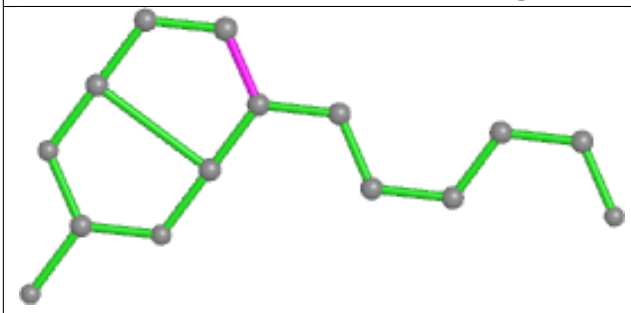
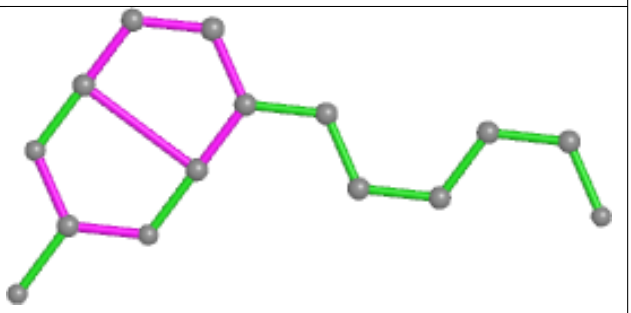
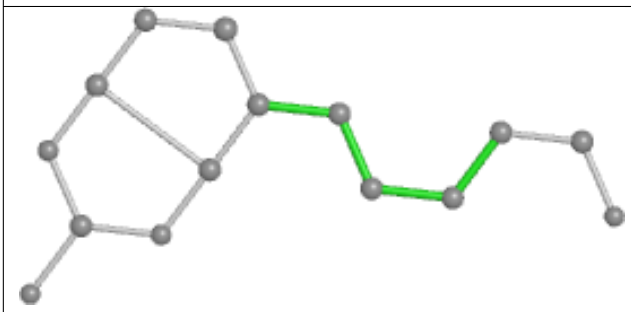
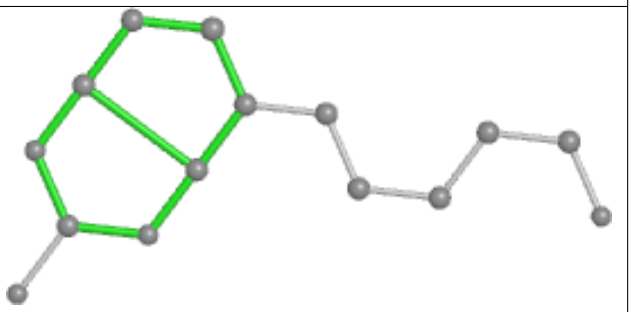
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2401	BTN	1	0

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

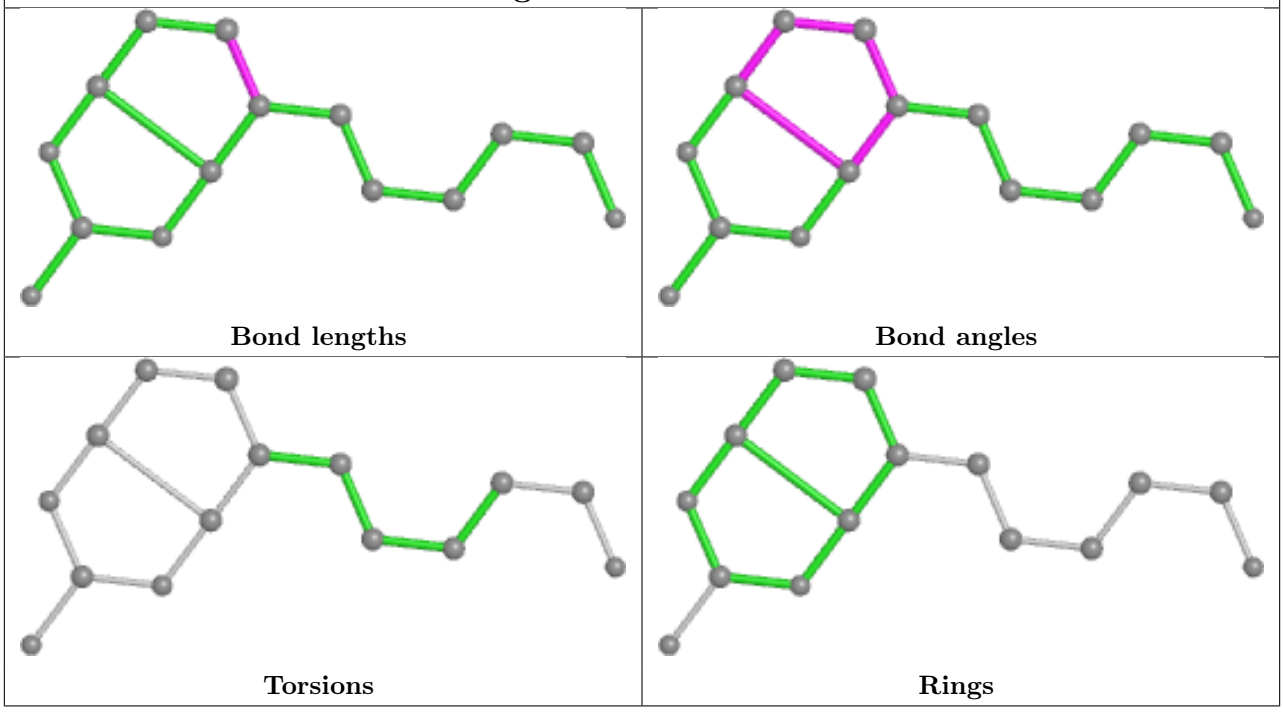
Ligand BTN C 2401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BTN B 2401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BTN E 2401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BTN D 2401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BTN A 2401



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.

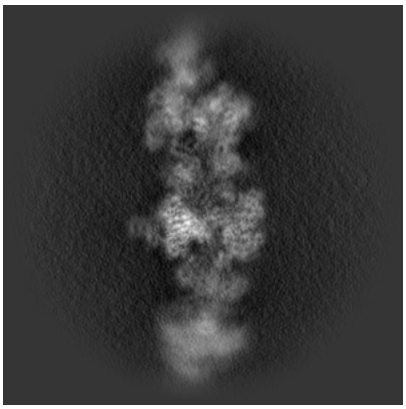
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38433. These allow visual inspection of the internal detail of the map and identification of artifacts.

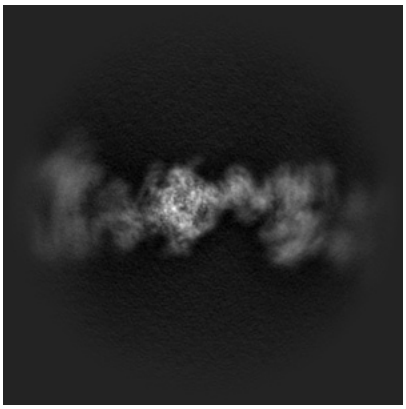
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

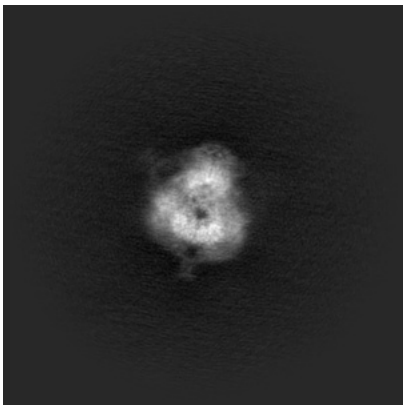
6.1.1 Primary map



X

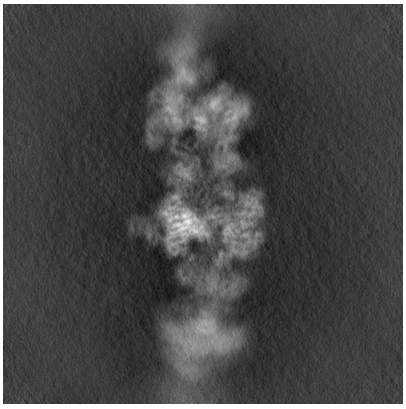


Y

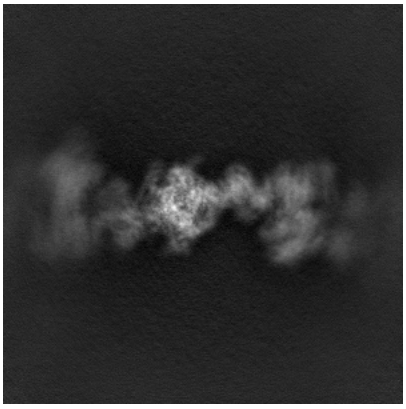


Z

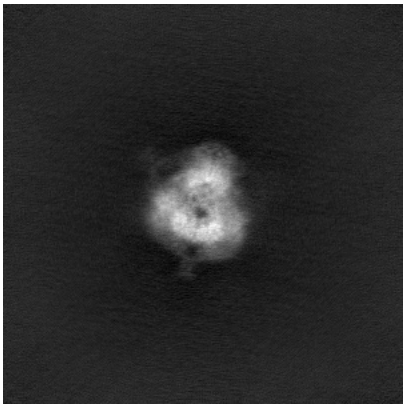
6.1.2 Raw map



X



Y

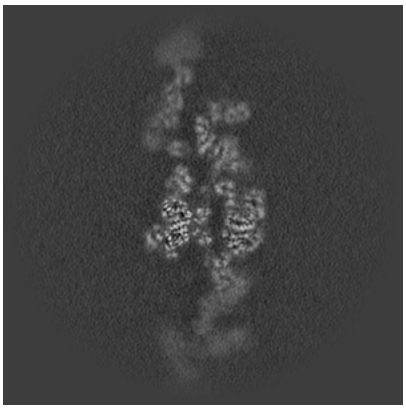


Z

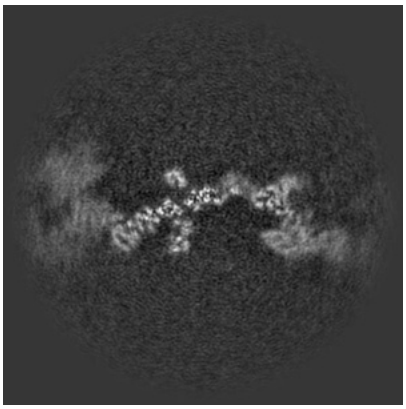
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

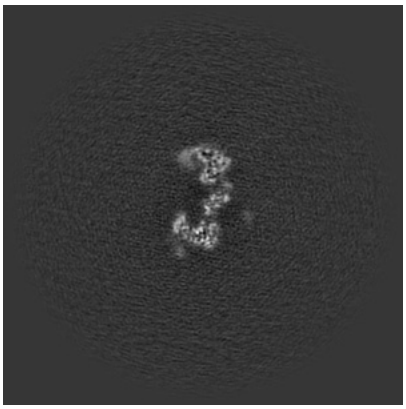
6.2.1 Primary map



X Index: 244

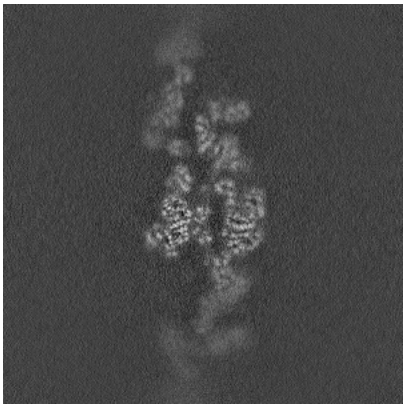


Y Index: 244

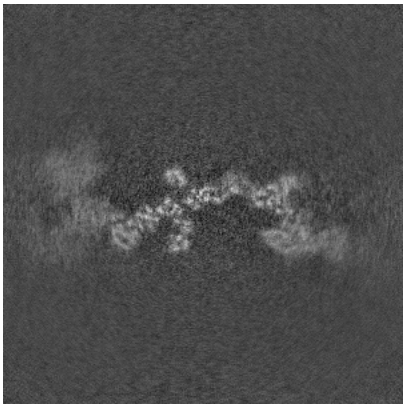


Z Index: 244

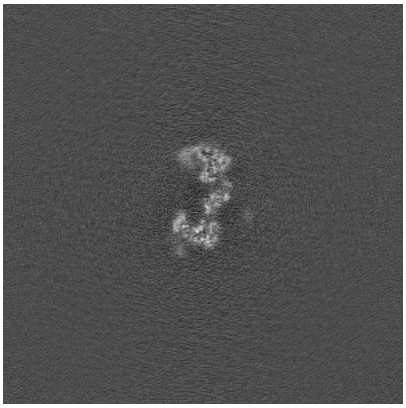
6.2.2 Raw map



X Index: 244



Y Index: 244

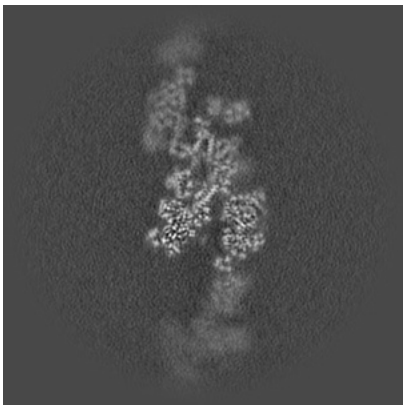


Z Index: 244

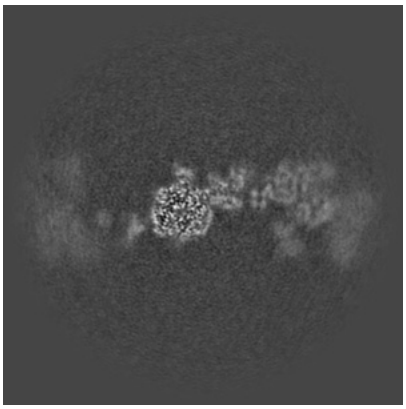
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

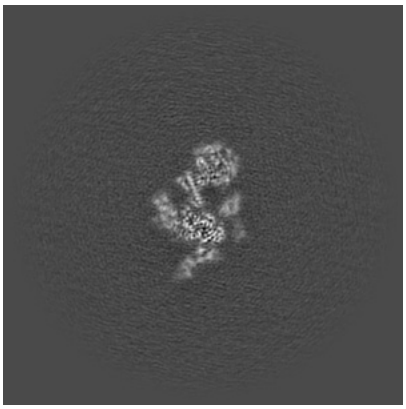
6.3.1 Primary map



X Index: 251

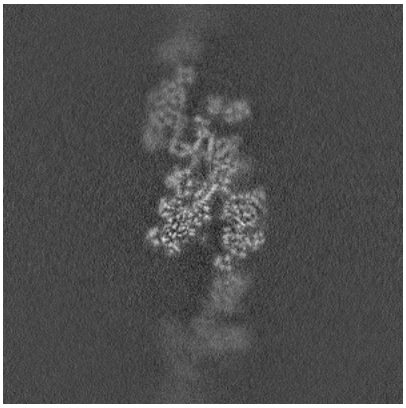


Y Index: 213

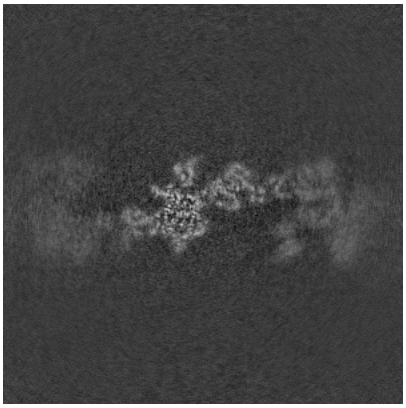


Z Index: 207

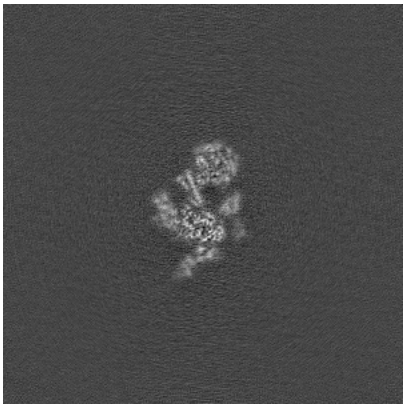
6.3.2 Raw map



X Index: 251



Y Index: 220

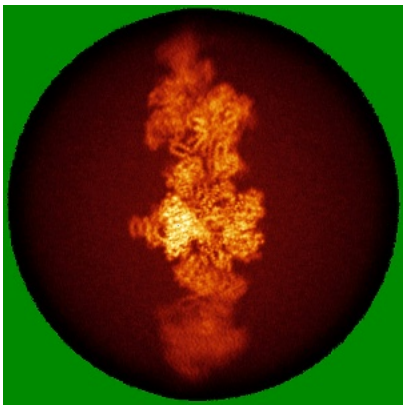


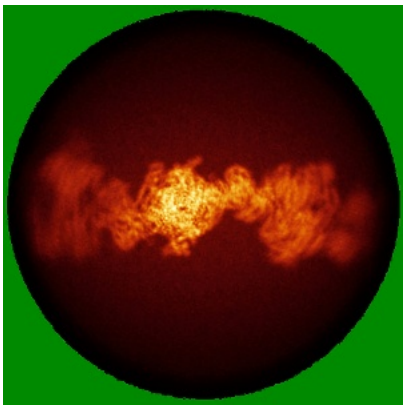
Z Index: 207

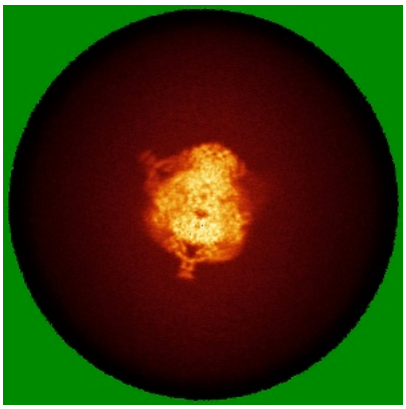
The images above show the largest variance slices of the map in three orthogonal directions.

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

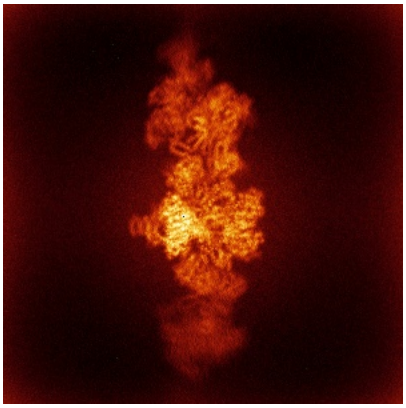
6.4.1 Primary map

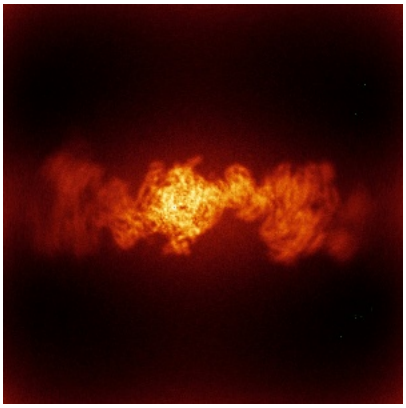

X

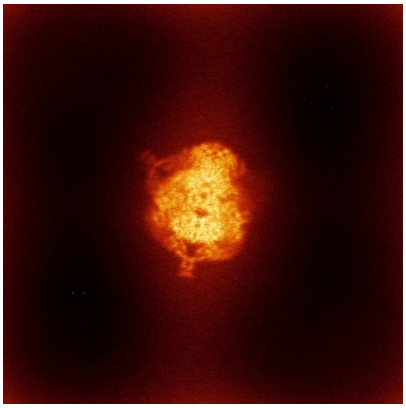

Y


Z

6.4.2 Raw map


X

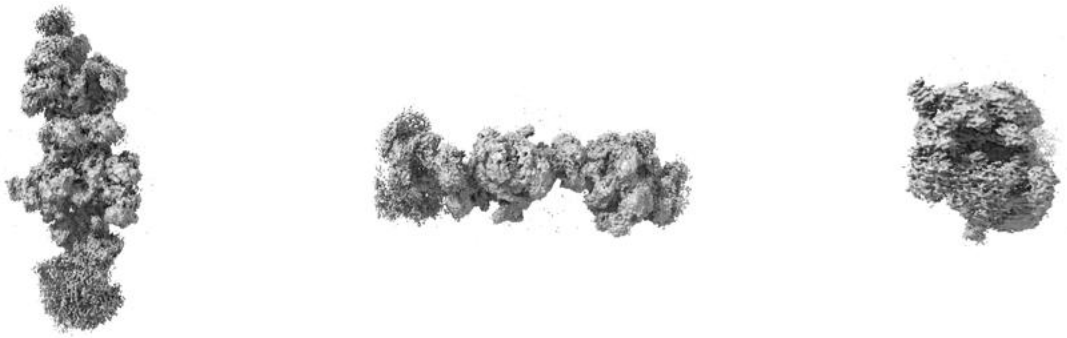

Y


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)

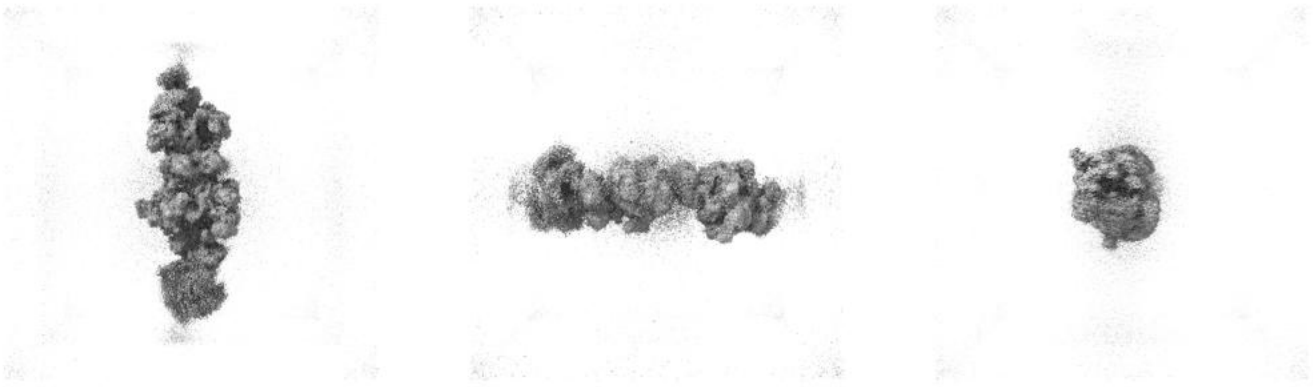
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

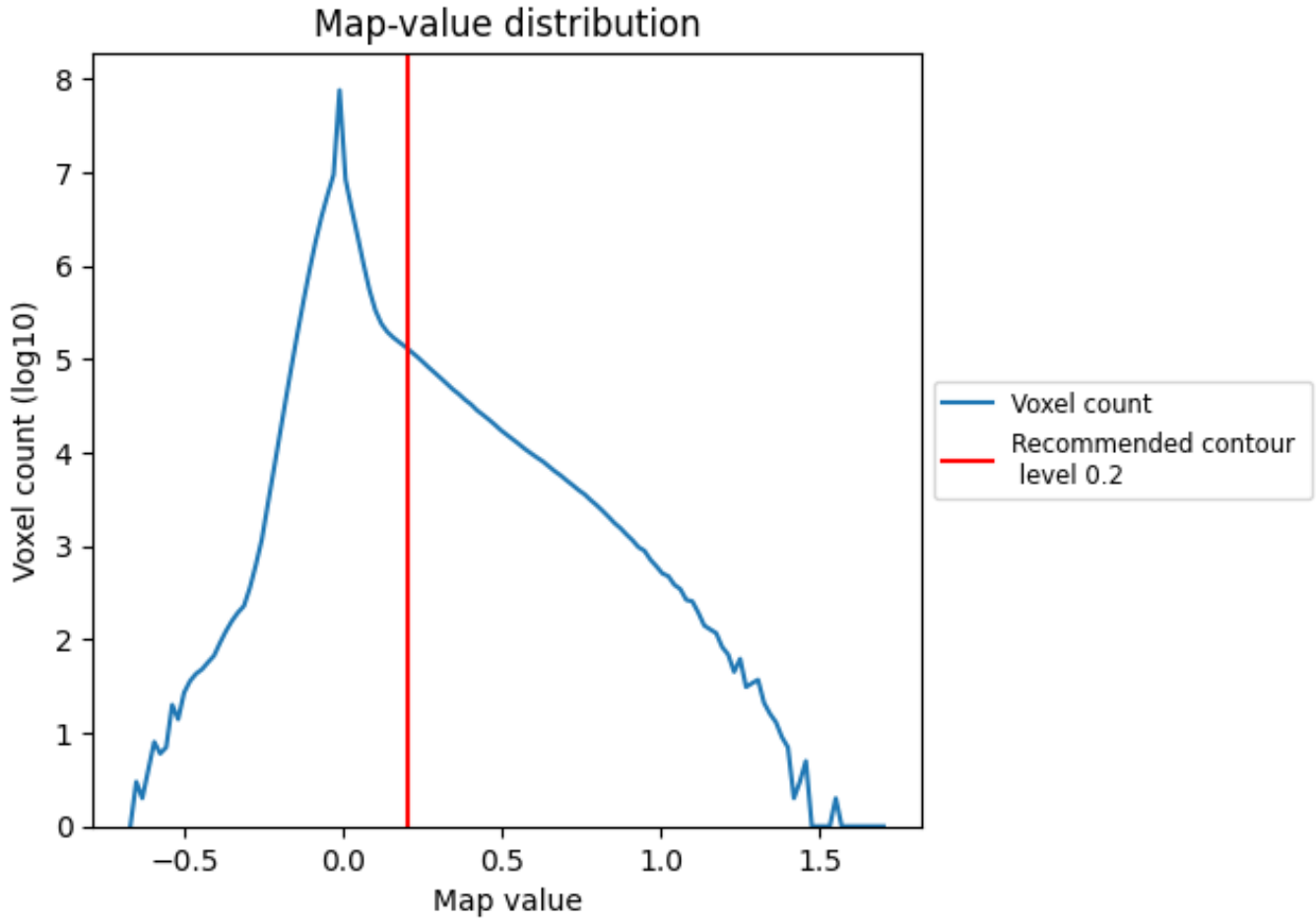
6.6 Mask visualisation (i)

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

7 Map analysis

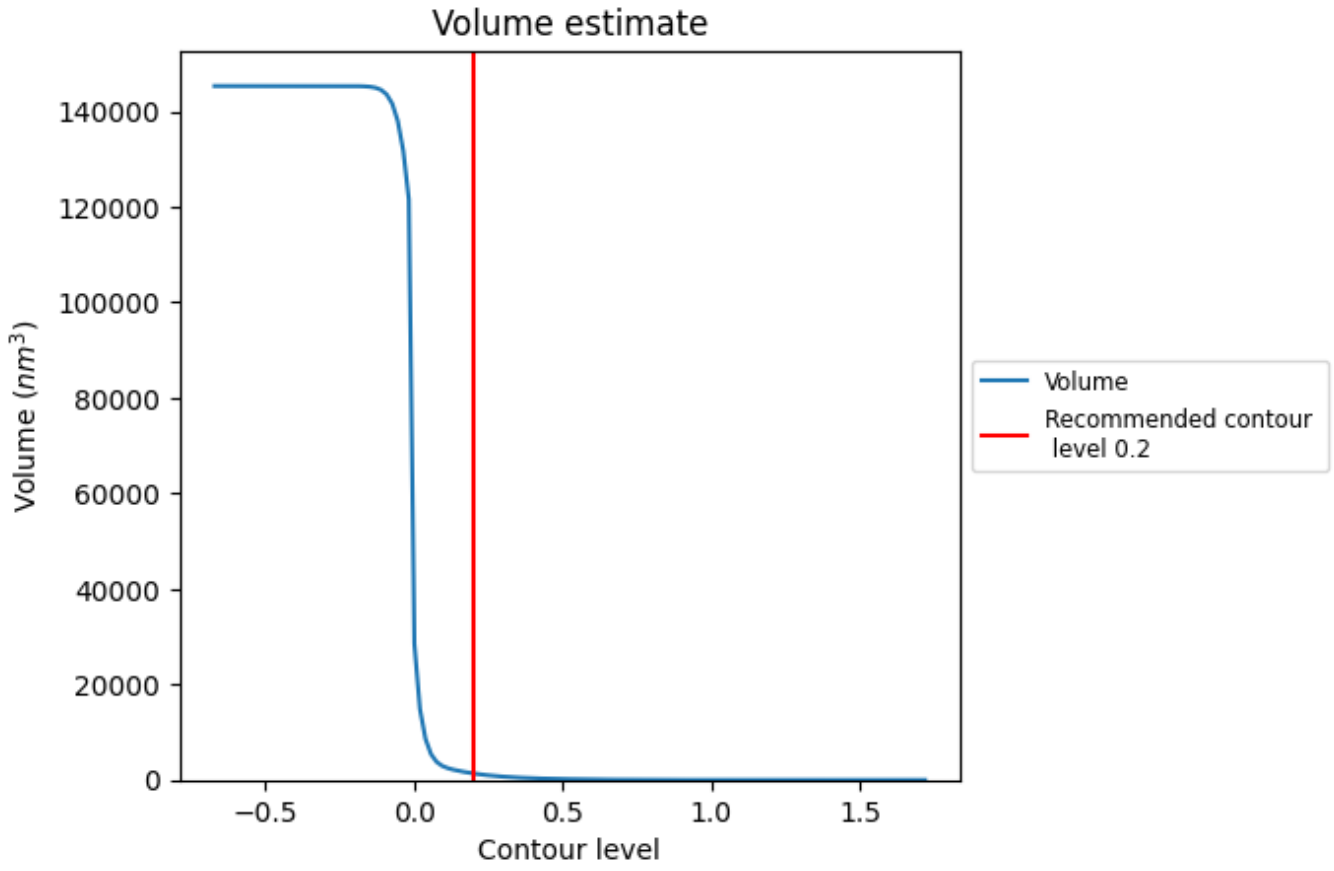
This section contains the results of statistical analysis of the map.

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.

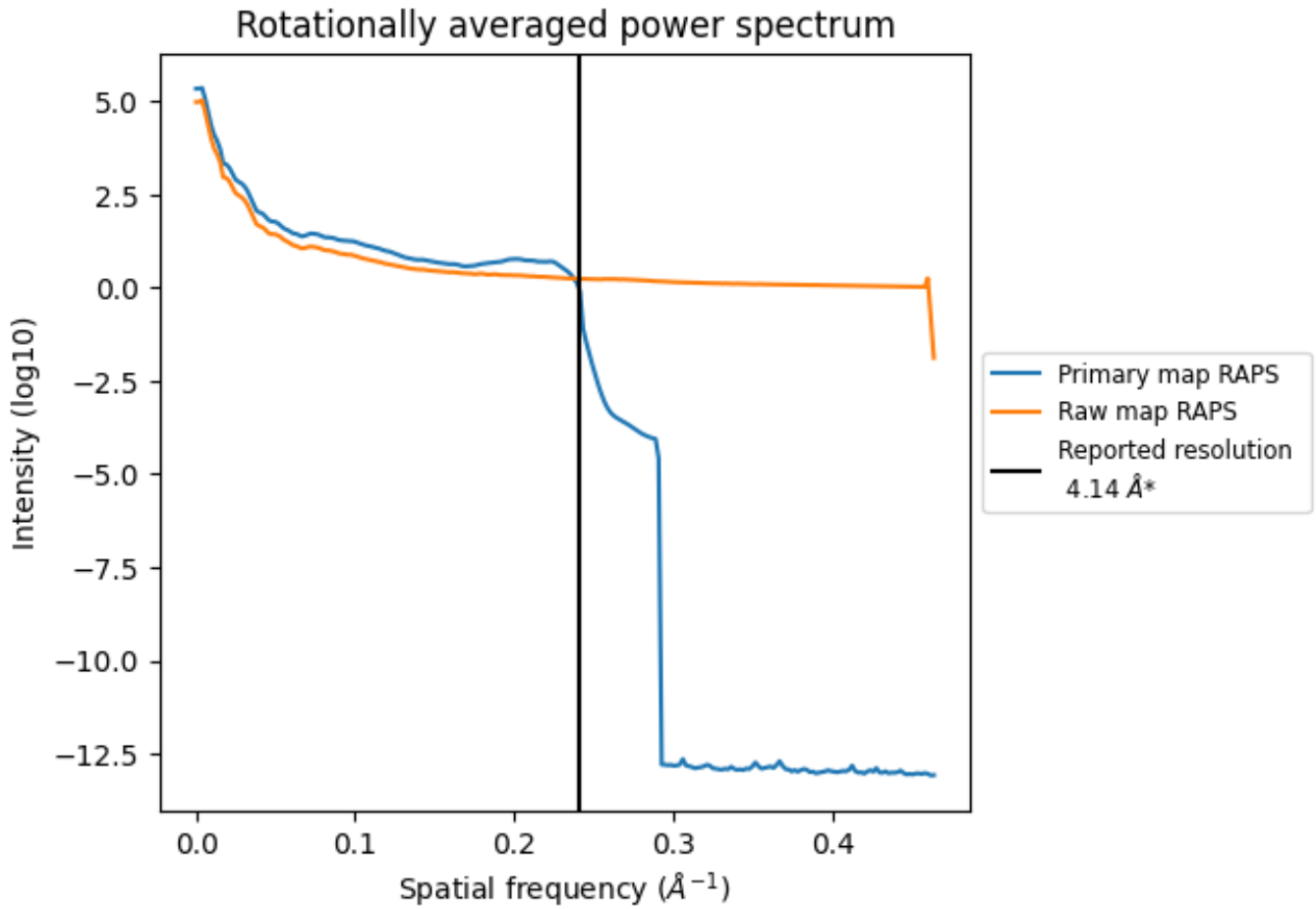
7.2 Volume estimate



The volume at the recommended contour level is 1379 nm^3; this corresponds to an approximate mass of 1246 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)

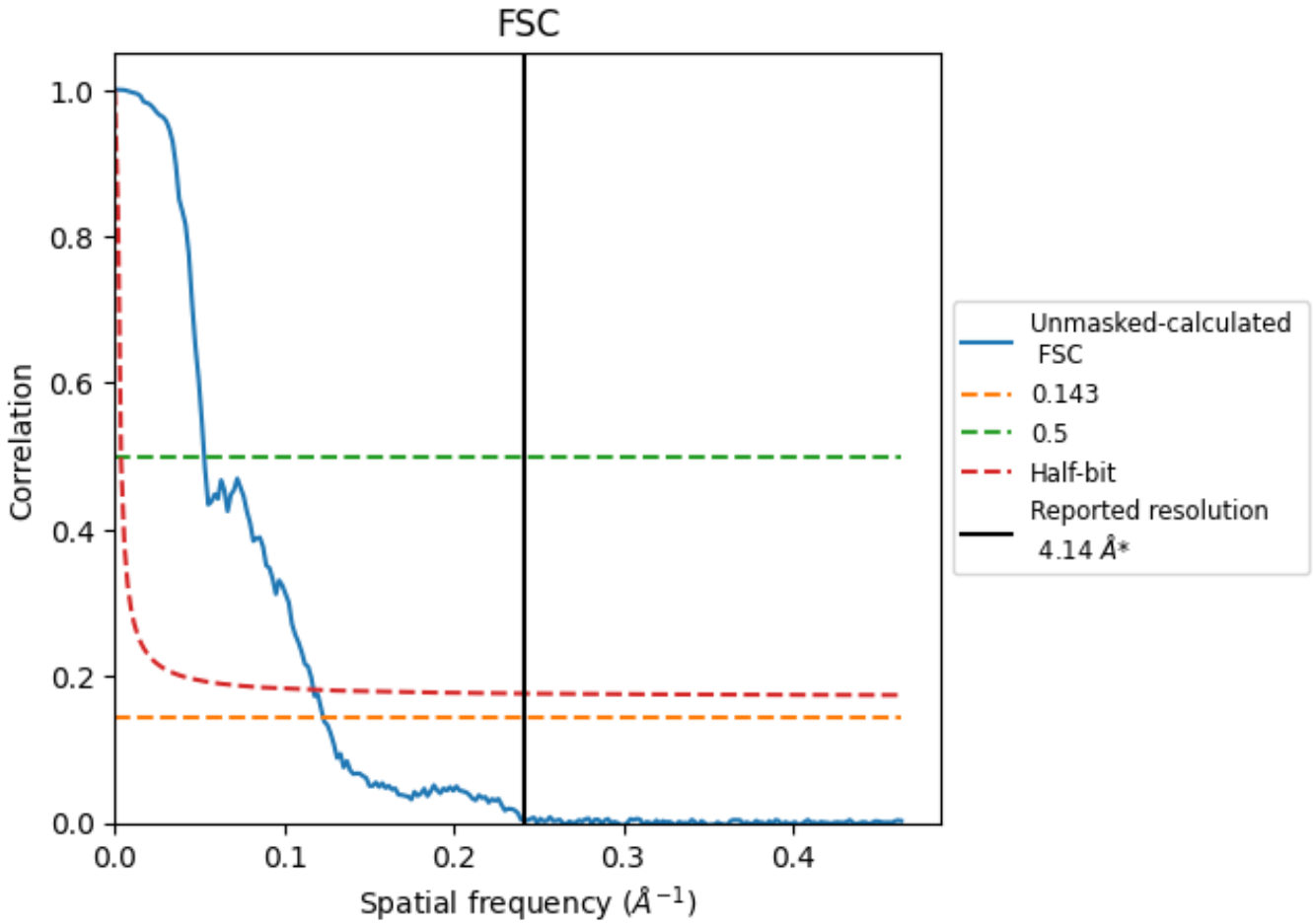


*Reported resolution corresponds to spatial frequency of 0.242 $Å^{-1}$

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 0.242 Å^{-1}

8.2 Resolution estimates (i)

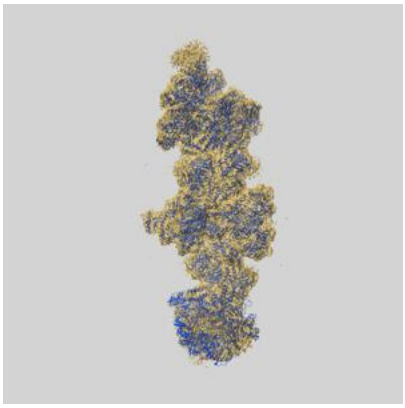
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.14	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.12	18.94	8.53

*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 8.12 differs from the reported value 4.14 by more than 10 %

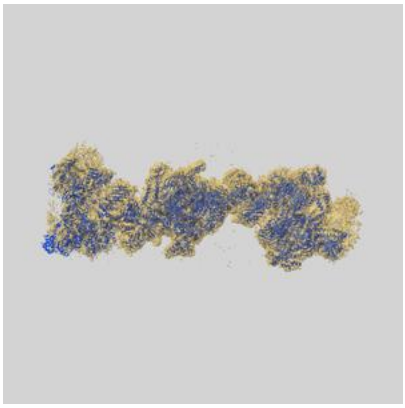
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38433 and PDB model 8XL0. Per-residue inclusion information can be found in section 3 on page 5.

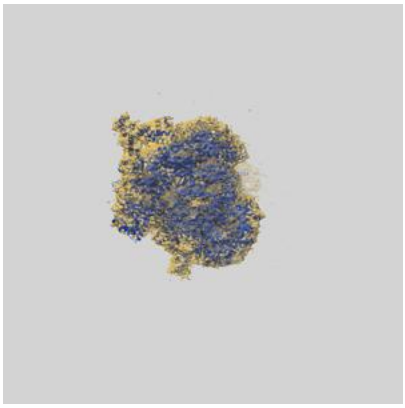
9.1 Map-model overlay



X



Y



Z

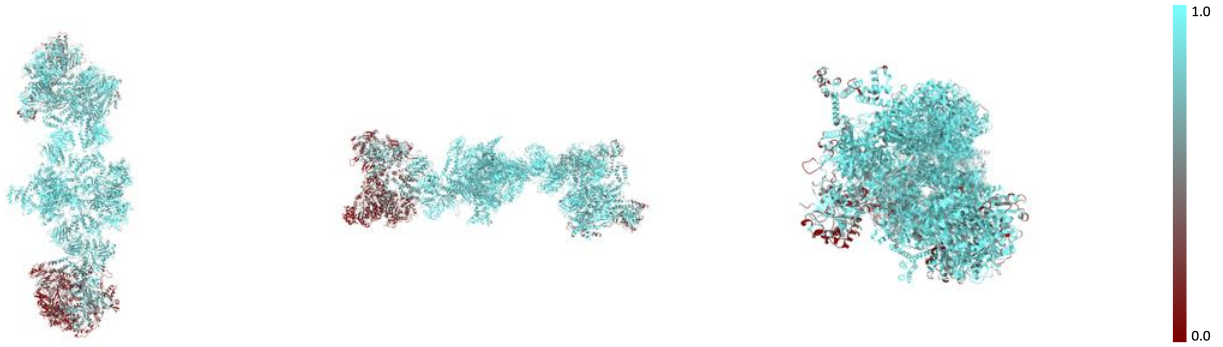
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

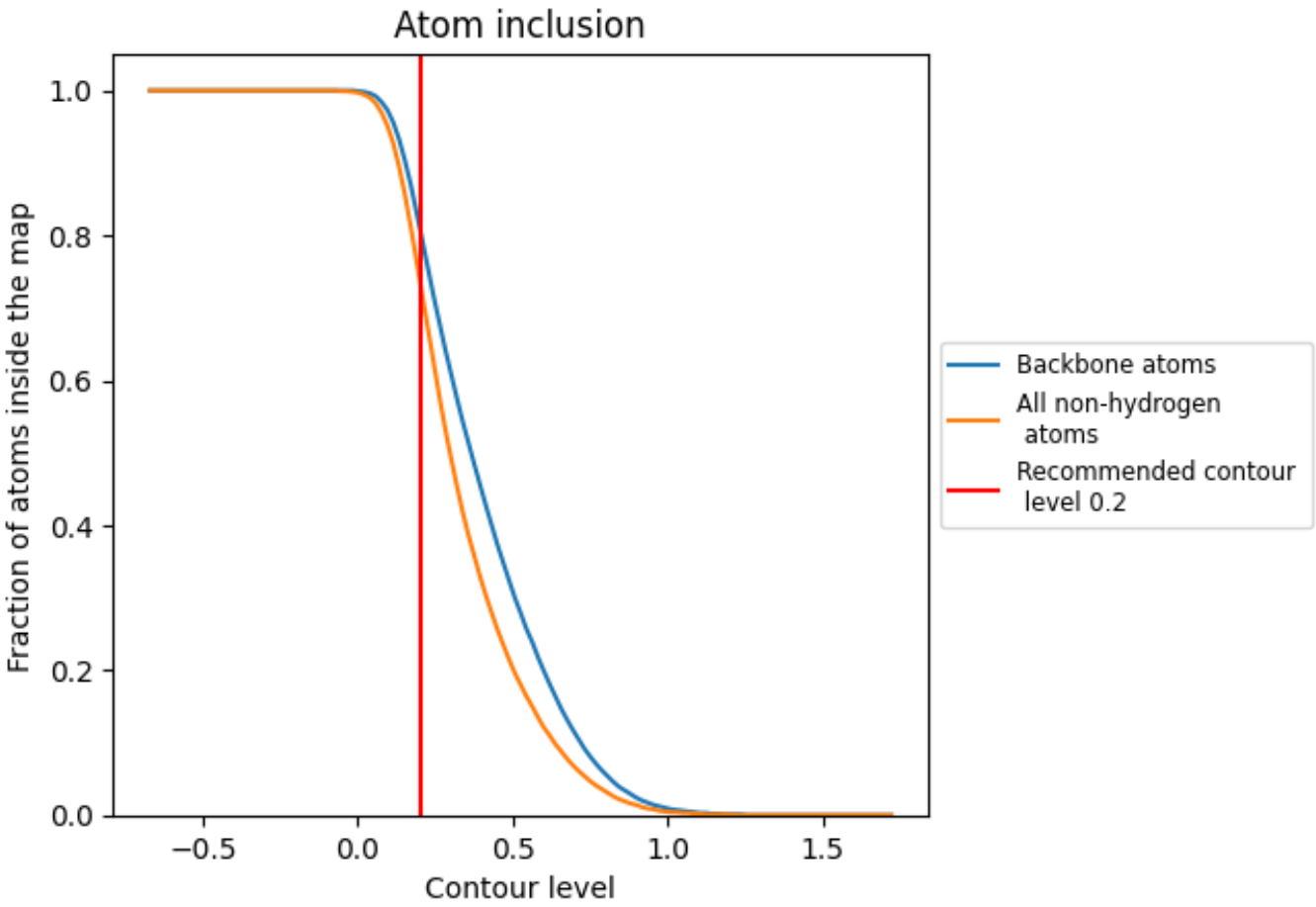
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 74% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7380	0.1620
A	0.7650	0.1060
B	0.8510	0.1530
C	0.9280	0.2830
D	0.9210	0.2770
E	0.4450	0.0520
F	0.2890	0.0270