wwPDB EM Validation Summary Report ⓘ

Jun 1, 2024 – 03:28 PM EDT

PDB ID	:	7TUI
EMDB ID	:	EMD-26132
Title	:	Structure of C. albicans FAS in an inhibited state
Authors	:	Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on	:	2022-02-02
Resolution	:	2.66 Å(reported)
Based on initial model	:	6U5V

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

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

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

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

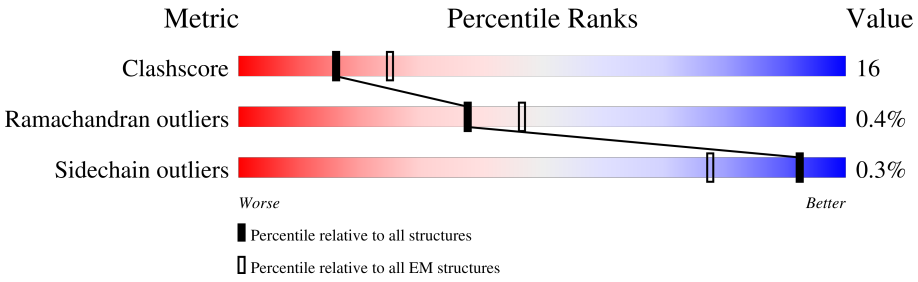
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.66 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	1885	11% 55% 21% 24%
2	B	2037	50% 62% 37% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27380 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 Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1433	11295	7171	1894	2185	45	0	0

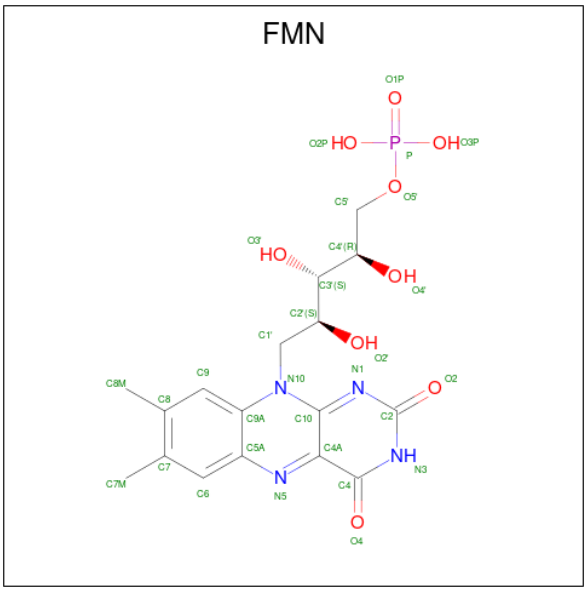
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	VAL	SER	conflict	UNP P43098
A	351	ASP	ARG	conflict	UNP P43098
A	353	ASN	LYS	conflict	UNP P43098
A	354	LYS	GLN	conflict	UNP P43098
A	357	ALA	LEU	conflict	UNP P43098
A	814	THR	PRO	conflict	UNP P43098
A	1067	LYS	GLN	conflict	UNP P43098
A	1124	VAL	ILE	conflict	UNP P43098
A	1445	GLU	LYS	conflict	UNP P43098
A	1743	SER	ASN	conflict	UNP P43098

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	2033	16054	10290	2665	3045	54	1	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



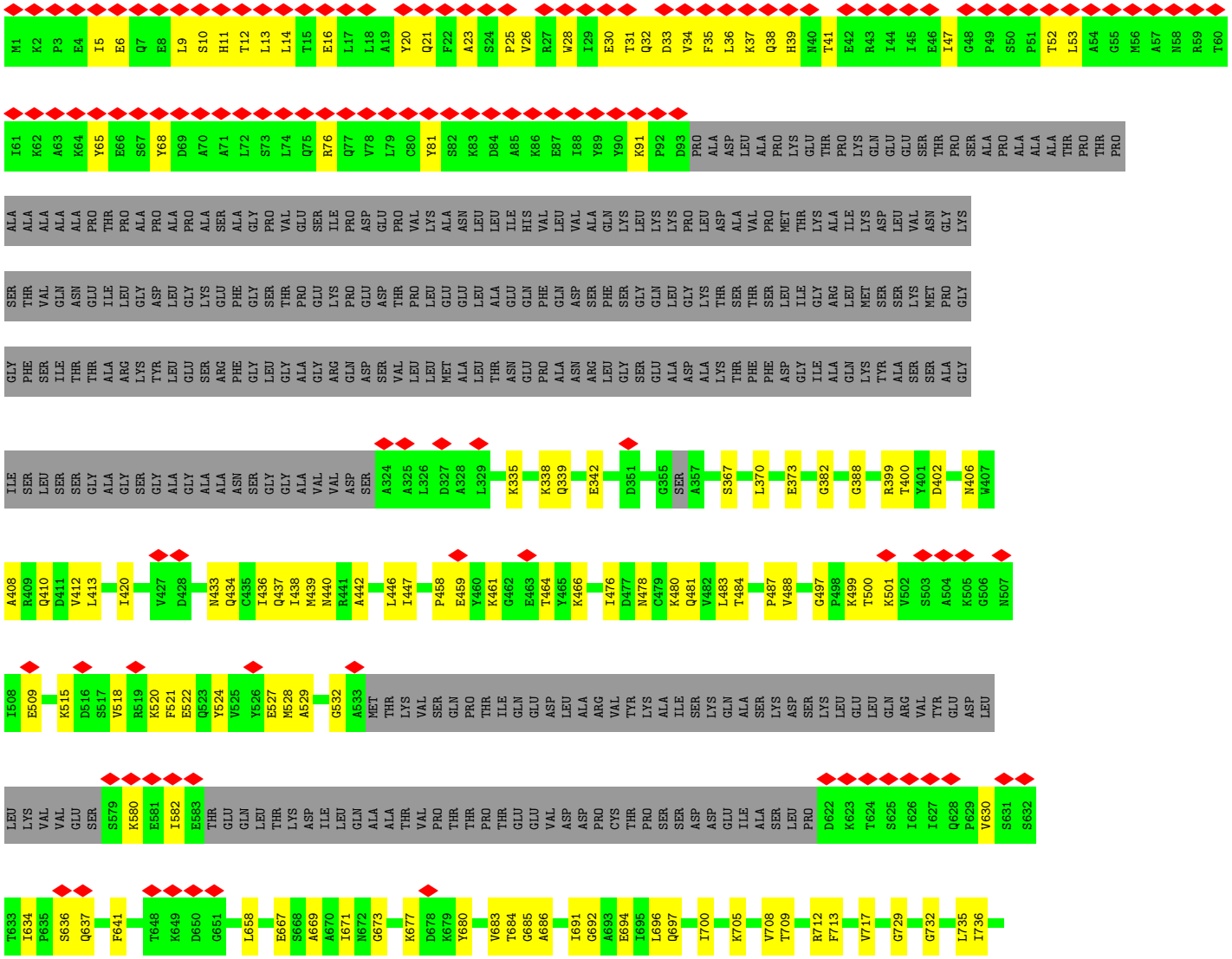
Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

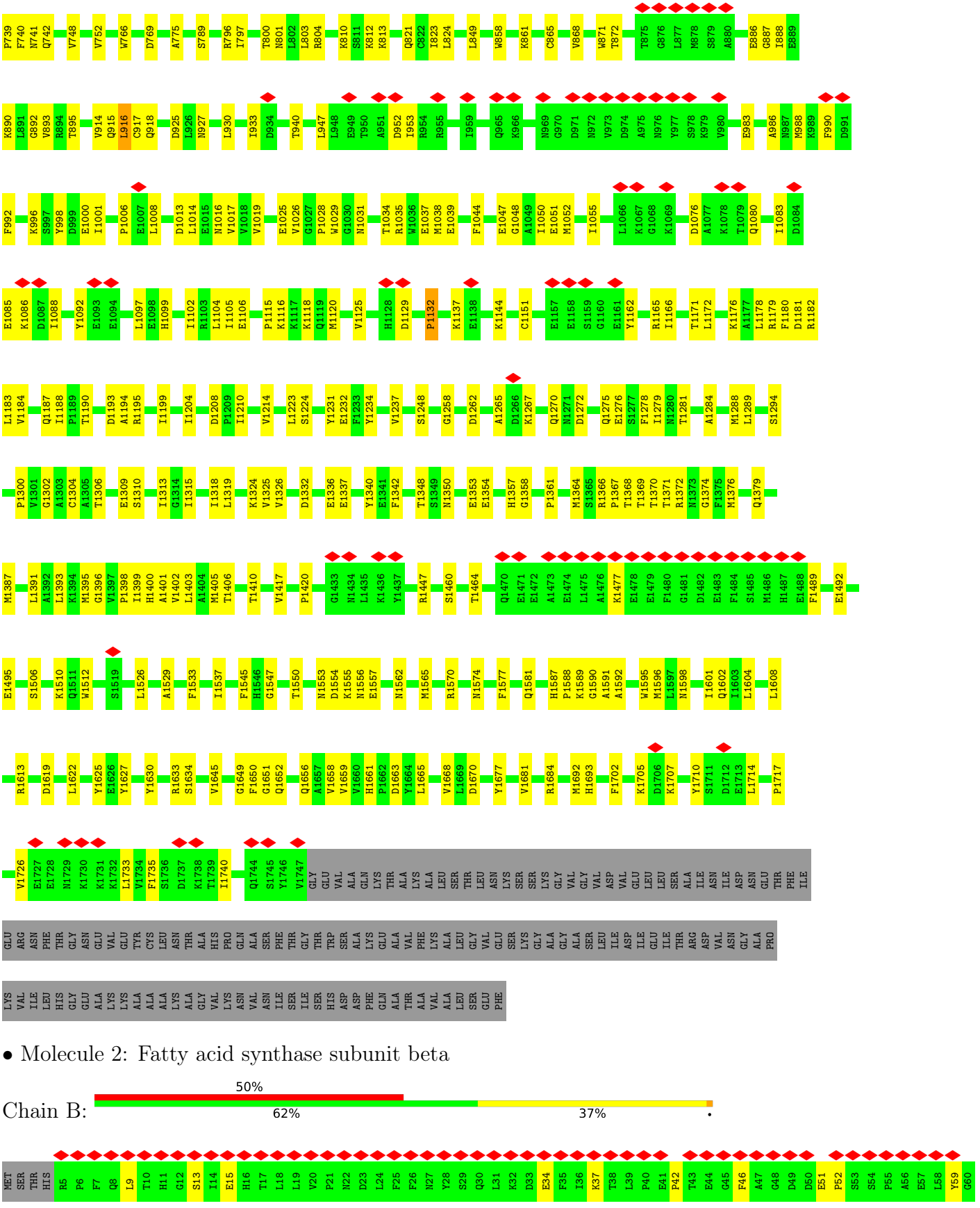
3 Residue-property plots (i)

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: Fatty acid synthase subunit alpha

Chain A:

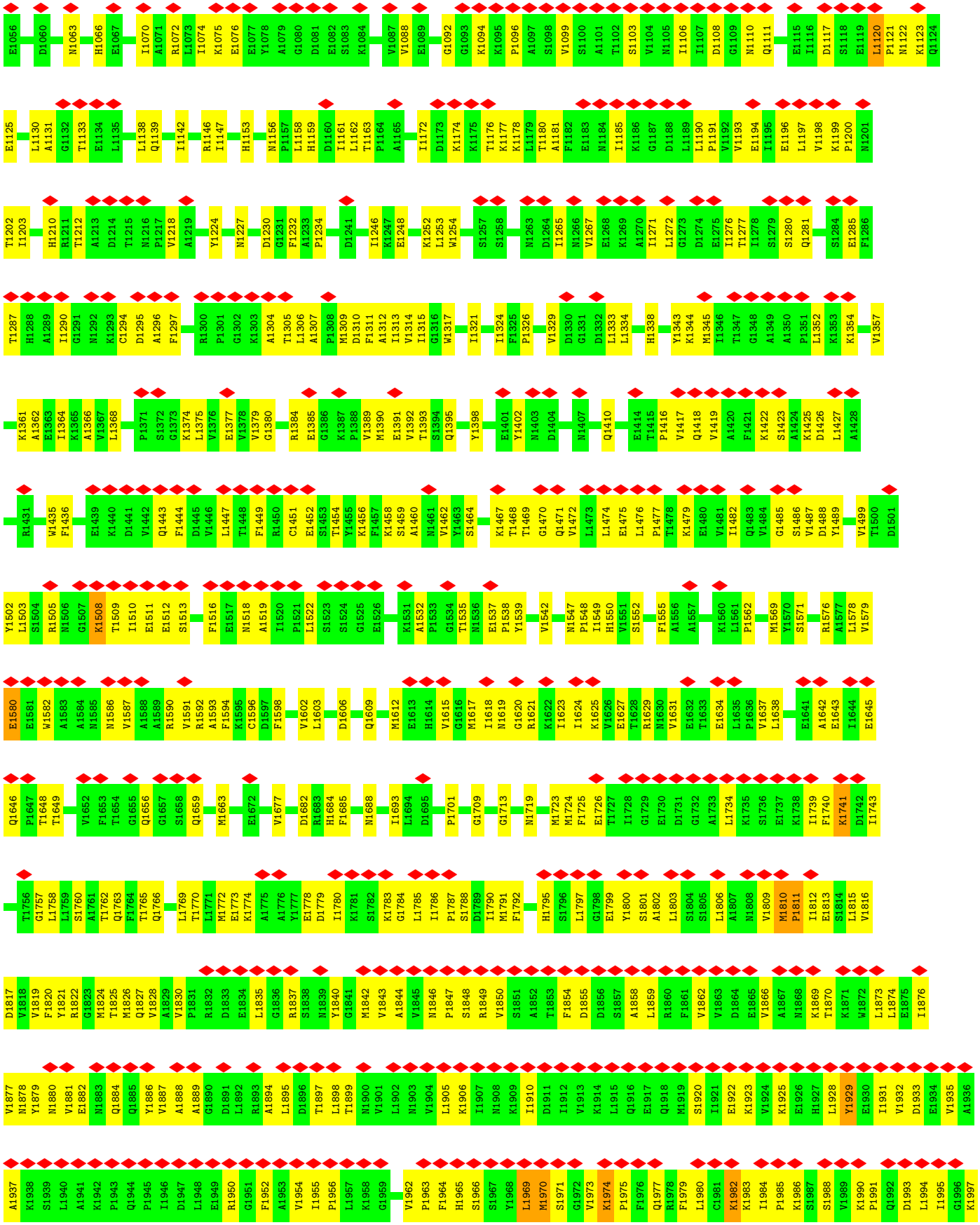




• Molecule 2: Fatty acid synthase subunit beta

Chain B:


K61 F62 I63 G64 F65 I66 S67 N68 A69 Q70 F71 P72 Q73 I74 V75 E76 L77 S78 L79 K80 D81 F82 E83 S84 R85 F86 L87 D88 N89 N90 N91 D92 N93 I94 H95 S96 F97 A98 V99 K100 L101 L102 D103 D104 E105 T106 Y107 P108 T109 T110 I111 A112 K113 V114 K115 E116 N117 I118 V119 K120
N121 Y122 Y123 K124 A125 V126 K127 S128 I129 N130 K131 V132 E133 S134 N135 L136 L137 Y138 H139 C140 K141 H142 D143 A144 K145 L146 V147 A148 I149 F150 Q153 G154 N155 T156 D157 D158 Y159 F160 E161 E162 L163 R164 E165 L166 Y167 T168 L169 Y170 Q171 G172 L173 I174 E175 D176 L177 L178 V179 S180 I181
A182 E183 K184 L185 N186 Q187 L188 H189 P190 S191 F192 D193 K194 I195 Y196 T197 Q198 G199 L200 N201 I202 L203 S204 V205 L206 K207 H208 P209 E210 T211 T212 P213 D214 Q215 D216 Y217 L218 L219 S220 V221 P222 V223 S224 C225 P226 V227 I228 C229 V230 I231 Q232 L233 C234 H235 Y236 T237 I238 T239 C240 K241
V242 L243 G244 L245 T246 P247 G248 E249 F250 R251 N252 S253 L254 K255 W256 S257 T258 G259 H260 S261 Q262 G263 L264 V265 T266 A267 V268 T269 I270 A271 A272 S273 D274 S275 W276 D277 S278 F279 L280 K281 N282 S283 L284 T285 A286 V287 S288 L289 L290 L291 F292 I293 G294 S295 R296 C297 L298 S299 T300 Y301
P302 R303 T304 S305 L306 P307 P308 T309 M310 L311 Q312 D313 S314 L315 D316 N317 G318 E319 G320 R321 P322 S323 P324 M325 L326 S327 D330 L331 S332 I333 K334 Q335 V336 E337 K338 F339 I340 E341 Q342 T343 N344 S345 H346 L347 P348 R349 E350 K351 H352 I353 A354 I355 S356 L357 G360 A361 R362
V365 L366 S367 G368 P369 P370 E371 S372 L373 Y374 G375 F376 N377 L378 N379 L380 R381 N382 Q383 K384 A385 P386 M387 G388 L389 D390 Q391 S392 R393 V394 P395 F396 S397 E398 R399 K400 L401 K402 C403 S404 N405 R406 F407 L408 P409 I410 F411 A412 P413 F414 H415 S416 H417 L418 L419 A420 D421 A422 T423 E424
L425 I426 L427 D428 D429 V430 K431 E432 H433 G434 L435 S436 F437 E438 G439 L440 K441 I442 P443 V444 Y445 D446 T447 F448 D449 G450 S451 D452 F453 Q454 A455 L456 K457 E458 P459 I460 I461 D462 R463 V464 V465 K466 L467 I468 T469 E470 L471 H474 W475 E476 E477 A478 T479 N480 H481 K482 A483 T484 H485
I486 L487 D488 F489 G490 P491 G492 G493 V494 S495 G496 L497 G498 V499 L500 T501 H502 R503 N504 K505 E506 G507 T508 G509 A510 R511 I512 I513 L514 A515 G516 T517 L518 D519 S520 N521 P522 I523 D524 D525 E526 Y527 G528 F529 K530 H531 E532 I533 F534 Q535 T536 S537 A538 D539 K540 A541 I542 K543 W544 A545
P546 D547 W548 L549 K550 E551 L552 R553 P554 T555 L556 V557 K558 N559 S560 E561 G562 K563 I564 Y565 V566 K567 T568 K569 F570 S571 Q572 L573 L574 G575 R576 A582 G583 M584 T585 P586 V589 I593 V594 S595 A596 S597 L598 N599 A600 G601 Y602 E605 L606 A607 G608 G609 G610 Y611 M616
R619 A620 I621 D622 D623 I624 R627 I628 K629 N637 L638 I639 Y640 V641 N642 P643 F644 M645 L646 Q647 W648 D655 L656 R657 E658 Y661 P662 I663 Q664 T667 I668 G669 A670 P673 E676 E680 Y681 I682 E683 D684 L685 G686 H689 L690 G691 L692 K693 P694 D698
A699 I700 V703 K708 A709 H710 F713 V716 L717 Q718 G721 G722 R723 G726 H727 H728 S729 F730 E731 D732 F733 H734 Q735 I738 Q739 M740 Y741 S742 K743 I744 R745 R746 C747 S748 N749 I750 V751 S756 G757 D763 I764 Y765 P766 Y767 W772 S773 E774 K775 Y778
P779 P780 M781 P782 V786 L787 F788 R791 E797 S798 H799 K805 V809 E810 C811 K812 G813 V814 P815 D816 Q817 Q818 W819 E820 Q821 T822 Y823 K824 K825 P826 T827 G828 G829 I830 I831 T832 V833 R834 S835 E836 M837 G838 E839 P840 I841 H842 K843 I844 A845 T846 R847 G848 V849 L855
D856 D857 T858 I859 F860 N861 L862 P863 K864 N865 K866 L867 L868 D869 K874 R875 I879 K880 K881 D885 F886 Q887 K888 P889 W890 F891 G892 K893 N896 E903 M904 R912 L913 V914 K920 S929 L930 R931 Y934 G935 D936 F937 L938 R939 E942 E943 R944 S948 A949
L961 N962 E963 F967 T968 A969 D970 K974 F975 P976 L982 E985 Y990 Q1000 V1006 D1010 E1011 R1012 F1013 E1014 K1019 D1020 E1026 D1027 L1028 E1029 V1032 D1033 E1034 D1035 V1036 Q1037 R1038 T1039 C1040 I1041 L1042 H1043 G1044 P1045 V1046 A1047 S1048 Q1049 K1053 V1054 D1055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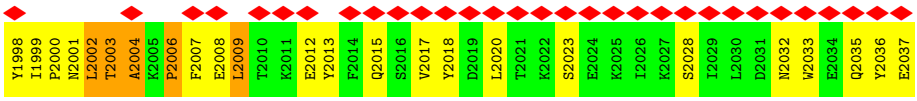
E1125 L1130 A1131 G1132 T1133 E1134 L1135 L1138 Q1139 I1142 R1146 I1147 H1153 N1156 P1157 L1158 H1159 D1160 I1161 L1162 T1163 P1164 A1165 I1172 D1173 K1174 K1175 T1176 K1177 K1178 L1179 T1180 A1181 F1182 E1183 N1184 I1185 K1186 G1187 D1188 L1189 L1190 P1191 V1192 V1193 E1194 I1195 E1196 L1197 V1198 K1199 P1200 N1201
T1202 I1203 H1210 R1211 T1212 A1213 D1214 T1215 N1216 P1217 V1218 A1219 Y1224 N1227 D1230 G1231 F1232 A1233 P1234 D1241 I1246 K1247 E1248 K1252 L1253 W1254 S1257 S1258 N1263 D1264 I1265 N1266 V1267 E1268 K1269 A1270 I1271 L1272 G1273 D1274 E1275 I1276 T1277 I1278 S1279 S1280 Q1281 S1284 E1285 F1286
T1287 H1288 A1289 I1290 G1291 N1292 K1293 C1294 D1295 A1296 F1297 R1300 P1301 G1302 K1303 A1304 T1305 L1306 A1307 P1308 M1309 D1310 F1311 A1312 I1313 V1314 I1315 G1316 W1317 I1321 I1324 F1325 P1326 V1329 D1330 G1331 D1332 L1333 L1334 H1338 Y1343 K1344 M1345 I1346 T1347 G1348 A1349 A1350 P1351 L1352 K1353 K1354 V1357
K1361 A1362 E1363 I1364 K1365 A1366 V1367 L1368 P1371 S1372 G1373 K1374 L1375 V1376 E1377 V1378 V1379 G1380 R1384 E1385 G1386 K1387 P1388 V1389 M1390 E1391 V1392 T1393 S1394 Q1395 Y1398 E1401 Y1402 N1403 D1404 N1407 Q1410 E1414 T1415 P1416 V1417 Q1418 V1419 A1420 F1421 K1422 S1423 A1424 K1425 D1426 L1427 A1428
R1431 W1435 F1436 E1439 K1440 D1441 V1442 Q1443 F1444 D1445 V1446 L1447 T1448 F1449 R1450 C1451 E1452 S1453 T1454 Y1455 K1456 F1457 K1458 S1459 A1460 N1461 V1462 Y1463 S1464 K1467 T1468 T1469 G1470 Q1471 V1472 L1473 L1474 E1475 L1476 P1477 T1478 K1479 E1480 V1481 I1482 Q1483 V1484 G1485 S1486 V1487 D1488 Y1489 V1499 T1500 D1501
Y1502 L1503 S1504 R1505 N1506 G1507 K1508 T1509 I1510 E1511 E1512 S1513 F1516 E1517 N1518 A1519 I1520 P1521 L1522 S1523 S1524 G1525 E1526 K1531 A1532 P1533 G1534 T1535 N1536 E1537 P1538 Y1539 V1542 N1547 P1548 I1549 H1550 V1551 S1552 F1555 A1556 A1557 K1560 L1561 P1562 M1569 Y1570 S1571 R1576 A1577 L1578 V1579
E1580 E1581 W1582 A1583 A1584 N1585 N1586 V1587 A1588 A1589 R1590 V1591 R1592 A1593 F1594 K1595 C1596 D1597 F1598 V1602 L1603 D1606 Q1609 M1612 E1613 H1614 V1615 G1616 M1617 I1618 N1619 G1620 R1621 K1622 I1623 I1624 K1625 V1626 E1627 T1628 R1629 N1630 V1631 E1632 T1633 E1634 L1635 P1636 V1637 L1638 E1641 A1642 E1643 I1644 E1645
Q1646 P1647 T1648 T1649 V1652 F1653 T1654 G1655 Q1656 G1657 S1658 Q1659 M1663 E1672 V1677 D1682 R1683 H1684 F1685 N1688 I1693 L1694 D1695 P1701 G1709 G1713 N1719 M1723 M1724 F1725 E1726 T1727 I1728 G1729 E1730 D1731 G1732 A1733 L1734 K1735 S1736 E1737 K1738 I1739 F1740 K1741 D1742 I1743
T1756 G1757 L1758 L1759 S1760 A1761 T1762 Q1763 F1764 T1765 Q1766 L1769 T1770 L1771 M1772 E1773 K1774 A1775 A1776 Y1777 E1778 D1779 I1780 K1781 S1782 K1783 G1784 L1785 I1786 P1787 S1788 D1789 I1790 M1791 F1792 H1795 S1796 L1797 G1798 E1799 Y1800 S1801 A1802 L1803 S1804 S1805 L1806 A1807 N1808 V1809 M1810 P1811 I1812 E1813 S1814 L1815 V1816
D1817 V1818 V1819 F1820 Y1821 R1822 G1823 M1824 T1825 M1826 Q1827 V1828 A1829 V1830 P1831 R1832 D1833 E1834 L1835 G1836 R1837 S1838 N1839 Y1840 G1841 M1842 V1843 A1844 V1845 N1846 P1847 S1848 R1849 V1850 S1851 A1852 T1853 F1854 D1855 D1856 S1857 A1858 L1859 R1860 F1861 V1862 V1863 D1864 E1865 V1866 A1867 N1868 K1869 T1870 K1871 W1872 L1873 L1874 E1875 I1876
V1877 N1878 Y1879 N1880 V1881 E1882 N1883 Q1884 Q1885 Y1886 V1887 A1888 A1889 G1890 D1891 L1892 R1893 A1894 L1895 D1896 T1897 L1898 T1899 N1900 V1901 L1902 N1903 V1904 L1905 K1906 I1907 N1908 K1909 I1910 D1911 I1912 V1913 K1914 L1915 Q1916 E1917 Q1918 M1919 S1920 I1921 E1922 K1923 V1924 K1925 E1926 H1927 L1928 Y1929 E1930 I1931 V1932 D1933 E1934 V1935 A1936
A1937 K1938 S1939 L1940 A1941 K1942 P1943 Q1944 P1945 I1946 D1947 L1948 E1949 R1950 G1951 F1952 A1953 V1954 I1955 P1956 L1957 K1958 G1959 V1962 P1963 F1964 H1965 S1966 S1967 Y1968 L1969 M1970 S1971 G1972 V1973 K1974 P1975 F1976 Q1977 R1978 F1979 L1980 C1981 K1982 K1983 I1984 P1985 K1986 S1987 S1988 V1989 K1990 P1991 Q1992 D1993 L1994 I1995 G1996 K1997


Y1998
I1999
P2000
M2001
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A2004
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F2014
Q2015
S2016
V2017
Y2018
D2019
L2020
T2021
K2022
S2023
E2024
K2025
I2026
K2027
S2028
I2029
L2030
D2031
N2032
W2033
E2034
Q2035
Y2036
E2037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	252339	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)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.743	Depositor
Minimum map value	-4.396	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.273	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	333.72, 333.72, 333.72	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.32	0/11522	0.53	2/15575 (0.0%)
2	B	0.28	0/16423	0.54	4/22279 (0.0%)
All	All	0.30	0/27945	0.54	6/37854 (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
2	B	0	3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1120	LEU	CA-CB-CG	7.00	131.41	115.30
1	A	1132	PRO	CA-N-CD	-5.94	103.18	111.50
2	B	2009	LEU	CA-CB-CG	5.71	128.44	115.30
2	B	2002	LEU	CA-CB-CG	5.60	128.18	115.30
2	B	1969	LEU	C-N-CA	5.09	134.44	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1810	MET	Peptide
2	B	1929	TYR	Peptide
2	B	1982	LYS	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	11295	0	11214	296	0
2	B	16054	0	16025	604	0
3	B	31	0	19	4	0
All	All	27380	0	27258	872	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 16.

The worst 5 of 872 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)
2:B:1780:ILE:HA	2:B:1783:LYS:HB2	1.54	0.88
2:B:1571:SER:HB3	2:B:1638:LEU:HD11	1.58	0.85
2:B:1620:GLY:HA2	2:B:1786:ILE:HB	1.57	0.85
1:A:709:THR:HG23	1:A:740:PHE:HB3	1.60	0.84
2:B:573:LEU:HB2	2:B:1096:PRO:HG3	1.61	0.83

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	1425/1885 (76%)	1383 (97%)	42 (3%)	0	100 100
2	B	2032/2037 (100%)	1824 (90%)	194 (10%)	14 (1%)	22 33
All	All	3457/3922 (88%)	3207 (93%)	236 (7%)	14 (0%)	38 48

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1032	VAL
2	B	1477	PRO
2	B	1580	GLU
2	B	1970	MET
2	B	1974	LYS

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	1220/1579 (77%)	1216 (100%)	4 (0%)	92	96
2	B	1780/1784 (100%)	1775 (100%)	5 (0%)	92	96
All	All	3000/3363 (89%)	2991 (100%)	9 (0%)	92	96

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1012	ARG
2	B	1508	LYS
1	A	1707	LYS
2	B	334	LYS
2	B	791	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	637	ASN
2	B	818	GLN
2	B	1827	GLN
2	B	1338	HIS
2	B	1550	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FMN	B	2101	-	33,33,33	1.10	2 (6%)	48,50,50	1.18	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	B	2101	-	-	3/18/18/18	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2101	FMN	C4A-N5	3.85	1.38	1.30
3	B	2101	FMN	C10-N1	2.44	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2101	FMN	C4-N3-C2	-2.99	120.12	125.64
3	B	2101	FMN	C4A-C4-N3	2.72	120.10	113.19
3	B	2101	FMN	O4-C4-C4A	-2.52	119.90	126.60
3	B	2101	FMN	C4A-C10-N10	2.41	120.00	116.48
3	B	2101	FMN	C10-C4A-N5	-2.25	120.08	124.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2101	FMN	C3'-C4'-C5'-O5'
3	B	2101	FMN	O4'-C4'-C5'-O5'
3	B	2101	FMN	C4'-C5'-O5'-P

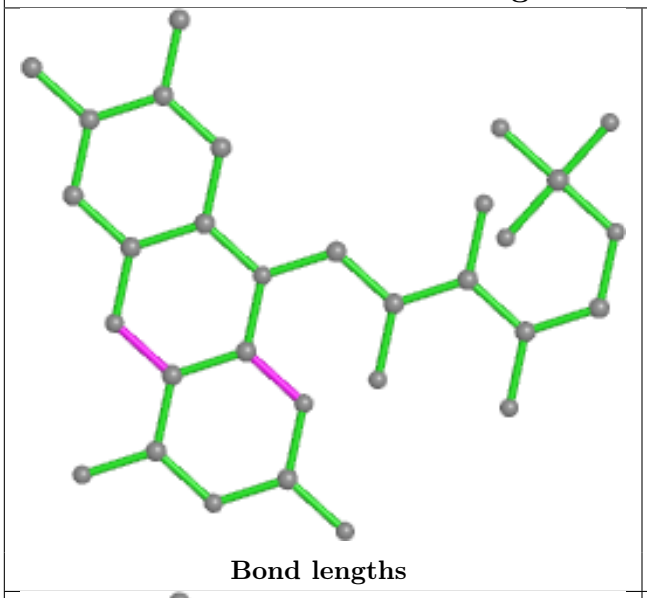
There are no ring outliers.

1 monomer is involved in 4 short contacts:

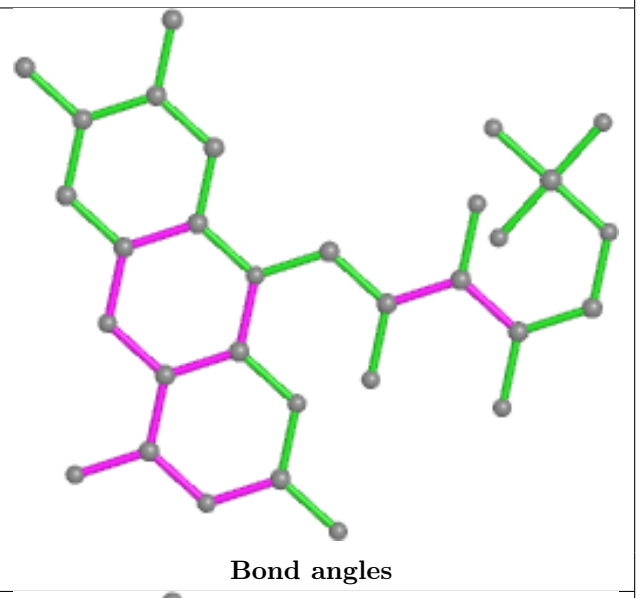
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2101	FMN	4	0

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.

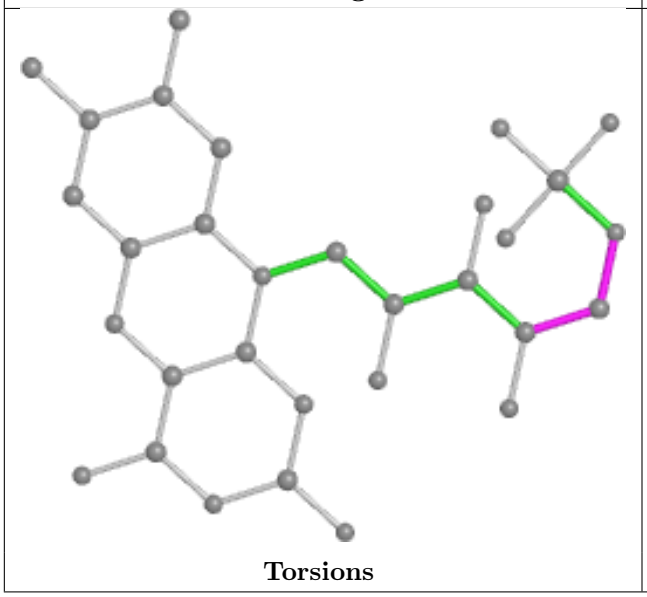
Ligand FMN B 2101



Bond lengths



Bond angles



Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

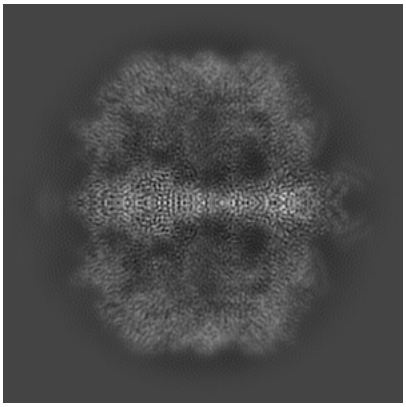
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26132. These allow visual inspection of the internal detail of the map and identification of artifacts.

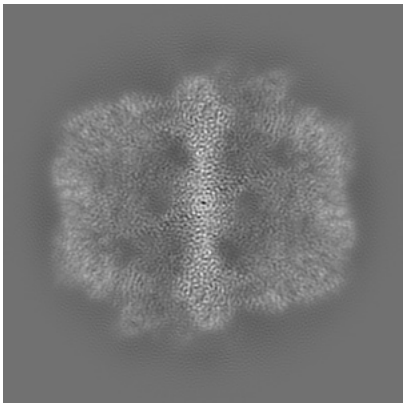
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

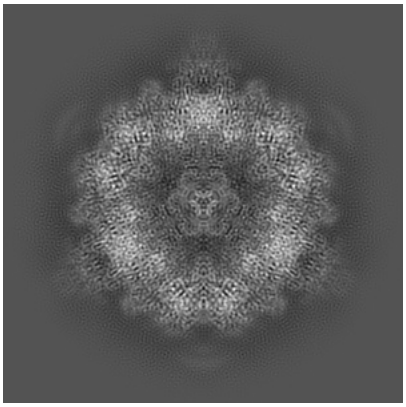
6.1.1 Primary map



X



Y

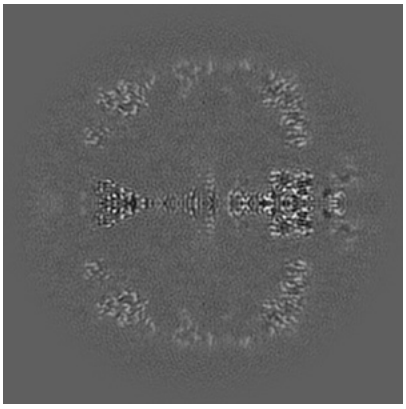


Z

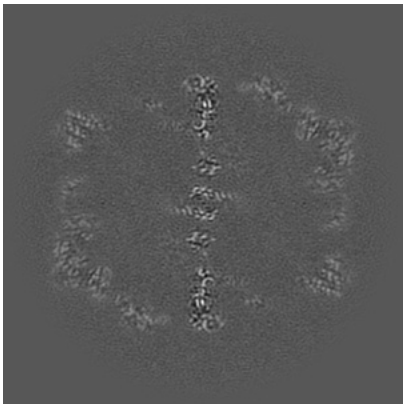
The images above show the map projected in three orthogonal directions.

6.2 Central slices

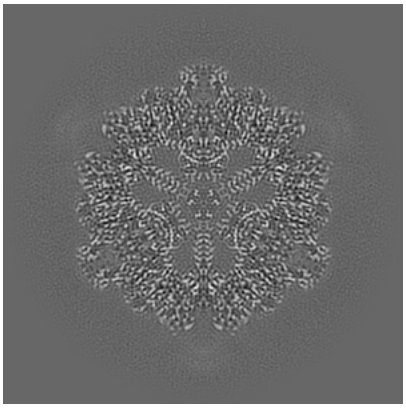
6.2.1 Primary map



X Index: 162



Y Index: 162

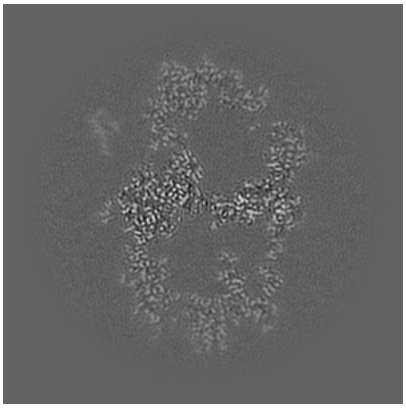


Z Index: 162

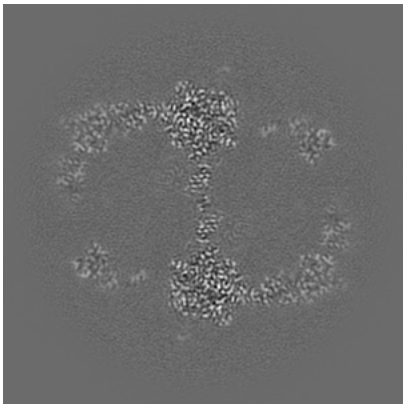
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

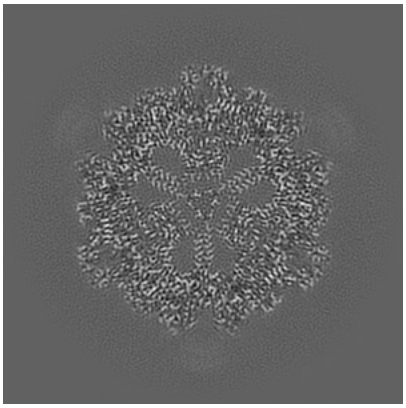
6.3.1 Primary map



X Index: 99



Y Index: 134

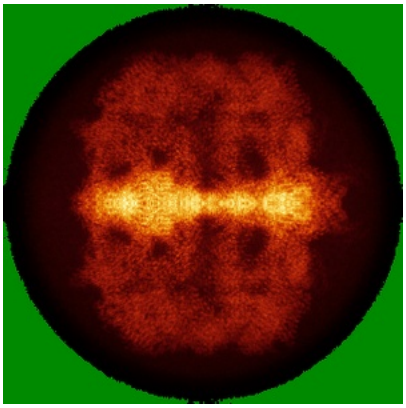


Z Index: 163

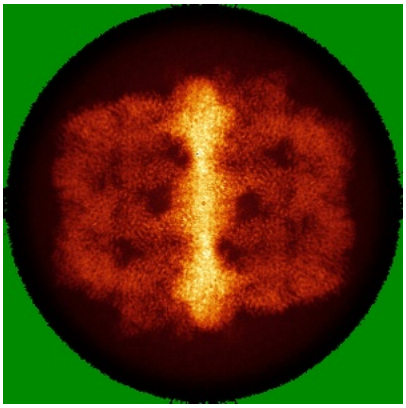
The images above show the largest variance slices of the map in three orthogonal directions.

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

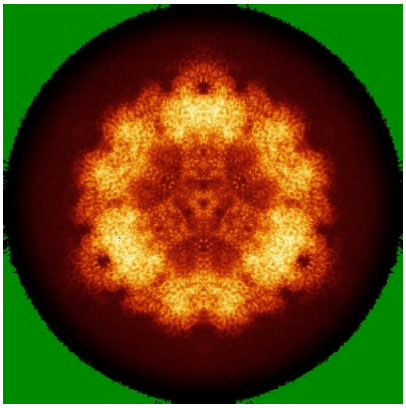
6.4.1 Primary map



X



Y

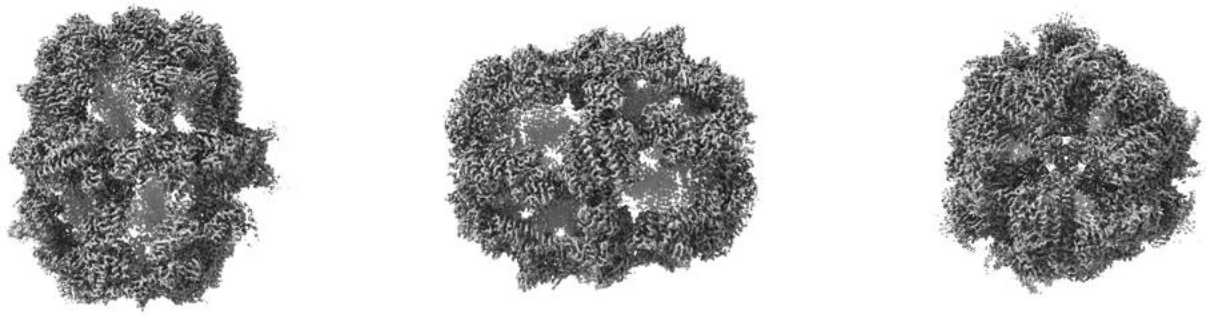


Z

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 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

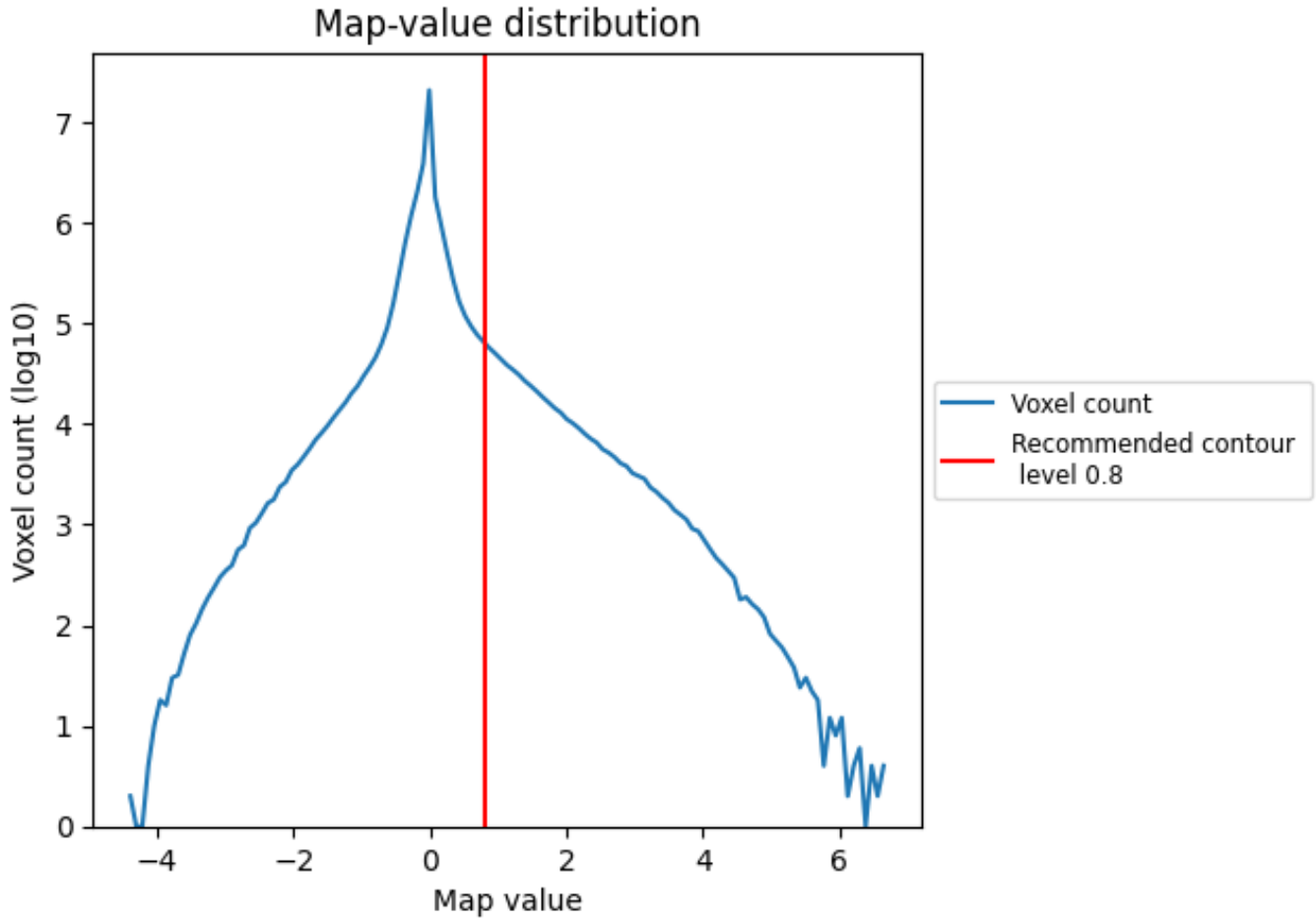
6.6 Mask visualisation (i)

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

7 Map analysis

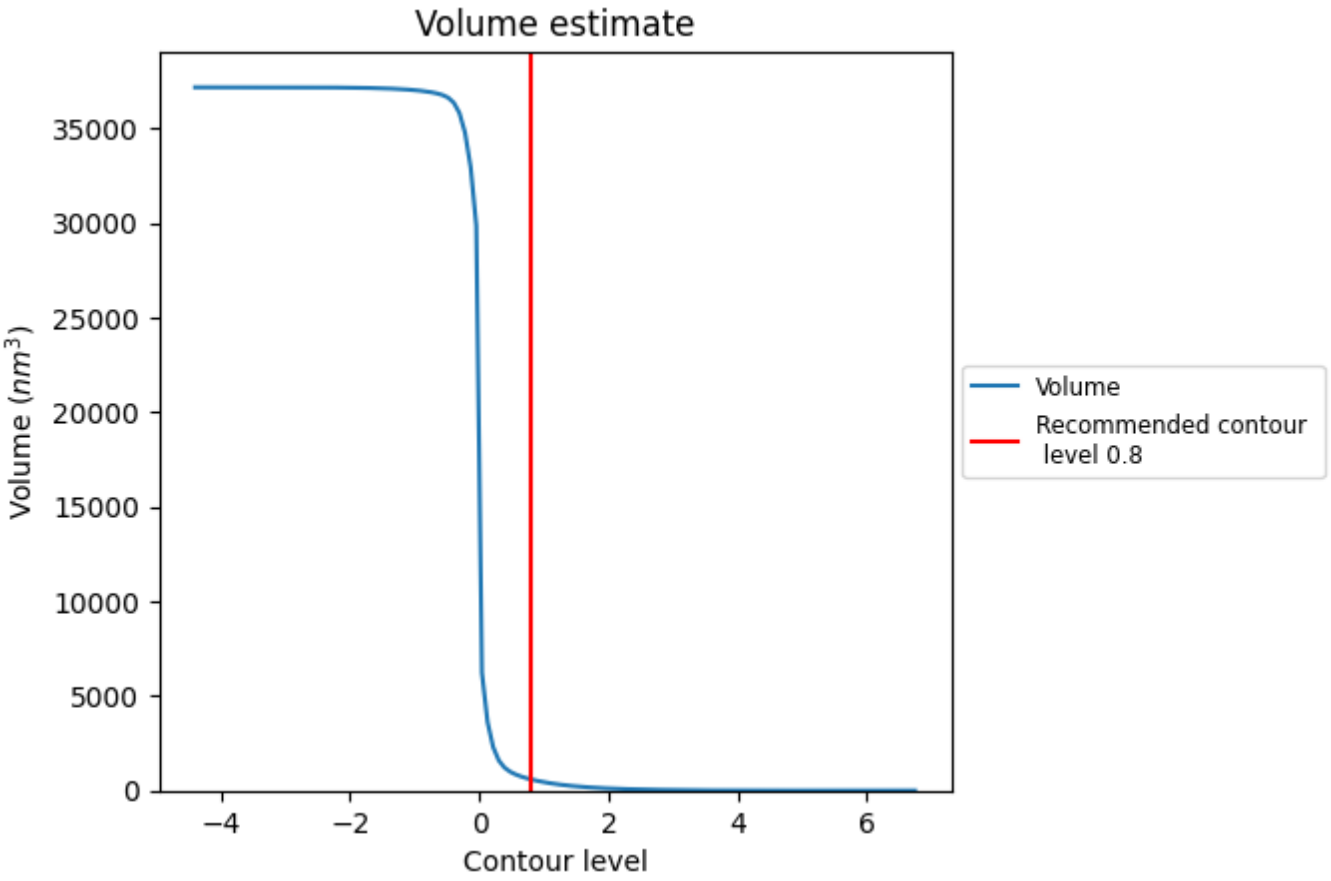
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

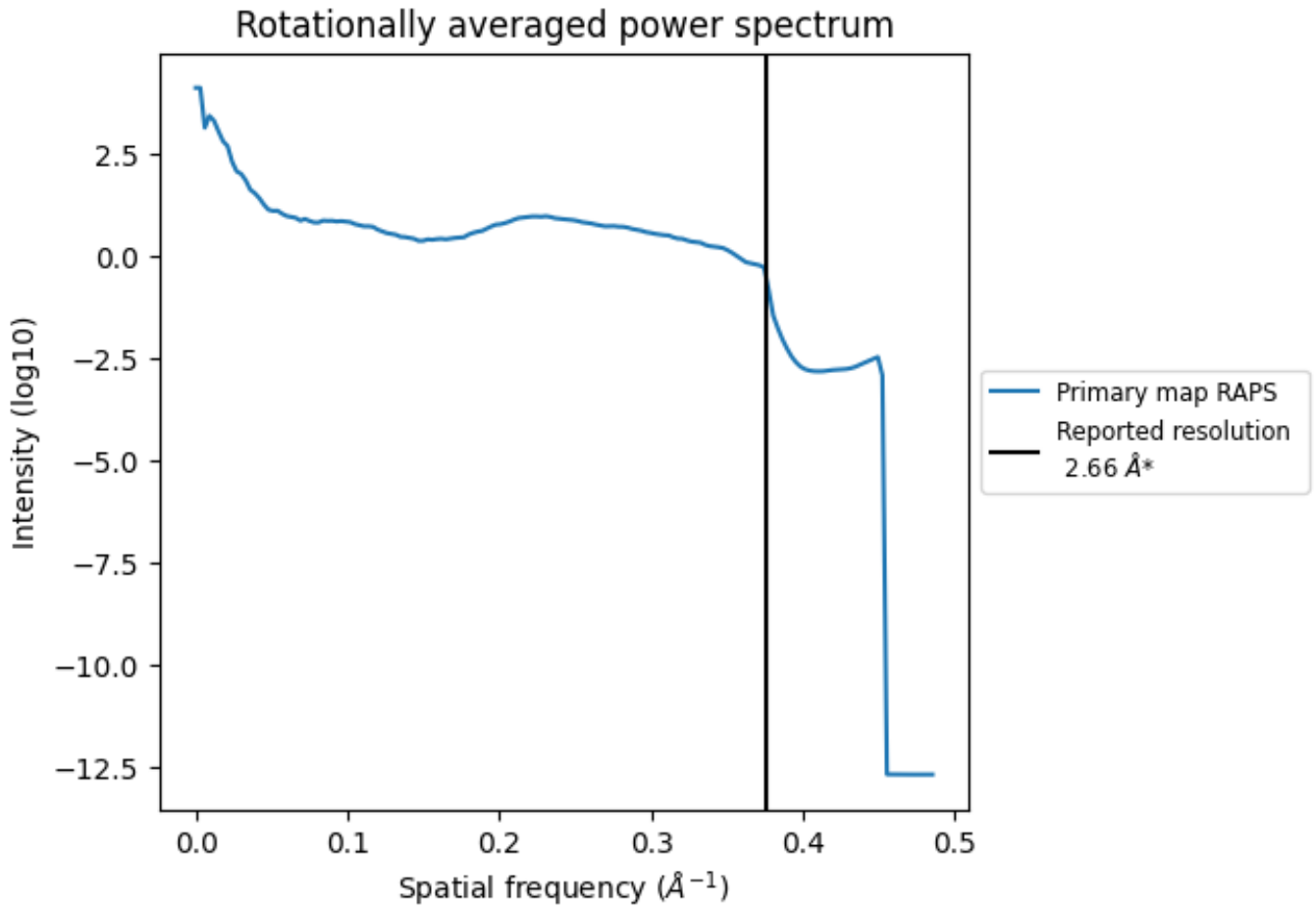
7.2 Volume estimate (i)



The volume at the recommended contour level is 593 nm^3; this corresponds to an approximate mass of 536 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 0.376 $Å^{-1}$

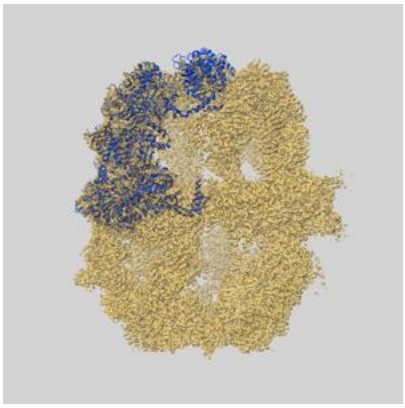
8 Fourier-Shell correlation

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

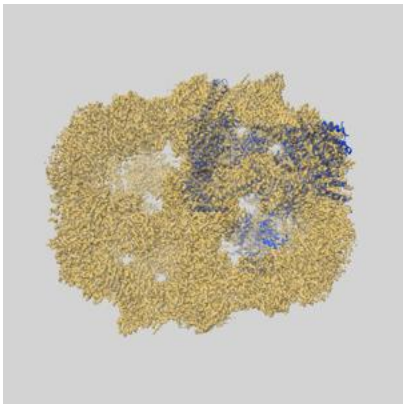
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26132 and PDB model 7TUI. Per-residue inclusion information can be found in section 3 on page 5.

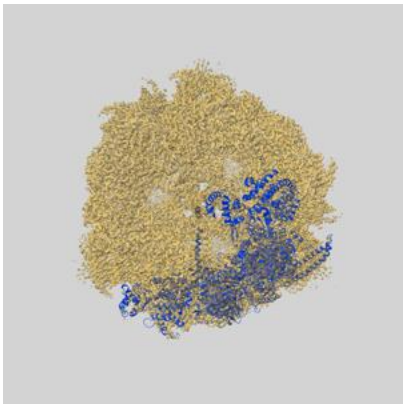
9.1 Map-model overlay



X



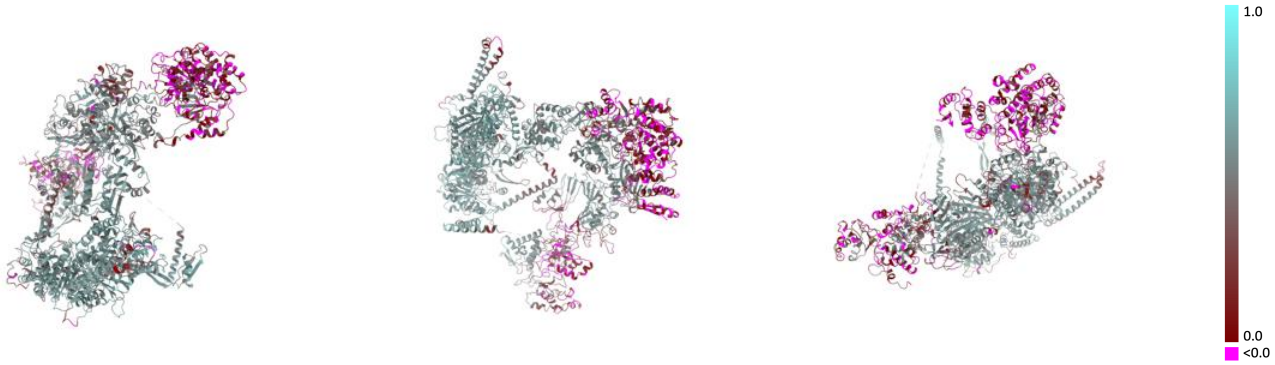
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

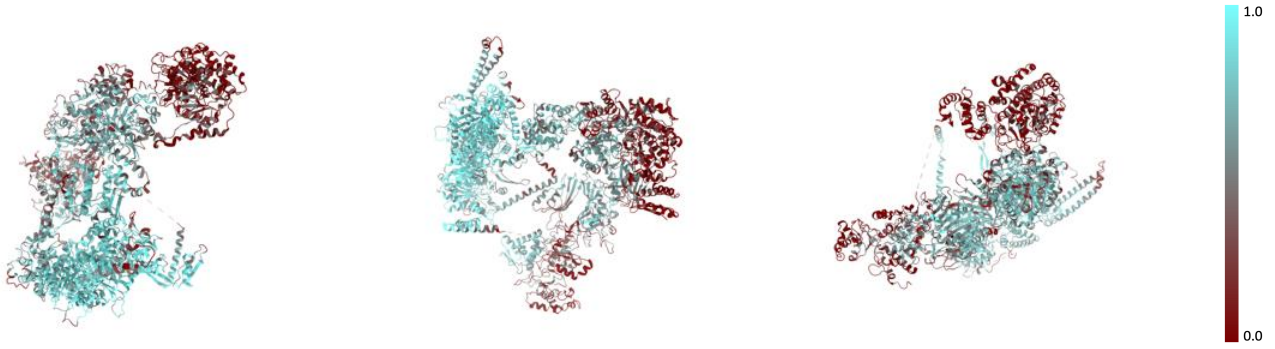
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

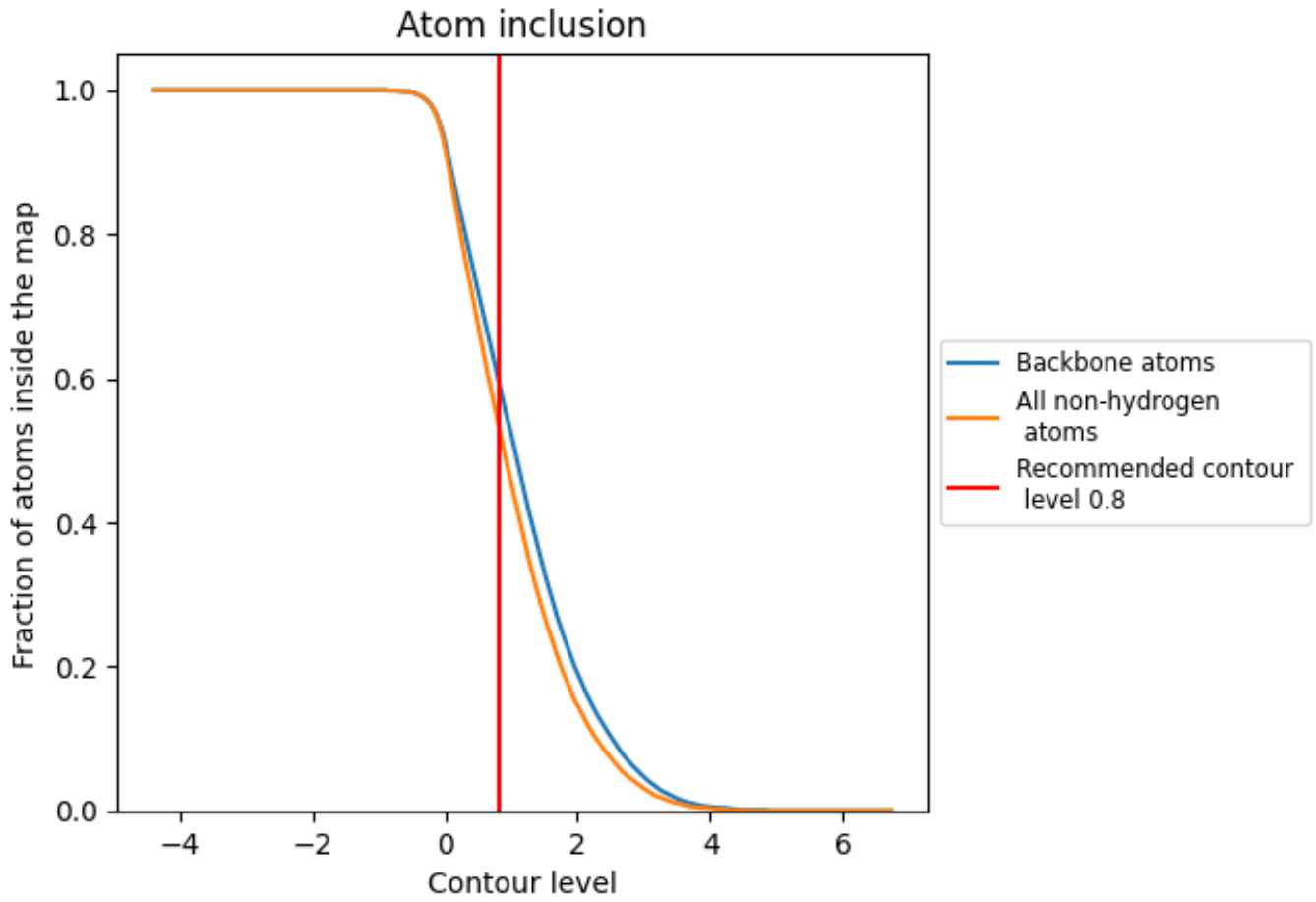
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 54% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5370	0.4130
A	0.7220	0.5220
B	0.4070	0.3370