wwPDB EM Validation Summary Report ⓘ

Mar 22, 2025 – 05:07 PM EDT

PDB ID	:	6U5T
EMDB ID	:	EMD-20655
Title	:	Electron cryomicroscopy Structure of S. cerevisiae FAS in the Apo state
Authors	:	Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on	:	2019-08-28
Resolution	:	2.90 Å(reported)
Based on initial model	:	2UV8

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:

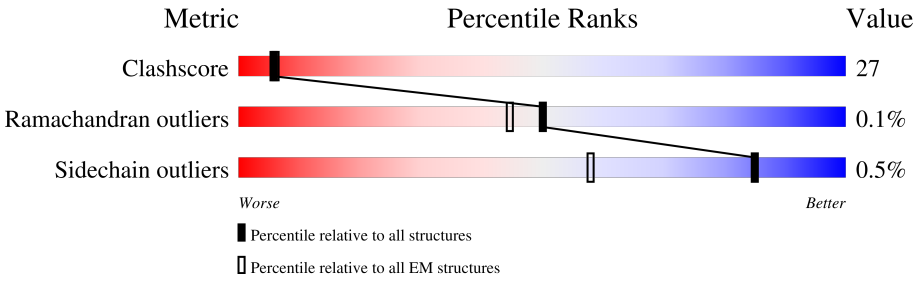
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.90 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	1887	26% 47% 38% 14%
2	G	2073	46% 50% 48% .

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28233 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	1616	12202	7703	2086	2368	45	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	2033	15995	10253	2660	3026	56	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	2052	ASP	-	expression tag	UNP P07149
G	2053	TYR	-	expression tag	UNP P07149
G	2054	LYS	-	expression tag	UNP P07149
G	2055	ASP	-	expression tag	UNP P07149
G	2056	HIS	-	expression tag	UNP P07149
G	2057	ASP	-	expression tag	UNP P07149
G	2058	GLY	-	expression tag	UNP P07149
G	2059	ASP	-	expression tag	UNP P07149
G	2060	TYR	-	expression tag	UNP P07149
G	2061	LYS	-	expression tag	UNP P07149
G	2062	ASP	-	expression tag	UNP P07149
G	2063	HIS	-	expression tag	UNP P07149
G	2064	ASP	-	expression tag	UNP P07149
G	2065	ILE	-	expression tag	UNP P07149
G	2066	ASP	-	expression tag	UNP P07149
G	2067	TYR	-	expression tag	UNP P07149
G	2068	LYS	-	expression tag	UNP P07149
G	2069	ASP	-	expression tag	UNP P07149
G	2070	ASP	-	expression tag	UNP P07149
G	2071	ASP	-	expression tag	UNP P07149
G	2072	ASP	-	expression tag	UNP P07149

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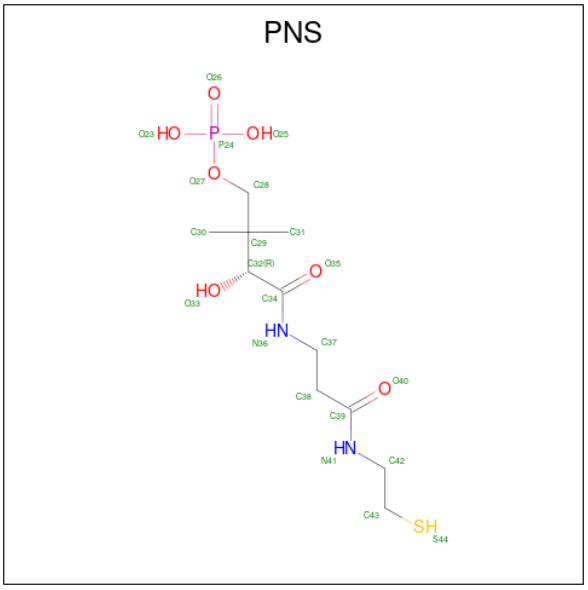
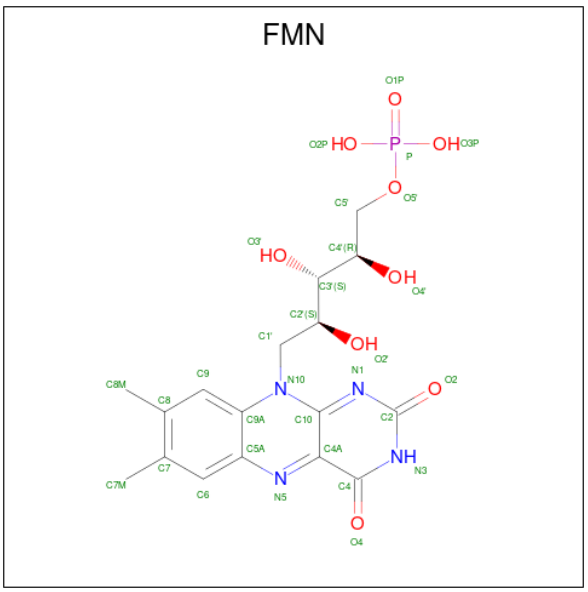
Chain	Residue	Modelled	Actual	Comment	Reference
G	2073	LYS	-	expression tag	UNP P07149

- Molecule 3 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	A	1	5	1	3	1	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



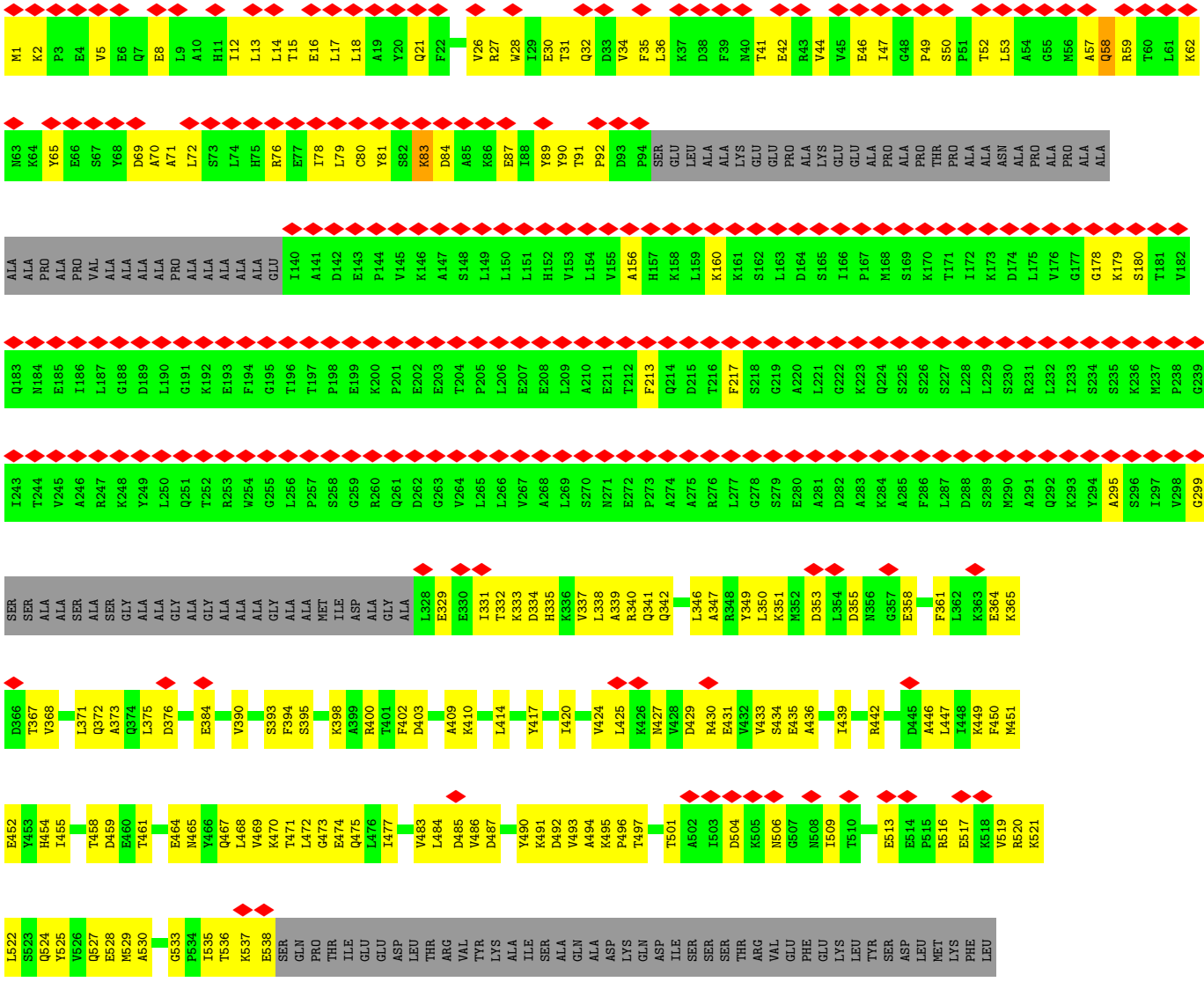
Mol	Chain	Residues	Atoms					AltConf
4	G	1	Total	C	N	O	P	0
			31	17	4	9	1	

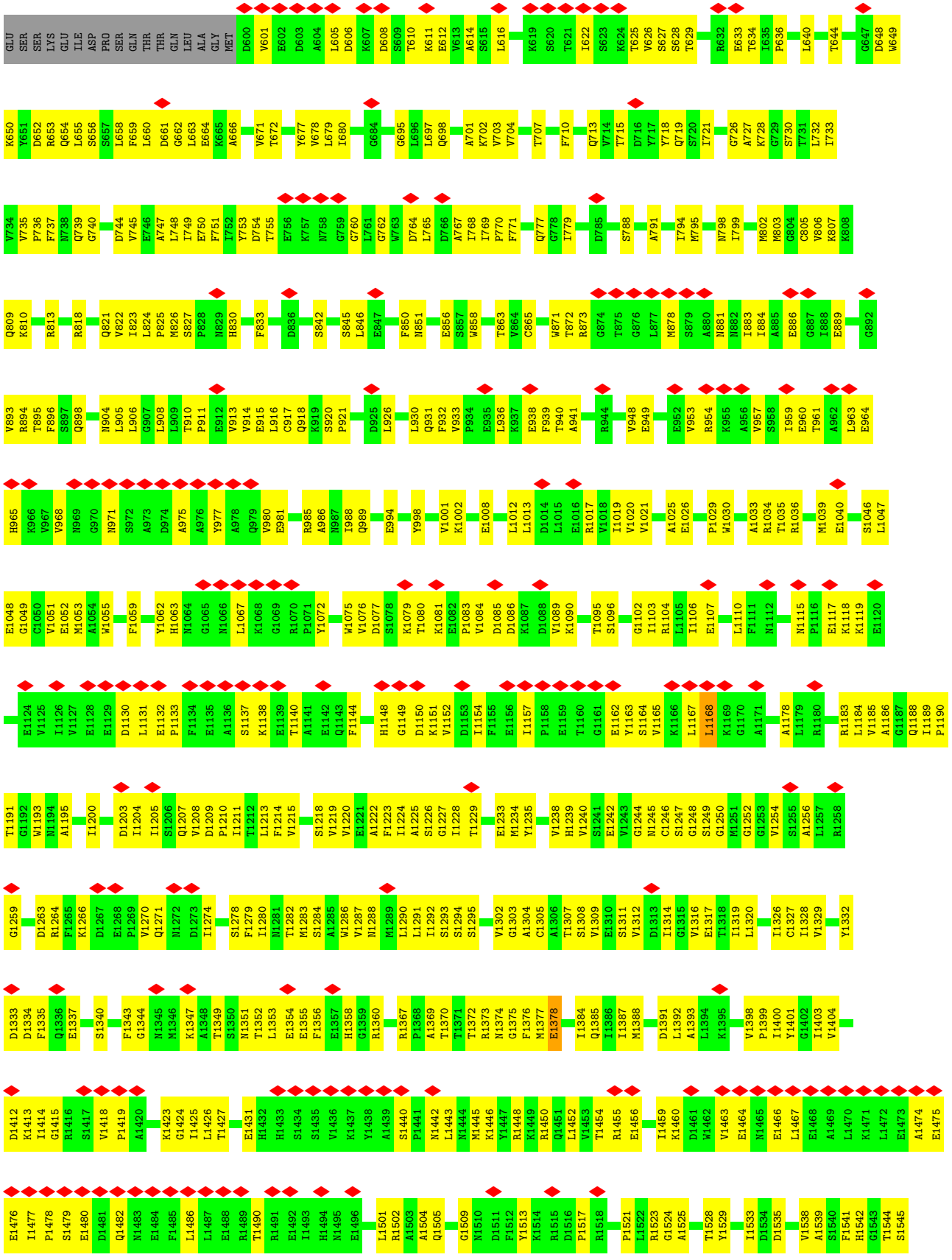
3 Residue-property plots (i)

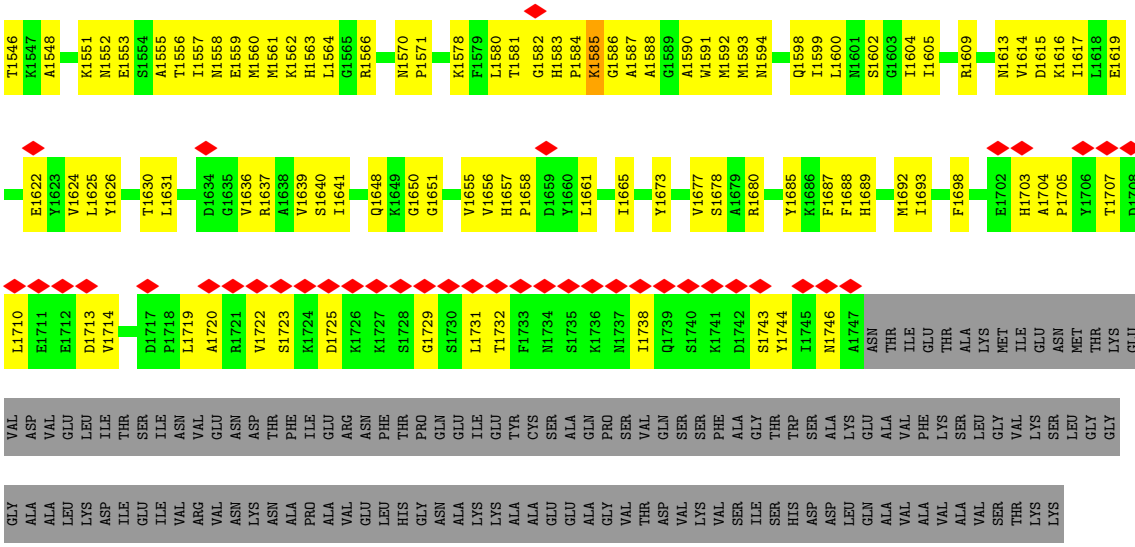
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

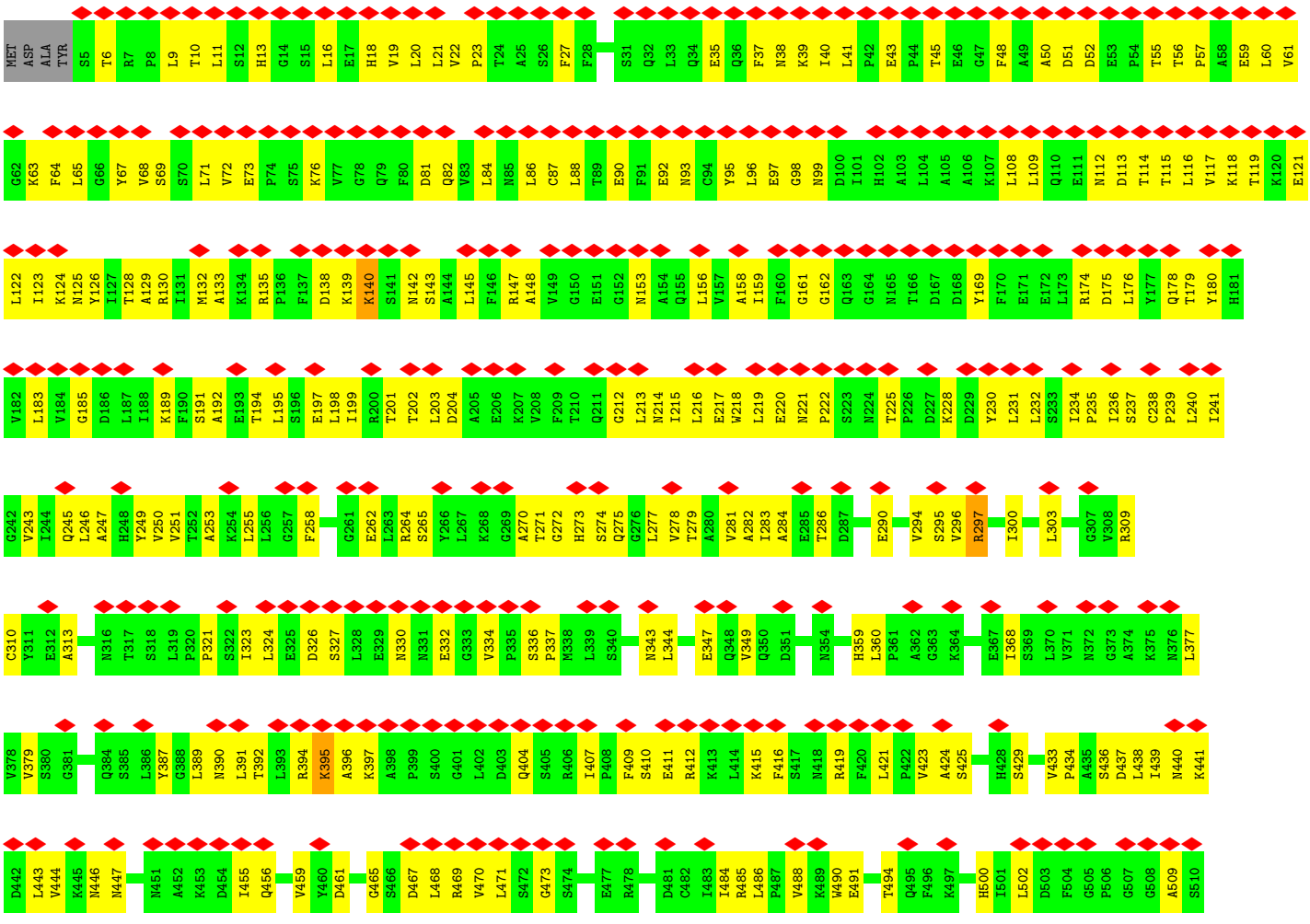


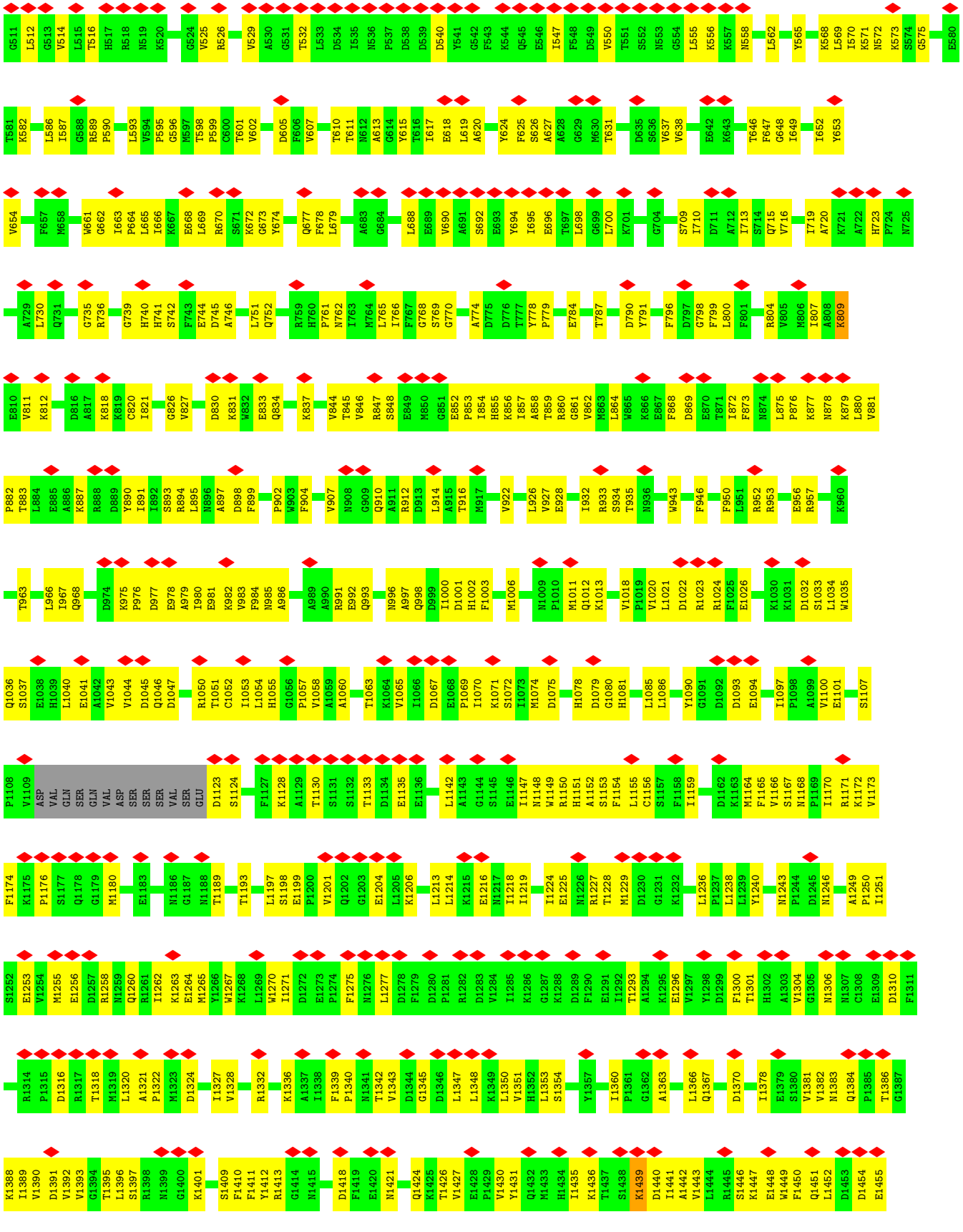

GLU SER SER LYS GLU ILE ASP PRO SER GLN THR THR GLN LEU ALA GLY MET D600 V601 E602 D603 A604 L605 D606 K607 D608 S609 T610 K611 E612 V613 A614 S615 L616 K619 S620 T621 I622 S623 K624 T625 V626 S627 S628 T629 R632 E633 T634 I635 P636 L640 T644 G647 D648 W649
K650 Y651 D652 R653 Q654 L655 S656 S657 L658 F659 L660 D661 G662 L663 E664 K665 A666 V671 T672 Y677 V678 L679 I680 G684 G695 L696 L697 Q698 A701 K702 V703 V704 T707 F710 Q713 V714 T715 D716 Y717 T718 Q719 S720 I721 G726 A727 K728 G729 S730 I731 L732 I733
V734 V735 P736 F737 N738 Q739 G740 D744 V745 E746 A747 L748 I749 E750 F751 I752 Y753 D754 T755 E756 K757 N758 G759 G760 L761 G762 W763 D764 L765 D766 A767 I768 I769 P770 F771 Q777 G778 I779 D785 S788 A791 I794 M795 N798 I799 M802 M803 G804 C805 V806 K807 K808
Q809 K810 R813 R818 Q821 V822 I823 L824 P825 M826 S827 P828 N829 H830 F833 D836 S842 S845 L846 E847 F850 N851 E856 S857 W858 T863 V864 C865 W871 T872 R873 G874 T875 G876 L877 M878 S879 A880 N881 N882 I883 I884 A885 E886 G887 I888 E889 G892
V893 R894 T895 F896 S897 Q898 N904 L905 L906 G907 L908 L909 T910 P911 E912 V913 V914 E915 L916 C917 Q918 K919 S920 P921 D925 L926 L930 Q931 F932 V933 P934 E935 L936 K937 E938 F939 T940 A941 R944 V948 E949 E952 V953 R954 K955 A956 V957 S958 I959 E960 T961 A962 L963 E964
H965 K966 V967 V968 N969 G970 N971 S972 A973 D974 A975 A976 Y977 A978 Q979 V980 E981 R985 A986 N987 I988 Q989 E994 Y998 V1001 K1002 E1008 L1012 L1013 D1014 L1015 E1016 R1017 V1018 I1019 V1020 V1021 A1025 E1026 P1029 W1030 A1033 R1034 T1035 R1036 M1039 E1040 S1046 L1047
E1048 G1049 C1050 V1051 E1052 M1053 A1054 W1055 F1059 Y1062 H1063 N1064 G1065 N1066 L1067 K1068 G1069 R1070 P1071 Y1072 W1075 V1076 D1077 S1078 K1079 T1080 K1081 E1082 P1083 V1084 D1085 D1086 K1087 D1088 V1089 K1090 T1095 S1096 G1102 I1103 R1104 L1105 I1106 E1107 L1110 F1111 N1112 N1115 P1116 E1117 K1118 K1119 E1120
E1124 V1125 I1126 V1127 E1128 E1129 D1130 L1131 E1132 P1133 F1134 E1135 A1136 S1137 K1138 E1139 T1140 A1141 E1142 Q1143 F1144 H1148 G1149 D1150 K1151 V1152 D1153 I1154 F1155 E1156 I1157 P1158 E1159 T1160 G1161 E1162 Y1163 S1164 V1165 K1166 L1167 L1168 K1169 G1170 A1171 A1178 L1179 R1180 R1183 L1184 V1185 A1186 G1187 Q1188 I1189 P1190
T1191 G1192 W1193 N1194 A1195 I1200 D1203 I1204 I1205 S1206 Q1207 V1208 D1209 P1210 I1211 T1212 L1213 F1214 V1215 S1218 V1219 V1220 E1221 A1222 F1223 I1224 A1225 S1226 G1227 I1228 T1229 E1233 M1234 Y1235 V1238 H1239 V1240 S1241 E1242 V1243 G1244 N1245 C1246 S1247 G1248 S1249 G1250 M1251 G1252 G1253 V1254 S1255 A1256 L1257 R1258
G1259 D1263 R1264 F1265 K1266 D1267 E1268 P1269 V1270 Q1271 N1272 D1273 I1274 S1278 F1279 I1280 N1281 T1282 M1283 S1284 A1285 W1286 V1287 N1288 M1289 L1290 L1291 I1292 S1293 S1294 S1295 V1302 G1303 A1304 C1305 A1306 T1307 S1308 V1309 E1310 S1311 V1312 D1313 I1314 G1315 V1316 E1317 T1318 I1319 L1320 I1326 C1327 I1328 V1329 Y1332
D1333 D1334 F1335 Q1336 E1337 S1340 F1343 G1344 N1345 M1346 K1347 A1348 T1349 S1350 N1351 T1352 L1353 E1354 E1355 F1356 E1357 H1358 G1359 R1360 R1367 P1368 A1369 T1370 T1371 T1372 R1373 N1374 G1375 F1376 M1377 E1378 I1384 Q1385 I1386 I1387 M1388 D1391 L1392 A1393 L1394 K1395 V1398 P1399 I1400 Y1401 G1402 I1403 V1404
D1412 K1413 I1414 G1415 R1416 S1417 V1418 P1419 A1420 K1423 G1424 I1425 L1426 T1427 E1431 H1432 H1433 S1434 S1435 V1436 K1437 Y1438 A1439 S1440 P1441 N1442 L1443 N1444 M1445 K1446 Y1447 R1448 K1449 R1450 Q1451 L1452 V1453 T1454 R1455 E1456 I1459 K1460 D1461 W1462 V1463 E1464 N1465 E1466 L1467 E1468 A1469 L1470 K1471 L1472 E1473 A1474 E1475
E1476 I1477 P1478 S1479 E1480 D1481 Q1482 N1483 E1484 F1485 L1486 L1487 E1488 R1489 T1490 R1491 E1492 I1493 H1494 N1495 E1496 L1501 R1502 A1503 A1504 Q1505 G1509 N1510 D1511 F1512 Y1513 K1514 R1515 D1516 P1517 R1518 P1521 L1522 R1523 G1524 A1525 T1528 Y1529 I1533 D1534 D1535 V1538 A1539 S1540 F1541 H1542 G1543 T1544 S1545



• Molecule 2: Fatty acid synthase subunit beta

Chain G:

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T581 K582 L586 I587 G588 R589 P590 L593 V594 P595 G596 K597 T598 P599 G600 T601 V602 D605 F606 V607 T610 T611 N612 A613 G614 Y615 T616 I617 E618 L619 A620 Y624 F625 S626 A627 A628 G629 M630 T631 D635 S636 V637 V638 E642 K643 T646 F647 G648 I649 I652 Y653
V654 F657 M658 W661 G662 I663 P664 L665 I666 K667 E668 L669 R670 S671 K672 G673 Y674 Q677 F678 L679 A683 G684 L688 E689 V690 A691 S692 E693 Y694 I695 E696 T697 L698 G699 L700 K701 G704 S709 I710 D711 A712 I713 S714 Q715 V716 I719 A720 K721 A722 H723 P724 N725
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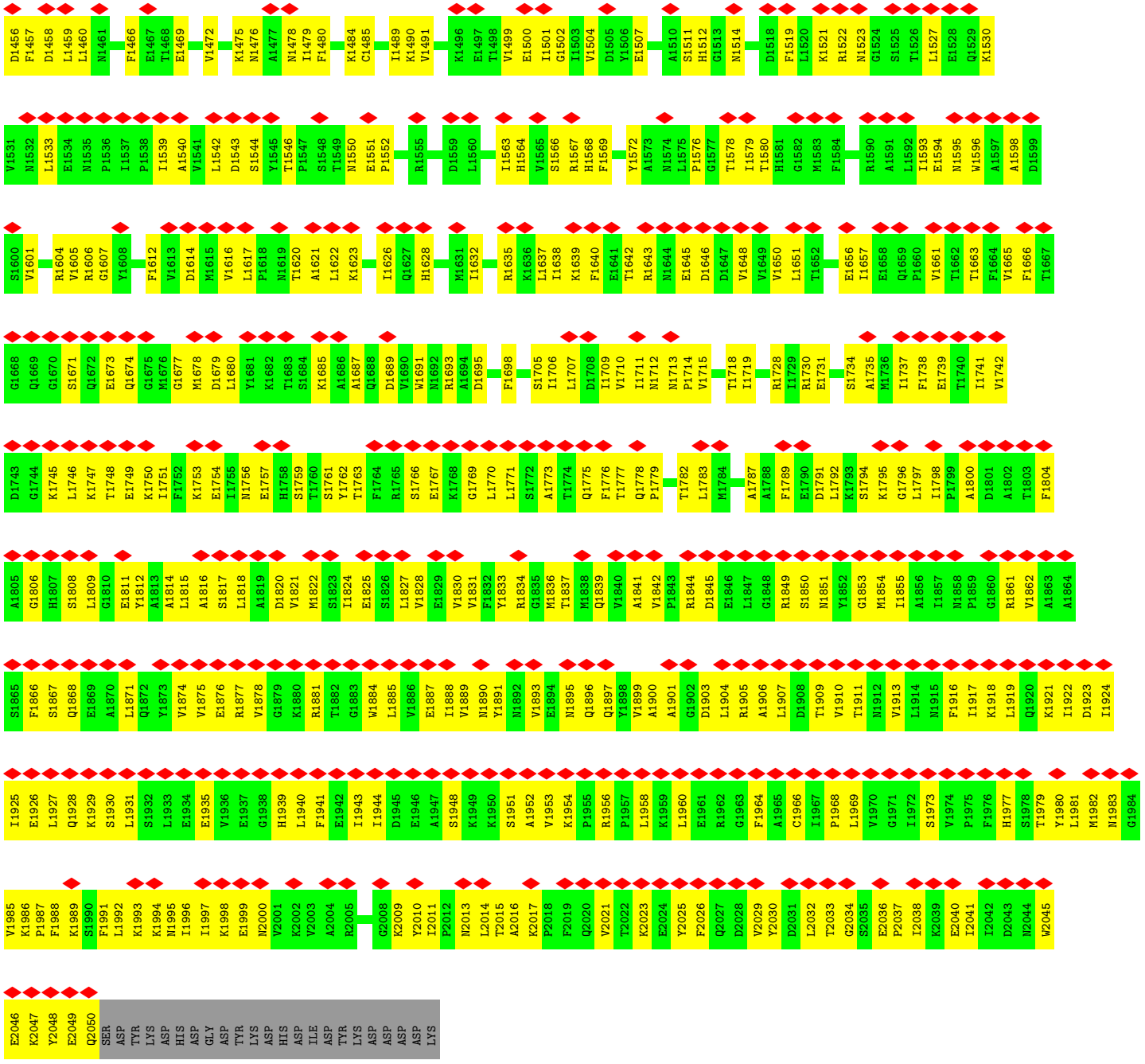
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S1865 F1866 S1867 Q1868 E1869 A1870 L1871 Q1872 Y1873 V1874 V1875 E1876 R1877 V1878 G1879 K1880 R1881 T1882 G1883 W1884 L1885 V1886 E1887 I1888 V1889 N1890 Y1891 N1892 V1893 E1894 N1895 Q1896 Q1897 Y1898 V1899 A1900 A1901 G1902 D1903 L1904 R1905 A1906 L1907 D1908 T1909 V1910 T1911 N1912 V1913 L1914 N1915 F1916 I1917 K1918 L1919 Q1920 K1921 I1922 D1923 I1924
I1925 E1926 L1927 Q1928 K1929 S1930 L1931 S1932 L1933 E1934 E1935 V1936 E1937 G1938 H1939 L1940 F1941 E1942 I1943 I1944 D1945 E1946 A1947 S1948 K1949 K1950 S1951 A1952 V1953 K1954 P1955 R1956 P1957 L1958 K1959 L1960 E1961 R1962 G1963 F1964 A1965 C1966 I1967 P1968 L1969 V1970 G1971 I1972 S1973 V1974 P1975 F1976 H1977 S1978 T1979 Y1980 L1981 M1982 N1983 G1984
V1985 K1986 P1987 F1988 K1989 S1990 F1991 L1992 K1993 K1994 N1995 I1996 I1997 K1998 E1999 N2000 V2001 K2002 V2003 A2004 R2005 G2008 K2009 Y2010 I2011 P2012 N2013 L2014 T2015 A2016 K2017 P2018 F2019 Q2020 V2021 T2022 K2023 E2024 Y2025 F2026 Q2027 D2028 V2029 Y2030 D2031 L2032 T2033 G2034 S2035 E2036 P2037 I2038 K2039 E2040 I2041 I2042 D2043 N2044 W2045
E2046 K2047 Y2048 E2049 Q2050 SER ASP TYR LYS ASP HIS ASP GLY ASP TYR LYS ASP HIS ASP ILE ASP TYR LYS ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	637823	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTFFIND4 within cryoSPARC2	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.591	Depositor
Minimum map value	-1.261	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.696	Depositor
Map size (Å)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PNS, 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	0.64	0/12424	0.54	0/16819
2	G	0.47	0/16360	0.49	0/22198
All	All	0.55	0/28784	0.51	0/39017

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1294	SER	Peptide
1	A	702	LYS	Peptide

5.2 Too-close contacts

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	12202	0	11715	648	0
2	G	15995	0	15978	878	0
3	A	5	0	0	0	0
4	G	31	0	19	1	0
All	All	28233	0	27712	1488	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 27.

The worst 5 of 1488 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1335:PHE:HD1	1:A:1378:GLU:HG3	1.07	1.12
1:A:1343:PHE:CE2	1:A:1585:LYS:NZ	2.18	1.10
1:A:1333:ASP:OD2	1:A:1585:LYS:HB2	1.52	1.09
1:A:1584:PRO:HB2	1:A:1587:ALA:HB3	1.34	1.04
1:A:1335:PHE:HD1	1:A:1378:GLU:CG	1.71	1.02

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	1608/1887 (85%)	1329 (83%)	275 (17%)	4 (0%)	44 73
2	G	2029/2073 (98%)	1771 (87%)	258 (13%)	0	100 100
All	All	3637/3960 (92%)	3100 (85%)	533 (15%)	4 (0%)	50 77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1585	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	179	LYS
1	A	1168	LEU
1	A	58	GLN

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	1233/1566 (79%)	1230 (100%)	3 (0%)	92 98
2	G	1772/1810 (98%)	1761 (99%)	11 (1%)	84 95
All	All	3005/3376 (89%)	2991 (100%)	14 (0%)	85 96

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

Mol	Chain	Res	Type
2	G	395	LYS
2	G	415	LYS
2	G	1439	LYS
2	G	1023	ARG
2	G	1128	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	1061	GLN
2	G	1383	ASN
2	G	1688	GLN
1	A	1345	ASN
1	A	1146	HIS

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)

2 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	$\#\|Z\| > 2$
3	PNS	A	1888	1	1,4,21	0.62	0	0,4,29	-	-
4	FMN	G	3051	-	33,33,33	1.15	2 (6%)	48,50,50	1.28	8 (16%)

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	PNS	A	1888	1	-	0/0/2/27	-
4	FMN	G	3051	-	-	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)
4	G	3051	FMN	C4A-N5	3.05	1.37	1.30
4	G	3051	FMN	C10-N1	2.21	1.37	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	3051	FMN	C4-N3-C2	-3.52	119.38	125.64
4	G	3051	FMN	C4A-C4-N3	2.74	120.23	113.25
4	G	3051	FMN	C5A-C9A-N10	2.69	120.40	117.97
4	G	3051	FMN	C4A-C10-N10	2.65	120.28	116.48
4	G	3051	FMN	O4-C4-C4A	-2.61	119.65	126.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	3051	FMN	C5'-O5'-P-O1P
4	G	3051	FMN	C5'-O5'-P-O2P
4	G	3051	FMN	C5'-O5'-P-O3P

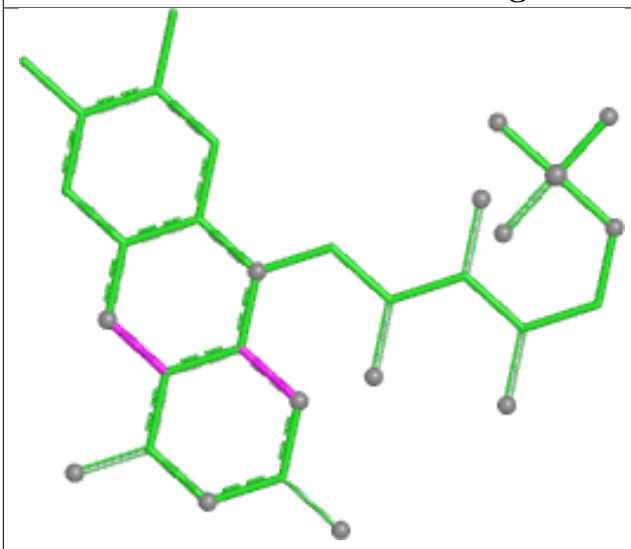
There are no ring outliers.

1 monomer is involved in 1 short contact:

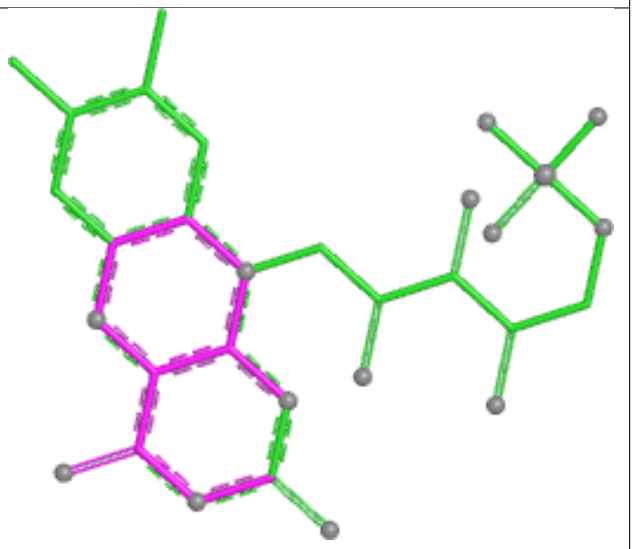
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3051	FMN	1	0

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.

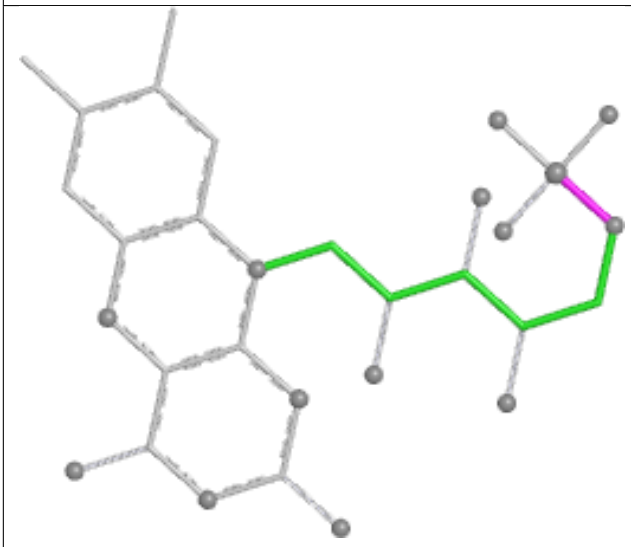
Ligand FMN G 3051



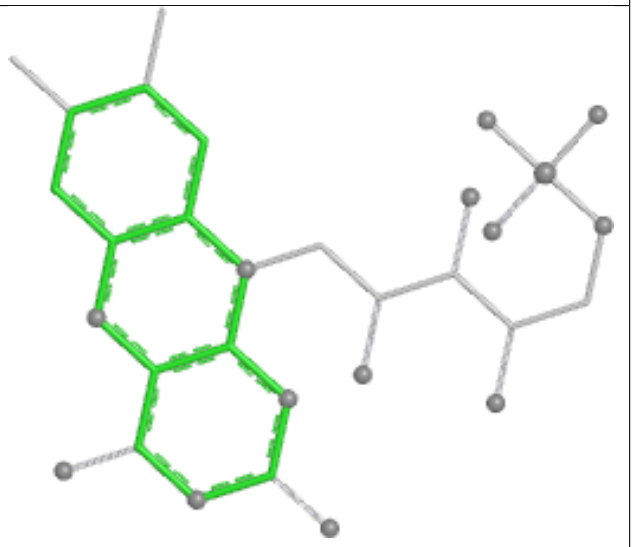
Bond lengths



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.

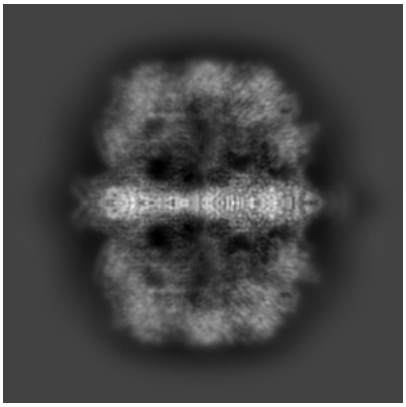
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20655. These allow visual inspection of the internal detail of the map and identification of artifacts.

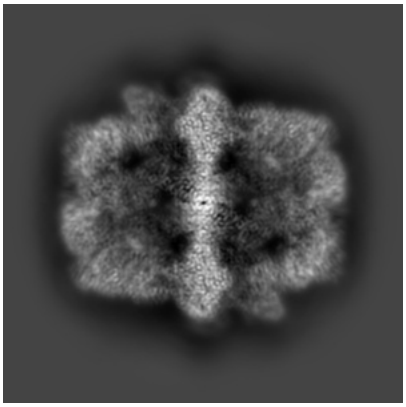
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

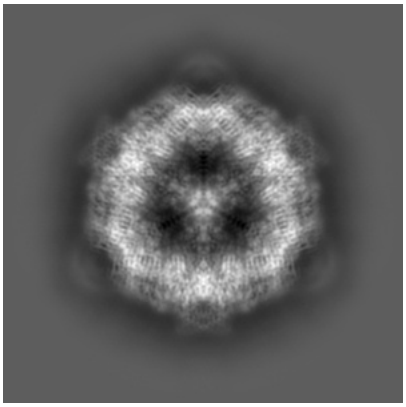
6.1.1 Primary map



X



Y

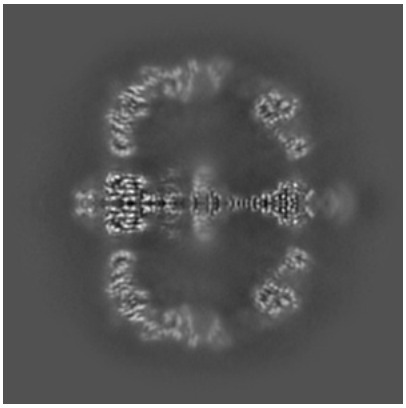


Z

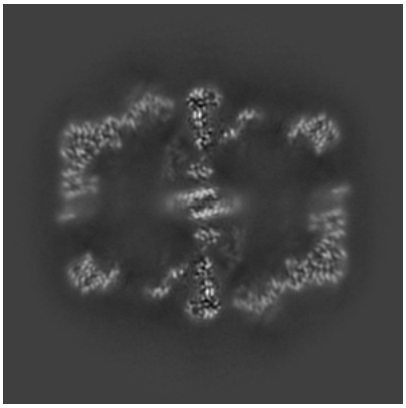
The images above show the map projected in three orthogonal directions.

6.2 Central slices

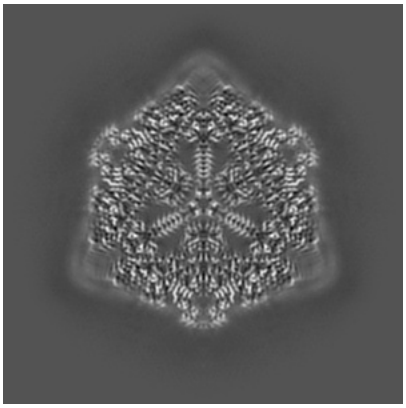
6.2.1 Primary map



X Index: 176



Y Index: 176

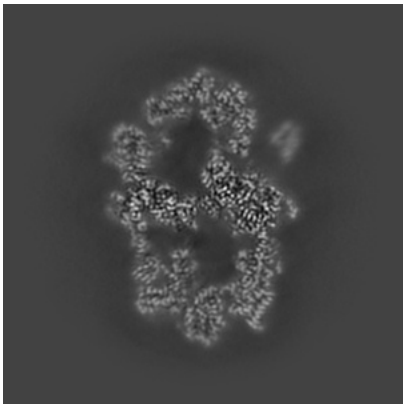


Z Index: 176

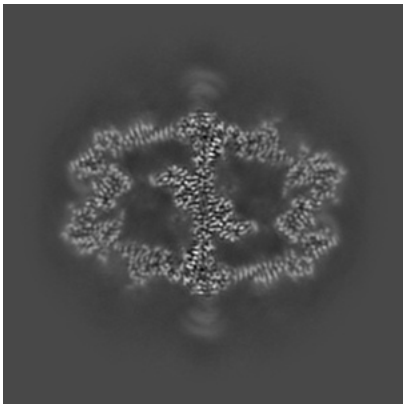
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

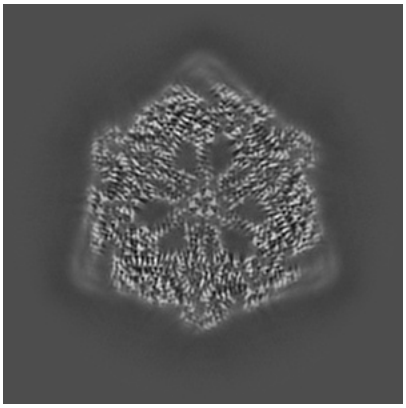
6.3.1 Primary map



X Index: 237



Y Index: 121

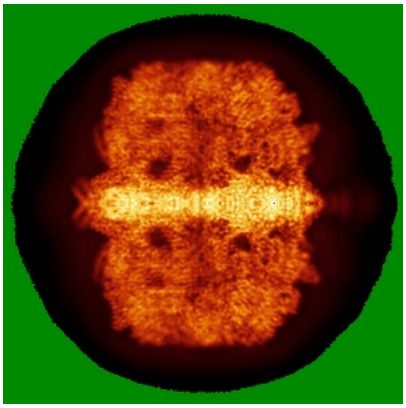


Z Index: 172

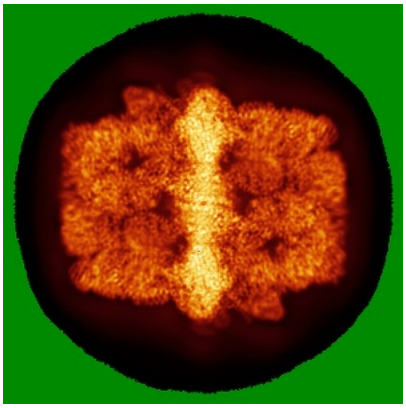
The images above show the largest variance slices of the map in three orthogonal directions.

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

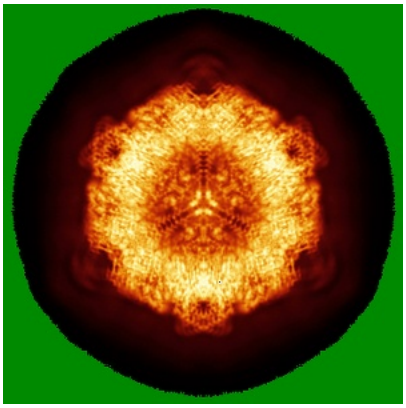
6.4.1 Primary map



X



Y

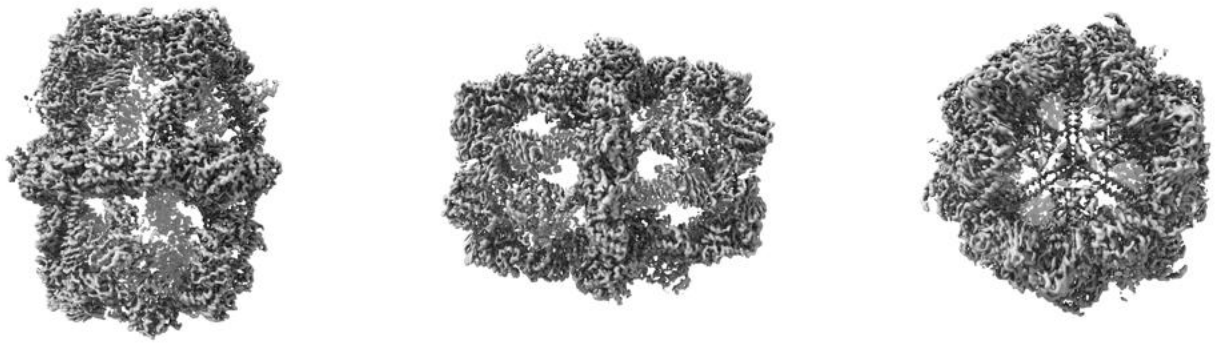


Z

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

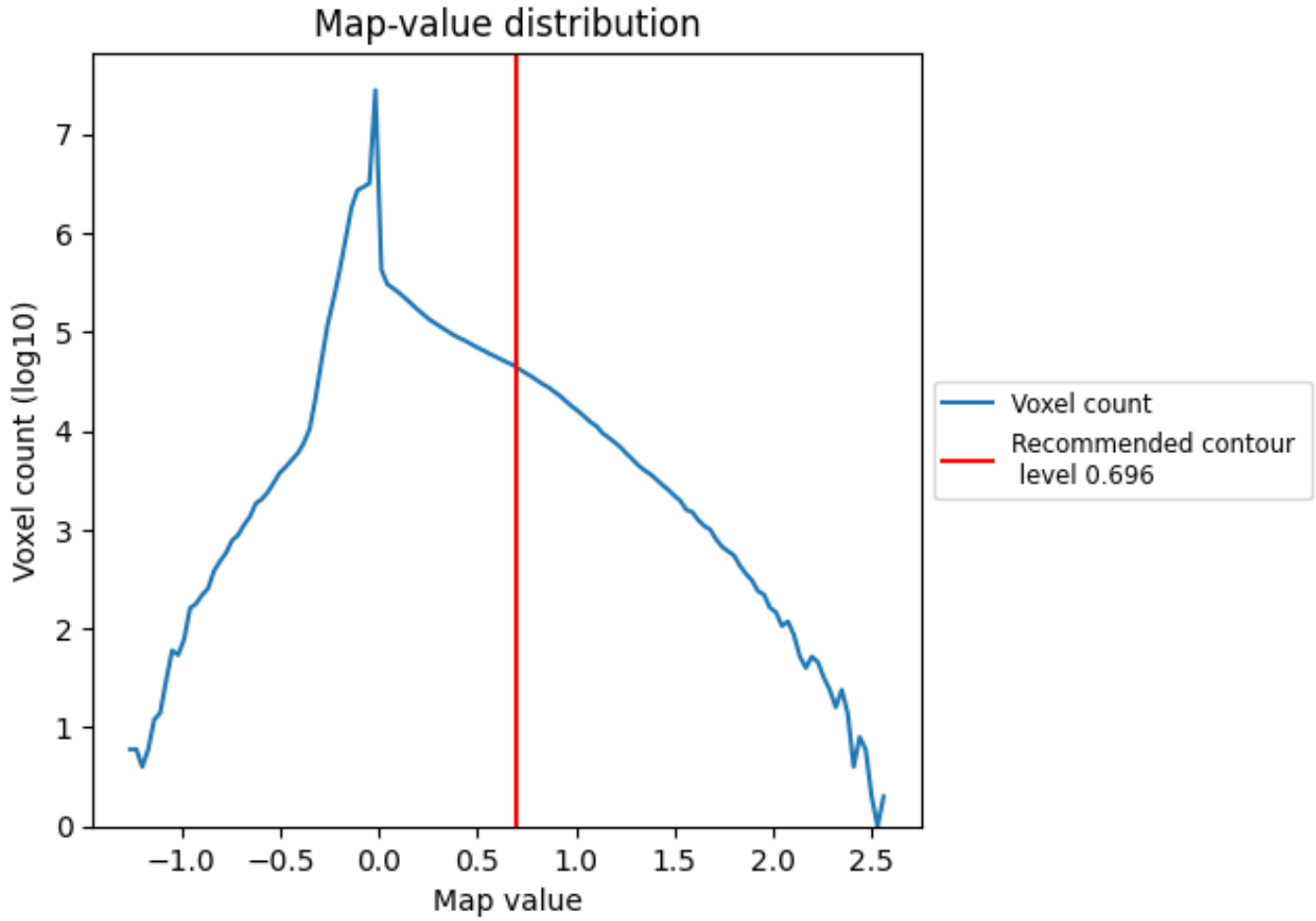
6.6 Mask visualisation (i)

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

7 Map analysis

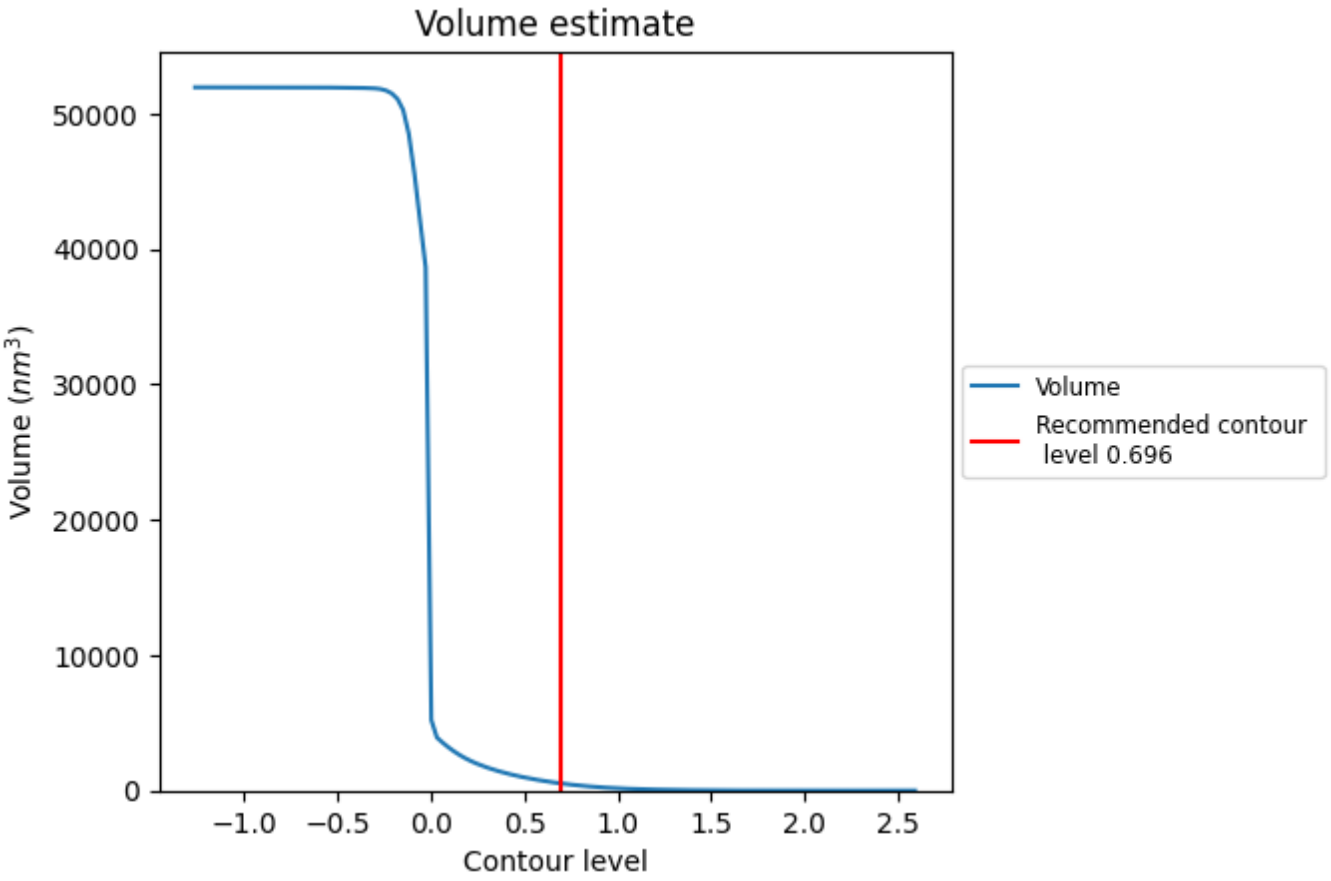
This section contains the results of statistical analysis of the map.

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.

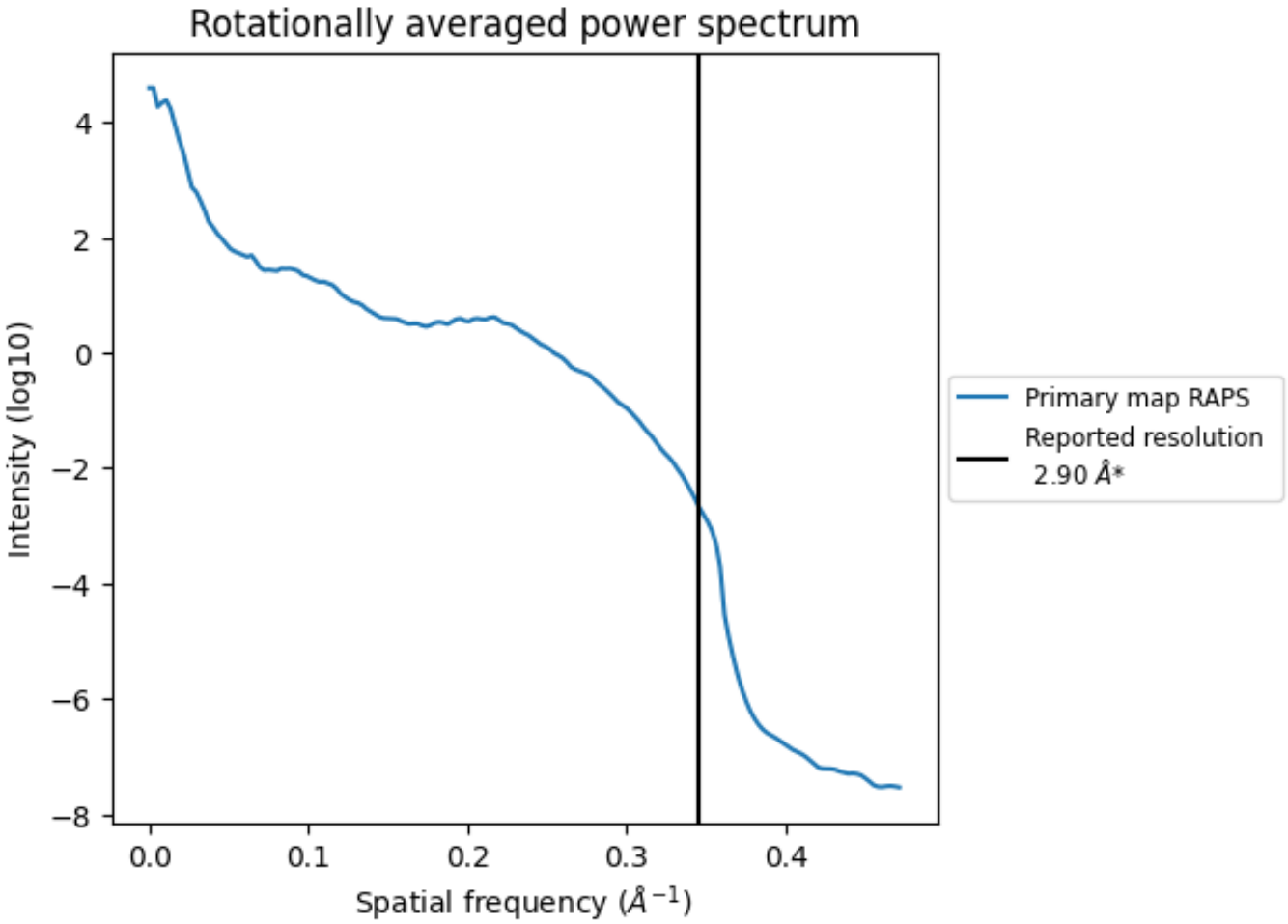
7.2 Volume estimate (i)



The volume at the recommended contour level is 528 nm^3; this corresponds to an approximate mass of 477 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 0.345 Å^{-1}

8 Fourier-Shell correlation

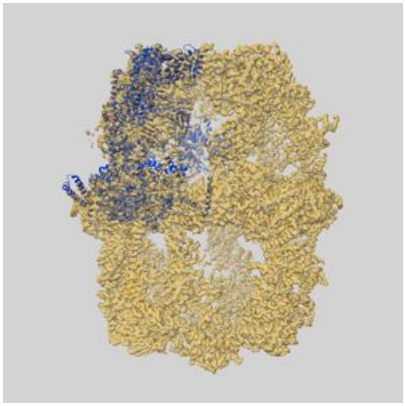
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

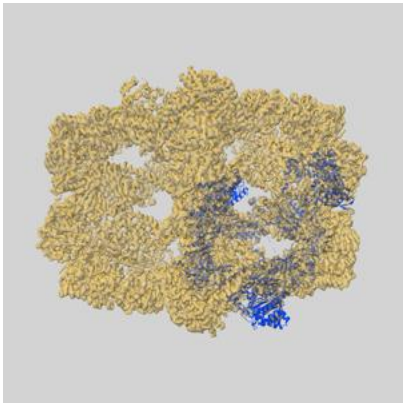
This section contains information regarding the fit between EMDB map EMD-20655 and PDB model 6U5T. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

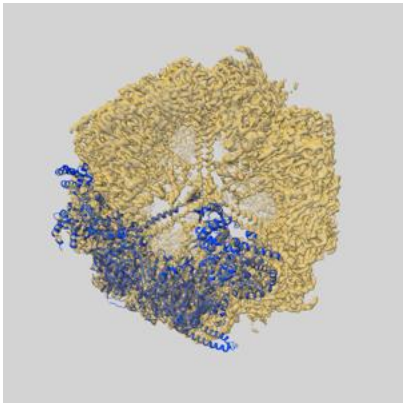
9.1.1 Map-model overlay



X

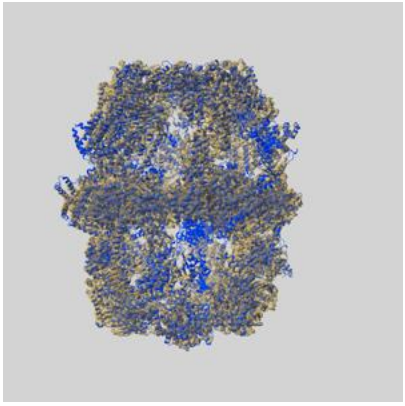


Y

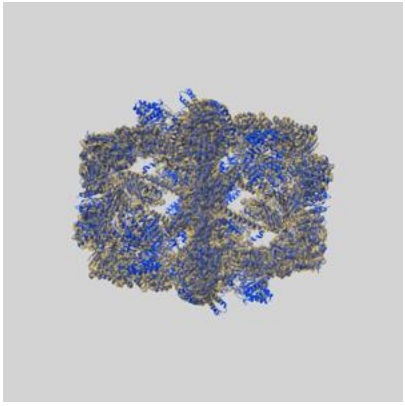


Z

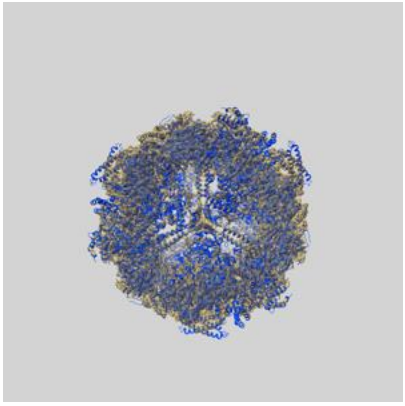
9.1.2 Map-model assembly overlay



X



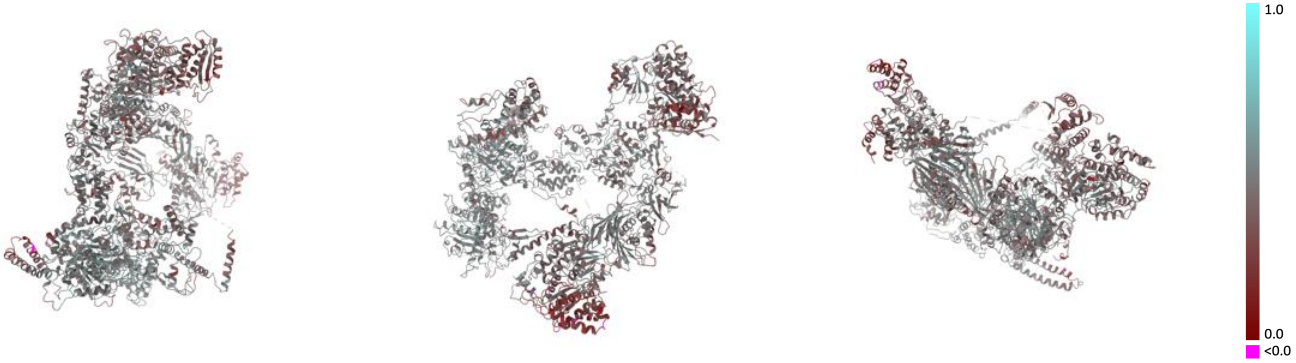
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.696 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.

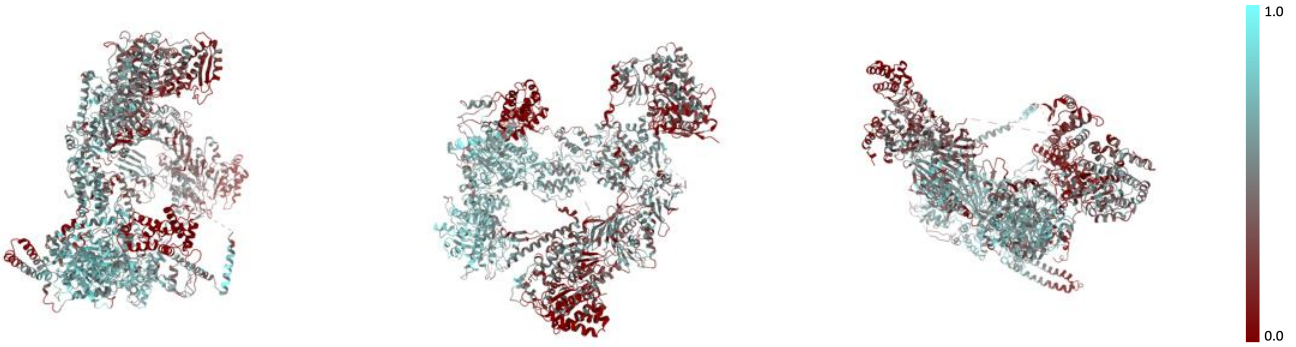
9.2 Q-score mapped to coordinate model (i)



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.

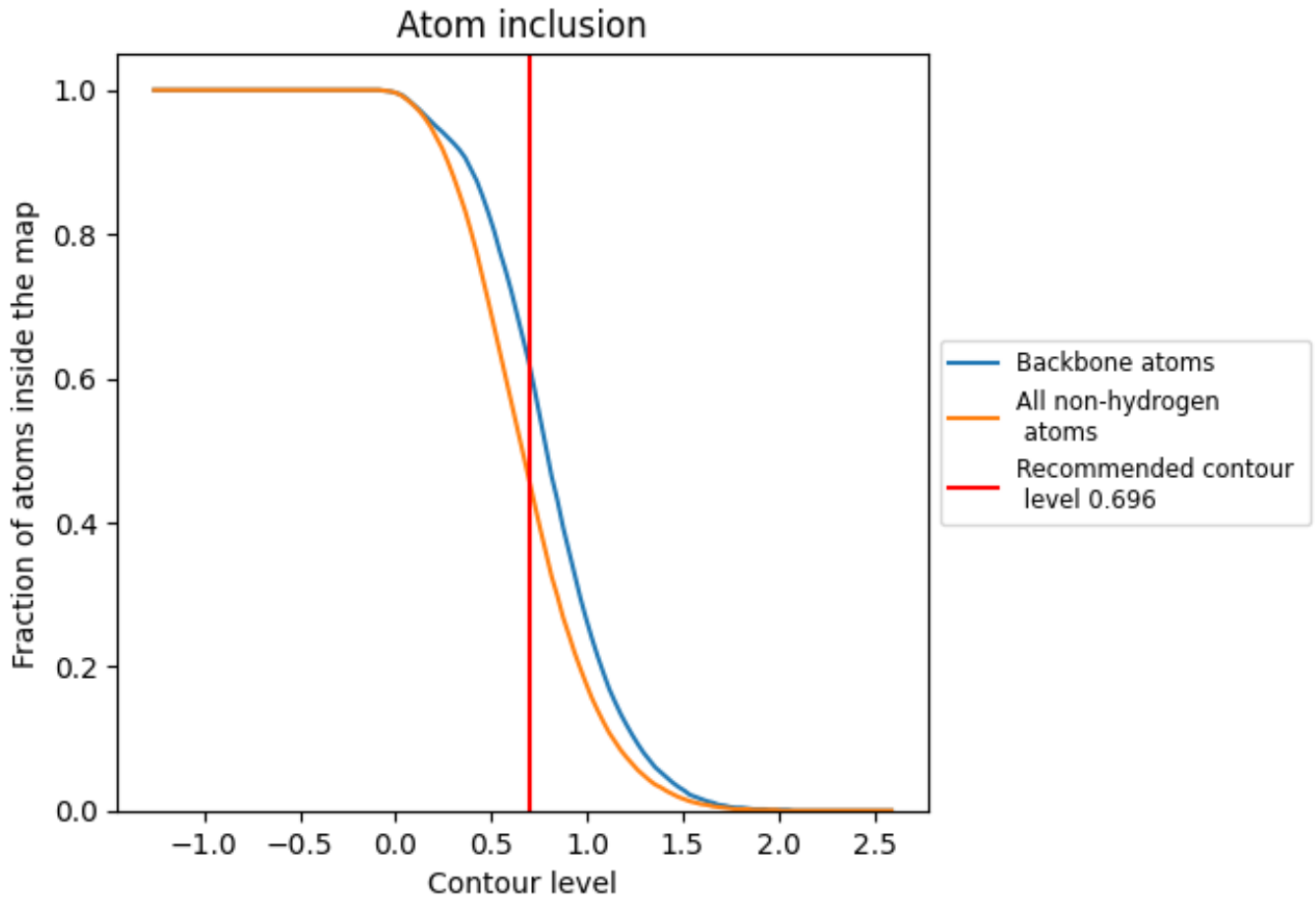
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.696).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 46% 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 (0.696) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4620	0.4420
A	0.5340	0.4690
G	0.4070	0.4210