wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 04:10 am GMT

PDB ID	:	6GJC
EMDB ID	:	EMD-0011
Title	:	Structure of Mycobacterium tuberculosis Fatty Acid Synthase - I
Authors	:	Elad, N.; Baron, S.; Shakked, Z.; Zimhony, O.; Diskin, R.
Deposited on	:	2018-05-16
Resolution	:	3.30 Å(reported)

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

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

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

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

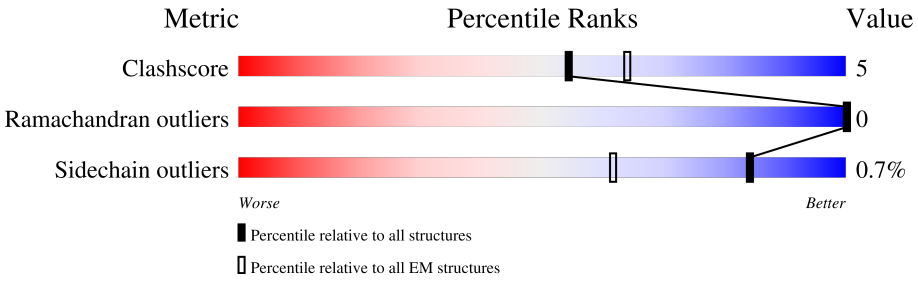
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	3092	7% 76% 13% 10%
1	B	3092	7% 76% 13% 10%
1	C	3092	7% 76% 13% 10%
1	D	3092	7% 76% 14% 10%
1	E	3092	7% 76% 13% 10%
1	F	3092	7% 76% 13% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 124992 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2770	Total	C	N	O	S	0	0
			20801	13078	3703	3955	65		
1	B	2770	Total	C	N	O	S	0	0
			20801	13078	3703	3955	65		
1	C	2770	Total	C	N	O	S	0	0
			20801	13078	3703	3955	65		
1	D	2770	Total	C	N	O	S	0	0
			20801	13078	3703	3955	65		
1	E	2770	Total	C	N	O	S	0	0
			20801	13078	3703	3955	65		
1	F	2770	Total	C	N	O	S	0	0
			20801	13078	3703	3955	65		

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A0T9Z6H1
A	-12	LYS	-	expression tag	UNP A0A0T9Z6H1
A	-11	LYS	-	expression tag	UNP A0A0T9Z6H1
A	-10	TRP	-	expression tag	UNP A0A0T9Z6H1
A	-9	SER	-	expression tag	UNP A0A0T9Z6H1
A	-8	HIS	-	expression tag	UNP A0A0T9Z6H1
A	-7	PRO	-	expression tag	UNP A0A0T9Z6H1
A	-6	GLN	-	expression tag	UNP A0A0T9Z6H1
A	-5	PHE	-	expression tag	UNP A0A0T9Z6H1
A	-4	GLU	-	expression tag	UNP A0A0T9Z6H1
A	-3	LYS	-	expression tag	UNP A0A0T9Z6H1
A	-2	GLY	-	expression tag	UNP A0A0T9Z6H1
A	-1	GLY	-	expression tag	UNP A0A0T9Z6H1
A	0	SER	-	expression tag	UNP A0A0T9Z6H1
A	1	ASP	-	expression tag	UNP A0A0T9Z6H1
A	2	TYR	-	expression tag	UNP A0A0T9Z6H1
A	3	LYS	-	expression tag	UNP A0A0T9Z6H1
A	4	ASP	-	expression tag	UNP A0A0T9Z6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ASP	-	expression tag	UNP A0A0T9Z6H1
A	6	ASP	-	expression tag	UNP A0A0T9Z6H1
A	7	ASP	-	expression tag	UNP A0A0T9Z6H1
A	8	LYS	-	expression tag	UNP A0A0T9Z6H1
A	9	PRO	-	expression tag	UNP A0A0T9Z6H1
A	10	ILE	-	expression tag	UNP A0A0T9Z6H1
A	11	CYS	-	expression tag	UNP A0A0T9Z6H1
B	-13	MET	-	initiating methionine	UNP A0A0T9Z6H1
B	-12	LYS	-	expression tag	UNP A0A0T9Z6H1
B	-11	LYS	-	expression tag	UNP A0A0T9Z6H1
B	-10	TRP	-	expression tag	UNP A0A0T9Z6H1
B	-9	SER	-	expression tag	UNP A0A0T9Z6H1
B	-8	HIS	-	expression tag	UNP A0A0T9Z6H1
B	-7	PRO	-	expression tag	UNP A0A0T9Z6H1
B	-6	GLN	-	expression tag	UNP A0A0T9Z6H1
B	-5	PHE	-	expression tag	UNP A0A0T9Z6H1
B	-4	GLU	-	expression tag	UNP A0A0T9Z6H1
B	-3	LYS	-	expression tag	UNP A0A0T9Z6H1
B	-2	GLY	-	expression tag	UNP A0A0T9Z6H1
B	-1	GLY	-	expression tag	UNP A0A0T9Z6H1
B	0	SER	-	expression tag	UNP A0A0T9Z6H1
B	1	ASP	-	expression tag	UNP A0A0T9Z6H1
B	2	TYR	-	expression tag	UNP A0A0T9Z6H1
B	3	LYS	-	expression tag	UNP A0A0T9Z6H1
B	4	ASP	-	expression tag	UNP A0A0T9Z6H1
B	5	ASP	-	expression tag	UNP A0A0T9Z6H1
B	6	ASP	-	expression tag	UNP A0A0T9Z6H1
B	7	ASP	-	expression tag	UNP A0A0T9Z6H1
B	8	LYS	-	expression tag	UNP A0A0T9Z6H1
B	9	PRO	-	expression tag	UNP A0A0T9Z6H1
B	10	ILE	-	expression tag	UNP A0A0T9Z6H1
B	11	CYS	-	expression tag	UNP A0A0T9Z6H1
C	-13	MET	-	initiating methionine	UNP A0A0T9Z6H1
C	-12	LYS	-	expression tag	UNP A0A0T9Z6H1
C	-11	LYS	-	expression tag	UNP A0A0T9Z6H1
C	-10	TRP	-	expression tag	UNP A0A0T9Z6H1
C	-9	SER	-	expression tag	UNP A0A0T9Z6H1
C	-8	HIS	-	expression tag	UNP A0A0T9Z6H1
C	-7	PRO	-	expression tag	UNP A0A0T9Z6H1
C	-6	GLN	-	expression tag	UNP A0A0T9Z6H1
C	-5	PHE	-	expression tag	UNP A0A0T9Z6H1
C	-4	GLU	-	expression tag	UNP A0A0T9Z6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	LYS	-	expression tag	UNP A0A0T9Z6H1
C	-2	GLY	-	expression tag	UNP A0A0T9Z6H1
C	-1	GLY	-	expression tag	UNP A0A0T9Z6H1
C	0	SER	-	expression tag	UNP A0A0T9Z6H1
C	1	ASP	-	expression tag	UNP A0A0T9Z6H1
C	2	TYR	-	expression tag	UNP A0A0T9Z6H1
C	3	LYS	-	expression tag	UNP A0A0T9Z6H1
C	4	ASP	-	expression tag	UNP A0A0T9Z6H1
C	5	ASP	-	expression tag	UNP A0A0T9Z6H1
C	6	ASP	-	expression tag	UNP A0A0T9Z6H1
C	7	ASP	-	expression tag	UNP A0A0T9Z6H1
C	8	LYS	-	expression tag	UNP A0A0T9Z6H1
C	9	PRO	-	expression tag	UNP A0A0T9Z6H1
C	10	ILE	-	expression tag	UNP A0A0T9Z6H1
C	11	CYS	-	expression tag	UNP A0A0T9Z6H1
D	-13	MET	-	initiating methionine	UNP A0A0T9Z6H1
D	-12	LYS	-	expression tag	UNP A0A0T9Z6H1
D	-11	LYS	-	expression tag	UNP A0A0T9Z6H1
D	-10	TRP	-	expression tag	UNP A0A0T9Z6H1
D	-9	SER	-	expression tag	UNP A0A0T9Z6H1
D	-8	HIS	-	expression tag	UNP A0A0T9Z6H1
D	-7	PRO	-	expression tag	UNP A0A0T9Z6H1
D	-6	GLN	-	expression tag	UNP A0A0T9Z6H1
D	-5	PHE	-	expression tag	UNP A0A0T9Z6H1
D	-4	GLU	-	expression tag	UNP A0A0T9Z6H1
D	-3	LYS	-	expression tag	UNP A0A0T9Z6H1
D	-2	GLY	-	expression tag	UNP A0A0T9Z6H1
D	-1	GLY	-	expression tag	UNP A0A0T9Z6H1
D	0	SER	-	expression tag	UNP A0A0T9Z6H1
D	1	ASP	-	expression tag	UNP A0A0T9Z6H1
D	2	TYR	-	expression tag	UNP A0A0T9Z6H1
D	3	LYS	-	expression tag	UNP A0A0T9Z6H1
D	4	ASP	-	expression tag	UNP A0A0T9Z6H1
D	5	ASP	-	expression tag	UNP A0A0T9Z6H1
D	6	ASP	-	expression tag	UNP A0A0T9Z6H1
D	7	ASP	-	expression tag	UNP A0A0T9Z6H1
D	8	LYS	-	expression tag	UNP A0A0T9Z6H1
D	9	PRO	-	expression tag	UNP A0A0T9Z6H1
D	10	ILE	-	expression tag	UNP A0A0T9Z6H1
D	11	CYS	-	expression tag	UNP A0A0T9Z6H1
E	-13	MET	-	initiating methionine	UNP A0A0T9Z6H1
E	-12	LYS	-	expression tag	UNP A0A0T9Z6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	LYS	-	expression tag	UNP A0A0T9Z6H1
E	-10	TRP	-	expression tag	UNP A0A0T9Z6H1
E	-9	SER	-	expression tag	UNP A0A0T9Z6H1
E	-8	HIS	-	expression tag	UNP A0A0T9Z6H1
E	-7	PRO	-	expression tag	UNP A0A0T9Z6H1
E	-6	GLN	-	expression tag	UNP A0A0T9Z6H1
E	-5	PHE	-	expression tag	UNP A0A0T9Z6H1
E	-4	GLU	-	expression tag	UNP A0A0T9Z6H1
E	-3	LYS	-	expression tag	UNP A0A0T9Z6H1
E	-2	GLY	-	expression tag	UNP A0A0T9Z6H1
E	-1	GLY	-	expression tag	UNP A0A0T9Z6H1
E	0	SER	-	expression tag	UNP A0A0T9Z6H1
E	1	ASP	-	expression tag	UNP A0A0T9Z6H1
E	2	TYR	-	expression tag	UNP A0A0T9Z6H1
E	3	LYS	-	expression tag	UNP A0A0T9Z6H1
E	4	ASP	-	expression tag	UNP A0A0T9Z6H1
E	5	ASP	-	expression tag	UNP A0A0T9Z6H1
E	6	ASP	-	expression tag	UNP A0A0T9Z6H1
E	7	ASP	-	expression tag	UNP A0A0T9Z6H1
E	8	LYS	-	expression tag	UNP A0A0T9Z6H1
E	9	PRO	-	expression tag	UNP A0A0T9Z6H1
E	10	ILE	-	expression tag	UNP A0A0T9Z6H1
E	11	CYS	-	expression tag	UNP A0A0T9Z6H1
F	-13	MET	-	initiating methionine	UNP A0A0T9Z6H1
F	-12	LYS	-	expression tag	UNP A0A0T9Z6H1
F	-11	LYS	-	expression tag	UNP A0A0T9Z6H1
F	-10	TRP	-	expression tag	UNP A0A0T9Z6H1
F	-9	SER	-	expression tag	UNP A0A0T9Z6H1
F	-8	HIS	-	expression tag	UNP A0A0T9Z6H1
F	-7	PRO	-	expression tag	UNP A0A0T9Z6H1
F	-6	GLN	-	expression tag	UNP A0A0T9Z6H1
F	-5	PHE	-	expression tag	UNP A0A0T9Z6H1
F	-4	GLU	-	expression tag	UNP A0A0T9Z6H1
F	-3	LYS	-	expression tag	UNP A0A0T9Z6H1
F	-2	GLY	-	expression tag	UNP A0A0T9Z6H1
F	-1	GLY	-	expression tag	UNP A0A0T9Z6H1
F	0	SER	-	expression tag	UNP A0A0T9Z6H1
F	1	ASP	-	expression tag	UNP A0A0T9Z6H1
F	2	TYR	-	expression tag	UNP A0A0T9Z6H1
F	3	LYS	-	expression tag	UNP A0A0T9Z6H1
F	4	ASP	-	expression tag	UNP A0A0T9Z6H1
F	5	ASP	-	expression tag	UNP A0A0T9Z6H1

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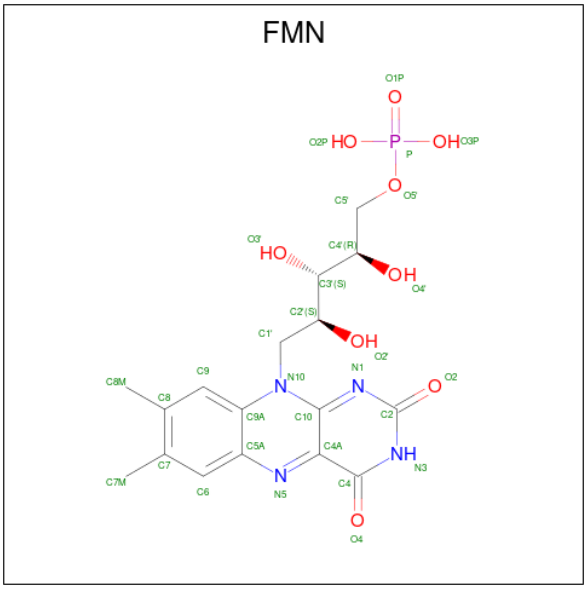
Chain	Residue	Modelled	Actual	Comment	Reference
F	6	ASP	-	expression tag	UNP A0A0T9Z6H1
F	7	ASP	-	expression tag	UNP A0A0T9Z6H1
F	8	LYS	-	expression tag	UNP A0A0T9Z6H1
F	9	PRO	-	expression tag	UNP A0A0T9Z6H1
F	10	ILE	-	expression tag	UNP A0A0T9Z6H1
F	11	CYS	-	expression tag	UNP A0A0T9Z6H1

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



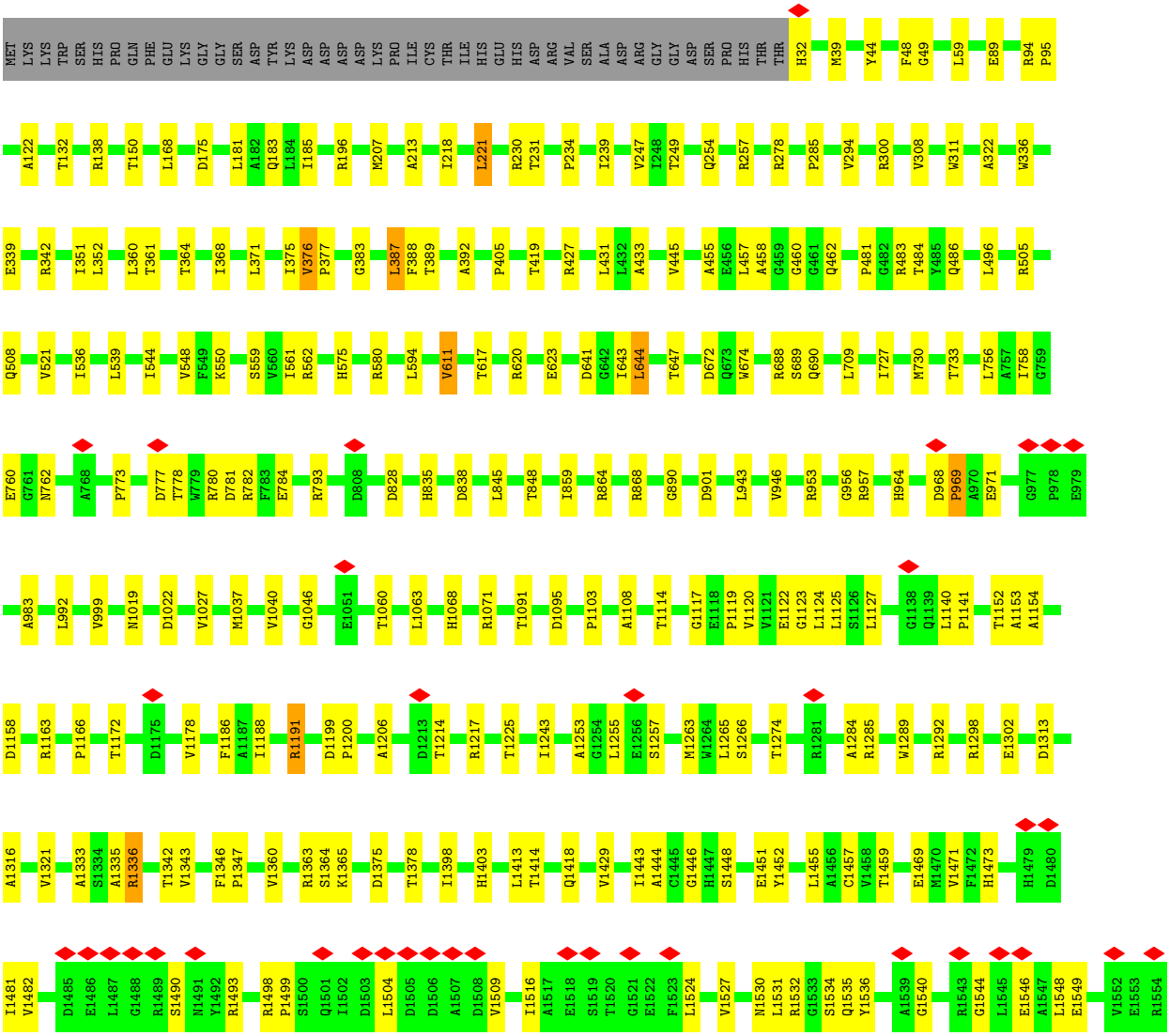
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	C	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	D	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

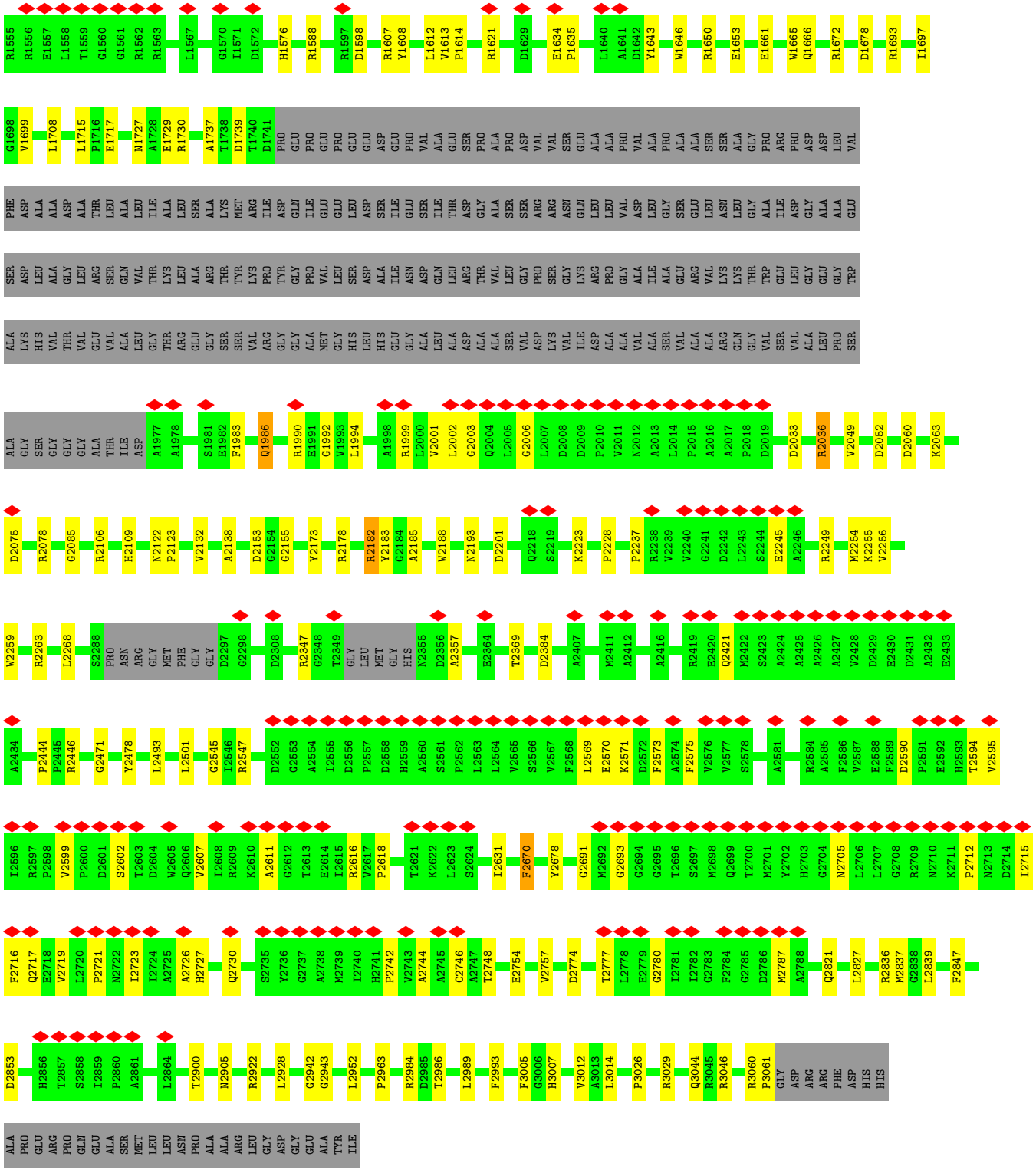
3 Residue-property plots (i)

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

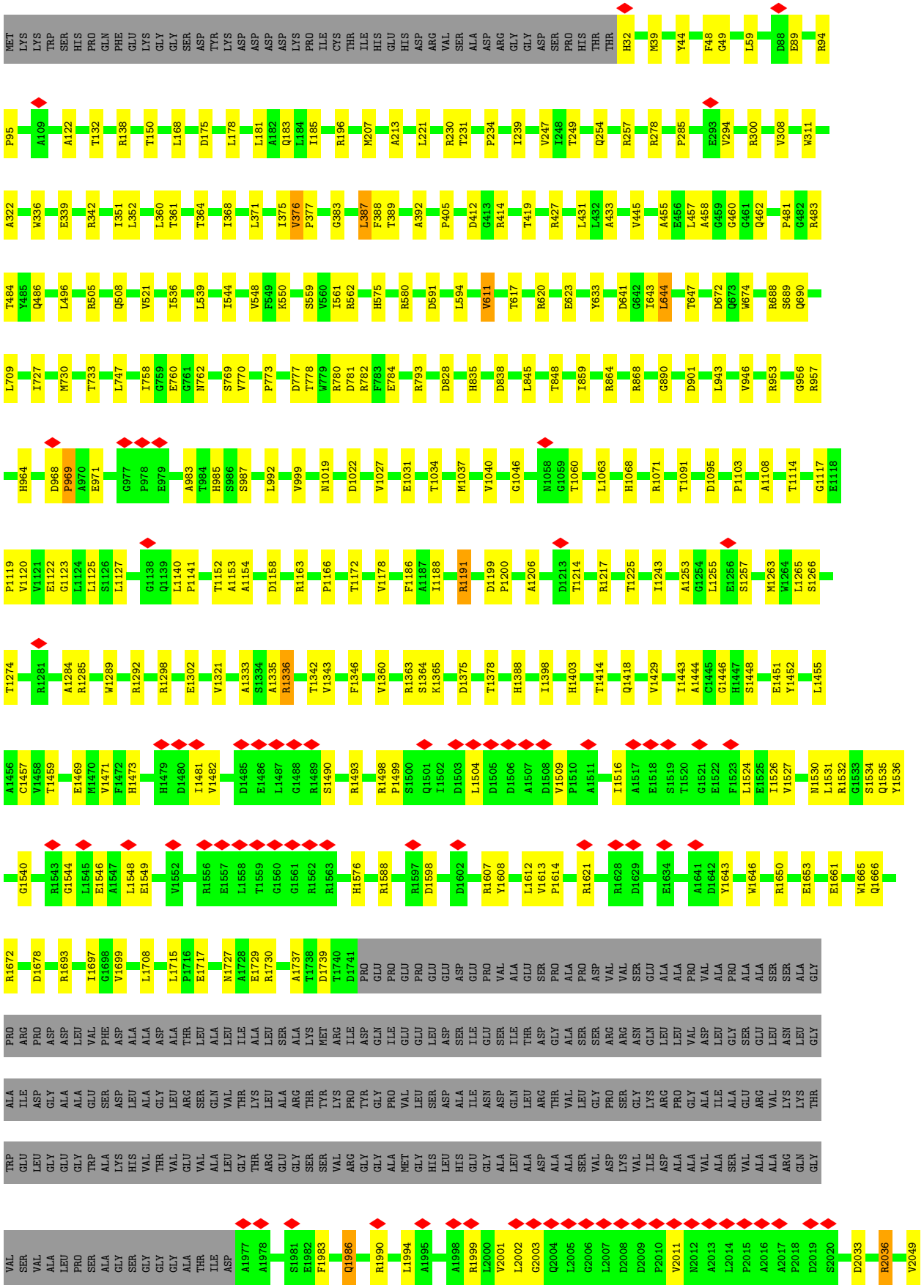
Chain A:

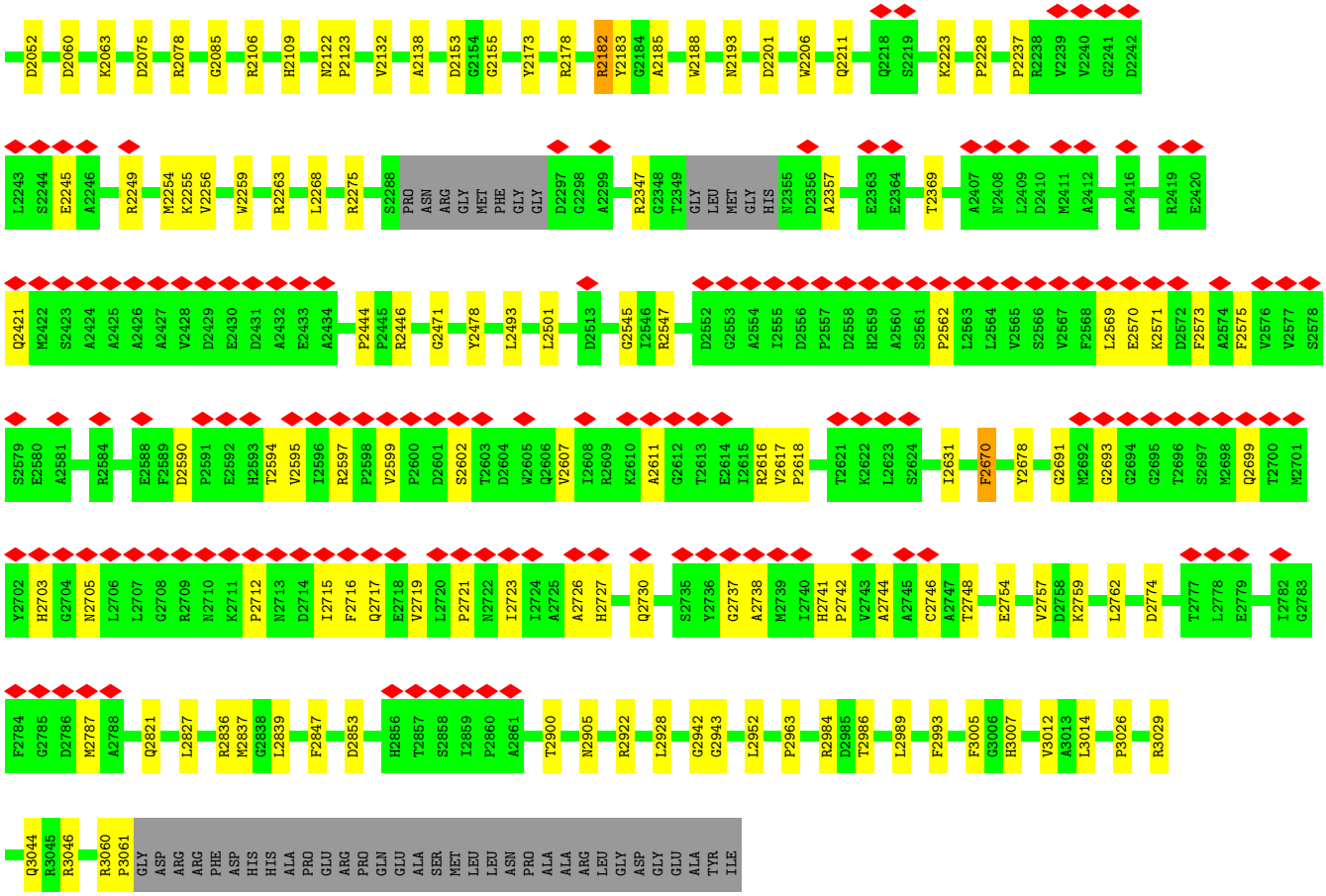




• Molecule 1: Fatty acid synthase

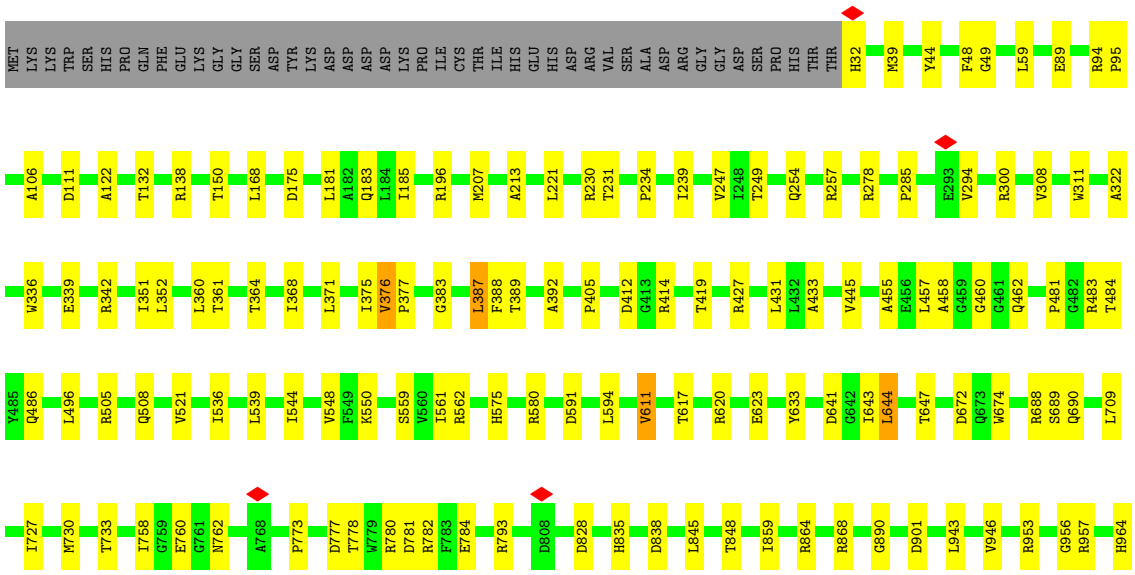
Chain B:

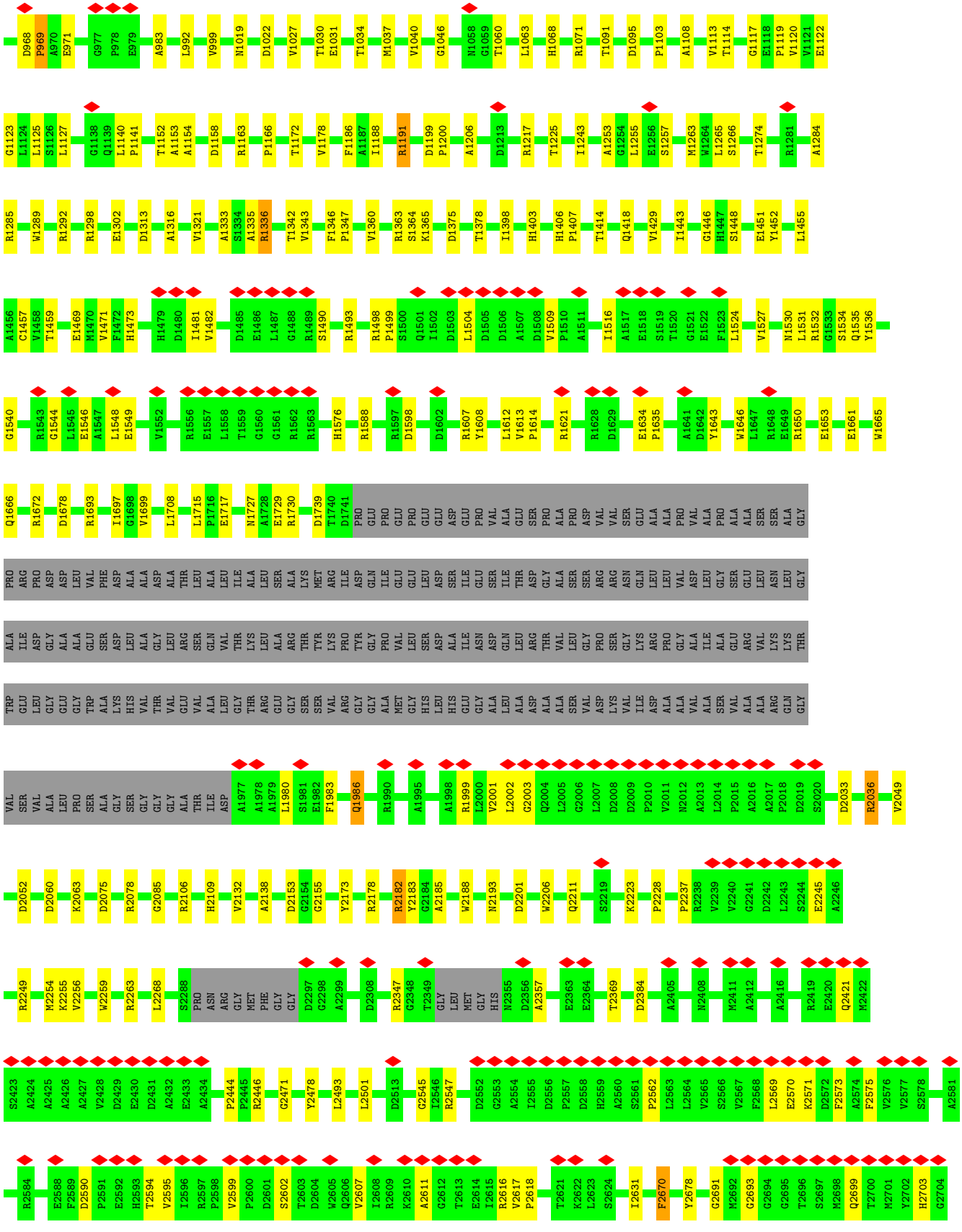

MET LYS LYS TRP SER HIS PRO GLN PHE GLU LYS GLY GLY SER ASP TYR LYS ASP ASP ASP LYS PRO ILE CYS THR ILE HIS GLU HIS ASP ARG VAL SER ALA ASP ARG GLY GLY ASP SER PRO HIS THR THR
H32 M39 Y44 F48 G49 L59 D88 E89 R94
P95 A109 A122 T132 R138 T150 L168 D175 L178 L181 A182 Q183 L184 I185 R196 M207 A213 L221 R230 T231 P234 I239 V247 T248 T249 Q254 R257 R278 P285 E293 V294 R300 V308 W311
A322 W336 E339 R342 I351 L352 L360 T361 T364 I368 L371 I375 V376 P377 G383 L387 F388 T389 A392 P405 D412 G413 R414 T419 R427 L431 L432 A433 V445 A455 E456 L457 A458 G459 G460 G461 Q462 P481 G482 R483
T484 Y485 Q486 L496 R505 Q508 V521 I536 L539 I544 V548 F549 K550 S559 V560 I561 R562 H575 R580 D591 L594 V611 T617 R620 E623 Y633 D641 G642 I643 L644 T647 D672 Q673 W674 R688 S689 Q690
L709 I727 M730 T733 L747 I758 G759 E760 G761 N762 S769 V770 P773 D777 T778 W779 R780 D781 R782 F783 E784 R793 D828 H835 D838 L845 T848 I859 R864 R868 G890 D901 L943 V946 R953 G956 R957
H964 D968 P969 A970 E971 G977 P978 E979 A983 T984 H985 S986 S987 L992 V999 N1019 D1022 V1027 E1031 T1034 M1037 V1040 G1046 N1058 G1059 T1060 L1063 H1068 R1071 T1091 D1095 P1103 A1108 T1114 G1117 E1118
P1119 V1120 V1121 E1122 G1123 L1124 L1125 S1126 L1127 G1138 Q1139 L1140 P1141 T1152 A1153 A1154 D1158 R1163 P1166 T1172 V1178 F1186 A1187 I1188 R1191 D1199 P1200 A1206 D1213 T1214 R1217 T1225 I1243 A1253 G1254 L1255 E1256 S1257 M1263 W1264 L1265 S1266
T1274 R1281 A1284 R1285 W1289 R1292 R1298 E1302 V1321 A1333 S1334 A1335 R1336 T1342 V1343 F1346 V1360 R1363 S1364 K1365 D1375 T1378 H1388 I1398 H1403 T1414 Q1418 V1429 I1443 A1444 C1445 G1446 H1447 S1448 E1451 Y1452 L1455
A1456 C1457 Y1458 T1459 E1469 M1470 V1471 F1472 H1473 H1479 D1480 I1481 V1482 D1485 E1486 L1487 G1488 R1489 S1490 R1493 R1498 P1499 S1500 Q1501 I1502 D1503 L1504 D1505 D1506 A1507 D1508 V1509 P1510 A1511 I1516 A1517 E1518 S1519 T1520 G1521 E1522 F1523 L1524 E1525 I1526 V1527 N1530 L1531 R1532 G1533 S1534 Q1535 Y1536
G1540 R1543 G1544 L1545 E1546 A1547 L1548 E1549 V1552 R1556 E1557 L1558 T1559 G1560 G1561 R1562 R1563 H1576 R1588 R1597 D1598 D1602 R1607 Y1608 L1612 V1613 P1614 R1621 R1628 D1629 E1634 A1641 D1642 Y1643 W1646 R1650 E1653 E1661 W1665 Q1666
R1672 D1678 R1693 I1697 G1698 V1699 L1708 L1715 P1716 E1717 N1727 A1728 E1729 R1730 A1737 T1738 D1739 T1740 D1741 PRO GLU PRO GLU PRO GLU GLU GLU ASP GLU GLU PRO VAL ALA GLU SER PRO ALA PRO ASP VAL VAL SER GLU ALA ALA PRO VAL ALA PRO ALA ALA SER SER ALA GLY
PRO ARG PRO ASP ASP LEU VAL PHE ASP ALA ALA ASP ALA THR LEU ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU GLU LEU ASP SER ILE GLU SER ILE THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU LEU VAL ASP LEU GLY SER GLU LEU ASN LEU GLY
ALA ILE ASP GLY ALA ALA GLU SER ASP LEU ALA ALA GLY LEU ARG SER GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO TYR GLY PRO VAL LEU SER ASP ALA ILE ASN ASP GLY GLN LEU ARG GLY PRO VAL LEU ALA ILE ALA GLU ARG VAL LYS LYS THR
TRP GLU LEU GLY GLU GLY VAL ALA LEU GLY THR ARG GLU GLY SER VAL ARG GLY GLY ALA MET GLY HIS LEU HIS GLU GLY ALA LEU ALA ASP ALA ALA SER VAL ASP LYS VAL ILE ASP ALA ALA VAL ALA SER VAL GLY LYS ARG PRO GLY ALA ILE ILE ALA GLU ARG VAL ALA ARG GLN GLY
VAL SER VAL ALA LEU PRO SER ALA GLY GLY GLY ALA THR ILE ASP A1977 A1978 S1981 E1982 F1983 Q1986 R1990 L1994 A1995 A1998 R1999 L2000 V2001 L2002 G2003 Q2004 L2005 G2006 L2007 D2008 D2009 P2010 V2011 N2012 A2013 L2014 P2015 A2016 A2017 P2018 D2019 S2020 D2033 R2036 V2049



• Molecule 1: Fatty acid synthase

Chain C:

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G1123 L1124 L1125 S1126 L1127 G1138 G1139 L1140 P1141 T1152 A1153 A1154 D1158 R1163 P1166 T1172 V1178 F1186 A1187 I1188 R1191 D1199 P1200 A1206 D1213 R1217 T1225 I1243 A1253 G1254 L1255 E1256 S1257 M1263 W1264 L1265 S1266 T1274 R1281 A1284
R1285 W1289 R1292 R1298 E1302 D1313 A1316 V1321 A1333 S1334 A1335 R1336 T1342 V1343 F1346 P1347 V1360 R1363 S1364 K1365 D1375 T1378 I1398 H1403 H1406 P1407 T1414 Q1418 V1429 I1443 G1446 H1447 S1448 E1451 Y1452 L1455
A1456 C1457 V1458 T1459 E1469 M1470 V1471 F1472 H1473 H1479 D1480 I1481 V1482 D1485 E1486 L1487 G1488 R1489 S1490 R1493 R1498 P1499 S1500 Q1501 I1502 D1503 L1504 D1505 D1506 A1507 D1508 V1509 P1510 A1511 I1516 A1517 E1518 S1519 T1520 G1521 E1522 F1523 L1524 V1527 N1530 L1531 R1532 G1533 S1534 Q1535 Y1536
G1540 R1543 G1544 L1545 E1546 A1547 L1548 E1549 V1552 R1556 E1557 L1558 T1559 G1560 G1561 R1562 R1563 H1576 R1588 R1597 D1598 D1602 R1607 Y1608 L1612 V1613 P1614 R1621 R1628 D1629 E1634 P1635 A1641 D1642 Y1643 W1646 L1647 R1648 E1649 R1650 E1653 E1661 W1665
Q1666 R1672 D1678 R1693 I1697 G1698 V1699 L1708 L1715 P1716 E1717 N1727 A1728 E1729 R1730 D1739 T1740 D1741 PRO GLU PRO GLU PRO GLU GLU ASP PRO VAL ALA GLU SER PRO ALA PRO ASP VAL VAL SER GLU ALA ALA PRO VAL ALA PRO ALA ALA SER SER ALA GLY
PRO ARG PRO ASP ASP LEU VAL PHE ASP ALA ALA ASP ALA THR LEU ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU GLU LEU ASP SER ILE GLU SER ILE THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU LEU VAL ASP LEU GLY SER GLU LEU ASN LEU GLY
ALA ILE ASP GLY ALA ALA GLU SER ASP LEU ALA GLY LEU ARG SER GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO TYR GLY PRO VAL LEU SER ASP ALA ILE ASN ASP GLN LEU ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO GLY ALA LEU ALA GLU ARG VAL LYS LYS THR
TRP GLU LEU GLY GLU GLY TRP ALA LYS HIS VAL THR VAL GLU VAL ALA LEU GLY THR ARG GLU GLY SER SER VAL ARG GLY GLY ALA MET GLY HIS LEU HIS GLU GLY GLY ALA LEU ALA ASP ALA ALA SER VAL ALA ASP LYS VAL ILE ASP ALA ALA ALA LEU LEU ALA SER VAL ALA ARG GLN GLY
VAL SER VAL ALA LEU PRO SER ALA GLY SER GLY GLY GLY ALA THR ILE ASP A1977 A1978 A1979 L1980 S1981 E1982 F1983 Q1986 R1990 A1995 A1998 R1999 L2000 V2001 L2002 G2003 Q2004 L2005 G2006 L2007 D2008 D2009 P2010 V2011 N2012 A2013 L2014 P2015 A2016 A2017 P2018 D2019 S2020 D2033 R2036 V2049
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S2423 A2424 A2425 A2426 A2427 V2428 D2429 E2430 D2431 A2432 E2433 A2434 P2444 P2445 R2446 G2471 Y2478 L2493 L2501 D2513 G2545 I2546 R2547 D2552 G2553 A2554 I2555 D2556 P2557 D2558 H2559 A2560 S2561 P2562 L2563 L2564 V2565 S2566 V2567 F2568 L2569 E2570 K2571 D2572 F2573 A2574 F2575 V2576 V2577 S2578 A2581
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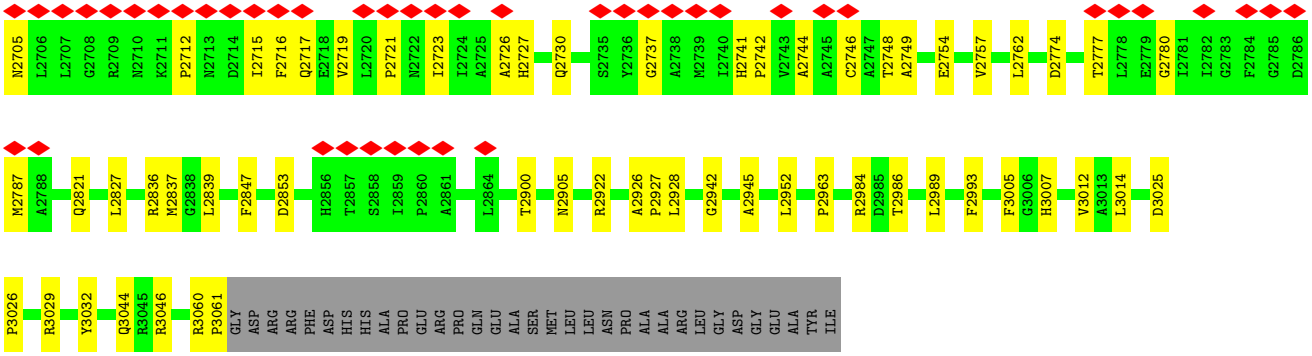
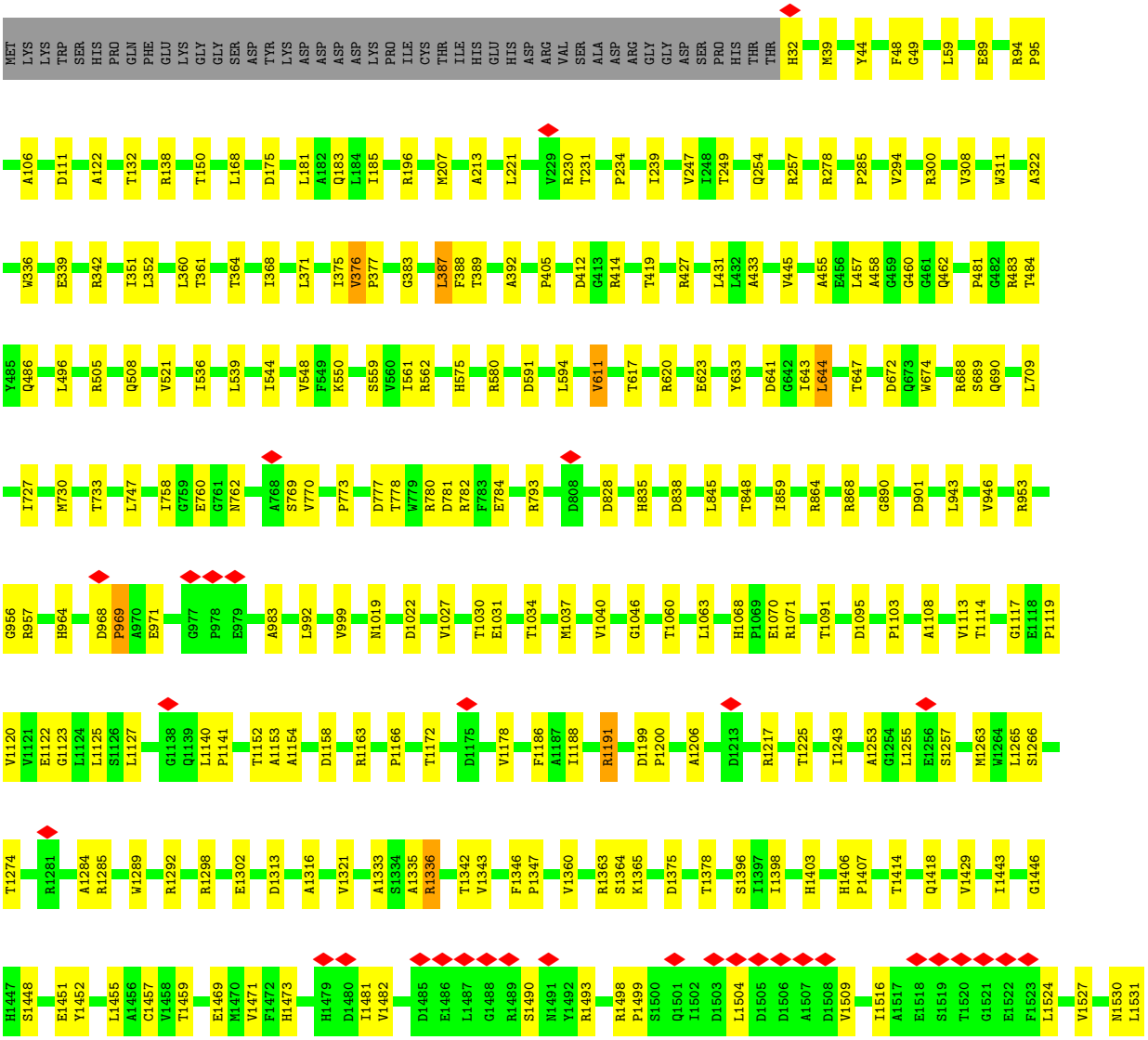
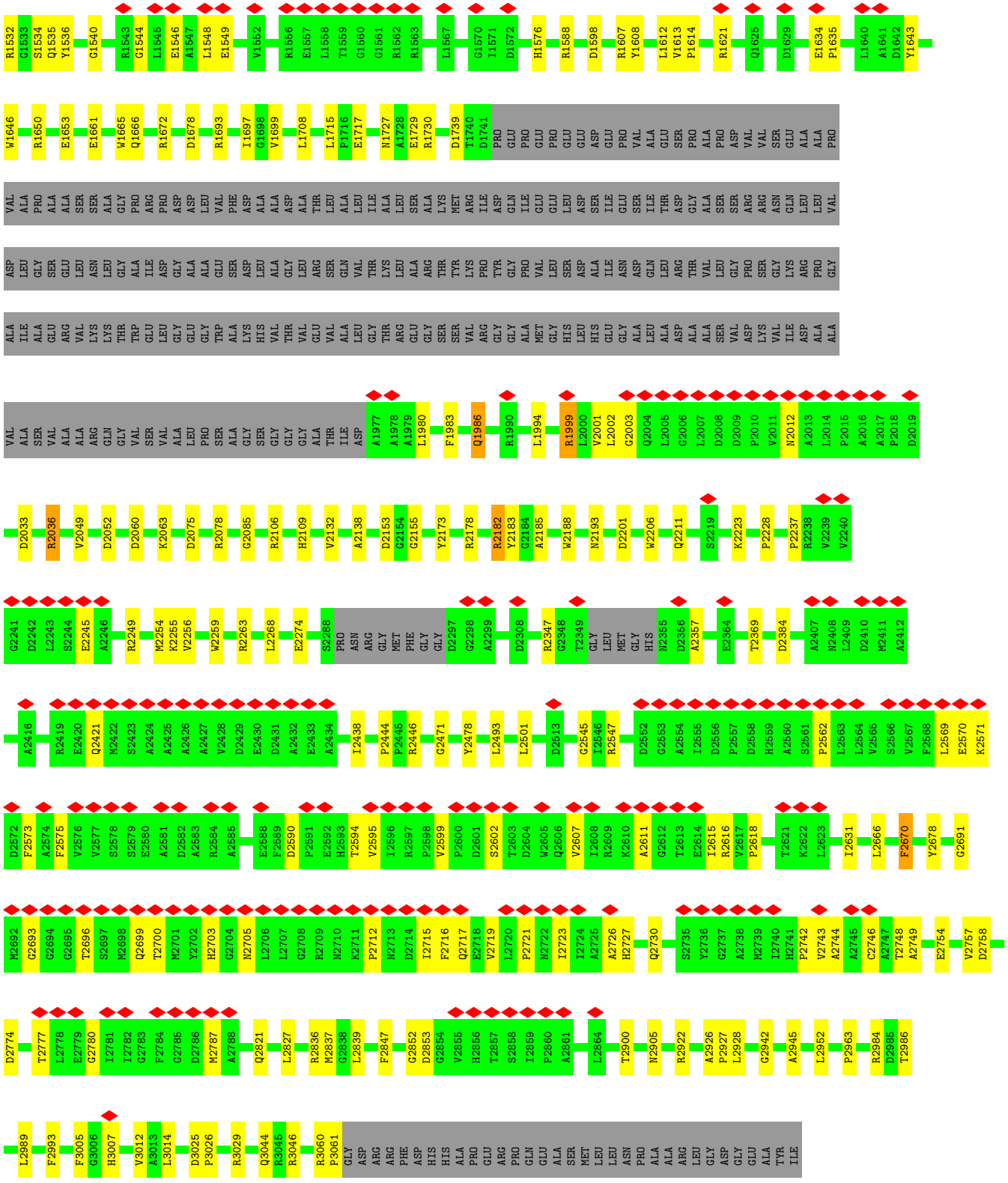


- Molecule 1: Fatty acid synthase

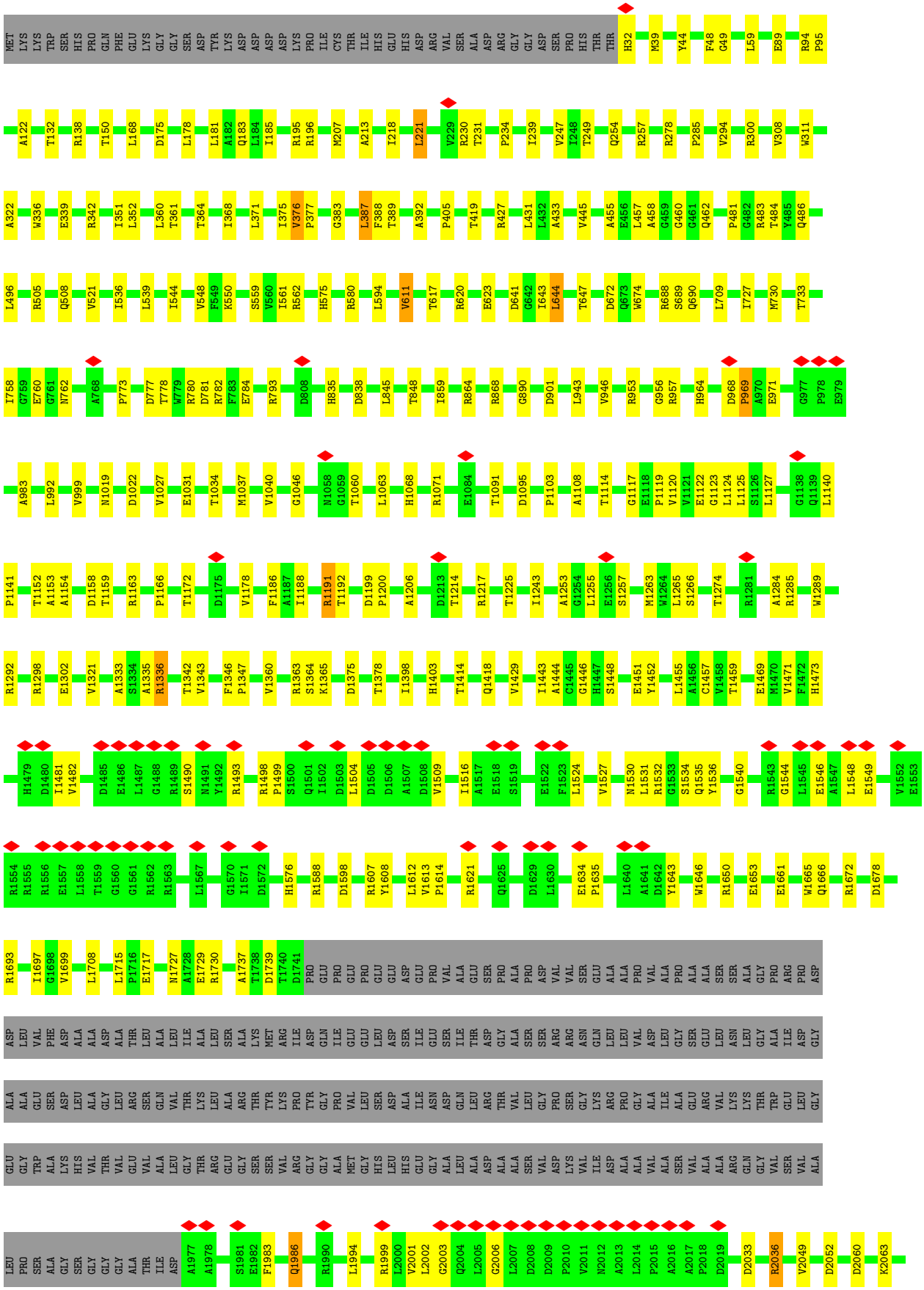
Chain D:





• Molecule 1: Fatty acid synthase

Chain E: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H32 M39 Y44 F48 G49 L59 E89 R94 P95
A122 T132 R138 T150 L168 D175 L178 L181 A182 Q183 L184 I185 R195 R196 M207 A213 I218 L221 V229 R230 T231 P234 I239 V247 I248 T249 Q254 R257 R278 P285 V294 R300 V308 W311
A322 W336 E339 R342 I351 L352 L360 T361 T364 I368 L371 I375 V376 P377 G383 L387 F388 T389 A392 P405 T419 R427 L431 L432 A433 V445 A455 E456 L457 A458 G459 G460 G461 Q462 P481 G482 R483 T484 Y485 Q486
L496 R505 Q508 V521 I536 L539 I544 V548 F549 K550 S559 V560 I561 R562 H575 R580 L594 V611 T617 R620 E623 D641 G642 I643 L644 T647 D672 Q673 W674 R688 S689 Q690 L709 I727 M730 T733
I758 G759 E760 G761 N762 A768 P773 D777 T778 W779 R780 D781 R782 F783 E784 R793 D808 H835 D838 L845 T848 I859 R864 R868 G890 D901 L943 V946 R953 G956 R957 H964 D968 P969 A970 E971 G977 P978 E979
A983 L992 V999 N1019 D1022 V1027 E1031 T1034 M1037 V1040 G1046 N1058 G1059 T1060 L1063 H1068 R1071 E1084 T1091 D1095 P1103 A1108 T1114 G1117 E1118 P1119 V1120 V1121 E1122 G1123 L1124 L1125 S1126 L1127 G1138 Q1139 L1140
P1141 T1152 A1153 A1154 D1158 T1159 R1163 P1166 T1172 D1175 V1178 F1186 A1187 I1188 R1191 T1192 D1199 P1200 A1206 D1213 T1214 R1217 T1225 I1243 A1253 G1254 L1255 E1256 S1257 M1263 W1264 L1265 S1266 T1274 R1281 A1284 R1285 W1289
R1292 R1298 E1302 V1321 A1333 S1334 A1335 R1336 T1342 V1343 F1346 P1347 V1360 R1363 S1364 K1365 D1375 T1378 I1398 H1403 T1414 Q1418 V1429 I1443 A1444 C1445 G1446 H1447 S1448 E1451 Y1452 L1455 A1456 C1457 V1458 T1459 E1469 M1470 V1471 F1472 H1473
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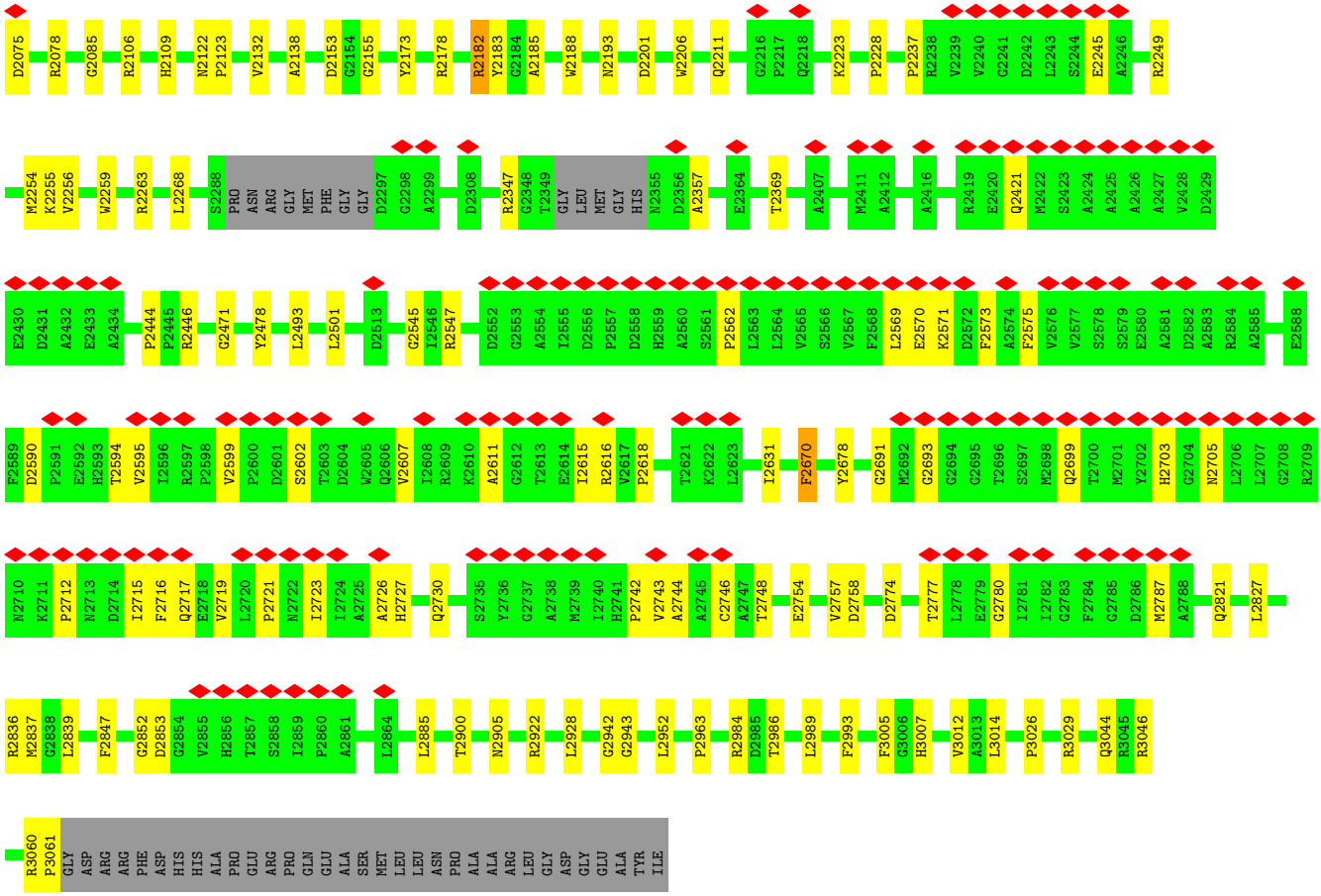
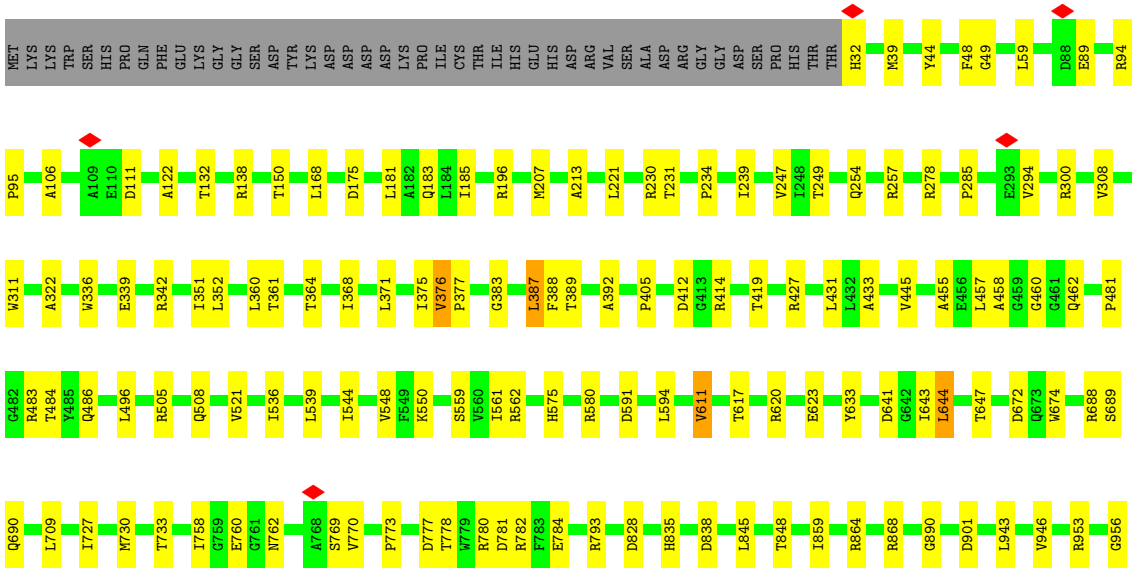
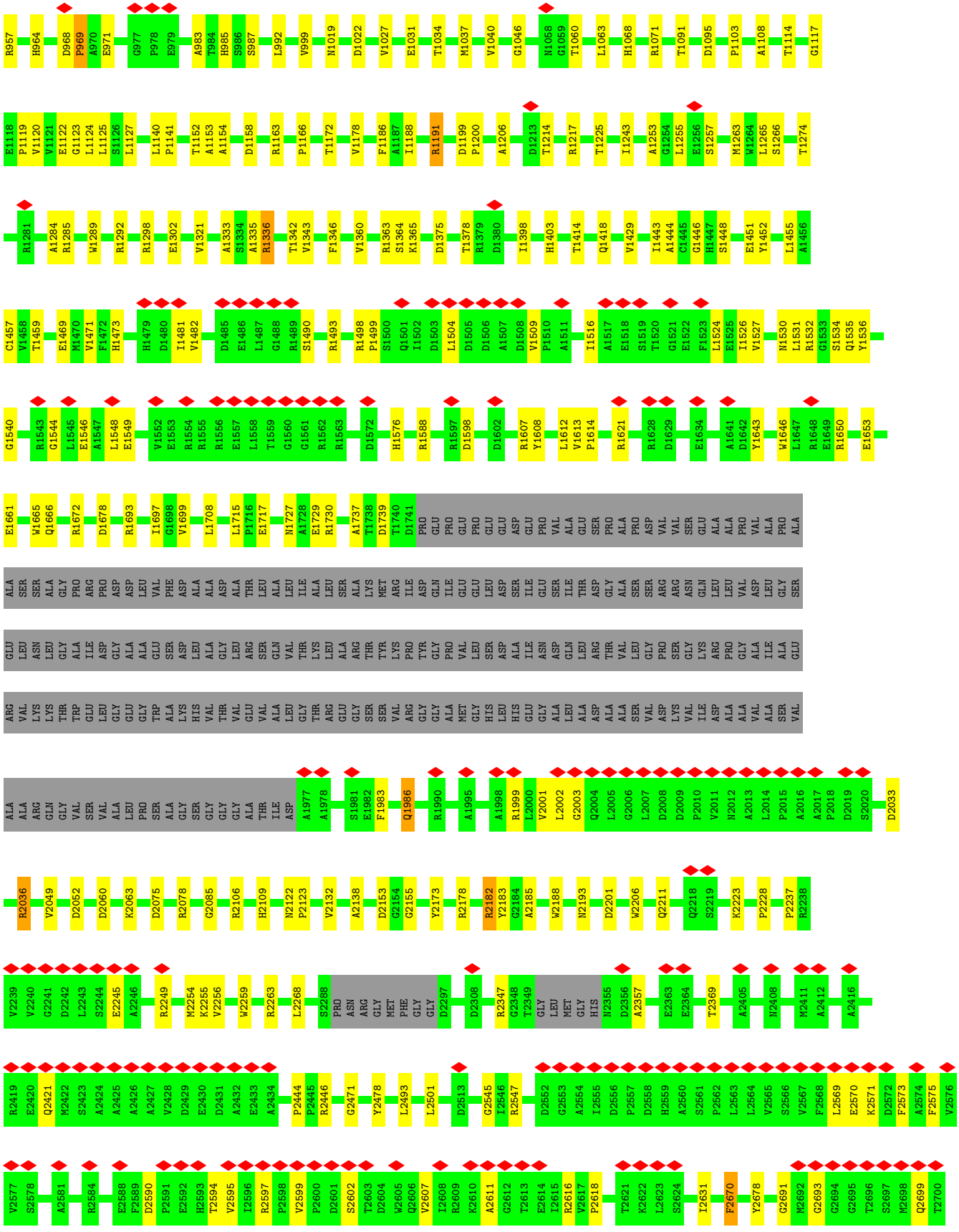
R1554 R1555 R1556 E1557 L1558 T1559 G1560 G1561 R1562 R1563 L1567 G1570 I1571 D1572 H1576 R1588 D1598 R1607 Y1608 L1612 V1613 P1614 R1621 Q1625 D1629 L1630 E1634 P1635 L1640 A1641 D1642 Y1643 W1646 R1650 E1653 E1661 W1665 Q1666 R1672 D1678
R1693 I1697 G1698 V1699 L1708 L1715 P1716 E1717 N1727 A1728 E1729 R1730 A1737 T1738 D1739 T1740 D1741 PRO GLU PRO GLU PRO GLU GLU ASP GLU PRO VAL ALA GLU SER PRO ALA PRO ASP VAL VAL SER GLU ALA ALA PRO VAL ALA PRO ALA ALA SER SER ALA GLY PRO ASP
ASP LEU VAL PHE ASP ALA ALA ASP ALA THR LEU ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU GLU LEU ASP SER ILE GLU SER ILE THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU VAL ASP LEU GLY SER GLU LEU ASN LEU GLY ALA ILE ASP GLY
ALA ALA GLU SER ASP LEU ALA ALA GLY LEU ARG SER GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO TYR GLY PRO VAL LEU SER ASP ALA ILE ASN ASP GLN LEU ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO GLY GLY ALA GLU ARG VAL LYS LYS THR TRP GLU LEU GLY
GLU GLY TRP ALA LYS HIS VAL THR VAL GLU VAL ALA LEU GLY THR ARG GLU GLY SER SER VAL ARG GLY GLY ALA MET GLY HIS LEU HIS GLU GLY ALA LEU ALA ASP ALA ALA SER VAL ASP LYS VAL ILE ASP ALA ALA ALA VAL ALA ALA SER VAL GLN GLY VAL ALA VAL
LEU PRO SER ALA GLY SER GLY GLY GLY ALA THR ILE ASP
A1977 A1978 S1981 E1982 F1983 Q1986 R1990 L1994 R1999 L2000 V2001 L2002 G2003 Q2004 L2005 G2006 L2007 D2008 D2009 P2010 V2011 N2012 A2013 L2014 P2015 A2016 A2017 P2018 D2019 D2033 R2036 V2049 D2052 D2060 K2063



• Molecule 1: Fatty acid synthase

Chain F:

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E1118 P1119 V1120 V1121 E1122 G1123 L1124 L1125 S1126 L1127 L1140 P1141 T1152 A1153 A1154 D1158 R1163 P1166 T1172 V1178 F1186 A1187 I1188 R1191 D1199 P1200 A1206 D1213 T1214 R1217 T1225 I1243 A1253 G1254 L1255 E1256 S1257 M1263 W1264 L1265 S1266 T1274
R1281 A1284 R1285 W1289 R1292 R1298 E1302 V1321 A1333 S1334 A1335 R1336 T1342 V1343 F1346 V1360 R1363 S1364 K1365 D1375 T1378 R1379 D1380 I1398 H1403 T1414 Q1418 V1429 I1443 A1444 C1445 G1446 H1447 S1448 E1451 Y1452 L1455 A1456
C1457 V1458 T1459 E1469 M1470 V1471 F1472 H1473 H1479 D1480 I1481 V1482 D1485 E1486 L1487 G1488 R1489 S1490 R1493 R1498 P1499 S1500 Q1501 I1502 D1503 L1504 D1505 D1506 A1507 D1508 V1509 P1510 A1511 I1516 A1517 E1518 S1519 T1520 G1521 E1522 F1523 L1524 E1525 I1526 V1527 N1530 L1531 R1532 G1533 S1534 Q1535 Y1536
G1540 R1543 G1544 L1545 E1546 A1547 L1548 E1549 V1552 E1553 R1554 R1555 R1556 E1557 L1558 T1559 G1560 G1561 R1562 R1563 D1572 H1576 R1588 R1597 D1598 D1602 R1607 Y1608 L1612 V1613 P1614 R1621 R1628 D1629 E1634 A1641 D1642 Y1643 W1646 L1647 R1648 E1649 R1650 E1653
E1661 W1665 Q1666 R1672 D1678 R1693 I1697 G1698 V1699 L1708 L1715 P1716 E1717 N1727 A1728 E1729 R1730 A1737 T1738 D1739 T1740 D1741 PRO GLU PRO GLU PRO GLU GLU ASP GLU PRO VAL ALA GLU SER PRO ALA PRO ASP VAL VAL SER GLU ALA ALA PRO VAL ALA
ALA SER SER ALA GLY PRO ARG PRO ASP ASP LEU VAL LEU PHE ASP ALA ALA ASP ALA THR LEU ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU GLU LEU ASP SER ILE GLU SER ILE THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU VAL ASP LEU GLY SER
GLU LEU ASN LEU GLY ALA ILE ASP GLY ALA ALA GLU SER ASP LEU ALA GLY LEU ARG SER GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO TYR GLY PRO VAL LEU LEU SER ASP ALA ILE ASN ASP GLN LEU ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO GLY ALA ILE ALA GLU
ARG VAL LYS LYS THR TRP GLU LEU GLY GLU GLY TRP ALA LYS HIS VAL THR VAL GLU VAL ALA LEU GLY THR ARG GLU GLY SER VAL ARG GLY GLY HIS LEU HIS GLU GLY GLY ALA LEU ALA ASP ALA ALA SER VAL ASP LYS VAL ILE ASP ALA ALA VAL ALA ALA SER VAL
ALA ALA ARG GLN GLY VAL SER VAL ALA LEU PRO SER ALA GLY SER GLY GLY GLY ALA THR ILE ASP A1977 A1978 S1981 E1982 F1983 Q1986 R1990 A1995 A1998 R1999 L2000 V2001 L2002 G2003 Q2004 L2005 G2006 L2007 D2008 D2009 P2010 V2011 N2012 A2013 L2014 P2015 A2016 A2017 P2018 D2019 S2020 D2033
R2036 V2049 D2052 D2060 K2063 D2075 R2078 G2085 R2106 H2109 N2122 P2123 V2132 A2138 D2153 G2154 G2155 Y2173 R2178 R2182 Y2183 G2184 A2185 W2188 N2193 D2201 W2206 Q2211 Q2218 S2219 K2223 P2228 P2237 R2238
V2239 V2240 G2241 D2242 L2243 S2244 E2245 A2246 R2249 M2254 K2255 V2256 W2259 R2263 L2268 S2288 PRO ASN ARG GLY MET PHE GLY GLY D2297 D2308 R2347 G2348 T2349 GLY LEU MET GLY HIS N2355 D2356 A2357 E2363 E2364 T2369 A2405 N2408 M2411 A2412 A2416
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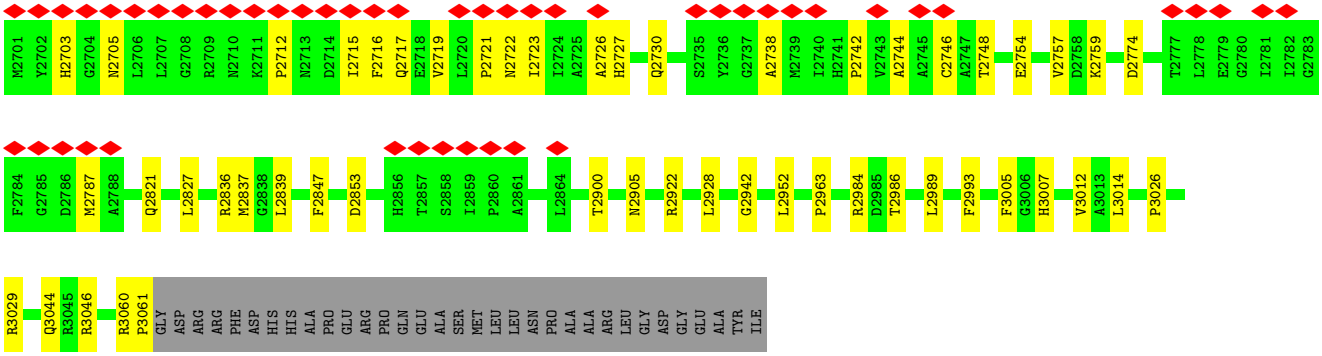
V2577 S2578 A2581 R2584 E2588 F2589 D2590 P2591 E2592 H2593 T2594 V2595 I2596 R2597 P2598 V2599 P2600 D2601 S2602 T2603 D2604 W2605 Q2606 V2607 I2608 R2609 K2610 A2611 G2612 T2613 E2614 I2615 R2616 V2617 P2618 T2621 K2622 L2623 S2624 I2631 F2670 Y2678 G2691 M2692 G2693 G2694 G2695 T2696 S2697 M2698 Q2699 T2700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F2784 G2785 D2786 M2787 A2788 Q2821 L2827 R2836 M2837 G2838 L2839 F2847 D2853 H2856 T2857 S2858 I2859 P2860 A2861 L2864 T2900 N2905 R2922 L2928 G2942 L2952 P2963 R2984 D2985 T2986 L2989 F2993 F3005 G3006 H3007 V3012 A3013 L3014 P3026
R3029 Q3044 R3045 R3046 R3060 P3061 GLY ASP ARG ARG PHE ASP HIS HIS ALA PRO GLU ARG PRO GLN GLU ALA SER MET LEU LEU ASN PRO ALA ALA ARG LEU GLY ASP GLY GLU ALA TYR ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	40160	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 ($e^-/Å^2$)	4.49	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	421.6, 421.6, 421.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/21223	0.62	7/28935 (0.0%)
1	B	0.39	0/21223	0.62	8/28935 (0.0%)
1	C	0.39	0/21223	0.62	7/28935 (0.0%)
1	D	0.39	0/21223	0.62	8/28935 (0.0%)
1	E	0.39	0/21223	0.62	7/28935 (0.0%)
1	F	0.39	0/21223	0.62	7/28935 (0.0%)
All	All	0.39	0/127338	0.62	44/173610 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	7
1	C	0	7
1	D	0	7
1	E	0	7
1	F	0	7
All	All	0	43

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2002	LEU	CA-CB-CG	6.40	130.01	115.30
1	D	2002	LEU	CA-CB-CG	6.38	129.98	115.30
1	C	2002	LEU	CA-CB-CG	6.37	129.96	115.30
1	E	2002	LEU	CA-CB-CG	6.37	129.96	115.30

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2002	LEU	CA-CB-CG	6.35	129.91	115.30

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1046	GLY	Peptide
1	A	1120	VAL	Peptide
1	A	1413	LEU	Peptide
1	A	848	THR	Peptide
1	A	969	PRO	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	20801	0	20660	223	0
1	B	20801	0	20660	233	0
1	C	20801	0	20660	231	0
1	D	20801	0	20660	243	0
1	E	20801	0	20660	230	0
1	F	20801	0	20660	221	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	1	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	0	0
All	All	124992	0	124074	1346	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 5.

The worst 5 of 1346 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:2228:PRO:HG3	1:A:2268:LEU:HD12	1.69	0.74
1:E:2228:PRO:HG3	1:E:2268:LEU:HD12	1.69	0.74
1:D:2228:PRO:HG3	1:D:2268:LEU:HD12	1.69	0.74
1:C:2228:PRO:HG3	1:C:2268:LEU:HD12	1.69	0.74
1:B:2715:ILE:O	1:B:2719:VAL:HB	1.88	0.74

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	2762/3092 (89%)	2555 (92%)	207 (8%)	0	100	100
1	B	2762/3092 (89%)	2556 (92%)	206 (8%)	0	100	100
1	C	2762/3092 (89%)	2555 (92%)	207 (8%)	0	100	100
1	D	2762/3092 (89%)	2556 (92%)	206 (8%)	0	100	100
1	E	2762/3092 (89%)	2557 (93%)	205 (7%)	0	100	100
1	F	2762/3092 (89%)	2556 (92%)	206 (8%)	0	100	100
All	All	16572/18552 (89%)	15335 (92%)	1237 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	2135/2381 (90%)	2120 (99%)	15 (1%)	84	90
1	B	2135/2381 (90%)	2120 (99%)	15 (1%)	84	90
1	C	2135/2381 (90%)	2120 (99%)	15 (1%)	84	90
1	D	2135/2381 (90%)	2120 (99%)	15 (1%)	84	90
1	E	2135/2381 (90%)	2120 (99%)	15 (1%)	84	90
1	F	2135/2381 (90%)	2120 (99%)	15 (1%)	84	90
All	All	12810/14286 (90%)	12720 (99%)	90 (1%)	84	90

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2193	ASN
1	E	2178	ARG
1	D	3046	ARG
1	E	1191	ARG
1	F	221	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2180	HIS
1	E	2109	HIS
1	D	2593	HIS
1	E	297	HIS
1	E	2680	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	FMN	D	3101	-	33,33,33	1.17	3 (9%)	48,50,50	1.34	7 (14%)
2	FMN	F	3101	-	33,33,33	1.19	3 (9%)	48,50,50	1.34	6 (12%)
2	FMN	C	3101	-	33,33,33	1.20	4 (12%)	48,50,50	1.36	7 (14%)
2	FMN	B	3101	-	33,33,33	1.21	3 (9%)	48,50,50	1.36	8 (16%)
2	FMN	A	3101	-	33,33,33	1.19	3 (9%)	48,50,50	1.31	7 (14%)
2	FMN	E	3101	-	33,33,33	1.19	2 (6%)	48,50,50	1.34	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
2	FMN	D	3101	-	-	1/18/18/18	0/3/3/3
2	FMN	F	3101	-	-	1/18/18/18	0/3/3/3
2	FMN	C	3101	-	-	2/18/18/18	0/3/3/3
2	FMN	B	3101	-	-	2/18/18/18	0/3/3/3
2	FMN	A	3101	-	-	2/18/18/18	0/3/3/3
2	FMN	E	3101	-	-	1/18/18/18	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3101	FMN	C4A-N5	3.42	1.37	1.30
2	F	3101	FMN	C4A-N5	3.36	1.37	1.30
2	E	3101	FMN	C4A-N5	3.32	1.37	1.30
2	C	3101	FMN	C4A-N5	3.31	1.37	1.30
2	D	3101	FMN	C4A-N5	3.24	1.37	1.30

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3101	FMN	C4-N3-C2	-3.80	118.62	125.64
2	B	3101	FMN	C4-N3-C2	-3.79	118.63	125.64
2	D	3101	FMN	C4-N3-C2	-3.77	118.67	125.64
2	A	3101	FMN	C4-N3-C2	-3.76	118.70	125.64
2	F	3101	FMN	C4-N3-C2	-3.74	118.73	125.64

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3101	FMN	C4'-C5'-O5'-P
2	E	3101	FMN	C4'-C5'-O5'-P
2	A	3101	FMN	C4'-C5'-O5'-P
2	F	3101	FMN	C4'-C5'-O5'-P
2	C	3101	FMN	C4'-C5'-O5'-P

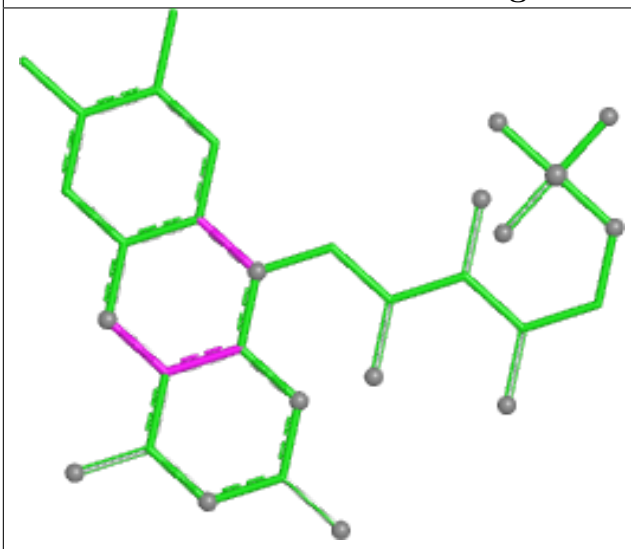
There are no ring outliers.

1 monomer is involved in 1 short contact:

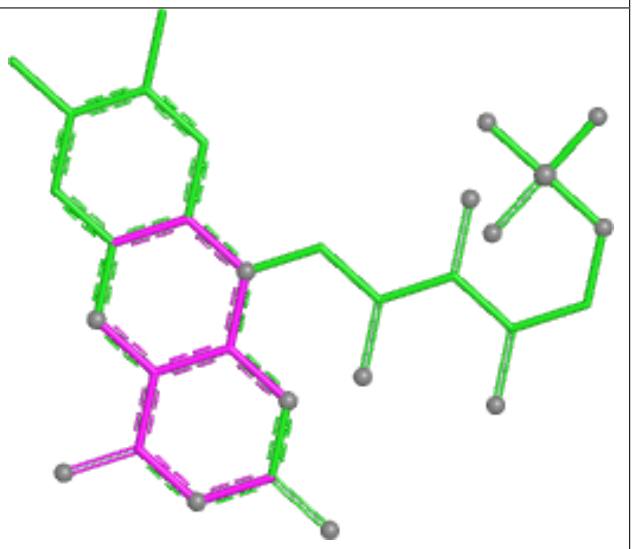
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3101	FMN	1	0

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.

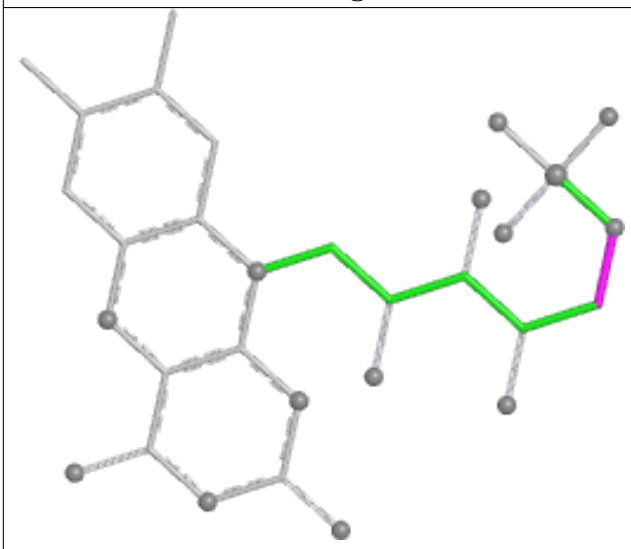
Ligand FMN D 3101



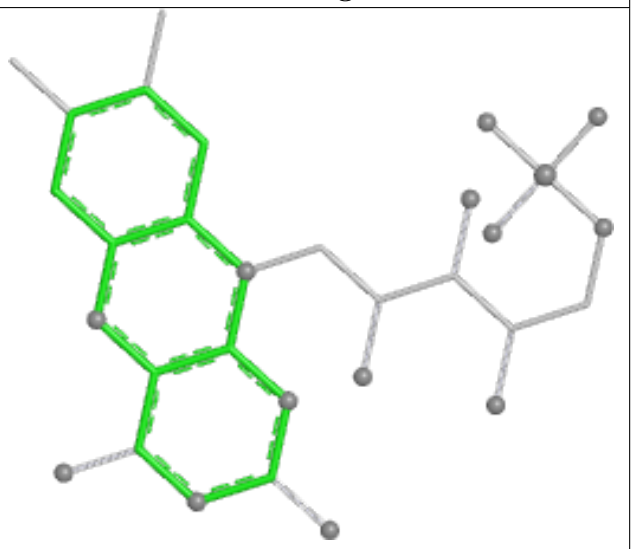
Bond lengths



Bond angles

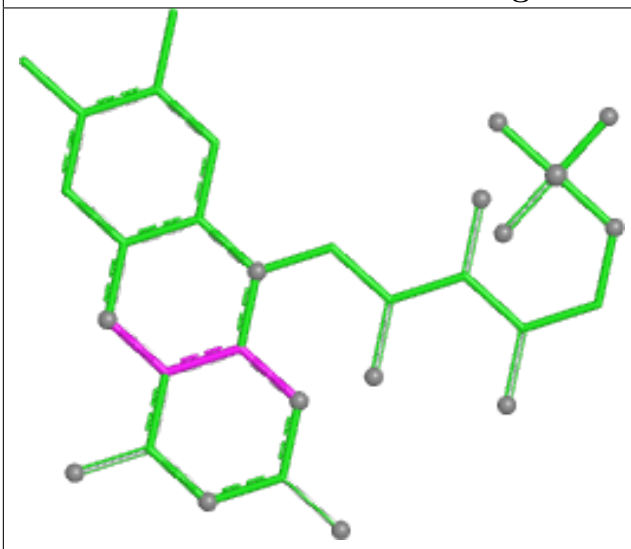


Torsions

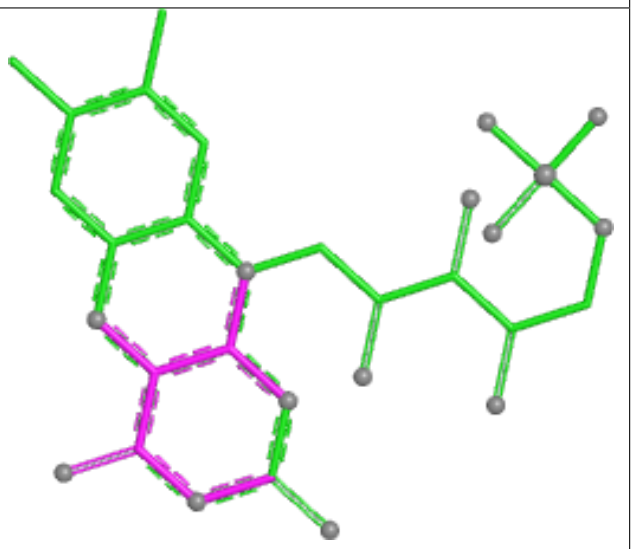


Rings

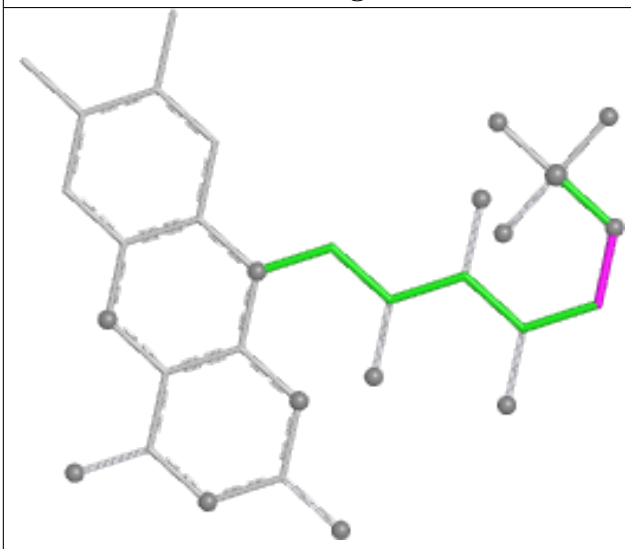
Ligand FMN F 3101



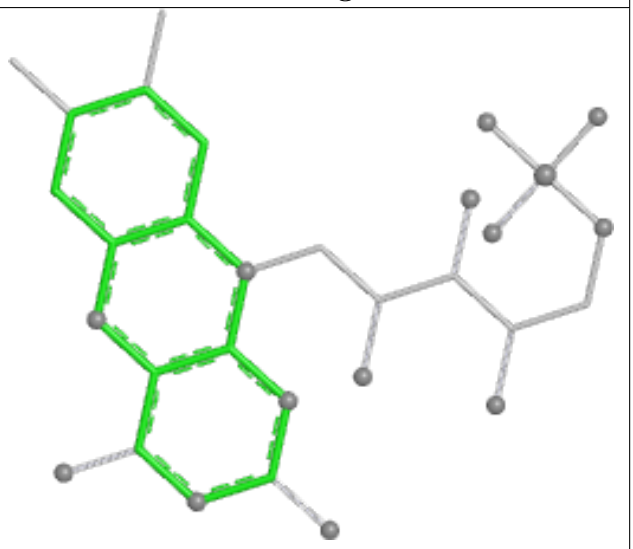
Bond lengths



Bond angles

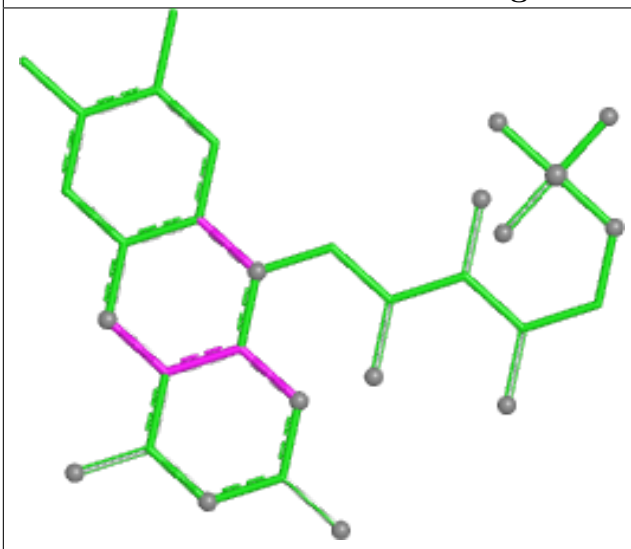


Torsions

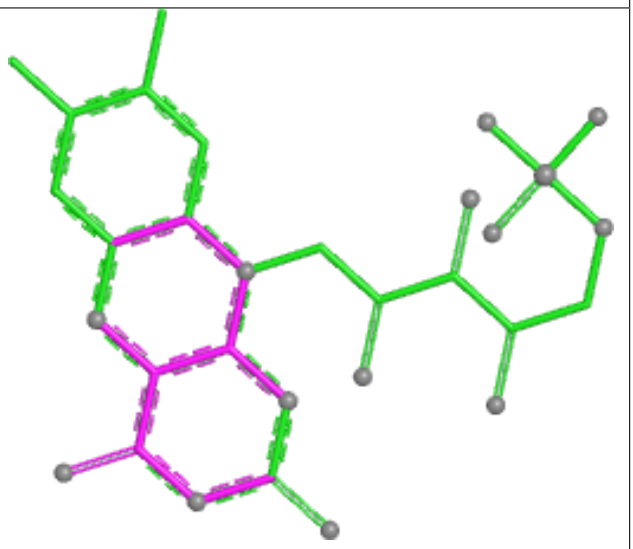


Rings

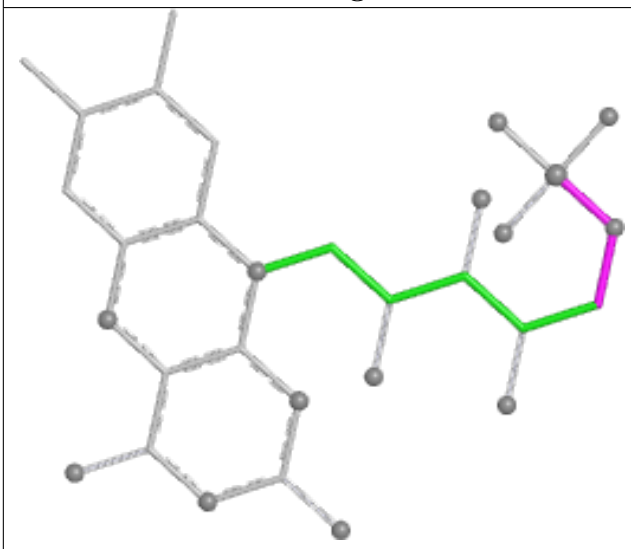
Ligand FMN C 3101



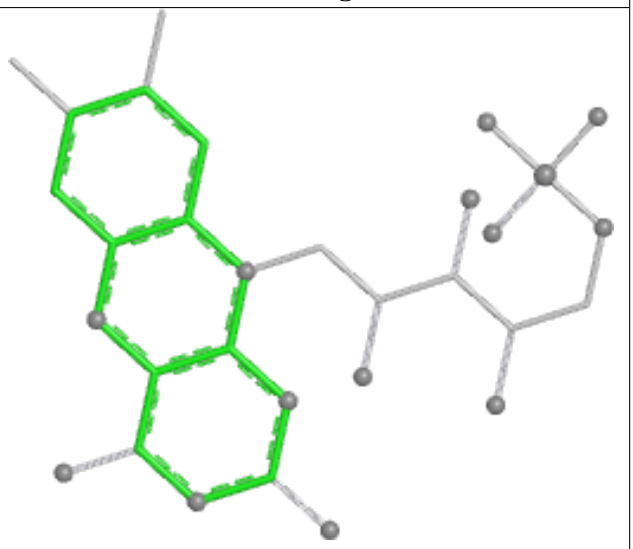
Bond lengths



Bond angles

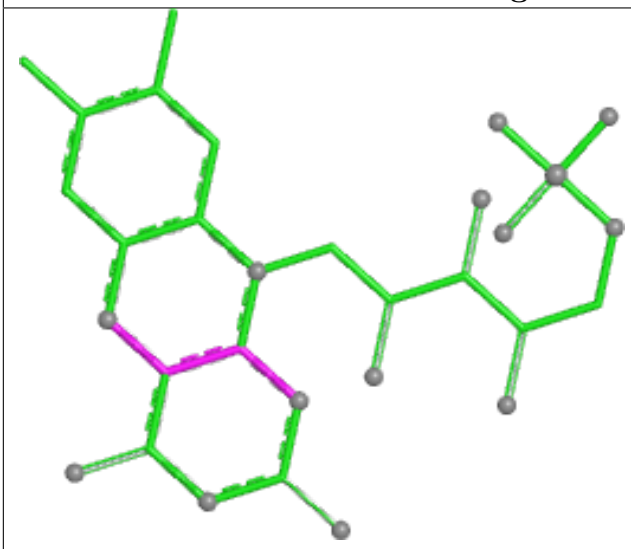


Torsions

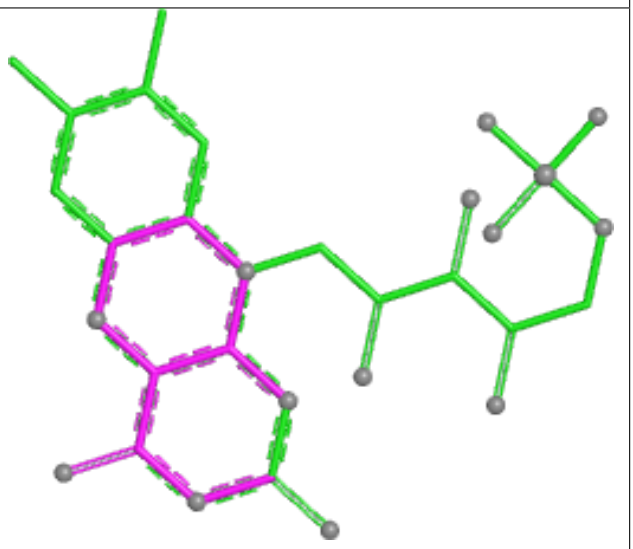


Rings

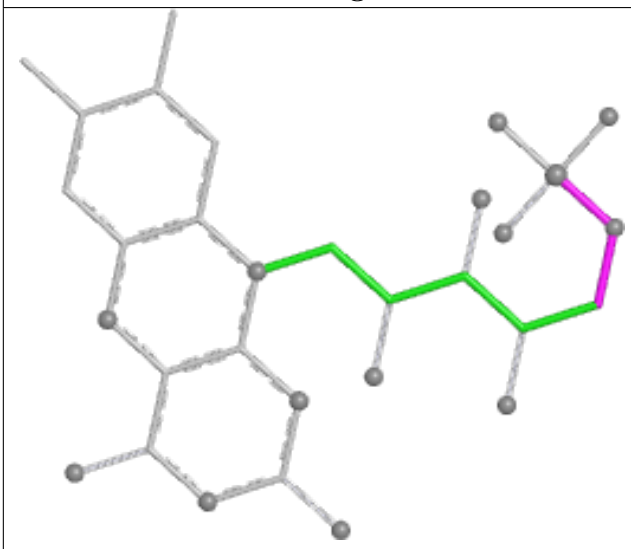
Ligand FMN B 3101



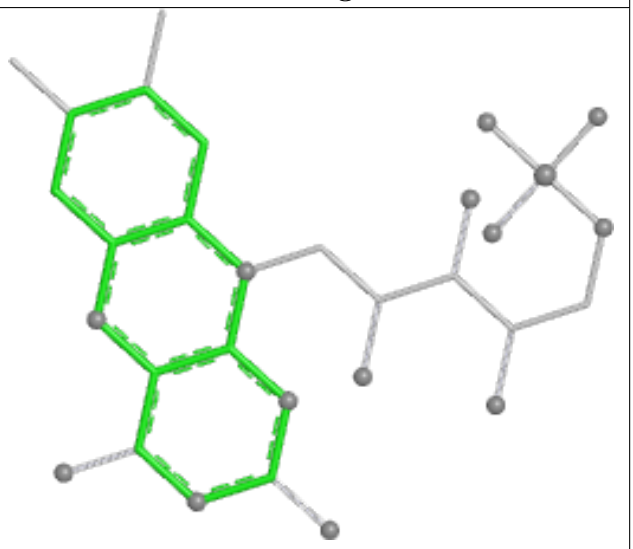
Bond lengths



Bond angles

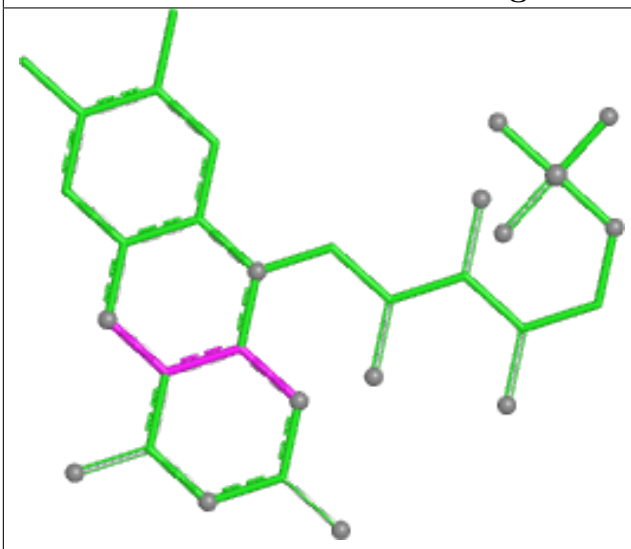


Torsions

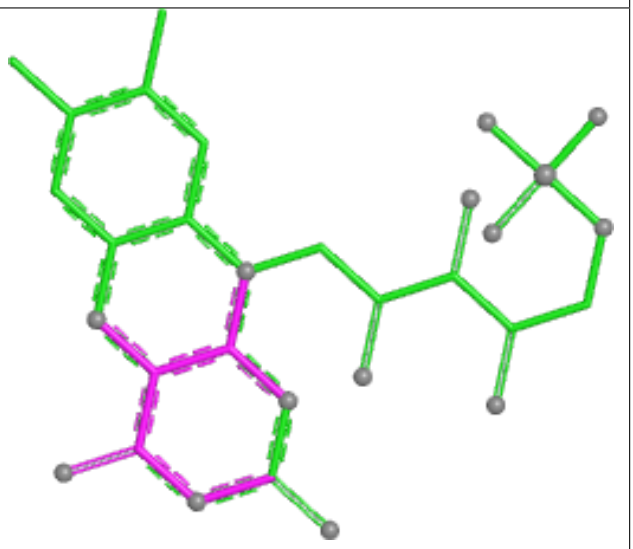


Rings

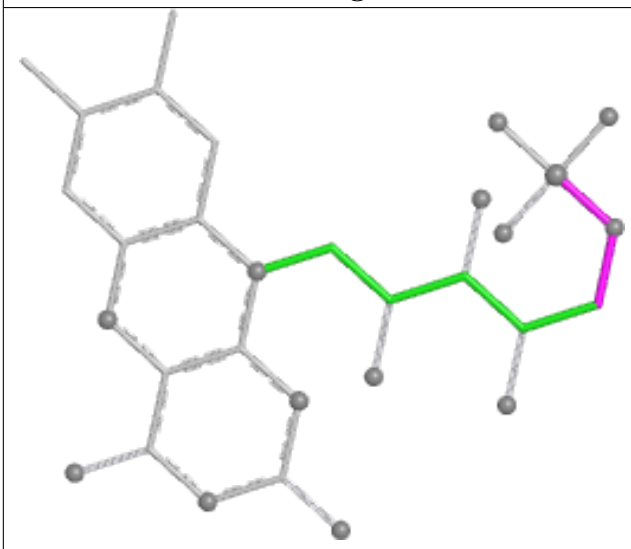
Ligand FMN A 3101



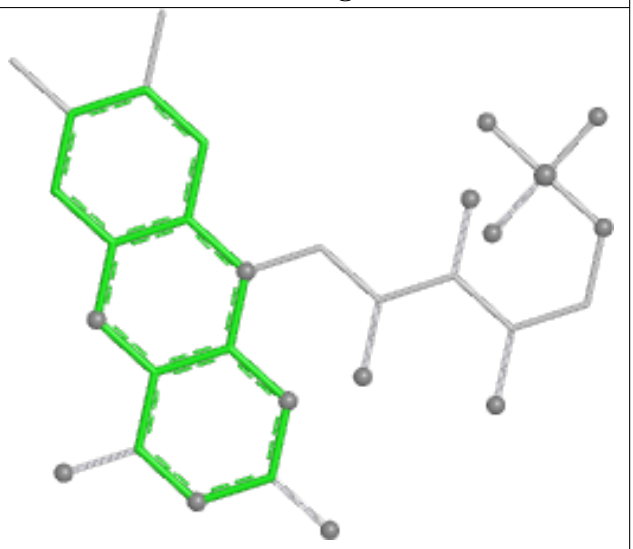
Bond lengths



Bond angles

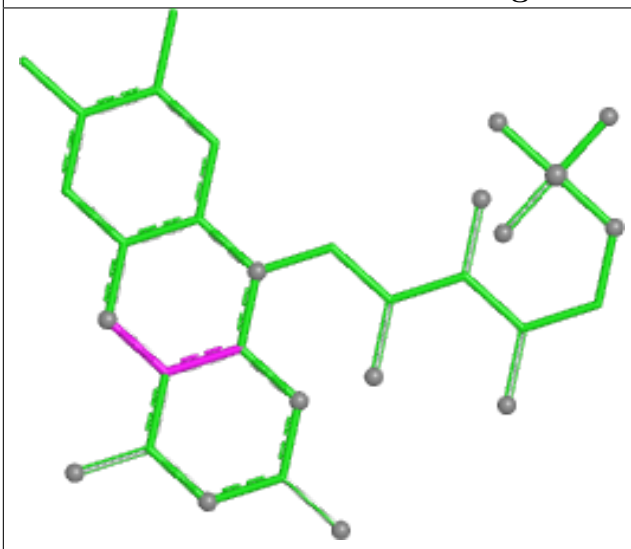


Torsions

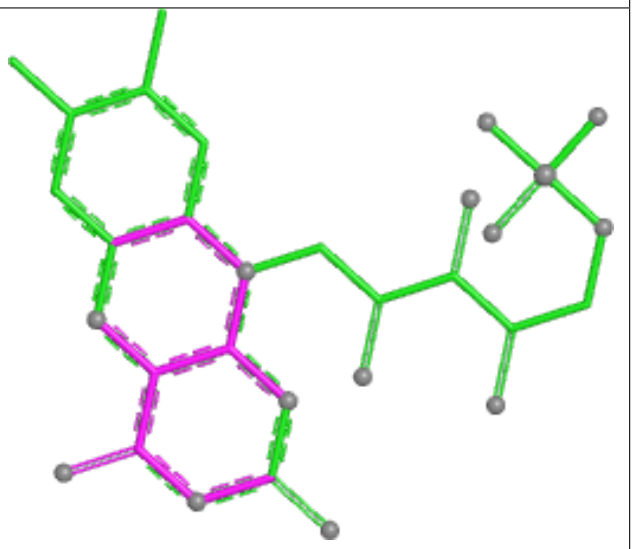


Rings

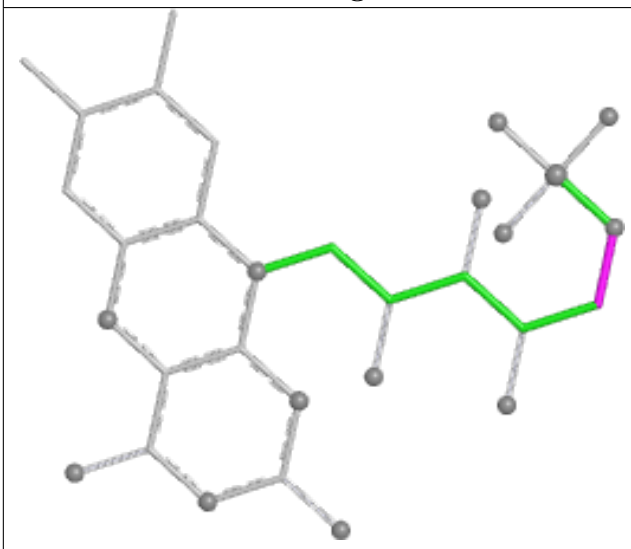
Ligand FMN E 3101



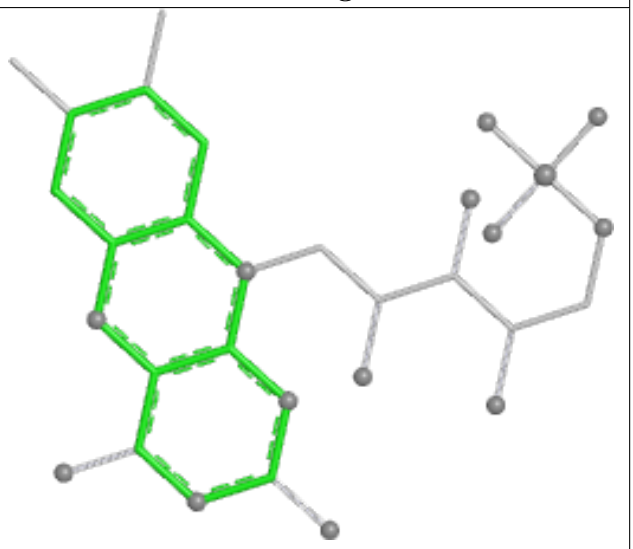
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

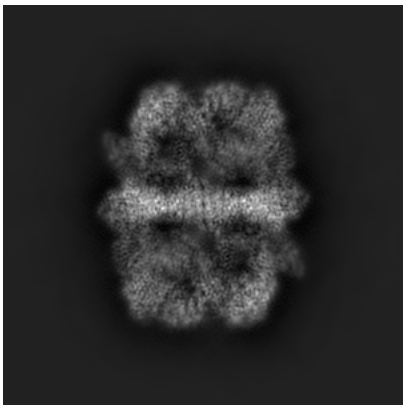
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0011. These allow visual inspection of the internal detail of the map and identification of artifacts.

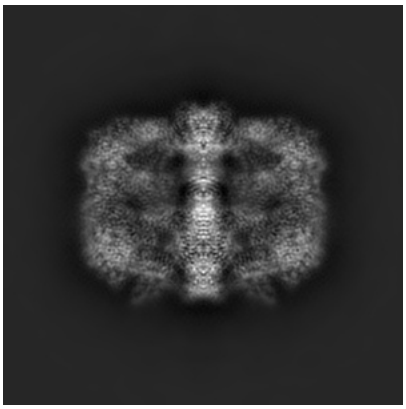
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

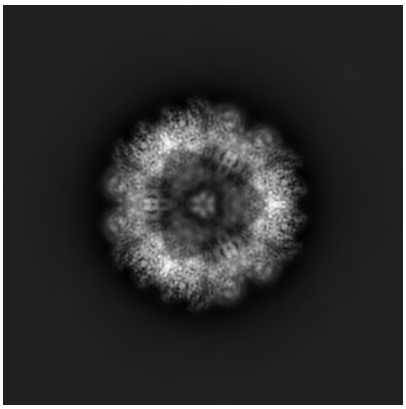
6.1.1 Primary map



X

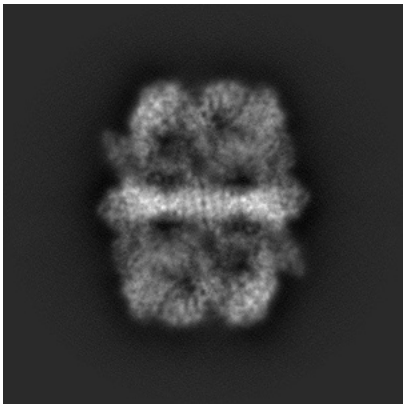


Y

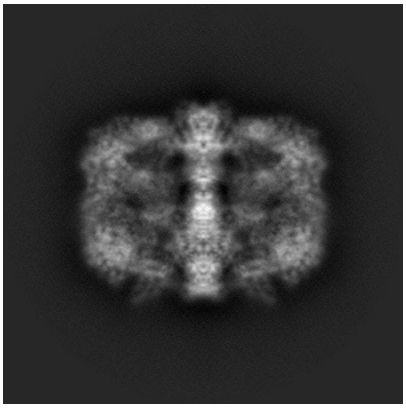


Z

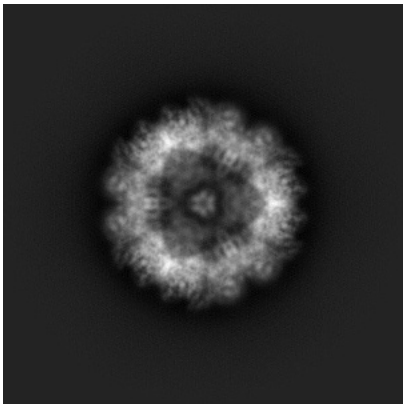
6.1.2 Raw map



X



Y

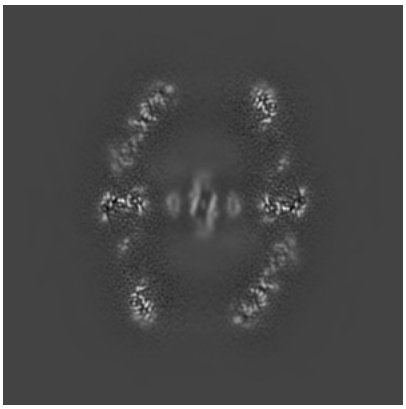


Z

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

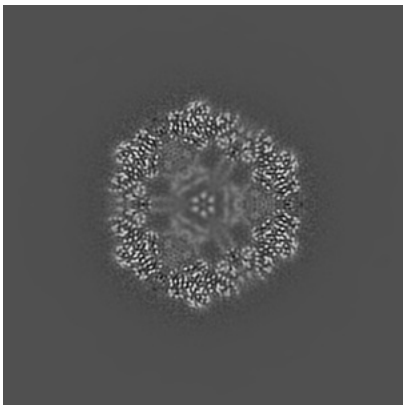
6.2 Central slices (i)

6.2.1 Primary map



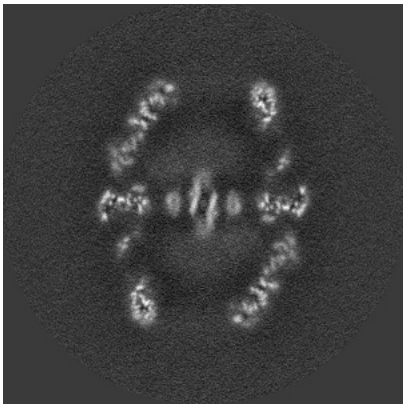
X Index: 200

Y Index: 200

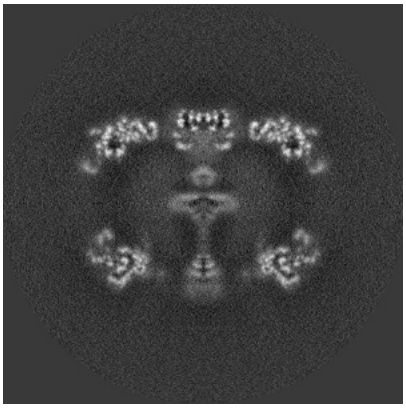


Z Index: 200

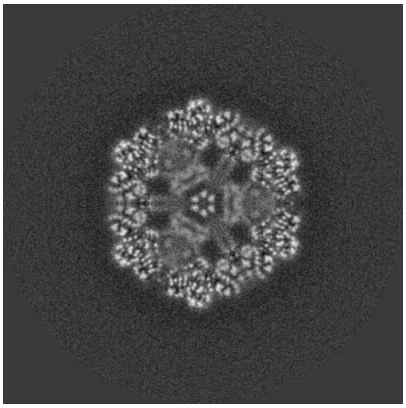
6.2.2 Raw map



X Index: 200



Y Index: 200

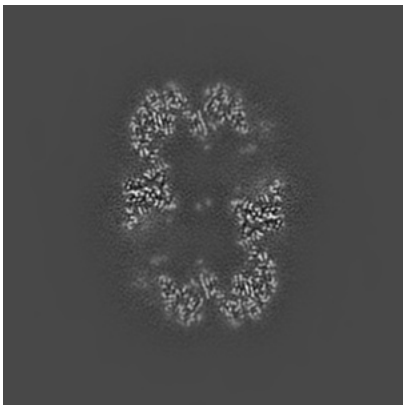


Z Index: 200

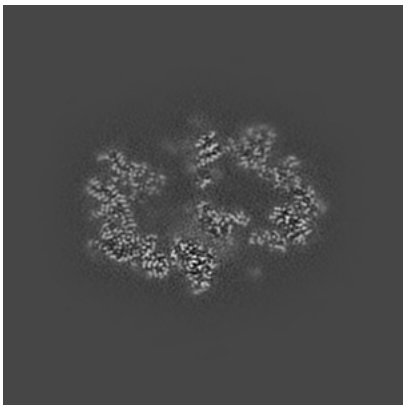
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

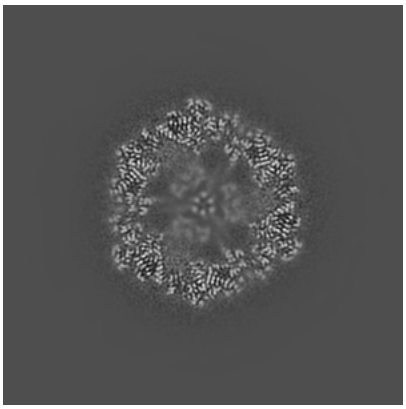
6.3.1 Primary map



X Index: 153

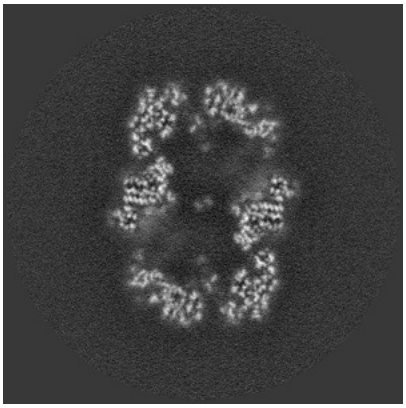


Y Index: 258

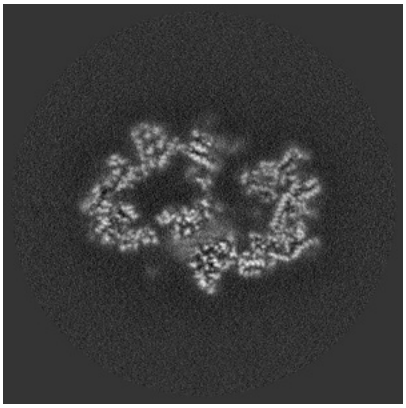


Z Index: 204

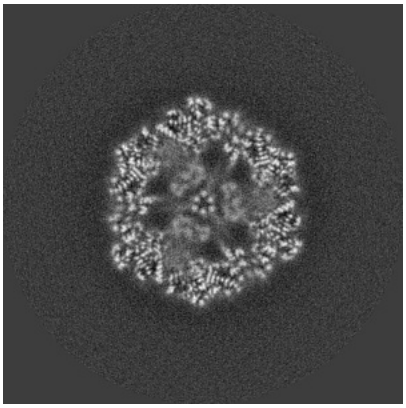
6.3.2 Raw map



X Index: 157



Y Index: 141

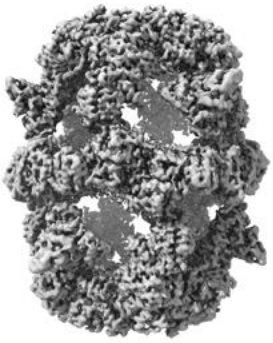


Z Index: 204

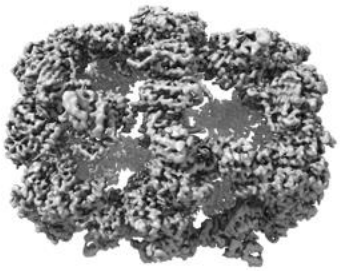
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

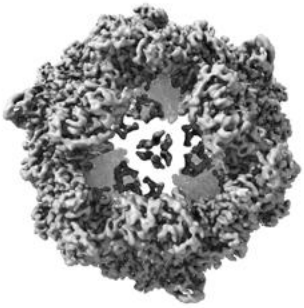
6.4.1 Primary map



X



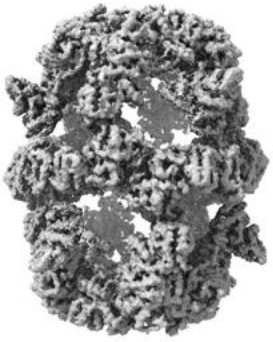
Y



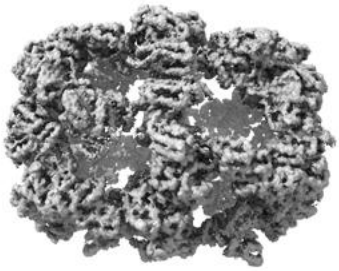
Z

The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

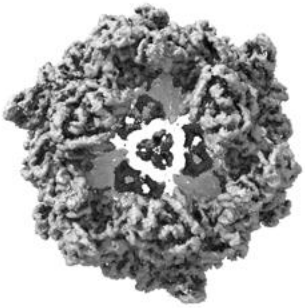
6.4.2 Raw map



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.

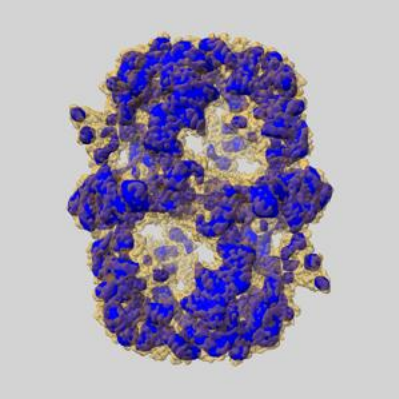
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

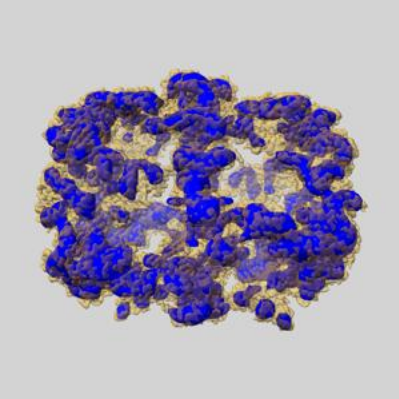
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

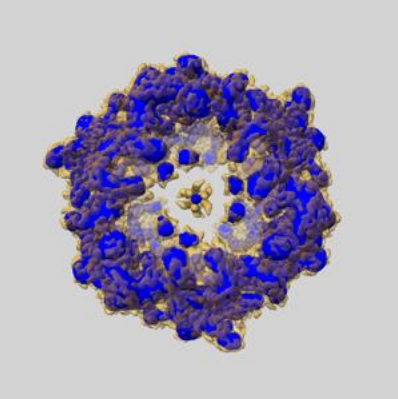
6.5.1 emd_0011_msk_1.map (i)



X



Y

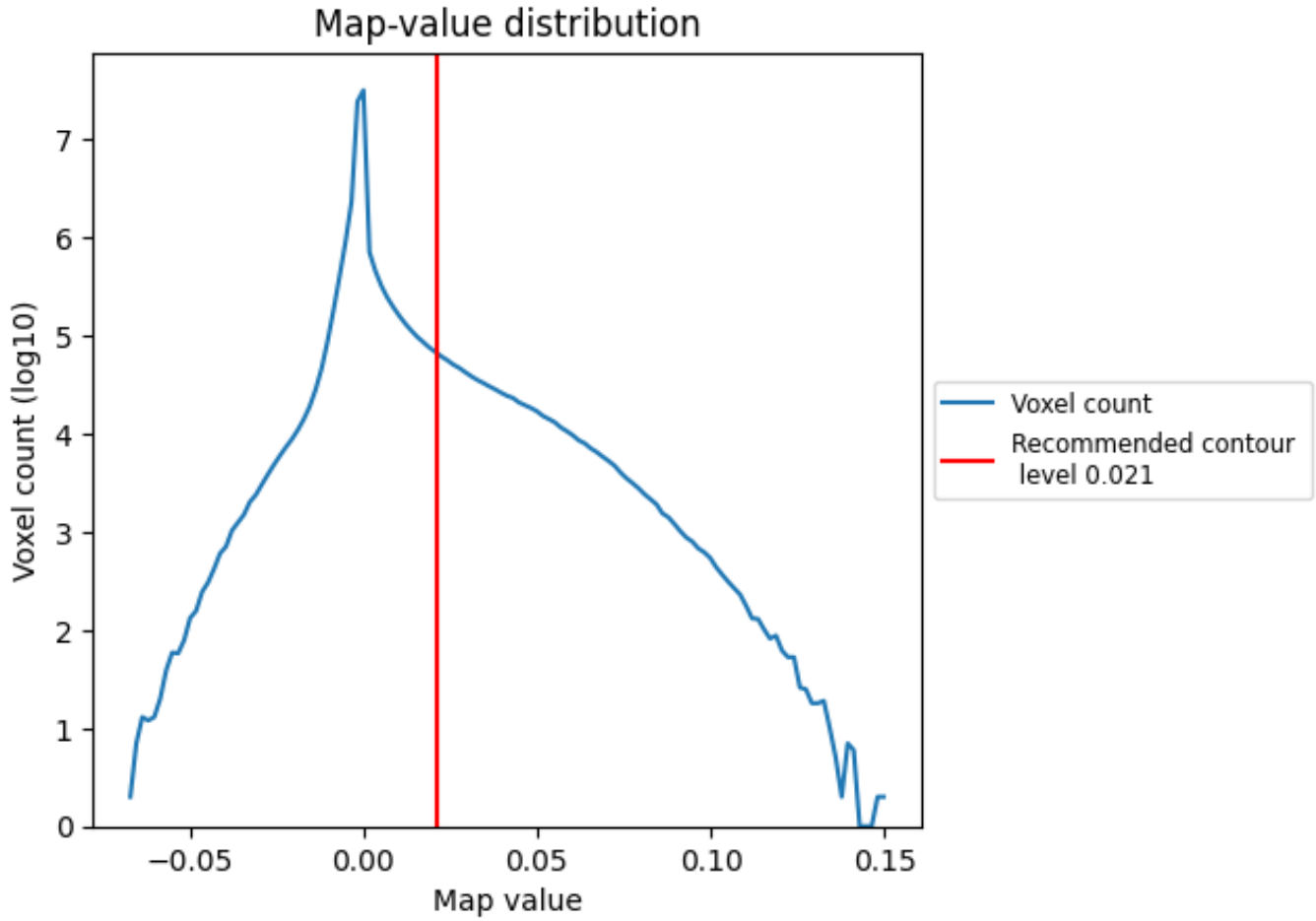


Z

7 Map analysis

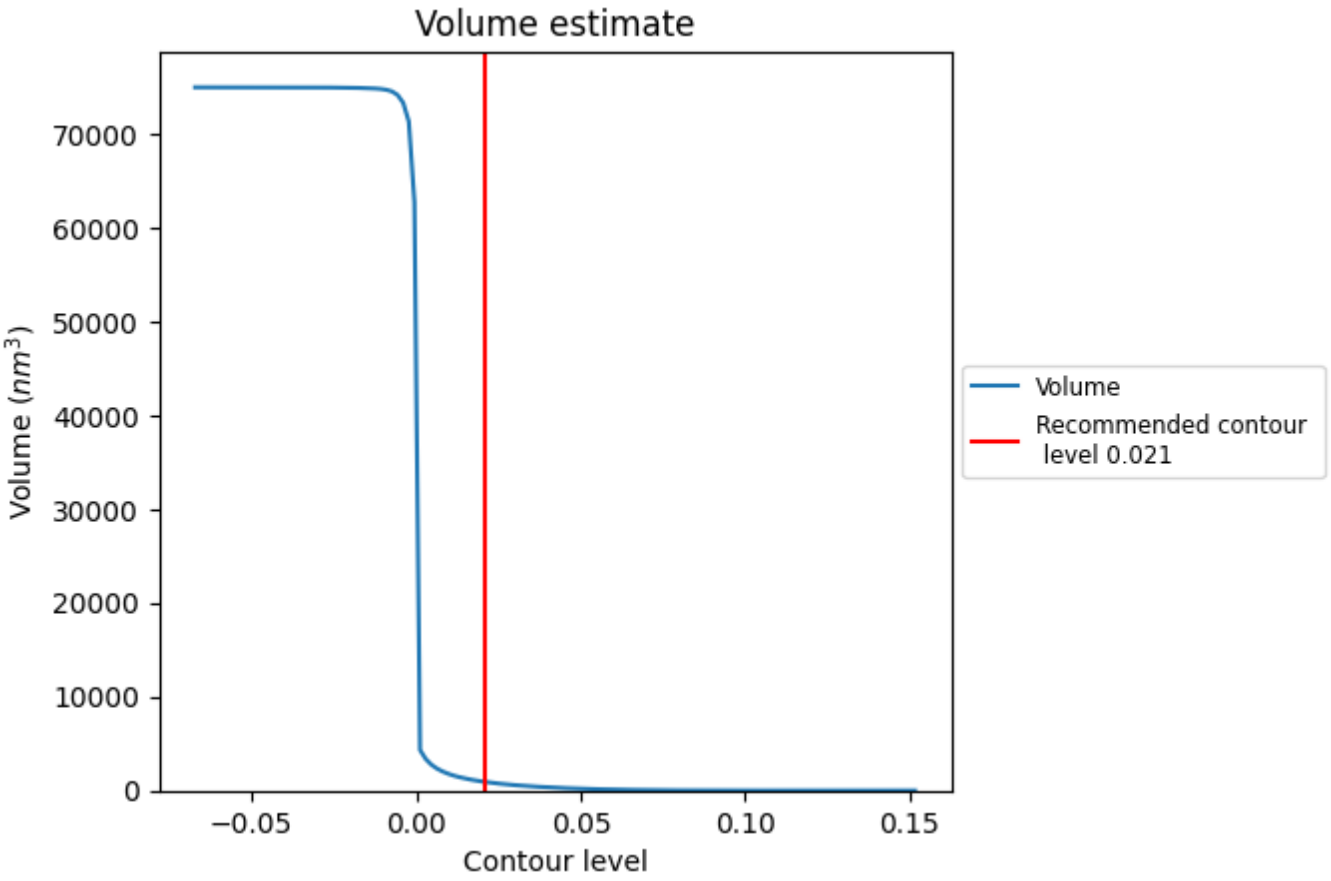
This section contains the results of statistical analysis of the map.

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.

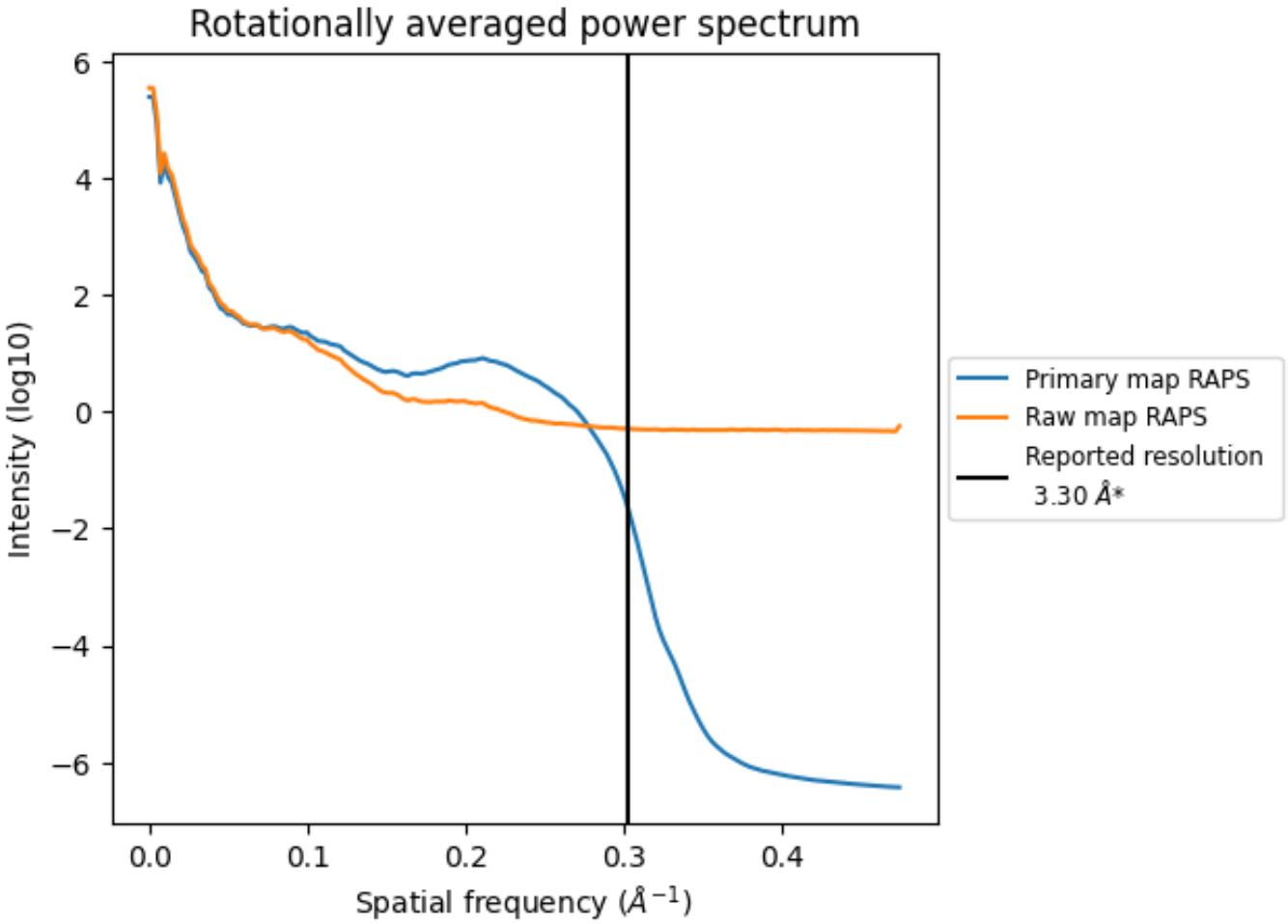
7.2 Volume estimate (i)



The volume at the recommended contour level is 919 nm^3; this corresponds to an approximate mass of 830 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)

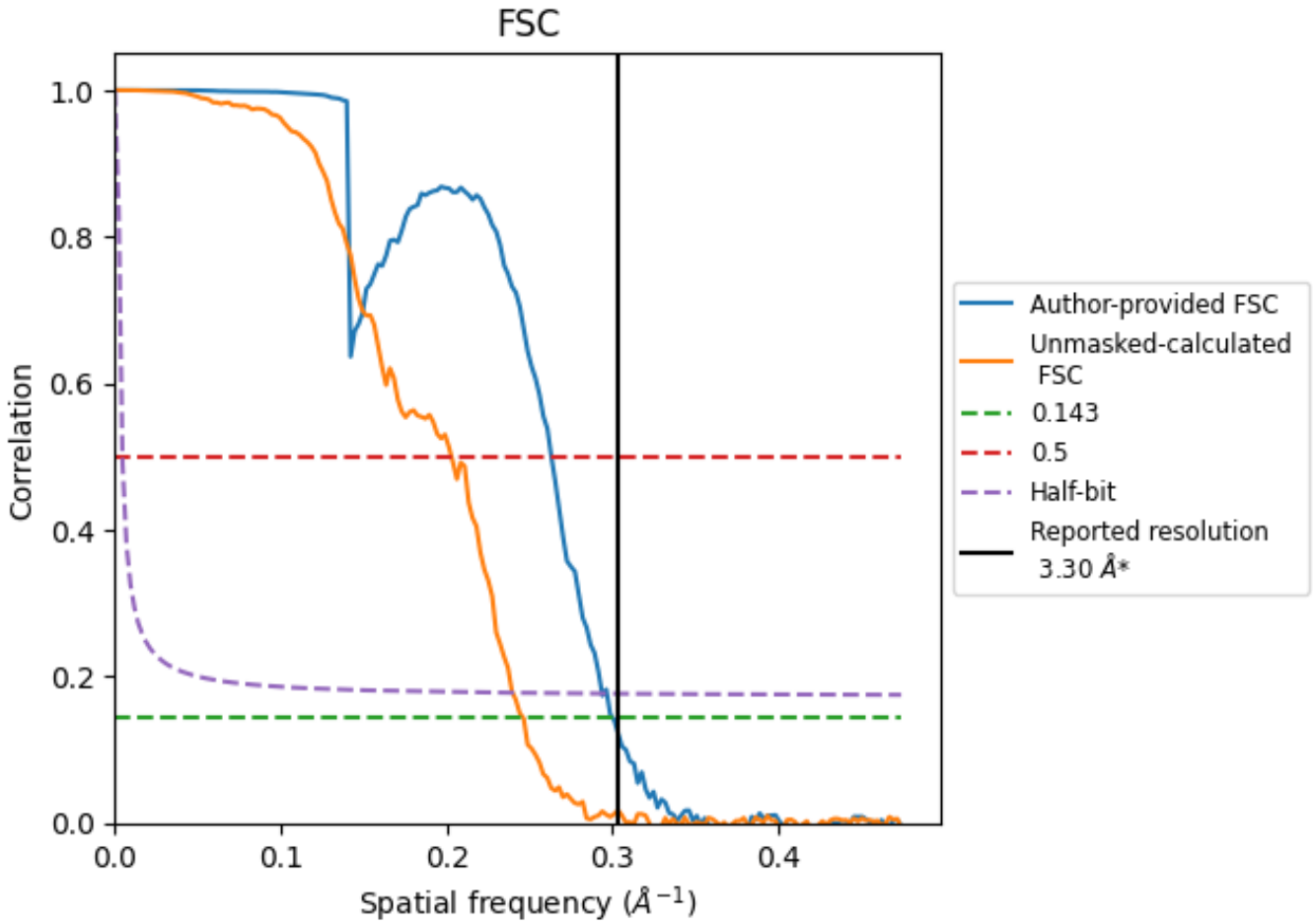


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

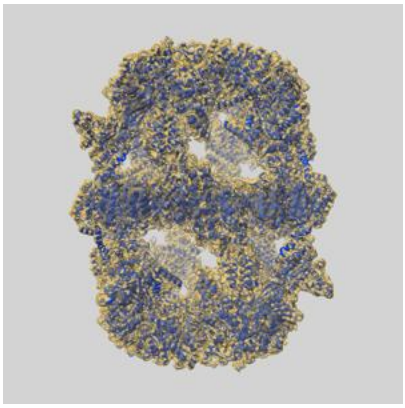
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.80	3.40
Unmasked-calculated*	4.06	4.92	4.17

*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 4.06 differs from the reported value 3.3 by more than 10 %

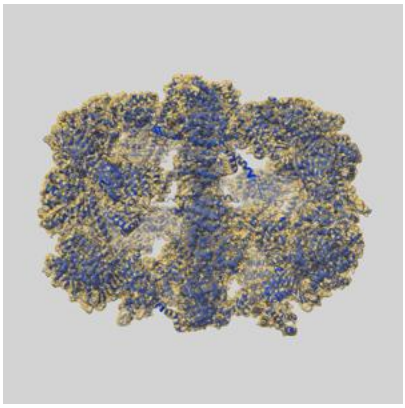
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0011 and PDB model 6GJC. Per-residue inclusion information can be found in section 3 on page 8.

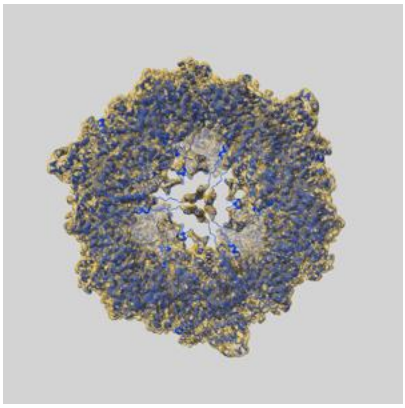
9.1 Map-model overlay



X



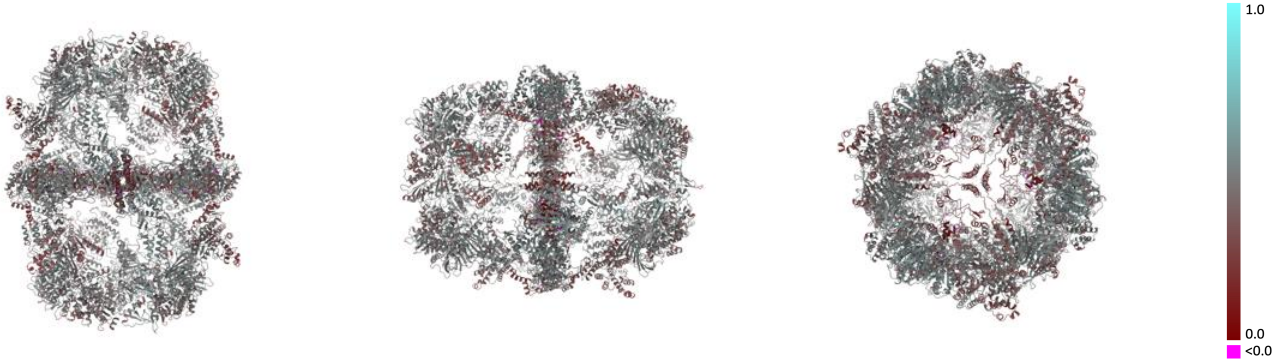
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.021 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.

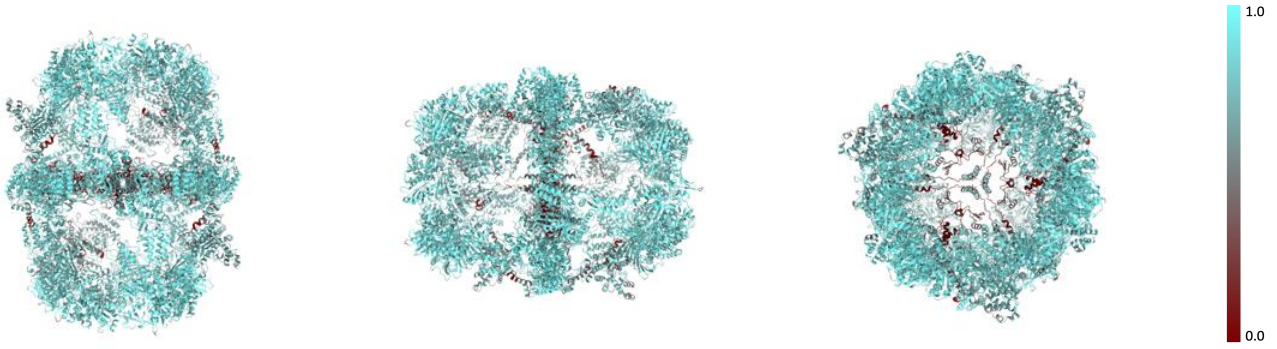
9.2 Q-score mapped to coordinate model



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.

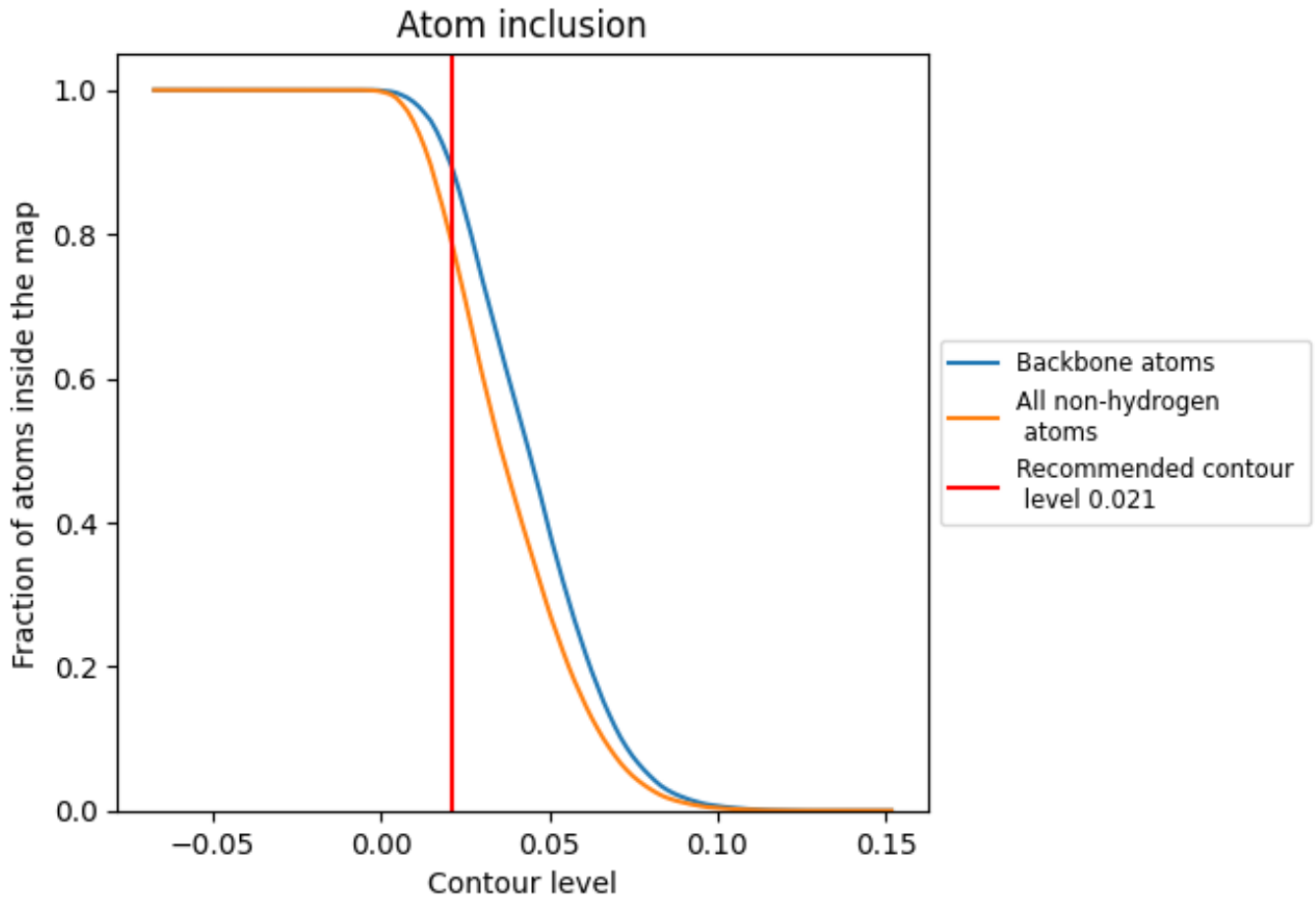
9.3 Atom inclusion mapped to coordinate model



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 (0.021).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 79% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7906	0.4430
A	0.7834	0.4370
B	0.7909	0.4420
C	0.7924	0.4440
D	0.7938	0.4450
E	0.7914	0.4430
F	0.7915	0.4440