wwPDB EM Validation Summary Report (i)

Mar 8, 2026 – 12:00 PM UTC

PDB ID	:	9P4W / pdb_00009p4w
EMDB ID	:	EMD-71285
Title	:	Atomic model of wild type S. cerevisiae Fatty Acid Synthase (FAS)
Authors	:	Hasan, N.S.M.; Keszei, F.A.A.; Mazhab-Jafari, M.T.
Deposited on	:	2025-06-17
Resolution	:	2.29 Å(reported)
Based on initial model	:	6TA1

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:

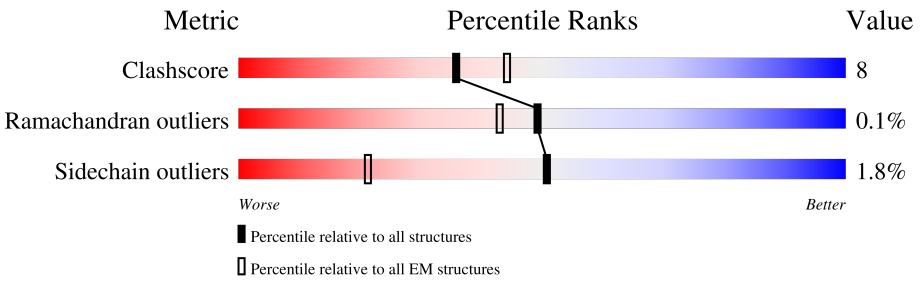
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

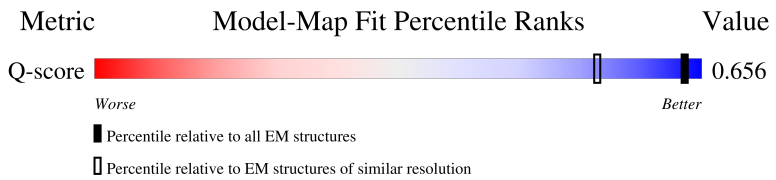
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.29 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3699 (1.79 - 2.79)

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	2051	9% 84% 14%
1	E	2051	9% 84% 14%
1	I	2051	9% 84% 14%
1	L	2051	9% 83% 14%

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Mol	Chain	Length	Quality of chain
1	O	2051	9% 83% 15%
1	R	2051	9% 84% 14%
2	B	1887	64% 10% 25%
2	D	1887	64% 10% 25%
2	H	1887	64% 11% 25%
2	K	1887	64% 11% 25%
2	N	1887	64% 11% 25%
2	Q	1887	64% 11% 25%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 165070 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.

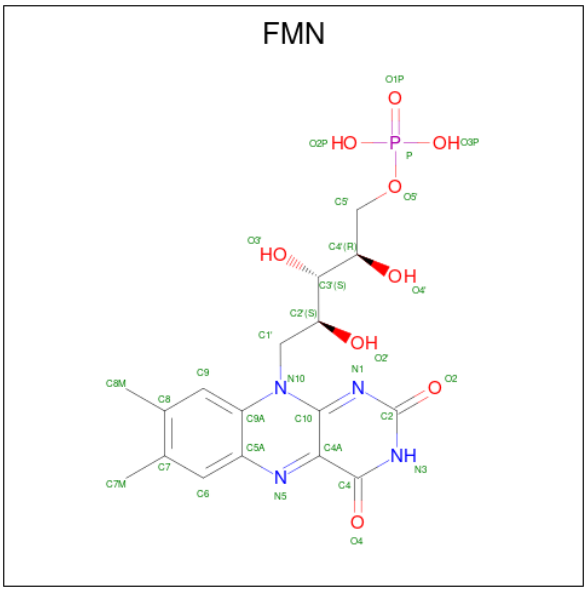
- Molecule 1 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2015	15605	10032	2610	2907	56	0	0
1	E	2015	15605	10032	2610	2907	56	0	0
1	I	2015	15605	10032	2610	2907	56	0	0
1	L	2015	15605	10032	2610	2907	56	0	0
1	O	2015	15605	10032	2610	2907	56	0	0
1	R	2015	15605	10032	2610	2907	56	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1417	10978	6975	1860	2098	45	0	0
2	D	1417	10978	6975	1860	2098	45	0	0
2	H	1417	10978	6975	1860	2098	45	0	0
2	K	1417	10978	6975	1860	2098	45	0	0
2	N	1417	10978	6975	1860	2098	45	0	0
2	Q	1417	10978	6975	1860	2098	45	0	0

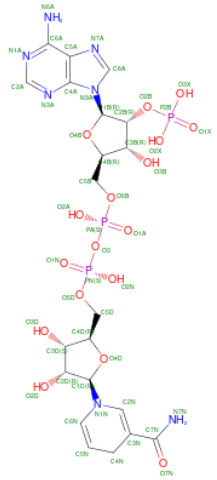
- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	I	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	L	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	O	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	R	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

NDP



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	B	1	48	21	7	17	3	0
4	D	1	48	21	7	17	3	0
4	H	1	48	21	7	17	3	0
4	K	1	48	21	7	17	3	0
4	N	1	48	21	7	17	3	0
4	Q	1	48	21	7	17	3	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
5	A	379	379	379	0
5	B	457	457	457	0
5	D	450	450	450	0
5	E	381	381	381	0
5	H	492	492	492	0
5	I	378	378	378	0

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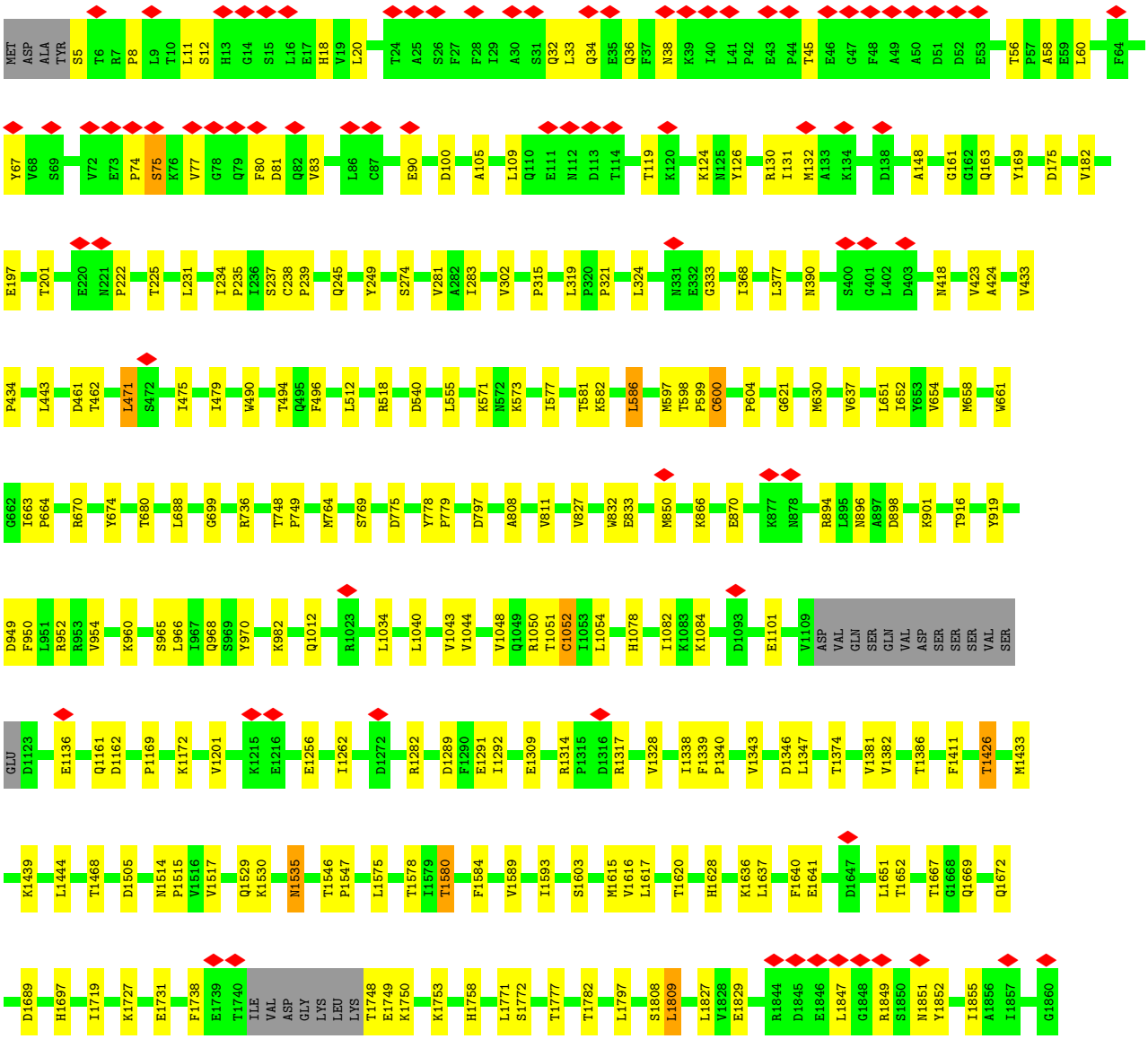
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
5	K	470	470	470	0
			Total	O	
5	L	378	378	378	0
			Total	O	
5	N	465	465	465	0
			Total	O	
5	O	381	381	381	0
			Total	O	
5	Q	489	489	489	0
			Total	O	
5	R	378	378	378	0

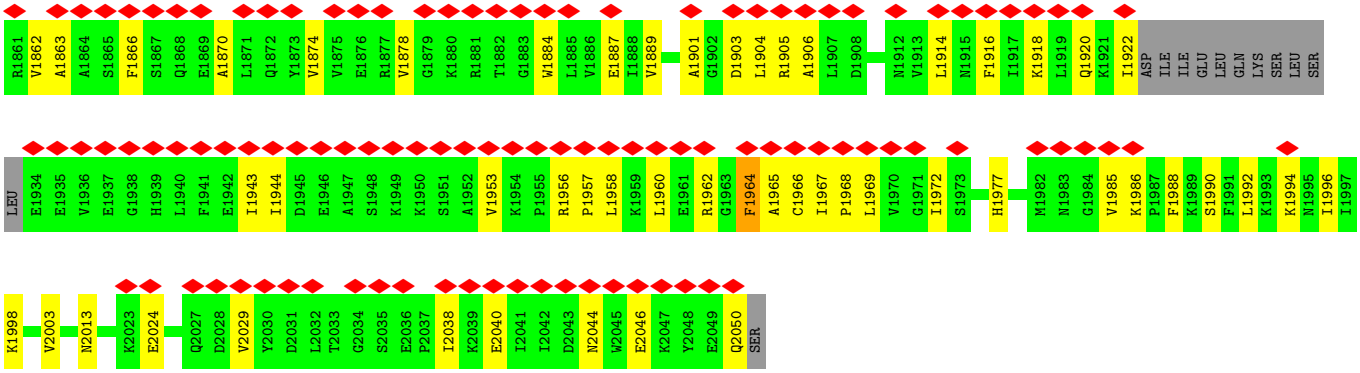
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fatty acid synthase subunit beta

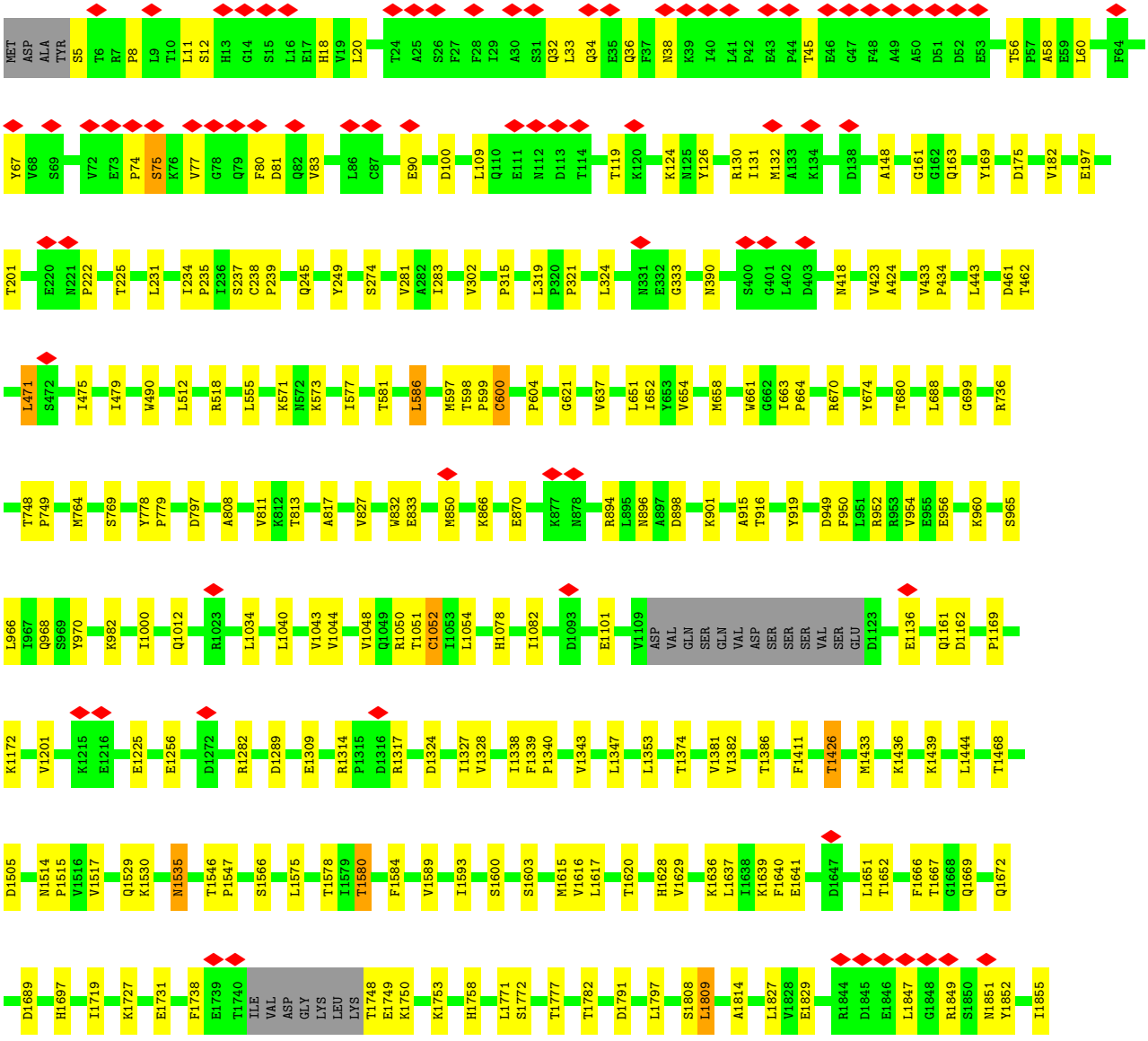
Chain A:

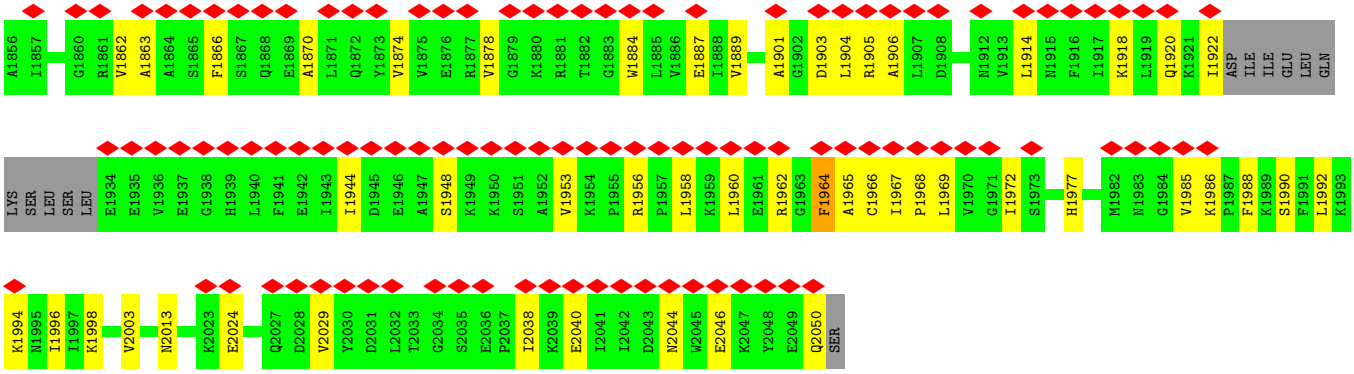




- Molecule 1: Fatty acid synthase subunit beta

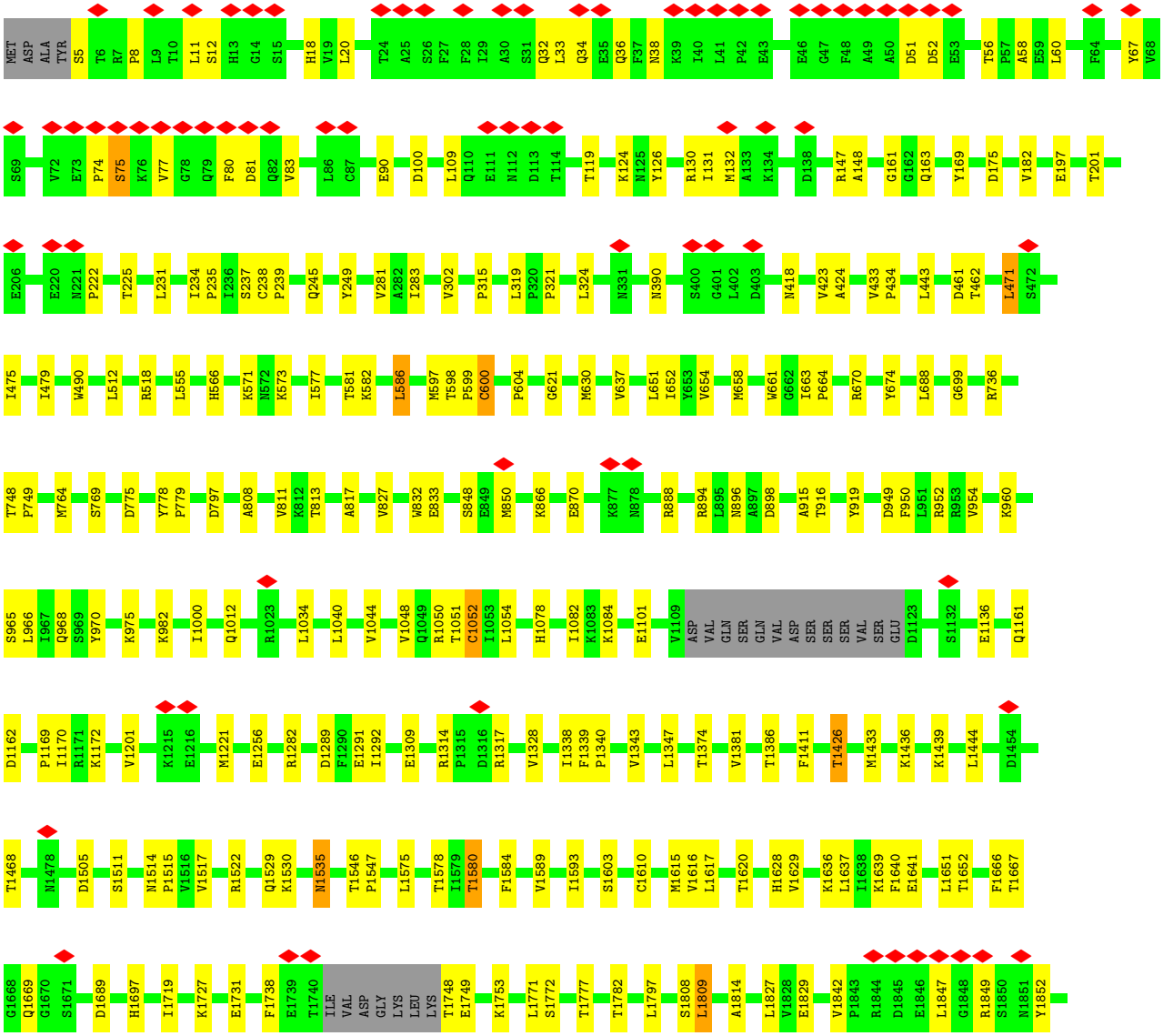
Chain E:

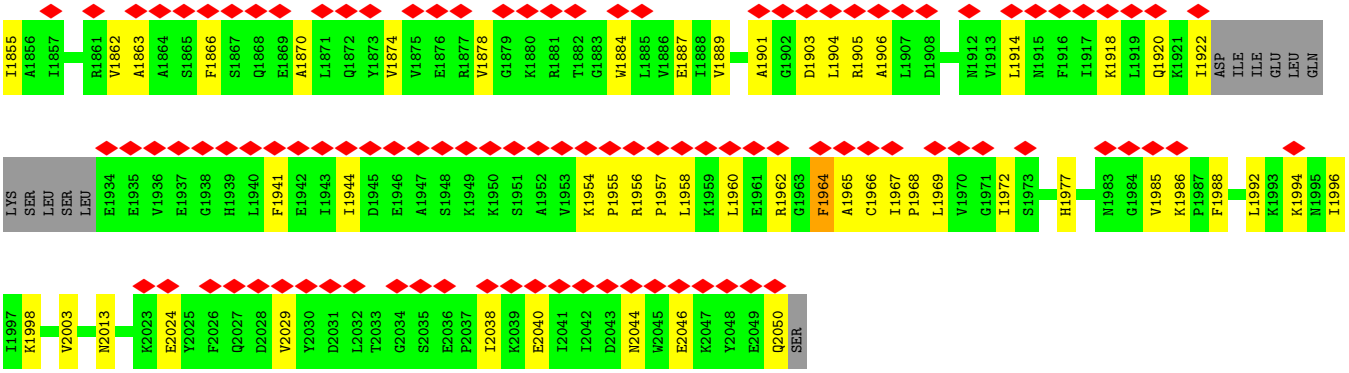




- Molecule 1: Fatty acid synthase subunit beta

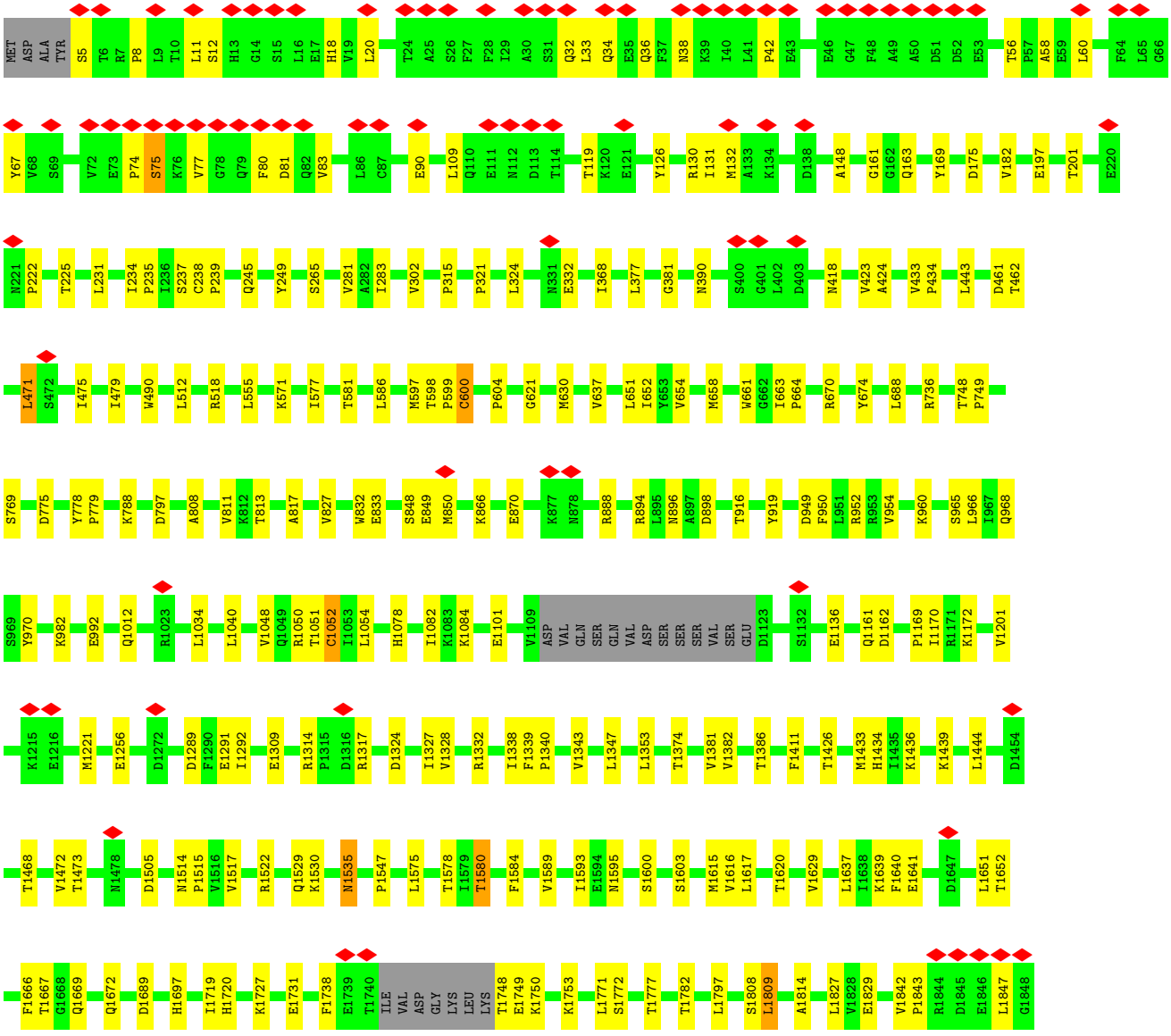
Chain I:

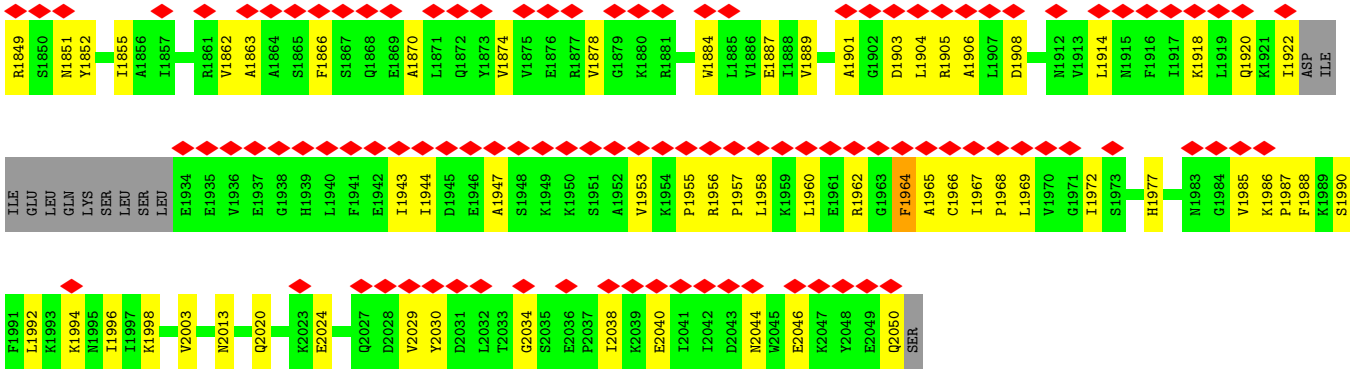




- Molecule 1: Fatty acid synthase subunit beta

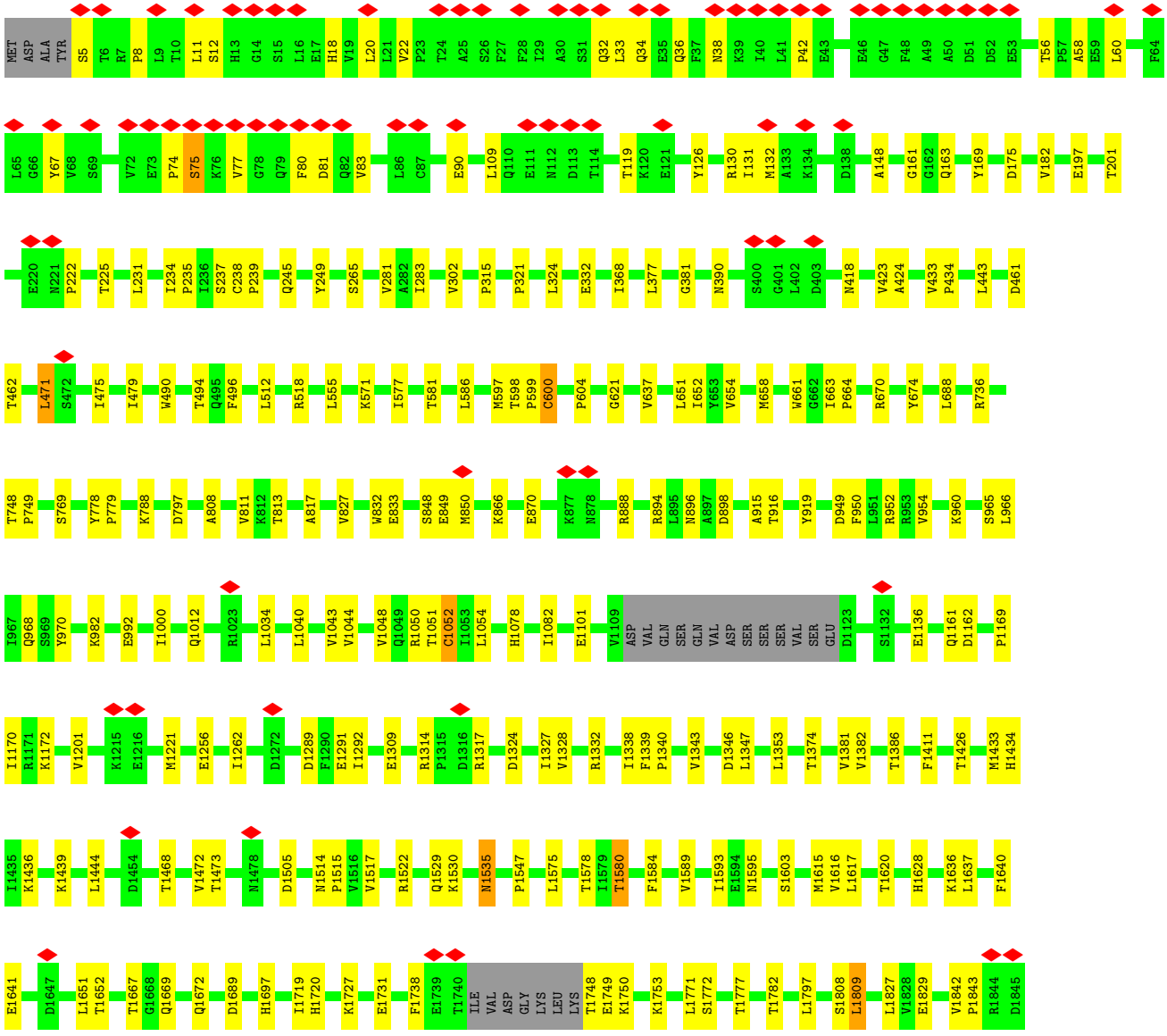
Chain L:

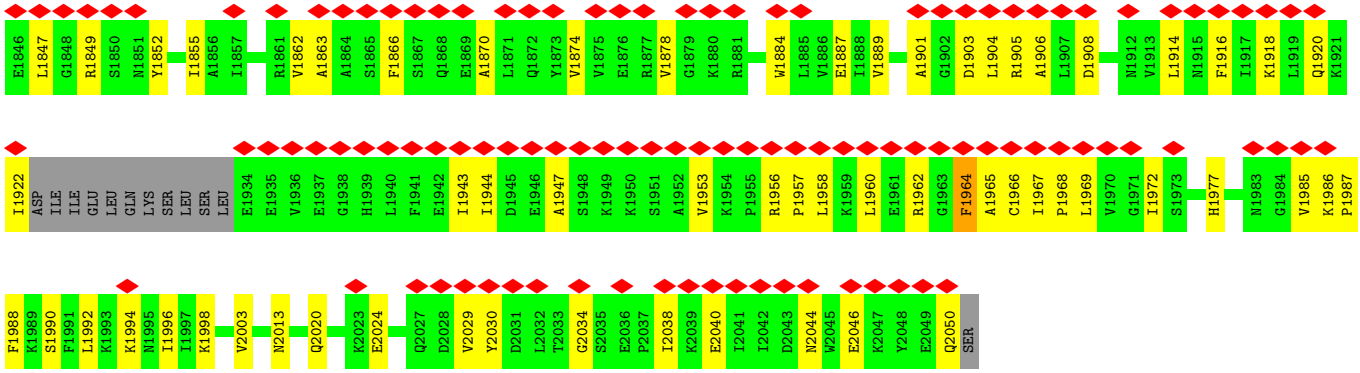




- Molecule 1: Fatty acid synthase subunit beta

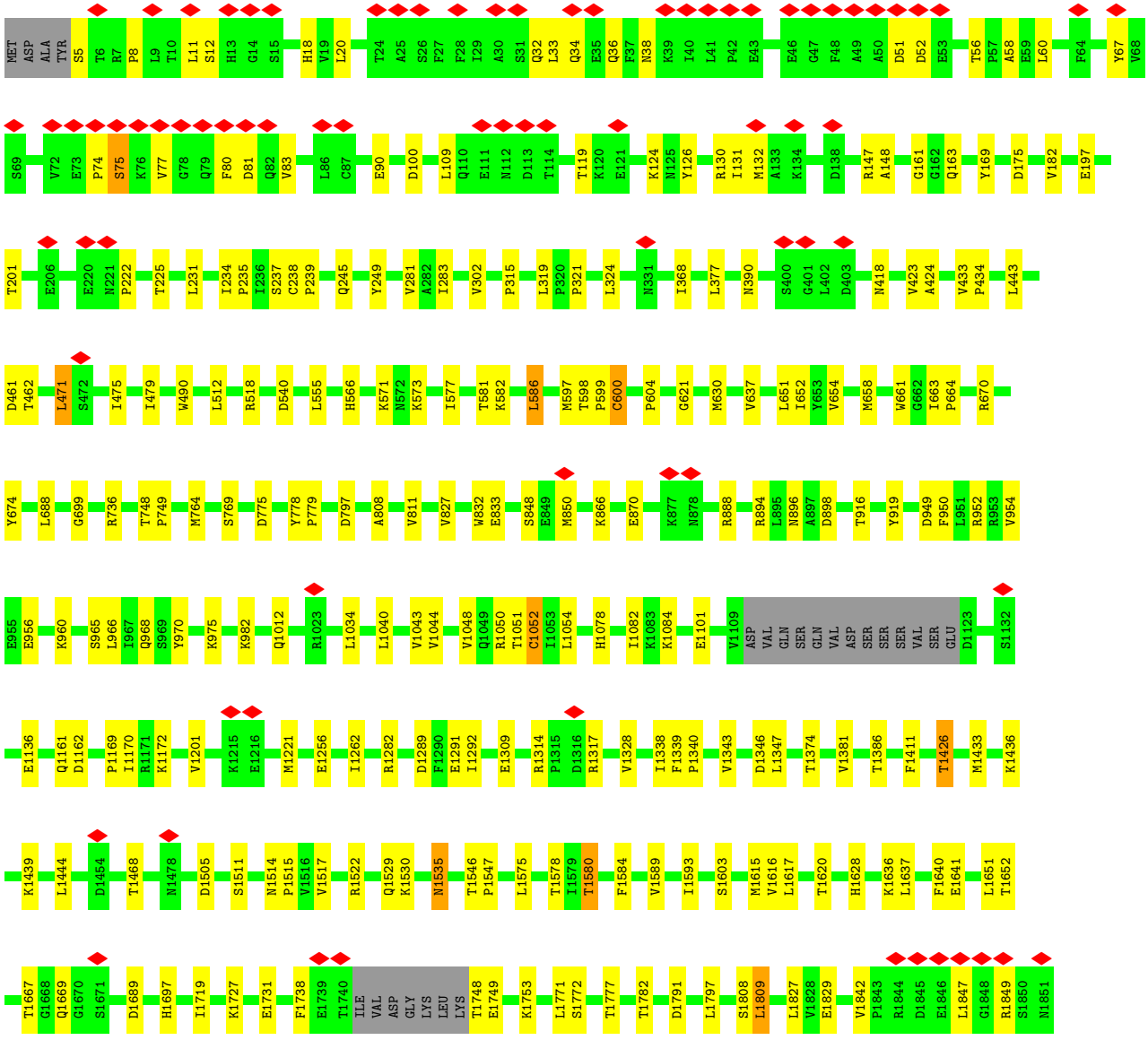
Chain O:

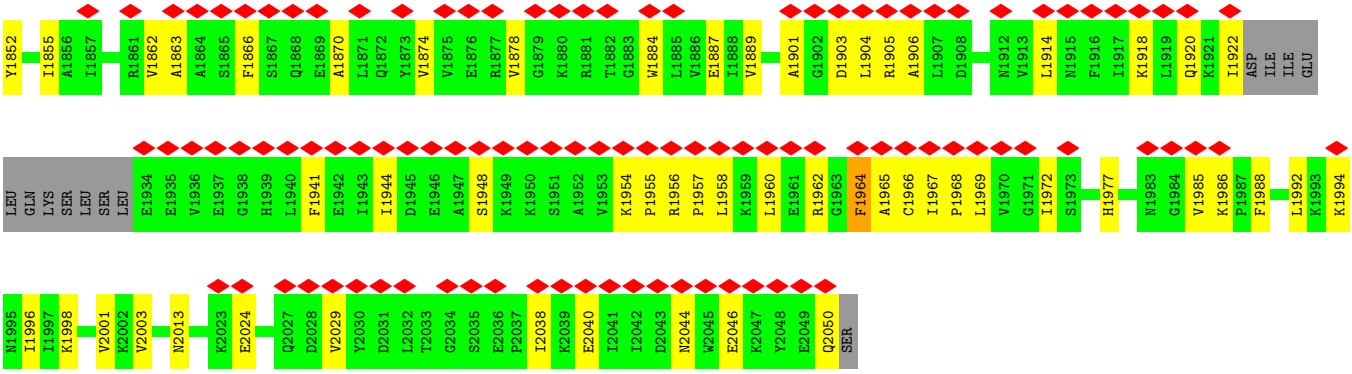




- Molecule 1: Fatty acid synthase subunit beta

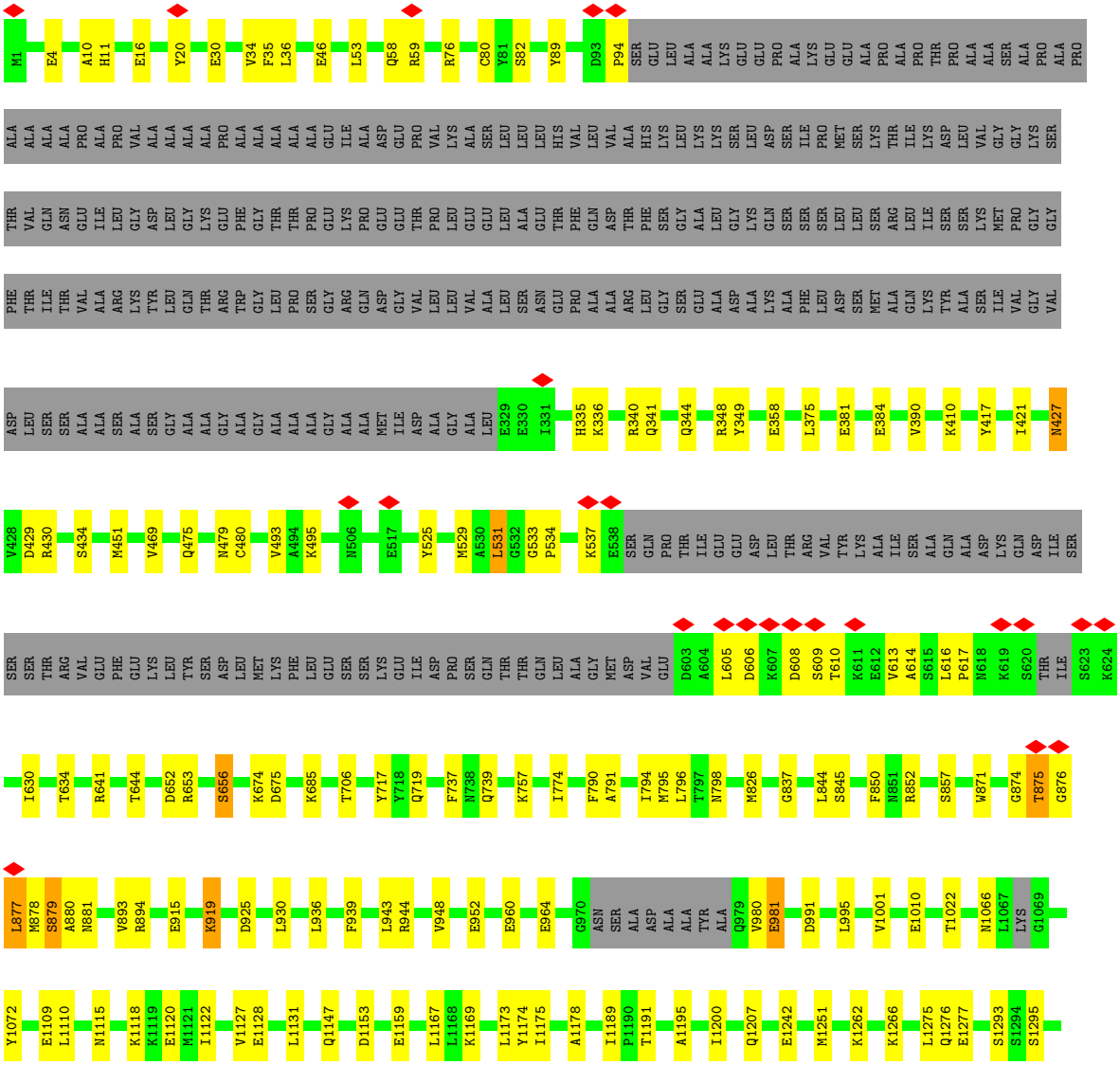
Chain R:

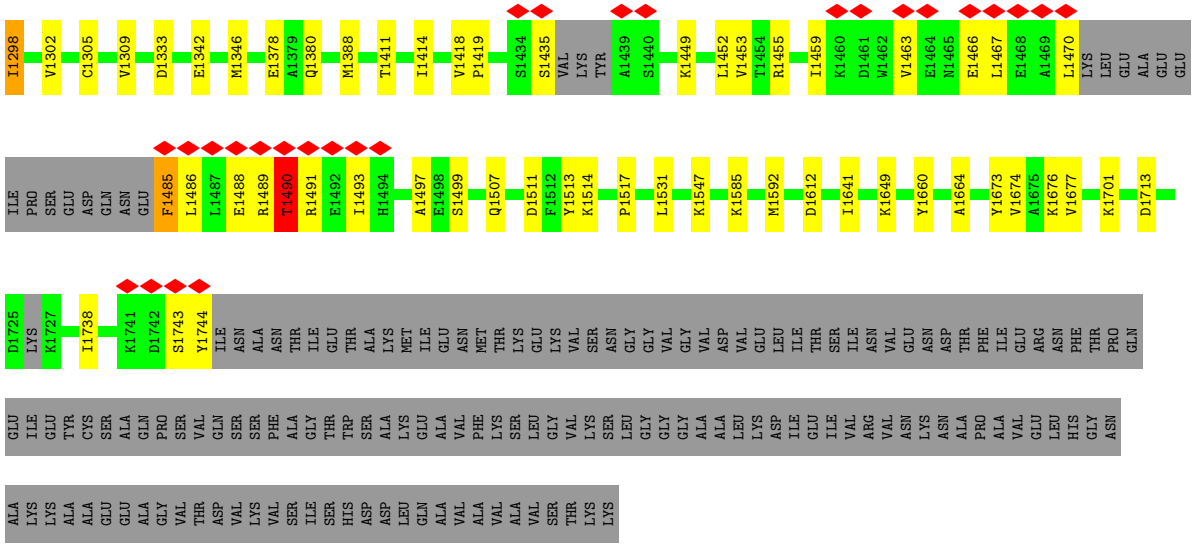




- Molecule 2: Fatty acid synthase subunit alpha

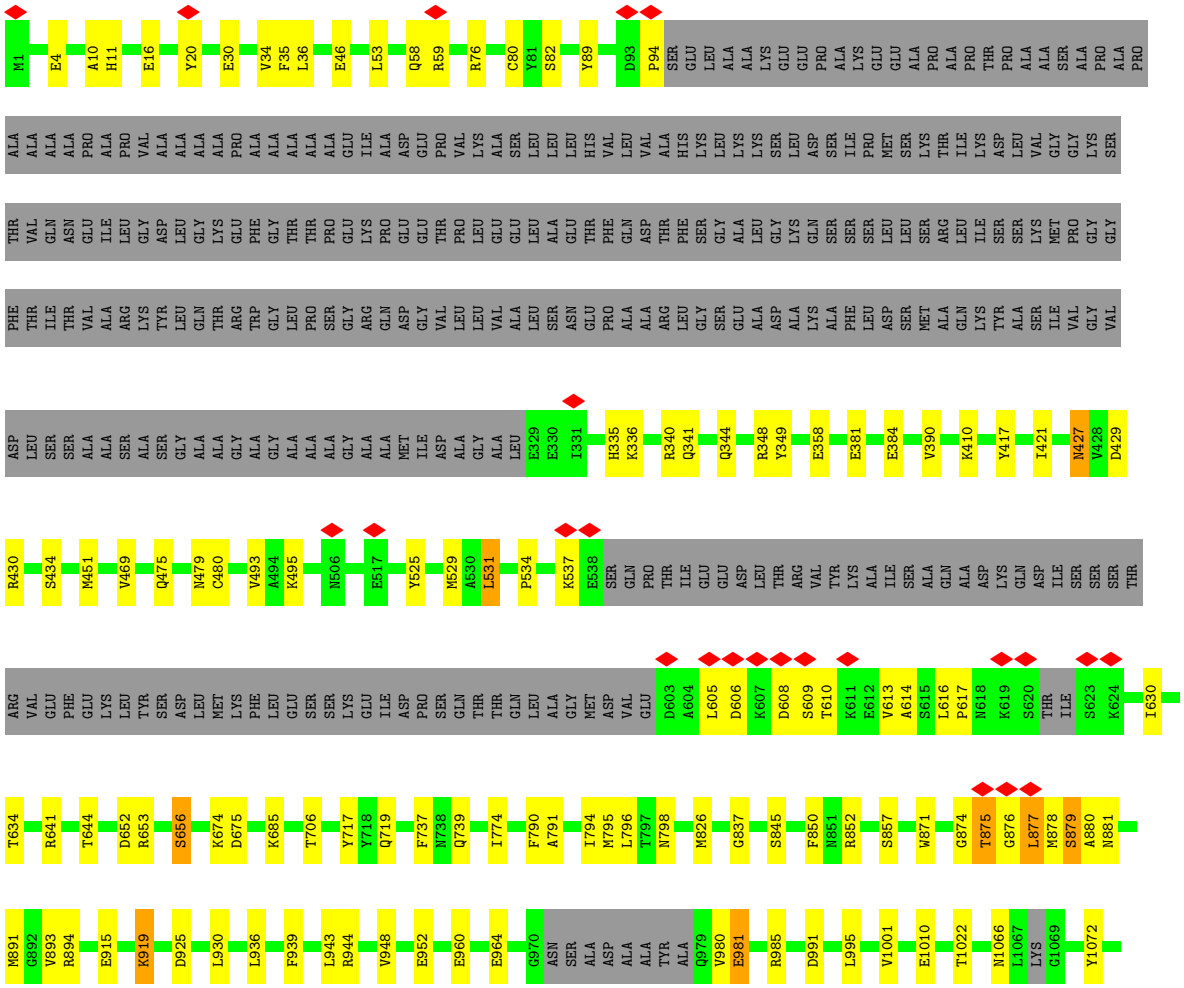
Chain B:

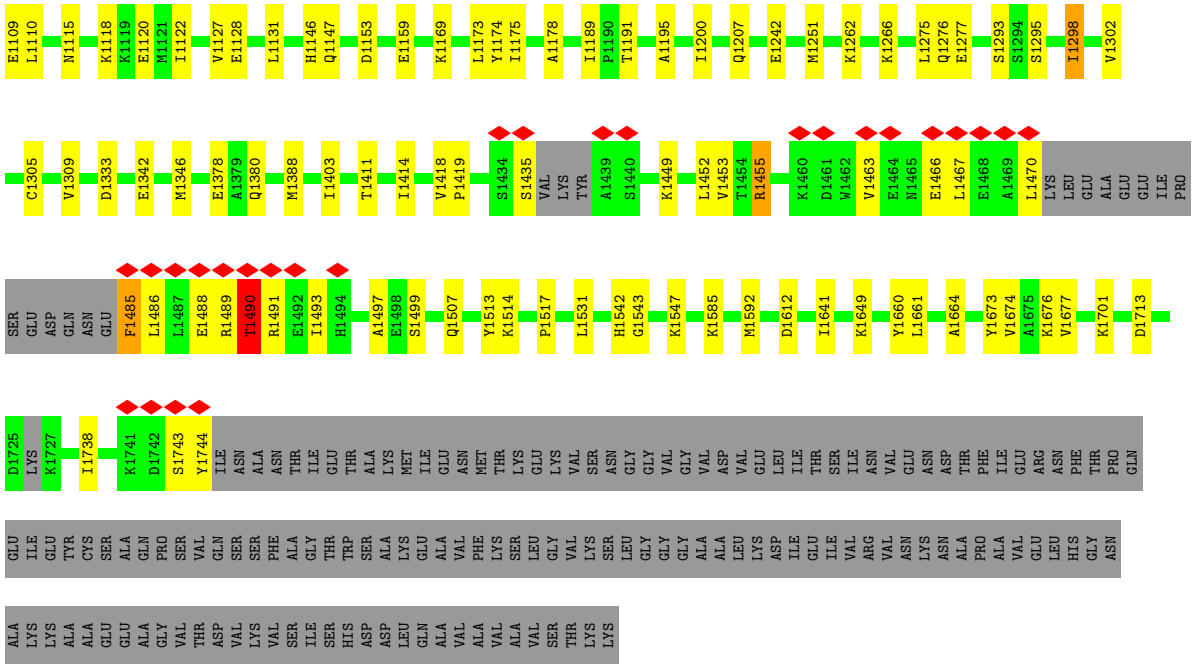




- Molecule 2: Fatty acid synthase subunit alpha

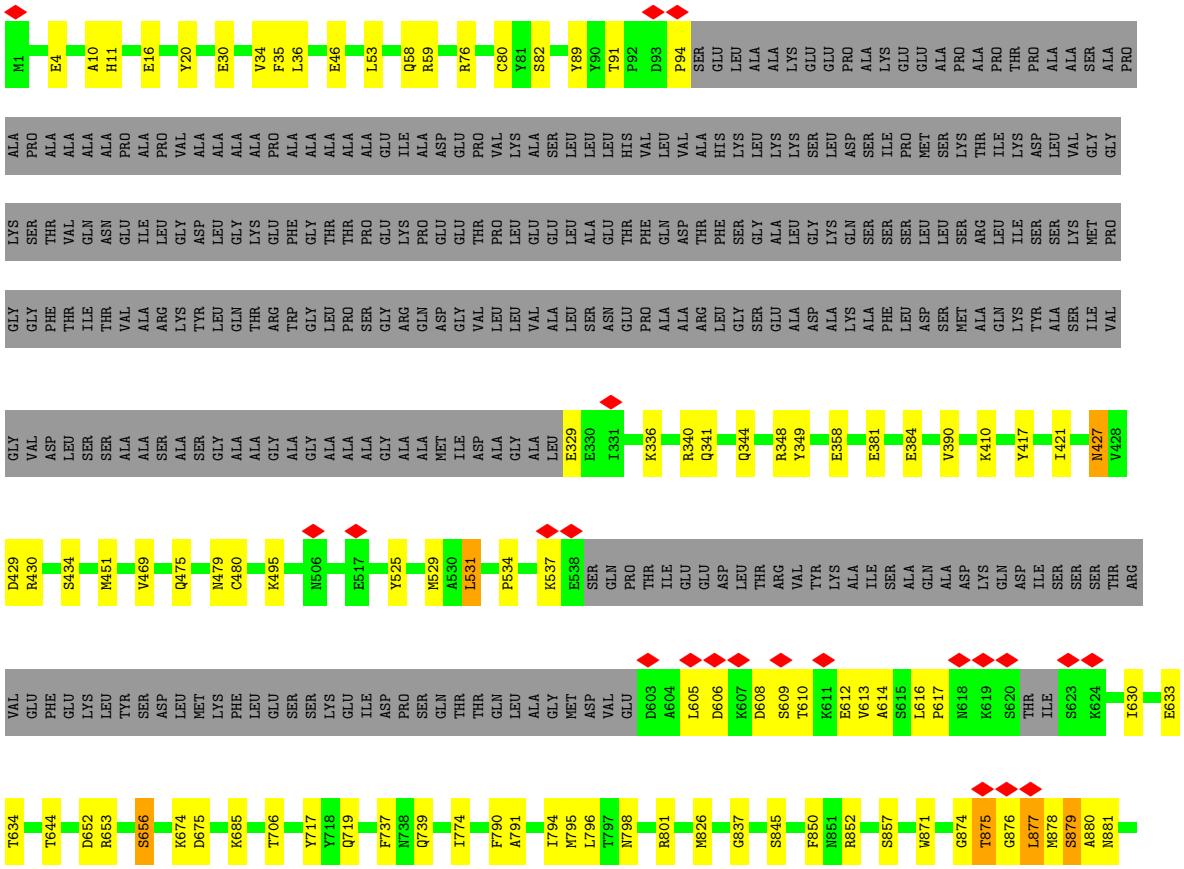
Chain D:

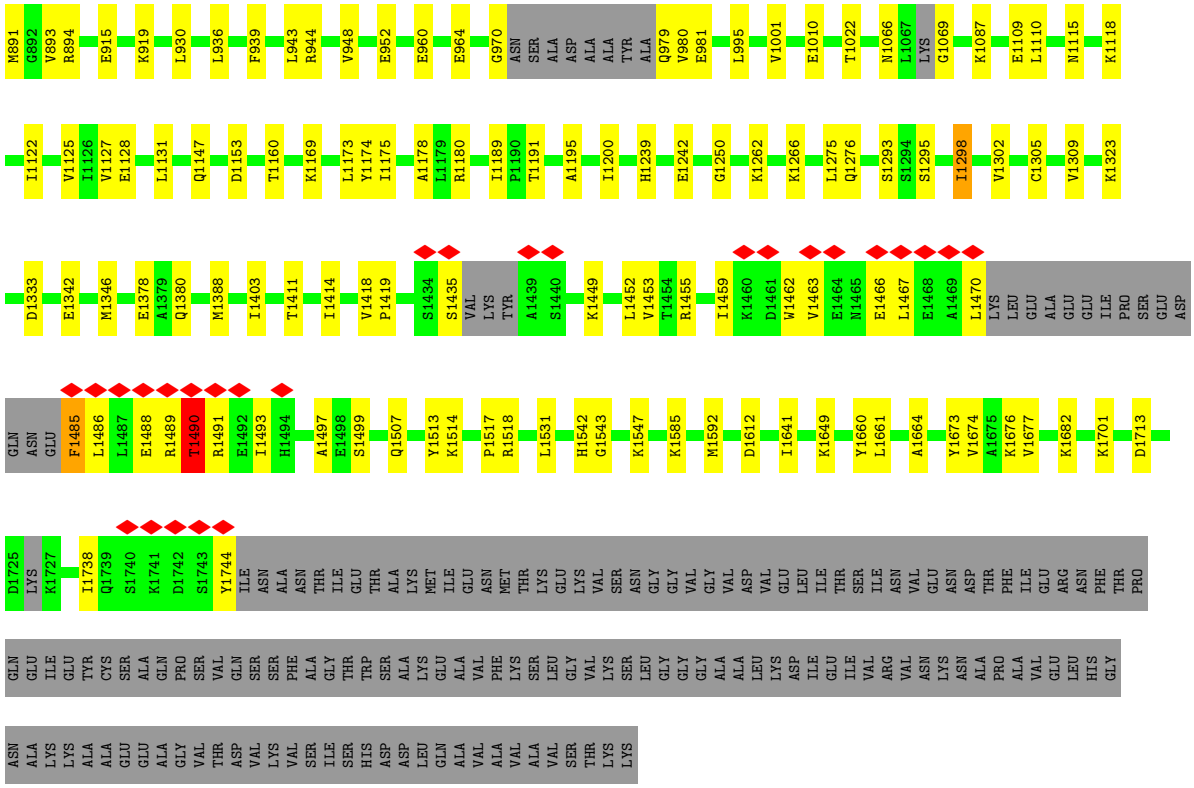




• Molecule 2: Fatty acid synthase subunit alpha

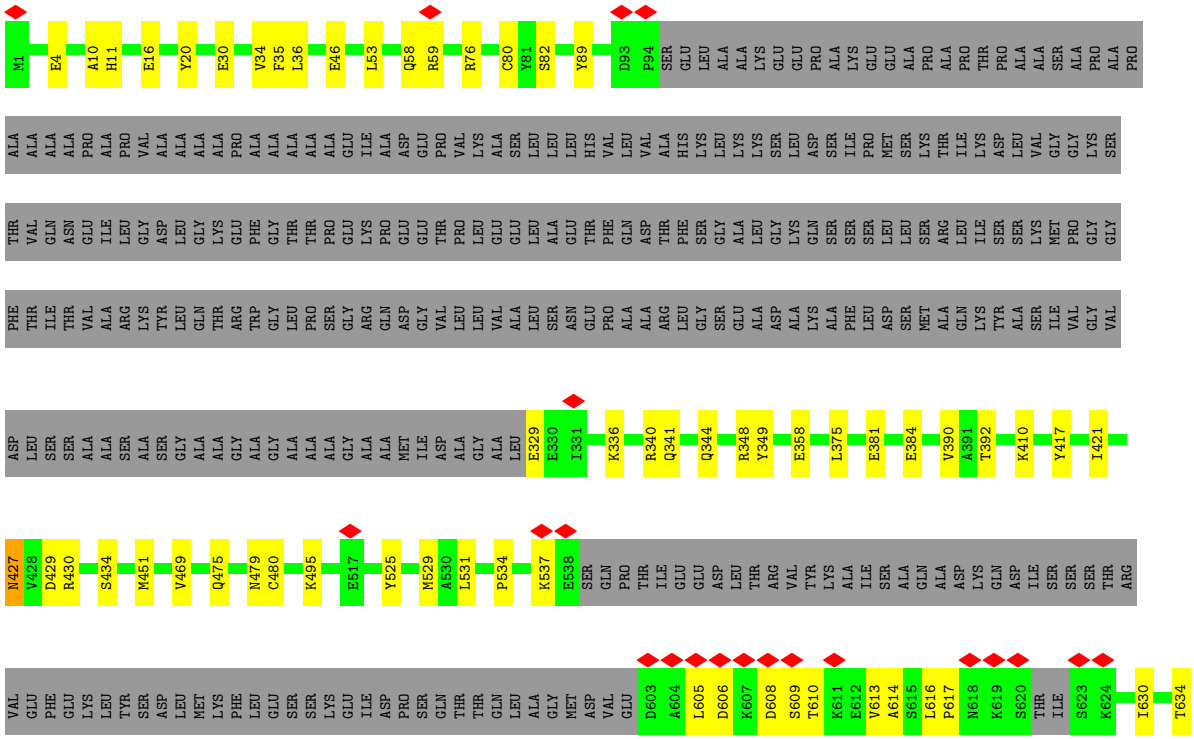
Chain H:

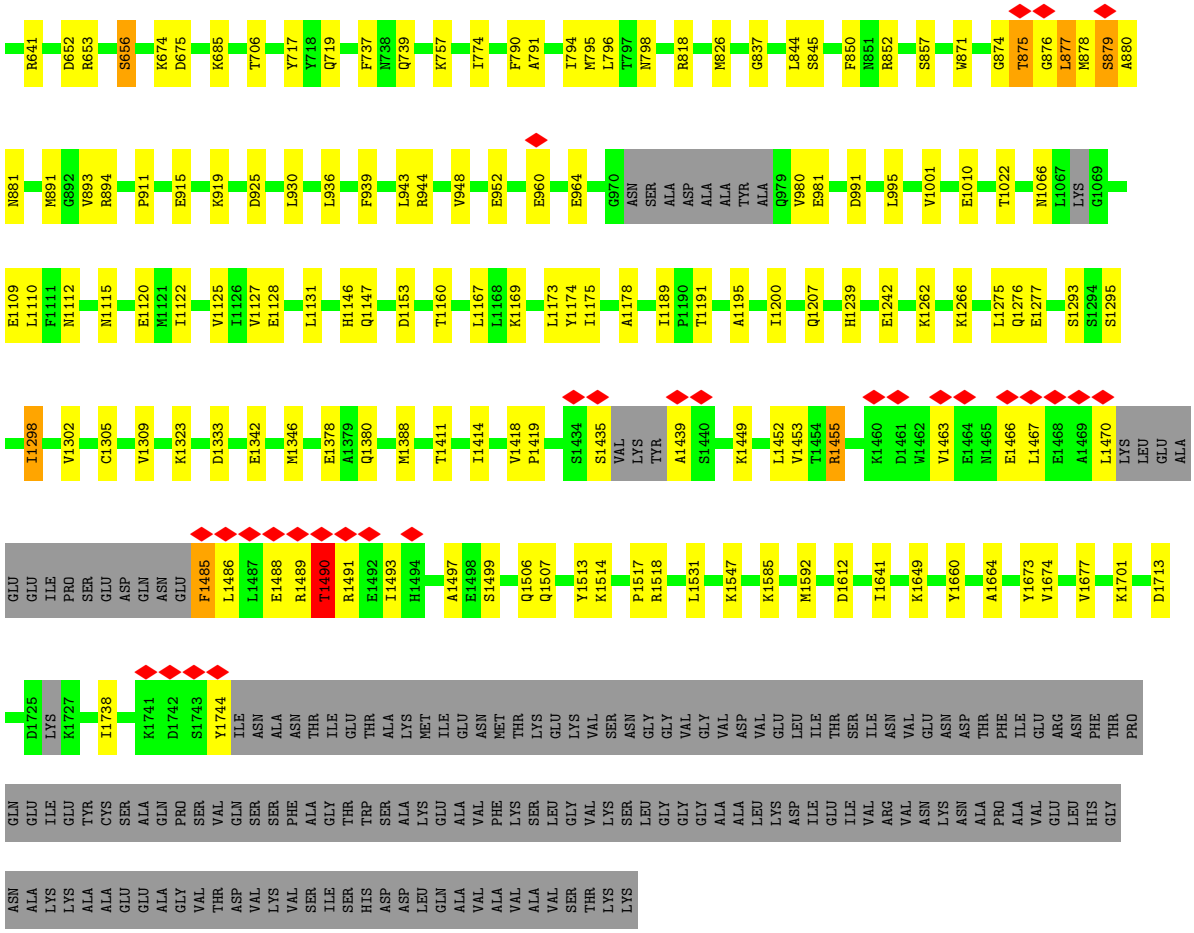




• Molecule 2: Fatty acid synthase subunit alpha

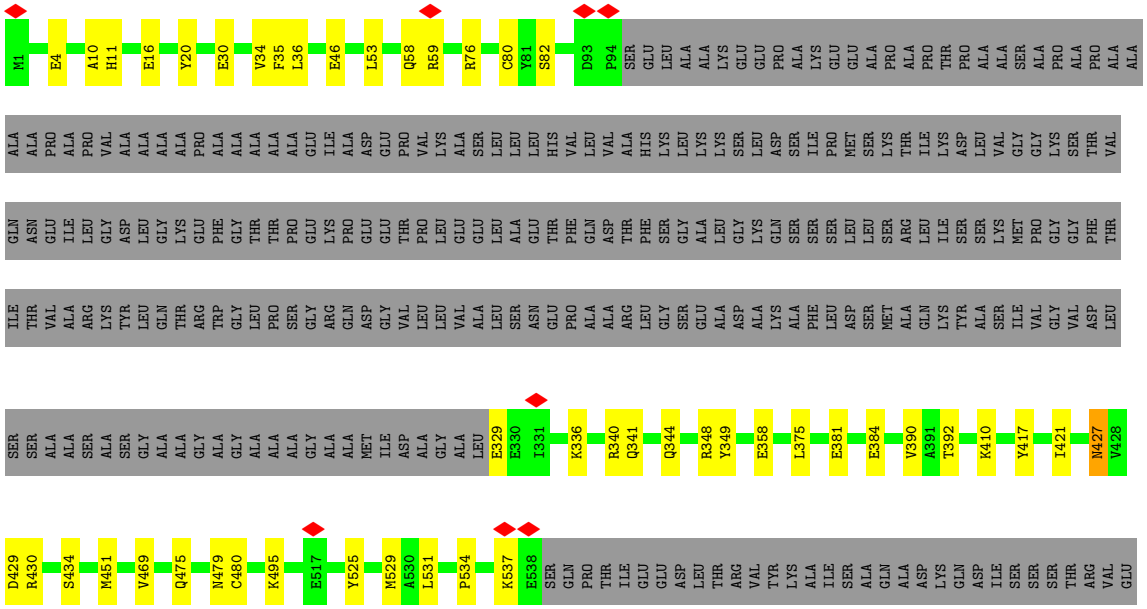
Chain K:

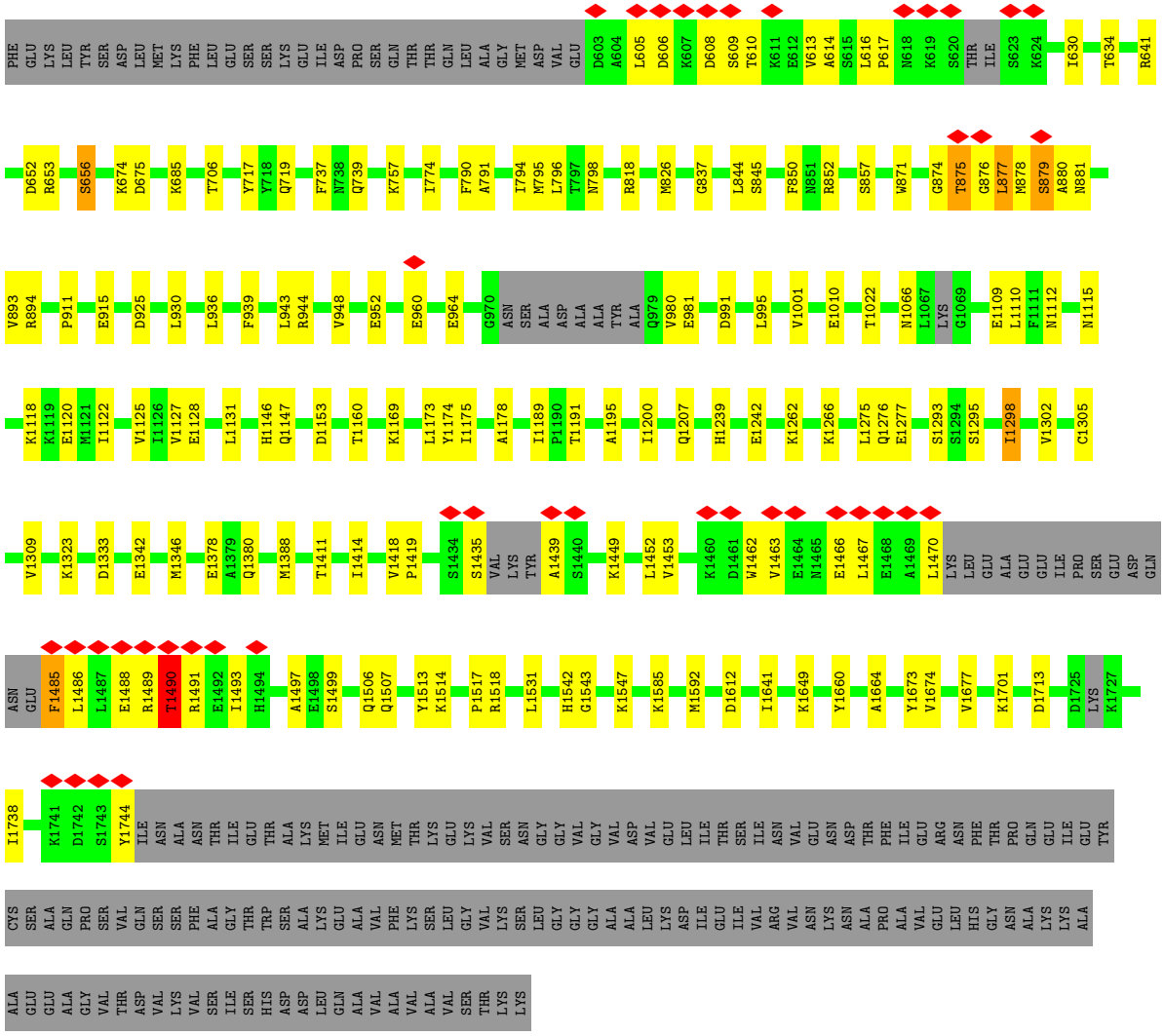




• Molecule 2: Fatty acid synthase subunit alpha

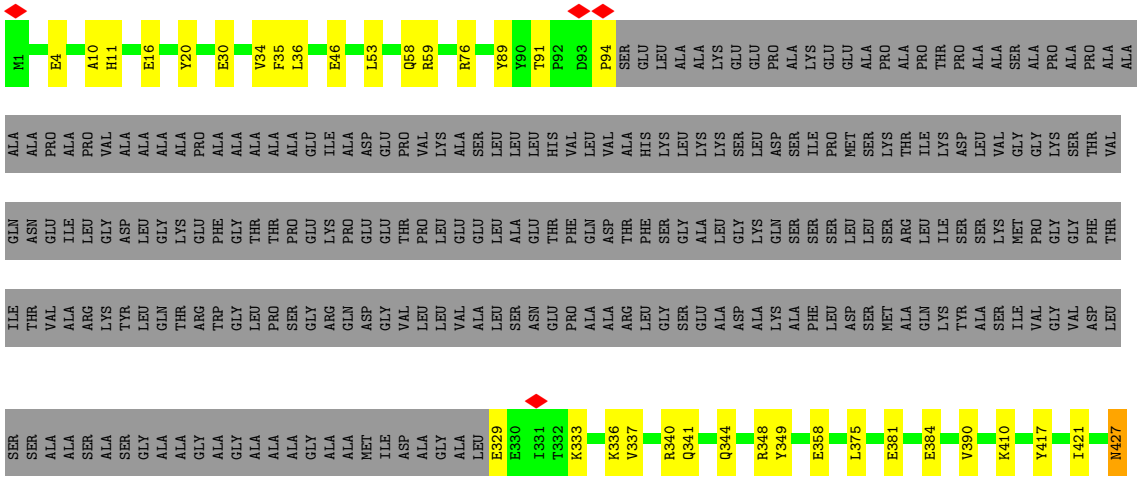
Chain N:

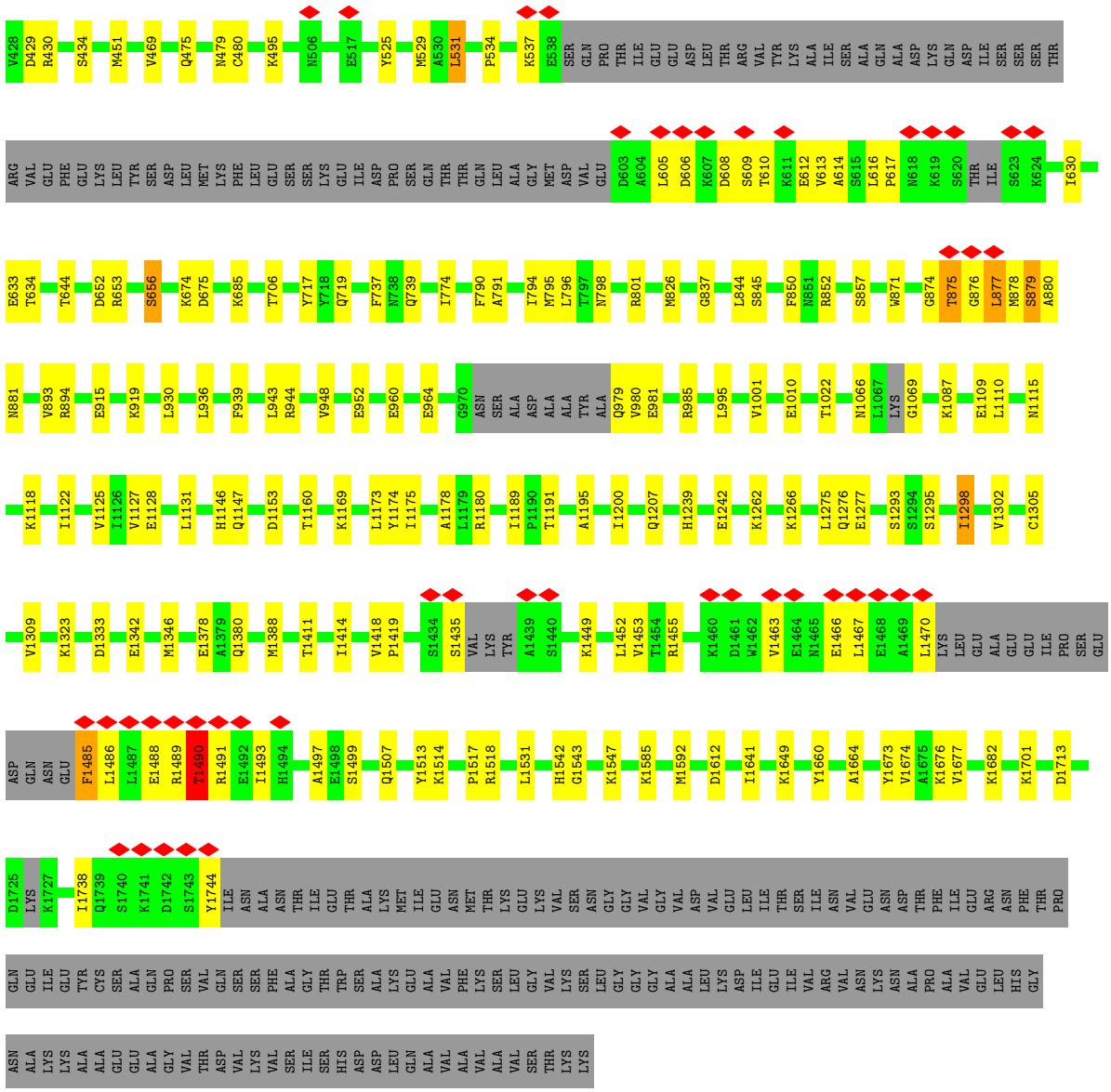




- Molecule 2: Fatty acid synthase subunit alpha

Chain Q:




V428 D429 R430 S434 M451 V469 Q475 N479 C480 K495 N506 E517 Y525 M529 A530 L531 P534 K537 E538 SER GLN PRO THR ILE GLU GLU ASP LEU THR ARG VAL TYR LYS ALA ILE SER ALA GLN ALA ASP LYS GLN ASP ILE SER SER SER THR
ARG VAL GLU PHE GLU LYS LEU TYR SER ASP LEU MET LYS PHE LEU GLU SER SER LYS GLU ILE ASP PRO SER GLN THR THR GLN LEU ALA GLY MET ASP VAL GLU D603 A604 L605 D606 K607 D608 S609 T610 K611 E612 V613 A614 S615 L616 P617 N618 K619 S620 THR ILE S623 K624 I630
E633 T634 T644 D652 R653 S656 K674 D675 K685 T706 Y717 Y718 Q719 F737 N738 Q739 I774 F790 A791 I794 M795 L796 T797 N798 R801 M826 G837 L844 S845 F850 N851 R852 S857 W871 G874 T875 G876 L877 M878 S879 A880
N881 V893 R894 E915 K919 L930 L936 F939 L943 R944 V948 E952 E960 E964 G970 ASN SER ALA ASP ALA ALA TYR ALA Q979 V980 E981 R985 L995 V1001 E1010 T1022 N1066 L1067 LYS G1069 K1087 E1109 L1110 N1115
K1118 I1122 V1125 I1126 V1127 E1128 L1131 H1146 Q1147 D1153 T1160 K1169 L1173 Y1174 I1175 A1178 L1179 R1180 I1189 P1190 T1191 A1195 I1200 Q1207 H1239 E1242 K1262 K1266 L1275 Q1276 E1277 S1293 S1294 S1295 I1298 V1302 C1305
V1309 K1323 D1333 E1342 M1346 E1378 A1379 Q1380 M1388 T1411 I1414 V1418 P1419 S1434 S1435 VAL LYS TYR A1439 S1440 K1449 L1452 V1453 T1454 R1455 K1460 D1461 V1462 V1463 E1464 N1465 E1466 L1467 E1468 A1469 L1470 LYS LEU GLU ALA GLU GLU ILE PRO SER GLU
ASP GLN ASN GLU F1485 L1486 L1487 E1488 R1489 T1490 R1491 E1492 I1493 H1494 A1497 E1498 S1499 Q1507 Y1513 K1514 P1517 R1518 L1531 H1542 G1543 K1547 K1585 M1592 D1612 I1641 K1649 Y1660 A1664 Y1673 V1674 A1675 K1676 V1677 K1682 K1701 D1713
D1725 LYS K1727 I1738 Q1739 S1740 K1741 D1742 S1743 Y1744 ILE ASN ALA ASN THR ILE GLU THR ALA LYS MET ILE GLU ASN MET THR LYS GLU LYS VAL SER ASN GLY GLY VAL GLY VAL ASP VAL GLU LEU ILE THR SER ILE ASN VAL GLU ASN ASP THR PHE ILE GLU ARG ASN PHE THR PRO
GLN GLU ILE GLU TYR CYS SER ALA GLN PRO SER VAL GLN SER SER PHE ALA GLY THR TRP SER ALA ALA LYS GLU ALA VAL PHE LYS SER SER LEU GLY VAL LYS SER LEU GLY GLY GLY ALA ALA LEU LYS ASP ILE GLU ILE VAL ARG VAL ASN LYS ASN ALA PRO ALA VAL GLU LEU HIS GLY
ASN ALA LYS LYS ALA ALA GLU GLU ALA GLY VAL THR ASP VAL LYS VAL SER ILE SER HIS ASP ASP LEU GLN ALA VAL ALA VAL ALA VAL SER THR LYS LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	260044	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.559	Depositor
Minimum map value	-0.823	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.209	Depositor
Map size (Å)	323.64, 323.64, 323.64	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93000007, 0.93000007, 0.93000007	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: NDP, 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	0.42	0/15968	0.49	6/21703 (0.0%)
1	E	0.42	0/15968	0.49	6/21703 (0.0%)
1	I	0.42	0/15968	0.49	6/21703 (0.0%)
1	L	0.42	0/15968	0.49	6/21703 (0.0%)
1	O	0.42	0/15968	0.49	6/21703 (0.0%)
1	R	0.42	0/15968	0.49	6/21703 (0.0%)
2	B	0.66	1/11192 (0.0%)	0.60	3/15140 (0.0%)
2	D	0.66	1/11192 (0.0%)	0.60	3/15140 (0.0%)
2	H	0.66	1/11192 (0.0%)	0.60	3/15140 (0.0%)
2	K	0.66	1/11192 (0.0%)	0.60	3/15140 (0.0%)
2	N	0.66	1/11192 (0.0%)	0.60	3/15140 (0.0%)
2	Q	0.66	1/11192 (0.0%)	0.60	3/15140 (0.0%)
All	All	0.53	6/162960 (0.0%)	0.54	54/221058 (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	1
1	E	0	1
1	I	0	1
1	L	0	1
1	O	0	1
1	R	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1115	ASN	C-O	-6.08	1.20	1.25
2	K	1115	ASN	C-O	-6.07	1.20	1.25
2	H	1115	ASN	C-O	-6.04	1.20	1.25
2	Q	1115	ASN	C-O	-6.04	1.20	1.25
2	B	1115	ASN	C-O	-6.00	1.20	1.25

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	600	CYS	N-CA-C	10.13	122.32	111.28
1	L	600	CYS	N-CA-C	10.10	122.29	111.28
1	R	600	CYS	N-CA-C	10.10	122.29	111.28
1	A	600	CYS	N-CA-C	10.08	122.26	111.28
1	E	600	CYS	N-CA-C	10.08	122.26	111.28

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	598	THR	Peptide
1	E	598	THR	Peptide
1	I	598	THR	Peptide
1	L	598	THR	Peptide
1	O	598	THR	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	15605	0	15434	218	0
1	E	15605	0	15434	223	0
1	I	15605	0	15434	224	0
1	L	15605	0	15434	253	0
1	O	15605	0	15434	252	0
1	R	15605	0	15434	225	0
2	B	10978	0	10833	227	0
2	D	10978	0	10833	221	0
2	H	10978	0	10833	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	10978	0	10833	228	0
2	N	10978	0	10833	225	0
2	Q	10978	0	10833	231	0
3	A	31	0	19	2	0
3	E	31	0	19	2	0
3	I	31	0	19	2	0
3	L	31	0	19	2	0
3	O	31	0	19	2	0
3	R	31	0	19	2	0
4	B	48	0	26	4	0
4	D	48	0	26	4	0
4	H	48	0	26	4	0
4	K	48	0	26	4	0
4	N	48	0	26	4	0
4	Q	48	0	26	4	0
5	A	379	0	0	35	0
5	B	457	0	0	39	0
5	D	450	0	0	34	0
5	E	381	0	0	37	0
5	H	492	0	0	43	0
5	I	378	0	0	43	0
5	K	470	0	0	40	0
5	L	378	0	0	69	0
5	N	465	0	0	40	0
5	O	381	0	0	71	0
5	Q	489	0	0	44	0
5	R	378	0	0	40	0
All	All	165070	0	157872	2468	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 8.

The worst 5 of 2468 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:475:GLN:NE2	2:N:614:ALA:CB	1.73	1.51
2:B:475:GLN:NE2	2:B:614:ALA:CB	1.73	1.50
2:D:475:GLN:NE2	2:D:614:ALA:CB	1.73	1.50
2:Q:475:GLN:NE2	2:Q:614:ALA:CB	1.73	1.50
2:H:475:GLN:NE2	2:H:614:ALA:CB	1.73	1.47

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	2007/2051 (98%)	1951 (97%)	53 (3%)	3 (0%)	48	60
1	E	2007/2051 (98%)	1950 (97%)	54 (3%)	3 (0%)	48	60
1	I	2007/2051 (98%)	1950 (97%)	54 (3%)	3 (0%)	48	60
1	L	2007/2051 (98%)	1951 (97%)	53 (3%)	3 (0%)	48	60
1	O	2007/2051 (98%)	1951 (97%)	53 (3%)	3 (0%)	48	60
1	R	2007/2051 (98%)	1950 (97%)	54 (3%)	3 (0%)	48	60
2	B	1399/1887 (74%)	1365 (98%)	34 (2%)	0	100	100
2	D	1399/1887 (74%)	1365 (98%)	34 (2%)	0	100	100
2	H	1399/1887 (74%)	1365 (98%)	34 (2%)	0	100	100
2	K	1399/1887 (74%)	1365 (98%)	34 (2%)	0	100	100
2	N	1399/1887 (74%)	1365 (98%)	34 (2%)	0	100	100
2	Q	1399/1887 (74%)	1365 (98%)	34 (2%)	0	100	100
All	All	20436/23628 (86%)	19893 (97%)	525 (3%)	18 (0%)	49	60

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	E	75	SER
1	I	75	SER
1	L	75	SER
1	O	75	SER

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	1667/1789 (93%)	1641 (98%)	26 (2%)	55	73
1	E	1684/1789 (94%)	1659 (98%)	25 (2%)	57	75
1	I	1684/1789 (94%)	1658 (98%)	26 (2%)	57	75
1	L	1684/1789 (94%)	1658 (98%)	26 (2%)	57	75
1	O	1684/1789 (94%)	1659 (98%)	25 (2%)	57	75
1	R	1684/1789 (94%)	1658 (98%)	26 (2%)	57	75
2	B	1166/1566 (74%)	1141 (98%)	25 (2%)	47	66
2	D	1166/1566 (74%)	1140 (98%)	26 (2%)	45	65
2	H	1166/1566 (74%)	1141 (98%)	25 (2%)	47	66
2	K	1166/1566 (74%)	1140 (98%)	26 (2%)	45	65
2	N	1166/1566 (74%)	1142 (98%)	24 (2%)	47	66
2	Q	1166/1566 (74%)	1140 (98%)	26 (2%)	45	65
All	All	17083/20130 (85%)	16777 (98%)	306 (2%)	51	70

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	163	GLN
1	R	586	LEU
1	O	827	VAL
2	Q	634	THR
1	R	1535	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 260 such sidechains are listed below:

Mol	Chain	Res	Type
2	Q	979	GLN
2	Q	1583	HIS
2	H	743	GLN
2	H	618	ASN

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Mol	Chain	Res	Type
1	R	660	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FMN	A	2101	-	33,33,33	1.49	5 (15%)	48,50,50	1.29	7 (14%)
4	NDP	D	1901	-	51,52,52	1.20	6 (11%)	71,80,80	1.59	12 (16%)
4	NDP	B	1901	-	51,52,52	1.20	6 (11%)	71,80,80	1.59	12 (16%)
4	NDP	H	1901	-	51,52,52	1.20	6 (11%)	71,80,80	1.59	12 (16%)
4	NDP	N	1901	-	51,52,52	1.20	6 (11%)	71,80,80	1.59	12 (16%)
3	FMN	I	2101	-	33,33,33	1.48	5 (15%)	48,50,50	1.29	8 (16%)
3	FMN	E	2101	-	33,33,33	1.49	5 (15%)	48,50,50	1.29	7 (14%)
4	NDP	K	1901	-	51,52,52	1.20	6 (11%)	71,80,80	1.58	12 (16%)
3	FMN	R	2101	-	33,33,33	1.48	5 (15%)	48,50,50	1.29	8 (16%)
4	NDP	Q	1901	-	51,52,52	1.20	6 (11%)	71,80,80	1.58	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FMN	O	2101	-	33,33,33	1.49	5 (15%)	48,50,50	1.30	7 (14%)
3	FMN	L	2101	-	33,33,33	1.48	5 (15%)	48,50,50	1.29	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	A	2101	-	-	2/18/18/18	0/3/3/3
4	NDP	D	1901	-	-	14/34/77/77	0/5/5/5
4	NDP	B	1901	-	-	14/34/77/77	0/5/5/5
4	NDP	H	1901	-	-	14/34/77/77	0/5/5/5
4	NDP	N	1901	-	-	14/34/77/77	0/5/5/5
3	FMN	I	2101	-	-	2/18/18/18	0/3/3/3
3	FMN	E	2101	-	-	2/18/18/18	0/3/3/3
4	NDP	K	1901	-	-	14/34/77/77	0/5/5/5
3	FMN	R	2101	-	-	2/18/18/18	0/3/3/3
4	NDP	Q	1901	-	-	14/34/77/77	0/5/5/5
3	FMN	O	2101	-	-	2/18/18/18	0/3/3/3
3	FMN	L	2101	-	-	2/18/18/18	0/3/3/3

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	2101	FMN	C9A-C5A	5.27	1.49	1.41
3	I	2101	FMN	C9A-C5A	5.27	1.49	1.41
3	A	2101	FMN	C9A-C5A	5.26	1.49	1.41
3	E	2101	FMN	C9A-C5A	5.26	1.49	1.41
3	R	2101	FMN	C9A-C5A	5.24	1.49	1.41

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1901	NDP	C5A-C4A-N3A	-5.69	118.88	126.72
4	D	1901	NDP	C5A-C4A-N3A	-5.65	118.93	126.72
4	B	1901	NDP	C5A-C4A-N3A	-5.65	118.94	126.72
4	K	1901	NDP	C5A-C4A-N3A	-5.64	118.95	126.72
4	N	1901	NDP	C5A-C4A-N3A	-5.64	118.95	126.72

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1901	NDP	C5B-O5B-PA-O1A
4	B	1901	NDP	C5B-O5B-PA-O2A
4	B	1901	NDP	C5B-O5B-PA-O3
4	B	1901	NDP	C5D-O5D-PN-O3
4	B	1901	NDP	C5D-O5D-PN-O1N

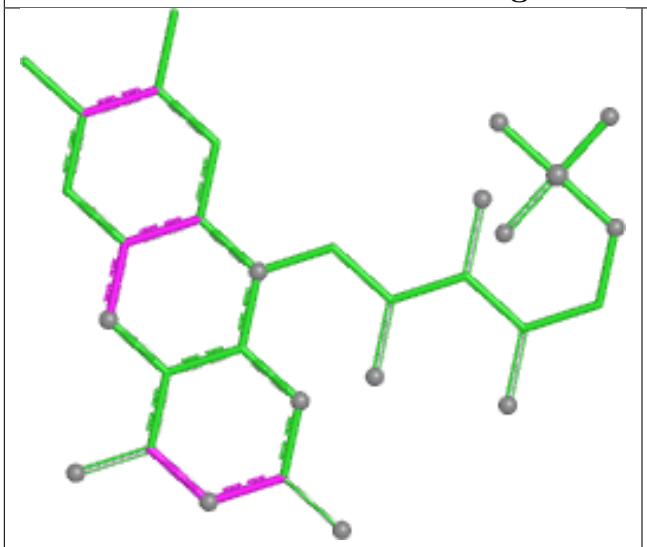
There are no ring outliers.

12 monomers are involved in 36 short contacts:

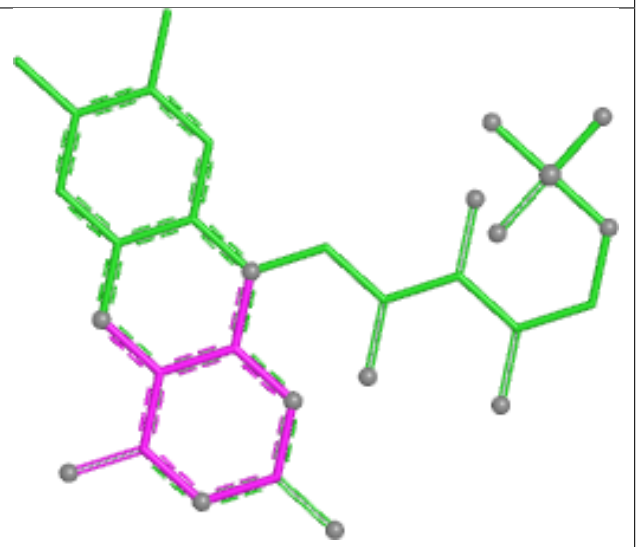
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2101	FMN	2	0
4	D	1901	NDP	4	0
4	B	1901	NDP	4	0
4	H	1901	NDP	4	0
4	N	1901	NDP	4	0
3	I	2101	FMN	2	0
3	E	2101	FMN	2	0
4	K	1901	NDP	4	0
3	R	2101	FMN	2	0
4	Q	1901	NDP	4	0
3	O	2101	FMN	2	0
3	L	2101	FMN	2	0

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.

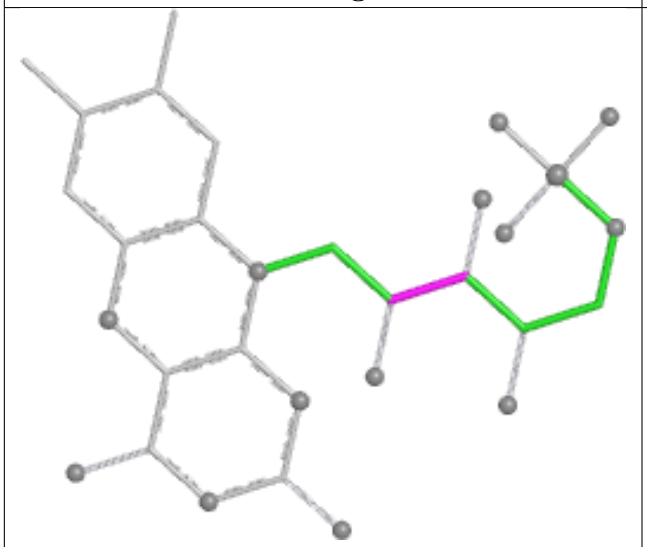
Ligand FMN A 2101



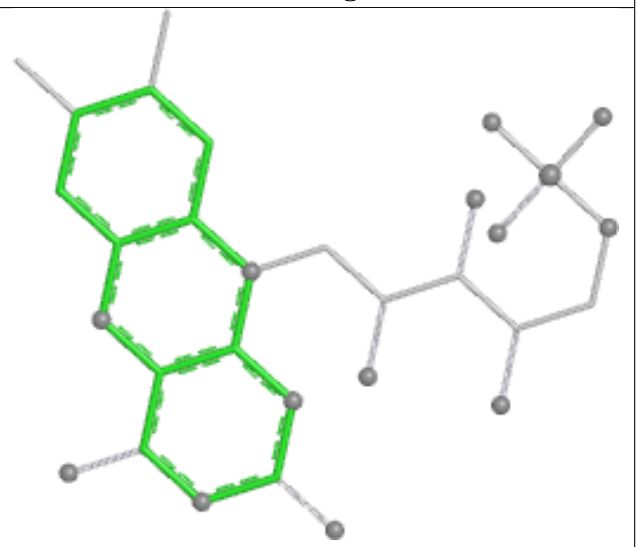
Bond lengths



Bond angles

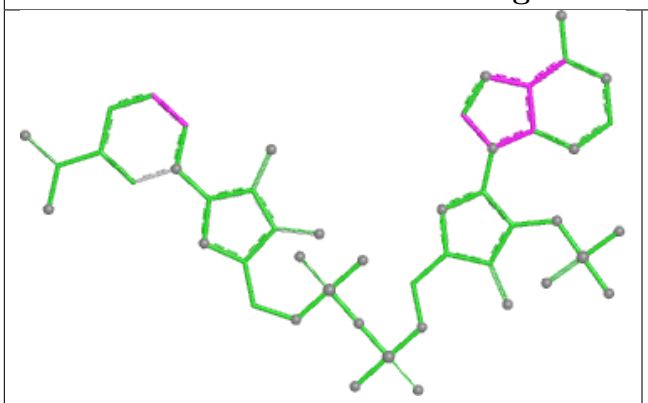


Torsions



Rings

Ligand NDP D 1901



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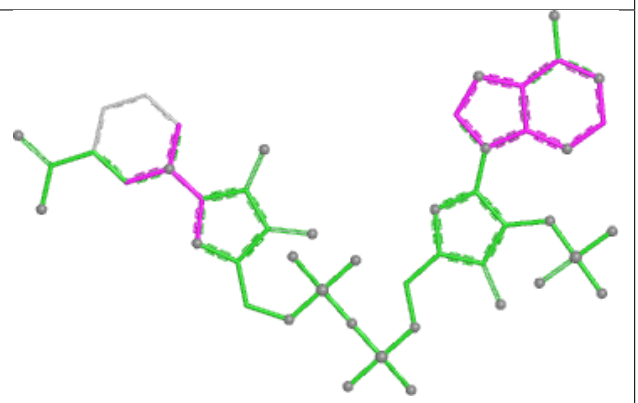

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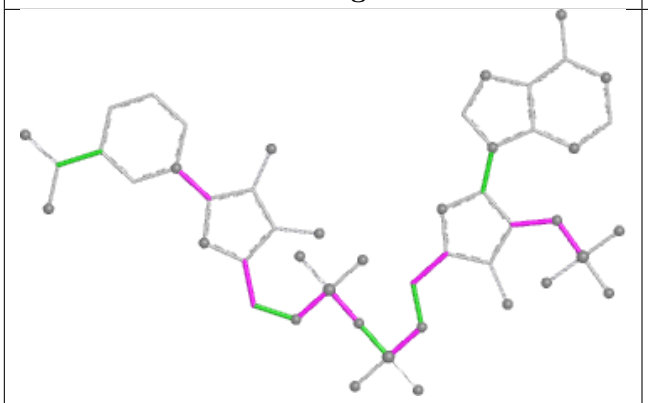
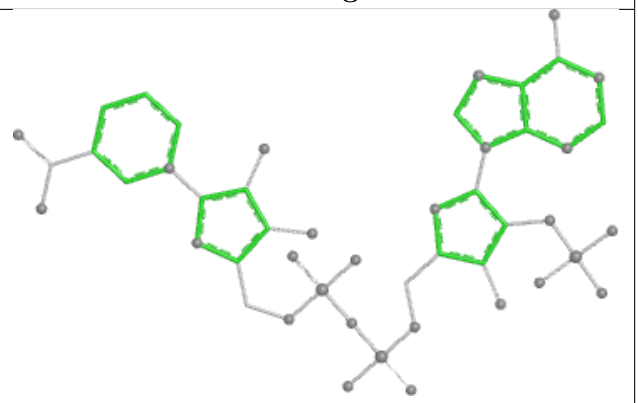
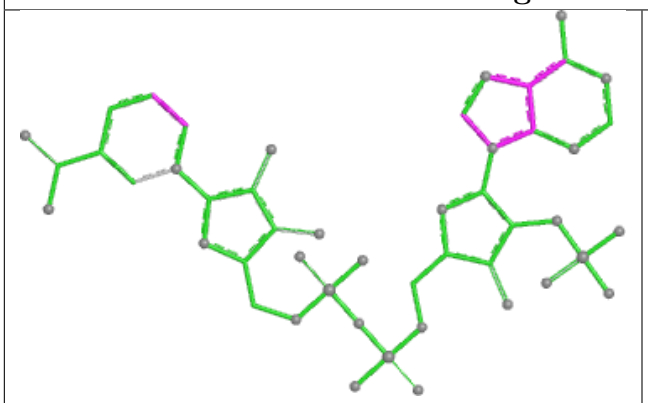


Torsions

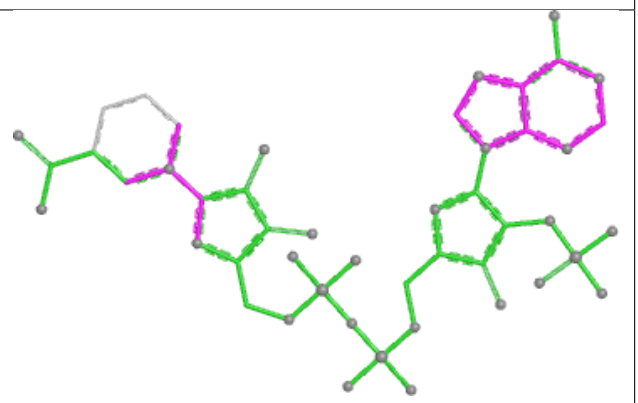


Rings

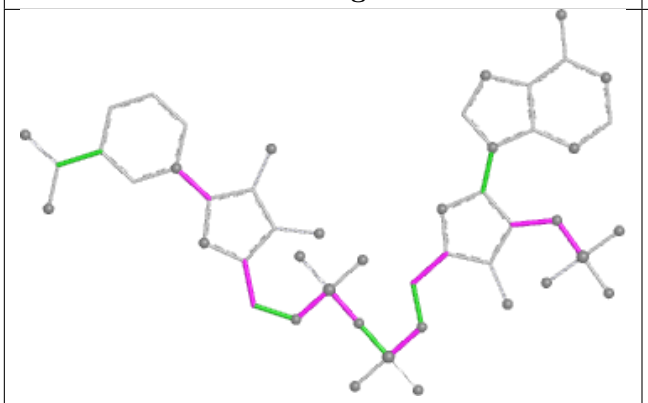
Ligand NDP B 1901



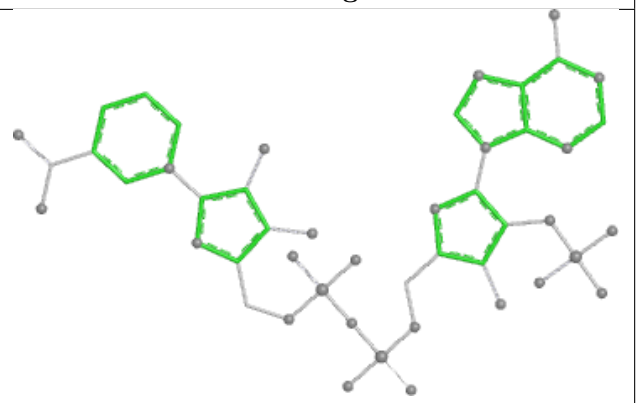
Bond lengths



Bond angles

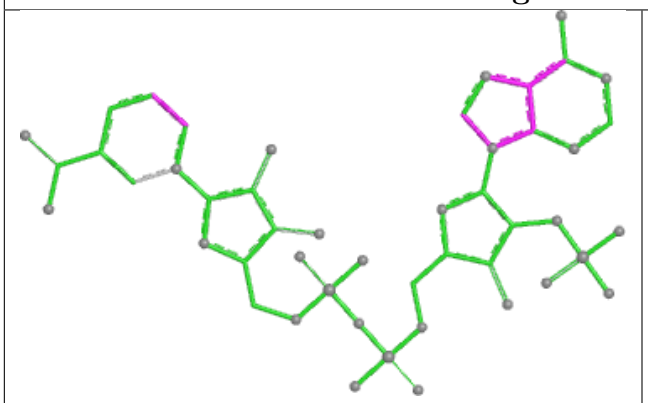


Torsions

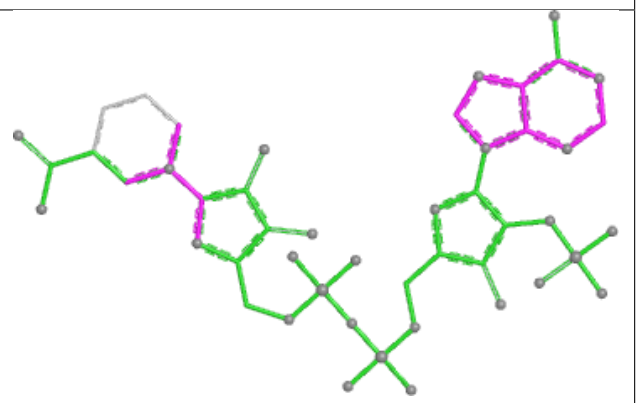


Rings

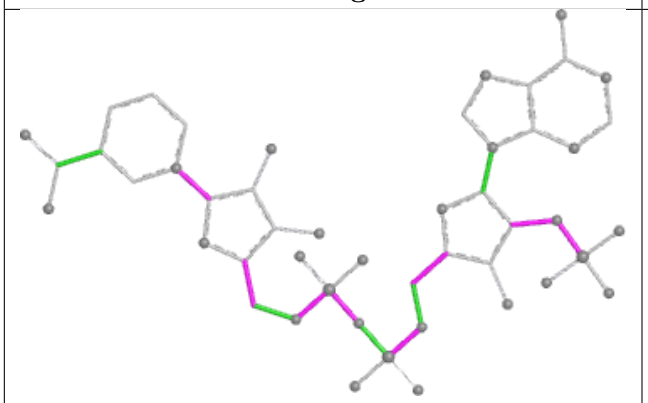
Ligand NDP H 1901



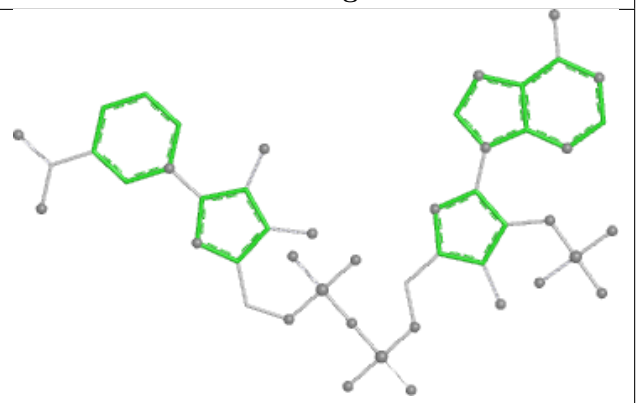
Bond lengths



Bond angles

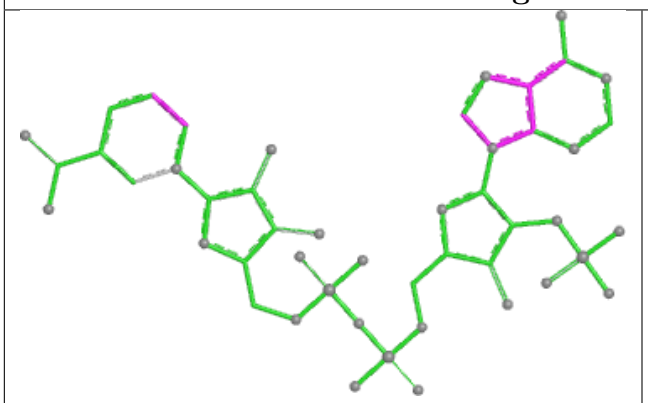


Torsions

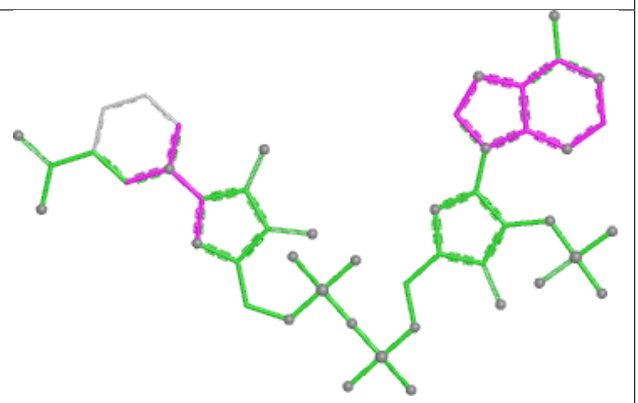


Rings

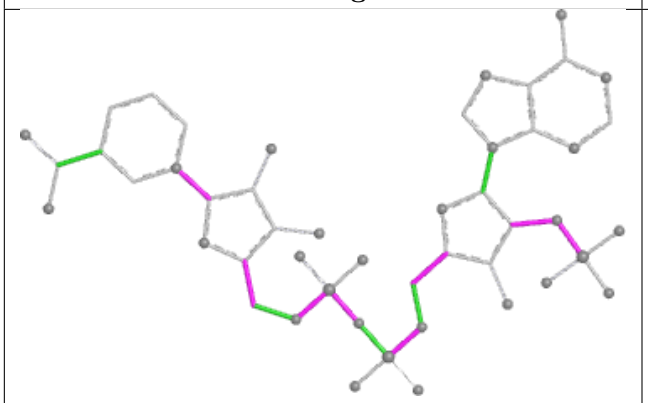
Ligand NDP N 1901



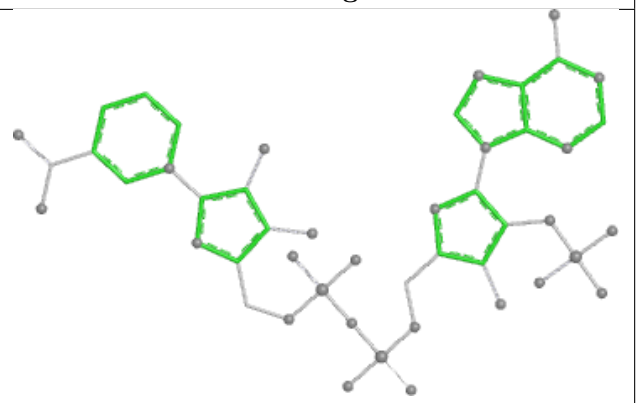
Bond lengths



Bond angles

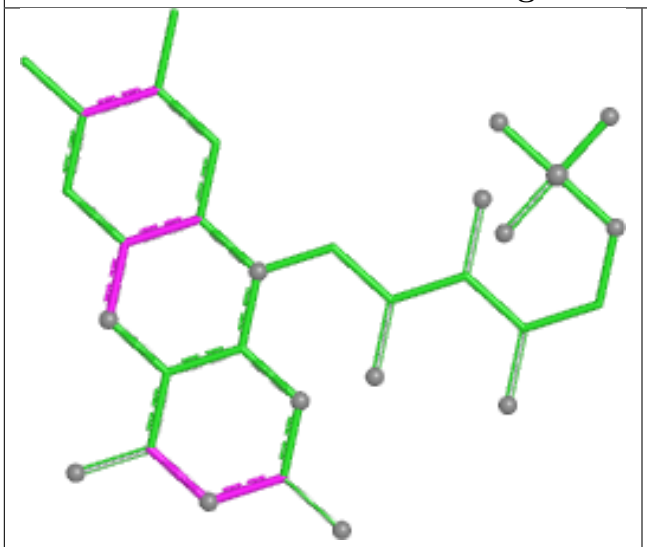


Torsions

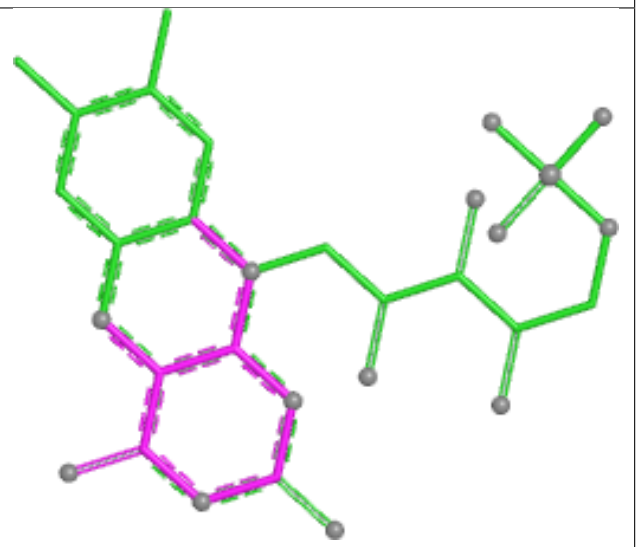


Rings

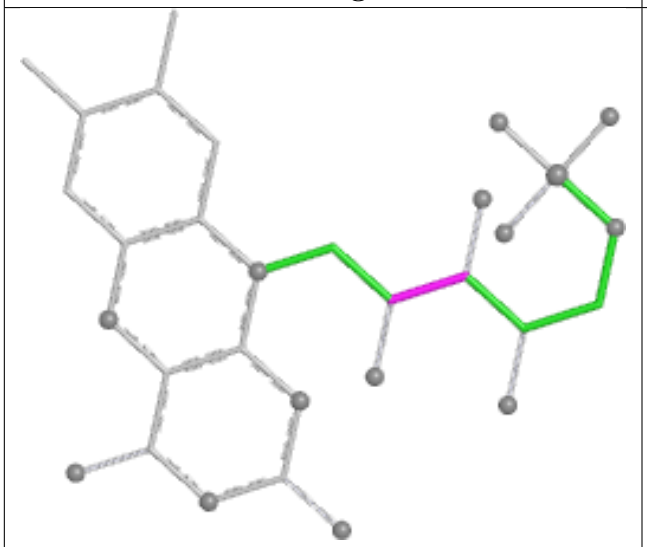
Ligand FMN I 2101



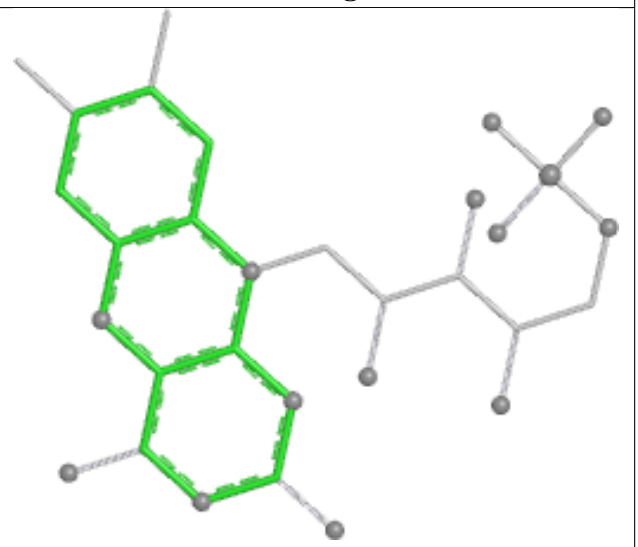
Bond lengths



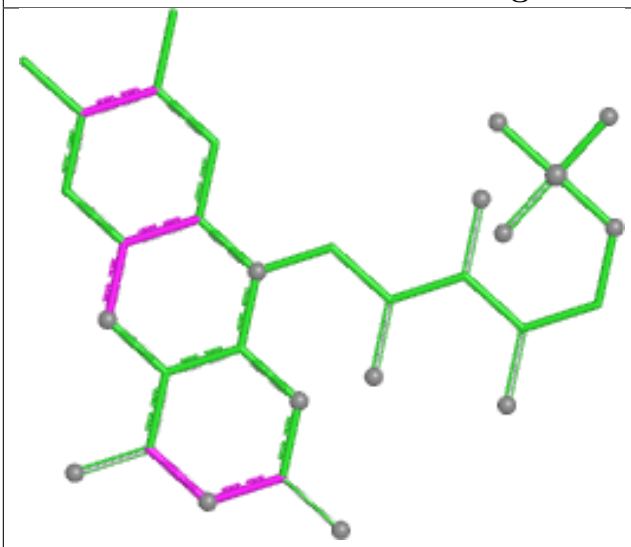
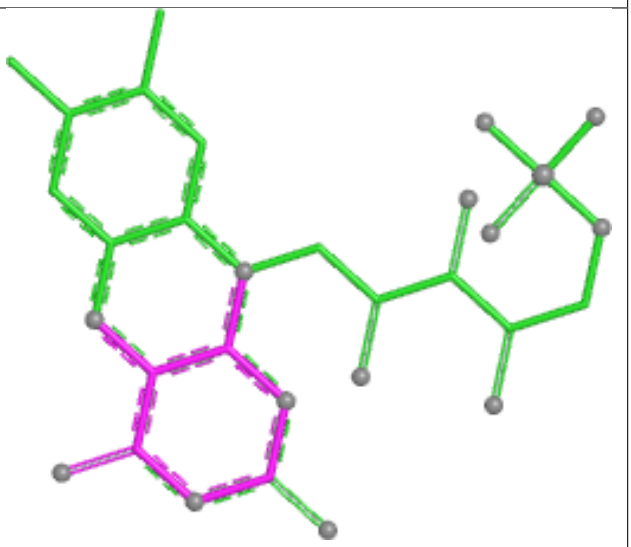
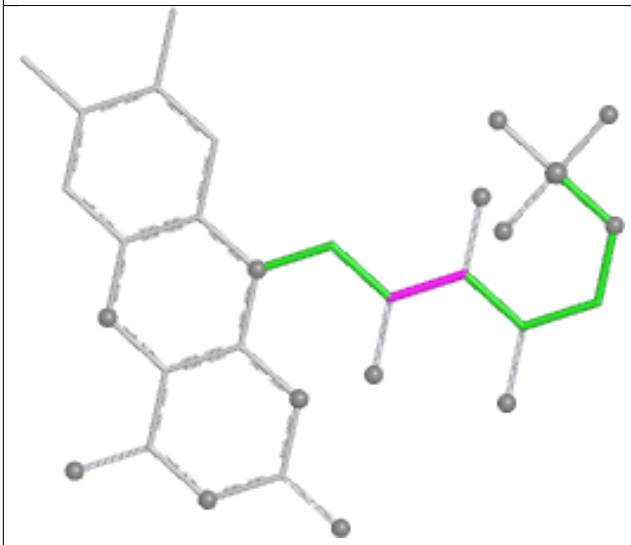
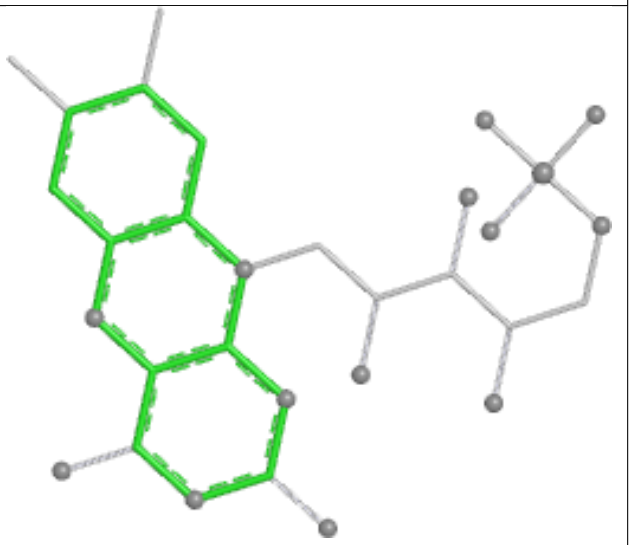
Bond angles

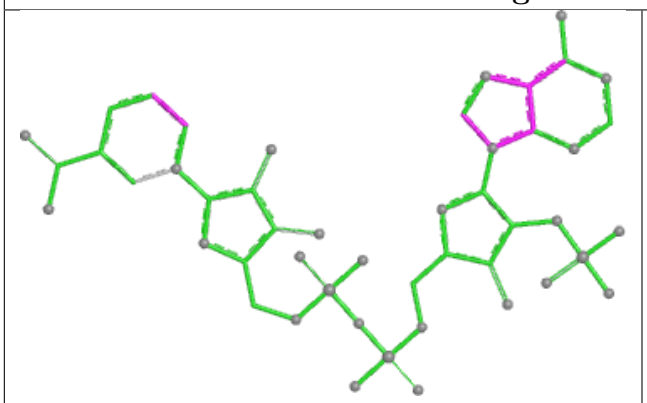
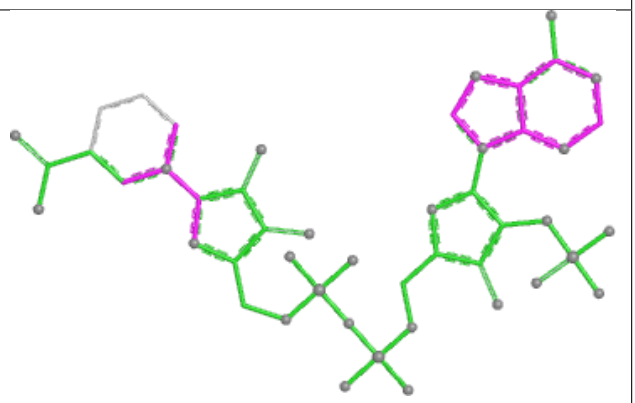
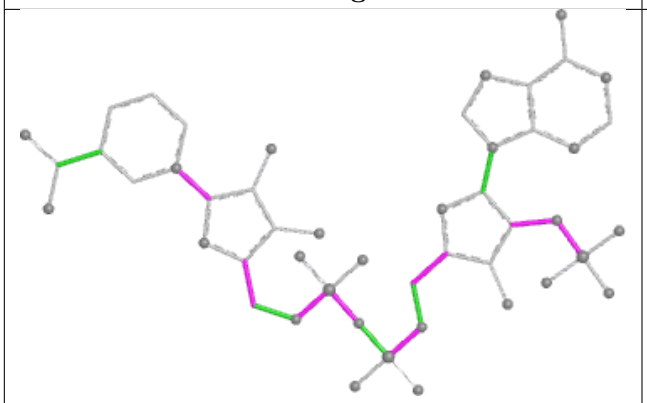
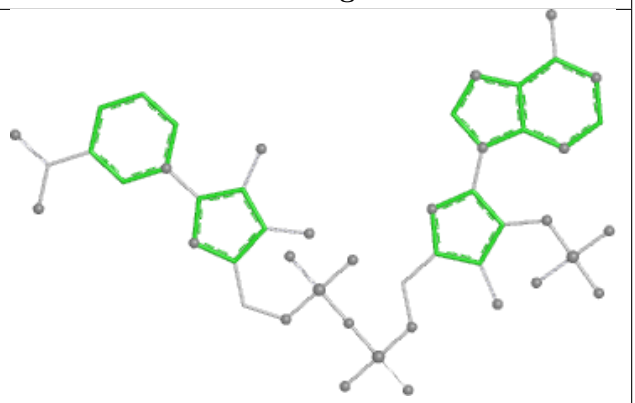


Torsions

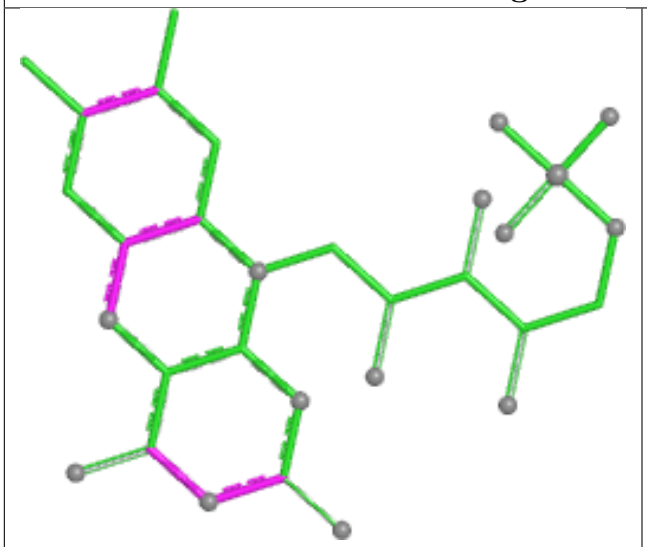


Rings

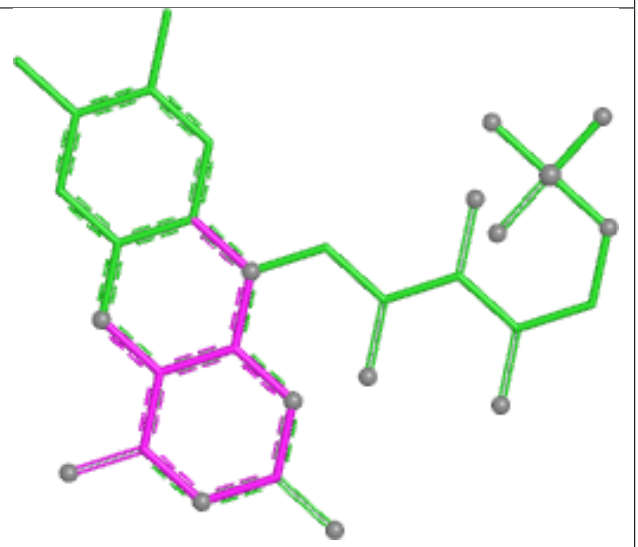
Ligand FMN E 2101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NDP K 1901	
 Bond lengths	 Bond angles
 Torsions	 Rings

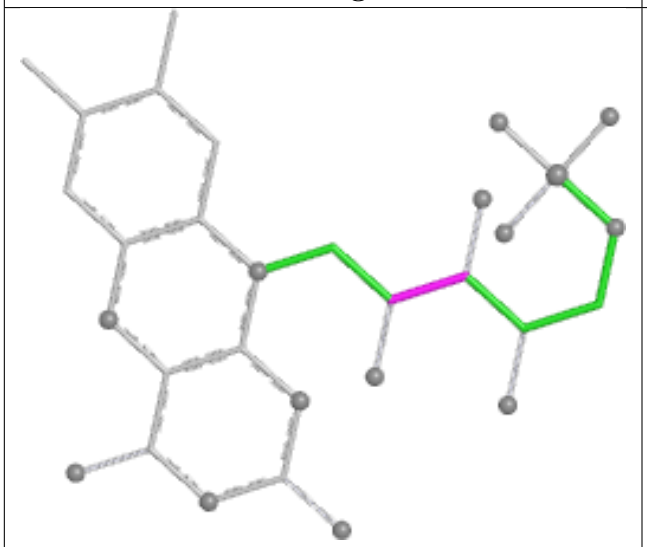
Ligand FMN R 2101



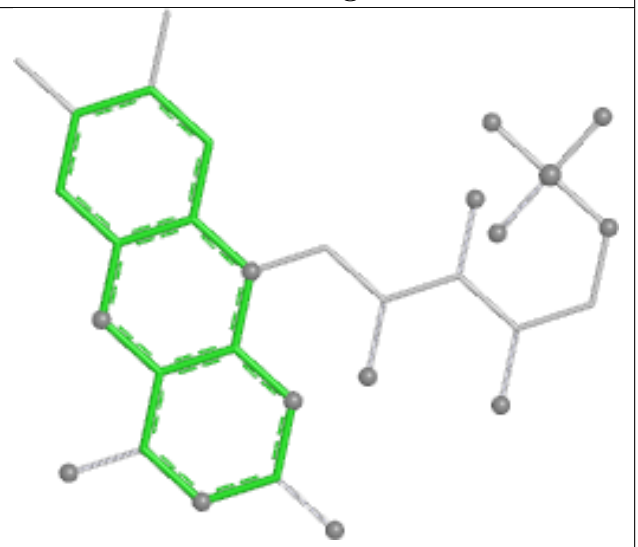
Bond lengths



Bond angles

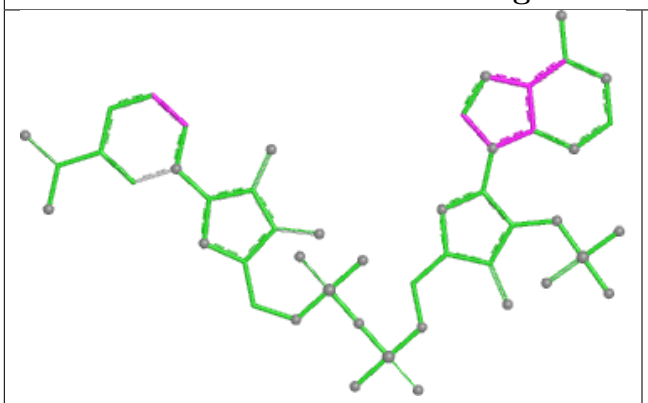


Torsions

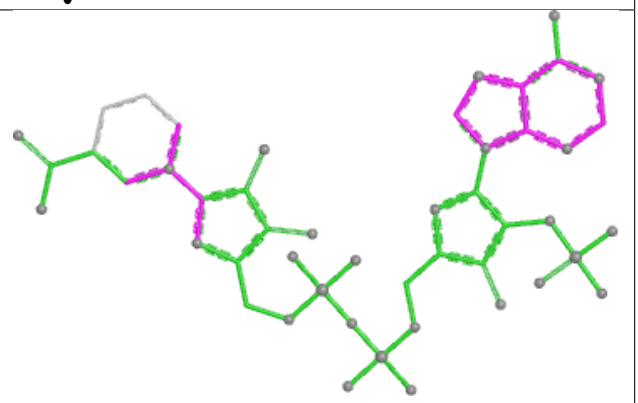


Rings

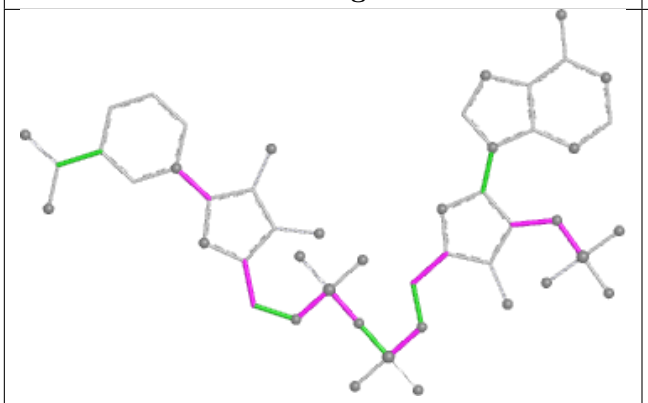
Ligand NDP Q 1901



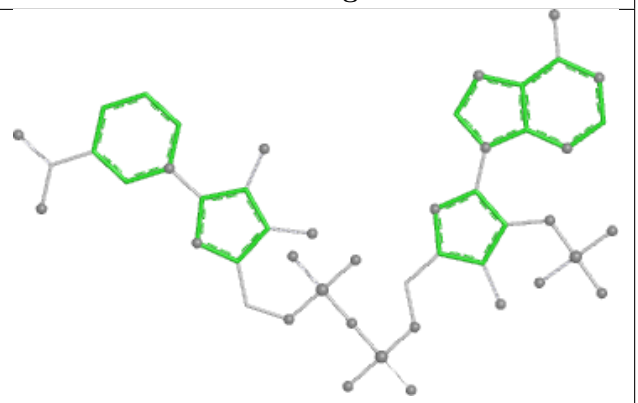
Bond lengths



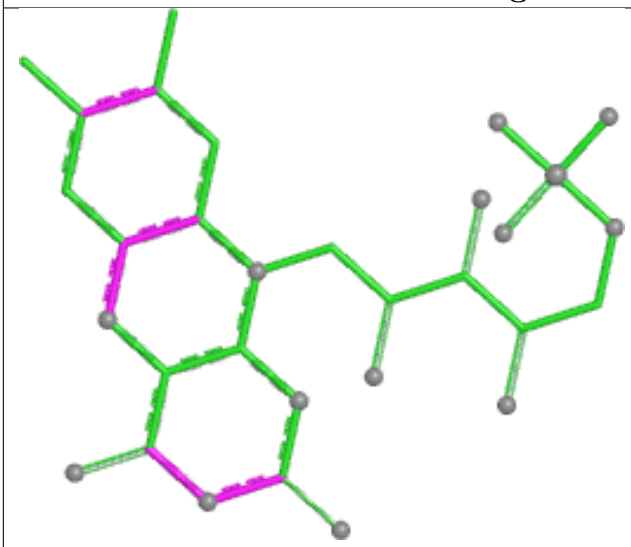
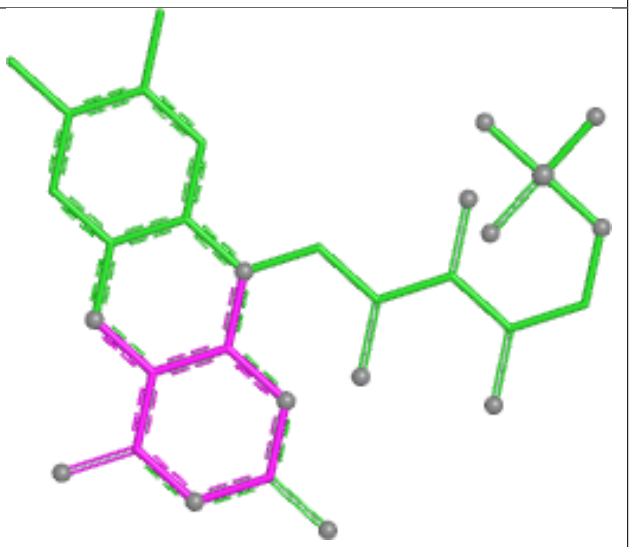
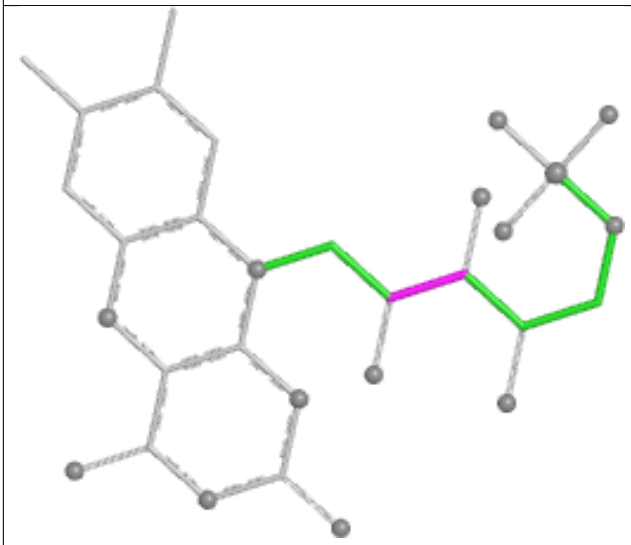
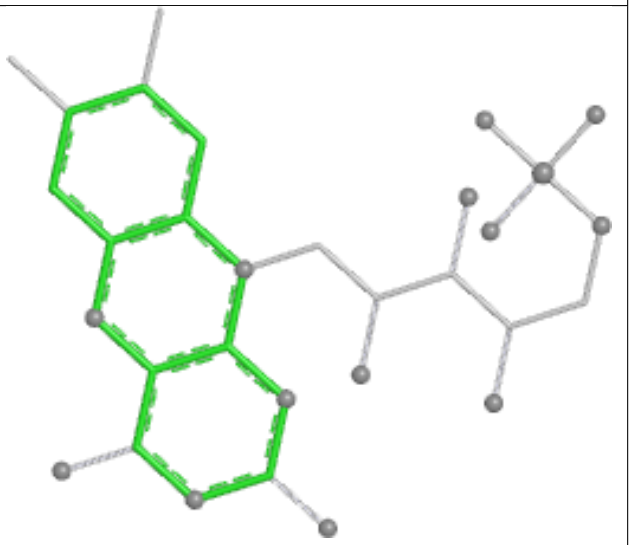
Bond angles

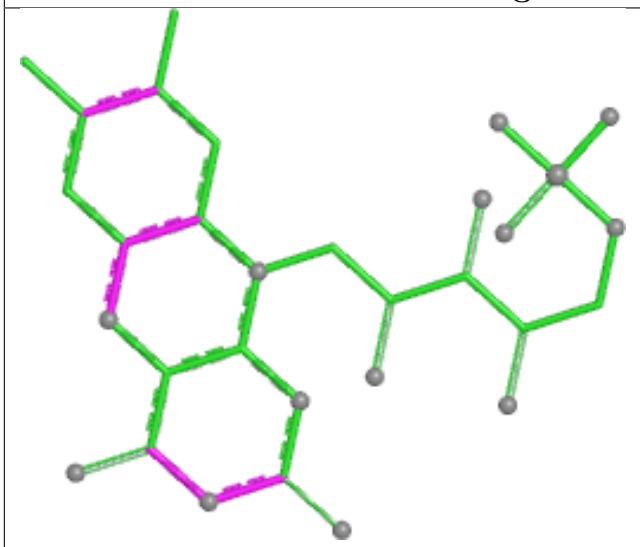
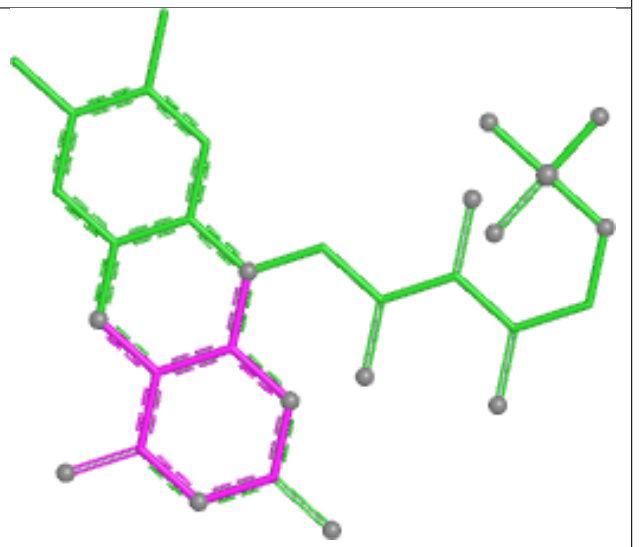
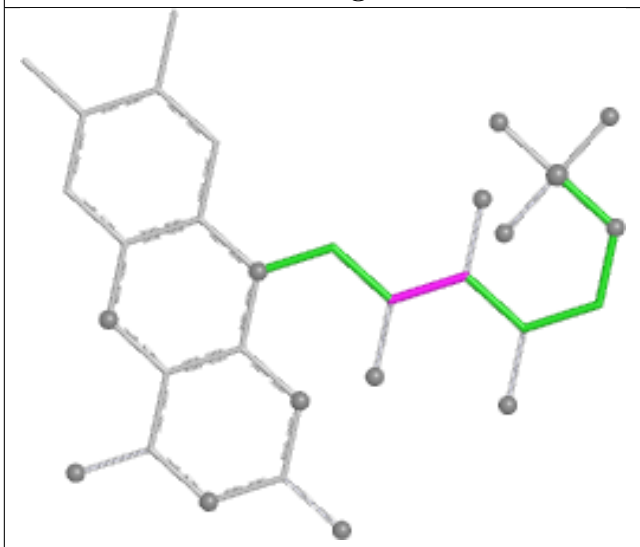
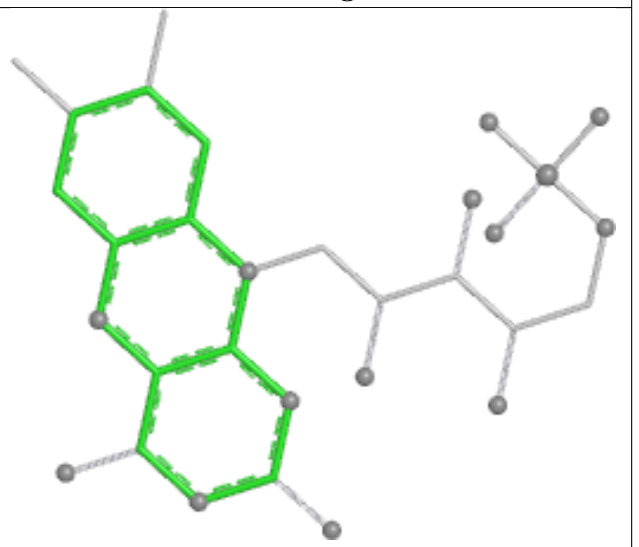


Torsions



Rings

Ligand FMN O 2101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FMN L 2101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

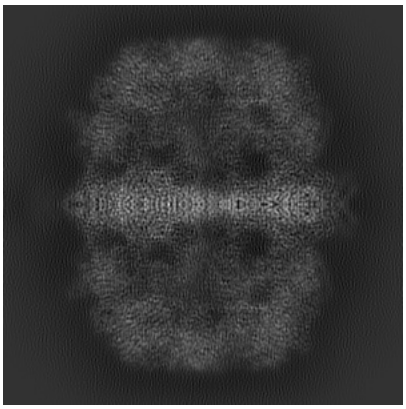
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-71285. These allow visual inspection of the internal detail of the map and identification of artifacts.

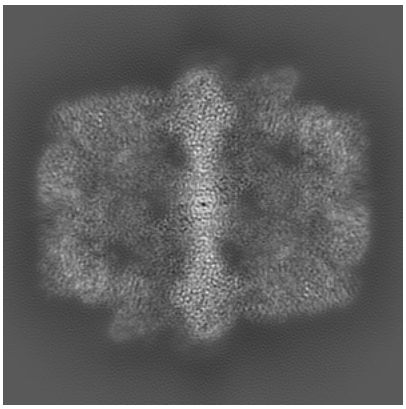
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

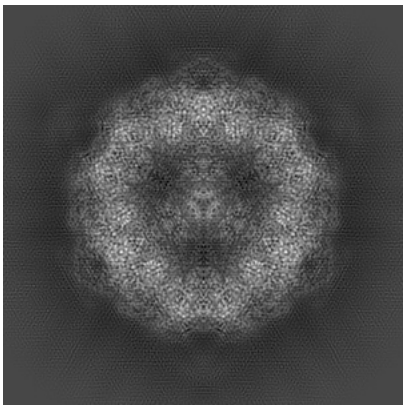
6.1.1 Primary map



X

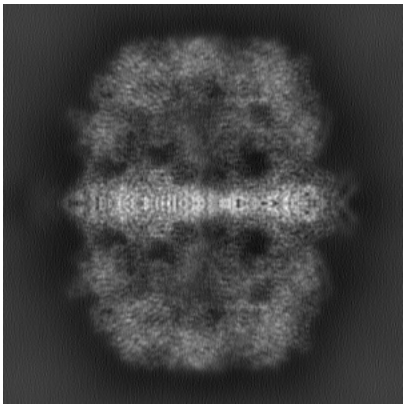


Y

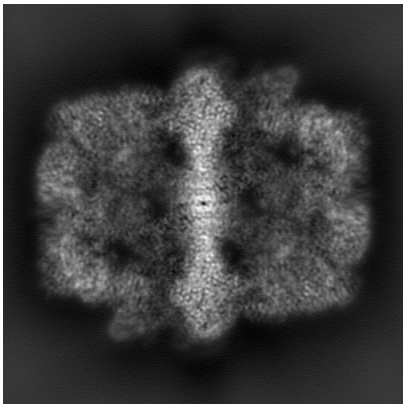


Z

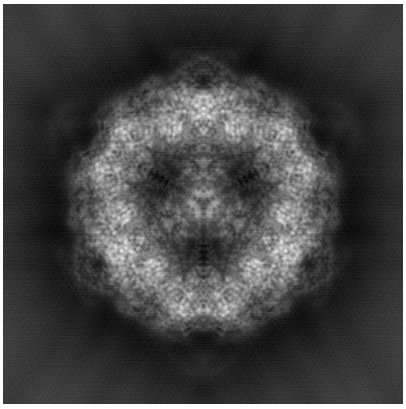
6.1.2 Raw map



X



Y

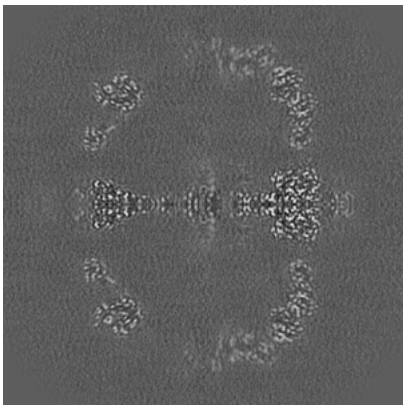


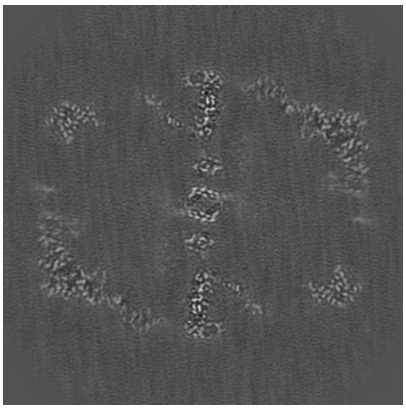
Z

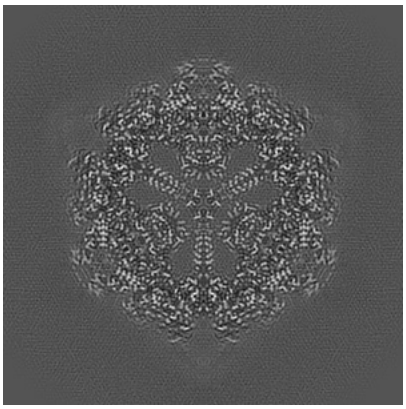
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

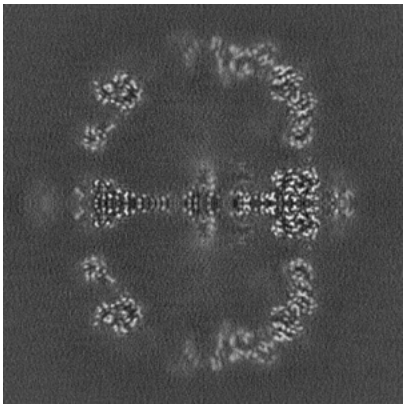
6.2.1 Primary map

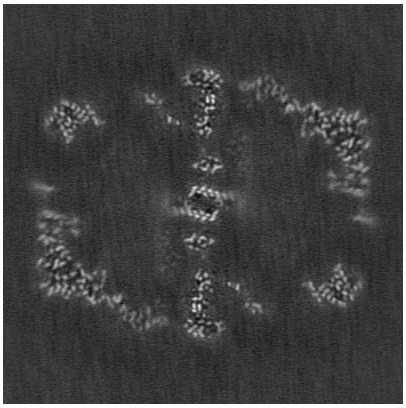

X Index: 174

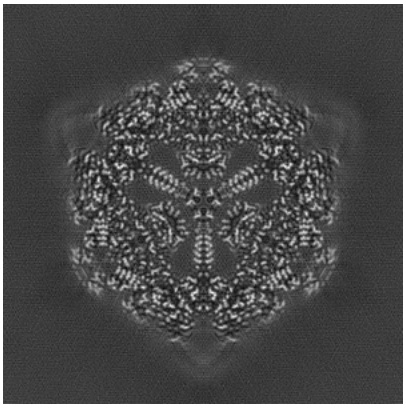

Y Index: 174


Z Index: 174

6.2.2 Raw map


X Index: 174

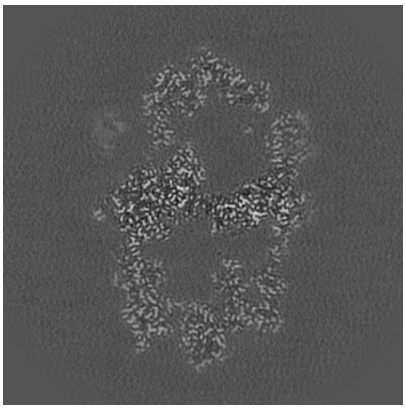

Y Index: 174

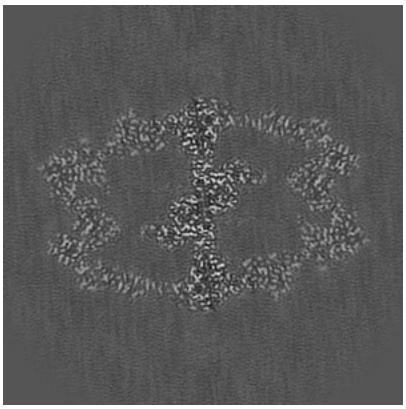

Z Index: 174

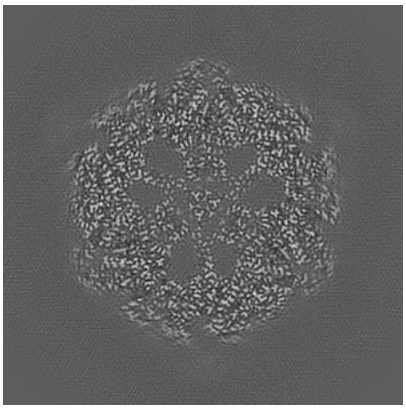
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

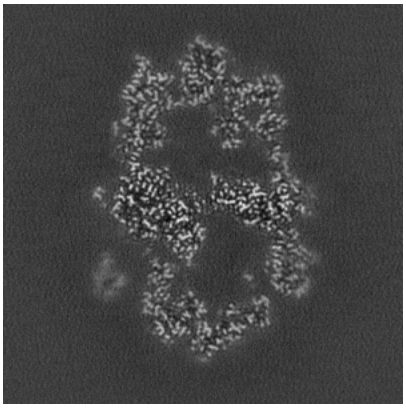
6.3.1 Primary map

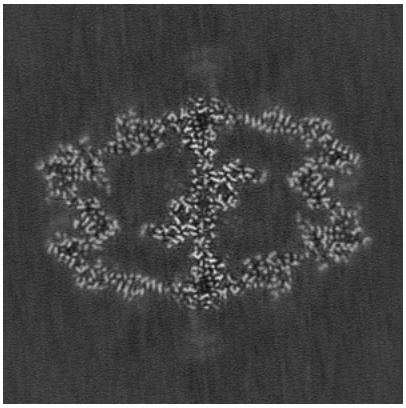

X Index: 103

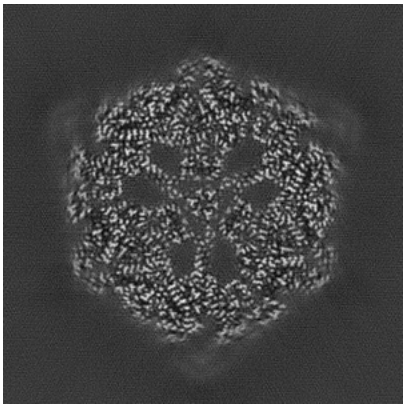

Y Index: 239


Z Index: 170

6.3.2 Raw map


X Index: 245

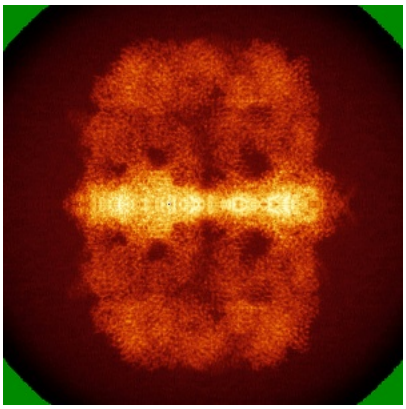

Y Index: 238

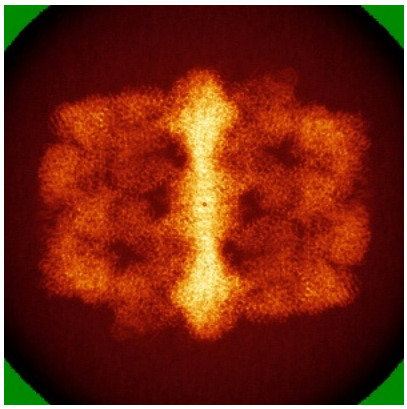

Z Index: 178

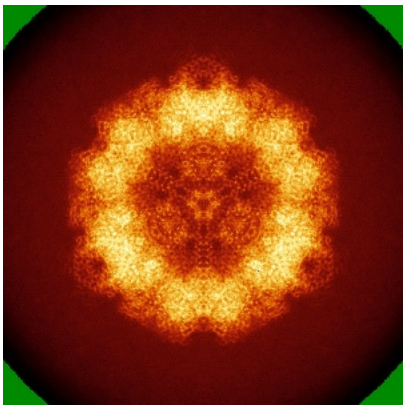
The images above show the largest variance slices of the map in three orthogonal directions.

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

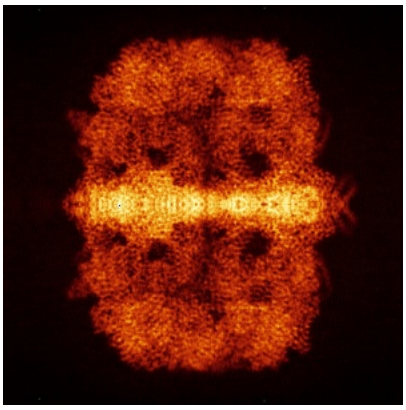
6.4.1 Primary map

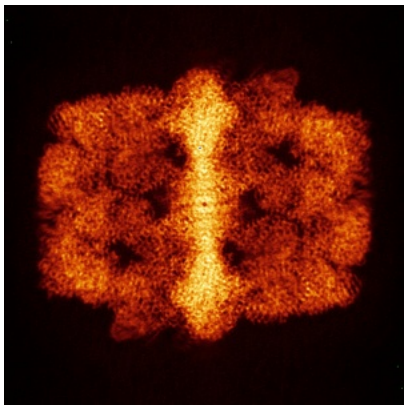

X

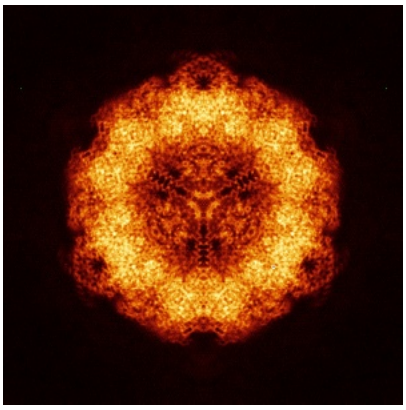

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

This section was not generated.

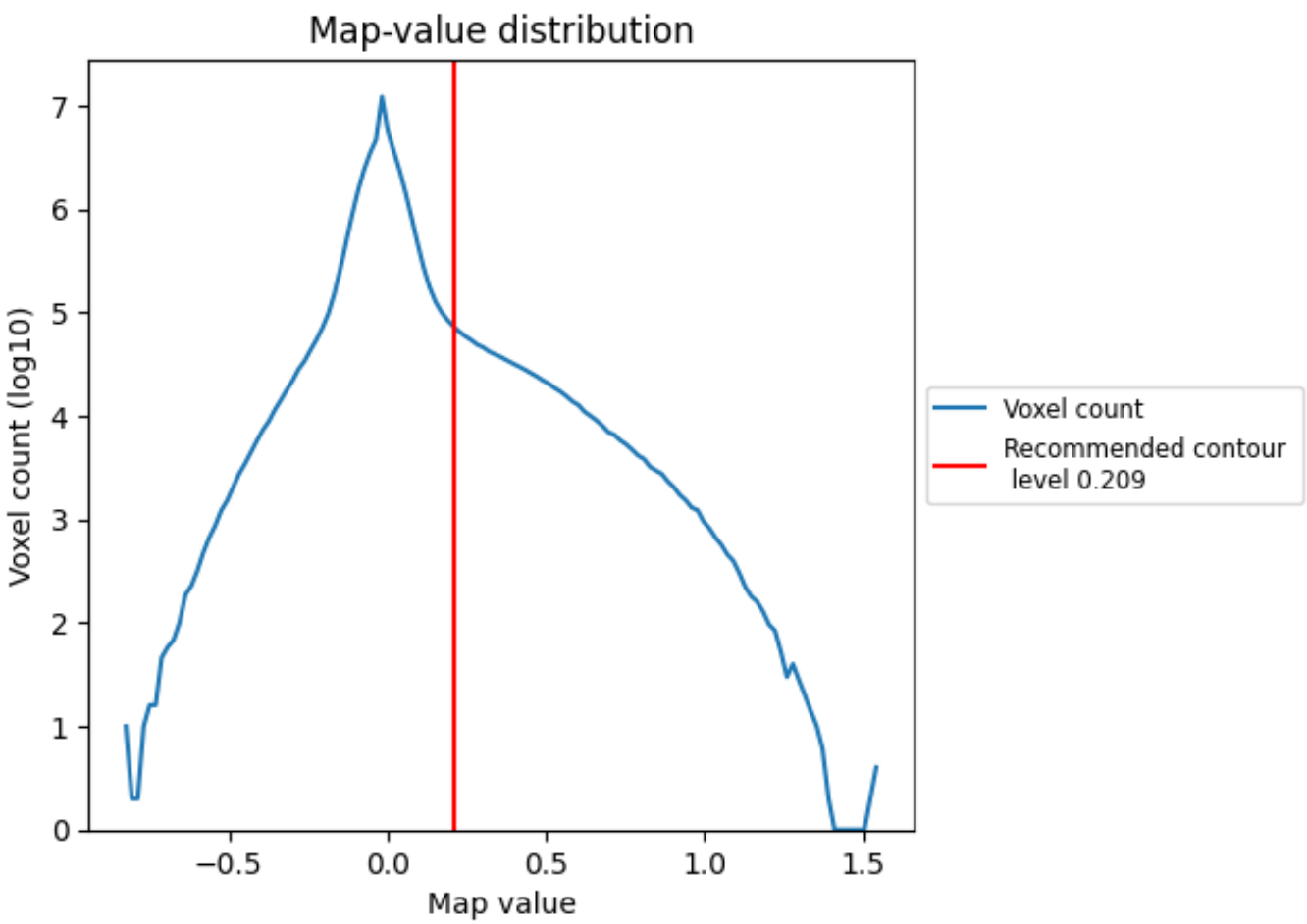
6.6 Mask visualisation (i)

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

7 Map analysis (i)

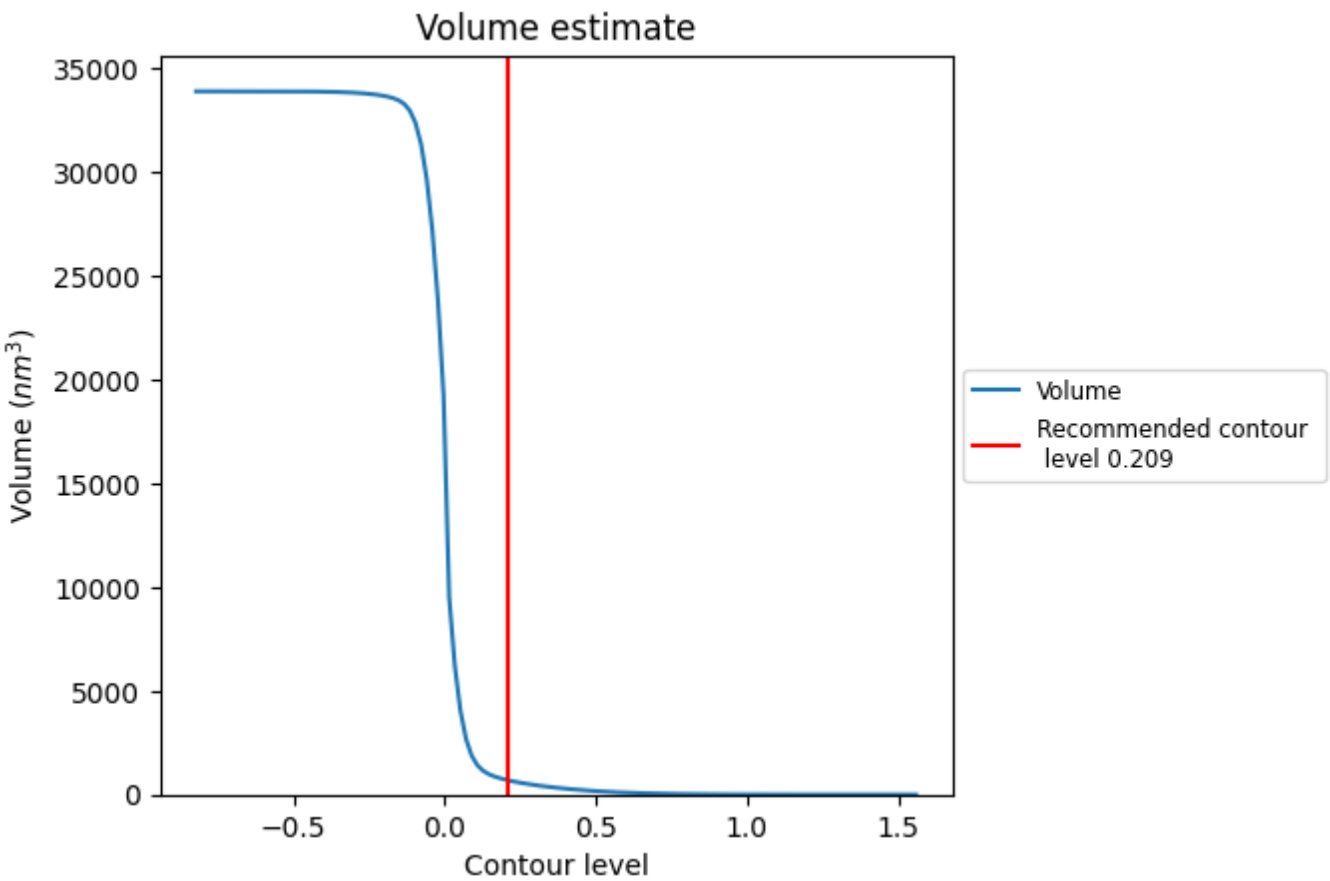
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

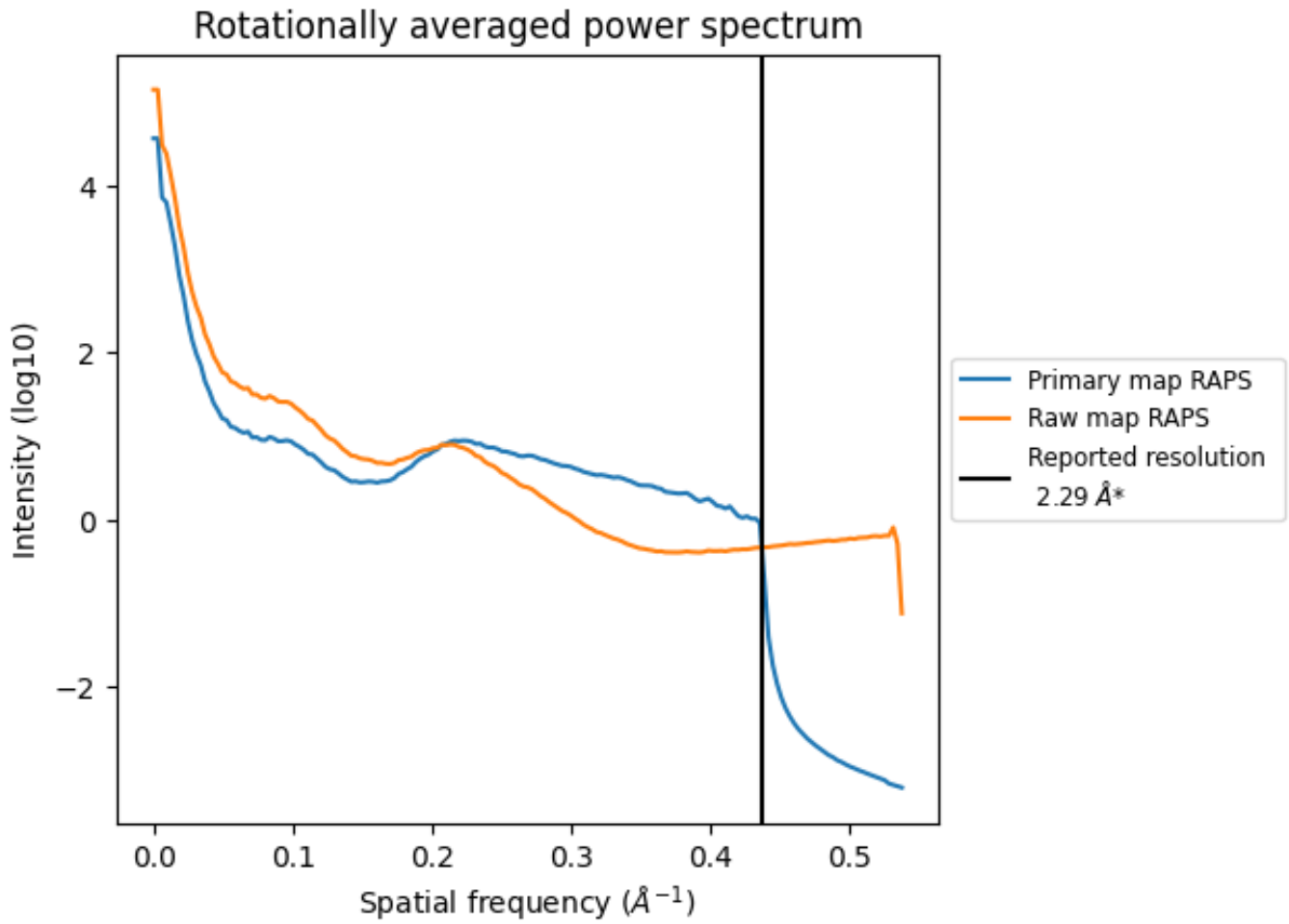
7.2 Volume estimate (i)



The volume at the recommended contour level is 688 nm^3; this corresponds to an approximate mass of 622 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)

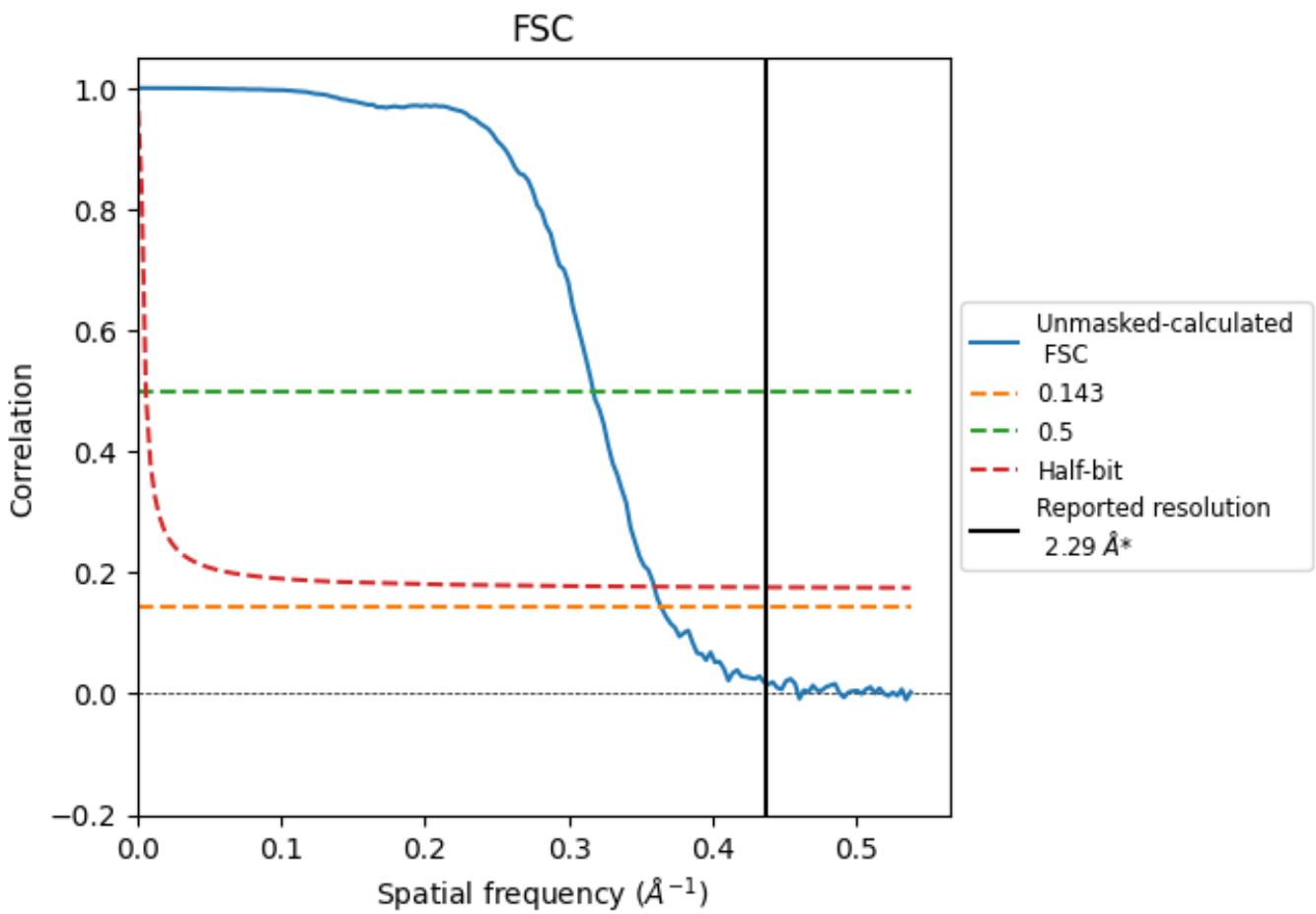


*Reported resolution corresponds to spatial frequency of 0.437 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.437 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.29	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.74	3.15	2.78

*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 2.74 differs from the reported value 2.29 by more than 10 %

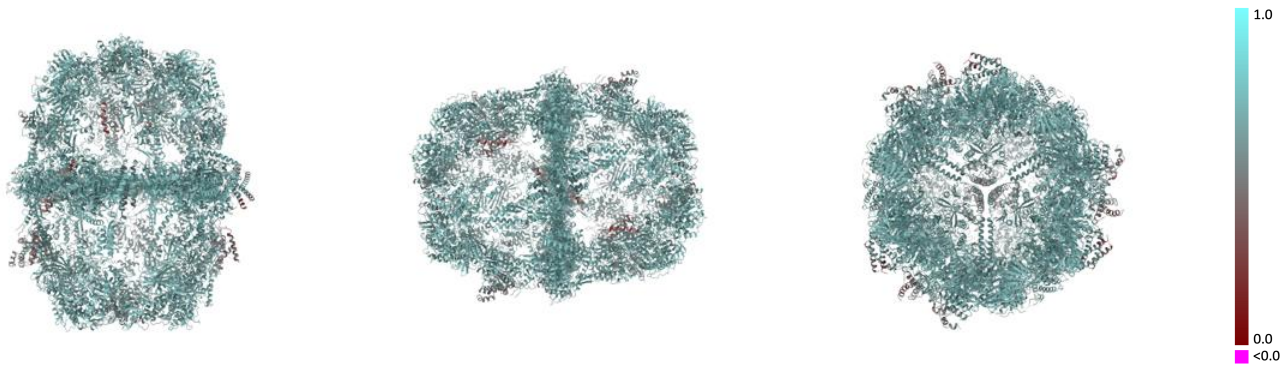
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-71285 and PDB model 9P4W. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)

This section was not generated.

9.2 Q-score mapped to coordinate model (i)



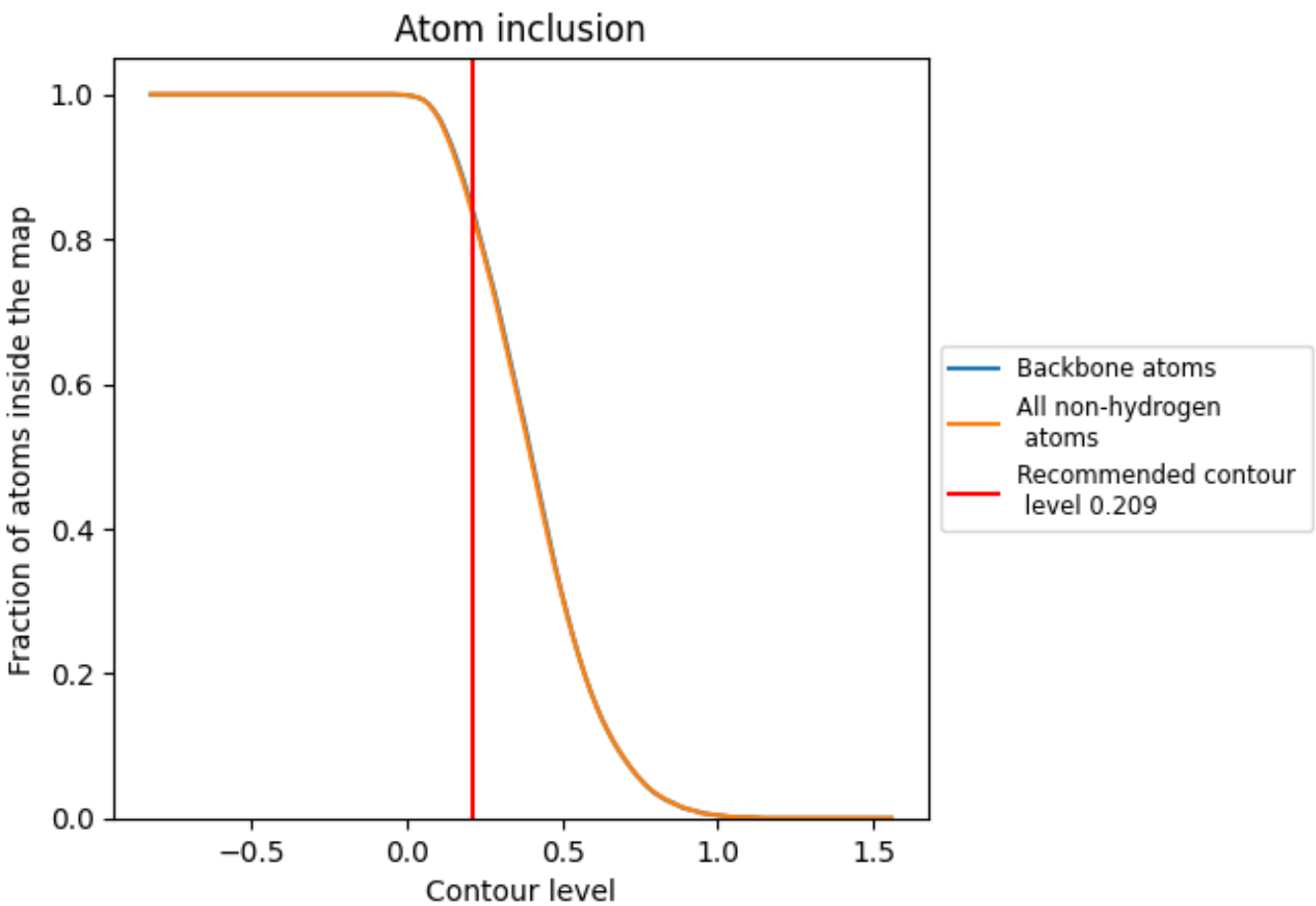
X Y Z

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)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.209) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8390	0.6560
A	0.8050	0.6420
B	0.8960	0.6810
D	0.8960	0.6810
E	0.8060	0.6420
H	0.8920	0.6780
I	0.8020	0.6400
K	0.8940	0.6770
L	0.8010	0.6400
N	0.8940	0.6770
O	0.8010	0.6400
Q	0.8920	0.6780
R	0.8020	0.6400