



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 2, 2020 – 08:02 am BST

PDB ID : 4V59
Title : Crystal structure of fatty acid synthase complexed with nadp+ from thermomyces lanuginosus at 3.1 angstrom resolution.
Authors : Jenni, S.; Leibundgut, M.; Boehringer, D.; Frick, C.; Mikolasek, B.; Ban, N.
Deposited on : 2007-03-09
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

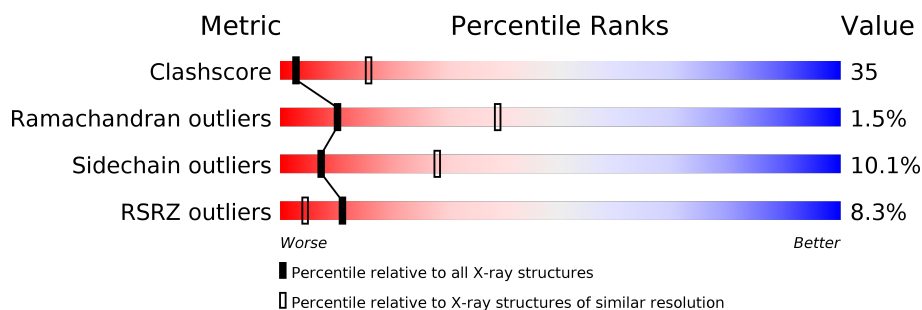
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1878	<div> <div>2%</div> <div> <div>39%</div> <div>35%</div> <div>•</div> <div>22%</div> </div> </div>
1	B	1878	<div> <div>2%</div> <div> <div>40%</div> <div>34%</div> <div>•</div> <div>22%</div> </div> </div>
1	C	1878	<div> <div>2%</div> <div> <div>39%</div> <div>34%</div> <div>•</div> <div>22%</div> </div> </div>
1	D	1878	<div> <div>3%</div> <div> <div>39%</div> <div>34%</div> <div>5%</div> <div>22%</div> </div> </div>
1	E	1878	<div> <div>3%</div> <div> <div>38%</div> <div>35%</div> <div>•</div> <div>22%</div> </div> </div>
1	F	1878	<div> <div>2%</div> <div> <div>40%</div> <div>33%</div> <div>•</div> <div>22%</div> </div> </div>
2	G	2060	<div> <div>8%</div> <div> <div>43%</div> <div>49%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	2060	
2	I	2060	
2	J	2060	
2	K	2060	
2	L	2060	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FMN	G	2101	-	-	X	-
4	FMN	H	2101	-	-	X	-
4	FMN	I	2101	-	-	X	-
4	FMN	J	2101	-	-	X	-
4	FMN	K	2101	-	-	X	-
4	FMN	L	2101	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 167247 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

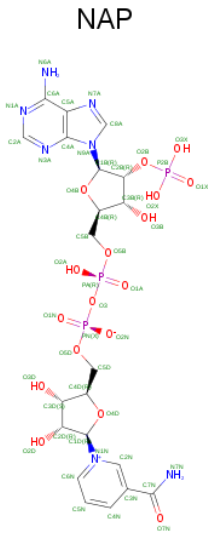
- Molecule 1 is a protein called FATTY ACID SYNTHASE ALPHA SUBUNITS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1457	Total	C	N	O	S	0	0	0
			11514	7290	2005	2170	49			
1	B	1464	Total	C	N	O	S	0	0	0
			11571	7323	2015	2183	50			
1	C	1462	Total	C	N	O	S	0	0	0
			11555	7312	2012	2181	50			
1	D	1467	Total	C	N	O	S	0	0	0
			11593	7336	2021	2186	50			
1	E	1456	Total	C	N	O	S	0	0	0
			11506	7285	2004	2169	48			
1	F	1461	Total	C	N	O	S	0	0	0
			11546	7307	2010	2179	50			

- Molecule 2 is a protein called FATTY ACID SYNTHASE BETA SUBUNITS.

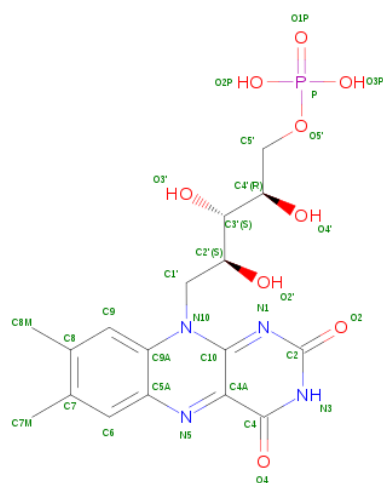
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	H	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	I	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	J	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	K	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	L	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	F	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	G	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	H	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	I	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	J	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	K	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	L	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



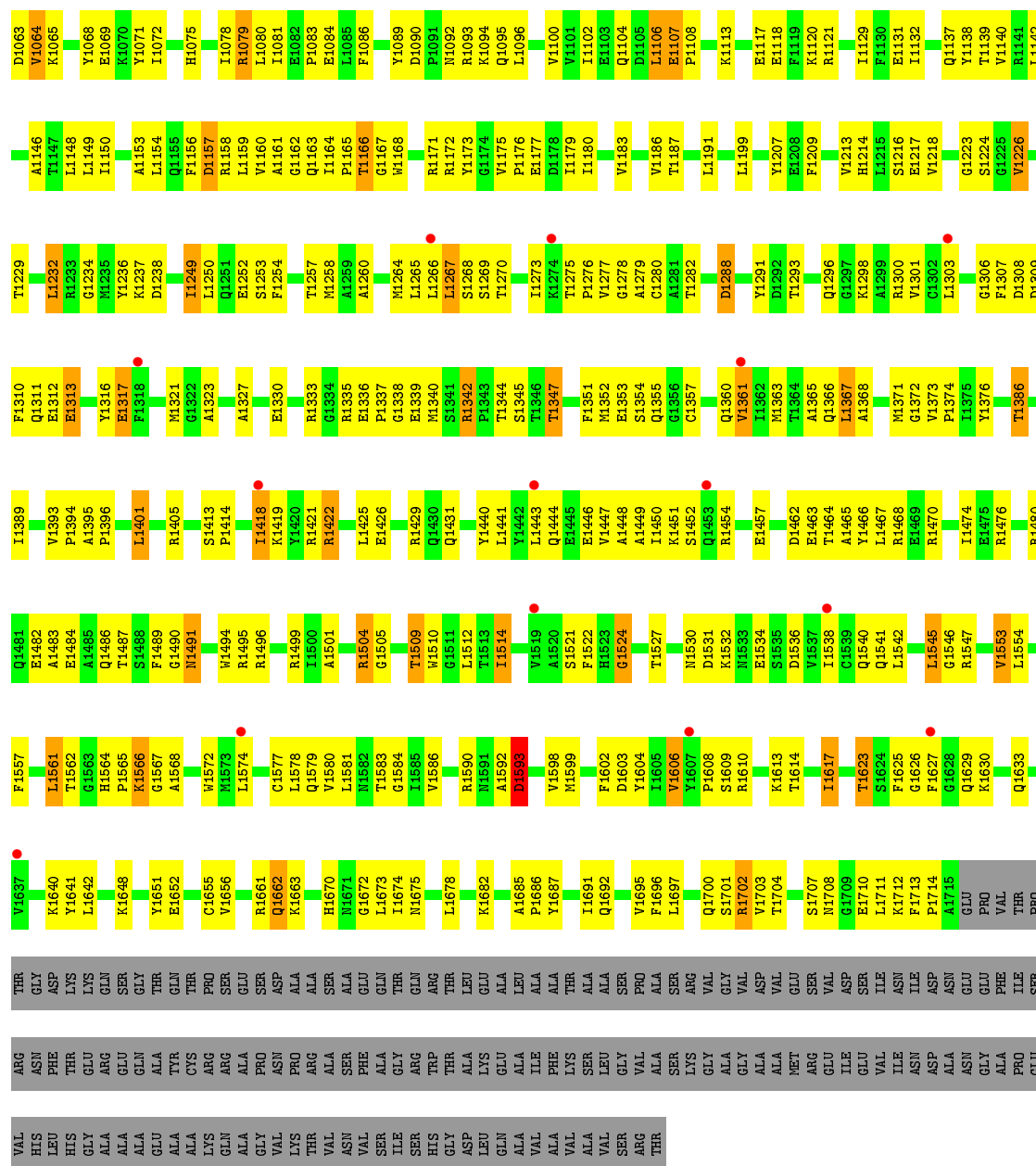
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	H	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	I	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	J	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	K	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	L	1	Total 31	C 17	N 4	O 9	P 1	0	0



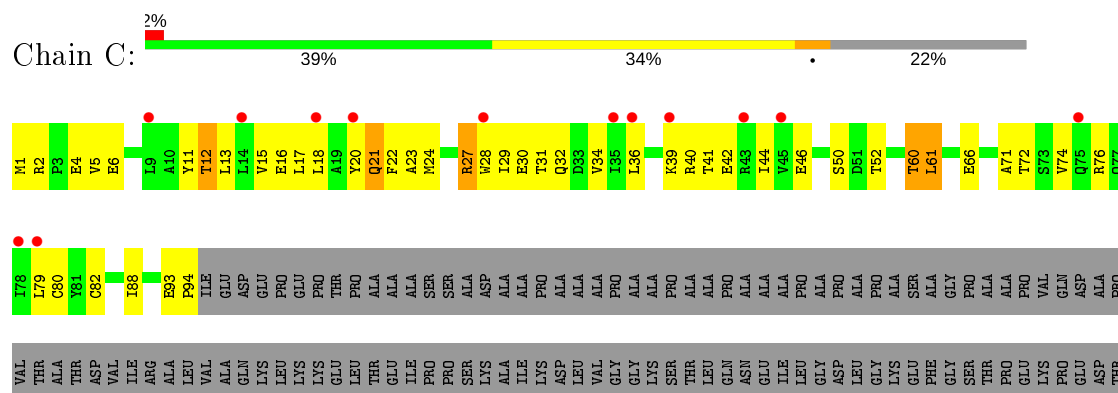
Chain B:

Sequence logo for Chain B, showing information content (bits) per position (1 to 250). The y-axis ranges from 0.00 to 2.00 bits. The x-axis ranges from 1 to 250. The logo shows a high peak at position 1 (approx. 1.8 bits) and a smaller peak at position 250 (approx. 0.8 bits).

Position	Residue	Information Content (bits)
1	M1	1.8
2	R2	1.5
3	P3	1.2
4	E4	1.0
5	V5	0.8
6	E6	0.6
7	L7	0.4
8	A10	0.3
9	Y11	0.2
10	T12	0.1
11	L13	0.1
12	L14	0.1
13	V15	0.1
14	E16	0.1
15	L17	0.1
16	L18	0.1
17	A19	0.1
18	Y20	0.1
19	Q21	0.1
20	F22	0.1
21	A23	0.1
22	M24	0.1
23	R27	0.1
24	W28	0.1
25	L29	0.1
26	T31	0.1
27	Q32	0.1
28	D33	0.1
29	V34	0.1
30	L35	0.1
31	L36	0.1
32	A37	0.1
33	E38	0.1
34	K39	0.1
35	T41	0.1
36	E42	0.1
37	R43	0.1
38	I44	0.1
39	V45	0.1
40	S50	0.1
41	D51	0.1
42	T52	0.1
43	R58	0.1
44	R59	0.1
45	T60	0.1
46	L61	0.1
47	E66	0.1
48	T72	0.1
49	S73	0.1
50	W74	0.1



• Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS



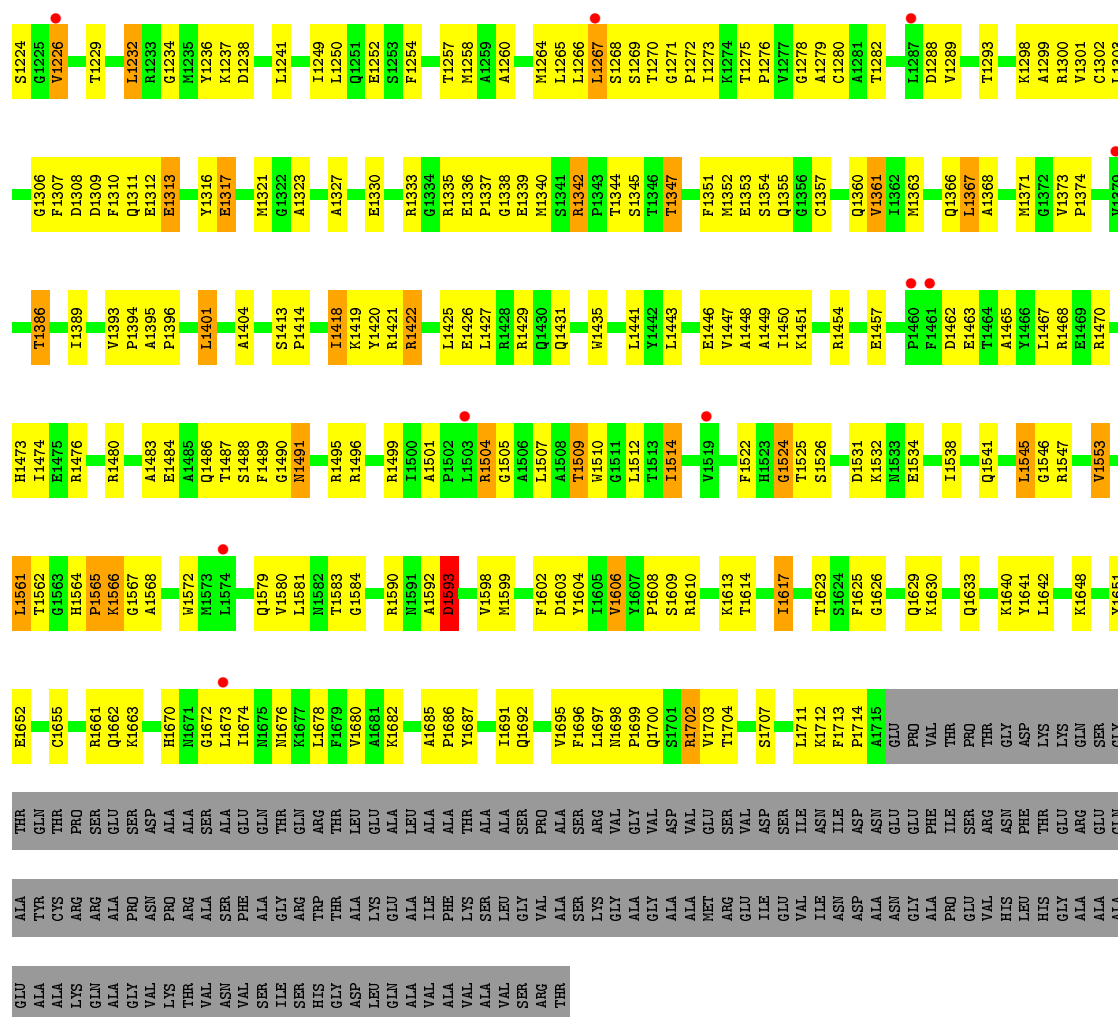






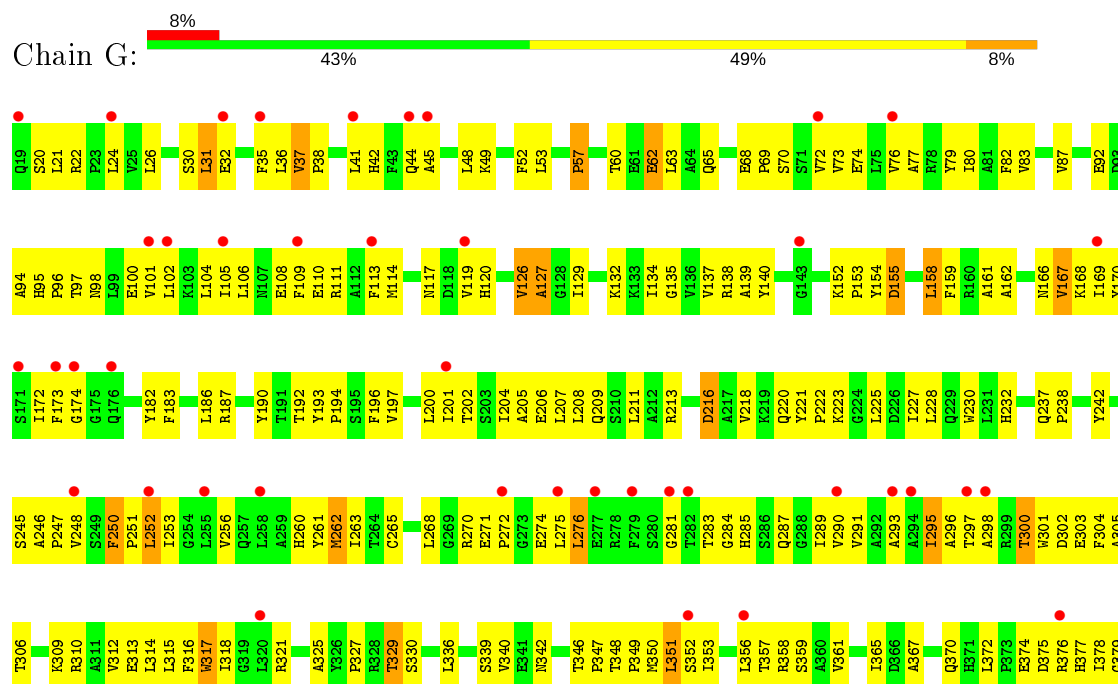


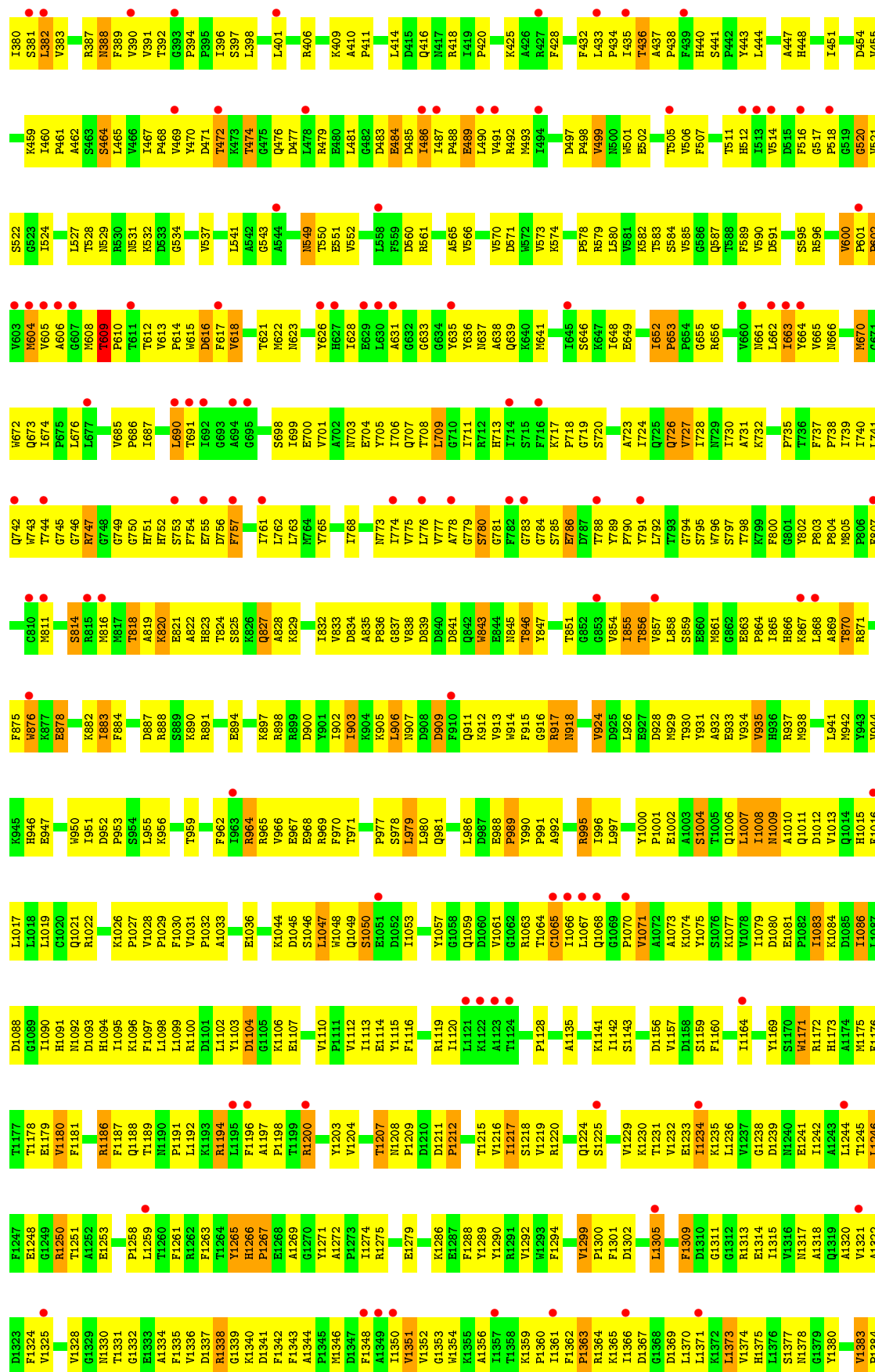


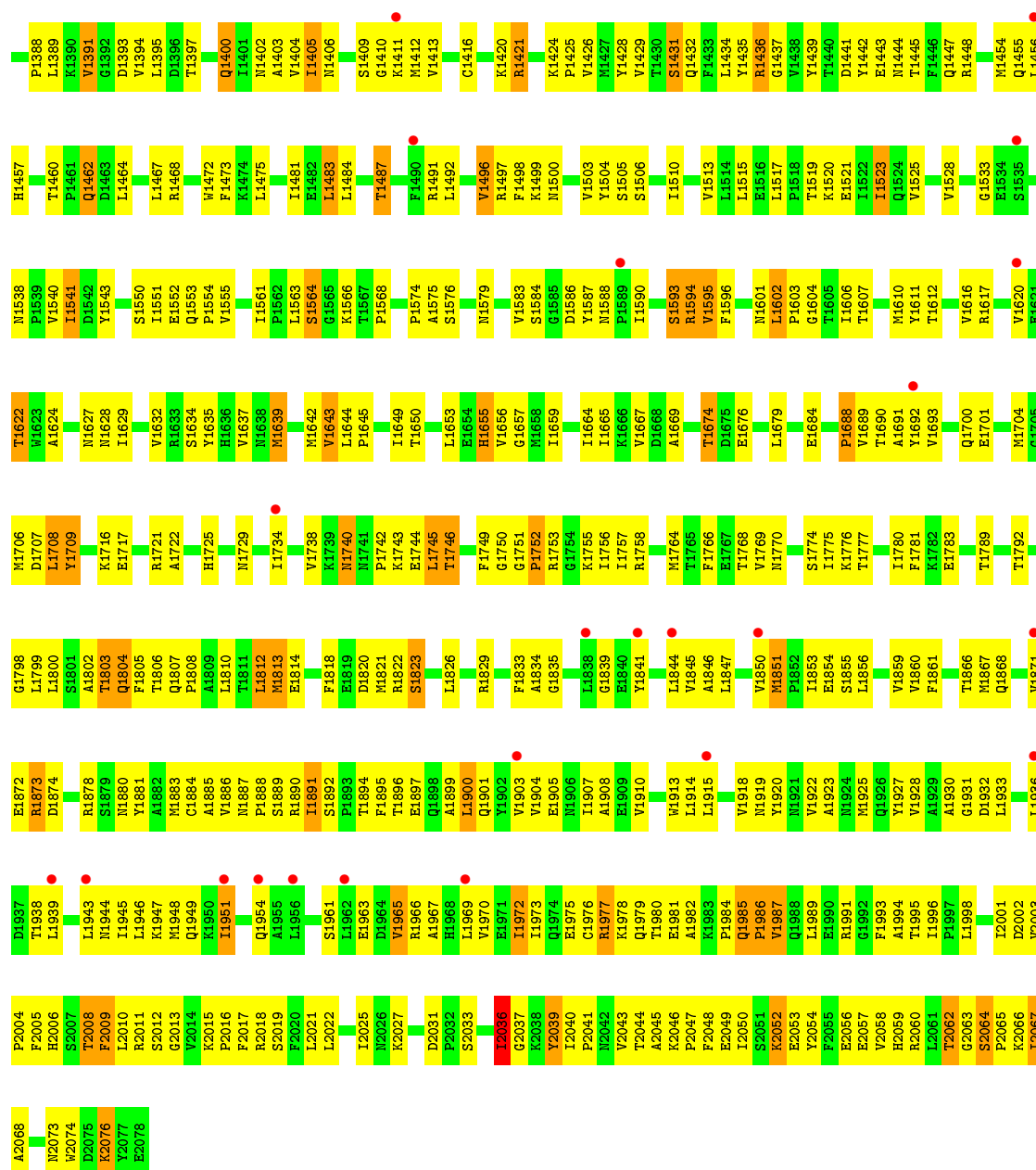


• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS

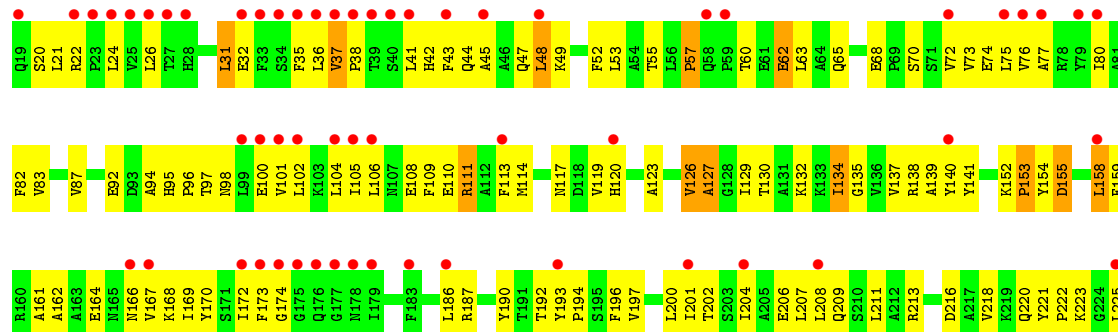
Chain G:

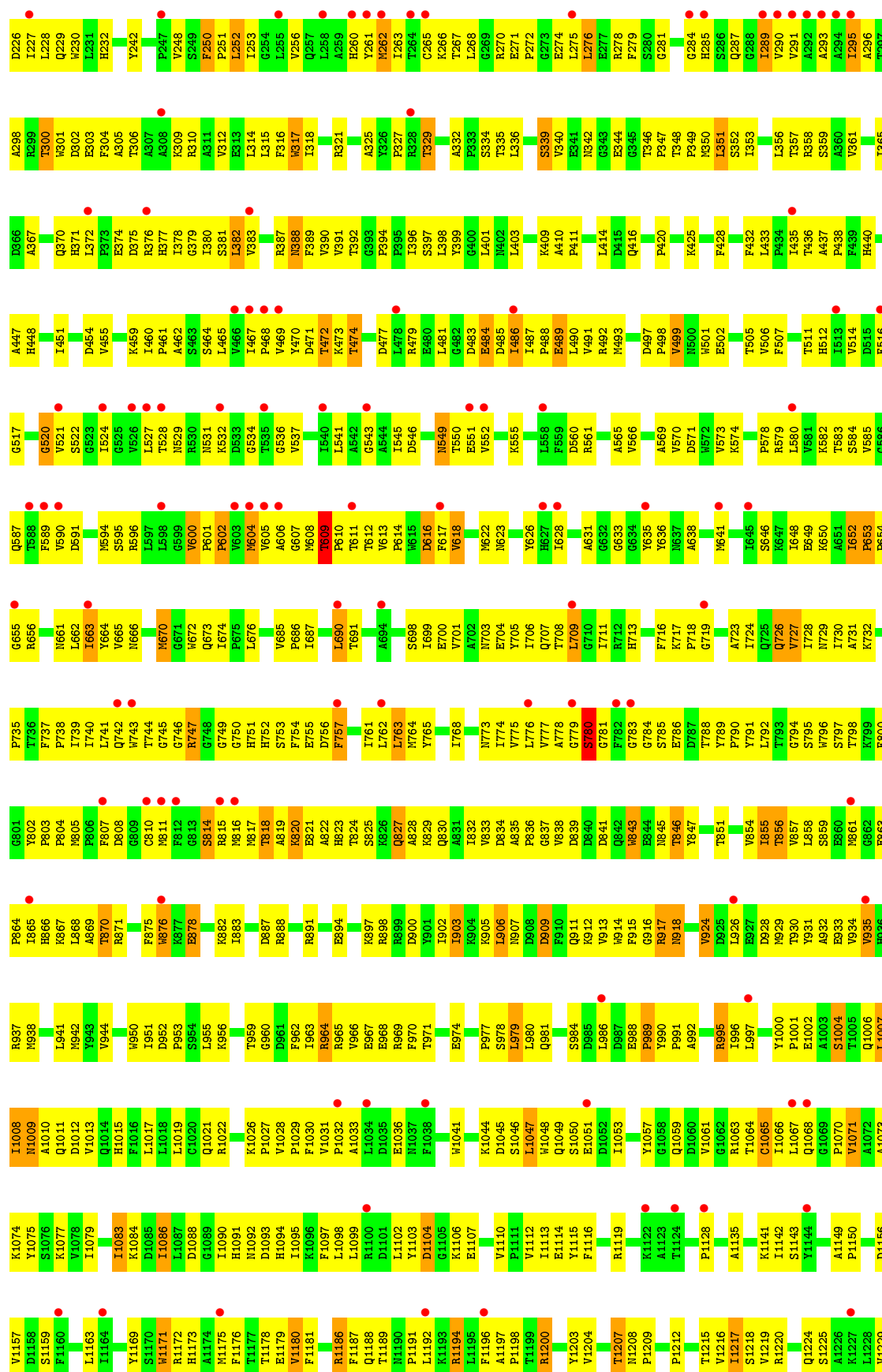


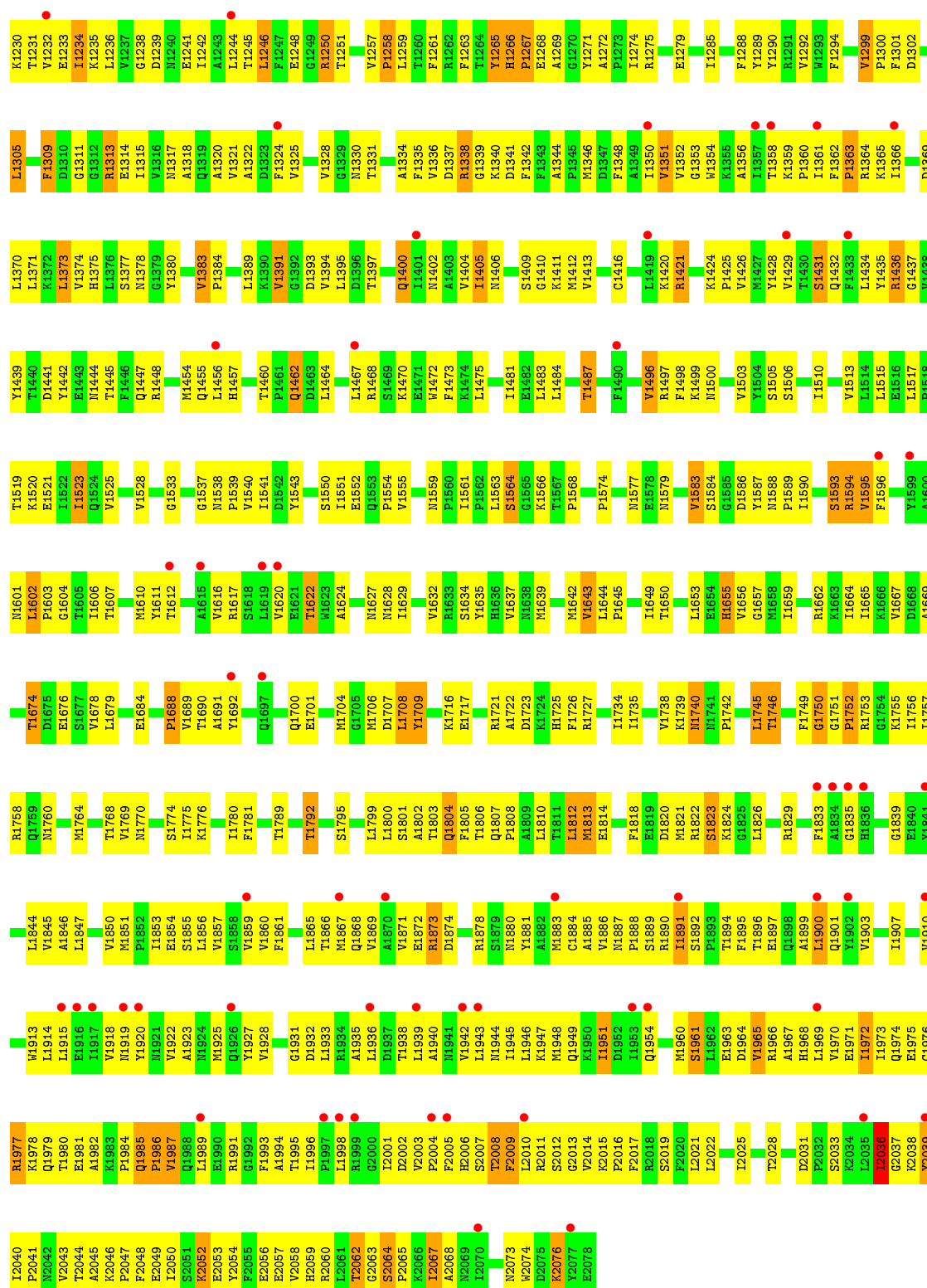




• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



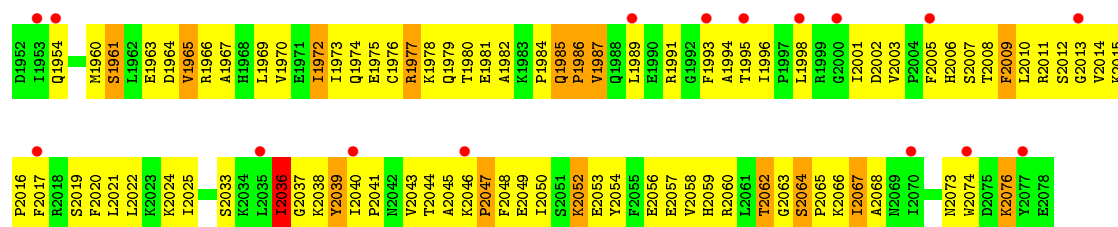




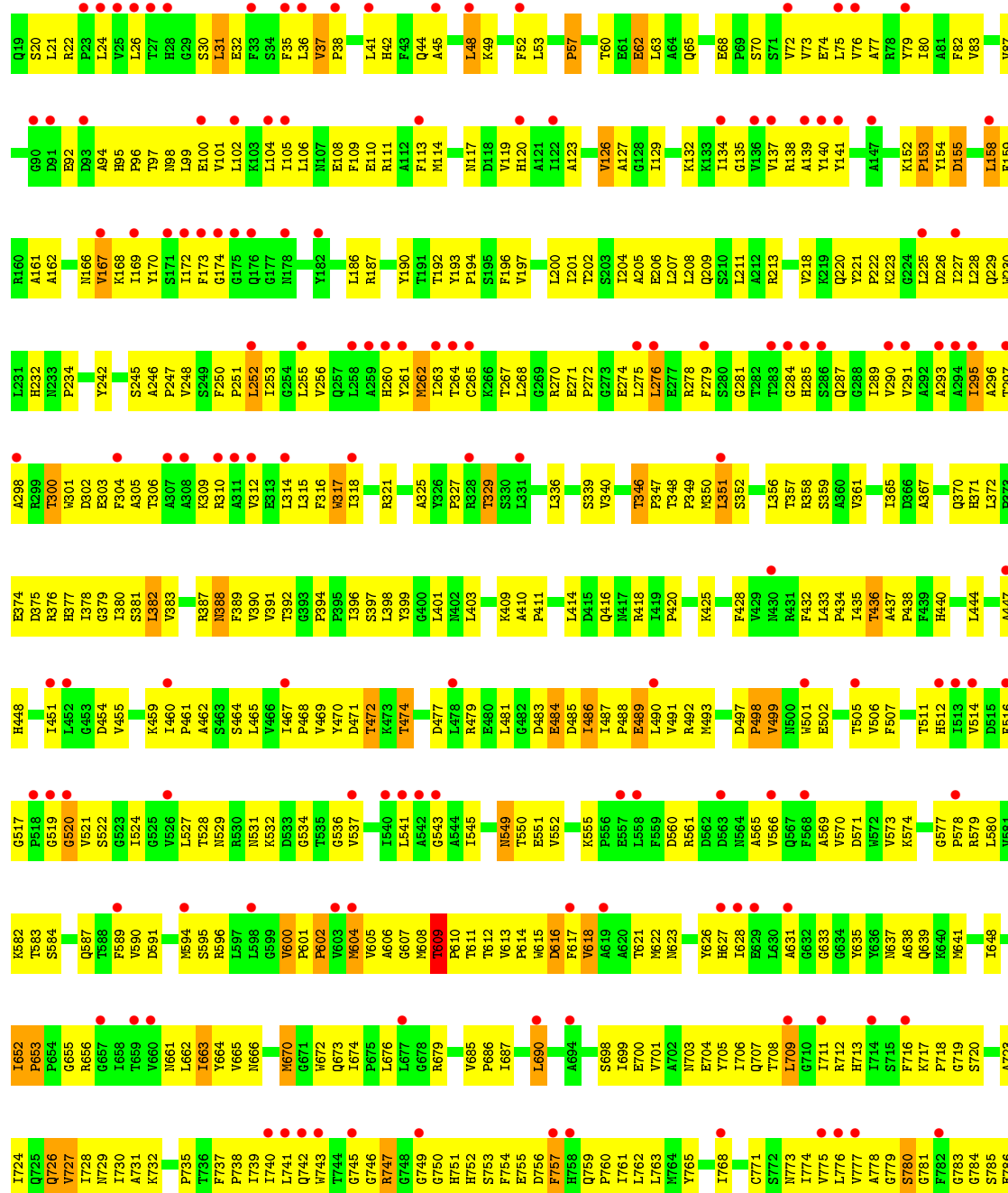
• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS

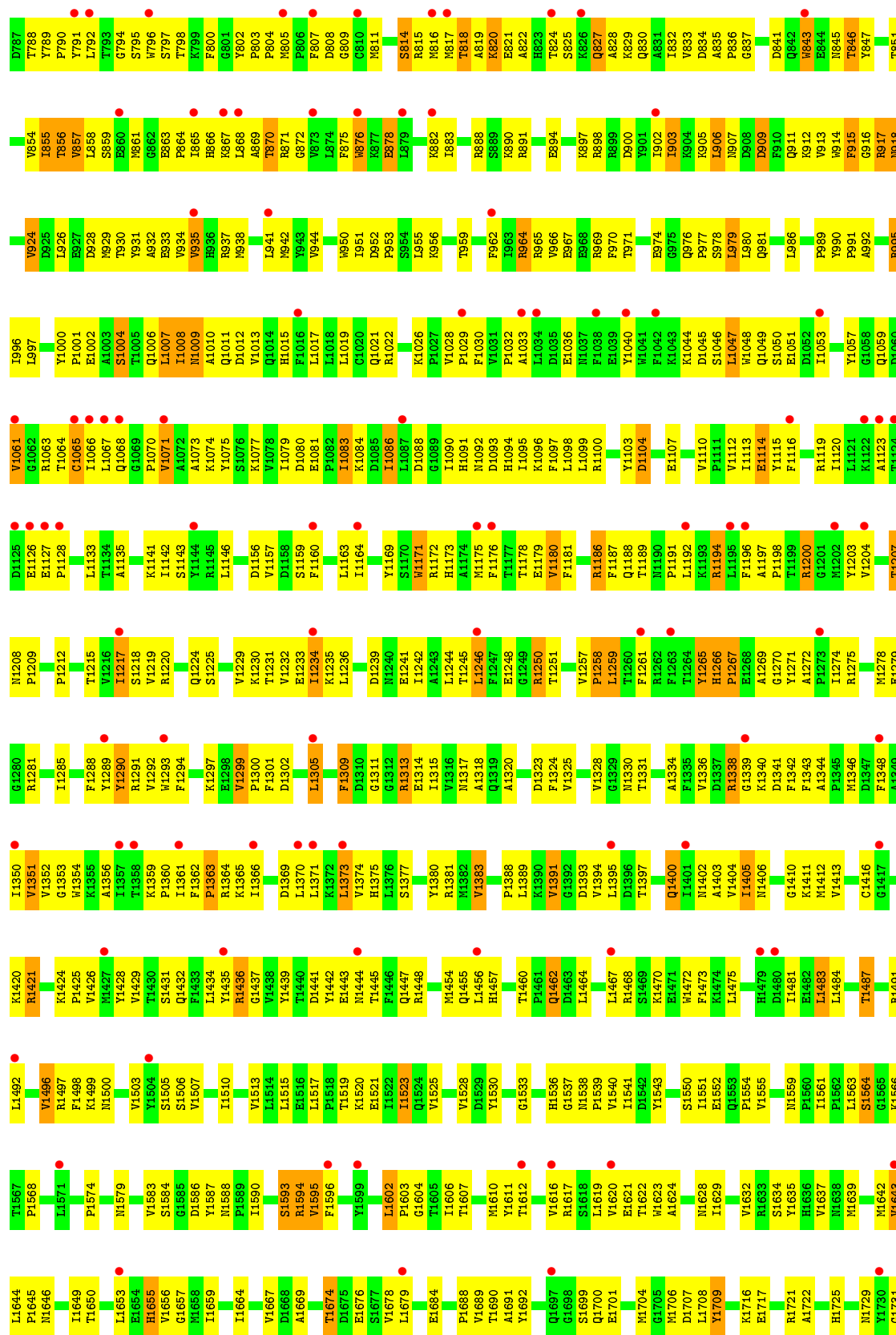


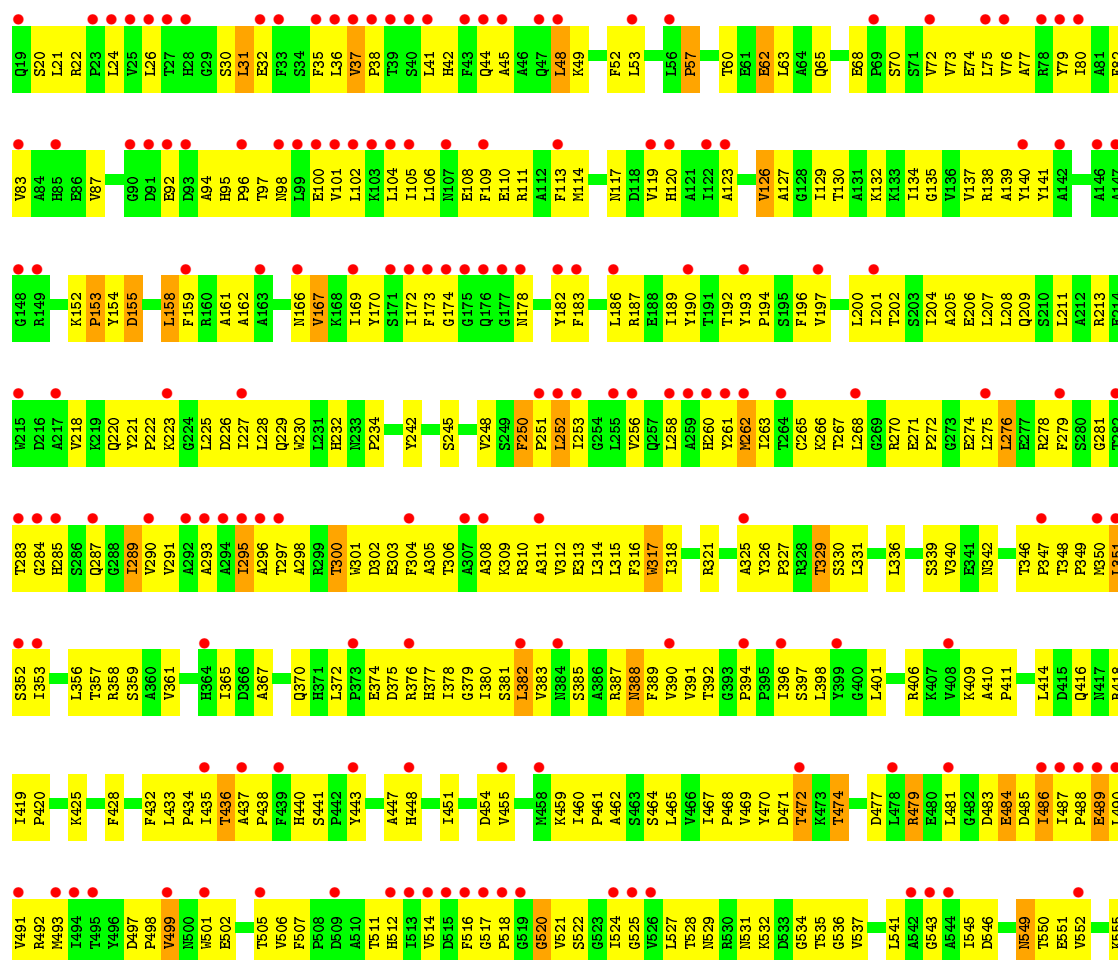
R1890	D1820	V1747	G1657	D1586	S1505	S1431	R1364	F1301	L1228	V1157	K1077	H1009
I1891	M1821	H1748	H1658	Y1587	S1506	Q1432	K1365	D1302	V1229	D1158	V1078	A1010
	S1822	F1749	I1659	M1588	V1507	F1433	I1366	T1303	K1230	F1160	I1079	Q1011
T1894	S1823	G1750		P1589		L1434	P1367	L1305	T1231	E1081	D1080	D1012
F1895		G1751	I1664	I1590	I1510	Y1435	G1368		E1233	Q1162	V1082	V1013
T1896	L1826	P1752				R1436	D1369	F1309	I1234	L1163	H1083	Q1014
E1897		R1753	V1687	S1593	V1513	G1437	L1370	D1310	I1235	L1164	K1084	H1015
Q1898	R1829	D1754	D1668	R1594	L1514	Y1438	L1371	G1311	L1236		F1016	L1017
A1899		K1755	L1515	V1595	L1515	Y1439	R1372	R1312	L1237		D1085	
Q1900	T1832	T1756		F1596	E1516	T1440	L1373	R1313	G1238	Y1169	L1086	L1018
Q1901	F1833	L1757	T1674		L1517	D1441	V1374	R1314	G1237	W1171	L1087	G1019
Y1902	A1834	R1758	D1675	Y1599	P1518	E1442	H1375	E1344	D1239	H1171	G1088	G1020
V1903	G1835		E1676	A1600	T1519	E1443	L1376	L1315	N1240	H1172	G1089	Q1021
Y1904	H1836	Y1761	S1677	H1601	K1520	N1444	S1377	V1316	E1241	H1173	I1090	A1022
E1905		M1762		L1602	E1521	T1446		M1317	I1242	A1174		R1023
N1906	G1839	S1763	L1678	P1603	I1522	F1446	Y1380	A1318	A1243	M1175	H1091	
I1907	E1840	M1764	L1679	G1604	O1523	Q1447	V1383	A1320	L1244	F1176	N1092	K1026
A1908	Y1941	T1765	E1684	T1605	Q1524	R1448	P1384	V1325	T1245	T1177	D1093	P1027
Y1909		F1766		I1606	V1525	H1456		V1321	L1246	T1178	H1094	V1028
V1910	L1844	E1767	P1688	T1607		H1457	P1388	D1323	F1247	E1179	K1096	P1029
V1911	V1845	T1768	V1689	M1610	Y1528	Q1455	L1389	A1329	E1248	V1180	F1097	F1030
G1912	A1846	V1769	A1691	Y1611	Y1530	M1455	K1390	F1324	G1249	F1181	L1098	V1031
V1913	L1847	N1770	Y1692	T1612		L1456	G1392	H1326	R1250		L1099	P1032
L1914					G1533	H1457	D1393	A1327	T1251	R1186	R1101	A1033
L1915	V1850	S1774	Q1700	V1616			D1393	V1328	V1257	F1187	L1102	E1036
E1916	M1851	T1775	E1701	S1617	H1536	T1460	L1393	G1329	P1258	Q1188	L1103	N1037
I1917	P1852	K1776	Q1702	A1618	G1537	P1461	L1395	L1330	L1259	T1189	D1104	F1038
V1918	T1853		G1703	L1619	M1538	Q1462	D1396	T1331	T1261	M1190	G1105	
N1919	E1854	K1779	M1704	V1620	P1539	D1463	T1397		G1263	P1191	K1106	K1044
Y1920	S1855	T1780	G1705	E1621	V1540	L1464		A1334	F1263	K1193	E1107	D1045
N1921	L1856	F1781	M1706	T1622	I1541	A1485	Q1400	F1335	R1263	R1194	S1046	S1046
Y1922	V1857	K1782	D1707	W1623	D1542	V1466	I1401	V1336	T1264	L1195	L1047	W1048
A1923	S1858	E1783	L1708	A1624	Y1543	L1487	A1403	D1337	H1265	A1197	V1112	Q1049
N1924	V1859	N1789	Y1709			S1469	A1404	G1339	P1267	T1198	I1113	S1050
Q1926	F1861	T1789		M1628	S1550		I1405	D1341	E1263	T1199	E1114	E1051
Y1927	K1716	T1792	K1716	I1629	I1551	W1472	M1406	F1342	G1270	R1200	Y1115	D1082
V1928	E1717	Y1793	E1717		E1552	F1473		F1343	I1271		F1116	I1083
A1929	T1866	R1794		V1632	Q1553	F1475	S1409	D1342	A1272	Y1203	I1120	Y1057
N1930	M1867	S1795	R1721	S1633	P1554	L1475	K1410	F1344	A1273	E1205	L1121	G1058
D1932	V1869		A1722	S1634	V1555		K1411	A1345	P1273	I1206	K1122	Q1059
L1933	H1725	L1799	H1725	Y1635	I1561	I1481	M1412	M1346	I1274	T1207	A1123	D1060
R1934	F1726	S1801	R1726	V1637	P1562	E1482	V1413	D1347	R1275	M1208	T1124	V1061
A1935	E1802	A1802	E1728	M1638	L1563	L1483	E1414	F1348	E1279	P1209	D1125	G1062
L1936	T1873	T1803	M1728	M1639	S1564	L1484	V1415	A1349			E1126	R1063
D1937	D1874	Q1804			K1565		C1416	I1350	I1285	P1212	E1127	T1064
T1938	R1878	F1805	Y1730	M1642	K1566	T1487	G1417	V1351	K1286	T1215	P1128	G1065
L1939	S1879	T1806	G1731	V1643	T1567	L1488	T1418	G1352	E1287	T1216	D1129	L1066
		Q1807	F1732	L1644	P1568	V1489	I1419	G1353	F1288	I1217	H1130	L1067
		P1808	S1733	P1645		F1490	K1420	K1354	Y1289	S1218	A1135	Q1069
		A1809	I1735	M1646	L1571		R1421	A1355	Y1290	V1219	G1069	P1070
V1942	M1880	L1810	I1735			V1496	K1424	A1356	R1291	K1141	V1071	A1072
N1943	N1881	T1811		I1649	P1574	R1497						
I1945	M1883	L1812		T1650		F1498	V1425	K1358	V1292	S1143	A1073	
L1946	A1884	K1739			M1579	K1499	V1426	K1359	H1293	T1142	K1074	
K1947	A1885	M1813		L1653		N1500	H1427	P1360	F1294	Q1224	S1143	
M1948	V1886	E1814		E1654	Y1583		L1428	F1361	V1299	S1225	Y1144	
N1949	N1887			H1655	S1584		V1429	F1362		K1227	D1156	
K1950	P1888	F1818	L1745			Y1503	T1430	P1363				
I1951	S1889	T1746		V1556	G1585	Y1504						



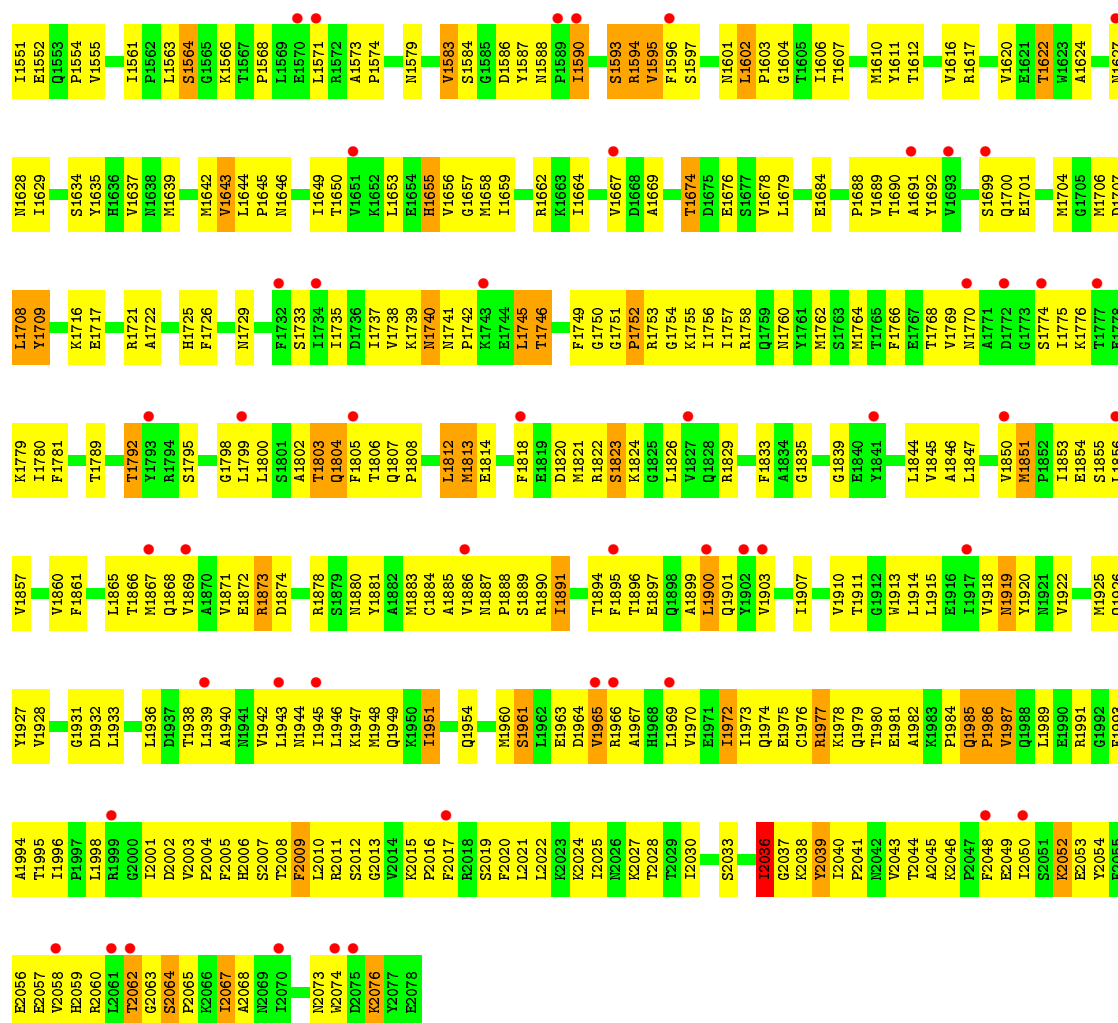
● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



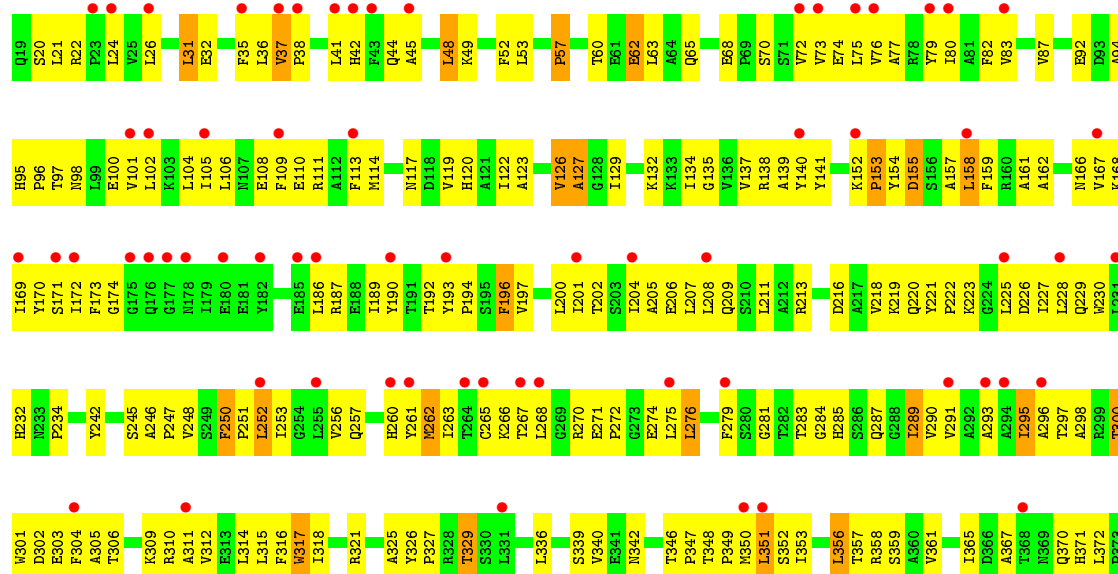




L1464	G1392	V1328	V1257	R1186	L1102	V966	K897	A828	V764	V701	I623	P556
A1465	D1393	G1329	V1258	F1187	Y1103	E967	R898	K829	Y765	A702	I626	E557
V1466	V1394	M1330	P1258	T1188	D1104	E968	R899	Q830	I768	I703	I627	L558
L1467	L1395	T1331	L1259	T1189	G1105	R969	D900	A831	I769	E704	H627	F559
R1468	D1396	G1332	T1260	N1190	K1006	F970	Y901	I832	N773	I705	I628	D560
S1469	T1397	E1333	F1261	P1191	E1107	S972	I902	V833	I774	I706	E629	R561
K1470		E1334	L1192	L1192	V1110		I903	D834	I775	Q707	L630	A565
E1471	Q1400	F1335	Y1265	K1193	P1111	Q976	K904	A835	V776	I708	A631	V566
I1401	I1401	V1336	H1266	R1194	F1112	S1046	K905	P836	L776	L709	A632	V567
N1402	N1402	D1337	E1267	F1196	L1047	P877	N906	G377	G710	I711	G633	A569
A1403	A1403	R1338	E1268	L1198	Y1113	S978	I907	V838	A778	G712	G634	V570
V1404	V1404	G1339	A1269	A1197	E1114	I979	D908	D839	G779	R712	V635	D571
L1405	L1405	K1340	G1270	P1198	Y1115	L380	D909	D840	S780	H713		
		D1341	Y1271	T1199	F1116	Q881	F910	D841	G781	I714	A638	H572
S1409	S1409	F1342	A1272	R1200	D1052	L866	Q911	Q842	F782	S715		V573
K1410	K1410	P1343	P1273	L1119	I1053	D887	K912	M843	G783	F716	K641	K574
K1411	K1411	A1344	I1274	I1120	Y1057	E988	W913	E944	G784	K717	S642	
M1412	M1412	F1345	R1275	V1204	G1058	P889	W914	N845	S785	P718	D643	P578
V1413	V1413	M1346			Q1059	Y990	F915	T846	E786	G719	A644	R579
		D1347	M1278	T1207	Q1060	Y991	G916	Y847	D787	S720		L580
C1416	C1416	F1348	E1279	N1208	D1061	A992	R917	T851	T788			V581
L1419	L1419	G1280	R1281	E1126	Y1061	A993	N918		Y789	A723		T583
K1420	K1420	P1282		E1127	T1064	D994		V854	Y791	Q726	A651	S584
R1421	R1421	Y1215		A1135	G1065	R995	D924	I855	L792	W727	L652	V585
		T1216			I1066	I996	L926	T856	L793	I728	P683	G586
K1424	K1424	I1217		K1141	L1067	I997	E927	V857	G794	I729	P654	Q587
P1425	P1425	S1218		T1142	Q1068	Y1000	D928	L858	S795	I730	P654	T588
V1426	V1426	Y1290		S1143	G1069	N929	W929	S859	W796	A731	R656	F589
H1427	H1427	R1291			P1070	E1002	T930	E860	S797	K732		V590
V1428	V1428	L1292		L1146	Y1071	E1003	Y931	M861	T798			D591
K1359	K1359	W1293			A1072	A1003	A932	G862	K799	P735		
P1360	P1360	F1294			S1004	E963	E933	E863	F800	I736	M594	M594
F1362	F1362	T1299		A1149	K1074	P864	V934	P864	Y802	F737	S595	S595
P1363	P1363	P1300		P1155	Y1075	Q1006	V935	I865	G801	L662	R596	R596
R1364	R1364	F1301		D1156	S1076	L1007	H936	H866	P803	I739	L597	L597
K1365	K1365	D1302		V1157	Y1078	I1008	R937	K867	P804	I740	L598	L598
						M1009	N938	L868	M805	L741	G599	G599
								A869	P806	Q742	V600	V600
								T870	F807	W743	P601	P601
								R871	D808	I744	P602	P602
								G872	G809	G745	V603	V603
								V873	C810	G746	M604	M604
								L874	M811	R747	V605	V605
								F875	F812	G746	A606	A606
								M876	G813	G749	G607	G607
								K877	S814	G750	M608	M608
								E878	R815	H751	T609	T609
									M816	H752	P610	P610
								K882	M817	S753	T611	T611
								I883	T818	F754	T612	T612
								D887	A819	E755	V613	V613
								K956	K820	D756	T614	T614
								T959	E821	F757	W615	W615
									S889	H758	D616	D616
									A822	Q759	F617	F617
									H823	P760	V618	V618
									T824	I761		
									K826	L762	T621	T621
									Q827	L763	M622	M622



• Molecule 2: FATTY ACID SYNTHASE BETA SUBUNITS



F1288	F1289	Y1290	Y1291	F1292	Y1293	F1294	V1216	I1217	S1218	V1219	R1220	Q1224	S1225	A1226	K1227	P1228	F1229	K1230	T1231	V1232	E1233	I1234	K1235	S1236	L1237	G1238	D1239	N1240	E1241	M1242	A1243	L1244	T1245	F1246	E1247	G1248	I1249	T1251	V1257	P1258	L1259	T1260	R1261	K1262	T1263	T1264	Y1265	H1266	P1267	A1268	G1269	Y1270	Y1271	A1272	P1273	I1274	R1275	N1207	N1208	P1209	L1133	P1212	T1134	T1215
K1141	I1142	S1143	V1144	L1145	L1146	D1156	V1157	D1158	S1159	F1160	M1161	T1164	M1167	S1168	Y1169	S1170	M1171	R1172	R1173	A1174	M1175	F1176	T1177	T1178	V1180	F1181	R1186	Q1188	T1189	N1190	P1191	L1192	K1193	R1194	F1196	A1197	F1198	T1199	R1200	G1201	M1202	Y1203	V1204	E1205	I1206	T1207	N1208	P1209	L1133	P1212	T1134	T1215												
A1073	K1074	Y1075	S1076	K1077	Y1078	I1079	D1080	E1081	P1082	I1083	K1084	D1085	I1086	L1087	G1089	H1091	D1093	H1094	I1095	K1096	F1097	L1098	L1099	Y1103	D1104	G1105	K1106	Q1107	V1110	P1111	Y1112	I1113	Y1115	F1116	R1119	I1120	L1121	K1122	A1123	T1124	D1125	E1126	P1127	D1128	T1207	N1208	P1209	L1133	P1212	T1134	T1215													
I1008	M1009	A1010	Q1011	D1012	Y1013	Q1014	H1015	L1016	L1017	L1018	L1019	C1020	Q1021	R1022	R1023	K1026	P1027	V1028	P1029	F1030	V1031	P1032	A1033	E1036	W1041	K1043	D1044	S1046	L1047	W1048	Q1049	S1050	E1051	D1052	I1053	A1054	V1056	Y1057	G1058	Q1059	V1061	G1062	R1063	T1064	C1065	I1066	L1067	Q1068	G1069	P1070	V1071	A1072												
R937	M938	L941	N942	Y943	Y944	R945	R946	E947	W950	L951	D952	P953	L955	K956	T959	F962	L963	R964	R965	V966	E967	E968	R969	F970	T971	E974	P977	S978	L979	L980	Q981	L986	D987	E988	P989	Y990	P991	A992	R995	L996	L997	Y1000	P1001	T1002	A1003	S1004	T1005	Q1006	L1007															
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K867	M805	N806	F807	D808	G809	C810	M811	F812	G813	S814	R815	M816	T818	A819	R820	E821	A822	H823	T824	S825	K826	Q827	A828	R829	Q830	L832	R833	D834	F836	G837	V838	D839	D840	D841	Q842	W843	E844	I845	T846	Y847	T851	R854	L855	R856	L858	S859	A861	G862	V863	R864													
H866	K																																																															

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	215.78Å 412.67Å 220.90Å 90.00° 111.57° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 96.48 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (12.00-3.10) 92.6 (96.48-3.10)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.270 , 0.300 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.078 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	167247	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.43	0/11744	0.60	1/15873 (0.0%)
1	B	0.43	0/11801	0.60	1/15949 (0.0%)
1	C	0.44	0/11785	0.59	0/15928
1	D	0.43	0/11824	0.60	0/15980
1	E	0.42	0/11736	0.59	0/15863
1	F	0.44	0/11776	0.60	5/15916 (0.0%)
2	G	0.36	0/16573	0.53	0/22516
2	H	0.35	0/16573	0.53	0/22516
2	I	0.35	0/16573	0.53	0/22516
2	J	0.36	0/16573	0.54	0/22516
2	K	0.39	0/16573	0.55	0/22516
2	L	0.36	0/16573	0.54	0/22516
All	All	0.39	0/170104	0.56	7/230605 (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	F	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	585	MET	N-CA-C	9.44	136.48	111.00
1	B	608	LYS	N-CA-C	-8.94	86.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	614	PHE	N-CA-C	6.04	127.30	111.00
1	F	613	PRO	CA-C-N	5.57	129.46	117.20
1	A	579	MET	N-CA-C	5.39	125.55	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	578	ALA	Peptide
1	F	613	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11514	0	11476	746	1
1	B	11571	0	11529	708	1
1	C	11555	0	11507	717	0
1	D	11593	0	11552	725	0
1	E	11506	0	11467	754	0
1	F	11546	0	11499	701	0
2	G	16200	0	16081	1290	1
2	H	16200	0	16081	1326	1
2	I	16200	0	16081	1344	0
2	J	16200	0	16081	1326	0
2	K	16200	0	16081	1391	0
2	L	16200	0	16081	1366	0
3	A	48	0	25	5	0
3	B	48	0	25	5	0
3	C	48	0	25	4	0
3	D	48	0	25	6	0
3	E	48	0	25	4	0
3	F	48	0	25	4	0
3	G	48	0	25	4	0
3	H	48	0	25	5	0
3	I	48	0	25	4	0
3	J	48	0	25	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	48	0	25	4	0
3	L	48	0	25	4	0
4	G	31	0	19	17	0
4	H	31	0	19	16	0
4	I	31	0	19	16	0
4	J	31	0	19	15	0
4	K	31	0	19	15	0
4	L	31	0	19	15	0
All	All	167247	0	165930	11767	2

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 35.

The worst 5 of 11767 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:GLN:HB3	1:D:579:MET:HE2	1.25	1.17
1:F:1443:LEU:HD21	1:F:1470:ARG:HB3	1.18	1.17
1:B:1268:SER:HB3	1:D:1389:ILE:HG13	1.23	1.16
1:F:1504:ARG:HH11	1:F:1504:ARG:HG3	1.04	1.15
1:D:1504:ARG:HH11	1:D:1504:ARG:HG3	1.02	1.15

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ARG:NH1	2:H:164:GLU:O[2_555]	2.01	0.19
1:B:1452:SER:O	2:G:1092:ASN:ND2[1_556]	2.18	0.02

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1451/1878 (77%)	1270 (88%)	164 (11%)	17 (1%)	13	44
1	B	1458/1878 (78%)	1278 (88%)	160 (11%)	20 (1%)	11	40
1	C	1456/1878 (78%)	1283 (88%)	156 (11%)	17 (1%)	13	44
1	D	1461/1878 (78%)	1276 (87%)	161 (11%)	24 (2%)	9	37
1	E	1450/1878 (77%)	1276 (88%)	155 (11%)	19 (1%)	12	42
1	F	1455/1878 (78%)	1282 (88%)	153 (10%)	20 (1%)	11	40
2	G	2058/2060 (100%)	1789 (87%)	237 (12%)	32 (2%)	9	37
2	H	2058/2060 (100%)	1791 (87%)	230 (11%)	37 (2%)	8	34
2	I	2058/2060 (100%)	1787 (87%)	238 (12%)	33 (2%)	9	37
2	J	2058/2060 (100%)	1784 (87%)	240 (12%)	34 (2%)	9	36
2	K	2058/2060 (100%)	1785 (87%)	239 (12%)	34 (2%)	9	36
2	L	2058/2060 (100%)	1780 (86%)	241 (12%)	37 (2%)	8	34
All	All	21079/23628 (89%)	18381 (87%)	2374 (11%)	324 (2%)	10	39

5 of 324 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	614	PHE
1	A	1566	LYS
1	B	614	PHE
1	B	624	GLY
1	B	1566	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1220/1527 (80%)	1107 (91%)	113 (9%)	9	32
1	B	1227/1527 (80%)	1117 (91%)	110 (9%)	9	34
1	C	1225/1527 (80%)	1110 (91%)	115 (9%)	8	32
1	D	1229/1527 (80%)	1107 (90%)	122 (10%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	1219/1527 (80%)	1106 (91%)	113 (9%)	9	32
1	F	1224/1527 (80%)	1111 (91%)	113 (9%)	9	33
2	G	1752/1752 (100%)	1569 (90%)	183 (10%)	7	27
2	H	1752/1752 (100%)	1569 (90%)	183 (10%)	7	27
2	I	1752/1752 (100%)	1565 (89%)	187 (11%)	6	26
2	J	1752/1752 (100%)	1567 (89%)	185 (11%)	6	26
2	K	1752/1752 (100%)	1566 (89%)	186 (11%)	6	26
2	L	1752/1752 (100%)	1563 (89%)	189 (11%)	6	25
All	All	17856/19674 (91%)	16057 (90%)	1799 (10%)	7	28

5 of 1799 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	1436	ARG
2	H	1564	SER
2	L	726	GLN
2	G	1707	ASP
2	H	616	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 492 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	1500	ASN
2	H	1655	HIS
2	L	448	HIS
2	G	1725	HIS
2	H	388	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

18 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	NAP	J	2102	-	45,52,52	1.30	4 (8%)	56,80,80	1.13	1 (1%)
3	NAP	C	1901	-	45,52,52	1.33	4 (8%)	56,80,80	1.20	2 (3%)
3	NAP	E	1901	-	45,52,52	1.28	3 (6%)	56,80,80	1.26	4 (7%)
4	FMN	K	2101	-	31,33,33	6.85	20 (64%)	40,50,50	1.69	4 (10%)
4	FMN	H	2101	-	31,33,33	6.61	19 (61%)	40,50,50	1.71	5 (12%)
4	FMN	I	2101	-	31,33,33	6.61	19 (61%)	40,50,50	1.75	6 (15%)
4	FMN	L	2101	-	31,33,33	6.62	19 (61%)	40,50,50	1.75	5 (12%)
4	FMN	G	2101	-	31,33,33	6.59	19 (61%)	40,50,50	1.84	6 (15%)
3	NAP	K	2102	-	45,52,52	1.22	4 (8%)	56,80,80	1.09	2 (3%)
3	NAP	I	2102	-	45,52,52	1.18	3 (6%)	56,80,80	1.14	1 (1%)
3	NAP	B	1901	-	45,52,52	1.25	3 (6%)	56,80,80	1.19	3 (5%)
3	NAP	G	2102	-	45,52,52	1.26	4 (8%)	56,80,80	1.12	2 (3%)
3	NAP	F	1901	-	45,52,52	1.30	3 (6%)	56,80,80	1.20	3 (5%)
4	FMN	J	2101	-	31,33,33	6.92	20 (64%)	40,50,50	1.88	4 (10%)
3	NAP	L	2102	-	45,52,52	1.24	4 (8%)	56,80,80	1.11	1 (1%)
3	NAP	D	1901	-	45,52,52	1.44	4 (8%)	56,80,80	1.26	2 (3%)
3	NAP	H	2102	-	45,52,52	1.27	4 (8%)	56,80,80	1.12	1 (1%)
3	NAP	A	1901	-	45,52,52	1.29	3 (6%)	56,80,80	1.18	3 (5%)

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	NAP	J	2102	-	-	10/31/67/67	0/5/5/5
3	NAP	C	1901	-	-	11/31/67/67	0/5/5/5
3	NAP	E	1901	-	-	11/31/67/67	0/5/5/5
4	FMN	K	2101	-	-	5/18/18/18	0/3/3/3
4	FMN	H	2101	-	-	5/18/18/18	0/3/3/3
4	FMN	I	2101	-	-	5/18/18/18	0/3/3/3
4	FMN	L	2101	-	-	5/18/18/18	0/3/3/3
4	FMN	G	2101	-	-	5/18/18/18	0/3/3/3
3	NAP	K	2102	-	-	11/31/67/67	0/5/5/5
3	NAP	I	2102	-	-	10/31/67/67	0/5/5/5
3	NAP	B	1901	-	-	11/31/67/67	0/5/5/5
3	NAP	G	2102	-	-	11/31/67/67	0/5/5/5
3	NAP	F	1901	-	-	11/31/67/67	0/5/5/5
4	FMN	J	2101	-	-	5/18/18/18	0/3/3/3
3	NAP	L	2102	-	-	10/31/67/67	0/5/5/5
3	NAP	D	1901	-	-	11/31/67/67	0/5/5/5
3	NAP	H	2102	-	-	10/31/67/67	0/5/5/5
3	NAP	A	1901	-	-	11/31/67/67	0/5/5/5

The worst 5 of 159 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2101	FMN	C4A-C10	15.95	1.54	1.38
4	K	2101	FMN	C4A-C10	15.01	1.53	1.38
4	I	2101	FMN	C4A-C10	14.92	1.53	1.38
4	L	2101	FMN	C4A-C10	14.89	1.53	1.38
4	H	2101	FMN	C4A-C10	14.71	1.53	1.38

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2101	FMN	C4-N3-C2	7.31	121.32	115.14
4	G	2101	FMN	C4-N3-C2	7.31	121.31	115.14
4	L	2101	FMN	C4-N3-C2	6.73	120.82	115.14
4	H	2101	FMN	C4-N3-C2	6.73	120.82	115.14
4	I	2101	FMN	C4-N3-C2	6.36	120.51	115.14

There are no chirality outliers.

5 of 158 torsion outliers are listed below:

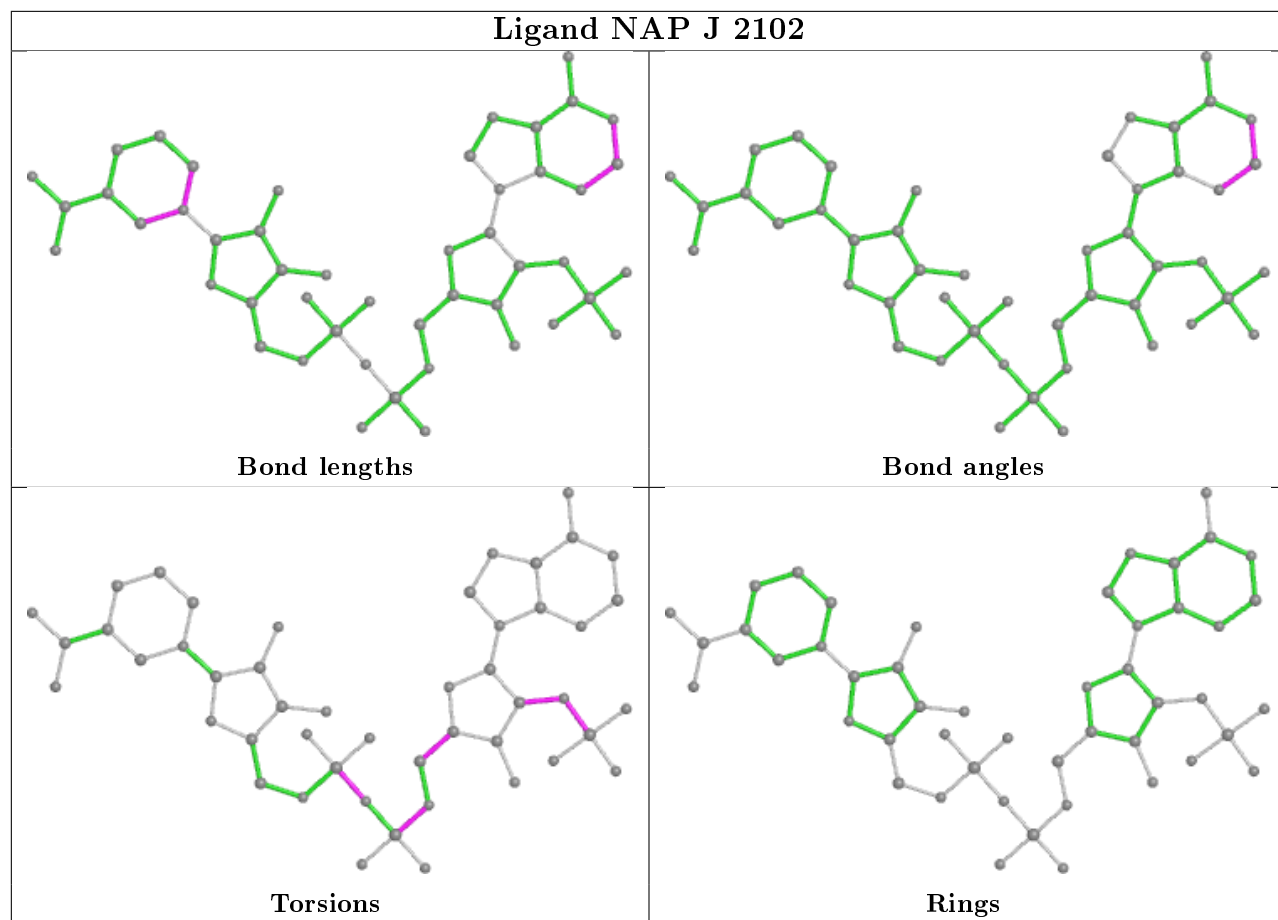
Mol	Chain	Res	Type	Atoms
3	J	2102	NAP	C5B-O5B-PA-O3
3	J	2102	NAP	C3B-C4B-C5B-O5B
3	J	2102	NAP	C2B-O2B-P2B-O1X
3	C	1901	NAP	C5B-O5B-PA-O3
3	C	1901	NAP	PA-O3-PN-O5D

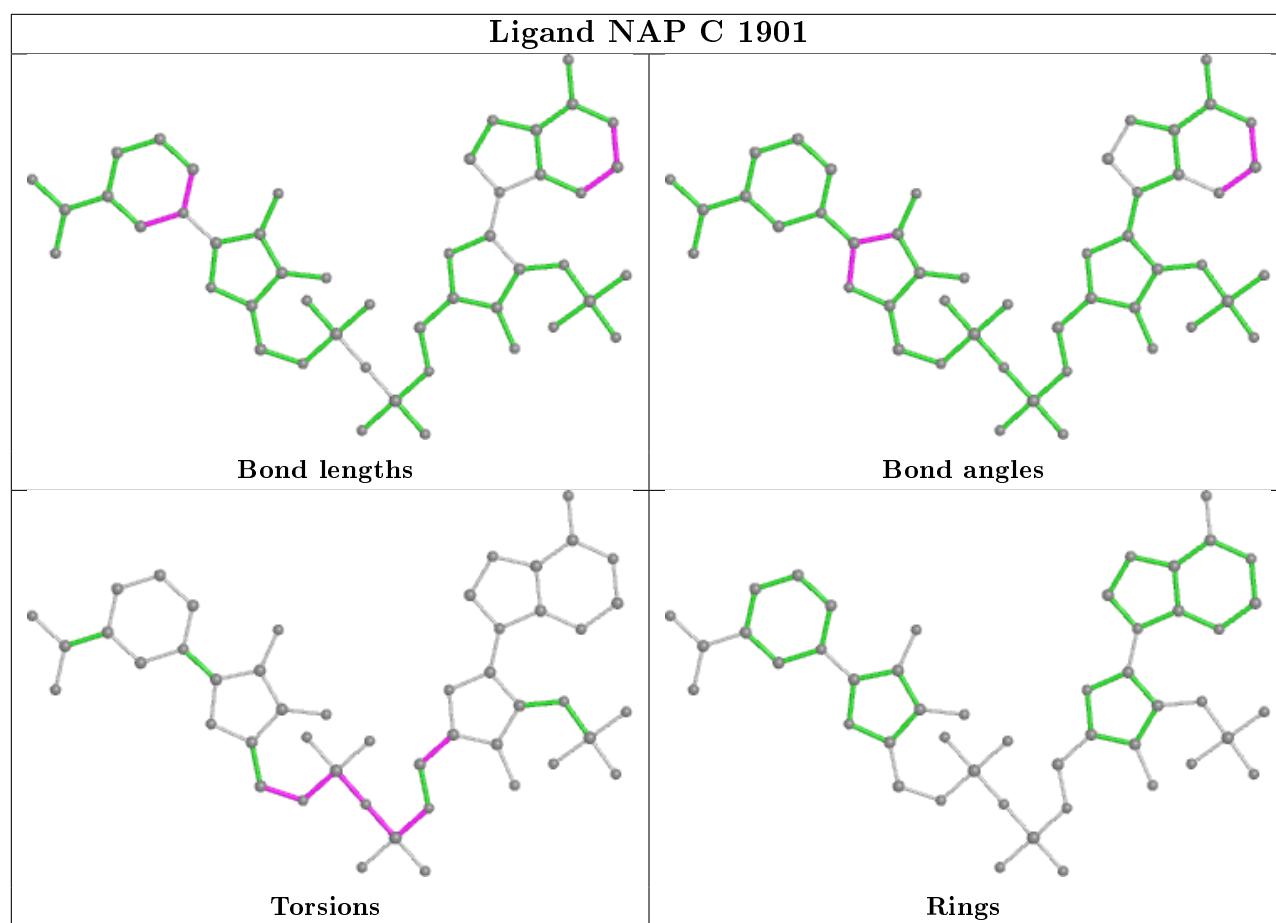
There are no ring outliers.

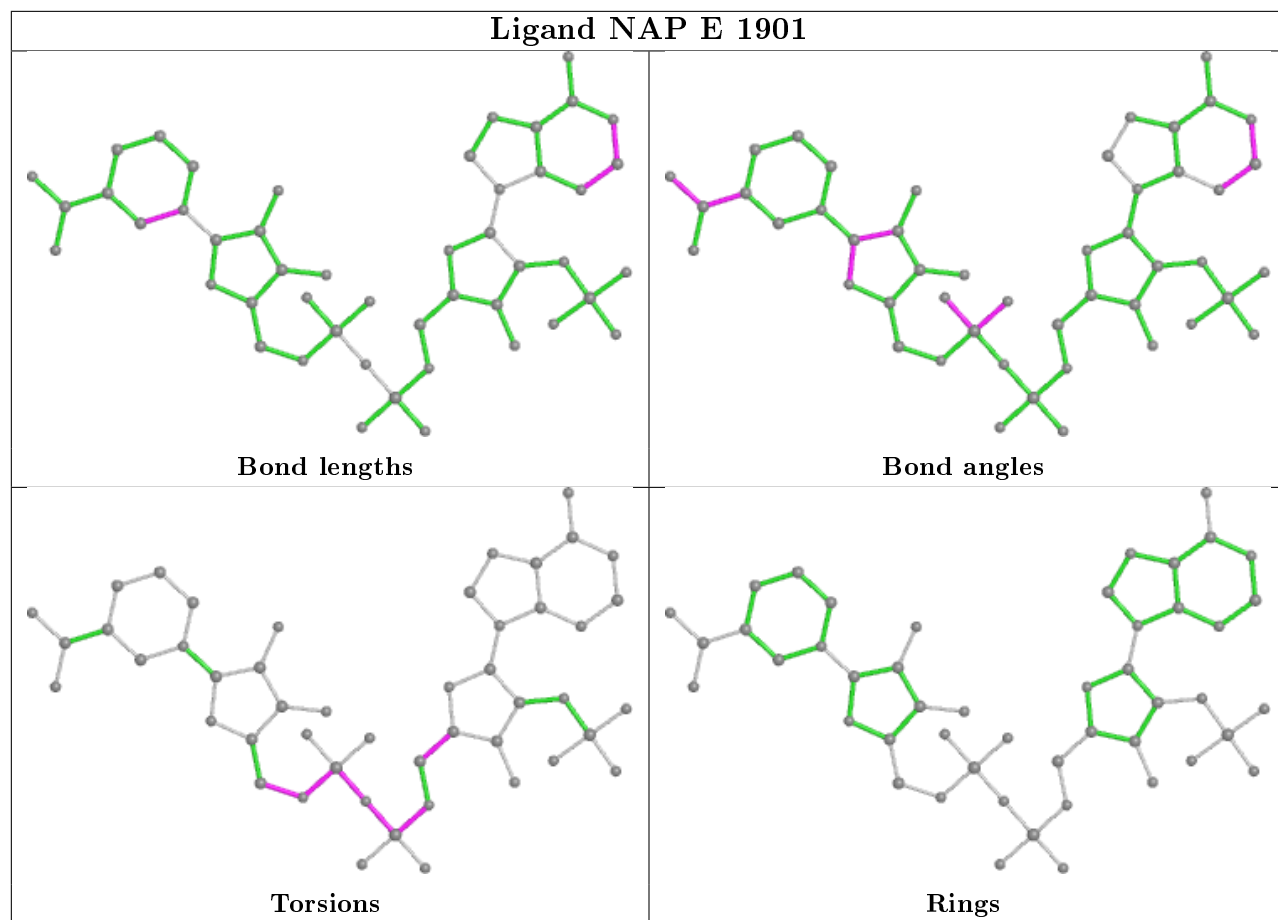
18 monomers are involved in 147 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2102	NAP	4	0
3	C	1901	NAP	4	0
3	E	1901	NAP	4	0
4	K	2101	FMN	15	0
4	H	2101	FMN	16	0
4	I	2101	FMN	16	0
4	L	2101	FMN	15	0
4	G	2101	FMN	17	0
3	K	2102	NAP	4	0
3	I	2102	NAP	4	0
3	B	1901	NAP	5	0
3	G	2102	NAP	4	0
3	F	1901	NAP	4	0
4	J	2101	FMN	15	0
3	L	2102	NAP	4	0
3	D	1901	NAP	6	0
3	H	2102	NAP	5	0
3	A	1901	NAP	5	0

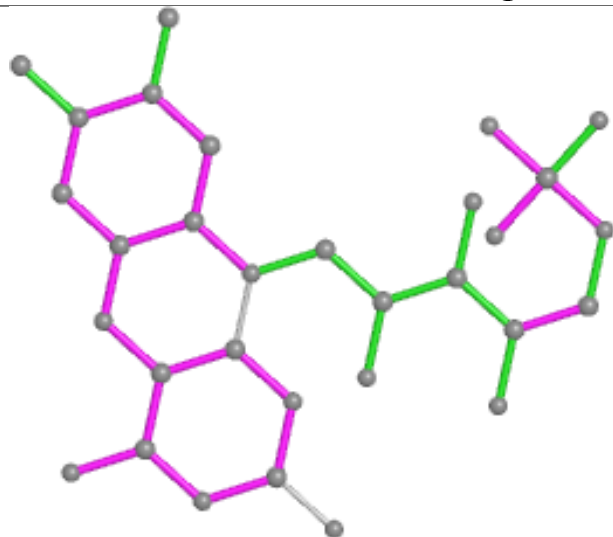
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



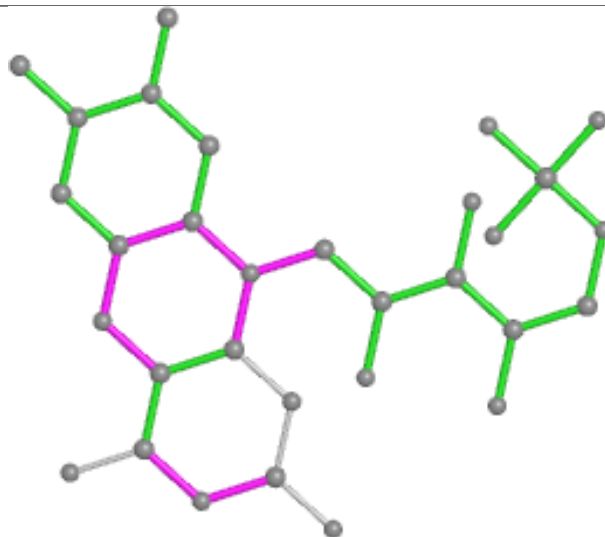




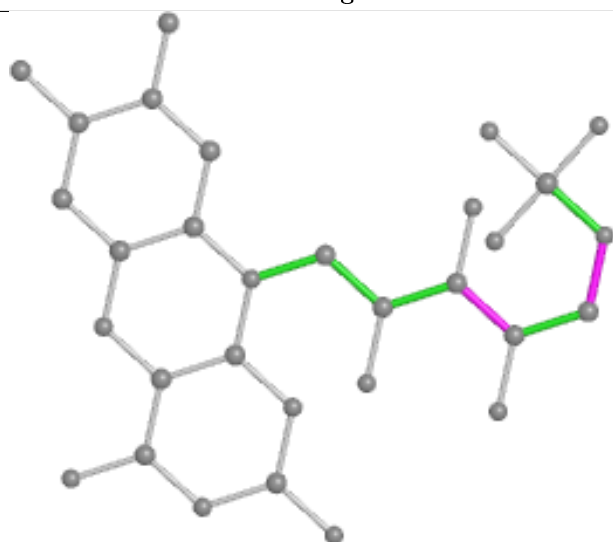
Ligand FMN K 2101



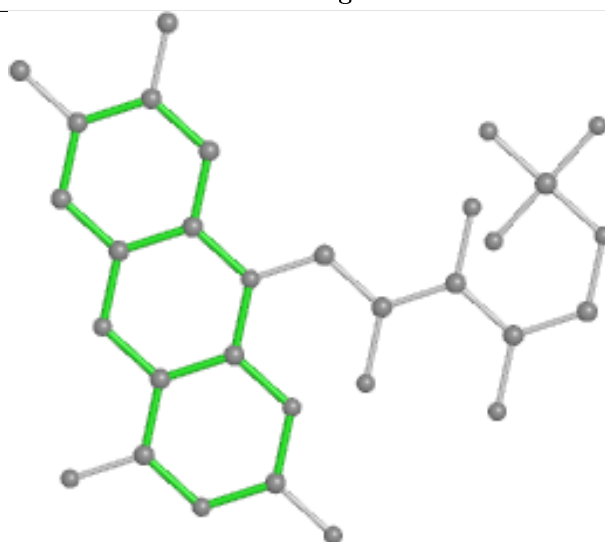
Bond lengths



Bond angles

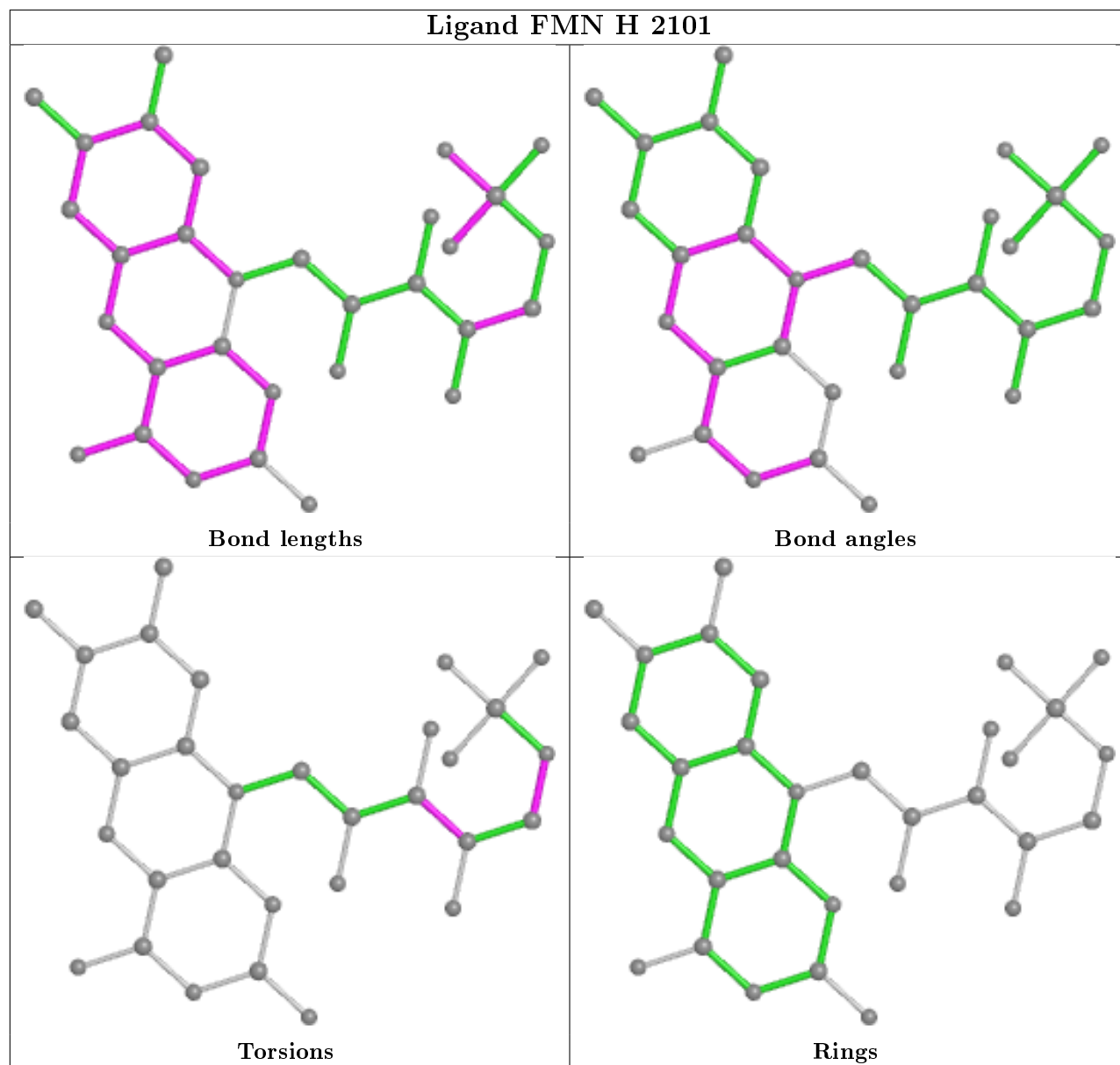


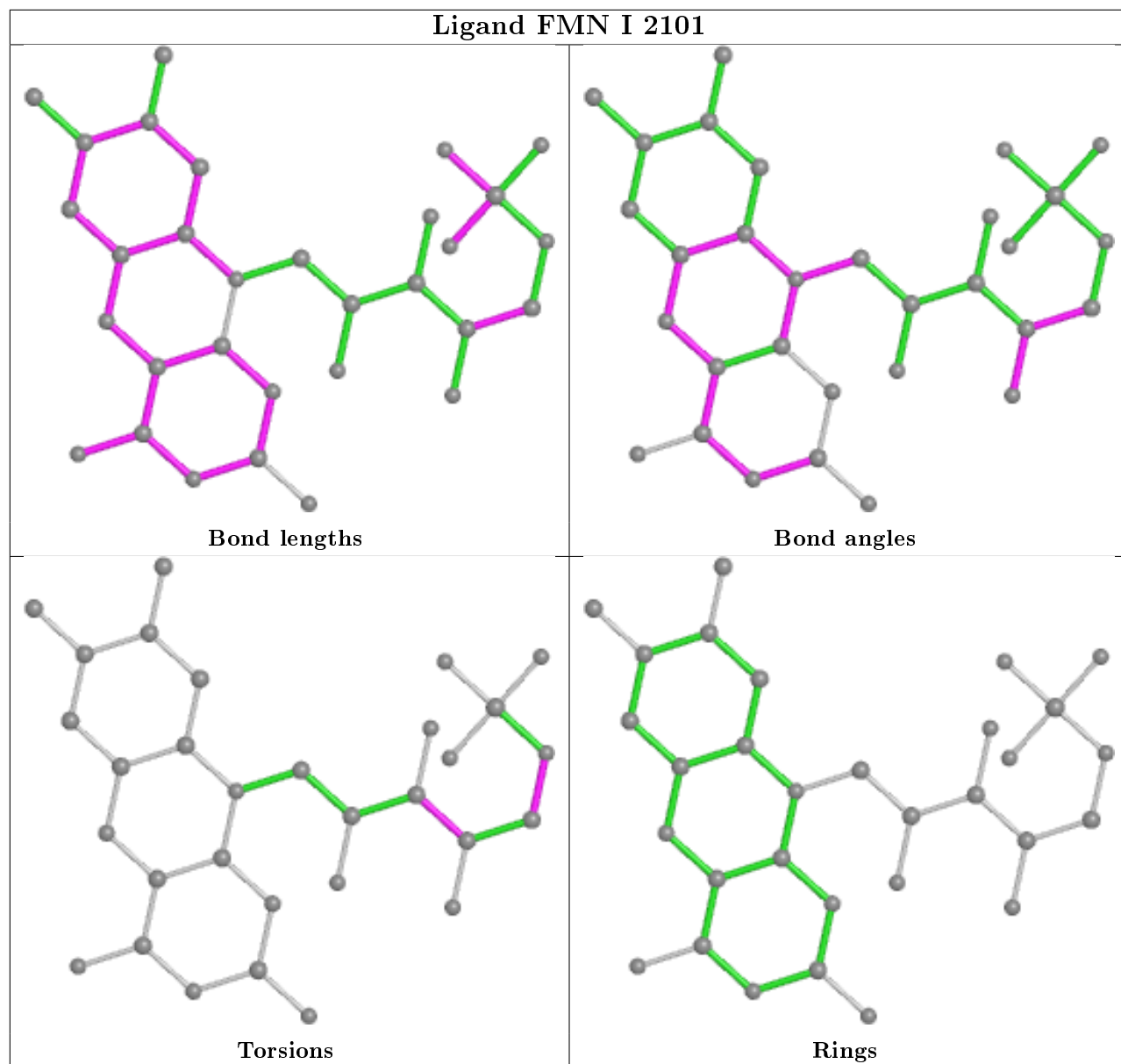
Torsions



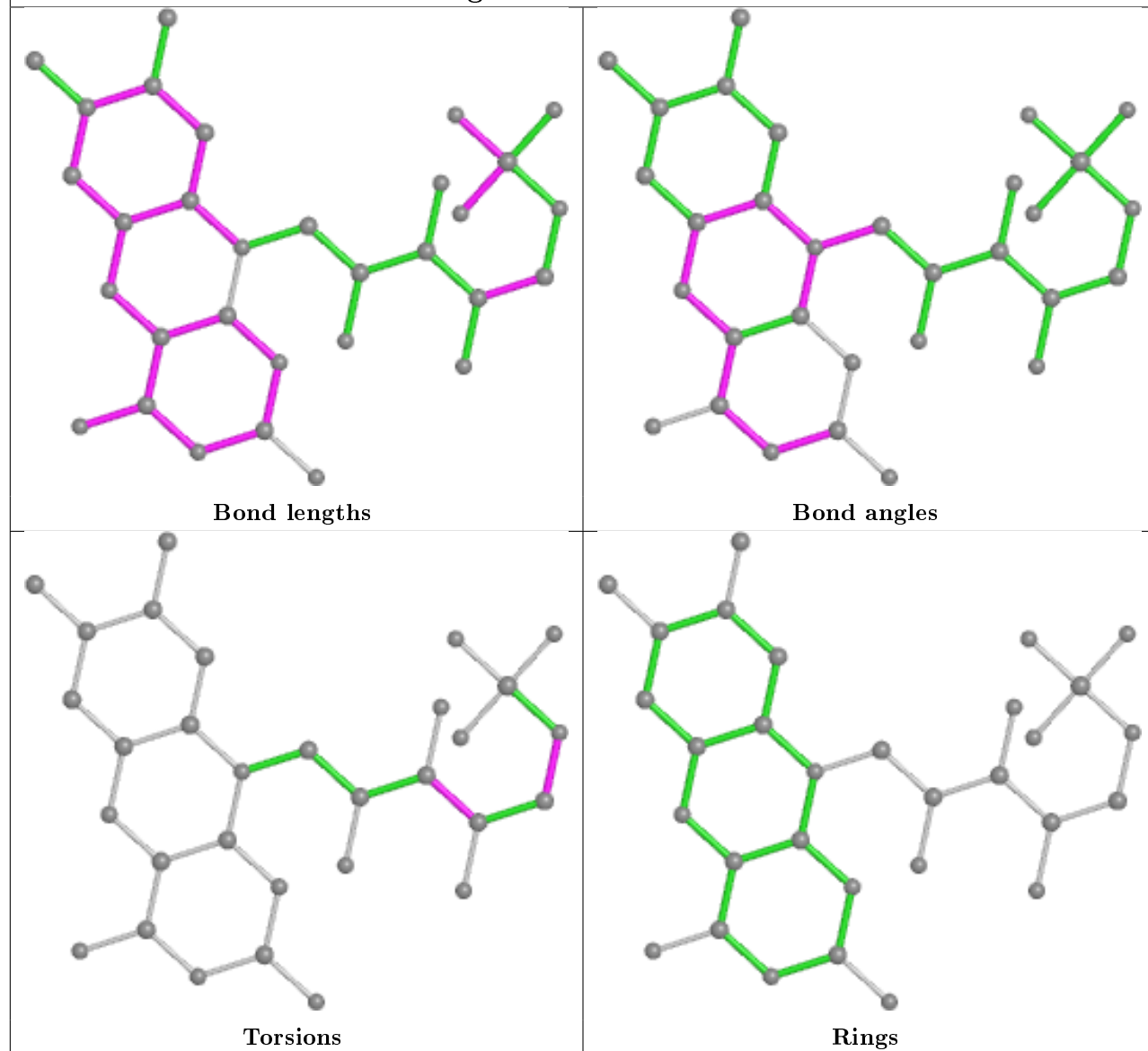
Rings

Ligand FMN H 2101

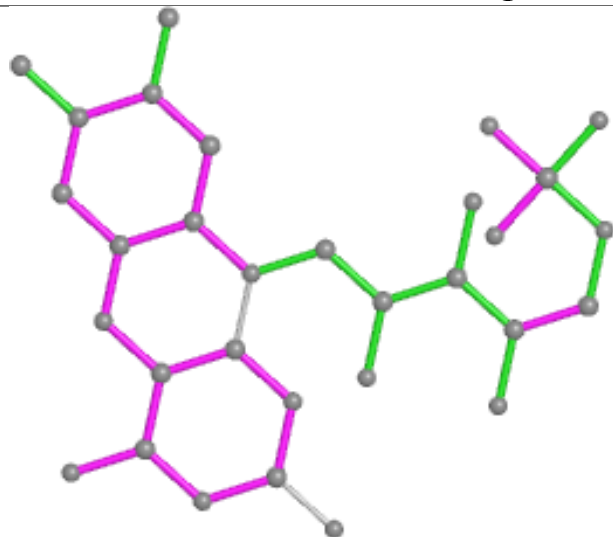




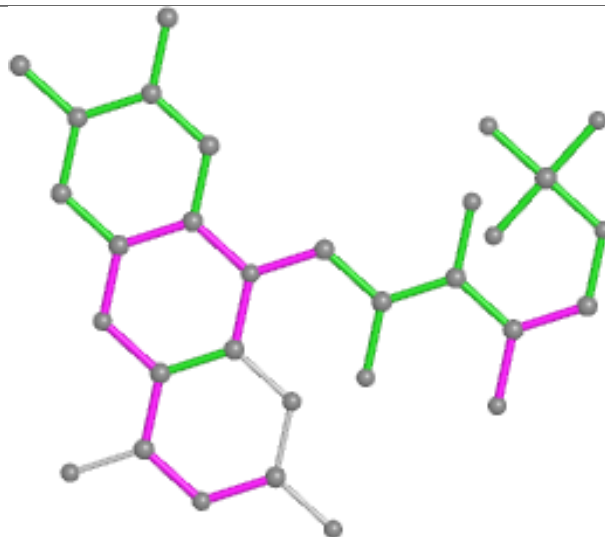
Ligand FMN L 2101



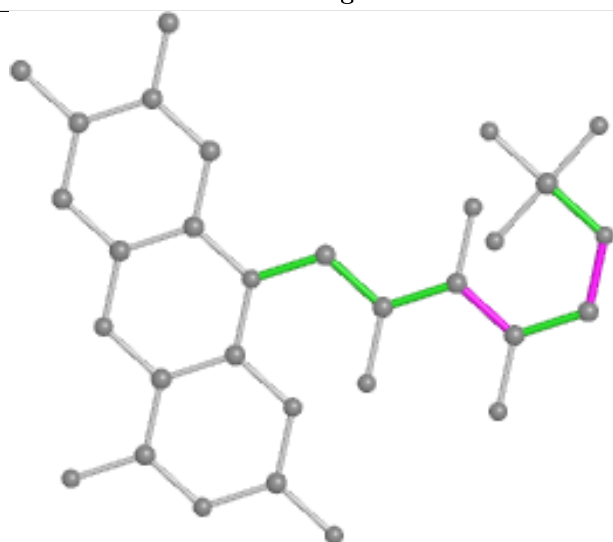
Ligand FMN G 2101



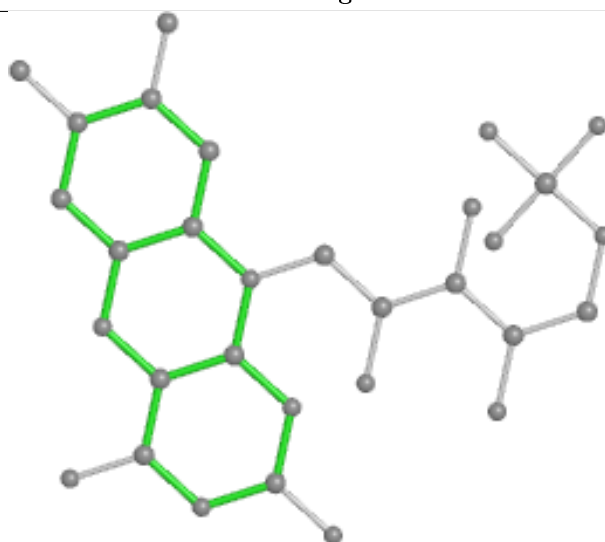
Bond lengths



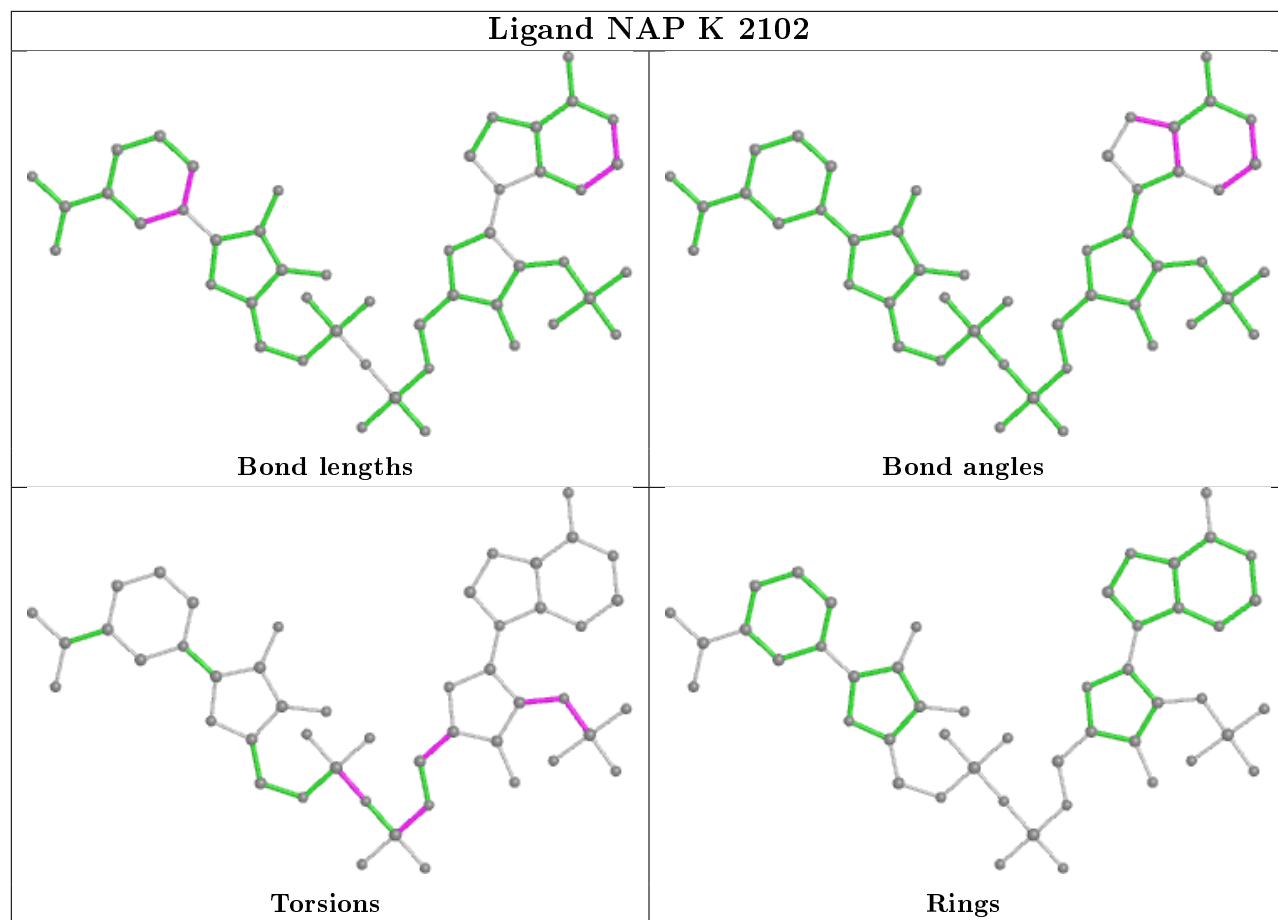
Bond angles

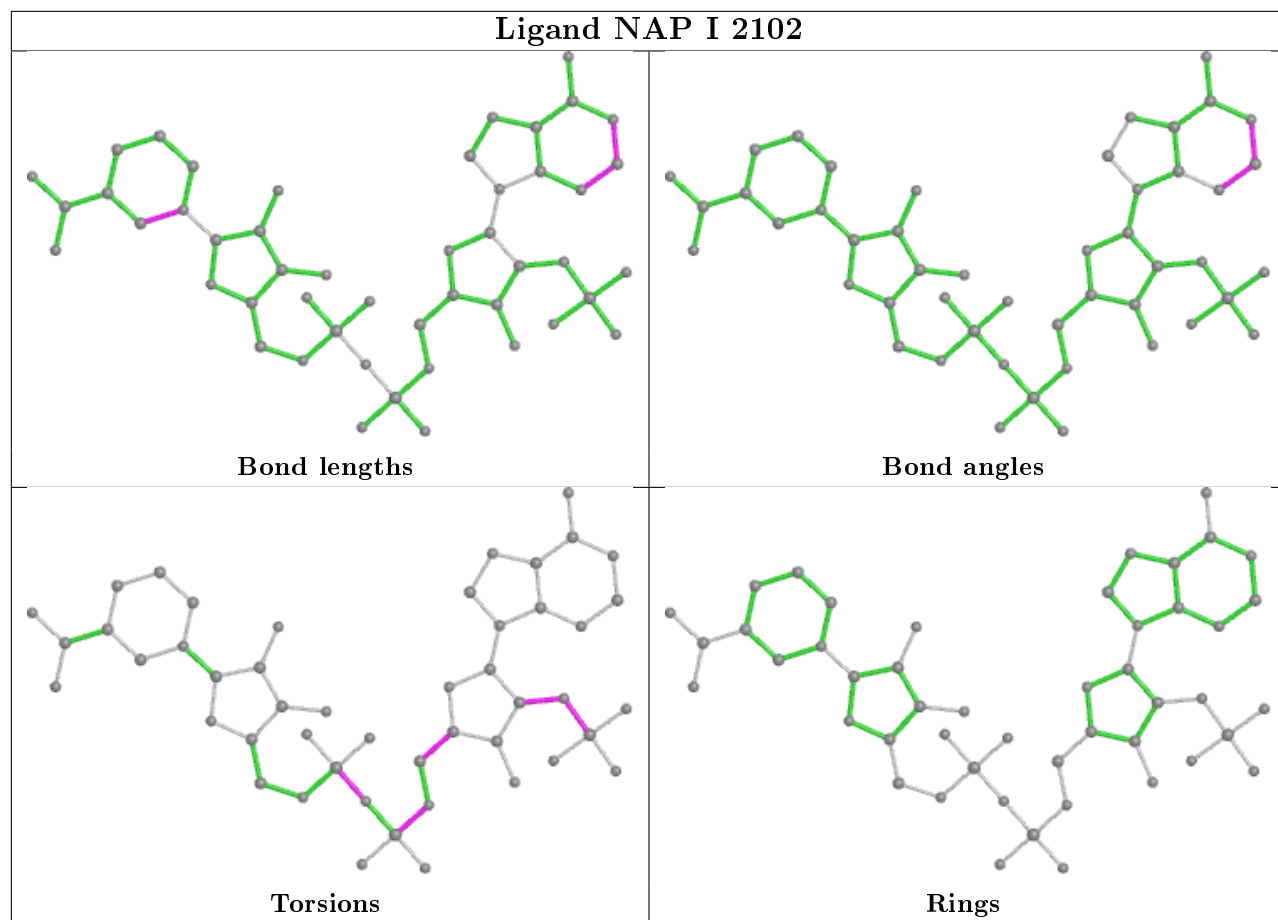


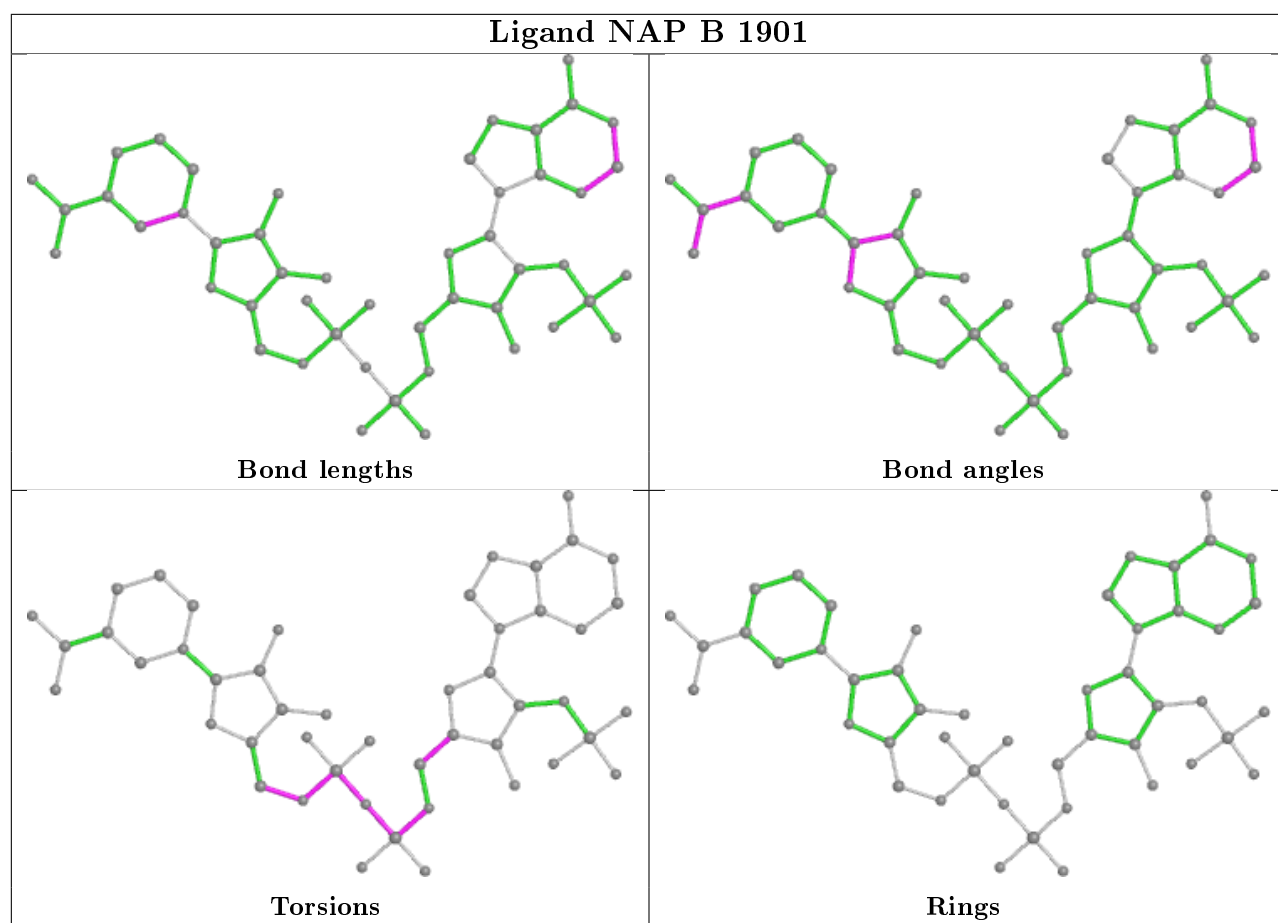
Torsions

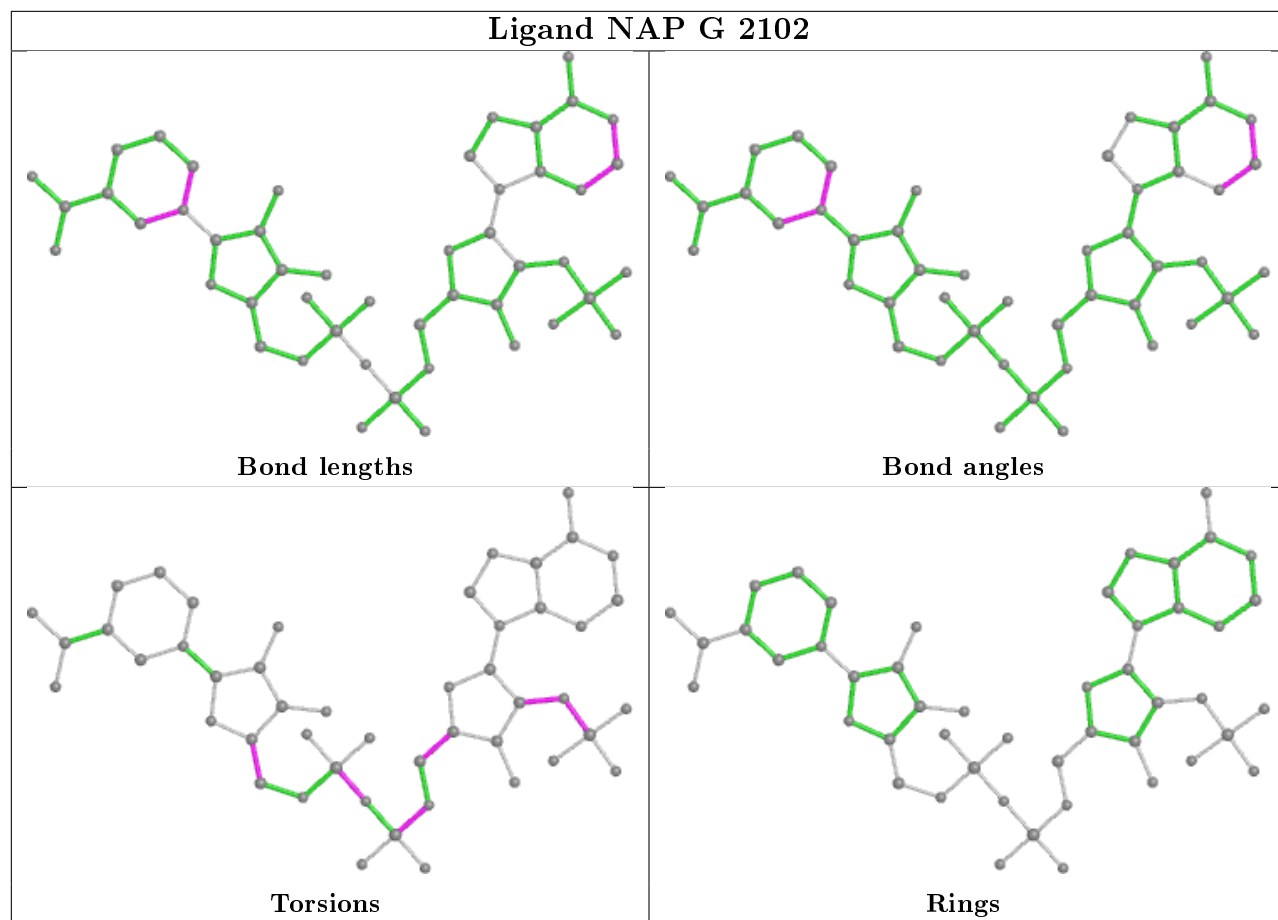


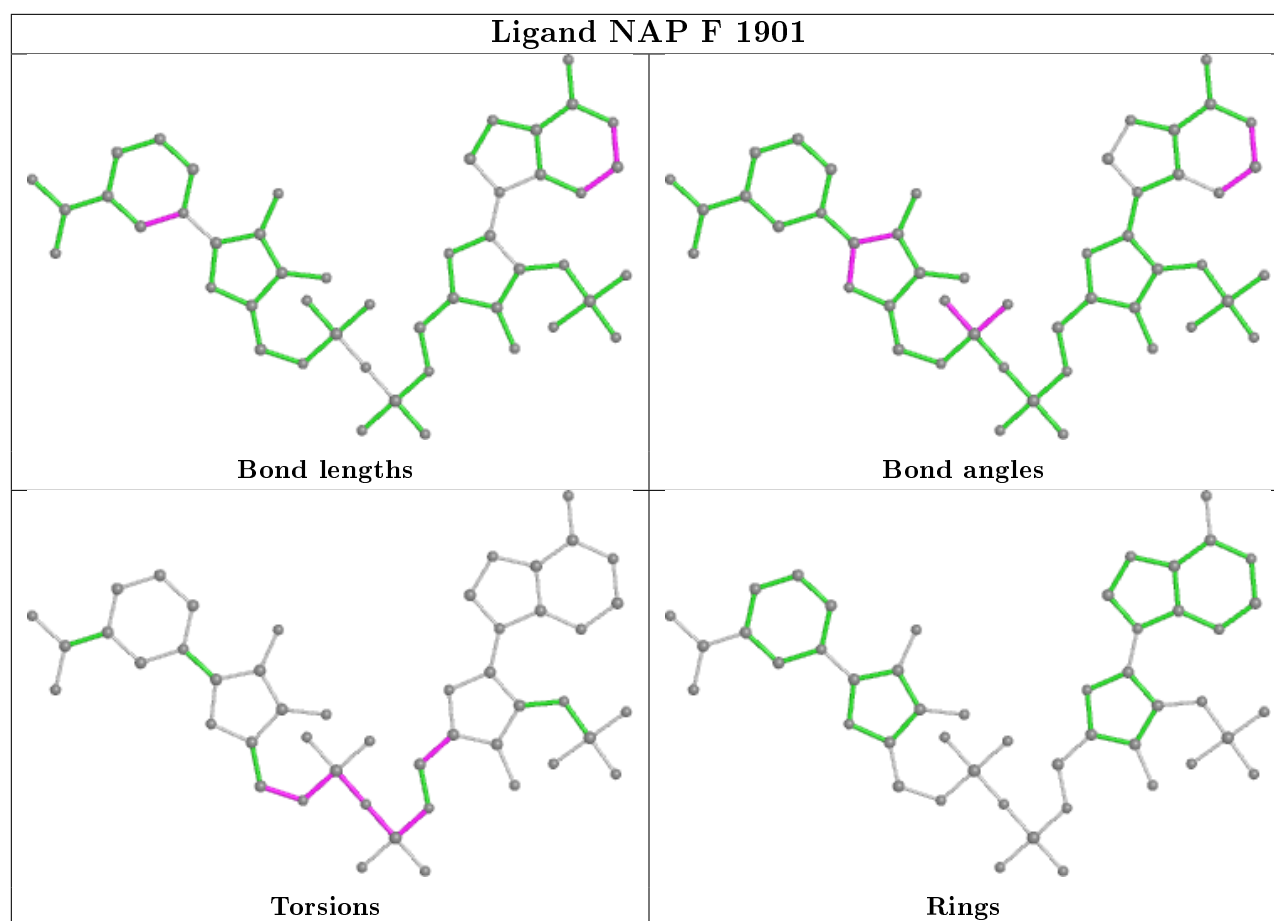
Rings



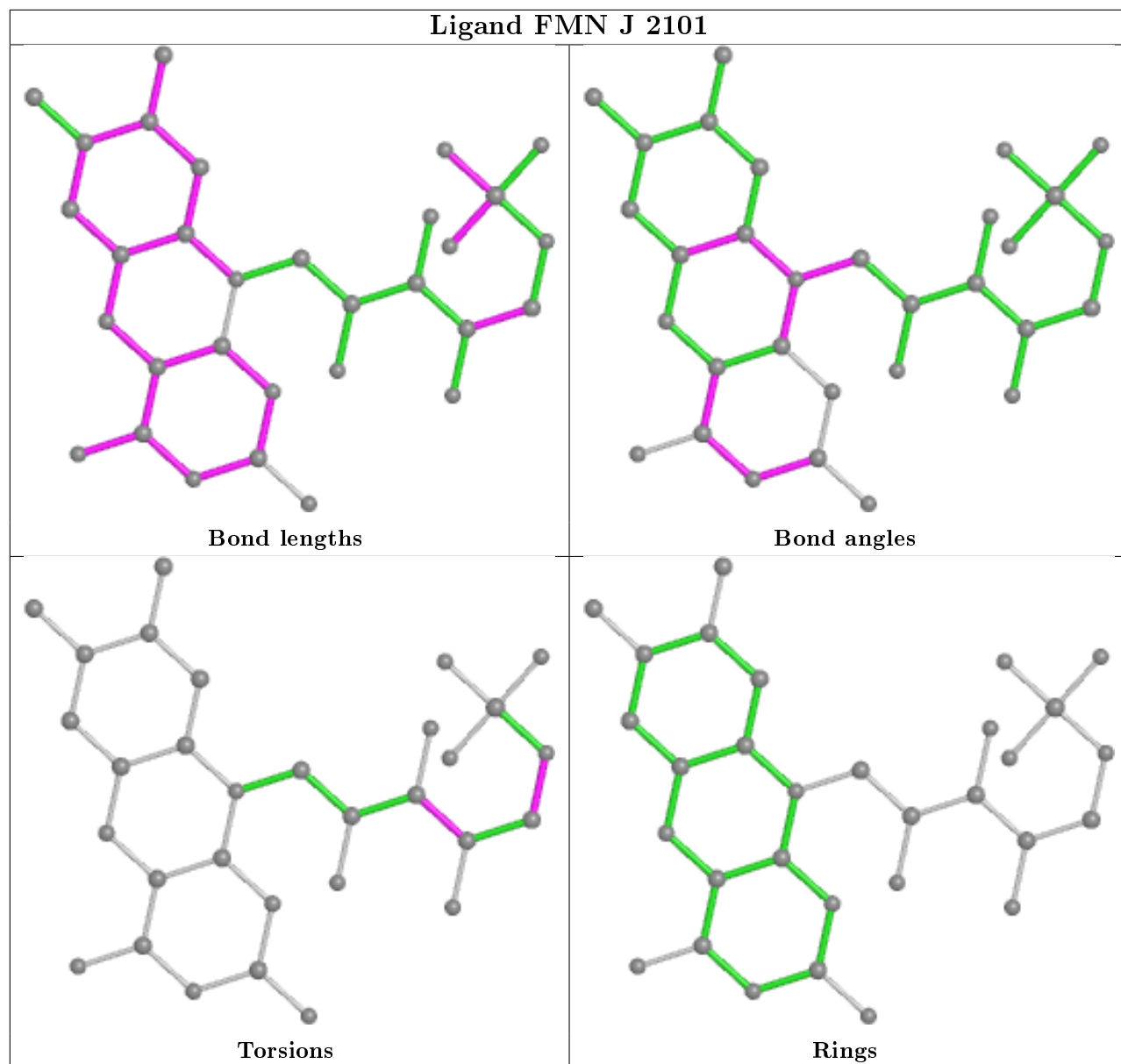


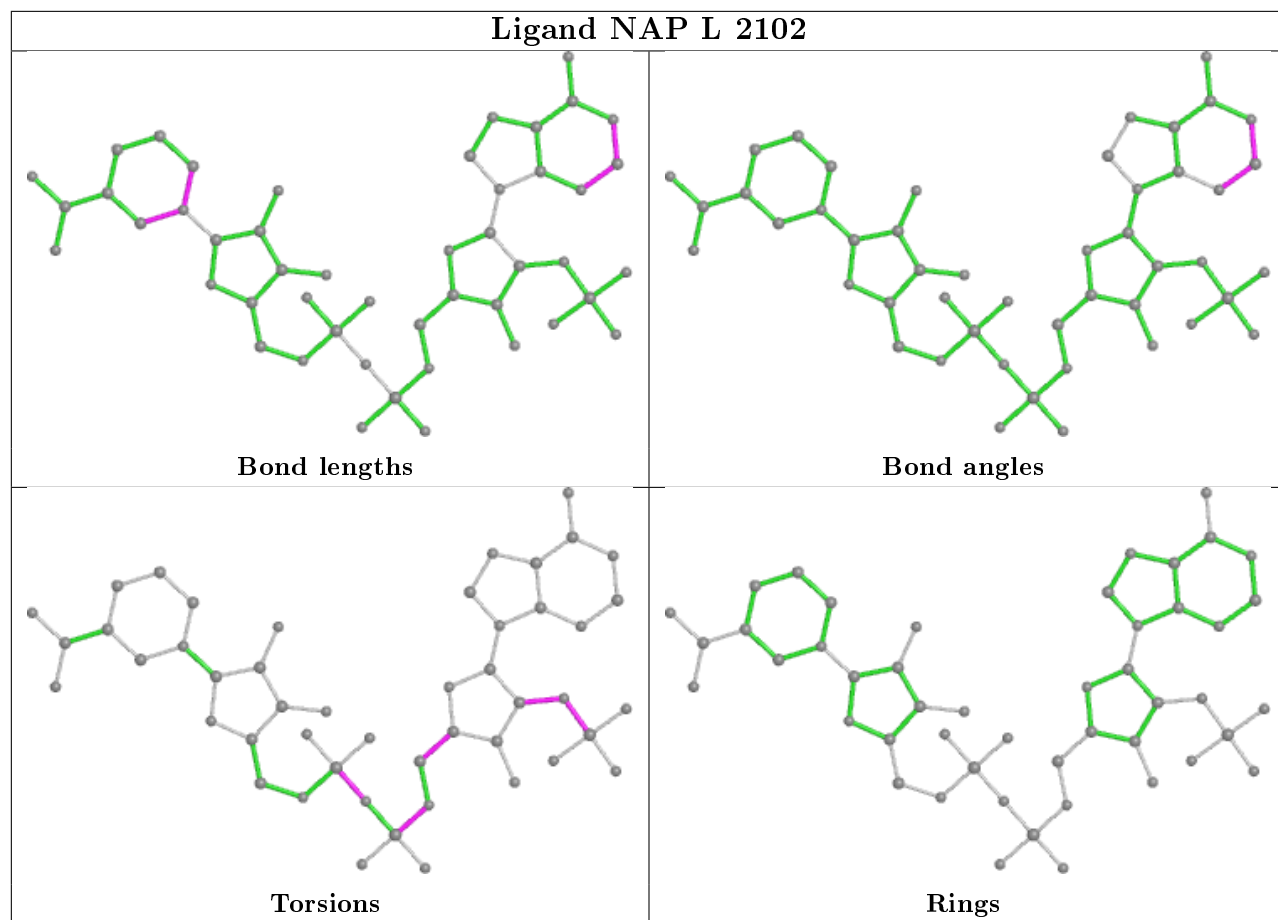


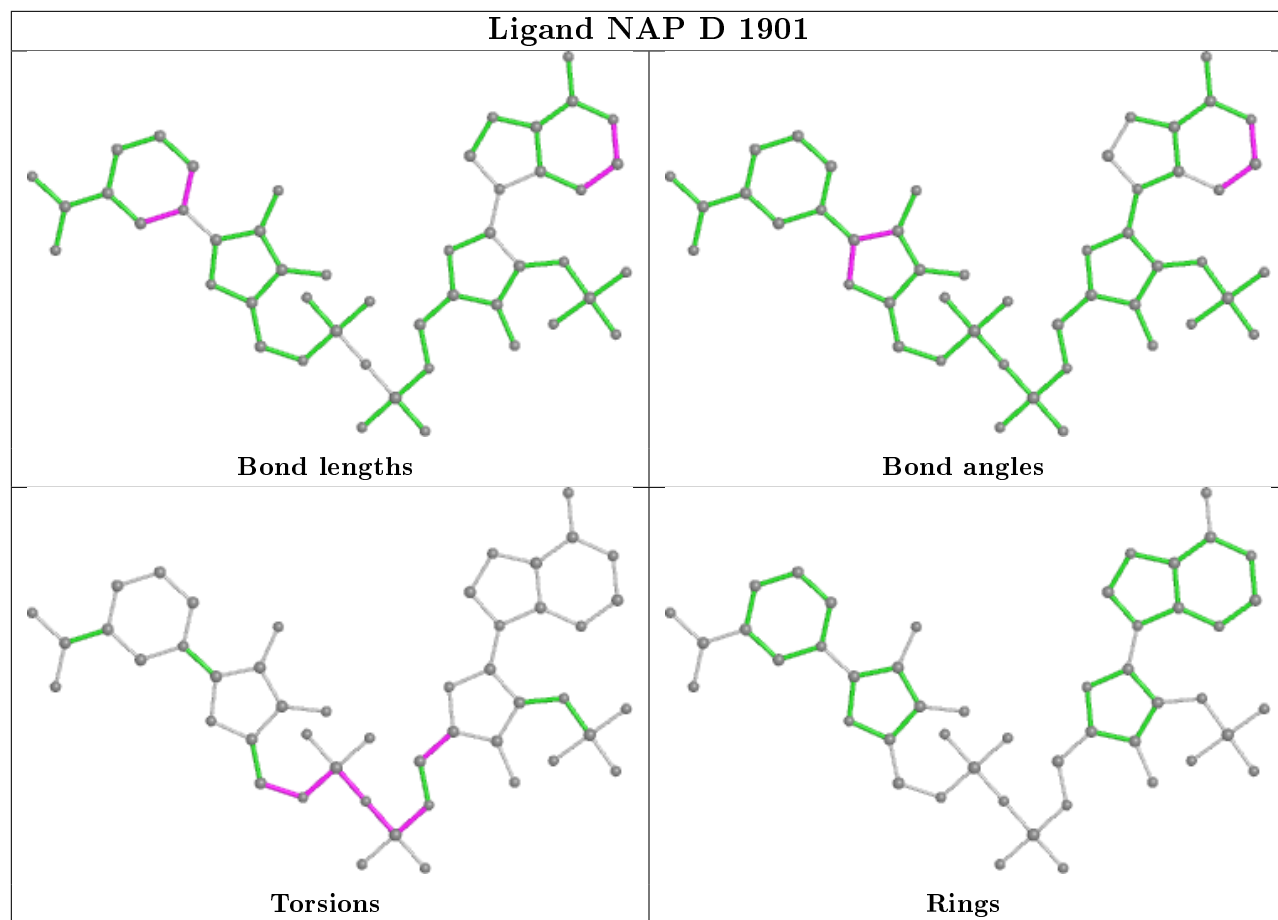


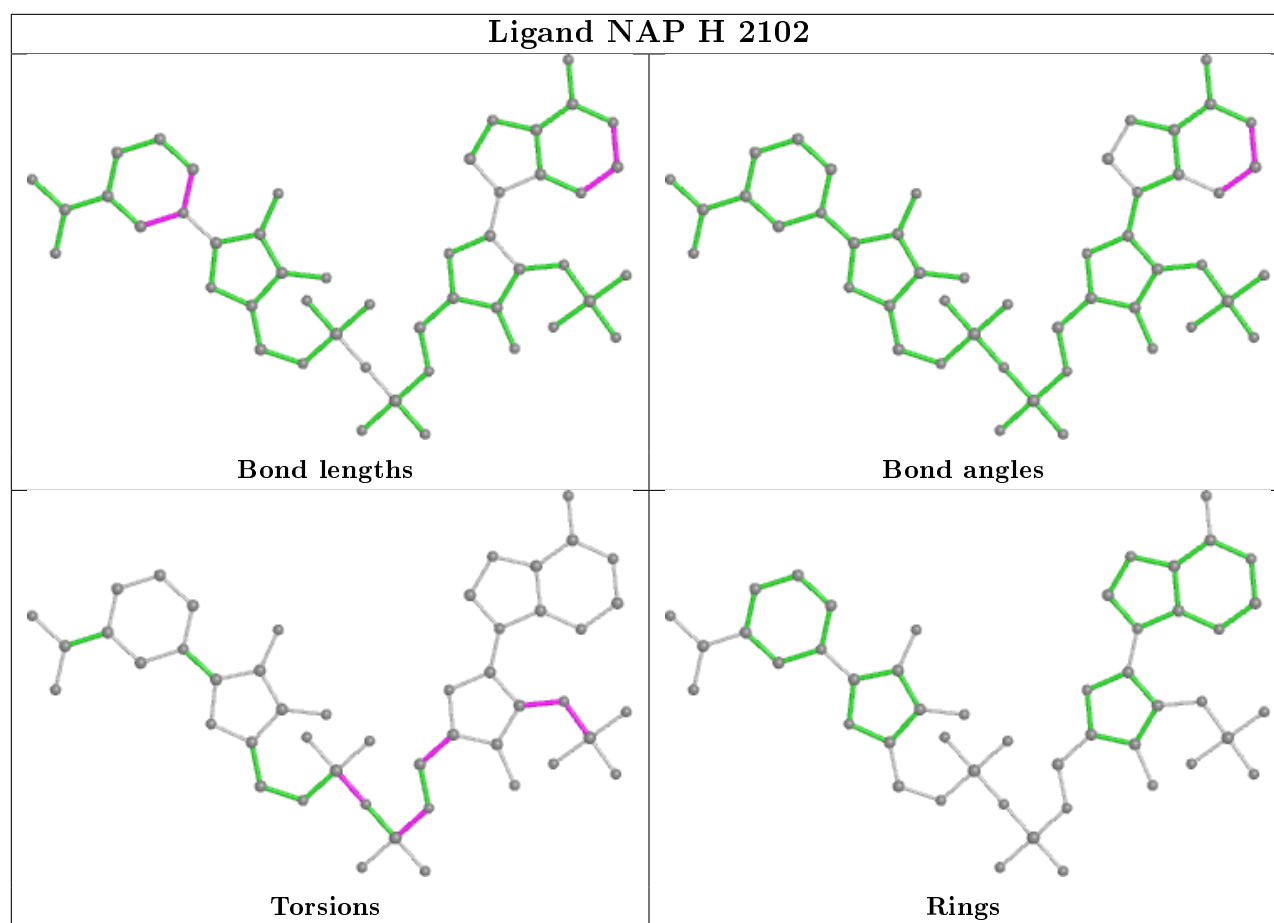


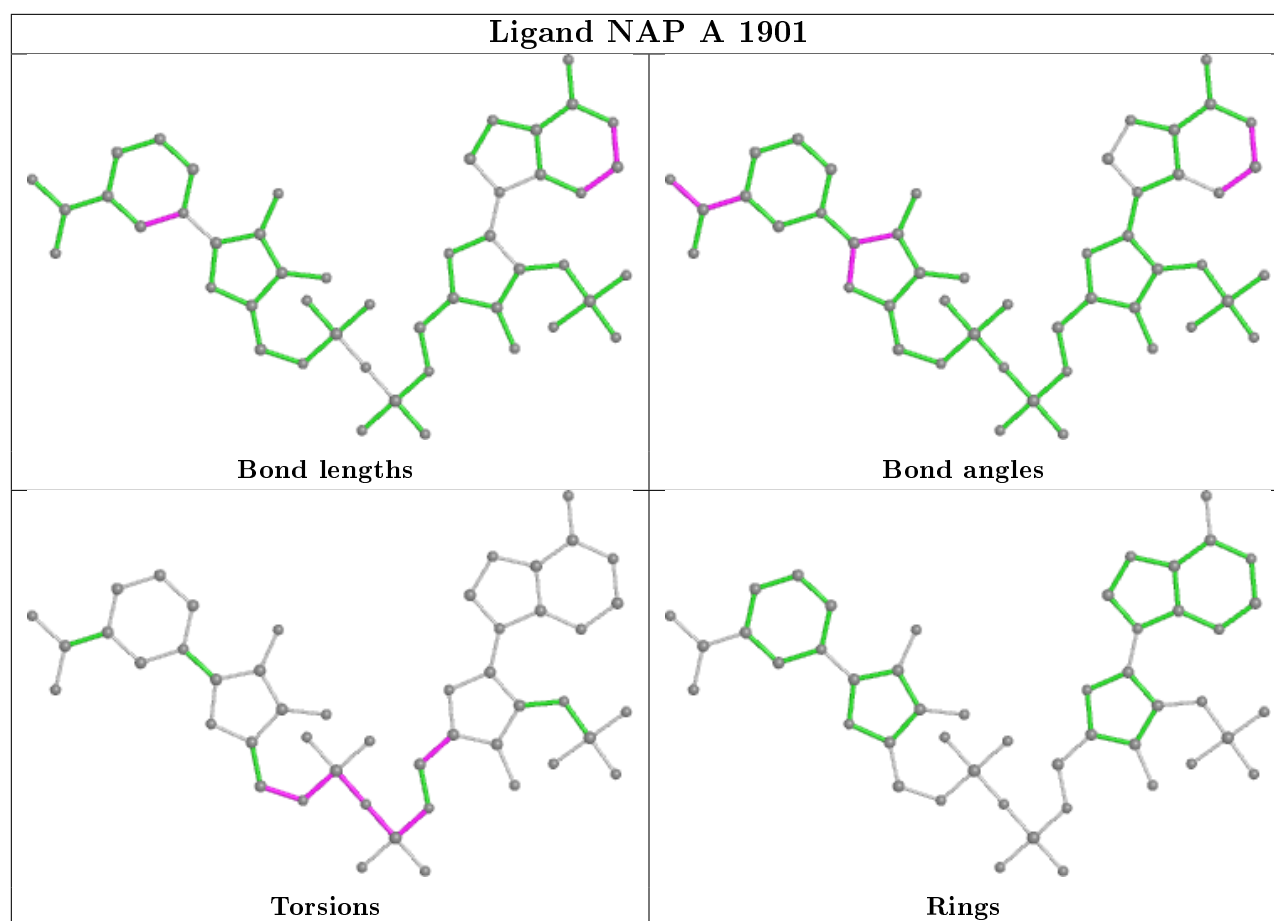
Ligand FMN J 2101











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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1457/1878 (77%)	0.30	44 (3%)	50	27	16, 50, 103, 146	0
1	B	1464/1878 (77%)	0.31	38 (2%)	56	33	17, 50, 106, 157	0
1	C	1462/1878 (77%)	0.33	44 (3%)	50	27	15, 48, 107, 155	0
1	D	1467/1878 (78%)	0.29	47 (3%)	47	25	17, 52, 106, 151	0
1	E	1456/1878 (77%)	0.31	47 (3%)	47	25	17, 50, 106, 152	0
1	F	1461/1878 (77%)	0.34	37 (2%)	57	34	17, 47, 106, 156	0
2	G	2060/2060 (100%)	0.48	170 (8%)	11	4	24, 83, 128, 156	0
2	H	2060/2060 (100%)	0.57	222 (10%)	5	2	24, 85, 129, 155	0
2	I	2060/2060 (100%)	0.51	212 (10%)	6	2	20, 85, 129, 158	0
2	J	2060/2060 (100%)	0.61	275 (13%)	3	1	27, 88, 132, 157	0
2	K	2060/2060 (100%)	0.85	353 (17%)	1	0	25, 90, 133, 157	0
2	L	2060/2060 (100%)	0.58	259 (12%)	3	1	22, 86, 131, 158	0
All	All	21127/23628 (89%)	0.48	1748 (8%)	11	4	15, 74, 125, 158	0

The worst 5 of 1748 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	176	GLN	16.8
2	H	178	ASN	14.1
2	K	178	ASN	14.0
2	K	175	GLY	12.8
2	K	516	PHE	12.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

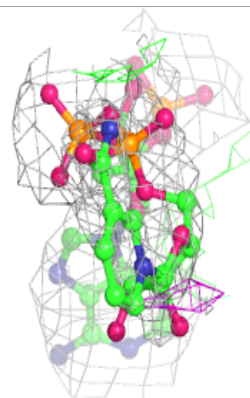
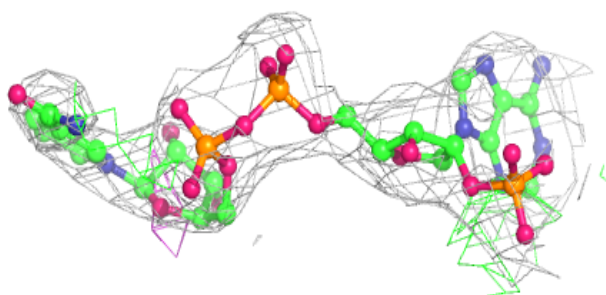
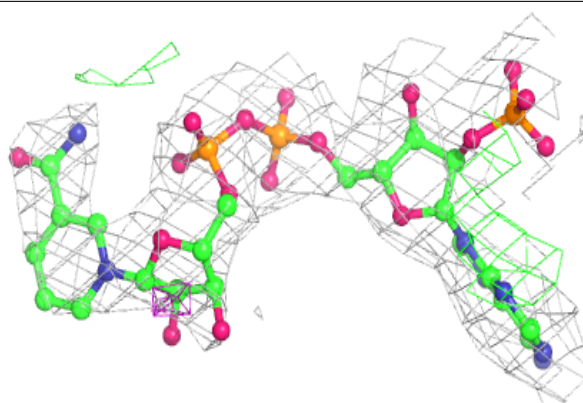
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAP	C	1901	48/48	0.87	0.34	23,81,130,171	0
3	NAP	F	1901	48/48	0.87	0.31	19,78,125,159	0
3	NAP	D	1901	48/48	0.87	0.34	21,83,127,174	0
3	NAP	J	2102	48/48	0.89	0.21	35,88,118,120	0
3	NAP	K	2102	48/48	0.90	0.29	43,94,127,131	0
3	NAP	A	1901	48/48	0.90	0.32	19,76,121,169	0
4	FMN	K	2101	31/31	0.92	0.36	27,66,110,123	0
3	NAP	B	1901	48/48	0.92	0.32	23,78,115,145	0
3	NAP	H	2102	48/48	0.92	0.25	37,85,113,122	0
3	NAP	G	2102	48/48	0.92	0.24	42,87,119,128	0
3	NAP	L	2102	48/48	0.93	0.31	37,84,116,120	0
3	NAP	E	1901	48/48	0.93	0.26	24,77,123,157	0
4	FMN	J	2101	31/31	0.94	0.32	23,61,101,113	0
4	FMN	G	2101	31/31	0.95	0.31	26,63,101,111	0
3	NAP	I	2102	48/48	0.95	0.26	29,80,104,116	0
4	FMN	L	2101	31/31	0.96	0.29	19,59,102,114	0
4	FMN	H	2101	31/31	0.96	0.32	25,49,105,113	0
4	FMN	I	2101	31/31	0.97	0.30	22,56,87,103	0

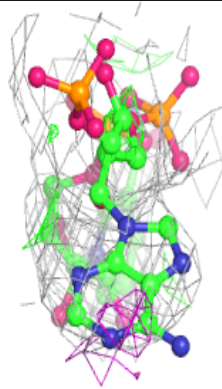
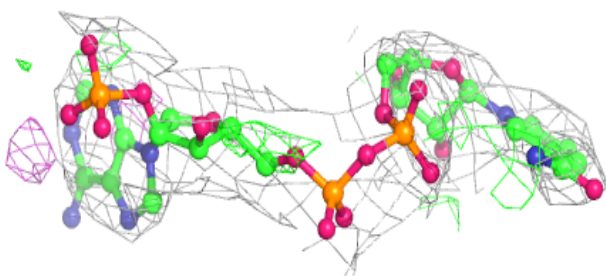
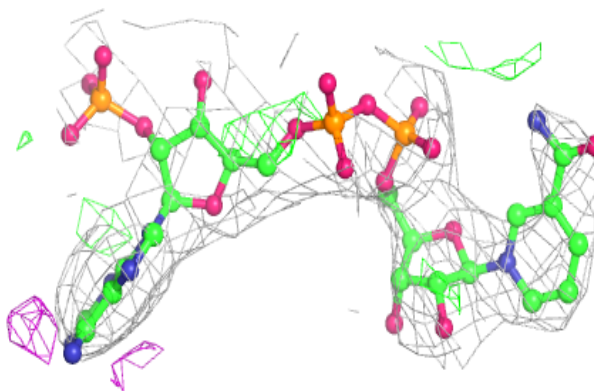
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAP C 1901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

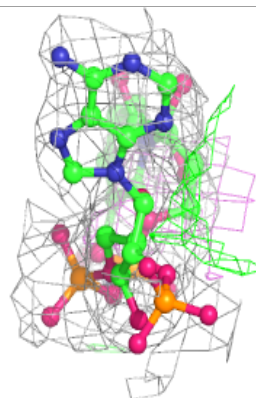
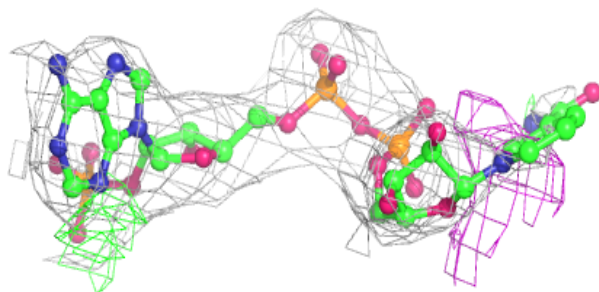
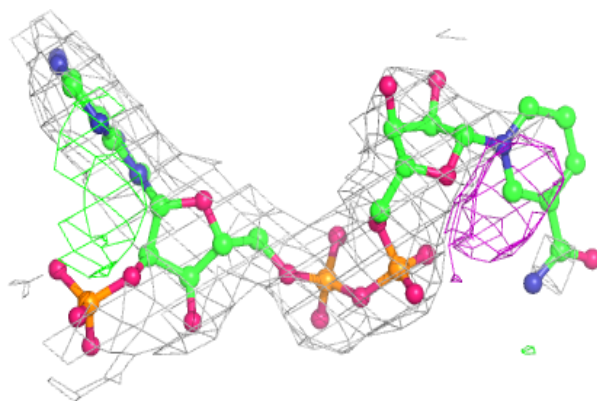
**Electron density around NAP F 1901:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

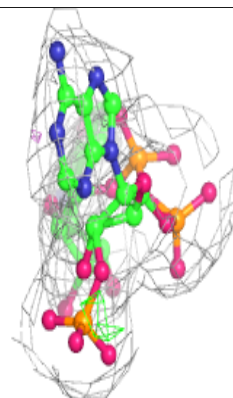
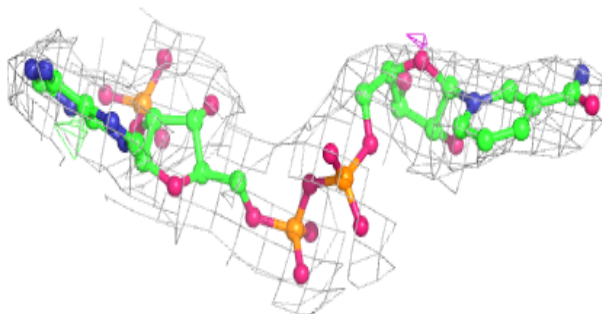
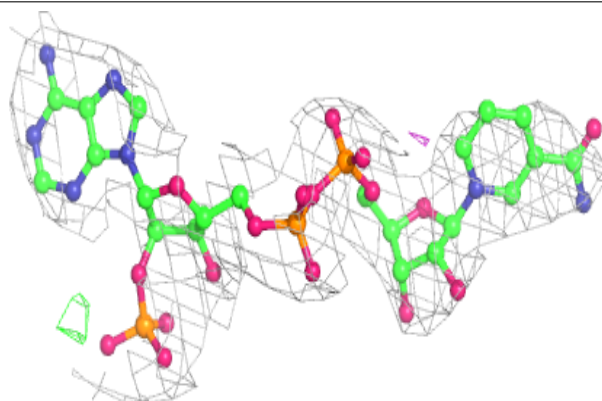


Electron density around NAP D 1901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

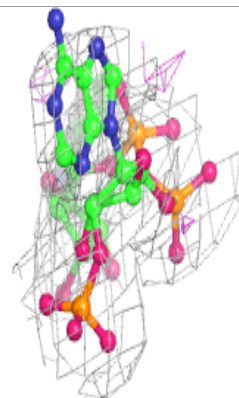
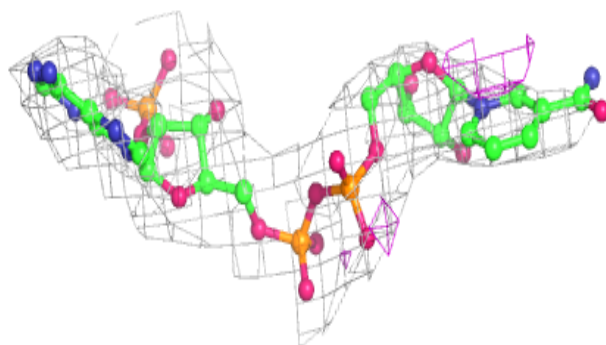
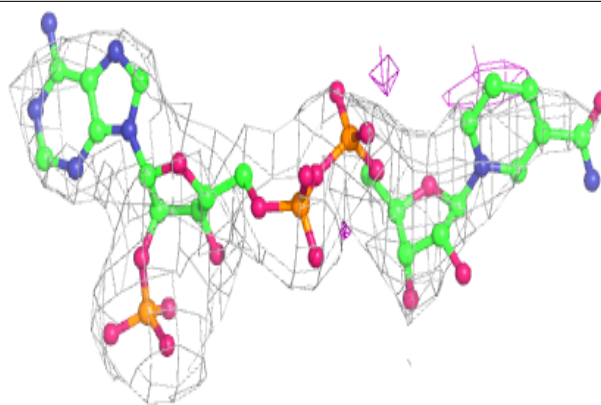
**Electron density around NAP J 2102:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

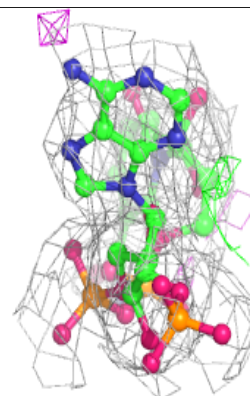
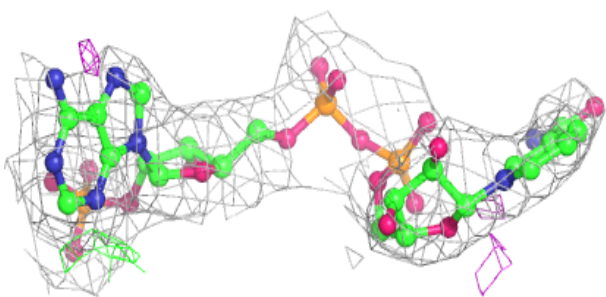
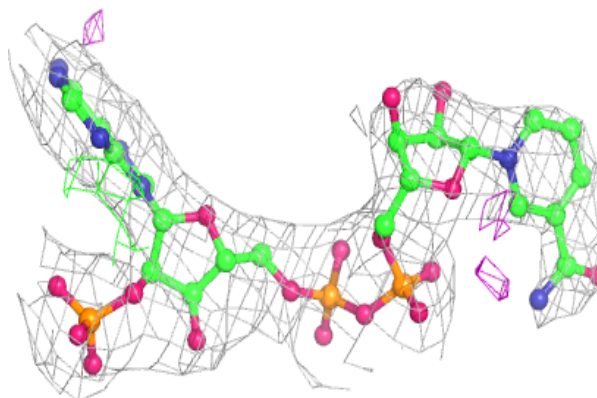


Electron density around NAP K 2102:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

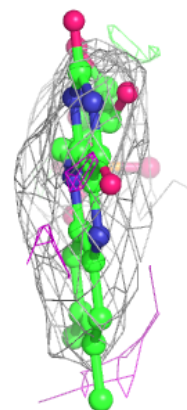
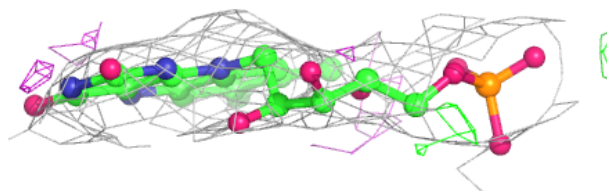
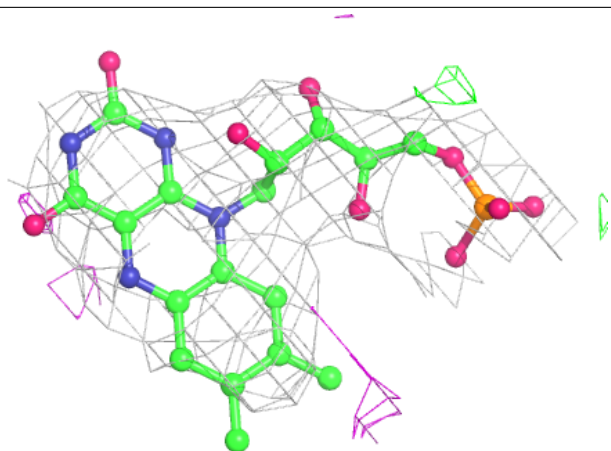
**Electron density around NAP A 1901:**

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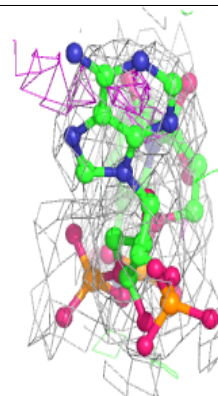
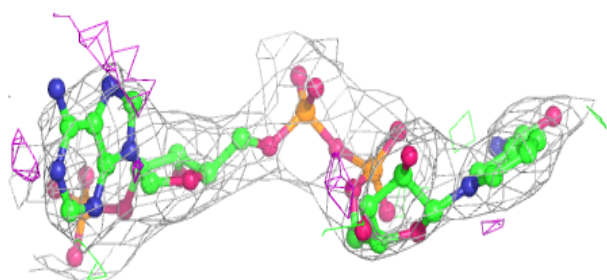
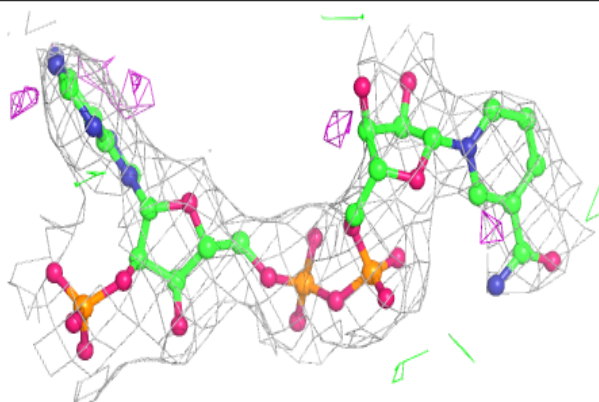


Electron density around FMN K 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

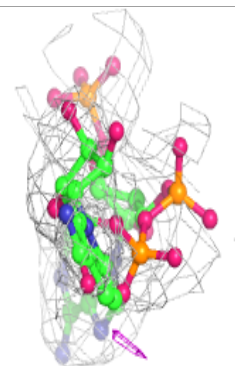
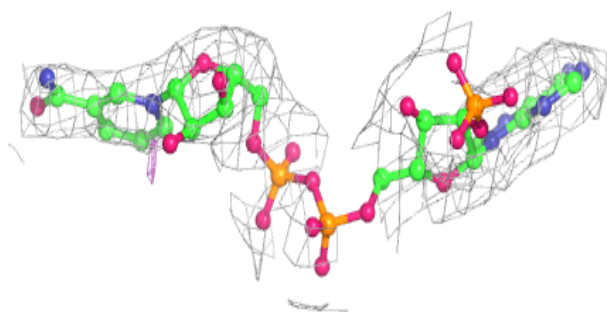
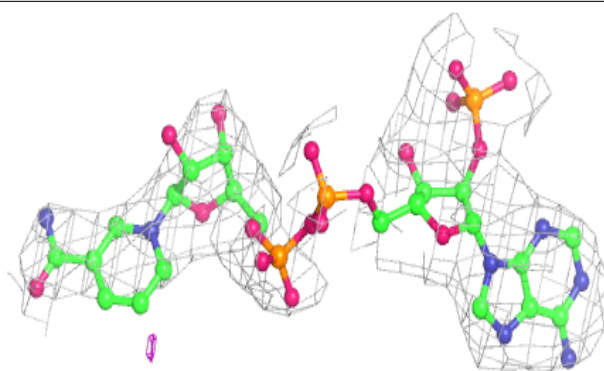
**Electron density around NAP B 1901:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

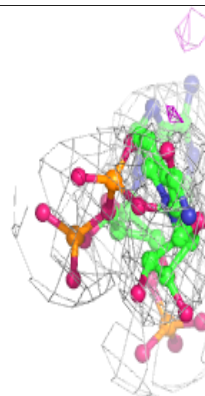
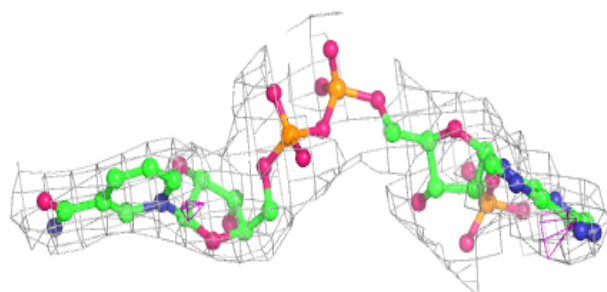
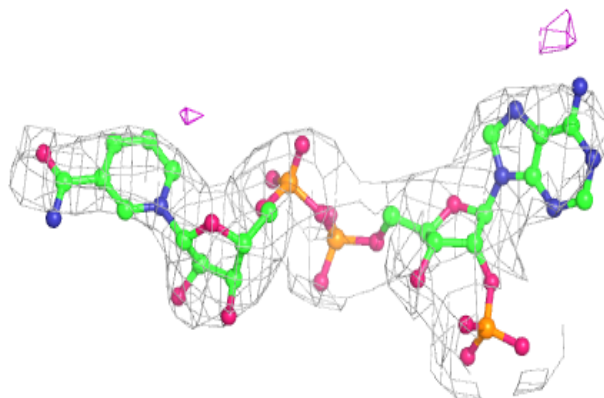


Electron density around NAP H 2102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

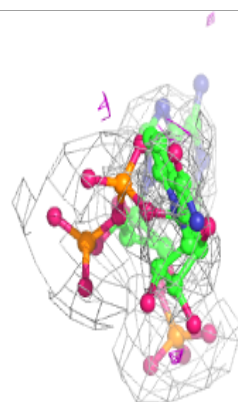
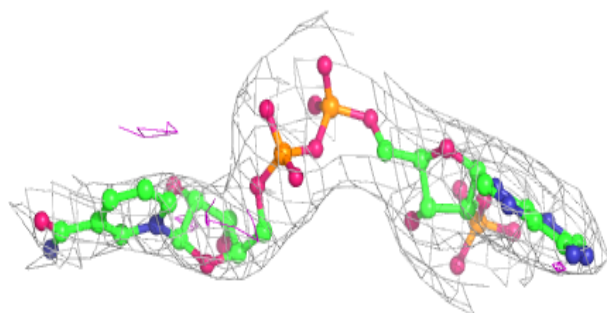
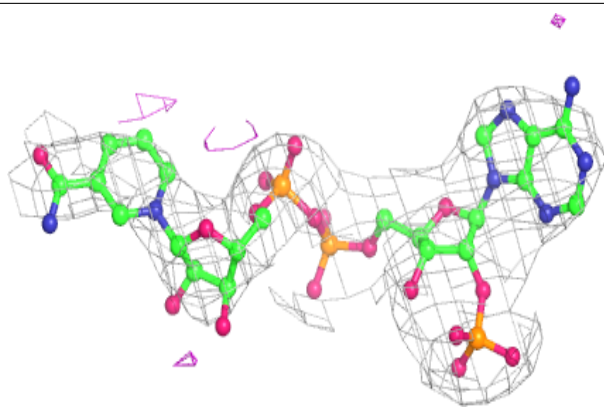
**Electron density around NAP G 2102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

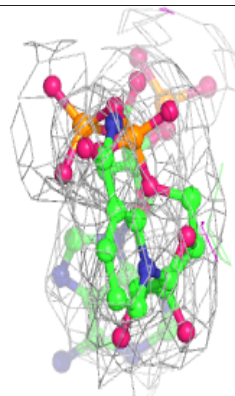
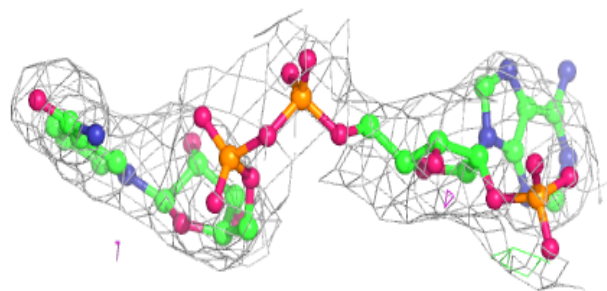
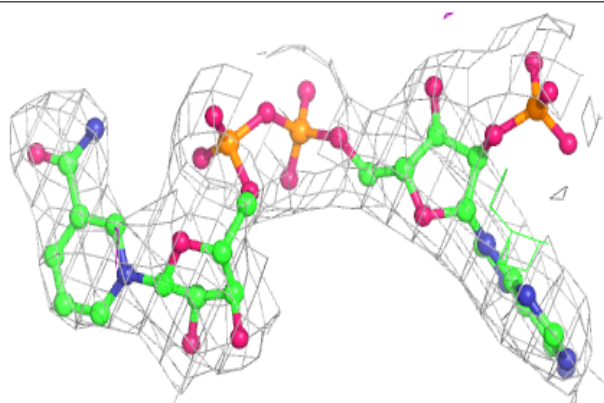


Electron density around NAP L 2102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

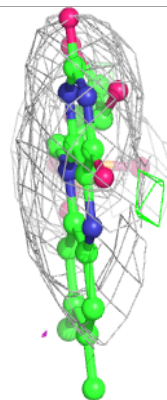
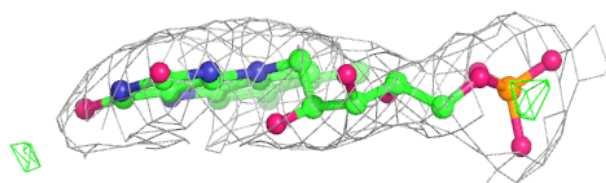
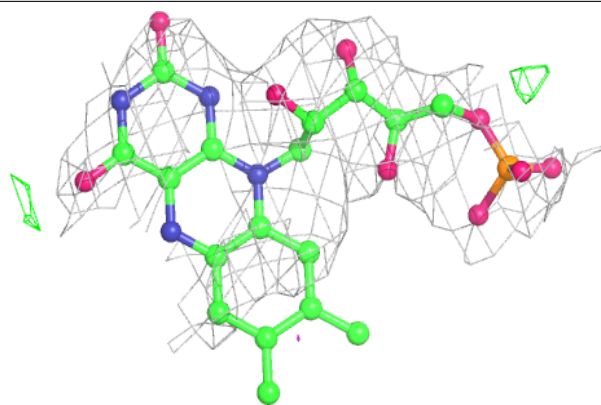
**Electron density around NAP E 1901:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

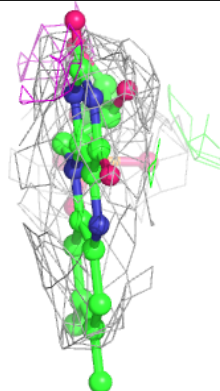
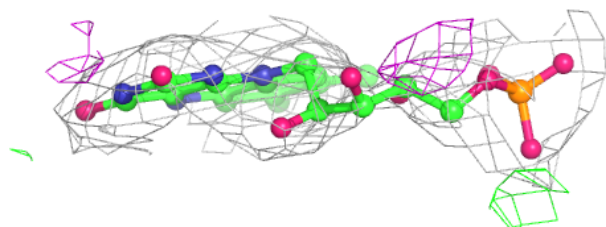
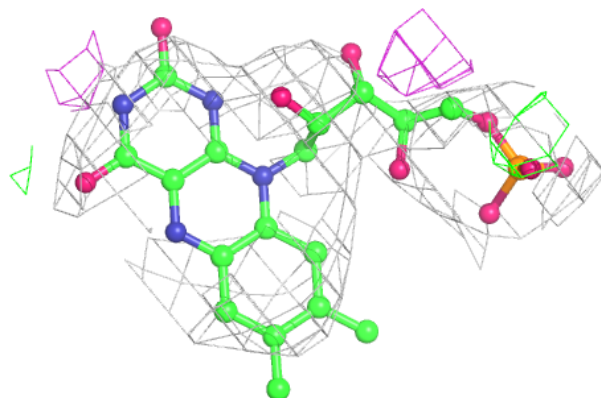


Electron density around FMN J 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

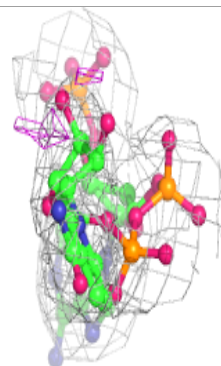
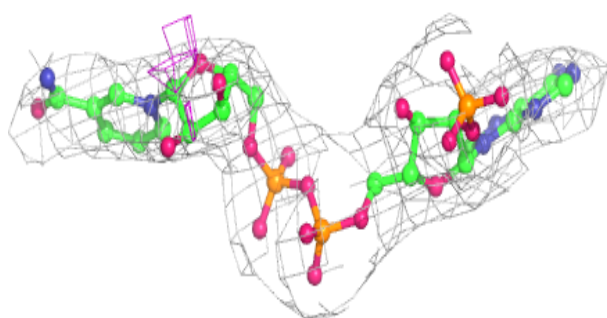
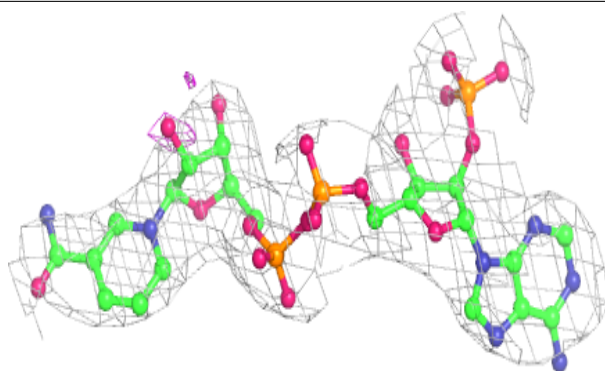
**Electron density around FMN G 2101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

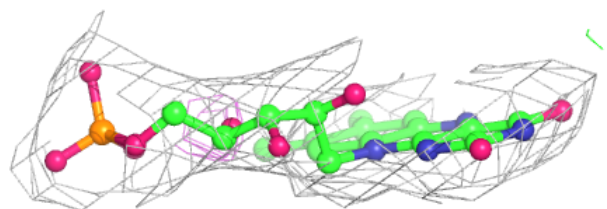
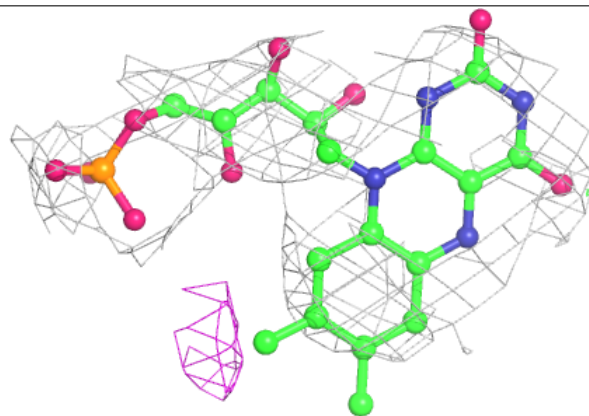


Electron density around NAP I 2102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

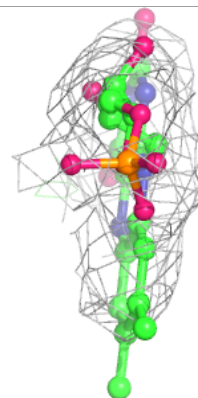
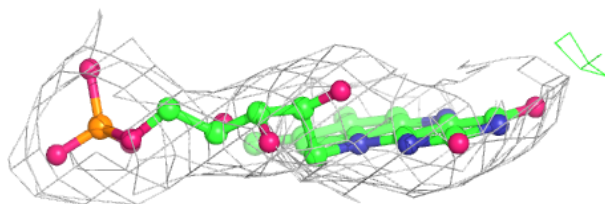
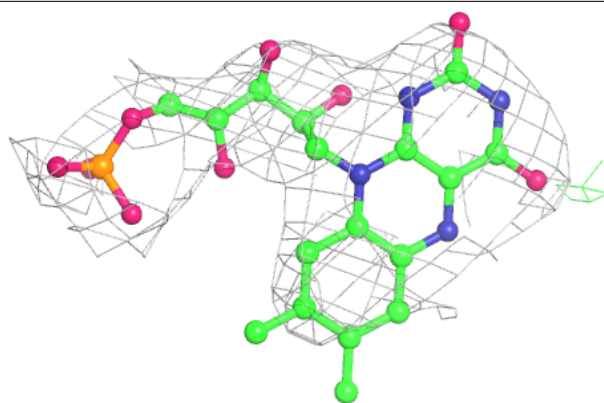
**Electron density around FMN L 2101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

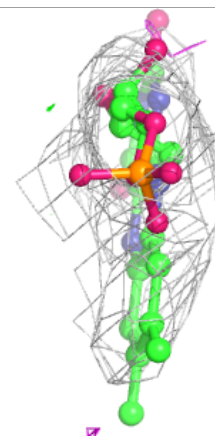
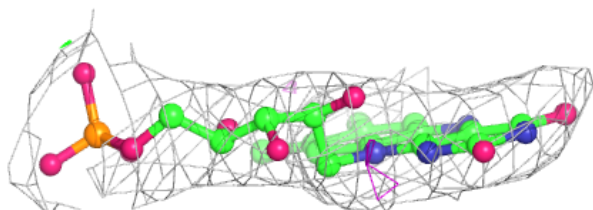
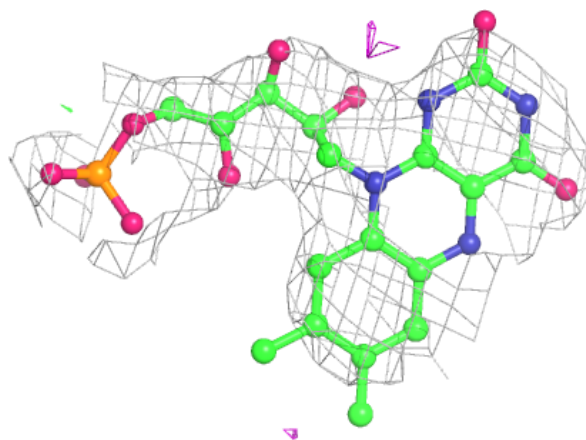


Electron density around FMN H 2101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FMN I 2101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.