



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 12:55 am BST

PDB ID : 3HMJ  
Title : Saccharomyces cerevisiae FAS type I  
Authors : Johansson, P.; Mulinacci, B.; Koestler, C.; Vollrath, R.; Oesterhelt, D.; Grininger, M.  
Deposited on : 2009-05-29  
Resolution : 4.00 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](mailto: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.

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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

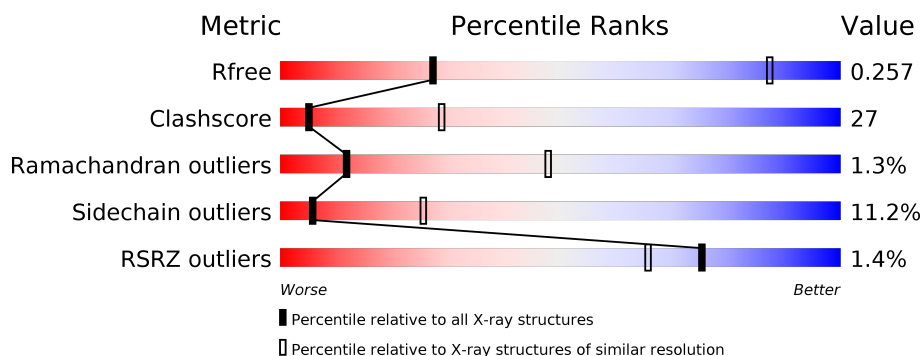
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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  $\geq 3$ , 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	1887	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>32%</div> <div>5%</div> <div>7%</div> </div> </div>
1	B	1887	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>32%</div> <div>5%</div> <div>7%</div> </div> </div>
1	C	1887	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>33%</div> <div>5%</div> <div>7%</div> </div> </div>
2	G	2051	<div> <div></div> <div> <div>51%</div> <div>40%</div> <div>8%</div> </div> </div>
2	H	2051	<div> <div></div> <div> <div>51%</div> <div>40%</div> <div>8%</div> </div> </div>
2	I	2051	<div> <div></div> <div> <div>51%</div> <div>40%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 88830 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.

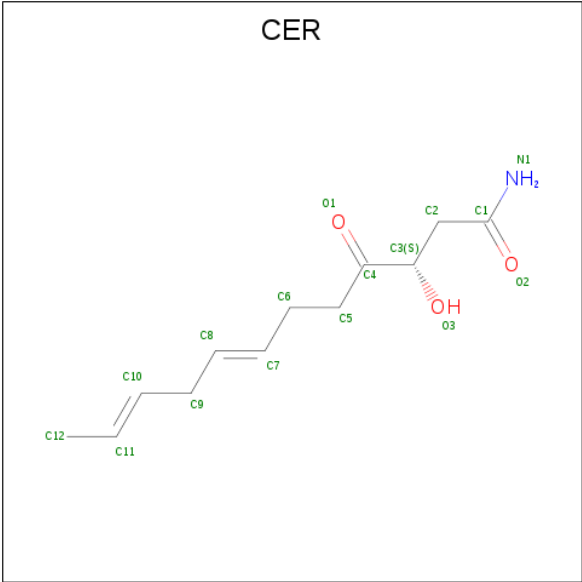
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1750	Total	C	N	O	S	0	0	0
			13572	8594	2292	2637	49			
1	B	1750	Total	C	N	O	S	0	0	0
			13572	8594	2292	2637	49			
1	C	1750	Total	C	N	O	S	0	0	0
			13572	8594	2292	2637	49			

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

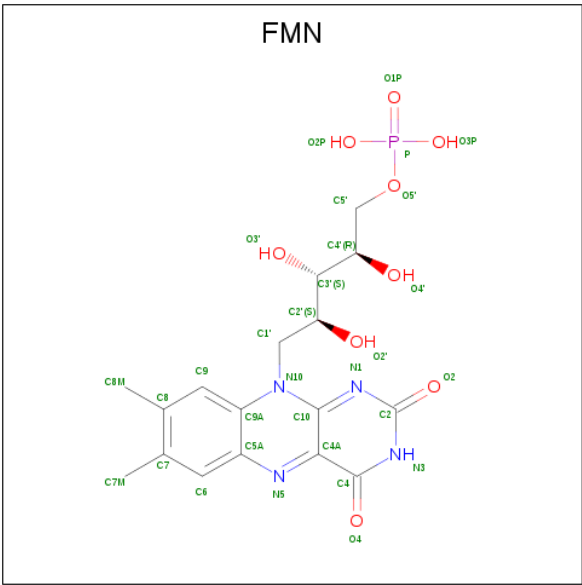
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	H	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	I	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			

- Molecule 3 is (2S, 3R)-3-HYDROXY-4-OXO-7,10-TRANS,TRANS-DODECADIENAMIDE (three-letter code: CER) (formula: C<sub>12</sub>H<sub>19</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	8	1	3		
3	B	1	Total	C	N	O	0	0
			12	8	1	3		
3	C	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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

Continued on next page...

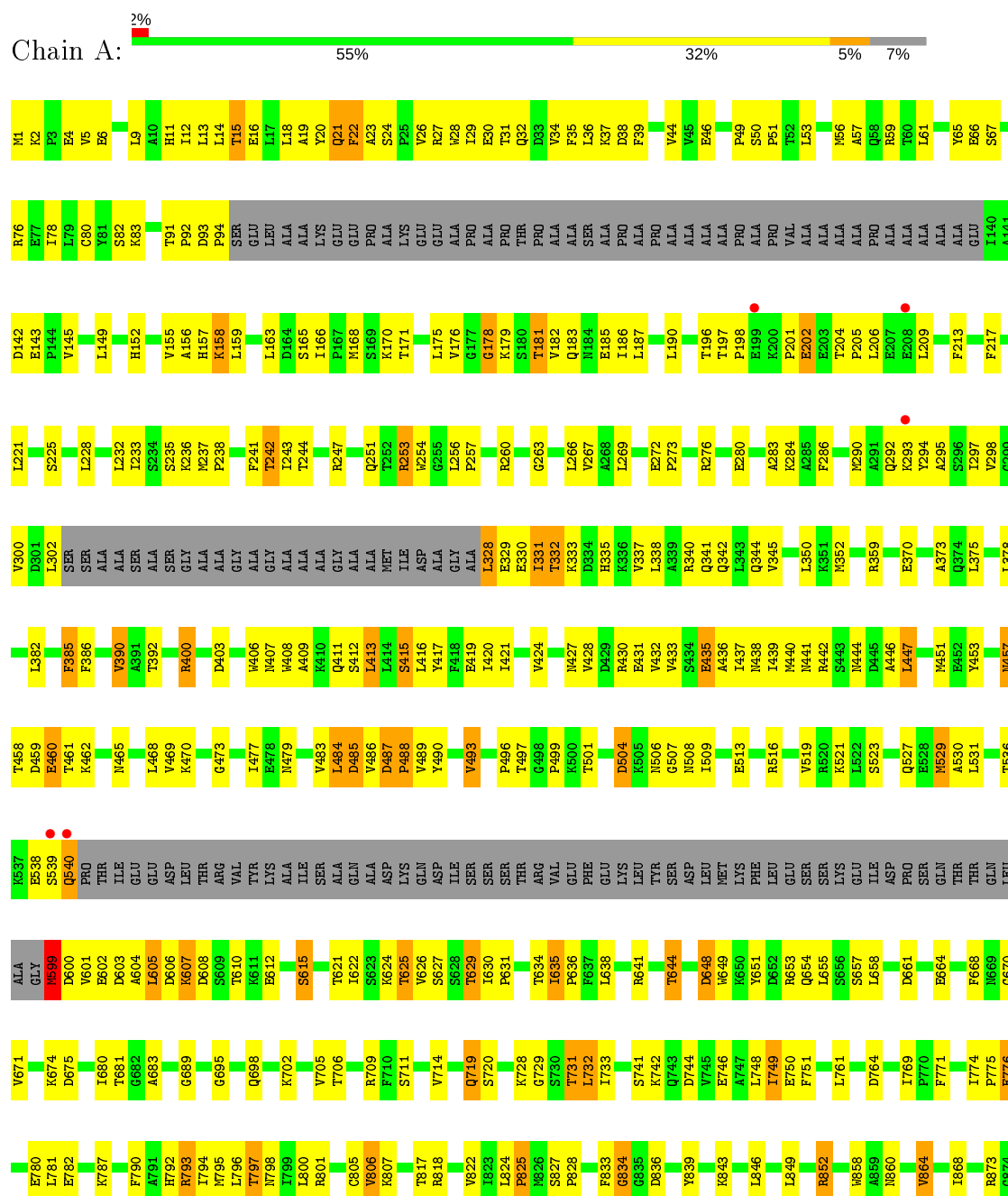
*Continued from previous page...*

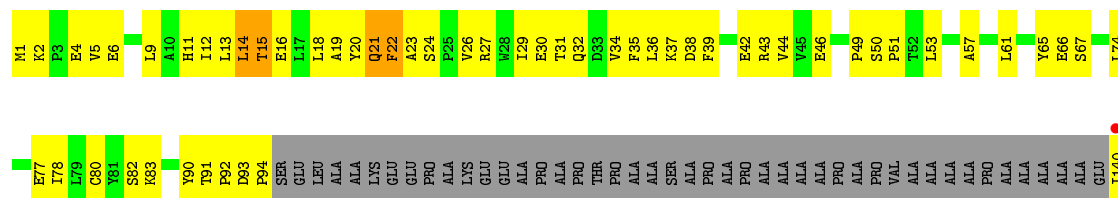
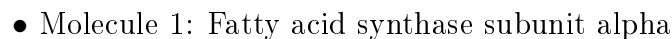
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fatty acid synthase subunit alpha





S1366	I1280	K1087	I982	SER	K787	G889	GLY	E533	D459	F386	L302	S225	A141
R1367	M1281	D1088	R985	ALA	S788	G695	R699	S539	E460	V390	SER	S226	D142
T1370	M1282	V1089	R985	R881	S788	G695	R699	S539	E460	V390	SER	S226	D142
T1371	M1283	V1089	R985	R881	S788	G695	R699	S539	E460	V390	SER	S226	D142
T1372	S1284	T1095	I988	I883	A790	Q698	E602	THR	K462	A391	ALA	L228	P144
R1373	K1196	T1096	Q989	I883	A790	Q698	E602	THR	K462	A391	ALA	L228	P144
H1374	T1197	I1097	F992	E886	H792	K702	A804	ILE	N465	T392	SER	L232	V145
F1376	T1200	S1101	F992	G887	H792	K702	A804	ILE	N465	T392	SER	L232	V145
Q1380	S1201	R1104	Y998	R888	H792	K702	A804	ILE	N465	T392	SER	L232	V145
I1384	D1202	R1104	Y998	R888	H792	K702	A804	ILE	N465	T392	SER	L232	V145
Q1386	D1202	R1104	Y998	R888	H792	K702	A804	ILE	N465	T392	SER	L232	V145
I1388	D1202	R1104	Y998	R888	H792	K702	A804	ILE	N465	T392	SER	L232	V145
L1392	V1208	L1105	I1004	M891	T797	R709	S609	ARG	G473	H406	GLY	P238	H152
M1396	D1209	Y1114	L1009	G892	N798	S711	T610	VAL	G473	H406	GLY	P238	H152
P1397	T1212	M1115	E1010	V893	R801	V714	E812	TTR	I477	H408	GLY	P241	A156
T1300	T1216	P1116	G1011	L906	R801	V714	E812	TTR	I477	H408	GLY	P241	A156
P1301	L1216	K1119	L1012	L906	R801	V714	E812	TTR	I477	H408	GLY	P241	A156
V1302	L1217	K1119	L1013	L908	C805	Q719	S615	ILE	N478	H409	ALA	T242	H157
G1303	S1218	D1014	D1014	L908	R806	S720	S615	ILE	N478	H409	ALA	T242	H157
A1304	V1219	L1015	L1015	V913	K807	S720	S615	ILE	N478	H409	ALA	T242	H157
C1305	S1226	E1124	E1016	V913	R818	G726	S623	GLN	P488	S415	ALA	R247	K168
T1307	T1229	V1125	I1019	L916	R818	G726	S623	GLN	P488	S415	ALA	R247	K168
S1308	T1229	V1125	I1019	L916	R818	G726	S623	GLN	P488	S415	ALA	R247	K168
V1309	T1229	V1125	I1019	L916	R818	G726	S623	GLN	P488	S415	ALA	R247	K168
E1310	Y1232	E1129	T1022	V922	R825	T731	S627	ASP	V493	F418	ALA	Q251	M168
S1311	E1233	D1130	V1021	V922	R825	T731	S627	ASP	V493	F418	ALA	Q251	M168
V1312	M1234	L1131	P1029	L930	R826	L732	T629	ILE	P496	I420	GLY	P257	T171
T1411	V1238	P1133	W1030	P934	R826	L732	T629	ILE	P496	I420	GLY	P257	T171
D1412	H1239	K1138	W1037	K937	R833	S741	I635	VAL	P499	V424	ALA	Q260	L175
T1318	V1240	K1138	W1037	K937	R833	S741	I635	VAL	P499	V424	ALA	Q260	L175
I1414	S1241	M1039	E1040	E938	R836	Q743	F637	PHE	A502	D429	K333	G263	G177
A1324	E1242	K1145	E1040	E938	R836	Q743	F637	PHE	A502	D429	K333	G263	G177
R1325	G1244	I1154	F1045	R944	R838	V745	T644	LYS	N506	S434	K336	L269	K178
P1419	S1247	P1158	S1046	L947	R839	E746	T644	LYS	N506	S434	K336	L269	K178
I1326	G1248	E1159	S1046	L947	R839	E746	T644	LYS	N506	S434	K336	L269	K178
A1420	S1249	Y1163	G1049	T950	L846	I749	D648	ASP	N508	E436	R340	E272	G178
P1421	S1249	Y1163	G1049	T950	L846	I749	D648	ASP	N508	E436	R340	E272	G178
L1426	G1252	K1166	V1051	S951	L849	F751	L655	LYS	T510	I437	Q342	R276	L190
T1427	G1253	K1166	V1051	S951	L849	F751	L655	LYS	T510	I437	Q342	R276	L190
R1429	S1255	T1172	I1056	R953	R852	L761	D661	PHE	N513	E513	Q344	E280	G195
E1431	A1256	L1173	M1057	R955	R858	D764	D661	PHE	N513	E513	Q344	E280	G195
H1432	L1257	Y1175	T1057	A956	R858	D764	D661	PHE	N513	E513	Q344	E280	G195
S1434	R1258	P1176	S1061	Y959	R858	D764	D661	PHE	N513	E513	Q344	E280	G195
N1442	G1259	K1177	Y1062	Y959	R858	D764	D661	PHE	N513	E513	Q344	E280	G195
M1445	D1263	A1178	M1066	E964	R864	I774	D661	PHE	N513	E513	Q344	E280	G195
K1446	R1264	L1179	M1066	E964	R864	I774	D661	PHE	N513	E513	Q344	E280	G195
Y1447	V1270	R1183	R1070	V968	R868	P775	D661	PHE	N513	E513	Q344	E280	G195
R1448	V1270	R1183	R1070	V968	R868	P775	D661	PHE	N513	E513	Q344	E280	G195
K1449	T1274	L1184	P1071	G970	R873	E776	D661	PHE	N513	E513	Q344	E280	G195
R1450	L1275	V1185	S1078	A976	R874	E780	D661	PHE	N513	E513	Q344	E280	G195
Q1451	Q1276	Q1188	T1079	A976	R874	E780	D661	PHE	N513	E513	Q344	E280	G195
E1364	E1364	Q1189	T1080	V980	GLY	H782	A683	GLN	T536	N457	L378	V300	G219
M1365	M1365	P1190	F1279	E981	GLY	H782	A683	GLN	T536	N457	L378	V300	G219
					MET	I784		ALA	R537	T458	F385	D301	L221





G689	K787	NET	R971	R1070	R1180	R1258	G1344	N1442	T1532	I1617	Y1706	V1805
G695	S788	SER	V980	V1076	F1181	G1259	K1347	L1443	I1533	L1618	T1707	G1811
E981	E789	ALA	R981	D1077	D1182	D1263	K1445	N1444	I1533	E1619	D1708	T1812
Q698	F790		H882	S1078	R1184	R1264	T1352	K1446	L1536	F1620	E1709	T1812
K702	A791		H883	K1081	V1185	V1270	T1352	R1450	G1537	E1622	V1714	K1816
V705	H792		R884	K1081	Q1188	I1274	R1360	Q1451	V1533	Y1623	A1720	F1820
T706	R793		R885	K1087	P1189	I1274	T1361	Q1451	A1539	E1623	R1721	K1821
	T794		A986	K1087	P1190	Q1276	A1363	R1455	S1540	V1624	V1722	S1822
	N795		A987	V1089	W1193	Q1276	E1364	R1455	G1543	Y1626	L1731	L1828
	L796		R888	V1089	M1194	F1279	M1365	T1544	T1544	P1627	G1732	G1829
	T797		E889	T1095	A1195	I1280	S1366	K1460	S1545	S1628	F1733	G1830
	N798		K890	T1095	K1196	I1281	R1367	D1461	T1546	V1639	F1733	G1831
	S711		G892	S1096	T1197	I1282	T1370	W1462	N1549	S1640	T1738	A1832
	V714		R893	I1097	K1197	T1282	T1371	E1463	K1551	I1641	Q1739	A1833
	C805		R894	S1101	I1200	S1284	T1372	V1463	M1552	T1642	Y1744	E1837
	Q719		L906	R1104	S1201	A1285	R1373	E1473	E1553	F1646	I1745	E1838
	S720		G907	R1105	D1202	M1289	R1374	A1474	S1554	K1649	ASN	I1839
	G726		L908	L1106	V1209	L1290	G1375	A1474	A1555	G1650	ALA	V1840
	K728		V913	E1107	D1209	L1291	F1376	I1477	T1556	Q1651	N1748	R1841
	T728		L916	P1108	T1212	I1292	Q1380	P1478	I1557	Q1652	T1749	V1842
	G729		P921	Y1114	T1212	G1296	G1381	S1479	L1564	V1655	I1750	N1843
	S730		V922	H1115	V1215	P1297	G1382	L1487	G1565	V1656	A1753	K1844
	T731		N927	P1116	V1215	P1297	G1383	E1488	G1566	V1656		N1845
	I732		N928	K1119	S1218	T1300	I1384	E1488	I1567	H1657		
	I733		G928	K1119	V1219	P1301	Q1385	E1489	I1573	P1658		
	F737		G929	Q1123	V1220	V1302	I1386	T1490	G1574	D1659		
	W738		L930	E1124	G1303	G1303	I1387	R1491	V1575	Y1660		
	Q739		Q931	E1125	I1224	A1304	M1388	E1492	F1576	L1661		
	G740		F932	V1126	C1305	C1305	M1388	I1493	Q1577	Y1662		
	S741		P933	V1127	A1226	A1306	L1392	E1494	L1580	G1663		
	K742		P934	V1127	S1226	T1307	M1396	N1495	E1496	A1664		
	Q743		R935	L1131	T1229	S1308	M1396	E1496	I1665	I1665		
	D744		R936	E1132		V1309	I1400	A1497	H1583	T1666		
	W745		A937	P1133	Y1232	E1310	I1400	E1498	P1584	E1667		
	E746		E938	K1138	E1233	S1311	Y1401	S1499	R1585	D1668		
	A747		F939	K1138	M1234	V1312	A1408	Q1500	R1585	L1669		
	L748							L1501	G1589	Y1670		
	I749							R1502	A1590			
	E750							Q1505	M1591	Y1673		
	F751								M1592	V1674		
	L761							N1510	N1593	V1677		
	D764							V1418	L1597	R1680		
	I769							P1419	Q1598	E1681		
	F770							A1420	I1599	K1682		
	F771							P1421	L1600	M1692		
	I774							L1426	P1606	I1693		
	P775							R1430	G1607	F1698		
	E776							E1431	N1603			
								H1433	R1609			
	E782							A1527	D1612	K1701		
	H783							L1528	N1613	P1705		
	GLY											
	LEU											

• Molecule 2: Fatty acid synthase subunit beta

Chain G:  51% 40% 8%



D1272	V1368	D1468	S1557	L1651	N1756	V1840	T1911	A2004	L84	I159	T234	P315
E1273	T1374	K1462	L1560	T1652	E1757	A1841	M1912	R2005	M85	F160	P235	M316
F1275	T1378	T1463	M1561	G1653	S1761	V1842	V1913	K2009	L86	G162	T236	T317
F1279	I1377	F1466	P1562	I1657	T1762	D1844	L1914	Y2010	S5	Q163	C238	S318
V1284	E1378	F1467	I1563	T1662	T1763	E1845	I1917	I2011	T89	T166	L240	L319
V1292	E1379	F1468	H1564	T1666	F1764	E1846	K1918	P2012	R7	D167	L241	P320
T1293	S1380	T1469	V1565	F1666	A1765	L1847	L1919	N2013	P8	G94	T244	P321
E1294	V1381	E1469	S1566	F1666	K1768	G1848	Q1920	L2014	L9	D168	Q245	L324
K1295	N1383	E1471	H1568	G1670	K1769	R1849	I1921	T2015	T10	F170	L246	L328
A1294	K1388	T1472	M1574	Q1671	L1770	S1850	I1922	A2016	L11	F170	A247	E322
E1296	I1389	T1473	L1575	S1672	L1771	M1854	L1931	K2017	S15	L173	E248	P335
F1300	V1390	F1474	L1579	E1673	S1772	I1855	S1932	T2022	L16	A174	V249	M338
A1303	S1397	K1475	T1580	Q1674	A1773	I1856	E1935	Y2025	H101	D175	V250	L339
C1308	V1403	S1481	M1583	M1676	Q1775	I1857	V1936	F2026	I102	L176	L251	S340
E1309	M1404	F1482	F1584	D1679	F1776	M1858	E1937	Y2029	A105	Y177	L255	S343
D1310	T1407	V1483	S1585	L1680	T1777	P1859	E1937	V2030	L109	Y178	F258	T344
V1311	T1408	V1489	S1586	T1683	M1678	R1861	L1940	Y2033	M112	T179	T259	T345
S1313	S1408	K1490	V1589	A1687	A1781	V1862	F1941	G2034	D113	V180	L259	T346
R1314	F1410	E1492	A1591	A1687	T1782	A1863	D1945	S2035	T114	H181	P260	T347
T1318	F1411	L1493	E1594	R1693	L1783	Q1868	K1949	E2036	T115	G185	T261	T348
M1319	Y1416	P1494	E1597	H1697	E1785	Q1868	V1953	P2037	L116	V186	L262	T349
L1320	T1417	T1495	A1597	T1706	P1799	L1871	V1953	K2038	V117	K187	L263	Q346
F1325	D1413	K1496	S1602	L1707	T1803	Y1872	K1955	K2039	K118	L188	R264	Q347
A1326	E1419	V1500	R1605	L1711	F1804	V1874	P1957	I2041	T119	K189	T271	Q348
I1327	M1421	G1502	R1606	M1712	A1805	V1875	L1958	D2043	I127	F190	H272	Q349
V1329	T1422	V1503	G1607	T1718	S1808	E1876	F1964	N2044	T128	S191	H273	Q350
G1330	Q1424	V1504	V1608	L1717	A1814	L1885	S1973	Y2047	I131	E197	S274	V353
V1331	K1425	A1504	T1609	I1719	L1815	L1885	V1974	K2048	M132	A50	Q275	R354
I1335	T1426	S1511	M1615	G1722	L1818	V1887	F1976	E2049	F1975	D51	G276	T355
F1339	E1428	H1512	V1616	G1726	A1819	I1888	H1977	Q2050	H1977	E53	L277	T356
P1340	Y1431	T1526	K1623	Q1726	V1820	V1889	S1978	SER	T1979	P54	L195	T278
V1343	H1434	L1527	T1624	F1738	V1821	I1890	I1888		Y1980	T55	L123	T279
D1344	I1435	E1528	S1625	E1739	M1822	M1891	V1893		M1980	T56	A192	A280
L1347	K1436	Q1529	Q1627	T1740	I1824	Y1891	E1894		L1981	E59	I127	L360
L1348	T1437	L1533	G1630	V1741	S1826	M1895	M1895		M1982	L60	L128	A281
K1349	S1438	D1543	M1631	V1742	V1828	Q1896	F1988		K1989	V61	L142	A282
L1350	I1441	P1547	I1632	K1745	E1829	Q1897	K1989		S1990	F64	L145	K288
V1351	A1442	S1548	T1637	L1746	V1830	Y1898	L1991		Y1899	L65	F146	A299
H1352	L1443	T1549	I1638	K1747	V1831	A1900	I1992		F1991	V68	V149	I300
N1355	R1445	N1550	K1639	T1748	R1834	A1901	K1993		K1993	V72	M153	L303
M1359	S1446	P1551	F1639	E1749	G1835	A1906	I1996		I1996	E73	D227	F303
L1360	L1452	P1552	F1640	F1752	M1836	L1907	I1997		I1997	K76	L231	F305
P1361	T1457	V1553	T1641	T1755	M1838	D1908	K1998		K1998	F80	L232	R309

• Molecule 2: Fatty acid synthase subunit beta

Chain H:  51% 40% 8%

MET	L84	I159	T234	P315
ASP	M85	F160	P235	M316
ALA	L86	G161	T236	T317
TYR	L87	Q163	C238	S318
S5	T89	T166	L240	L319
R7	M93	D167	L241	P320
P8	G94	D168	T244	P321
L9	Y95	F169	Q245	L324
T10	L11	F170	L246	L328
L11	M99	L173	A247	E322
S15	D100	A174	E248	P335
L16	I101	D175	V249	M338
V22	H102	L176	L250	L339
P23	A105	Y177	V251	S340
P23	L109	T178	L255	S343
T24	M112	V180	F258	T344
A25	V182	H181	T259	T345
S26	D113	L183	P260	T346
F27	T114	T115	L261	T347
F28	L115	G185	L262	T348
L33	L116	V186	L263	T349
M38	V117	K187	R264	Q346
A39	K118	L188	T271	Q347
L40	T119	K189	H272	Q348
L41	K120	F190	H273	Q349
P42	E121	S191	S274	Q350
L45	L122	A192	Q275	V353
T45	I123	E193	L276	R354
E46	K124	T194	G277	T355
G47	L127	L195	L278	N357
F48	T128	S196	T279	S358
A49	I131	E197	A280	R359
A50	M132	L198	V281	L360
D51	A133	I199	A282	P361
D52	K134	L203	L283	S369
E53	R135	P209	T286	L370
P54	P136	T210	V371	A374
T55	F137	L213	E289	R375
T56	D138	M214	E290	M376
E59	K139	I215	S295	L377
L60	N142	L216	V296	S380
V61	M145	E217	K298	L389
G62	L145	V146	A299	R390
K63	F146	V149	I300	T392
F64	V149	M153	L303	L393
L65	V149	E154	F304	R394
V68	V149	Q155	F305	R397
V72	M153	D227	L231	
E73	Q155	L156	L232	
K76	V157	L157	S233	
F80	A158			

V1556	D1458	T1374	F1279	L1197	VAL	L1040	T945	A858	E784	I717	P567	I483	L402
S1557	K1462	V1377	D1280	S1198	GLN	E1041	F945	T859	W785	I718	K568	I484	D403
L1560	T1463	I1378	P1281	E1199	GLN	A1042	G948	R860	S786	I719	L569	R485	Q404
P1561			V1284	L1205	VAL	V1043	D949	W865	T787	A720	I641	L486	
T1563	T1468	V1381	I1282	L1206	ASP	D1045	F950	F866	K788	K721	N572	V487	P408
H1564	E1469	V1382	T1293	K1206	SER	Q1046	R952	F867	F789	A722	K573	K489	P409
P1565	T1470	M1382	I1294	I1210	VAL	D1047	R953	F868	T791	H723	K574	W490	
S1566	E1471	V1383	K1295	L1211	VAL	Q1048	V954	D869	P792	F726	K575	E491	F416
T1567	T1472	K1295	K1212	K1212	VAL	Q1049	R954	T870	P793	P727	I577	S417	S417
H1568	F1473	K1295	L1213	L1213	VAL	R1050	E955	T871	M794	T492	T492	T492	N418
	F1474	K1388	L1214	L1214	GLU	T1051	E956	T872	T794	T493	W579	R419	T494
	K1475	V1389			D1123	C1052		F873	F795	T494	P580	Q495	P420
N1574		V1390	F1300			T1052			T796	L730	T581	Q496	L421
L1575	S1481		A1303	I1219	K1128	I1053	K960	K879	D797	Q731	K582	F496	
L1576	S1482	L1396	A1303	Q1220	M1221	L1054	L964	R880	F798	W732	P584	Q422	V423
L1579	V1483	S1397	C1308	M1221	T1130	V1058		W881	F799	T733	M558	H500	A424
T1580			E1309	M1223		A1059	I967	P882	L800	R736	K585	S425	S425
M1583	F1486	V1403	D1310	M1227	T1133	A1060		K887	R804		L586	P504	P426
F1584		M1404	F1311	T1228	D1134	Q1061	Y970	R888	P805	G739	W587	G505	F427
S1585	T1407	S1408	V1312	T1228	E1135	F1062	S971		W806	H740	G583	G506	H428
S1586	S1408	S1408	R1314			T1063	L972	I892	I807	H741	P664	P506	
	S1409	S1409	R1314	G1231	W1138		L973			S742	P590	P591	L431
	F1410	S1409	T1318	K1232	S1145	I1066	Y987	S893	E810		L665	L512	L432
K1496	F1410	S1409	M1319	V1234	E1146	D1067		R894	W811	D745	I666	L512	L433
E1497	F1411		K1320	S1235	E1147	P1069	Q993	L895	K812	A746	K667	T516	P434
T1498	G1414		A1321	L1236	N1148	T1077		A897	T813	H747	P595	H517	I439
V1499	T1415		P1322	P1237	W1149	D1078	F994	F994	D816	T748	G596	K520	N440
E1500	T1416		L1238	L1238		D1079	L995	D898	A817	P749	M597	K520	N441
I1501	T1417		F1325		H1151	G1080	Q998	F899	D817	M750	T598	D821	D442
G1502	D1418		A1326	N1241	A1152	H1081	Q999	Q900	K818	L751	P599	G822	L443
I1503	T1419		I1327	F1242		D1075	D999	K901		Q752	G600	V827	V444
V1504	E1420		V1329	P1243	I1159	I1077	I1000	P902	I821	Y754	T601	I533	N446
Y1506	T1421		G1330	P1244	T1160	H1078	D1002	W903	A823		V602	N446	
	T1422		W1331		Q1161	D1079	F1004	A905	G824	I757	S603	L533	N447
A1510	K1425		I1335	G1247	D1162	G1080	L1004	T906	T825	I758	F606	N536	V448
S1511	T1426		I1338	S1262	K1163	H1081	S1006	Q907	G826	R759	V607	P837	I485
H1512	V1427		F1339		V1166	I1082	M1006	Q910	P828	H760	T610	D538	Q456
P1515	E1428		P1340		S1167	K1084	P1010	A911	W832	N762	T611	D540	I459
					N1168	L1085	M1011	R912	E693	M764	N612	F543	Y460
T1526	Y1431				P1169	L1086	Q1012	D913	E694	L765	Y615	K544	D461
L1527			V1343	W1259	I1170	Y1090	V1015	T916	T835	I766	T616	Q545	T462
E1528	H1434		D1344	Q1260	K1171	G1091	P1016		T836	F767	I617	Q545	F463
Q1529	I1435			I1262	K1172	D1092	F1017	E921	Y836	G768	T551	V550	D464
K1530	F1436		L1347	I1263	V1173	D1093	V1018	P839	P839	S769	L619	T551	G465
	T1437		L1348	E1264	K1175	K1096	P1019	L926	T840		A620	S552	S466
	S1438		K1349	M1265	P1176	K1096	V1020	L926	T840		G621	N553	
			L1350	Y1266	S1177	I1097	L1021	L929	W844	G772	G622	R469	
	I1441		V1351						T845	S773	G623	V470	
D1543	A1442		H1352	L1269	M1180	V1100	R1024	I932	A774	D775	Y624	L471	
P1547	L1444		W1270	M1270	V1181	E1101	F1025		T846	D776	P707	N560	
K1634	T1548		N1355	I1271	T1189	F1102	I1026	W938	E852	T777	G629	W561	S476
R1635	T1549			D1272		F1103	I1027	P939	P853	Y778	M630	I562	E477
L1637	S1446		M1359	E1273	T1189				I854	P779	T631	E563	R478
L1638	L1452		I1360	F1274	V1194	P1108	K1031	T942	H855	L781	A632	E564	
K1639			V1368	F1275	V1195	W109	K1032	R944	W943		A633	Y565	D481
F1640					T1196	ASP			I857		V716	H566	C482





Y2029	Y2030
T2033	G2034
S2035	E2036
P2037	I2038
K2039	E2040
I2041	I2042
D2043	I2044
W2045	E2046
K2047	Y2048
E2049	Q2050
SER	



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.88Å 231.88Å 756.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-4.00) 97.3 (20.00-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.94Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.266 , 0.267 0.257 , 0.257	Depositor DCC
$R_{free}$ test set	8521 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	130.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 74.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	88830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, CER

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	5/13822 (0.0%)	0.59	6/18682 (0.0%)
1	B	0.43	3/13822 (0.0%)	0.61	9/18682 (0.0%)
1	C	0.43	4/13822 (0.0%)	0.59	4/18682 (0.0%)
2	G	0.41	7/16360 (0.0%)	0.58	6/22198 (0.0%)
2	H	0.40	7/16360 (0.0%)	0.57	3/22198 (0.0%)
2	I	0.40	5/16360 (0.0%)	0.58	10/22198 (0.0%)
All	All	0.42	31/90546 (0.0%)	0.59	38/122640 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1
2	H	0	2
2	I	0	1
All	All	0	4

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	992	PHE	C-N	13.35	1.59	1.34
1	C	992	PHE	C-N	13.18	1.59	1.34
2	I	842	GLY	C-N	11.12	1.59	1.34
2	G	315	PRO	C-N	10.45	1.58	1.34
1	C	485	ASP	C-N	9.61	1.56	1.34

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1116	PRO	O-C-N	-11.67	104.02	122.70
2	I	1982	MET	O-C-N	-9.44	107.59	122.70
2	G	842	GLY	O-C-N	-8.86	108.52	122.70
2	G	1053	ILE	O-C-N	-8.58	108.97	122.70
1	B	992	PHE	O-C-N	8.47	137.19	121.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1108	PRO	Peptide
2	H	1108	PRO	Peptide
2	H	1256	GLU	Mainchain
2	I	1108	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	13572	0	13489	663	15
1	B	13572	0	13490	618	6
1	C	13572	0	13490	638	22
2	G	15995	0	15978	1026	32
2	H	15995	0	15978	1023	7
2	I	15995	0	15977	983	26
3	A	12	0	10	3	0
3	B	12	0	10	4	0
3	C	12	0	10	4	0
4	G	31	0	19	7	0
4	H	31	0	19	6	0
4	I	31	0	19	8	0
All	All	88830	0	88489	4773	54

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 4773 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1749:THR:CB	1:A:1874:ASP:HB3	1.53	1.37
1:B:1749:THR:CB	1:B:1874:ASP:HB3	1.56	1.34
1:B:1749:THR:CB	1:B:1873:HIS:O	1.75	1.32
1:A:1464:GLU:HG3	1:A:1773:VAL:CG1	1.58	1.32
1:C:1749:THR:CB	1:C:1874:ASP:HB3	1.62	1.29

The worst 5 of 54 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:C:1784:ASP:CA	2:G:1087:HIS:CE1[7_655]	0.16	2.04
1:A:1784:ASP:CG	2:I:1087:HIS:CE1[7_545]	0.52	1.68
1:C:1784:ASP:C	2:G:1087:HIS:NE2[7_655]	0.54	1.66
1:C:1784:ASP:CB	2:G:1087:HIS:ND1[7_655]	0.56	1.64
1:A:1784:ASP:OD2	2:I:1087:HIS:ND1[7_545]	0.58	1.62

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	1736/1887 (92%)	1614 (93%)	100 (6%)	22 (1%)	12	48
1	B	1736/1887 (92%)	1619 (93%)	100 (6%)	17 (1%)	15	53
1	C	1736/1887 (92%)	1618 (93%)	96 (6%)	22 (1%)	12	48
2	G	2029/2051 (99%)	1825 (90%)	173 (8%)	31 (2%)	10	45
2	H	2029/2051 (99%)	1826 (90%)	173 (8%)	30 (2%)	10	45
2	I	2029/2051 (99%)	1829 (90%)	174 (9%)	26 (1%)	12	48
All	All	11295/11814 (96%)	10331 (92%)	816 (7%)	148 (1%)	12	48

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	PRO
1	A	504	ASP
1	A	538	GLU
1	A	605	LEU
1	A	834	GLY

### 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	1460/1566 (93%)	1308 (90%)	152 (10%)	7	28
1	B	1460/1566 (93%)	1312 (90%)	148 (10%)	7	29
1	C	1460/1566 (93%)	1310 (90%)	150 (10%)	7	28
2	G	1772/1789 (99%)	1563 (88%)	209 (12%)	5	24
2	H	1772/1789 (99%)	1560 (88%)	212 (12%)	5	23
2	I	1772/1789 (99%)	1561 (88%)	211 (12%)	5	24
All	All	9696/10065 (96%)	8614 (89%)	1082 (11%)	6	25

5 of 1082 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	344	LEU
2	G	1452	LEU
2	I	1145	SER
2	G	471	LEU
2	G	857	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 294 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	989	GLN
2	G	418	ASN
2	I	900	GLN
1	C	1064	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1542	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	FMN	H	3051	-	31,33,33	6.73	18 (58%)	40,50,50	1.91	8 (20%)
4	FMN	G	3051	-	31,33,33	6.88	18 (58%)	40,50,50	1.96	7 (17%)
3	CER	A	2748	-	10,11,15	4.19	3 (30%)	9,13,17	3.18	3 (33%)
3	CER	C	2748	-	10,11,15	4.21	3 (30%)	9,13,17	3.18	3 (33%)
4	FMN	I	3051	-	31,33,33	6.74	21 (67%)	40,50,50	1.81	7 (17%)
3	CER	B	2748	-	10,11,15	4.19	3 (30%)	9,13,17	3.05	3 (33%)

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
4	FMN	H	3051	-	-	5/18/18/18	0/3/3/3
4	FMN	G	3051	-	-	5/18/18/18	0/3/3/3
3	CER	A	2748	-	-	5/12/12/16	-
3	CER	C	2748	-	-	5/12/12/16	-
4	FMN	I	3051	-	-	5/18/18/18	0/3/3/3
3	CER	B	2748	-	-	5/12/12/16	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3051	FMN	C4A-C10	16.06	1.54	1.38
4	H	3051	FMN	C4A-C10	15.15	1.53	1.38
4	I	3051	FMN	C4A-C10	14.86	1.53	1.38
4	G	3051	FMN	C4A-N5	12.70	1.51	1.33
4	I	3051	FMN	C4A-N5	12.26	1.50	1.33

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2748	CER	O1-C4-C5	-7.72	107.97	121.70
3	A	2748	CER	O1-C4-C5	-7.67	108.06	121.70
4	H	3051	FMN	C4-N3-C2	7.46	121.44	115.14
3	B	2748	CER	O1-C4-C5	-7.34	108.64	121.70
4	G	3051	FMN	C4-N3-C2	7.33	121.33	115.14

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	3051	FMN	C2'-C3'-C4'-C5'
4	H	3051	FMN	O3'-C3'-C4'-C5'
4	G	3051	FMN	C2'-C3'-C4'-C5'
4	G	3051	FMN	O3'-C3'-C4'-C5'
3	A	2748	CER	C2-C3-C4-O1

There are no ring outliers.

6 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	3051	FMN	6	0

*Continued on next page...*

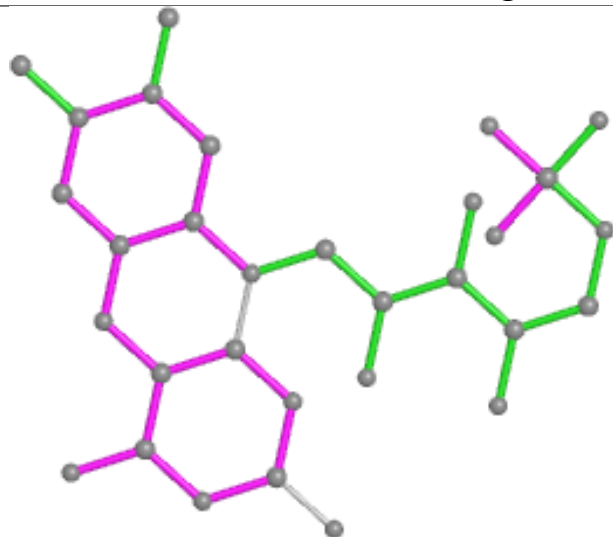
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3051	FMN	7	0
3	A	2748	CER	3	0
3	C	2748	CER	4	0
4	I	3051	FMN	8	0
3	B	2748	CER	4	0

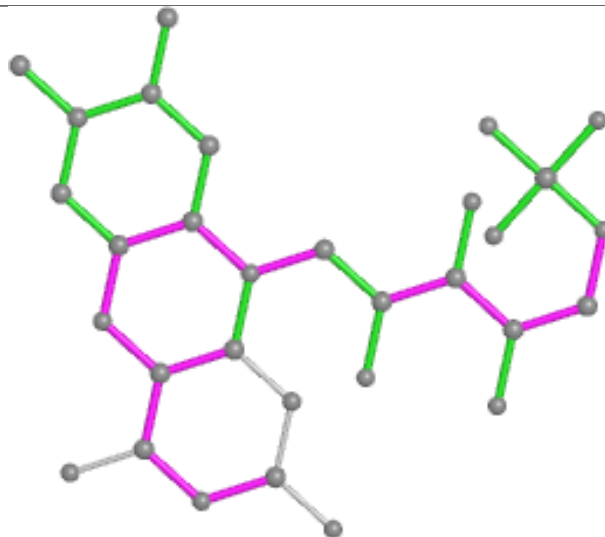
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



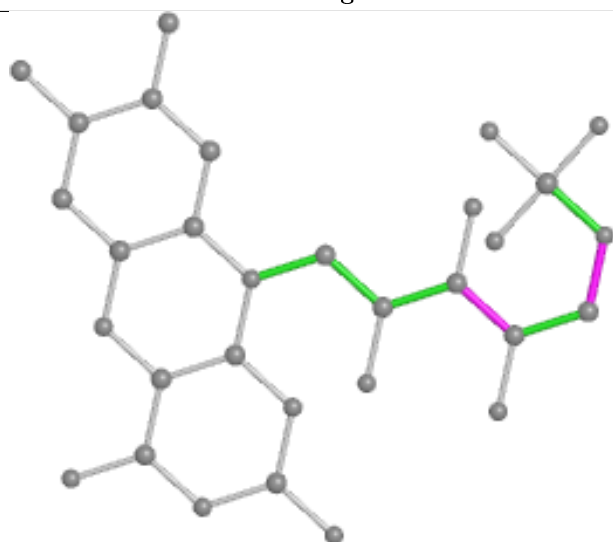
## Ligand FMN H 3051



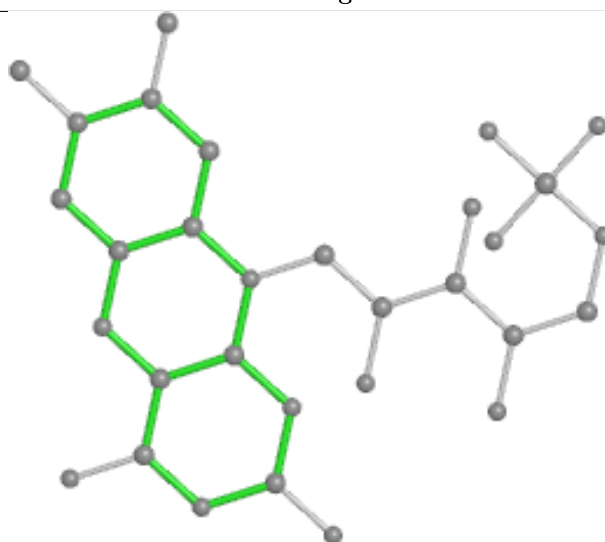
Bond lengths



Bond angles

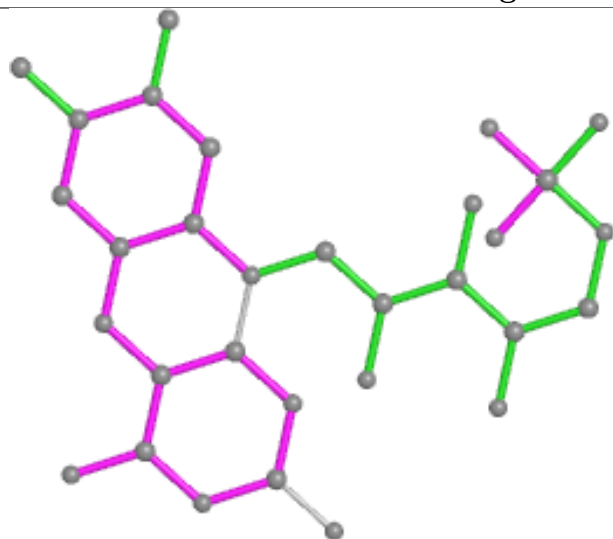


Torsions

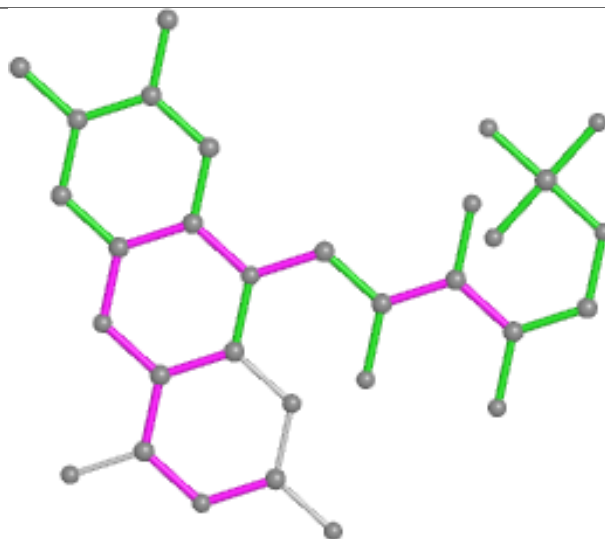


Rings

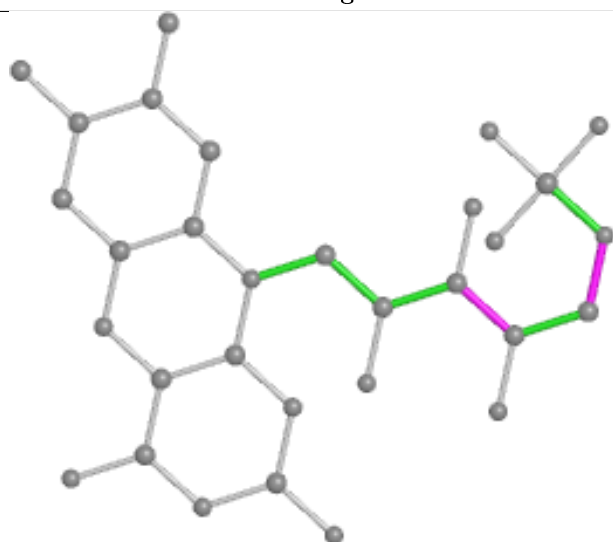
## Ligand FMN G 3051



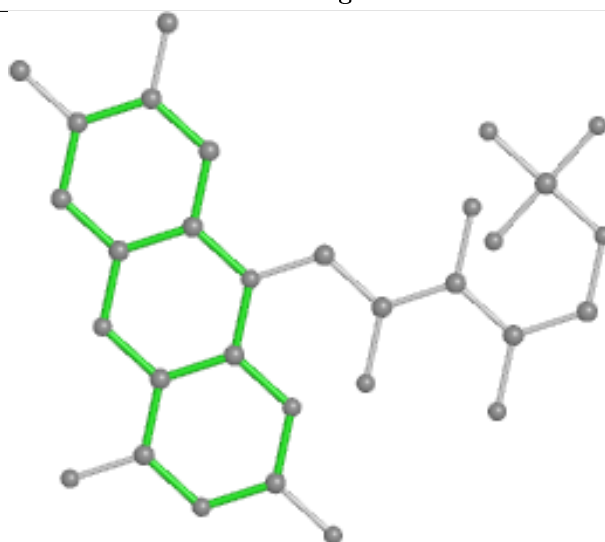
Bond lengths



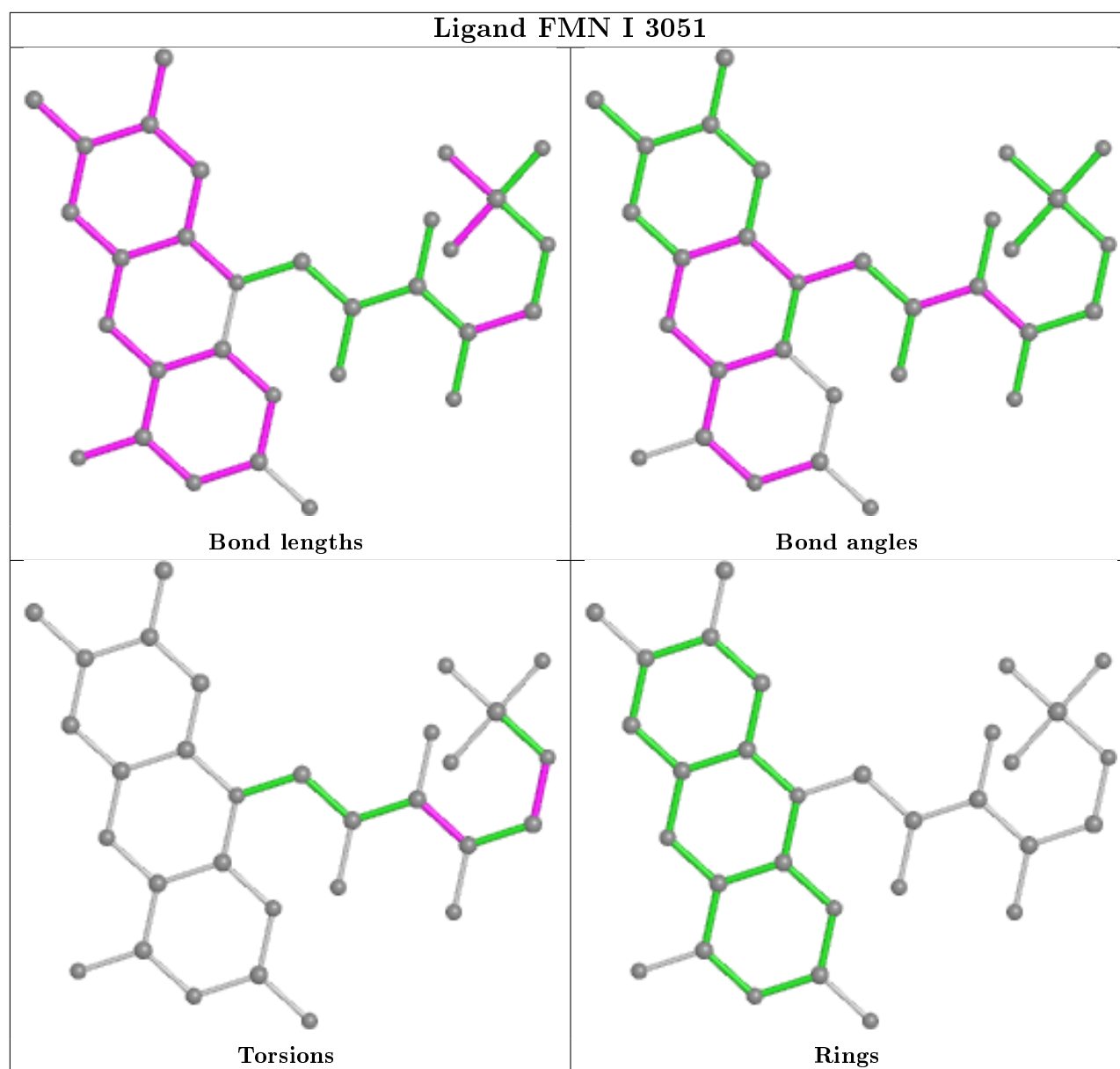
Bond angles



Torsions



Rings



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1750/1887 (92%)	-0.30	46 (2%) 56 46	95, 134, 347, 457	0
1	B	1750/1887 (92%)	-0.34	32 (1%) 68 59	96, 133, 302, 419	0
1	C	1750/1887 (92%)	-0.26	62 (3%) 44 35	98, 135, 423, 568	0
2	G	2033/2051 (99%)	-0.45	1 (0%) 100 100	131, 169, 218, 267	0
2	H	2033/2051 (99%)	-0.36	10 (0%) 91 85	130, 170, 215, 265	0
2	I	2033/2051 (99%)	-0.43	6 (0%) 94 90	131, 171, 215, 261	0
All	All	11349/11814 (96%)	-0.36	157 (1%) 75 65	95, 162, 239, 568	0

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1882	ALA	10.4
1	C	1831	GLY	9.1
1	A	1829	GLY	8.0
1	C	1830	GLY	7.7
1	C	1870	SER	7.6

### 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 [i](#)

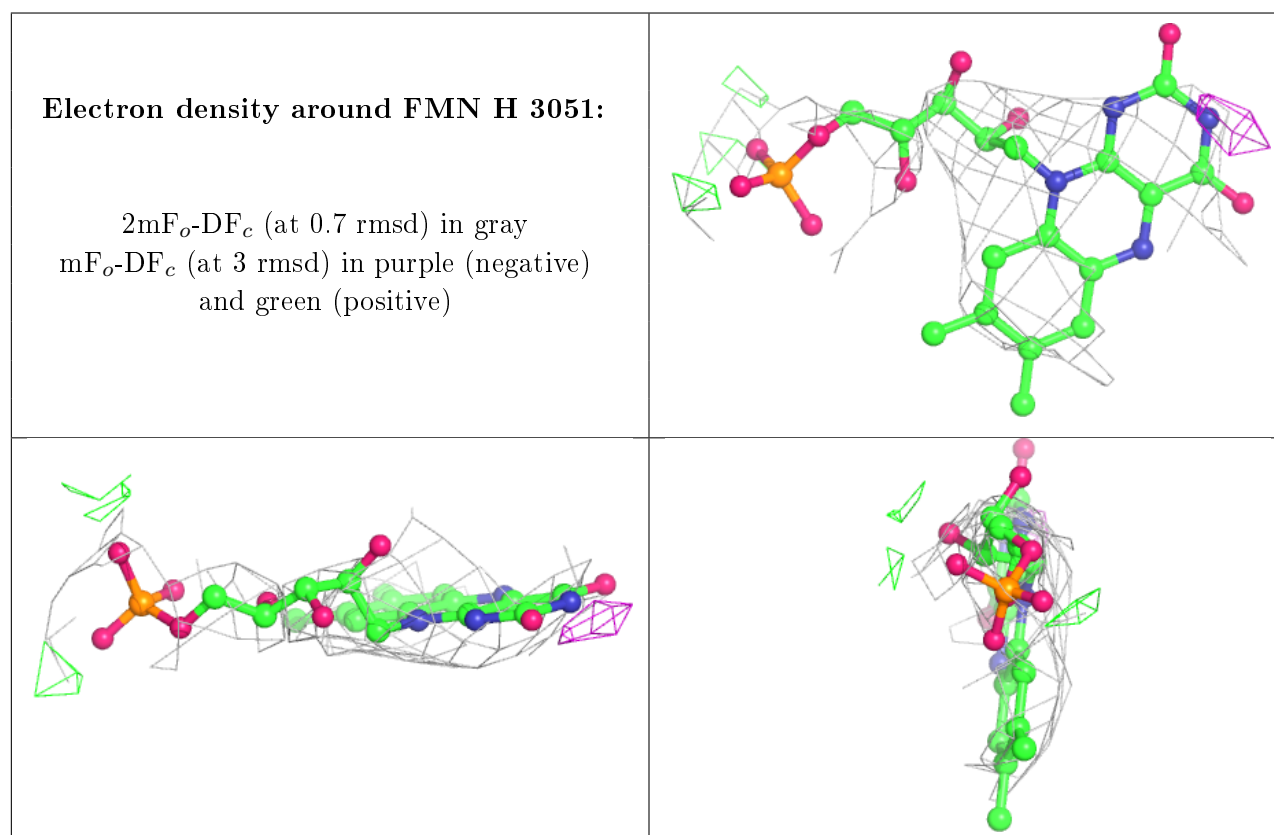
There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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.

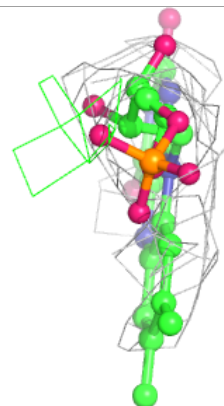
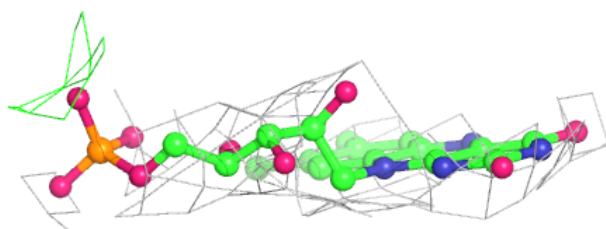
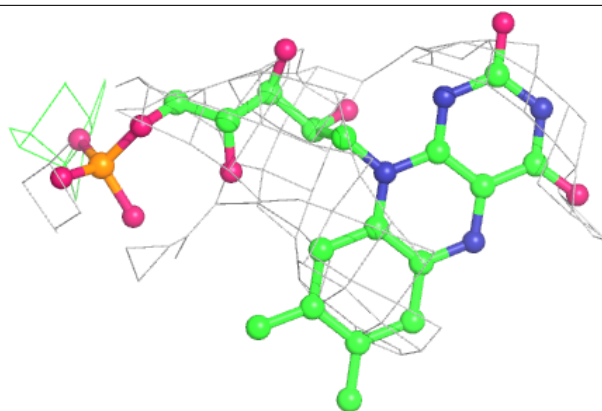
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FMN	H	3051	31/31	0.80	0.32	131,157,181,186	0
4	FMN	G	3051	31/31	0.82	0.27	135,158,184,203	0
4	FMN	I	3051	31/31	0.82	0.26	129,161,178,201	0
3	CER	A	2748	12/16	0.84	0.30	67,131,240,249	0
3	CER	C	2748	12/16	0.90	0.34	67,131,249,250	0
3	CER	B	2748	12/16	0.91	0.20	67,131,249,250	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.

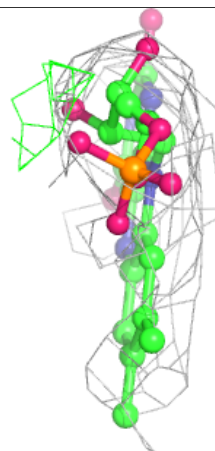
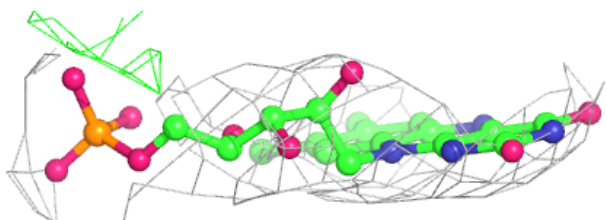
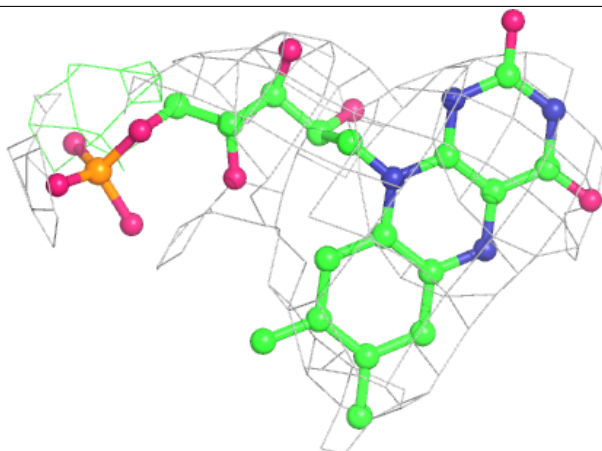


**Electron density around FMN G 3051:**

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

**Electron density around FMN I 3051:**

$2mF_o-DF_c$  (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.