



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:30 PM UTC

PDB ID : 2VKZ / pdb_00002vkz
Title : Structure of the cerulenin-inhibited fungal fatty acid synthase type I multienzyme complex
Authors : Johansson, P.; Wiltshi, B.; Kumari, P.; Kessler, B.; Vonrhein, C.; Vonck, J.; Oesterhelt, D.; Grininger, M.
Deposited on : 2008-01-07
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

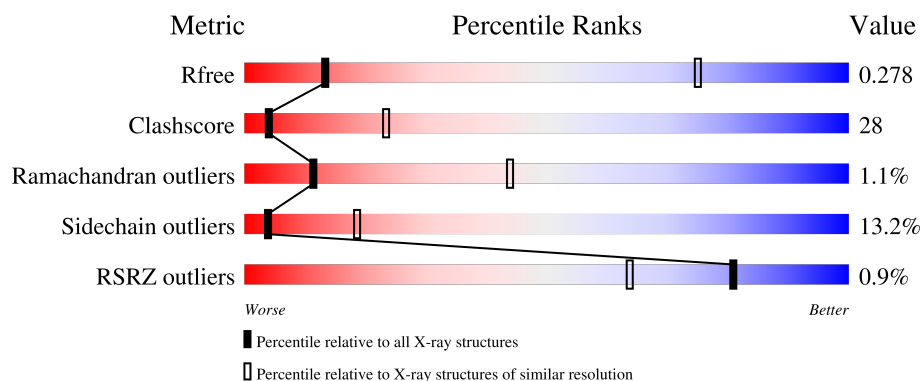
1 Overall quality at a glance

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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 of 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	1887	% 49% 31% 6% 14%
1	B	1887	48% 31% 6% 14%
1	C	1887	% 47% 32% 6% 14%
2	G	2051	% 49% 41% 9% .

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Mol	Chain	Length	Quality of chain
2	H	2051	% 48% 41% 9%
2	I	2051	% 49% 41% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 85959 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.

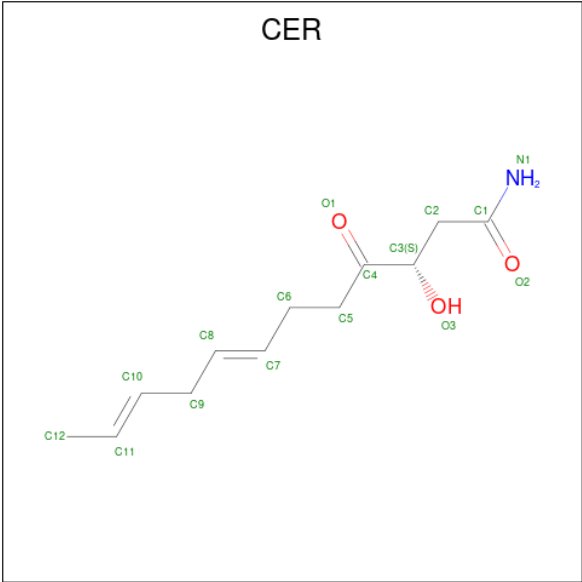
- Molecule 1 is a protein called FATTY ACID SYNTHASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1614	Total	C	N	O	S	0	0	0
			12615	7997	2127	2443	48			
1	B	1614	Total	C	N	O	S	0	0	0
			12615	7997	2127	2443	48			
1	C	1614	Total	C	N	O	S	0	0	0
			12615	7997	2127	2443	48			

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

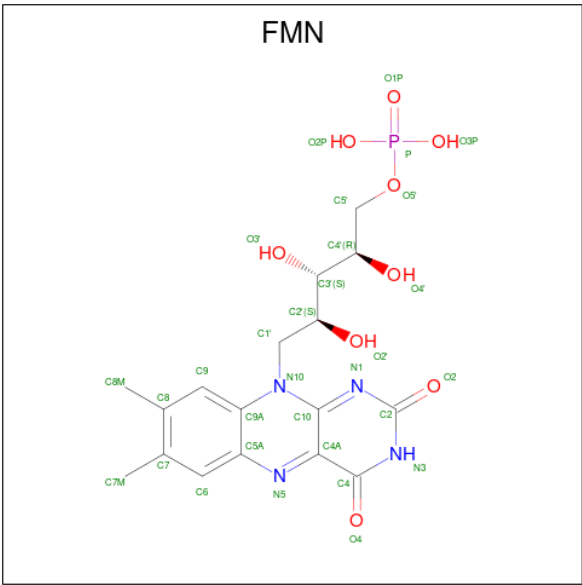
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	H	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	I	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			

- Molecule 3 is (2S, 3R)-3-HYDROXY-4-OXO-7,10-TRANS,TRANS-DODECADIENTAMIDE (CCD ID: CER) (formula: C₁₂H₁₉NO₃).



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 (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

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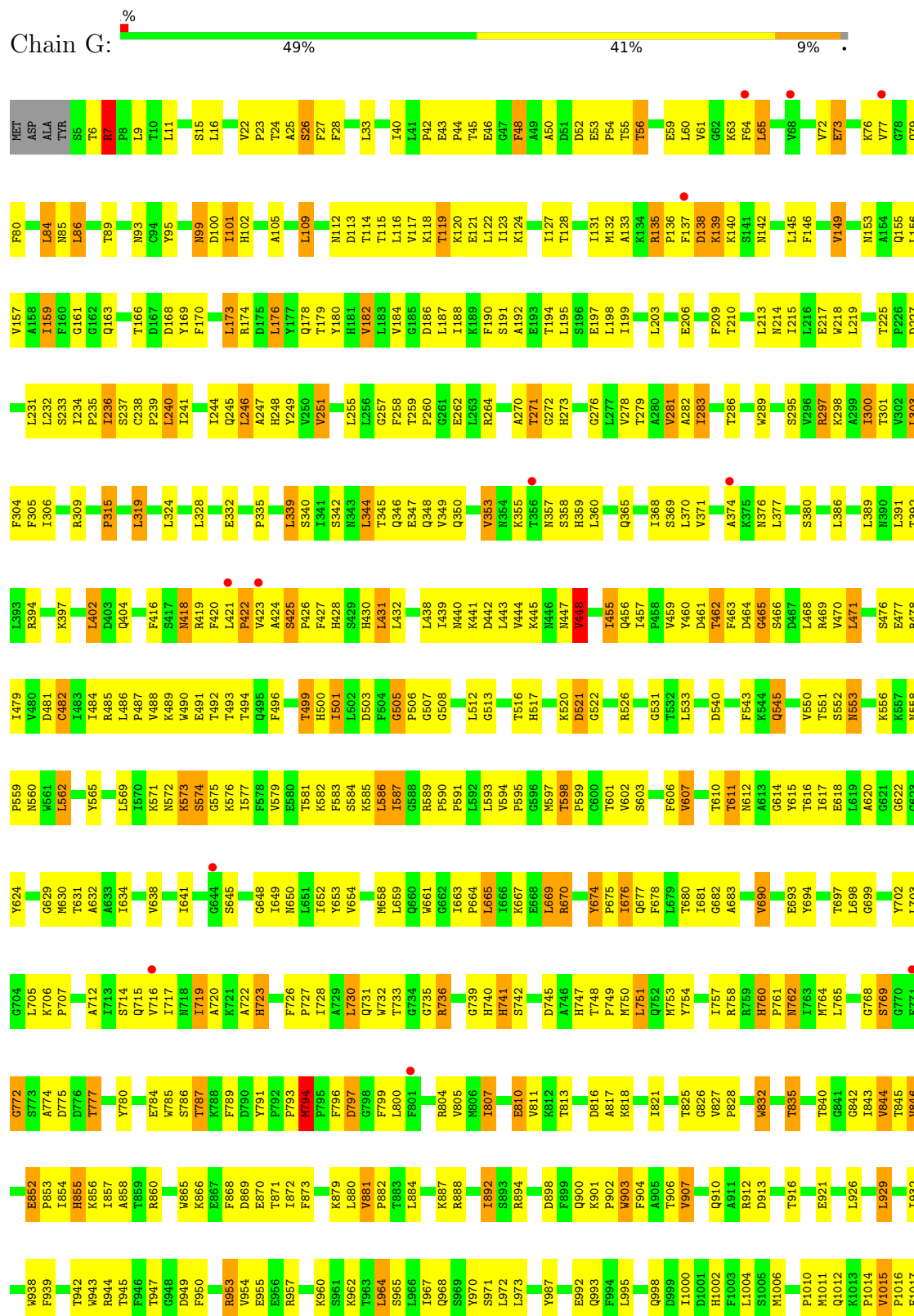
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

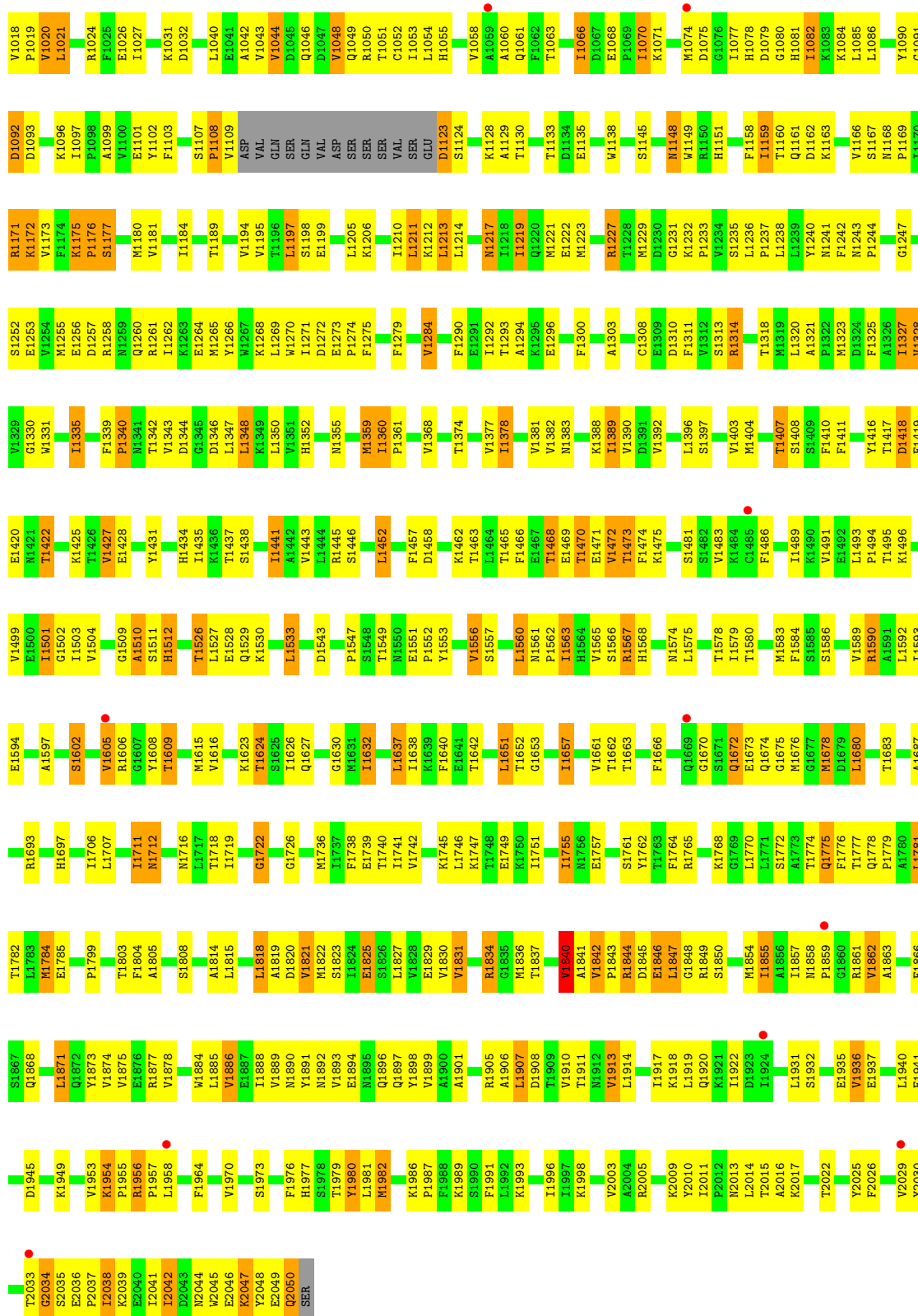
I1326	C1327	I1328	V1329	Y1332	G1252	G1253	V1254	A1255	A1256	F1341	G1344	M1345	M1346	K1347	T1352	R1360	T1361	P1362	E1363	E1364	M1365	S1366	R1367	T1370	T1371	T1372	R1373	H1374	G1375	F1376	Q1380	I1384	Q1385	F1386	I1387	M1388	L1392	M1396	P1399	T1400	Y1401	M1406	T1411	D1412	K1413	I1414	A1324	R1325																			
I1056	M1057	S1061	Y1062	N1066	L1067	R1070	P1071	Y1072	T1073	V1076	D1077	T1078	K1079	T1080	Q1188	I1189	P1190	W1193	M1194	A1195	K1196	T1197	R1198	L1199	I1200	S1201	D1202	M1203	V1204	D1205	T1206	T1207	Q1208	T1209	T1210	I1211	Q1212	L1216	V1217	S1218	V1219	G1220	P1221	W1222	L1223	S1224	T1225	P1226	L1227	T1228	S1229	T1230	P1231	V1232	G1233	A1234	C1235	A1236	L1237	S1238	E1239	S1240	S1241	E1242	V1243	G1244	
V953	R954	R955	A956	I959	E964	V968	H969	G970	V980	E981	R982	Q983	P984	R985	I986	G987	I988	E989	K990	M991	G992	V993	R994	I1004	L1009	E1010	G1011	L1012	P1013	D1014	I1019	V1020	T1021	T1022	G1028	P1029	W1030	R1036	W1037	E1038	M1039	E1040	F1045	S1046	L1047	E1048	G1049	C1050	E949	T950	V1051	E1052	Y1163														
K1166	L1167	T1172	L1173	Y1174	L1175	P1176	K1177	A1178	L1179	R1180	F1181	D1182	L1183	L1184	V1185	Q1188	I1189	P1190	W1193	M1194	A1195	K1196	T1197	R1198	L1199	I1200	S1201	D1202	M1203	V1204	D1205	T1206	T1207	Q1208	T1209	T1210	I1211	Q1212	L1216	V1217	S1218	V1219	G1220	P1221	W1222	L1223	S1224	T1225	P1226	L1227	T1228	S1229	T1230	P1231	V1232	G1233	A1234	C1235	A1236	L1237	S1238	E1239	S1240	S1241	E1242	V1243	G1244
S1247	I1248	S1249	G1252	G1253	V1254	A1255	A1256	F1257	R1258	G1259	D1263	R1264	T1265	V1270	T1274	L1275	Q1276	F1279	I1280	M1281	T1282	M1283	S1284	T1285	W1286	T1287	H1288	M1289	I1292	P1297	T1300	P1301	V1302	G1303	A1304	C1305	A1306	T1307	S1308	V1309	E1310	S1311	V1312	V1316	E1317	T1318	I1319	K1413	I1414	A1324	R1325																
D142	E143	P144	V145	L149	H152	V155	A156	H157	K158	L163	D164	S165	A166	I166	P167	M168	S169	K170	T171	L175	V176	G177	G178	K179	S180	T181	V182	Q183	E184	I186	L187	L190	T196	T197	P198	P201	E202	A203	T204	P205	L206	L209	F213	F217	V218	G219	V300	S225																			
L228	L232	I233	S234	S235	K236	P238	F241	T242	I243	T244	A246	R247	Q251	T252	R253	W254	G255	L256	P257	R260	G263	L266	V267	A268	L269	S270	N271	E272	P273	R276	T277	E280	A283	K284	A285	F286	M290	A291	Q292	K293	Y294	L297	V298	G299	V300	D301																					
L302	SER	SER	ALA	ALA	SER	ALA	GLY	ALA	GLY	ALA	ALA	ALA	ALA	ALA	ALA	ALA	MET	ILE	ASP	ALA	GLY	ALA	ALA	L328	E329	E330	T331	T332	K333	D334	R335	V337	L338	A339	R340	Q341	Q342	L343	Q344	V345	L350	K351	M352	D353	L354	R359	E370	A373	Q374	L375	V300	L378															
F385	F386	V390	T461	A391	T392	R400	T401	F402	D403	W406	W407	W408	A409	E410	Q411	S412	L413	L414	S415	L416	Y417	F418	E419	I420	I421	W424	N427	V428	A502	R430	E431	V432	V433	S434	E435	A436	I437	N438	I439	N440	R442	S443	N444	D445	A446	L447	W451	E452	Y453	H454	I455	S456															
N457	T458	D459	E460	T461	K462	N465	L468	W469	K470	G473	L476	I477	E478	N479	W483	L484	D485	P488	W489	V483	A494	K495	P496	T497	T501	A502	R430	E431	V432	V433	S434	E435	A436	I437	N438	I439	N440	R442	S443	N444	D445	A446	L447	W451	E452	Y453	H454	I455	S456																		
T536	R537	E538	S539	Q540	PRO	THR	ILE	GLU	GLU	ASP	LEU	THR	ARG	VAL	TYR	LYS	ALA	ILE	SER	ALA	GLN	ASP	GLN	ASP	ILE	SER	VAL	R335	PHE	GLU	LYS	LEU	TYR	SER	ASP	LEU	MET	LYS	PHE	LEU	GLU	SER	LYS	GLU	ILE	ASP	PRO	SER	GLN	THR	THR	GLN															
LEU	ALA	GLY	E589	D600	V601	E602	D603	A604	L605	D606	K607	D608	S609	T610	R611	E612	S615	T621	ALA	L622	S623	G624	T625	W626	S627	G628	T629	L630	P631	T634	T635	P636	F637	L638	T644	D648	V651	Q654	L655	D661	G662	L663	E664	F668	G669	G670	V671	K674	D675																		
T680	T681	A683	G689	G695	G698	S788	K702	V705	T706	R709	W710	S711	K712	W714	Q719	S720	I721	G726	A727	K728	G729	S730	I731	P636	F637	L638	S741	K742	Q743	D744	V745	E746	K747	L748	I749	E750	F751	L761	D764	I769	F770	V771	A772	A773	I774																						
P775	E776	E780	L781	E782	H783	I784	K787	S788	E789	F790	A791	H792	T793	I794	W795	L796	T797	R801	C805	W806	R807	R813	E816	T817	R818	W822	L823	L824	P825	H826	S827	P828	F833	G834	G835	D836	G837	H838	Y839	K843	L846	L849	F850	H851	R852	A858																					
A859	N860	V864	I868	R873	G874	GLY	LEU	MET	SER	N881	A882	I883	E886	G887	I888	E889	K890	M891	G892	V893	R894	L906	G907	L908	L909	T910	V913	L916	P921	V922	L930	Q931	F932	V933	P934	K937	F938	F939	R944	L947	V948	E949	T950	S951	E952																						
V953	R954	R955	A956	I959	E964	V968	H969	G970	V980	E981	R982	Q983	P984	R985	I986	G987	I988	E989	K890	M891	G892	V893	R894	I1004	L1009	E1010	G1011	L1012	P1013	D1014	I1019	V1020	T1021	T1022	G1028	P1029	W1030	R1036	W1037	E1038	M1039	E1040	F1045	S1046	L1047	E1048	G1049	C1050	E949	T950	V1051	E1052															
I1056	M1057	S1061	Y1062	N1066	L1067	R1070	P1071	Y1072	T1073	V1076	D1077	T1078	K1079	T1080	Q1188	I1189	P1190	W1193	M1194	A1195	K1196	T1197	R1198	L1199	I1200	S1201	D1202	M1203	V1204	D1205	T1206	T1207	Q1208	T1209	T1210	I1211	Q1212	L1216	V1217	S1218	V1219	G1220	P1221	W1222	L1223	S1224	T1225	P1226	L1227	T1228	S1229	T1230	P1231	V1232	G1233	A1234	C1235	A1236	L1237	S1238	E1239	S1240	S1241	E1242	V1243	G1244	
S1247	I1248	S1249	G1252	G1253	V1254	A1255	A1256	F1257	R1258	G1259	D1263	R1264	T1265	V1270	T1274	L1275	Q1276	F1279	I1280	M1281	T1282	M1283	S1284	T1285	W1286	T1287	H1288	M1289	I1292	P1297	T1300	P1301	V1302	G1303	A1304	C1305	A1306	T1307	S1308	V1309	E1310	S1311	V1312	V1316	E1317	T1318	I1319	K1413	I1414	A1324	R1325																

SER	GLU	A1664	H1583	Q1500	M1406	V1316	D1153	L1047	R852	F771	K674	V601
LEU	LYS	T1665	P1584	L1501	A1407	E1317	I1154	E1048	E956	F771	K674	E602
GLY	VAL	T1666	K1585	L1501	A1408	T1318	P1158	G1049	E949	A772	D676	D603
VAL	ASN	E1667	G1589	Q1505	T1411	I1319	E1159	C1050	E957	A773	D676	A604
ASN	GLN	G1668	G1590	M1510	D1412	A1324	E1163	E1052	E958	T774	I680	L605
LEU	GLY	Y1670	V1591	M1510	K1413	R1326	Y1163	E1052	E959	P775	A683	D606
VAL	VAL	Y1673	M1592	R1515	D1412	I1327	K1166	I1056	E953	E776	A683	K607
GLY	VAL	V1674	M1593	R1516	K1413	C1327	K1167	M1057	E954	E780	G689	D608
ALA	ASP	V1674	N1594	P1517	I1414	I1328	L1167	M1057	E955	L781	G689	S609
ALA	VAL	V1677	N1594	P1517	V1418	V1329	L1173	S1061	E956	E782	G695	T610
GLU	GLU	V1677	L1597	A1520	P1419	Y1332	L1173	Y1062	E957	H783	G695	K611
LEU	LEU	Q1598	Q1598	A1520	A1420	Y1332	Y1174	H1063	E958	I784	G698	E612
LYS	LEU	L1599	L1599	P1521	P1421	E1337	Y1174	L1067	E964	K787	K702	A614
ASP	ILE	L1600	L1600	L1522	L1426	E1338	P1176	L1067	E964	S788	K702	S615
ILE	THR	K1682	L1600	R1523	L1426	E1338	P1176	R1070	E968	E789	K702	L616
GLU	SER	P1606	G1607	G1524	T1427	F1341	K1177	E1070	E969	F790	T706	P617
ILE	ILE	G1607	G1607	G1524	T1428	F1341	K1177	E1070	E969	F790	T706	T621
VAL	ASN	N1608	N1608	A1527	R1429	G1344	L1179	T1073	E970	H791	K709	L622
ARG	VAL	R1609	R1609	T1528	R1430	G1344	R1180	V1076	E980	H792	K709	S623
VAL	VAL	D1612	D1612	T1532	E1431	M1346	R1181	D1077	E981	K793	F710	K624
ASN	ASN	N1613	N1613	T1532	H1432	M1346	R1182	D1077	E981	L794	S711	T625
ASN	ASN	N1613	N1613	T1532	H1432	M1346	R1183	D1077	E981	M795	K712	T625
THR	THR	N1613	N1613	T1532	S1434	K1347	L1184	K1079	E983	L796	U713	V626
ALA	PHE	I1617	I1617	L1536	S1434	T1352	V1185	T1080	E985	T797	U714	S627
PRO	ILE	L1618	L1618	G1537	M1442	T1352	V1185	K1081	E985	H798	U714	S628
GLU	GLU	E1619	E1619	G1537	L1443	R1360	Q1188	K1081	E985	H798	U714	S628
ALA	ALA	A1620	A1620	A1539	L1443	R1360	Q1188	K1081	E985	H798	U714	S628
LEU	LEU	F1621	F1621	S1540	M1445	T1361	P1190	V1089	E987	R801	Q719	T629
THR	PHE	E1622	E1622	F1541	K1446	A1363	L1275	E989	E988	S720	S720	P631
HIS	THR	Y1623	Y1623	F1541	K1446	A1363	L1275	E989	E988	I721	I721	P631
PRO	GLN	Y1624	Y1624	G1543	R1460	M1364	Y1193	S1096	E991	C805	G726	T634
ASN	GLN	L1625	L1625	T1644	Q1461	S1366	N1194	I1097	E992	H806	K727	L635
ALA	ALA	R1721	R1721	T1644	Q1461	S1366	N1194	I1097	E992	K807	K727	L635
LYS	LYS	P1627	P1627	T1546	V1463	P1367	A1196	S1101	E993	E816	K728	P636
LYS	LYS	S1628	S1628	T1546	V1463	P1367	T1197	S1101	E993	T817	G729	F637
TYR	CYS	T1633	T1633	M1549	R1455	T1370	Y1104	I1004	E994	R818	S730	L638
CYS	SER	T1633	T1633	D1550	R1455	T1370	Y1104	I1004	E994	R818	S730	L638
GLU	GLU	T1633	T1633	K1551	Q1468	T1372	L1109	L1009	E995	V822	I733	R641
ALA	ALA	V1639	V1639	M1552	T1469	R1373	E1010	L1009	E995	L824	F737	T644
GLY	GLY	S1640	S1640	E1553	T1469	R1373	G1011	E1010	E995	L824	F737	T644
VAL	VAL	T1642	T1642	S1554	D1461	G1375	L1012	L1012	E995	P825	N738	D648
THR	THR	Y1744	Y1744	T1556	V1463	F1376	Y1114	D1014	E995	N826	Q739	V649
ASP	VAL	A1747	A1747	I1557	E1464	Q1380	N1115	P1116	E995	S827	G740	K650
VAL	SER	THR	THR	M1561	M1465	G1381	T1212	P1116	E995	P828	S741	Y651
VAL	PHE	THR	THR	M1561	M1465	G1381	T1212	P1116	E995	P828	S741	Y651
ALA	ALA	ILE	ILE	L1564	E1473	I1384	Y1215	K1119	E995	F833	G743	Q654
ILE	GLY	Q1652	Q1652	G1565	A1474	G1383	S1218	K1119	E995	G834	G743	Q654
SER	THR	THR	THR	R1566	I1477	I1386	V1219	T1022	E995	G835	V746	L655
HIS	THR	THR	THR	R1566	I1477	I1386	V1219	T1022	E995	G835	V746	L655
ASP	ASP	LYS	LYS	I1573	P1478	T1387	T1224	P1029	E995	L930	L747	S657
ASP	ASP	LYS	LYS	G1574	S1479	M1388	T1226	P1029	E995	L930	L747	S657
LEU	LEU	P1658	P1658	V1575	L1487	L1392	T1229	W1030	E995	Y839	L749	L658
GLN	GLN	F1576	F1576	F1576	L1487	L1392	T1229	W1030	E995	Y839	L749	L658
ALA	ALA	ASN	ASN	Q1577	R1491	M1396	Y1232	R1036	E995	S842	E750	D661
VAL	VAL	THR	THR	L1580	E1492	M1396	E1233	W1037	E995	K843	F751	G662
VAL	VAL	LYS	LYS	L1580	E1496	Y1401	M1234	E1040	E995	K937	L761	L663
										E938	L761	E664
										F939	D764	F668
										R944	I769	V671

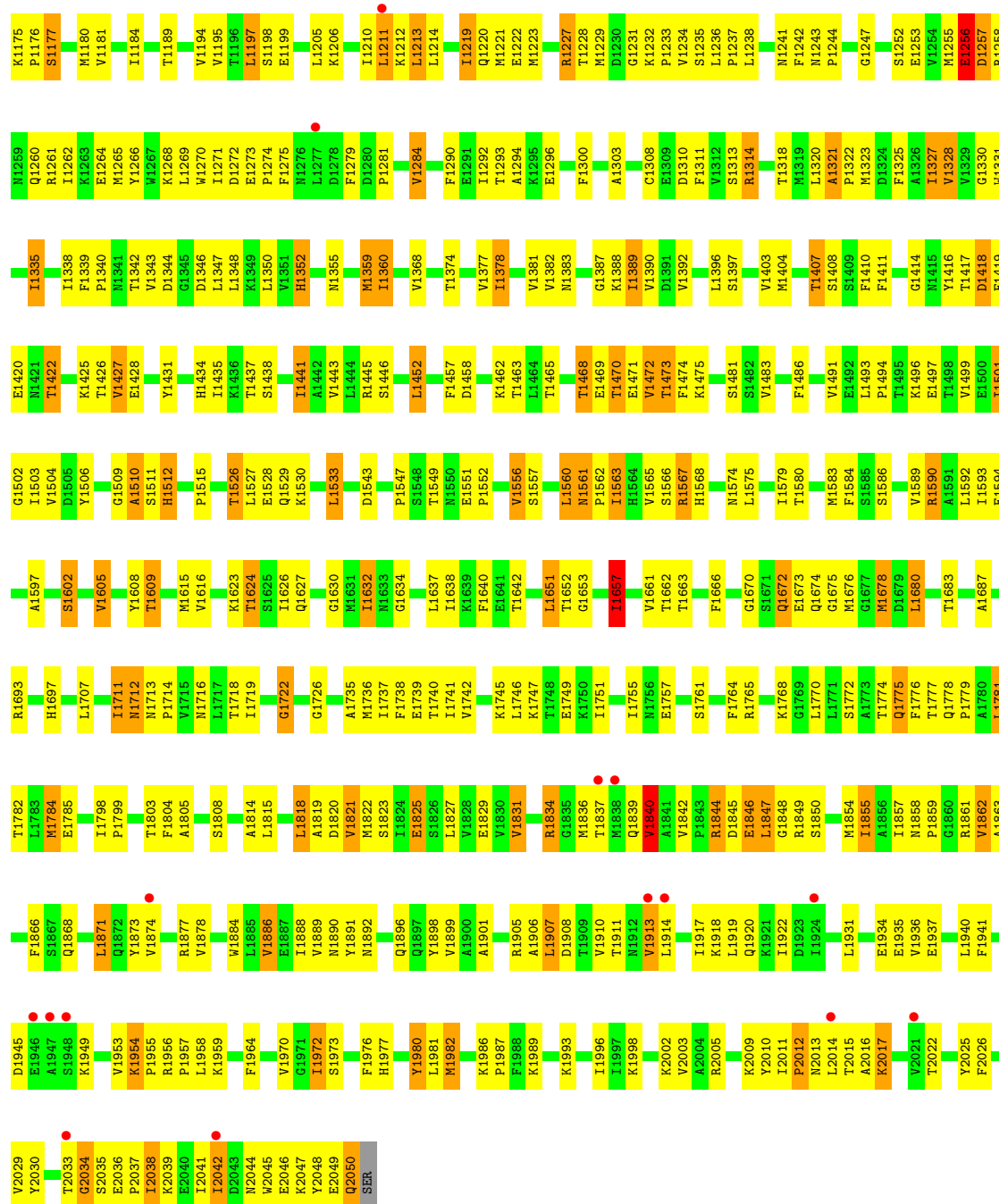
ALA
VAL
SER
THR
LYS
LVS

● Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA





I1097	R1024	T845	S773	L703	G623	K556	E477	L393	F305	L231	A158	F80	MET
V1100	F1025	V846	A774	G704	Y624	K557	R478	R394	I306	L232	I159	L84	ASP
E1101	E1026	E852	D776	L705	G629	N558	V480	K397	R309	S233	F160	N85	ALA
Y1102	I1027	P853	T777	K706	M630	P559	D481	L402	P315	L234	G161	L86	TYR
F1103	F939	I854	Y778	P707	T631	N560	C482	D403	P315	P235	Q163	T89	S5
		H855	P779	A712	A632	L562	I483	Q404	S318	T236	T166		T6
		K856	Y780	I713	A633	Y565	I484	P408	S319	S237	D167		R7
		I857	E784	S714	I634		R485	P408	P320	C238	D168		P8
		A858	W785	Q715	V638	L569	L486	P409	P321	L9	Y169		T10
		T859	W786	V716			P487	F409		Y95	F170		L11
		R860	S787	I717	I641	N572	V488	F416	L324	T244			S15
			K788	I718	E842	K573	K489	S417		Q245	L173		L16
			F789	I719	K643	K574	W490	M418	L328	L246	R174		D100
			A720	K721	G644	S574	W490	R419		A247	D175		V22
			D790	K722	S645	G575	T492	F420	E332	H248	L176		P23
			Y791	A723		K576	T493	F420	E332	Y249	Y177		T24
			P792	H723	I577	I577	T494	P422	P335	V250	Q178		A25
			P793		G648	F578	Q495	V423		V251	T179		S26
			K794	F726	I649	V579	F496	A424	K339	L255	I190		F27
			P795	P727	I652	E590		A424	L339	H181			F28
			F796	I728	Y653	T581	T499	S425	S340	L256	V182		L33
			W797	A729	V654	K582	H500	P426		G257	L183		N38
			G798	L730		F583	I501	F427	S342	T259	V184		K39
			L800	W732	M658	K585	F504	H428	K343	P260	G185		I40
				T733	L659	L586	G505	L431	L344	G261	D186		L39
			R804		Q660	I587	P506	L432	T345	L187	L187		L41
			W805	R736	G661	G588	G507	V433	Q346	E262	I188		P42
			M806		G662	G589	G508	P434	E347	L263	K189		E43
			I807	G739	I663	P590		Q348	Q348	R264	F190		
				H740	P664	P591	L512	L438	V349		S191		P44
			E810	H741	L665			L439	Q350	T271	A192		T45
			V811	S742	K667	V594	T516	M440		G272	E193		E46
			T813		E668	G596	H517	K441	V353	S274	L194		G47
			D816	D745	L669	M597	K520	D442	K354	Q275	L195		F48
			A817	H747	R670	T598	D821	V444	K355	G276	E197		A49
			K818	I748	Y674	P599	G522	K445	K356	L277	L198		A50
				P749	P675	G600	R526	M445	N357	V278	I131		D51
			I821	M750	I676	T601	R527	N447	H359	T279	M132		D52
			A822	Q752	Q677	V802	V527	V449	L360	A280	A133		E53
			C824	Y754	F678	S603		T455	P361	V281	K134		P54
			T825		L679	F606	L533	Q456		A282	R135		T55
			G826	I757	T680	V607	N536		T368	L283	F136		T56
			V827	R758	I681	G607	P537	V459	S369	F209	F137		E59
			P828	R759	G682	T610	D539	Y460	L370	T210	K139		L60
				H760	A683	N612	D540	D461	V371	T286			V61
			W832	P761	V690	A613		T462	A374	V289	L213		G62
			E833	N762		G614	F543	D464	K375	E290	N214		K63
			Q834	I763	E693	Y615	K544	G465	L377	S295	L215		P84
			T835	M764	Y694	T616	Q545	S466		V296	E217		L85
			Y836	L765		I617			S380	R297	W218		V68
					T697	E618	V550	R469		K298	L219		
			P839	G768	L698	L819	T551	V470	L389	T300	T225		V72
			T840	S769	G699	A620	N551	L471	K390	L303	P226		E73
						G621	N553		L391	L303	D227		K76
			V844	G772	Y702	G622		S476	T392	F304			



P1244	V1186	I1082	M1011	L926	T845	G772	Y702	A620	N553	V480	L383	F304	L231	A158
G1247	S1167	K1083	Q1012	L929	V846	G773	L703	G621	K556	D481	K394	F305	L232	I189
	N1168	K1084		L929	E852	S773	L705	G622	K557	C482	K397	I306	S233	G161
S1252	R1171	L1086	V1015	I932	P853	A774	L706	G623	K558	I483		R309	I234	G162
E1253	R1170		F1017	I932	P854		K706	Y824	N558	R485			P235	Q163
V1254	K1172	Y1090	F1018	Q938	H855	T777	P707		L562	R486	L402	P315	I236	T166
M1255	K1173	G1091	V1019	F939	K866	Y778	A712	G629	L562	F487	D403		S237	D167
E1256	F1174	D1092	P1020	T942	T857	Y790	I713	M630	Y565	V488	Q404	L319	D168	D169
D1257	K1175	D1093	Y943	T942	H859	E784	Q715	A632	H566	K489	F416		P239	Y169
R1258	P1176		R944	R945	R860	W785	Q716	A633	P567	W490	S417	L324	L240	F170
K1259	S1177	K1096	F1025	T945	R860	S786	W717	I634	K568	E491	R418		L241	
Q1260		I1097	F1026	F946	L864	T787	W718	V638	L569	T492	R419	L328		
R1261	M1180	E1101	E1026	T947	W885	F788	I719		N572	T494	F420			L178
K1263	I1184	Y1102	I1027	G948	K866	F789	W720	I641	K573	L422	L421	E332	Q245	R174
E1264	F1103	F1103	K1031	D949	E867	W790	K721	S874	K574	Q495	P422		L246	R175
M1265	T1189		D1032	F950	F888	Y791	K722	S645	G575	F496	V423	P335	A247	L176
Y1266		P1108		R951	D869	W792	A722		K576	T499	A424		H248	Y177
W1267	V1194	V1109	S1037	R952	E870	F793	R723	G648	I577	H500	P426	K338	Y249	Q178
K1268	V1195	ASP	L1040	R953	T871	R794	F726	I649	F578	L501	F427	S340	V251	T179
L1269	T1196	VAL	L1041	S961	L880	F795	P727		V579	D502	H428	S342		V182
W1270	L1197	GLN	E1041	E955	F873	F796	I728	I652	E580	L502	H429	S343	L255	L183
S1198	S1198	SER	A1042	E956	R874	D797	A729	Y653	T581	F504	H430	R343	G257	V184
D1271	E1199	GLN	V1043	R957	L875	G798	L730	V654	K582	G505	H431	L344	F258	G185
E1273		VAL	Y1044			F799	Q731		F583	P506	L432	T345	T259	D186
P1274	L1205	ASP	D1045	K960	K879	L800	W732	M658	S584	G507	L438	Q346	P260	L187
F1275	K1206	SER	Q1046	S961	L880	R804	W733	E659	K585	G508	N440	Q348	E262	L188
		SER	Y881	T963	P882	R805	R736	Q661	I587	L512	N441	Q350	G263	F190
F1279	T1210	SER	V1048	K964	P882	M806		G662	G588		D442		R264	S191
V1284	L1211	VAL	Q1049	S965	K887	I807	Q739	I663	R589	T516	D443	V353		A192
F1290	L1212	GLU	R1050	L966		E810	H740	P664	P590	H517	V444	K354	T271	E193
I1292	L1213	D1123	K1052	T967	E892	R811	H741	I665	L591	R518	V445	K355	G272	L194
T1293	A1129		L1054	Q969	S893	K812	S742	I666	L592	N519	K446	T356	H273	L195
	T1130		H1055	S971	L895	T813	D745	K667	L593	K520	N447	N357	S274	S196
				S971	N896		A746	E668	V594	D521	N447	S358	Q275	E197
E1296	T1133	T1133	V1058	L972	A897	D816	A747	L669	P595	G524	V448	H359	G276	L198
F1300	D1134	E1135	A1059	L973	D898	A817	H748	R670	G596	V525	L455	L360	L277	L199
	E1222		Q1061	A979	F899	K818	P749	P675	M597	R526	Q456	P361	L203	D204
A1303	W1138		F1062	Y987	Q900	L821	W750	I676	P599	A530	V459	V368	T278	A205
C1308	S1145		T1063		P902	A822	Q752	Q677	C600	G531	Y460	F367	T279	E206
E1309	M1148	M1148	I1066	Q993	W903	A823	M753	F678	T601	T832	D461	I368	A281	A206
D1310	W1149	E1068	E1067	F994	A905	T825	Y754	I680	V602	L533	T462	S369	A282	E207
F1311	R1150	P1069	T906	L995	T906	Q826	Y754	I681	S903		F463	L370	I283	V208
V1312	H1151	P1069	W827	Q998	V907	V827	I757	G682	F606	N536	D464	V371	T286	F209
S1313	A1152	I1070	P828	Q998		P828	R759	A683	V607	P537	Q465			T210
R1314	S1153	K1071		D999	Q910		H760		T610	D538	S466	A374	W289	L213
					A911	W832	P761	V690	T611	D539	D467	K375		N214
T1318	M1074	D1075	R912	I1000	A911		P761		N612	D540	L468	K376	S296	L215
M1319	F1158	H1002	D913	H1001	R912	T835	I762	E893	A613	F543	R469	L377	V296	L216
L1320	D1075	F1003	D913	H1002	D913	T835	I762	Y694	G614				R297	E217
A1321	G1076	L1004	L914	F1003	L914	T840	M764		Y615	Q545	L471	S380	K298	W218
L1249	L1077	L1004	A915	L1004	A915	T840	L765		T616				A299	L219
Y1240	H1078	S1085	T916	S1085	T916	G841	I766	T697	L617	V550	S476	L389	I300	T225
P1322	D1079	M1006	E921	M1006	E921	G842	F767	L698	E477	K390	R478	L391	T301	P226
M1323	G1080	K1163				I843	G768	G699	E518	T551			V302	F1324
F1325				P1010		V844	S769		L619	S552	L479		L303	D227

F2026	L1940	S1867	L1781	D1679	A1591	K1496	F1410	A1326
V2029	F1941	Q1868	T1782	L1680	L1592		F1411	I1327
Y2030		L1871	L1783	T1683	I1593	V1499	Y1416	V1329
T2033	D1945	Y1872	M1784	S1684	E1594	I1501	Y1417	G1330
G2034	K1949	Y1873	E1785	A1687	M1596	G1502	D1418	T1417
S2035		V1874	P1799	Q1688	A1597	I1503	F1419	W1331
E2036	V1953	R1877	T1803	R1693	A1598	V1504	E1420	I1385
P2037	K1954	G1878	F1804	R1693	D1599	G1509	N1421	I1338
I2038	P1955	G1879	A1805	H1697	S1600	A1510	T1422	F1339
K2039	R1956	K1880	S1808	L1707	V1601	H1512	K1425	P1340
P2040	P1957	W1884		I1711	S1602	G1513	T1426	N1341
I2041	L1958	L1885	A1814	N1712	V1605	P1515	V1427	T1342
D2042	L1959	V1886	L1815	N1716	R1606	M1514	E1428	V1343
D2043	E1887	I1888	L1818	T1717	G1607	G1515	Y1431	D1344
N2044	V1889	D1820	A1819	L1717	T1608	T1526	H1434	L1347
W2045	N1890	V1821	D1820	T1717	M1615	L1527	L1435	L1348
E2046	Y1891	M1822	V1821	I1719	V1616	E1528	I1436	K1349
K2047	S1973	N1892	S1823	I1719	K1623	K1530	F1436	L1350
Y2048	F1976	V1893	I1824	G1722	T1624	L1533	T1437	V1351
E2049	H1977	Q1896	E1825	G1726	S1625	D1543	S1438	H1352
Q2050	Y1980	Q1897	S1826	A1735	I1626		I1441	N1355
SER	L1981	Y1898	L1827	M1736	Q1627		A1442	G1356
	M1982	A1900	V1828	I1737	G1630	P1547	V1443	Y1357
	K1986	A1901	V1830	F1738	M1631	S1548	R1445	K1358
	P1987	R1905	V1831	E1739	I1632	N1550	S1446	M1359
	F1988	A1906	R1834	I1740	L1637	E1551	L1452	V1368
	K1989	L1907	G1835	T1741	T1638	P1552	F1457	G1369
	K1993	D1908	M1836	V1742	K1639	Y1553	D1458	D1370
		T1909	T1837	K1745	F1640	V1556	L1459	T1374
		V1910		L1746	F1641	L1560	K1462	V1377
	I1996	V1913	V1840	K1747	T1642	M1561	T1463	I1378
	I1997	L1914	V1842	I1751	L1651	P1562		
			P1843	I1755	T1652	I1563	T1468	V1381
	V2003	I1917	R1844	I1755	G1653	H1564	E1469	V1382
	A2004	K1918	D1845	N1756	I1657	V1565	T1470	N1383
	R2005	L1919	E1846	E1757		S1566	E1471	K1388
		Q1920	L1847	S1761	V1661	H1568	V1472	I1389
	K2009	K1921	G1848		T1662		F1474	V1390
	Y2010	I1922	R1849		T1663	N1574	K1475	D1391
	I2011	D1923	S1850	F1764	F1666	L1575		V1392
	P2012	I1924	M1854	R1765			S1481	L1396
	N2013	L1927	I1855	L1770	G1670	T1579	S1482	S1397
	L2014	Q1928	A1956	T1774	S1671	T1580	F1486	V1403
	T2015	K1929	I1857	Q1775	Q1672	M1583		M1404
	A2016	N1958	N1858	Q1776	E1673	F1584	V1491	E1405
	K2017	S1930	P1859	T1777	G1675	S1585	E1492	V1406
		L1931	G1860	Q1778	M1676		L1493	T1407
	Q2020	S1932	R1861		G1677	V1589	P1494	S1408
	V2021	E1935	V1862	A1780			T1495	S1409
	T2022	V1936	F1866					
		E1937						

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	231.90Å 231.90Å 756.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 4.00 24.99 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.99-4.00) 96.8 (24.99-4.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.97Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.268 , 0.268 0.276 , 0.278	Depositor DCC
R_{free} test set	8547 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	130.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 85.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	85959	wwPDB-VP
Average B, all atoms (Å ²)	164.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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, 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	0.71	9/12855 (0.1%)	0.95	40/17369 (0.2%)
1	B	0.58	9/12855 (0.1%)	0.96	35/17369 (0.2%)
1	C	0.68	12/12855 (0.1%)	0.94	32/17369 (0.2%)
2	G	0.59	16/16360 (0.1%)	0.95	44/22198 (0.2%)
2	H	0.82	16/16360 (0.1%)	0.98	54/22198 (0.2%)
2	I	0.56	13/16360 (0.1%)	0.95	56/22198 (0.3%)
All	All	0.66	75/87645 (0.1%)	0.96	261/118701 (0.2%)

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	3
2	I	0	1
All	All	0	5

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1657	ILE	C-N	-55.01	0.58	1.33
2	H	559	PRO	C-N	32.88	1.87	1.33
1	A	485	ASP	C-N	32.60	1.77	1.33
1	C	181	THR	C-N	-27.09	1.05	1.34
2	H	1422	THR	C-N	-24.89	1.03	1.33

The worst 5 of 261 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1657	ILE	O-C-N	-26.14	95.13	123.10
1	B	992	PHE	CA-C-N	-17.47	102.73	120.03
1	B	992	PHE	C-N-CA	-17.47	102.73	120.03
2	H	1657	ILE	CA-C-N	17.04	149.68	121.39
2	H	1657	ILE	C-N-CA	17.04	149.68	121.39

There are no chirality outliers.

All (5) 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	H	1657	ILE	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	12615	0	12590	631	1
1	B	12615	0	12592	606	6
1	C	12615	0	12590	619	0
2	G	15995	0	15977	1037	10
2	H	15995	0	15974	1044	7
2	I	15995	0	15977	1014	12
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	8	0
4	H	31	0	19	5	0
4	I	31	0	19	4	0
All	All	85959	0	85787	4772	18

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 28.

The worst 5 of 4772 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:485:ASP:C	1:A:486:VAL:N	1.77	1.42
2:H:559:PRO:C	2:H:560:ASN:N	1.87	1.31
2:H:1956:ARG:HB2	2:H:1957:PRO:HD3	1.24	1.18
2:G:28:PHE:CE2	2:H:7:ARG:HD2	1.80	1.16
2:G:1859:PRO:HG3	2:G:1871:LEU:HD12	1.29	1.15

The worst 5 of 18 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:B:1480:GLU:OE2	2:H:290:GLU:CB[6_555]	0.75	1.45
1:B:1480:GLU:CD	2:H:290:GLU:CB[6_555]	1.29	0.91
2:G:77:VAL:CB	2:I:1929:LYS:CD[6_455]	1.32	0.88
1:B:1480:GLU:OE2	2:H:290:GLU:CG[6_555]	1.43	0.77
2:G:77:VAL:CG2	2:I:1929:LYS:NZ[6_455]	1.47	0.73

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	1604/1887 (85%)	1498 (93%)	92 (6%)	14 (1%)	14	48
1	B	1604/1887 (85%)	1497 (93%)	94 (6%)	13 (1%)	16	52
1	C	1604/1887 (85%)	1499 (94%)	90 (6%)	15 (1%)	14	48
2	G	2029/2051 (99%)	1836 (90%)	167 (8%)	26 (1%)	9	41
2	H	2029/2051 (99%)	1836 (90%)	170 (8%)	23 (1%)	11	44
2	I	2029/2051 (99%)	1833 (90%)	171 (8%)	25 (1%)	10	42
All	All	10899/11814 (92%)	9999 (92%)	784 (7%)	116 (1%)	11	44

5 of 116 Ramachandran outliers are listed below:

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

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	1367/1566 (87%)	1197 (88%)	170 (12%)	4	20
1	B	1367/1566 (87%)	1200 (88%)	167 (12%)	5	21
1	C	1367/1566 (87%)	1196 (88%)	171 (12%)	4	20
2	G	1772/1789 (99%)	1528 (86%)	244 (14%)	3	17
2	H	1772/1789 (99%)	1529 (86%)	243 (14%)	3	17
2	I	1772/1789 (99%)	1527 (86%)	245 (14%)	3	17
All	All	9417/10065 (94%)	8177 (87%)	1240 (13%)	4	18

5 of 1240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	1468	THR
2	I	1327	ILE
2	H	1663	THR
2	H	1465	THR
2	I	344	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 299 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	910	GLN
2	I	1352	HIS
2	H	1260	GLN
2	I	418	ASN

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Mol	Chain	Res	Type
1	B	1552	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
3	CER	A	2748	1	11,11,15	4.18	3 (27%)	11,13,17	4.44	4 (36%)
3	CER	B	2748	1	11,11,15	4.17	3 (27%)	11,13,17	4.27	4 (36%)
3	CER	C	2748	1	11,11,15	4.19	3 (27%)	11,13,17	4.43	4 (36%)
4	FMN	I	3051	-	33,33,33	6.45	24 (72%)	48,50,50	1.36	8 (16%)
4	FMN	H	3051	-	33,33,33	6.35	21 (63%)	48,50,50	1.36	7 (14%)
4	FMN	G	3051	-	33,33,33	6.45	22 (66%)	48,50,50	1.36	6 (12%)

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	CER	A	2748	1	-	4/12/12/16	-
3	CER	B	2748	1	-	4/12/12/16	-
3	CER	C	2748	1	-	4/12/12/16	-
4	FMN	I	3051	-	-	5/18/18/18	0/3/3/3
4	FMN	H	3051	-	-	5/18/18/18	0/3/3/3
4	FMN	G	3051	-	-	5/18/18/18	0/3/3/3

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3051	FMN	C6-C7	13.44	1.57	1.39
4	I	3051	FMN	C6-C7	13.08	1.57	1.39
4	H	3051	FMN	C6-C7	12.77	1.57	1.39
4	I	3051	FMN	C6-C5A	12.55	1.59	1.40
4	I	3051	FMN	C9-C8	12.37	1.56	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2748	CER	O1-C4-C3	-11.11	108.66	120.07
3	C	2748	CER	O1-C4-C3	-11.09	108.69	120.07
3	B	2748	CER	O1-C4-C3	-10.73	109.06	120.07
3	C	2748	CER	O1-C4-C5	-8.10	107.97	121.68
3	A	2748	CER	O1-C4-C5	-8.05	108.06	121.68

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 28 short contacts:

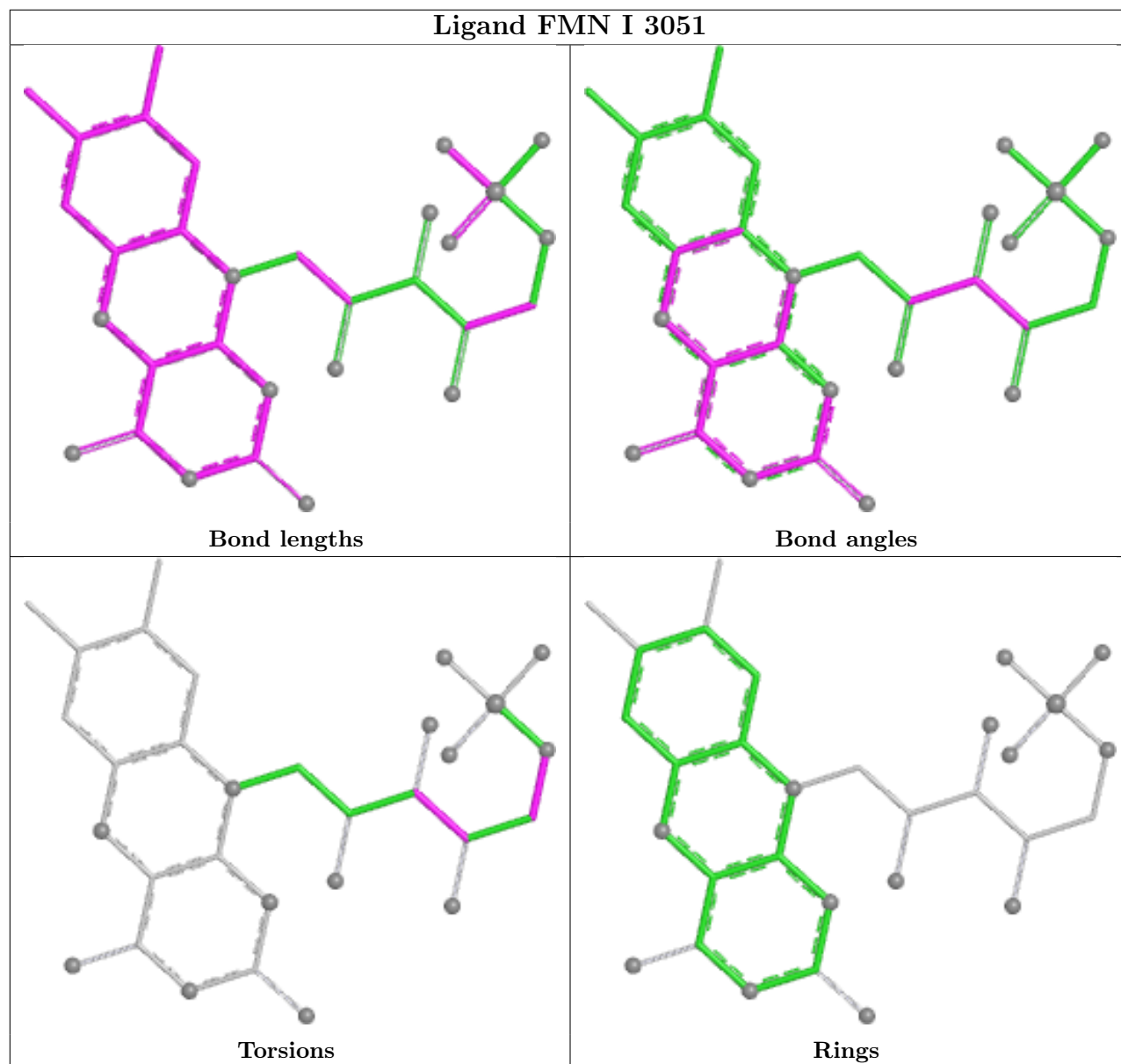
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2748	CER	3	0

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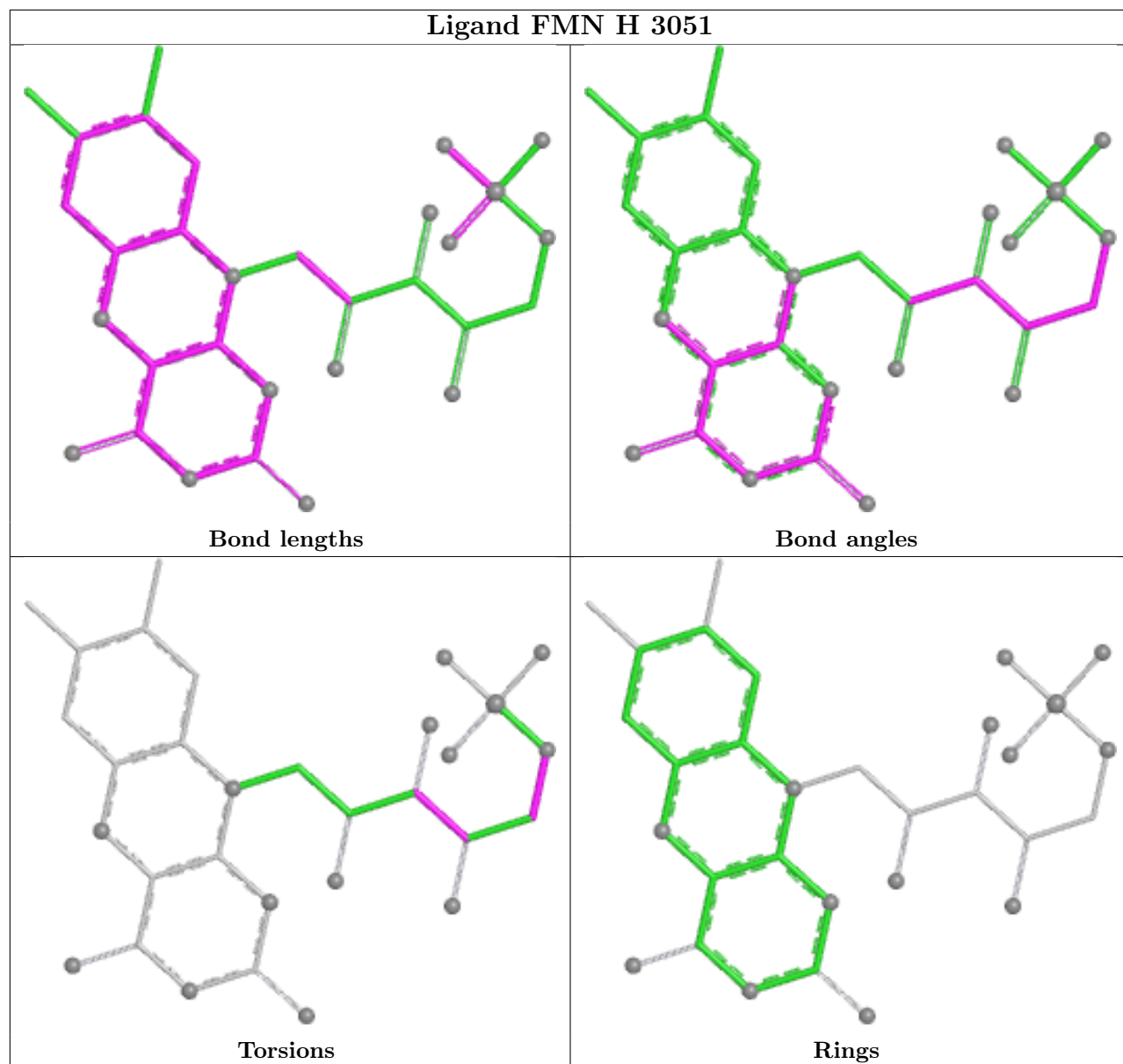
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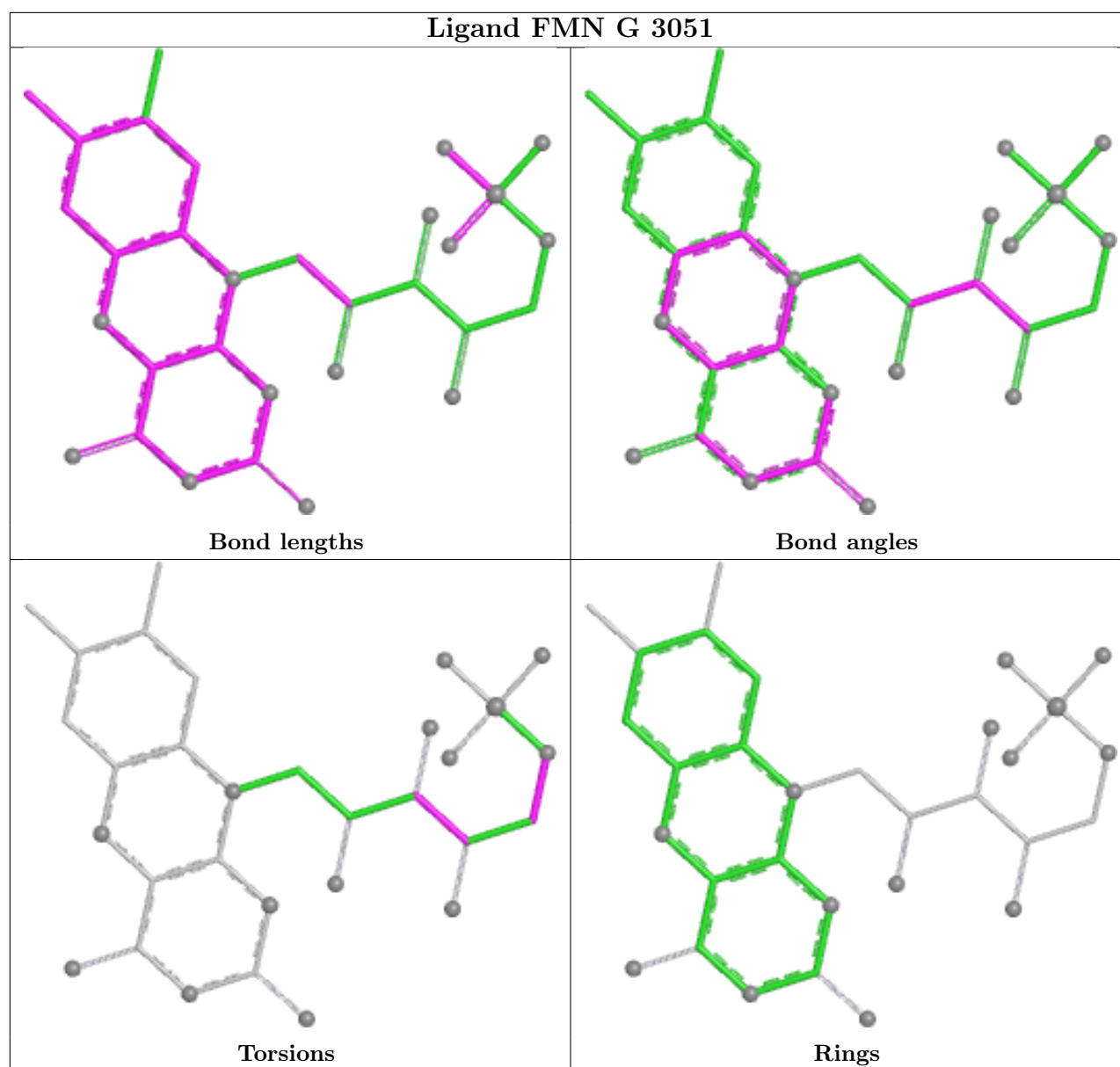
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2748	CER	4	0
3	C	2748	CER	4	0
4	I	3051	FMN	4	0
4	H	3051	FMN	5	0
4	G	3051	FMN	8	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	6
1	C	4
1	A	3

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Mol	Chain	Number of breaks
2	G	3
2	I	2

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	559:PRO	C	560:ASN	N	1.87
1	A	485:ASP	C	486:VAL	N	1.77
1	H	315:PRO	C	316:ASN	N	1.64
1	H	1530:LYS	C	1531:VAL	N	1.60
1	C	932:PHE	C	933:VAL	N	1.19

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	1614/1887 (85%)	0.01	10 (0%) 85 71	98, 134, 233, 288	0
1	B	1614/1887 (85%)	-0.01	4 (0%) 91 81	99, 133, 233, 296	0
1	C	1614/1887 (85%)	0.03	16 (0%) 79 61	100, 135, 233, 294	0
2	G	2033/2051 (99%)	0.02	22 (1%) 78 60	134, 172, 221, 270	0
2	H	2033/2051 (99%)	0.06	19 (0%) 81 64	133, 173, 218, 268	0
2	I	2033/2051 (99%)	0.04	26 (1%) 75 57	134, 173, 218, 264	0
All	All	10941/11814 (92%)	0.03	97 (0%) 81 64	98, 164, 226, 296	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	1924	ILE	8.2
2	H	2014	LEU	5.8
2	I	205	ALA	4.6
2	H	1924	ILE	4.1
2	I	1219	ILE	3.7

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

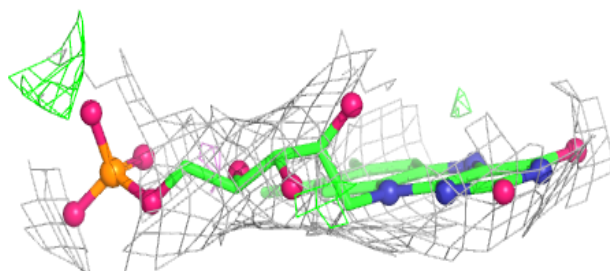
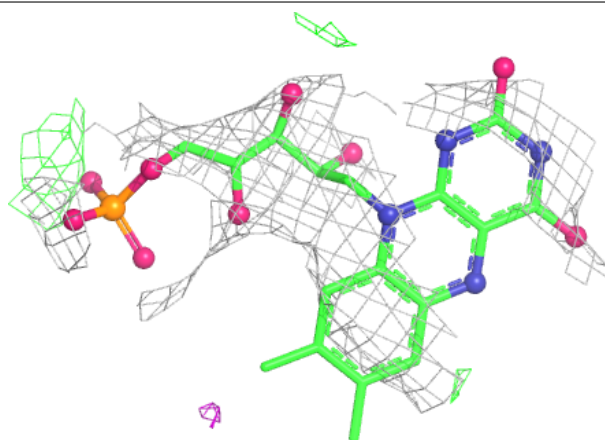
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	CER	A	2748	12/16	0.82	0.24	70,134,243,252	0
4	FMN	G	3051	31/31	0.85	0.12	137,161,187,206	0
4	FMN	H	3051	31/31	0.88	0.09	133,160,184,188	0
3	CER	C	2748	12/16	0.91	0.14	70,134,252,253	0
4	FMN	I	3051	31/31	0.91	0.10	132,164,181,204	0
3	CER	B	2748	12/16	0.92	0.15	70,134,252,253	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.

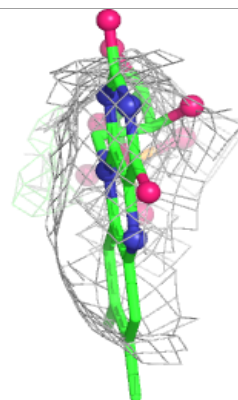
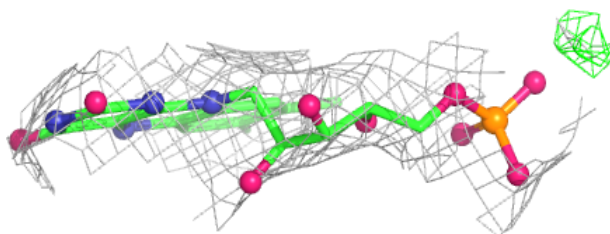
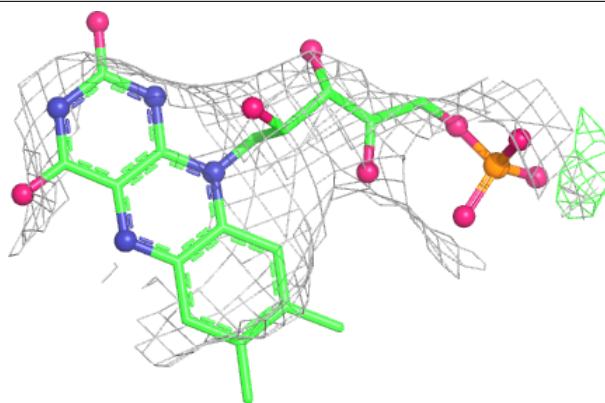
Electron density around FMN G 3051:

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

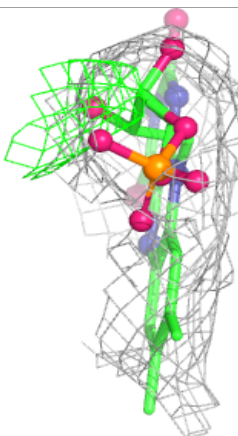
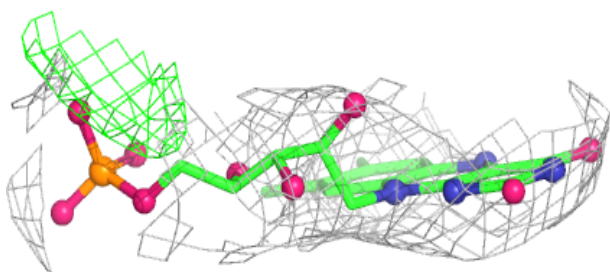
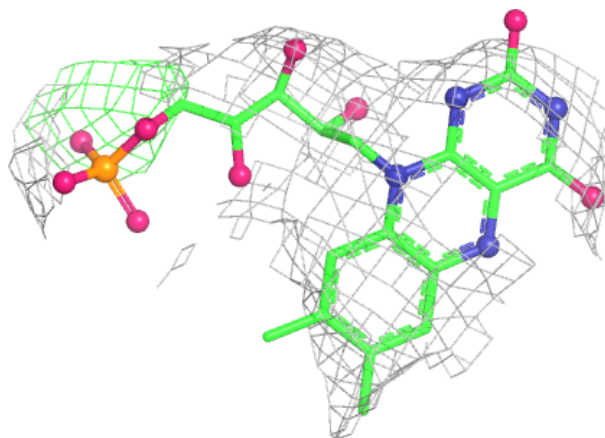


Electron density around FMN H 3051:

$2mF_o-DF_c$ (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.