



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 9, 2024 – 10:42 am GMT

PDB ID : 2VKZ
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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

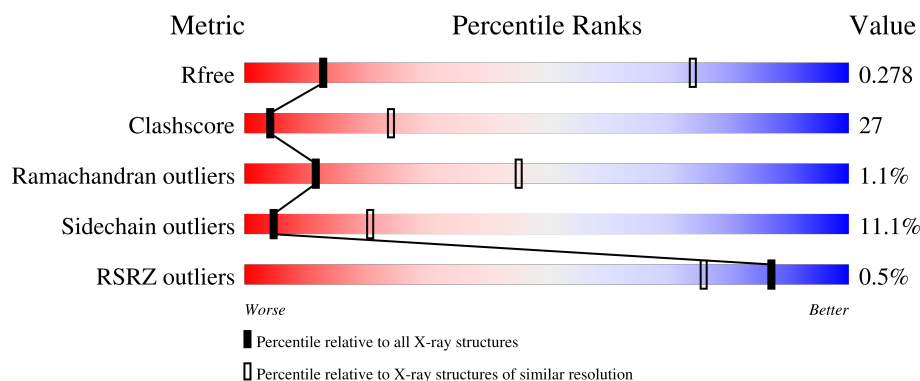
1 Overall quality at a glance

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}	164625	1028 (4.22-3.78)
Clashscore	180529	1055 (4.20-3.80)
Ramachandran outliers	177936	1004 (4.20-3.80)
Sidechain outliers	177891	1027 (4.22-3.78)
RSRZ outliers	164620	1029 (4.22-3.78)

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	
1	B	1887	
1	C	1887	
2	G	2051	

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Mol	Chain	Length	Quality of chain
2	H	2051	<div><div></div><div>51%40%8% .</div></div>
2	I	2051	<div>%<div><div></div><div>51%40%8% .</div></div></div>

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.

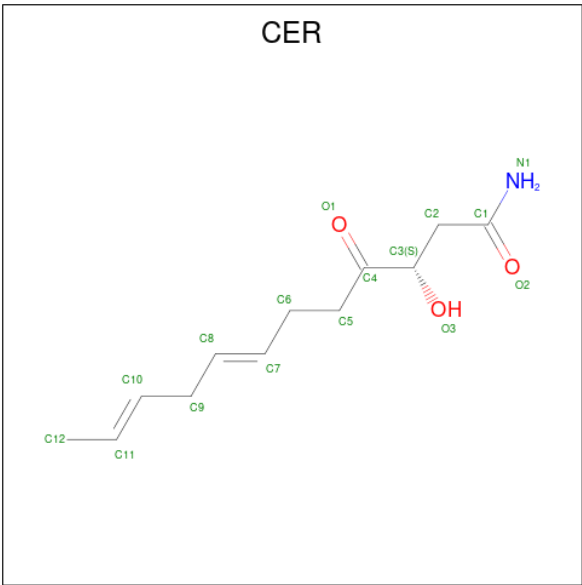
- Molecule 1 is a protein called FATTY ACID SYNTHASE SUBUNIT ALPHA.

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.

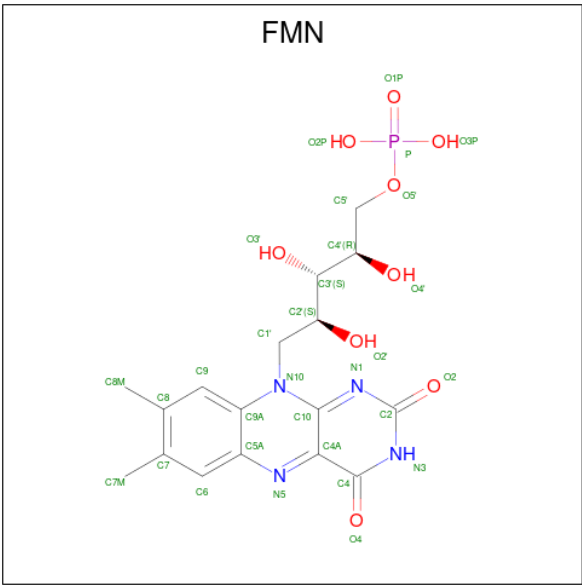
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	H	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	I	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			

- Molecule 3 is (2S, 3R)-3-HYDROXY-4-OXO-7,10-TRANS,TRANS-DODECADIENAMIDE (three-letter code: 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 (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

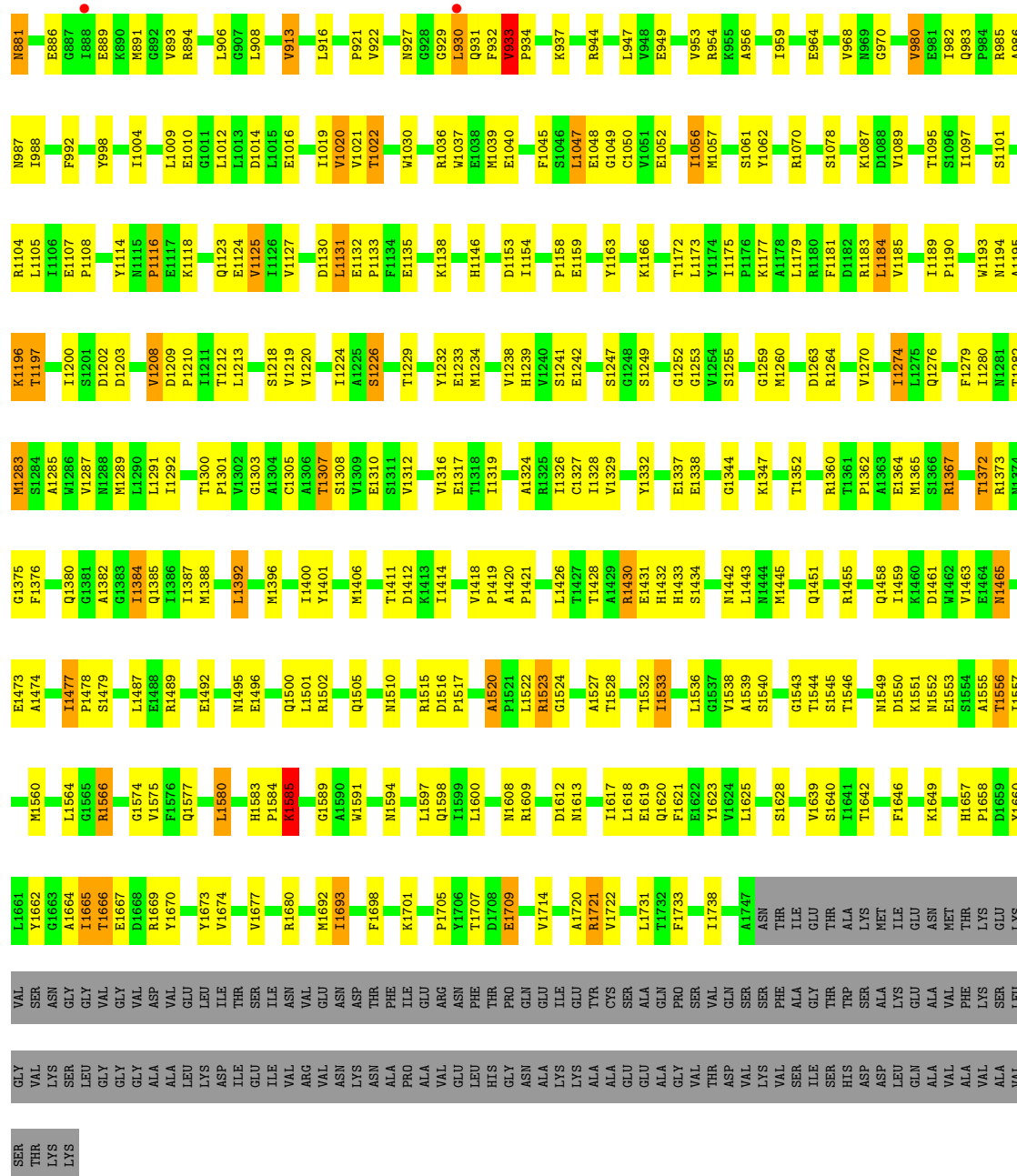


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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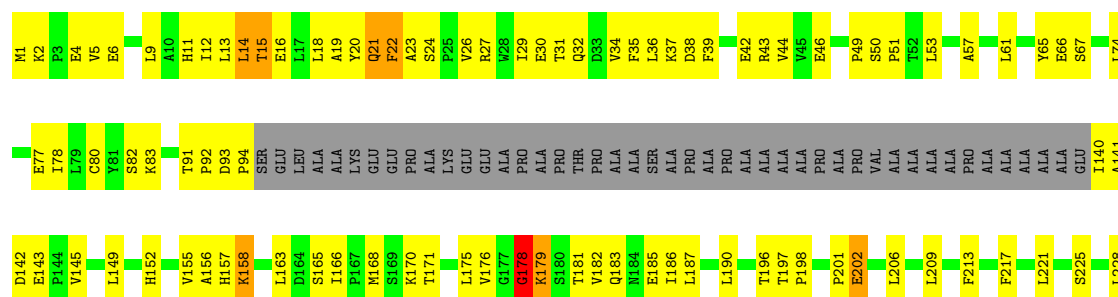
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		



• Molecule 1: FATTY ACID SYNTHASE SUBUNIT ALPHA

Chain B: 50% 30% 5% 14%



V1463	E1464	N1465	E1473	A1474	I1477	P1478	S1479	E1480	E1492	E1496	Q1500	L1501	R1502	Q1505	W1508	G1509	N1510	R1515	P1517	A1520	P1521	L1522	G1523	G1524	A1527	T1528	T1532	I1533	D1534	V1538	A1539	S1540	G1543	T1544	S1545	T1546	N1549	D1550	K1551	N1552	E1553	S1554	A1555	T1556												
R1373	N1374	G1375	F1376	Q1380	I1384	Q1385	I1386	I1387	M1388	L1392	M1396	P1399	T1400	Y1401	M1406	T1411	D1412	K1413	I1414	V1418	P1419	A1420	P1421	L1426	T1427	T1428	R1430	E1431	H1432	S1433	N1442	M1445	K1446	R1447	R1448	K1449	R1450	Q1451	R1455	Q1458	I1459	D1460	S1461	W1462												
W1286	V1287	M1288	M1289	I1292	P1297	T1300	P1301	G1302	V1303	A1304	C1305	T1307	S1308	V1309	E1310	S1311	V1312	V1316	E1317	T1318	I1319	A1324	R1325	I1326	C1327	G1328	Y1332	E1337	E1338	F1341	G1344	K1347	T1352	R1360	T1361	P1362	A1363	A1364	M1365	S1366	T1367	T1370	N1552	E1553	S1554	A1555	T1556									
I1200	S1201	D1202	V1208	D1209	T1212	L1216	V1217	S1218	V1219	S1226	V1225	T1229	Y1232	E1233	M1234	V1238	H1239	W1240	S1241	G1242	G1243	G1244	S1247	G1248	S1249	G1252	G1253	S1254	S1255	L1257	R1258	G1259	D1263	R1264	V1270	I1274	L1275	Q1276	F1279	M1280	W1281	T1282	M1283	T1370	N1552	E1553	S1554	A1555	T1556							
I1097	F992																																																							
S1101	Y998																																																							
R1104	L1105																																																							
L1114	N1115																																																							
P1116	L1012																																																							
K1119	L1013																																																							
Q1123	A1014																																																							
E1128	L1015																																																							
E1129	E1016																																																							
E1130	L1012																																																							
L1131	L1013																																																							
E1132	L1014																																																							
P1133	E1038																																																							
K1138	M1039																																																							
K1145	E1040																																																							
T1184	F1045																																																							
P1158	S1046																																																							
E1159	L1047																																																							
Y1163	G1049																																																							
K1186	C1050																																																							
R1187	V1051																																																							
T1172	E1052																																																							
L1173	I1056																																																							
Y1174	M1057																																																							
L1175	K955																																																							
R1177	A956																																																							
P1176	Y1062																																																							
A1178	N1066																																																							
L1179	M1066																																																							
R1183	R1070																																																							
L1184	P1071																																																							
V1185	R969																																																							
S1078	S1078																																																							
K1079	K1079																																																							
L1189	T1080																																																							
T1189	T1080																																																							
P1190	P1190																																																							
L1199	L1199																																																							
M1365	M1365																																																							
S1366	S1366																																																							
T1367	T1367																																																							
Q1455	Q1455																																																							
K1551	K1551																																																							
N1552	N1552																																																							
E1553	E1553																																																							
S1554	S1554																																																							
A1555	A1555																																																							
T1556	T1556																																																							
ALA	SER	ALA	SER	GLY	ALA	GLY	ALA	ALA	ALA	ALA	GLY	ALA	ALA	ALA	ALA	ASP	ILE	ASP	GLN	ASP	GLN	ASP	GLY	ALA	L328	E329	E330	I331	T332	K333	D334	H335	K336	V337	L338	A339	R340	Q341	Q342	L343	Q344	V345	L350	K351	M352	R359	E370	A373	Q374	L375	L378	F385	F386	V390	SER	ALA

L1567	V1655	LYS	LEU
L1564	V1656	VAL	GLY
G1565	P1657	SER	VAL
R1566	P1658	ASN	VAL
	D1659	LYS	VAL
G1574	Y1660	GLY	LEU
V1575	L1661	GLY	GLY
F1576	Y1662	GLY	GLY
Q1577	G1663	VAL	GLY
	A1664	ASP	ALA
L1580	I1665	VAL	ALA
T1581	T1666	GLU	LEU
G1582	E1667	LEU	LYS
H1583	D1668	ILE	ASP
P1584	R1669	THR	ASP
K1585	Y1673	SER	ILE
	Y1673	ILE	ILE
G1589	V1677	ASN	VAL
A1590		VAL	ARG
W1590	R1680	GLU	VAL
M1592	E1681	ASN	ASN
M1593	K1682	ASP	LYS
N1594	T1682	THR	ASN
G1595	P1682	ALA	ASN
A1596	M1692	PHE	PRO
L1597	I1693	ILE	PRO
Q1598	K1701	GLU	ALA
I1599	P1705	ARG	VAL
L1600	Y1706	LEU	GLU
N1608	T1707	THR	HIS
R1609	D1708	GLY	GLY
	E1709	ASN	ASN
D1612	V1714	ALA	ALA
N1613		ALA	ALA
	R1721	SER	GLU
L1618	V1722	ALA	GLU
E1619		ALA	GLU
L1731		GLN	ALA
F1620	T1732	PRO	GLY
F1621	F1733	VAL	VAL
E1622		THR	THR
Y1623		ASP	ASP
V1624	A1747	VAL	VAL
L1625	ASN	SER	LYS
	THR	PHE	VAL
S1628	ILE	SER	VAL
	ALA	ILE	ILE
V1639	GLU	THR	SER
S1640	ALA	THR	HIS
I1641	LYS	TRP	ASP
T1642	MET	ASP	ASP
	ILE	ALA	ASP
F1646	GLY	LYS	LEU
	ASN	GLN	GLN
K1649	MET	ALA	ALA
	THR	VAL	VAL
Q1652	GLU	PHE	VAL
		LYS	VAL
		SER	ALA

● Molecule 1: FATTY ACID SYNTHASE SUBUNIT ALPHA

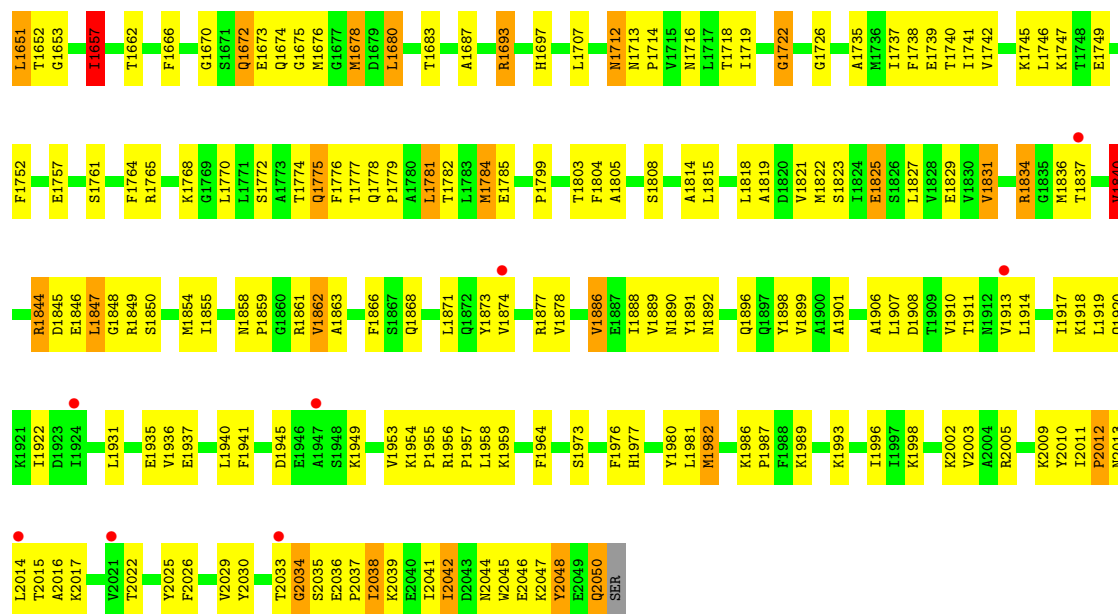
Chain C:  49% 32% 5% 14%

K1	V81	H152	M237	ALA	W408	I477	VAL	T610	V705
K2	S82		P238	GLY	A409	E478	TYR	A611	T706
F3		V155	F241	ALA	Q410	M479	LYS	B612	
E4	D93	A156	F241	ALA	Q411		ALA	V613	
V5	P94	H157	T242	ALA	S412		ILE	A614	
E6	SER	K158	I243	GLY	L413		SER	S615	
	GLU	L159	T244	ALA	L414		ALA	L616	
	LEU			ALA	S415		GLN	P617	
L9	ALA	L163	R247	MET	L416	P488	ALA	T621	V714
A10	ALA	D164		ILE	L417	V489	ASP	T622	
H11	LYS	S165	Q251	ASP	F418		LYS	Q719	
I12	ALA	I166	T252	ALA	E419	V493	GLN	S720	
L13	GLU	T167	R253	GLY	I420	A494	ASP	K624	
L14	GLU	M168	W254	ALA	I421	K495	ILE	T625	G726
T15	PRO	S169	G255	ALA	L328	P496	SER	V626	A727
L18	LYS	K170	P257	L329	E329	T497	SER	K728	K728
A19	ALA	T171		E330	E330	G498	SER	S628	G729
Y20	GLU			T332	M427	P499	THR	T629	S730
Q21	ALA	L175	R260	T332	V428	K500	ARG	T630	T731
F22	PRO	V176	G263	K333	D429	T501	VAL	P631	I733
A23	PRO	G178		H335	R430	A502	GLU		
S24	THR	K179	L266	K336	E431	I503	PHE	T634	F737
	PRO	S180	V267	K336	V432	D504	GLU	T635	N738
R27	PRO	T181	A268	L338	V433	K505	LYS	P636	Q739
K28	ALA	V182	L269	A339	S434	G507	LEU	L638	G740
I29	ALA	Q183		R340	E435	N508	TYR	H639	S741
T30	SER	N184	E272	Q341	I437	I509	ASP	K742	K742
Q32	PRO	E185	P273	Q342	M438		LEU	Q743	R641
D33	ALA	I186	R276	L343	I439	E513	MET	D744	
V34	PRO	L187		Q344	M440		LYS	T644	
F35	ALA		E280	V345	N441	R516	PHE	D648	E746
L36	ALA	L190		R348	R442	V519	LEU	W649	A747
K37	ALA	T196	F286		S443	S520	GLU	L748	L748
D38	ALA	T197		E370	D445	K521	SER	Y651	I749
F39	PRO	P198	M290		A446	I522	SER	E750	E750
	ALA		A291		L447	S523	LYS	F751	
R43	PRO	P201	Q292	A373	M451	V526	ILE	L655	L761
V44	VAL	E202	K293	Q374	Q452	Q527	ASP	S656	
E46	ALA	L206	Y294	D376	E453	E528	PRO	S657	D764
	ALA		A295	Y377	Y453	M529	SER	L658	
P49	ALA	L209	S296	L378	M457	A530	GLN	D661	D661
S50	PRO	F213	I297	N379	T458	A530	THR	E664	E664
P51	ALA	F217	V298	A380	D459	T536	GLN	K674	I774
L53	ALA	F217	V300	E381	E460	K537	LEU	D675	P775
	ALA	L221	L302	F386	T461	E538	ALA	E776	
M56	ALA		SER		K462	S539	GLY	L680	
A57	GLU				M465	Q540	GLY		
Q58		S225	SER	V390			ASP	E683	E782
R59	ALA		ALA	A391	L468		THR	H783	H783
T60	ALA	L228	ALA	T392	V469		ILE	I784	I784
L61	D142		SER		K470		GLU	Q689	Q689
	E143		ALA	R400			GLU	G695	G695
P144	V145	L232	SER	D403	G473		ASP	E788	E788
		T233	GLY		E474		LEU	Q698	Q698
S149	L149	S234	ALA	W406	Q475		THR	A791	A791
L78	L79	K236	GLY	N407	L476		ARG	H792	H792
C80									

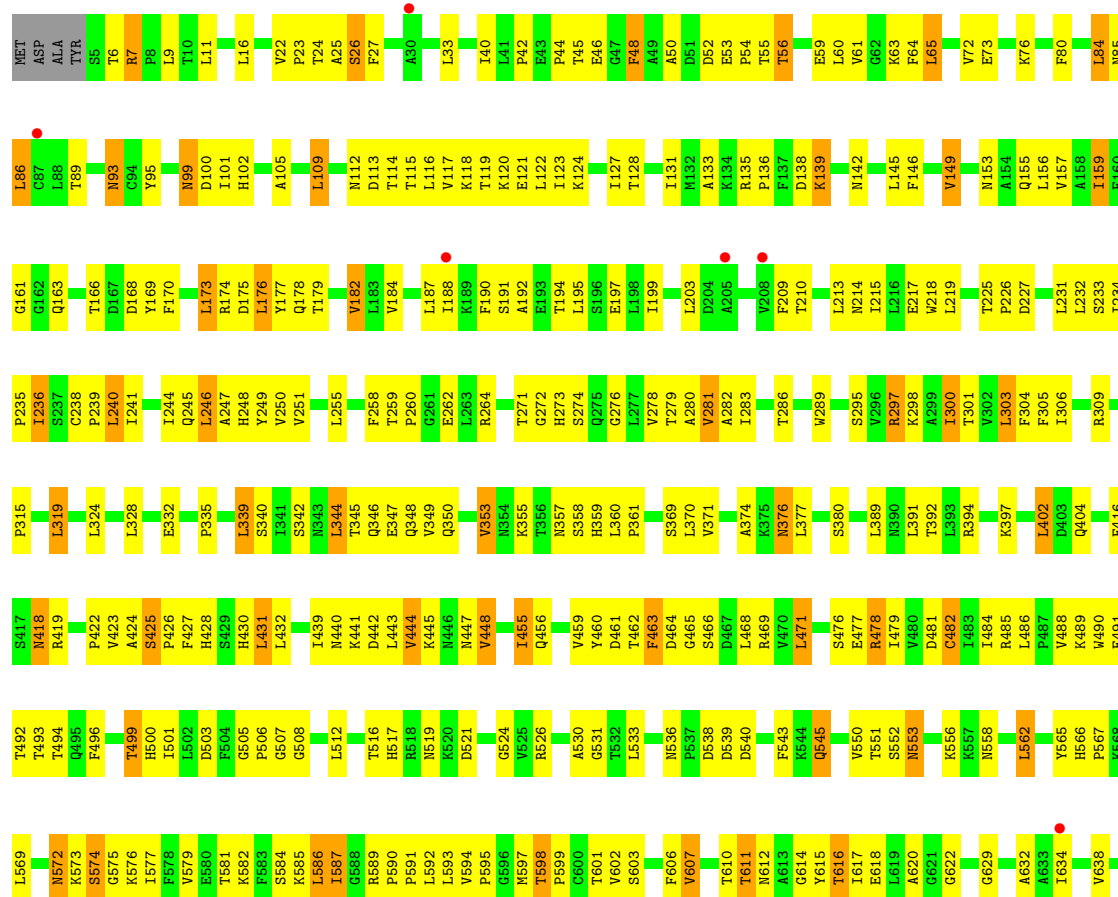
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F1103	P1108	V1109	A1101	V1102	G1103	S1104	G1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147							
K1031	D1032	L1040	E1041	A1042	V1043	V1044	G1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	V1058	A1059	A1060	Q1061	T1062	T1063	I1066	D1067	E1068	E1069	I1070	M1074	D1075	G1076	I1077	H1078	G1079	H1080	H1081	I1082	K1083	K1084	L1085	L1086	Y1090	G1091	D1092	D1093	K1096	P1097	P1098	A1099	V1101	Y1102					
D949	F950	R951	R952	R953	R954	E955	E956	R957	K960	S961	K962	R963	L964	S965	L966	I967	Q968	S969	Y970	S983	S984	S985	S986	S987	E992	Q993	Q994	L995	Q998	D999	I1000	H1001	H1002	F1003	L1004	S1005	M1006	P1010	M1011	Q1012	K1013	P1014	V1015	P1016	F1017	V1018	P1019	I1020	L1021	R1024	F1025	E1026	Y1027	G948		
W885	K886	E887	F888	D889	E890	T891	R892	R893	L894	K897	W898	R899	I892	S893	R894	D898	F899	Q900	K901	E902	A903	Y904	A905	T906	Y907	Q910	A911	R912	D913	S1005	T916	E921	M1011	L926	K1013	L929	V1015	P1016	F1017	N938	F939	T854	R885	T942	Y943	R944	T945	F946	T947	G948						
W785	S786	T787	F788	D789	E790	Y791	F792	P793	W794	F795	A796	D797	F798	F799	L800	R804	W805	K806	I807	D816	A817	Q818	L819	T813	D816	T748	P749	W750	L751	Q752	M753	Y754	I757	R758	F759	H760	P761	W762	I763	M764	L765	F766	F767	G768	T845	W846	E882	P883	I884	R885	K886	R887	A888	T889	R890	G948
V638	I641	G644	S645	G648	N650	L651	I652	Y653	V654	M658	L659	Q660	W661	E662	P663	P664	L665	K666	E667	E668	R670	Y674	P675	I676	Q677	F678	G682	A683	V690	E693	Y694	T697	L698	G699	Y702	L703	G704	L705	K706	P707	A712	I713	S714	Q715	W716	E784										
I570	K571	N572	K573	S574	T575	K576	I577	F578	E579	E580	T581	K582	F583	S584	K585	L586	I587	G588	R589	P590	P591	L592	L593	V594	P595	G596	K597	T598	P599	C600	T601	V602	S603	F606	V607	T610	T611	N612	A613	G614	Y615	T616	E617	E618	L619	A620	G621	G622	Y624	G629	M630	T631	A632	I634		
V488	K489	W490	E491	T492	T493	T494	Q495	F496	T499	H500	I501	L502	F503	F504	G505	P506	G507	G508	L512	G513	T515	H517	K520	D521	G522	R526	G531	L532	L533	D539	D540	F543	K544	Q545	V550	T551	S552	N553	K556	K557	N558	P559	N560	N561	L562	Y565	L569									
Q404	F416	R417	N418	M419	F420	L421	P422	V423	A424	S425	A426	F427	H428	S429	H430	N431	L432	T439	M440	E441	D442	L443	V444	K445	M446	N447	V448	L455	Q456	P458	V459	D461	T462	F463	D464	G465	S466	D467	L468	R469	V470	L471	S476	E477	R478	D481	C482	N483	I484	R485	L486	P487				
L234	P235	I236	G237	C238	P239	L240	L241	T244	Q245	L246	A247	H248	Y249	V251	L255	F258	T259	P260	G261	E262	L263	R264	A270	T271	P278	T279	A280	V281	A282	I283	T286	W289	S295	V296	R297	K298	A299	T301	L302	V302	L303	F304	F305	I306	R309											
F80	A158	I159	F160	G161	N85	L86	Q163	T166	D167	D168	Y169	F170	L173	R174	I175	L176	Y177	Q178	T179	Y180	H181	V182	G183	V184	L187	I188	K189	T271	P278	T279	A280	V281	A282	I283	T286	W289	S295	V296	R297	K298	A299	T301	L302	V302	L303	F304	F305	I306	R309							
L84	N85	L86	Q163	T166	D167	D168	Y169	F170	L173	R174	I175	L176	Y177	Q178	T179	Y180	H181	V182	G183	V184	L187	I188	K189	T271	P278	T279	A280	V281	A282	I283	T286	W289	S295	V296	R297	K298	A299	T301	L302	V302	L303	F304	F305	I306	R309											
F137	D138	K139	N142	L145	F146	V149	N153	A154	Q155	L156	S233																																													



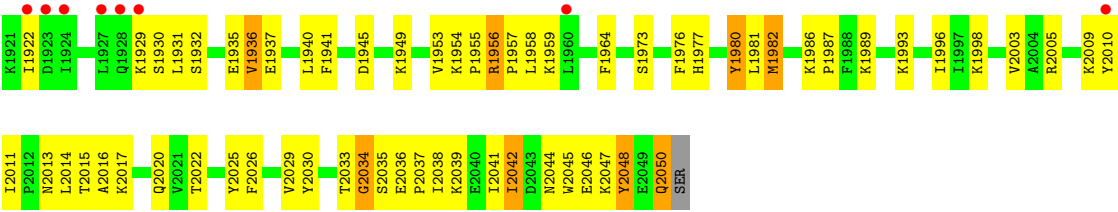




• Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA







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 , 85.5	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: CER, FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	9/12855 (0.1%)	0.61	8/17369 (0.0%)
1	B	0.44	3/12855 (0.0%)	0.62	9/17369 (0.1%)
1	C	0.48	8/12855 (0.1%)	0.61	7/17369 (0.0%)
2	G	0.42	11/16360 (0.1%)	0.58	7/22198 (0.0%)
2	H	0.55	13/16360 (0.1%)	0.61	9/22198 (0.0%)
2	I	0.42	8/16360 (0.0%)	0.59	12/22198 (0.1%)
All	All	0.47	52/87645 (0.1%)	0.60	52/118701 (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	3
2	I	0	1
All	All	0	5

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1657	ILE	C-N	-32.81	0.58	1.34
2	H	559	PRO	C-N	23.37	1.87	1.34
1	A	485	ASP	C-N	18.89	1.77	1.34
1	C	1430	ARG	C-N	-13.61	1.02	1.34
2	H	1422	THR	C-N	-13.47	1.03	1.34

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1657	ILE	O-C-N	-17.23	95.13	122.70
2	H	1657	ILE	CA-C-N	12.14	143.92	117.20
1	B	1116	PRO	O-C-N	-11.67	104.02	122.70
2	H	1657	ILE	C-N-CA	11.19	149.68	121.70
1	C	178	GLY	O-C-N	10.12	138.89	122.70

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	12589	601	1
1	B	12615	0	12591	582	6
1	C	12615	0	12587	588	0
2	G	15995	0	15975	998	10
2	H	15995	0	15974	997	7
2	I	15995	0	15976	977	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	7	0
4	H	31	0	19	6	0
4	I	31	0	19	8	0
All	All	85959	0	85779	4568	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 27.

The worst 5 of 4568 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	1.36
2:H:559:PRO:C	2:H:560:ASN:N	1.87	1.26
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	49
1	B	1604/1887 (85%)	1497 (93%)	94 (6%)	13 (1%)	16	53
1	C	1604/1887 (85%)	1499 (94%)	90 (6%)	15 (1%)	14	49
2	G	2029/2051 (99%)	1836 (90%)	167 (8%)	26 (1%)	10	42
2	H	2029/2051 (99%)	1836 (90%)	170 (8%)	23 (1%)	12	45
2	I	2029/2051 (99%)	1833 (90%)	171 (8%)	25 (1%)	11	43
All	All	10899/11814 (92%)	9999 (92%)	784 (7%)	116 (1%)	12	45

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%)	1224 (90%)	143 (10%)	5	22
1	B	1367/1566 (87%)	1225 (90%)	142 (10%)	5	22
1	C	1367/1566 (87%)	1227 (90%)	140 (10%)	6	23
2	G	1772/1789 (99%)	1567 (88%)	205 (12%)	4	19
2	H	1772/1789 (99%)	1566 (88%)	206 (12%)	4	19
2	I	1772/1789 (99%)	1562 (88%)	210 (12%)	4	19
All	All	9417/10065 (94%)	8371 (89%)	1046 (11%)	5	21

5 of 1046 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	767	PHE
2	I	993	GLN
2	I	762	ASN
2	I	2003	VAL
1	C	1283	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 288 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	1355	ASN
2	I	2013	ASN
2	H	1896	GLN
2	I	740	HIS

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Mol	Chain	Res	Type
1	B	1577	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	2748	1	10,11,15	4.19	3 (30%)	9,13,17	3.05	3 (33%)
4	FMN	H	3051	-	33,33,33	6.23	21 (63%)	48,50,50	1.31	8 (16%)
4	FMN	G	3051	-	33,33,33	6.32	21 (63%)	48,50,50	1.30	5 (10%)
3	CER	C	2748	1	10,11,15	4.21	3 (30%)	9,13,17	3.18	3 (33%)
4	FMN	I	3051	-	33,33,33	6.32	24 (72%)	48,50,50	1.30	7 (14%)
3	CER	A	2748	1	10,11,15	4.19	3 (30%)	9,13,17	3.18	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
3	CER	B	2748	1	-	5/12/12/16	-
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	C	2748	1	-	5/12/12/16	-
4	FMN	I	3051	-	-	5/18/18/18	0/3/3/3
3	CER	A	2748	1	-	5/12/12/16	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3051	FMN	C6-C7	12.51	1.57	1.39
4	G	3051	FMN	C9-C9A	12.29	1.59	1.39
4	I	3051	FMN	C6-C7	12.18	1.57	1.39
4	I	3051	FMN	C6-C5A	12.15	1.59	1.40
4	H	3051	FMN	C9-C9A	12.15	1.59	1.39

The worst 5 of 29 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
3	B	2748	CER	O1-C4-C5	-7.34	108.64	121.70
3	A	2748	CER	C5-C4-C3	-3.86	110.87	117.94
3	B	2748	CER	C5-C4-C3	-3.77	111.03	117.94

There are no chirality outliers.

5 of 30 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 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2748	CER	4	0

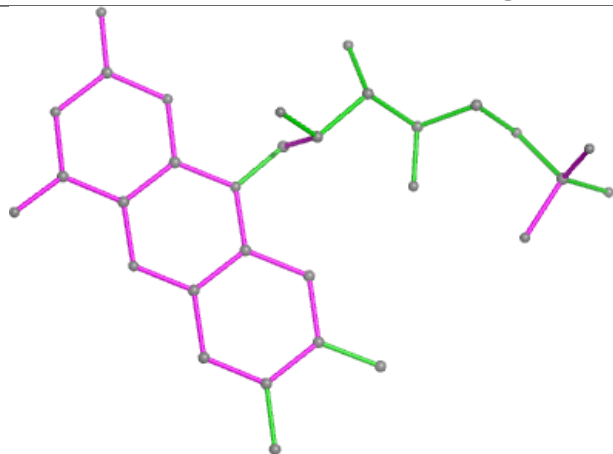
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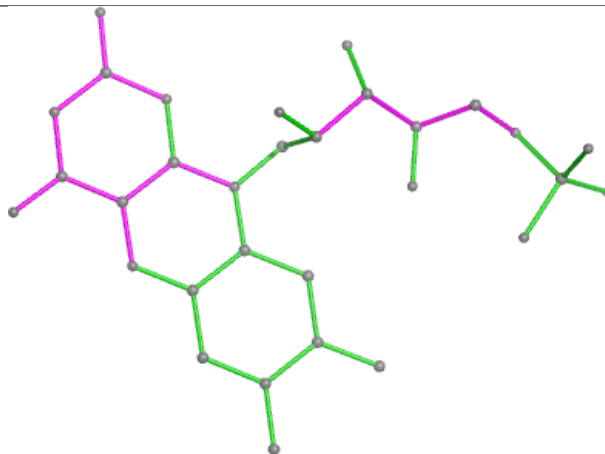
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	3051	FMN	6	0
4	G	3051	FMN	7	0
3	C	2748	CER	4	0
4	I	3051	FMN	8	0
3	A	2748	CER	3	0

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.

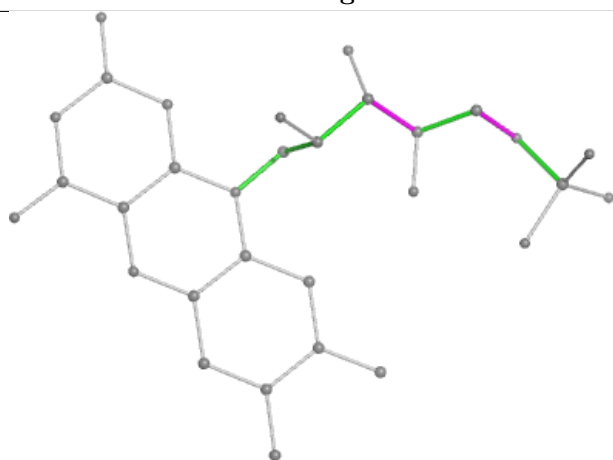
Ligand FMN H 3051



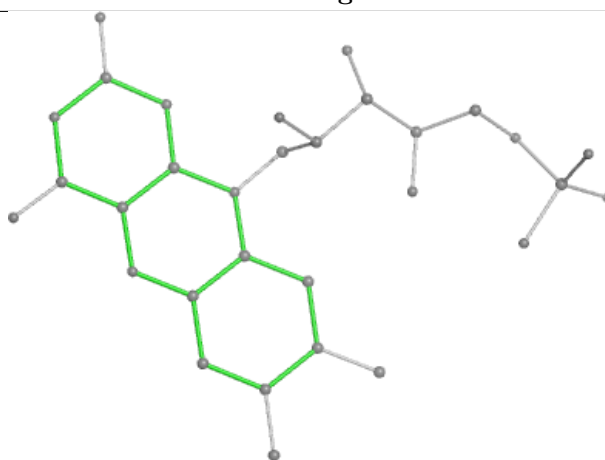
Bond lengths



Bond angles

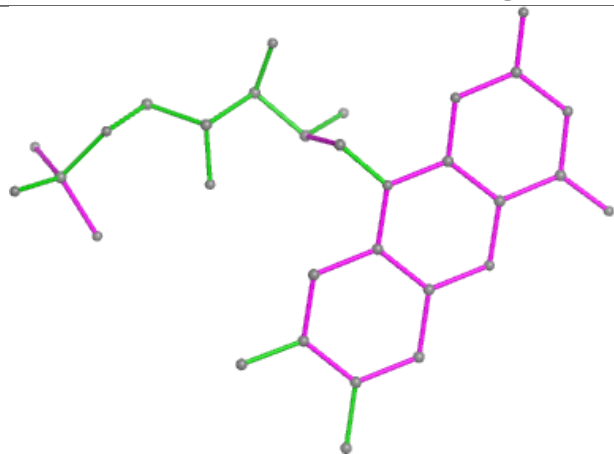


Torsions

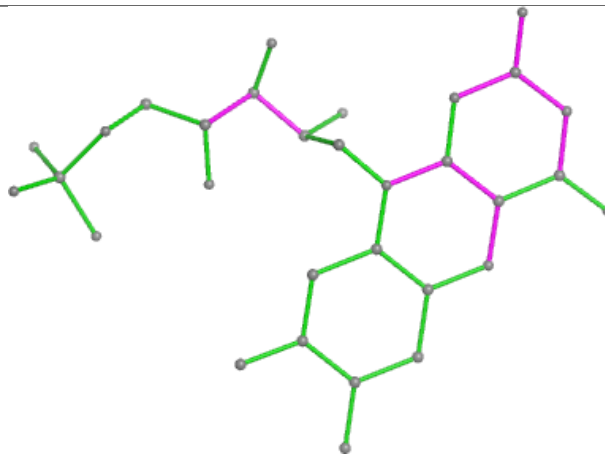


Rings

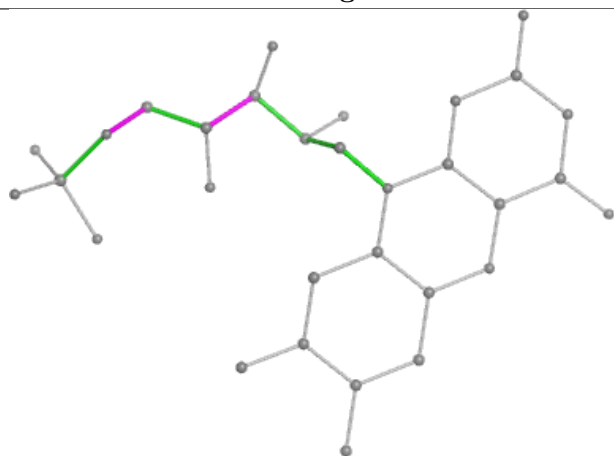
Ligand FMN G 3051



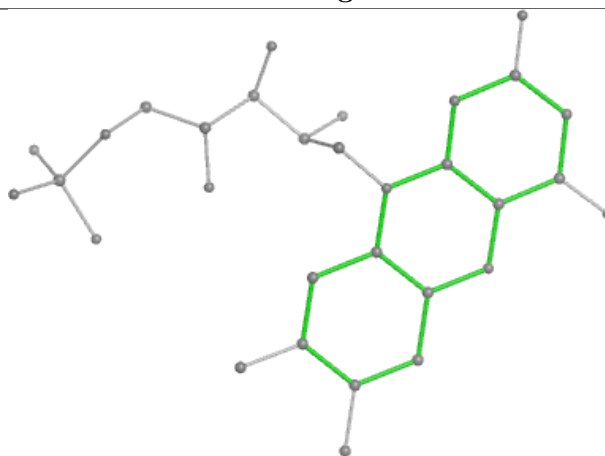
Bond lengths



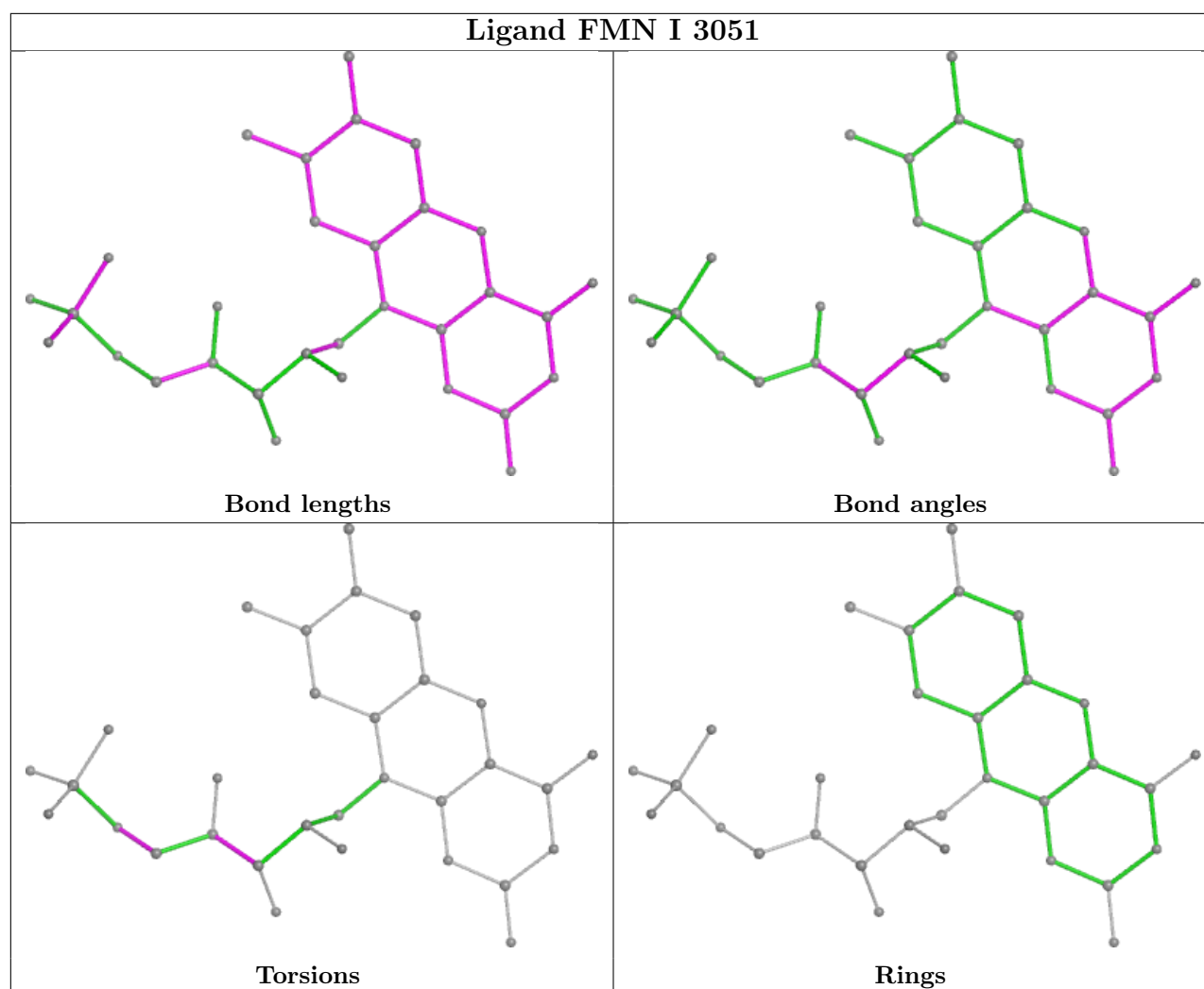
Bond angles



Torsions



Rings



5.7 Other polymers [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
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%)	-0.12	2 (0%) 92 89	98, 134, 233, 288	0
1	B	1614/1887 (85%)	-0.14	2 (0%) 92 89	99, 133, 233, 296	0
1	C	1614/1887 (85%)	-0.10	9 (0%) 85 73	100, 135, 233, 294	0
2	G	2033/2051 (99%)	-0.11	13 (0%) 85 73	134, 172, 221, 270	0
2	H	2033/2051 (99%)	-0.07	10 (0%) 87 76	133, 173, 218, 268	0
2	I	2033/2051 (99%)	-0.09	19 (0%) 81 67	134, 173, 218, 264	0
All	All	10941/11814 (92%)	-0.11	55 (0%) 87 76	98, 164, 226, 296	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	1924	ILE	7.5
2	H	2014	LEU	5.3
2	I	205	ALA	4.1
2	H	1924	ILE	3.7
2	I	87	CYS	3.3

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 monosaccharides in this entry.

6.4 Ligands [i](#)

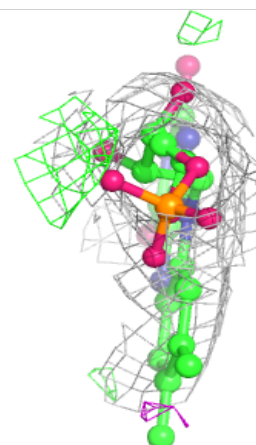
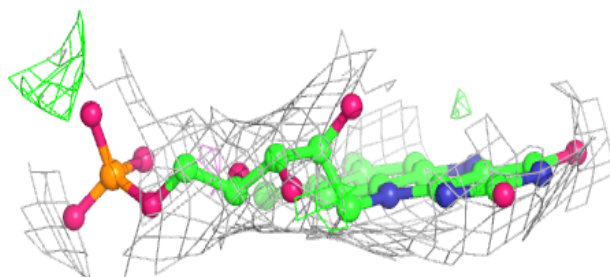
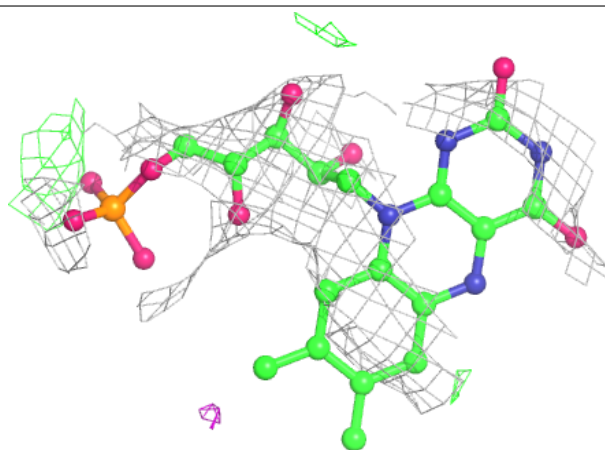
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^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.

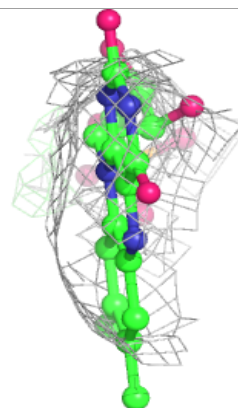
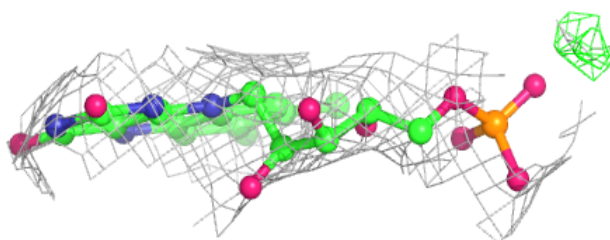
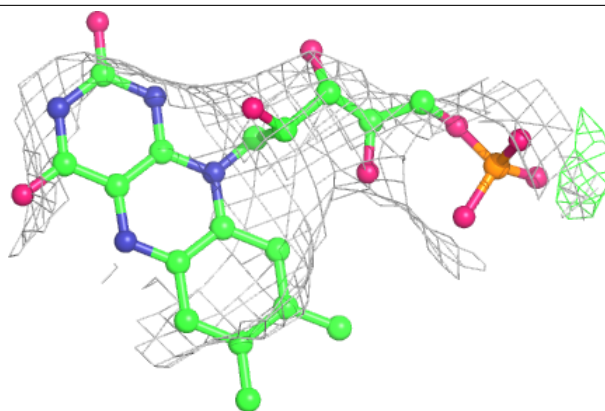
Electron density around FMN G 3051:

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

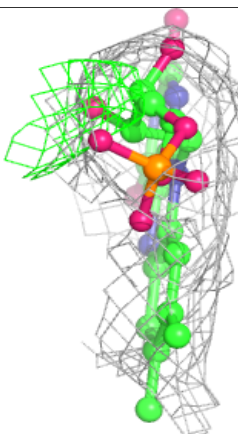
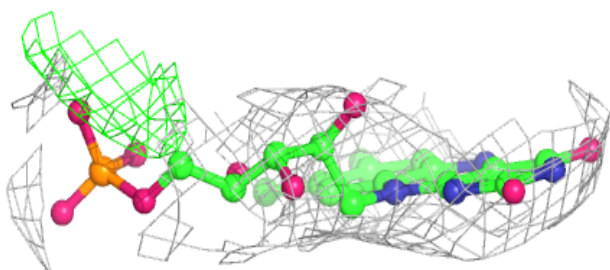
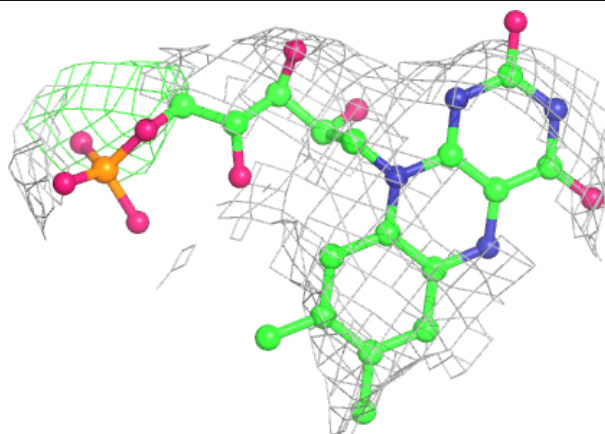


Electron density around FMN H 3051:

$2mF_o-DF_c$ (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.