



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:45 PM GMT

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 validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

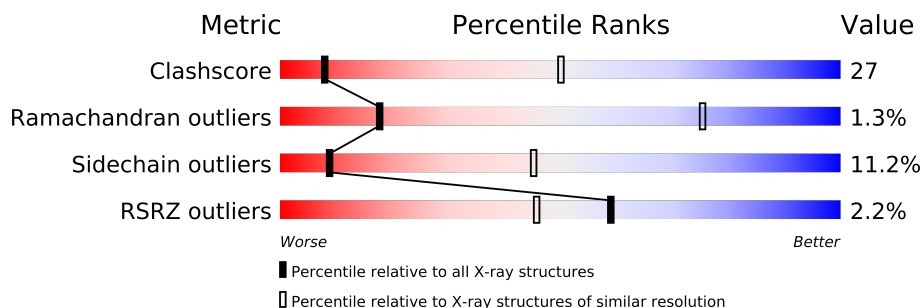
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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))
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1887	
1	B	1887	
1	C	1887	
2	G	2051	
2	H	2051	
2	I	2051	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CER	C	2748	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 88830 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

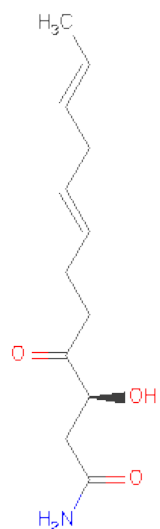
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

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.

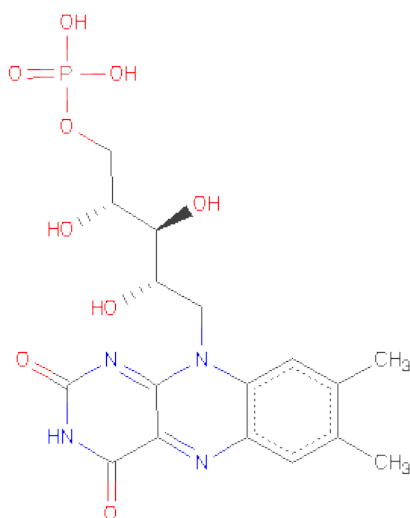
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	H	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	I	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			

- Molecule 3 is (2S, 3R)-3-HYDROXY-4-OXO-7,10-TRANS,TRANS-DODECADIENAMIDE (three-letter code: CER) (formula: 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: $C_{17}H_{21}N_4O_9P$).

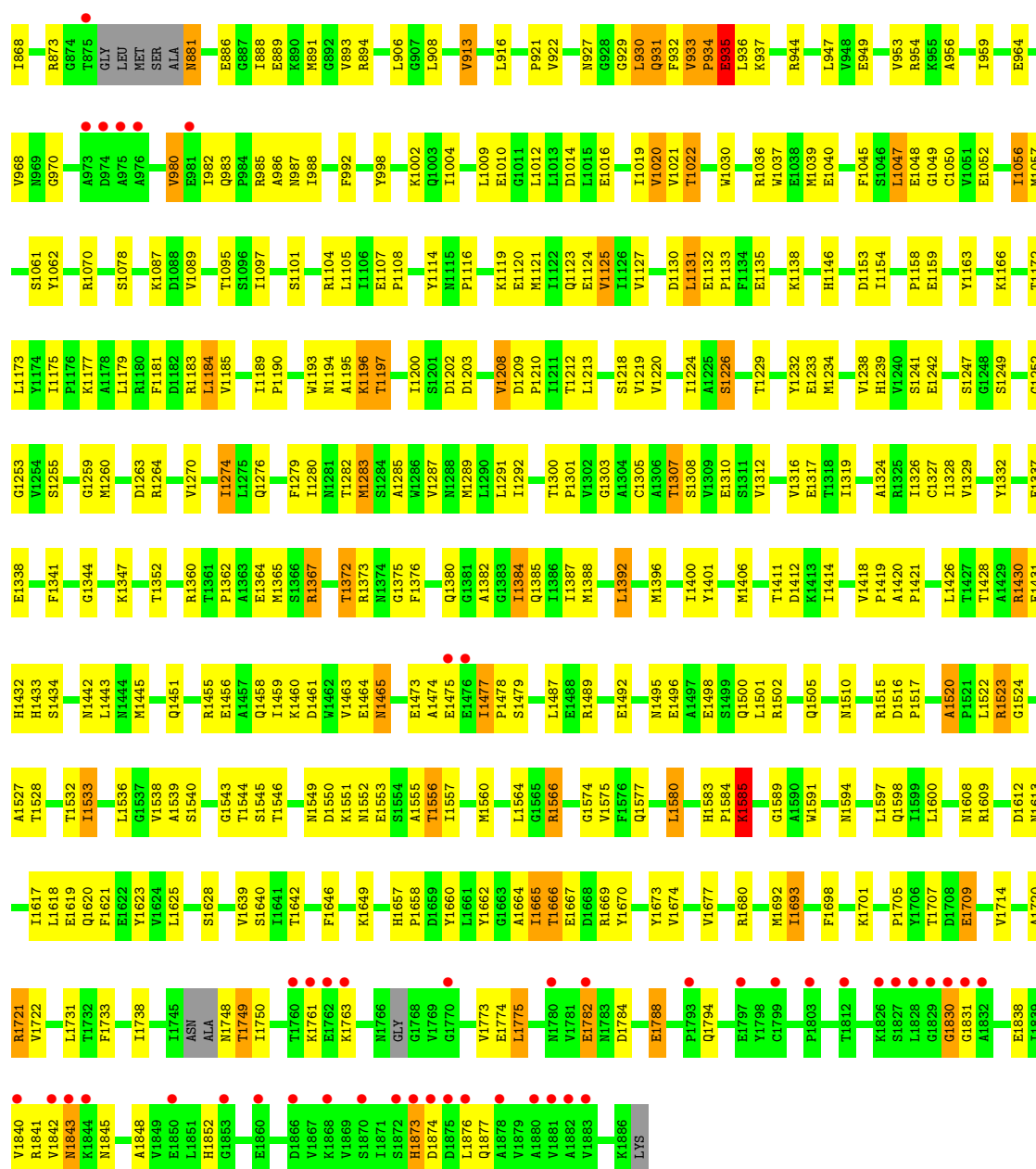


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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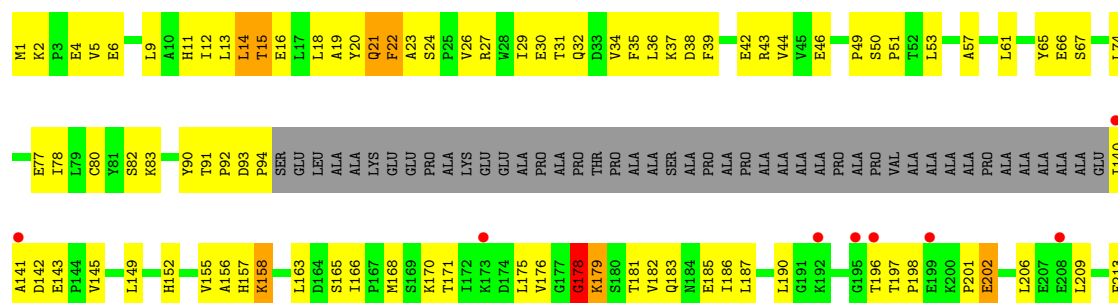
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

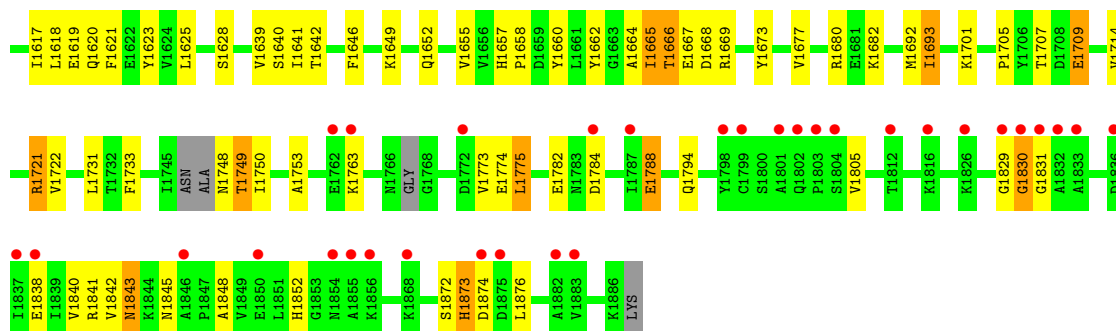


● Molecule 1: Fatty acid synthase subunit alpha

Chain B:

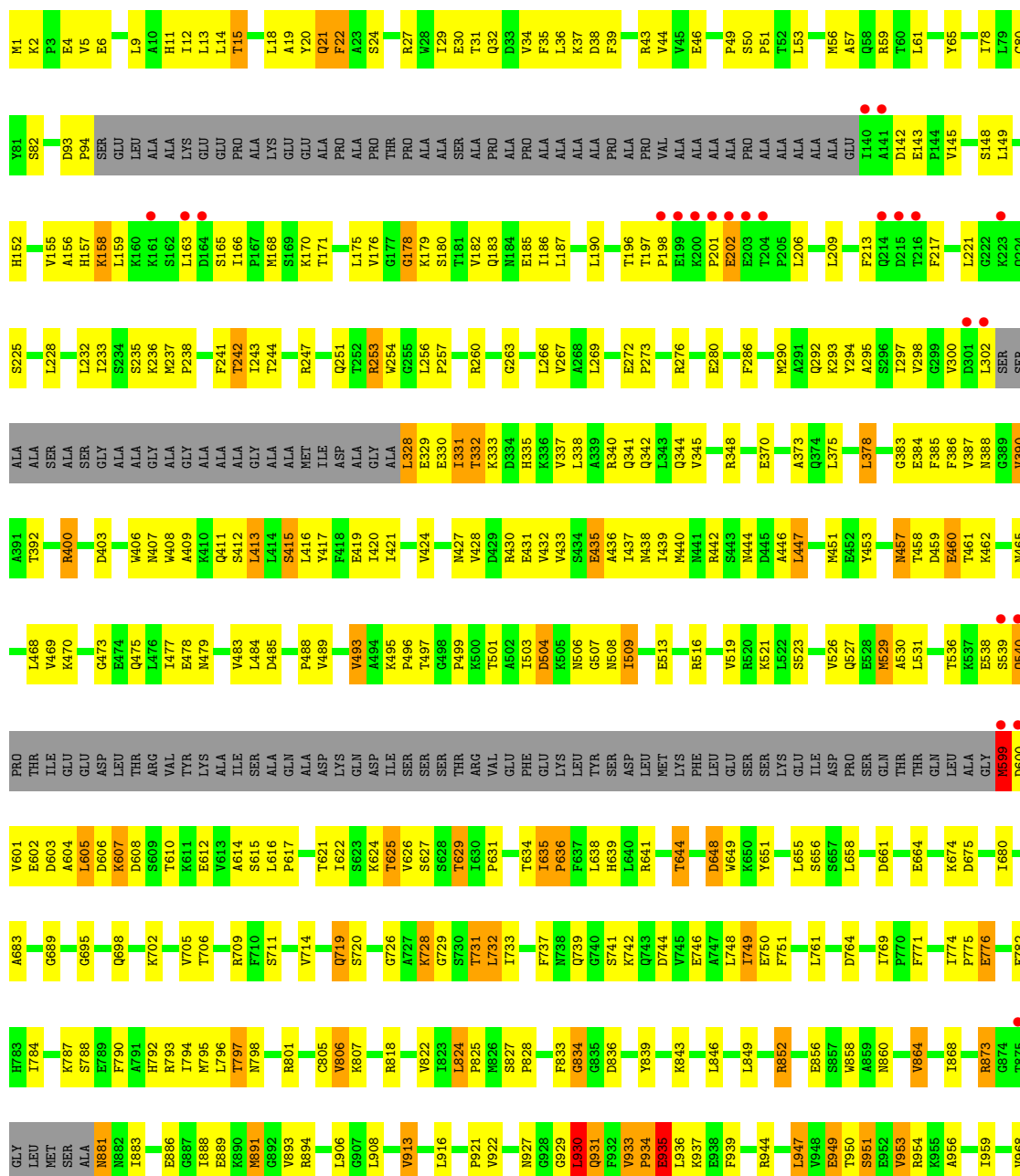


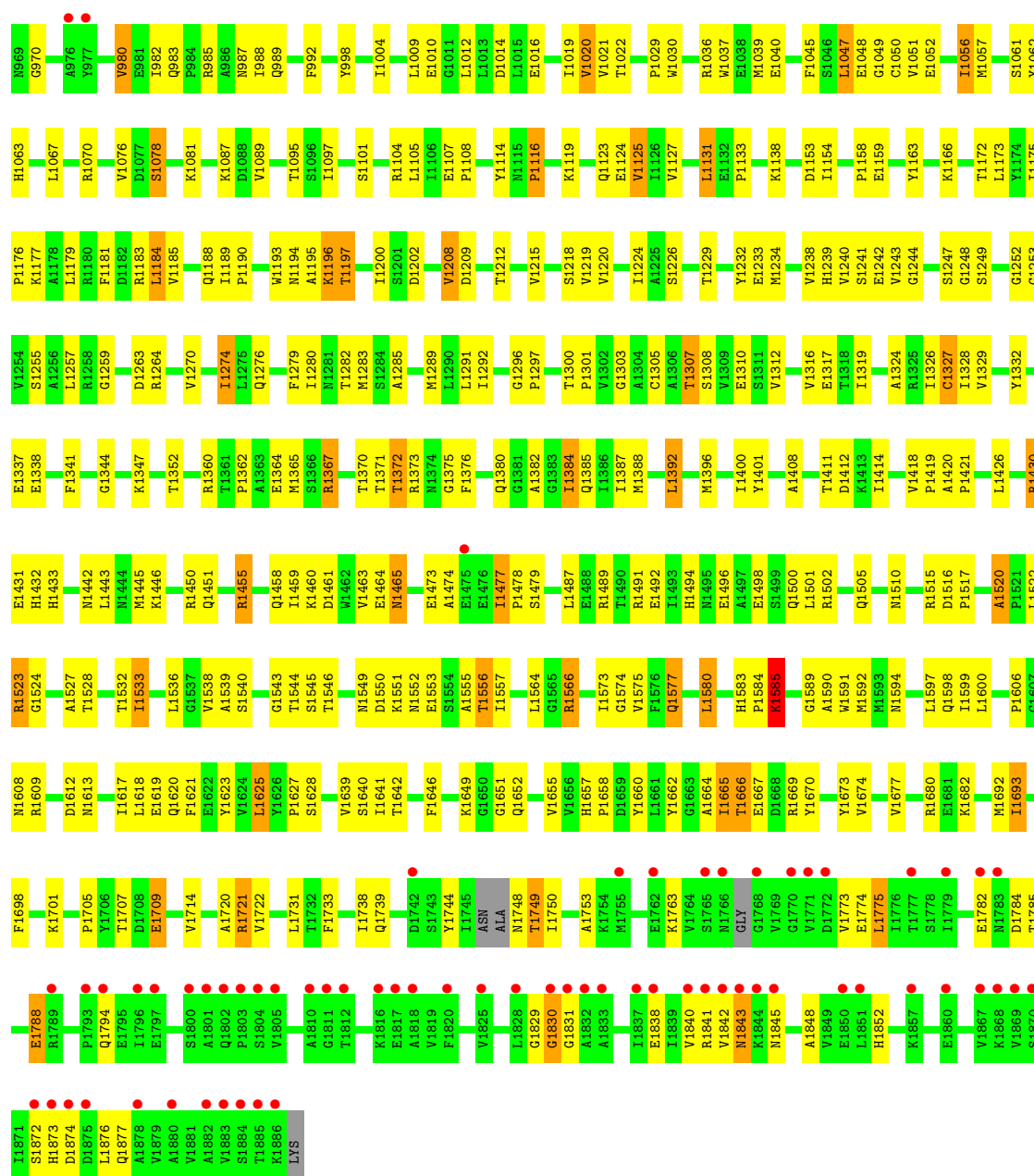
A1527	H1432	A1256	E964	V884	I774	G670	ASP	Q527	M451	E370	Q292	Q214
T1528	H1433	L1257	V968	T888	I774	K674	PRD	Q528	E452	A373	K293	D215
T1532	S1434	R1258	N969	T888	E776	D675	SER	M529	Y453	P775	Y294	D216
D1534	N1442	G1259	G970	R873	E776	D675	GLN	A530	H454	L375	F217	F217
V1538	M1445	D1263	A976	R874	E780	I680	THR	L531	L455	L378	I297	S218
A1539	K1446	R1264	A976	T875	L781	T681	THR	T536	S456	L378	Q219	Q219
S1540	K1448	V1270	A977	GLY	E782	G683	GLN	K537	M457	L378	A220	A220
G1543	K1449	I1274	V980	GLY	H783	A683	LEU	E538	F385	F385	G299	G299
Q1450	K1450	I1274	V980	GLY	H783	A683	ALA	E539	F386	F386	V300	V300
Q1451	Q1451	Q1276	V982	GLY	H783	A683	ALA	E539	F386	F386	L302	L302
R1455	R1455	F1279	V985	SER	I784	G689	GLY	Q540	E460	E460	SER	SER
E1456	E1456	I1280	R985	ALA	K787	G695	D600	PRD	T461	T461	L228	L228
N1549	Q1457	N1281	V988	ALA	S788	G695	V601	THR	K462	K462	ALA	ALA
D1550	Q1458	D1088	V988	R881	E789	G695	E602	THR	M485	M485	L232	L232
K1551	I1459	V1089	Q989	R882	E789	G695	D603	THR	T392	T392	L233	L233
N1552	K1460	T1089	Q989	R883	E789	G695	A604	THR	T392	T392	ALA	ALA
E1553	K1461	T1089	Q989	R883	E789	G695	A604	THR	T392	T392	S234	S234
S1554	V1462	S1096	V992	R883	E789	G695	D606	THR	T392	T392	S235	S235
V1463	V1463	I1097	V998	R883	E789	G695	D606	THR	T392	T392	GLY	GLY
A1555	V1463	I1097	V998	R883	E789	G695	D606	THR	T392	T392	K236	K236
T1556	E1464	S1101	V998	R883	E789	G695	D606	THR	T392	T392	M237	M237
I1557	N1465	D1202	I1004	R883	E789	G695	D606	THR	T392	T392	P238	P238
L1564	E1473	V1208	L1009	L906	R801	V714	S615	THR	T392	T392	F241	F241
G1565	G1565	D1209	E1010	L906	R801	V714	S615	THR	T392	T392	T242	T242
R1566	A1474	D1209	E1010	L906	R801	V714	S615	THR	T392	T392	A243	A243
G1574	I1477	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
V1575	P1478	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
F1576	S1479	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
Q1577	A1480	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
L1580	E1492	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
T1581	E1496	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
G1582	E1497	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
H1583	E1498	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
P1584	S1499	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
K1585	Q1500	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
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W1591	Q1505	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
M1592	W1508	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
M1593	G1509	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
N1594	G1509	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
G1595	N1510	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
A1596	R1515	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
L1597	D1516	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
Q1598	P1517	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
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L1597	P1517	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
Q1598	P1517	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
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L1597	P1517	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
Q1598	P1517	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
I1599	P1517	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
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A1596	P1517	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
L1597	P1517	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
Q1598	P1517	T1212	G1011	V913	R818	G726	G624	THR	T392	T392	ALA	ALA
I1599	P1517	T1212	G1011	V913	R818	G726	G624	THR</				



● Molecule 1: Fatty acid synthase subunit alpha

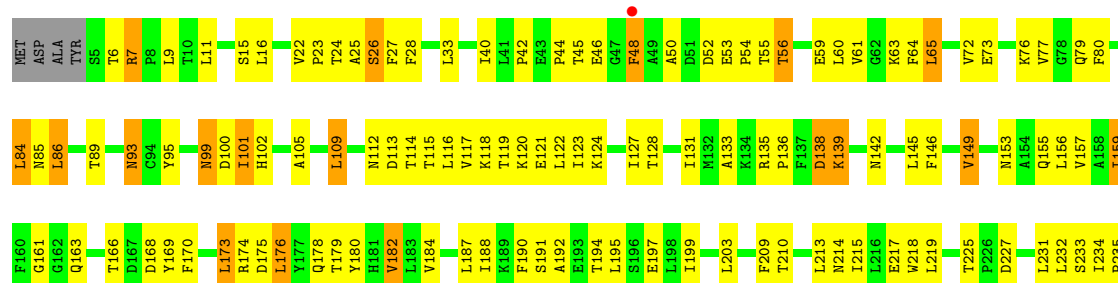
Chain C:



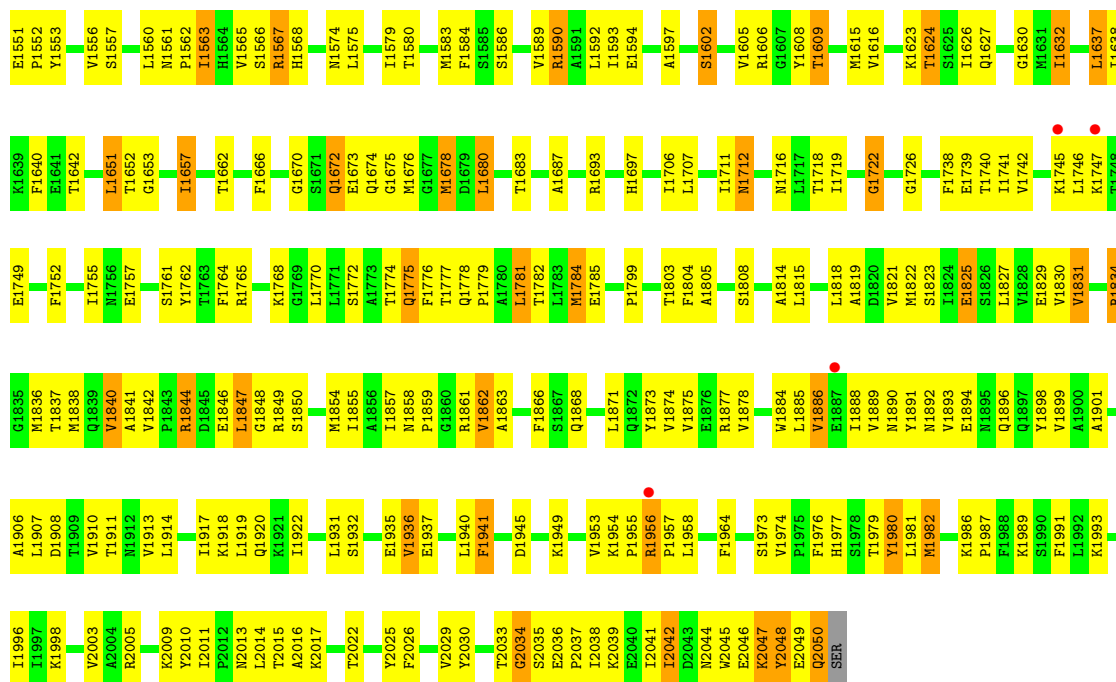


• Molecule 2: Fatty acid synthase subunit beta

Chain G:





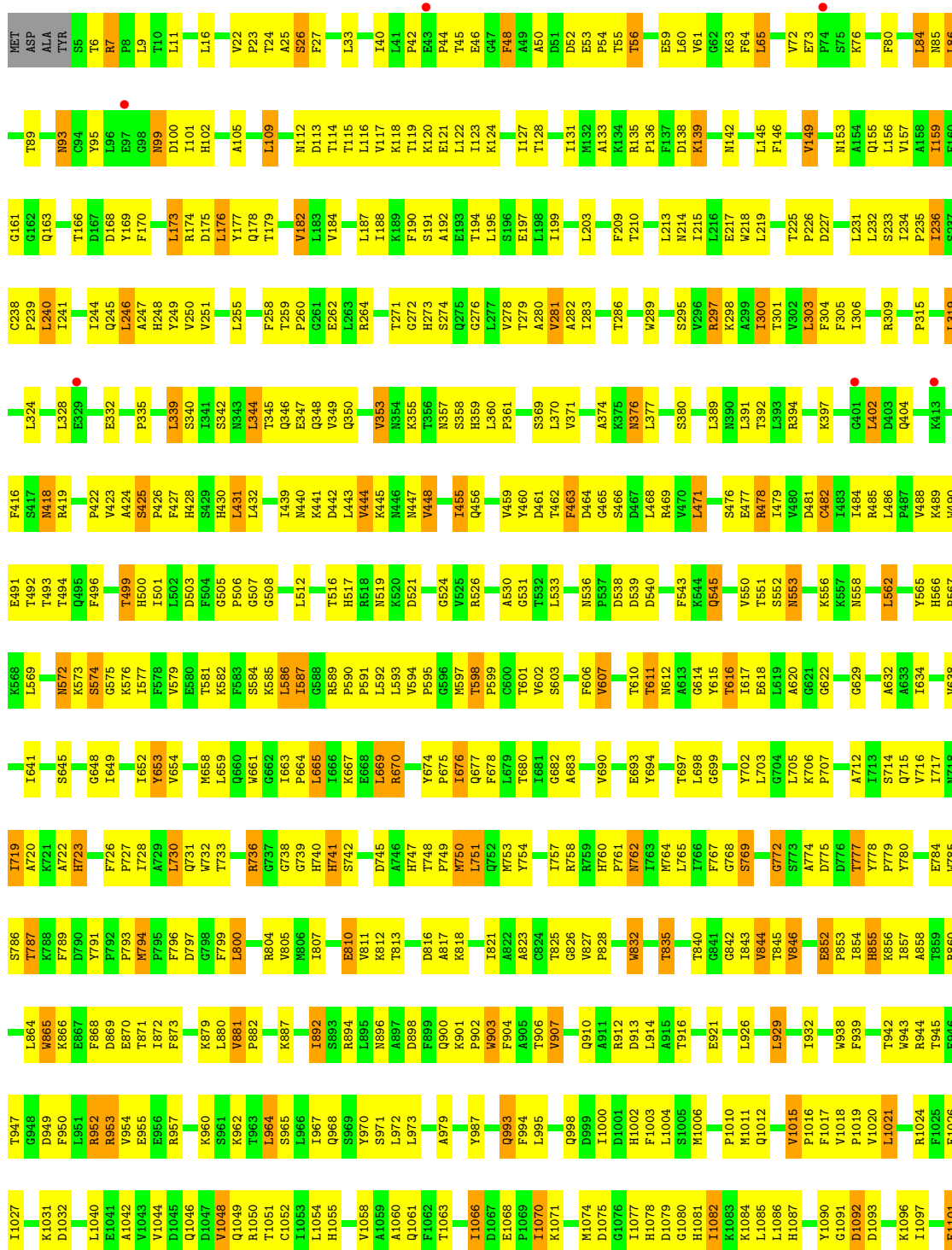


D1908	E1829	T1740	M1550	M1359	E1273	V1194	P1108	K1031	T942	K856	L781	Q715
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T1911	V1831	F1640	P1552	V1368	F1275	T1196	ASP		R944	T859	W785	I718
N1913	R1834	E1641	S1557	T1374	F1279	L1197	GLM	E1040	F946	R860	T787	A720
L1914	G1835	T1642	S1557	V1377	D1280	S1198	GLM	E1041	T947	K865	F788	K721
T1917	M1851	L1651	L1560	V1378	V1284	L1205	GLM	V1043	G948	K866	D790	A722
K1918	T1652	T1652	N1561	I1378	I1292	K1206	GLM	V1044	D949	E967	D790	H723
L1919	G1653	F1457	P1562	V1381	I1293	K1206	ASP	V1044	VAL	F868	F791	F726
Q1920	I1657	T1470	H1563	V1382	T1293	I1210	ASP	Q1046	F950	D869	P792	F726
K1921	E1658	T1470	H1564	N1383	A1294	L1211	ASP	Q1046	L951	F950	P792	P727
T1922	Q1659	V1472	S1566	V1383	K1285	K1212	ASP	Q1047	R952	F870	P793	L728
E1926	P1660	T1473	H1567	G1387	E1296	K1213	ASP	Q1048	R953	T871	M794	L728
L1927	T1661	F1474	H1568	K1388	E1296	L1214	ASP	Q1049	V954	I872	F795	A729
Q1928	T1662	K1475	H1568	V1389	F1300	L1214	ASP	Q1050	E955	F873	F796	L730
K1929	F1666	S1481	M1574	V1390	A1303	I1219	D1123	T1051	E956	K879	T797	Q731
L1931	G1670	S1482	L1575	L1396	A1303	Q1220	K1128	C1052	K960	L880	F799	W732
E1935	S1671	T1483	T1579	S1397	C1308	M1221	A1129	I1053	L964	V881	L800	T733
V1936	Q1672	F1486	T1580	V1403	E1309	M1223	T1130	V1058	I967	K887	R804	R736
E1937	Q1674	V1491	M1583	M1404	D1310	M1223	T1133	A1059	Y970	R888	M806	G739
R1861	G1675	E1492	S1585	T1407	F1311	R1227	D1134	Q1061	S971	K894	I807	H741
V1862	M1676	E1493	S1586	S1408	S1313	T1228	E1135	F1062	L972	S893		S742
A1863	G1677	L1493	S1586	S1408	R1314	G1231	W1138	T1063	L973	R894	B810	D745
F1866	M1678	T1495	R1589	F1410	T1318	V1233	S1145	I066	Y987	L895	K812	A746
S1867	Q1679	E1497	R1590	F1411	M1319	P1234	E1146	E1067		N896	T813	H747
Q1868	L1680	T1498	A1591	G1414	L1320	S1235	I1147	P1069	Q993	D898	D816	T748
K1949	T1683	E1500	L1592	G1414	A1321	L1236	M1148	P1069	F994	F899	K817	P749
V1953	L1781	E1501	E1594	Y1416	P1322	L1238	W1149	K1071	L995	Q900	K818	M750
K1954	T1782	G1502	E1594	Y1416	F1325	N1241	R1150	M1074	Q998	K901		L751
P1955	L1783	G1503	E1594	D1418	I1327	F1242	H1151	D1075	D999	P902	I821	W753
R1956	M1784	I1503	A1597	F1419	V1328	N1243	A1152	G1076	I1000	F904	A823	Y754
P1957	P1779	D1505	S1602	E1420	V1329	P1244	I1159	I1077	D1001	A905	C824	I757
L1958	H1697	Y1506	V1605	T1422	G1330	G1247	T1160	H1078	H1002	T906	T825	R758
K1959	L1707	A1510	V1605	K1425	W1331	G1247	Q1161	G1080	L1162	V907	V826	R759
F1964	M1712	S1511	T1609	T1426	I1335	S1252	K1163	H1081	S1005	Q910	P828	H760
S1973	P1714	P1515	M1615	V1427	I1338	E1256	V1166	I082	M1006	A911	W832	P761
F1976	V1715	V1616	V1616	V1427	F1339	D1257	S1167	K1084	P1010	R912	E833	L763
H1977	L1717	E1528	T1624	E1428	P1340	R1258	N1168	L1085	M1011	D913	Q834	L765
Y1980	L1718	Q1529	K1623	Y1431	V1343	N1259	I1170	L1086	Q1012	T916	T835	I766
L1981	L1719	L1626	S1625	H1434	D1344	Q1260	R1172	Y1090	P1015	E921	Y836	F767
M1982	G1722	Q1627	L1626	K1436	L1347	R1261	V1173	D1093	F1017	L926	P839	S769
Q1896	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772
Q1897	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772
V1888	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772
V1889	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772
V1890	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772
M1992	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772
K1996	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772
V1997	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772
F1998	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772
K1999	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772
L1993	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772
K1993	G1726	G1630	G1630	K1436	L1347	E1264	F1174	D1093	P1016	L926	T840	G772



• Molecule 2: Fatty acid synthase subunit beta

Chain I:



Q2020	Y1102	V1194	H1270	N1355	L1452	Y1553	F1640	K1747	L1847	K1929	Q2020
Y2021	F1103	V1196	I1271	G1356	L1452	V1556	E1641	K1747	G1848	S1930	Y2021
T2022	P1108	T1196	D1272	K1358	F1457	L1560	T1642	F1752	R1849	L1931	T2022
Y2025	V1109	L1197	E1273	M1359	D1458	L1561	L1661	E1757	S1850	S1932	Y2025
T2026	ASP	E1199	P1274	I1360	L1459	P1562	T1652	S1761	M1854	E1935	T2026
Y2029	VAL	L1205	F1275	V1368	K1462	I1563	G1653	S1761	I1855	V1936	Y2029
Y2030	GLN	K1206	F1279	T1374	T1463	H1564	T1657	F1764	P1859	E1937	Y2030
T2033	SER	L1210	R1282	T1374	T1463	V1565	H1564	R1765	G1860	L1940	T2033
G2034	GLN	I1211	D1283	V1377	T1468	S1566	T1662	R1765	R1861	F1941	G2034
S2035	VAL	K1212	V1284	I1378	E1469	R1567	F1666	L1770	V1862	D1945	S2035
E2036	ASP	L1213	L1292	L1378	E1471	H1568	F1666	T1774	F1866	K1949	E2036
P2037	SER	L1214	T1293	V1381	V1472	M1574	G1670	Q1775	S1967	K1949	P2037
K2038	SER	K1215	E1296	V1382	T1473	L1575	S1671	F1776	Q1868	F1941	K2038
E2040	SER	N1216	L1296	V1389	F1474	I1579	E1672	Q1777	L1871	V1953	E2040
I2041	VAL	N1217	F1300	I1389	K1475	T1580	E1673	Q1778	P1872	K1954	I2041
T2042	GLU	I1219	F1300	V1390	S1481	T1583	G1674	P1779	A1780	P1955	T2042
P2043	D1123	Q1220	A1303	L1396	S1482	F1584	G1675	A1780	L1781	R1956	P2043
N2044	S1124	E1222	C1308	S1397	V1483	F1585	M1676	T1782	V1874	P1957	N2044
W2045	A1129	M1221	E1309	F1403	F1486	S1586	G1677	L1783	R1877	K1958	W2045
E2046	T1130	M1223	D1310	M1404	F1486	S1586	E1678	M1784	V1878	L1959	E2046
K2047	T1133	M1223	F1311	V1405	V1491	V1589	L1680	E1785	G1879	F1964	K2047
Y2048	D1134	R1227	V1312	E1406	E1492	R1590	T1683	P1799	K1880	S1973	Y2048
E2049	E1135	T1228	G1313	T1407	E1492	A1591	S1684	T1803	V1886	F1976	E2049
Q2050	W1138	G1231	R1314	S1408	P1494	L1592	A1687	F1804	I1888	H1977	Q2050
SER	S1145	P1233	T1318	S1409	T1495	I1593	Q1688	A1805	V1889	K1980	SER
		V1234	H1319	F1410	K1496	E1594			N1890	L1981	
	M1148	S1236	L1320	F1411	V1499	A1597	R1693	S1808	T1891	M1982	
	W1149	A1321	L1320	T1417	E1500	D1599	H1697	A1814	V1893	K1986	
	H1151	P1237	P1322	D1418	G1502	S1602	L1707	L1815	Q1896	P1987	
		L1238	F1325	F1419	I1503				G1897	F1988	
	T1159	Y1240	A1326	E1420	V1504	V1605	M1712	L1818	Y1898	K1989	
	T1160	N1241	I1327	N1421	A1510	R1606	D1820	A1819	V1899		
	Q1161	F1242	V1329	F1423	S1511	G1607	N1716	M1821	M1900	K1993	
	D1162	M1244	G1330	F1427	H1512	Y1608	L1717	M1822	A1901		
	K1163	P1244	W1331	V1428	G1513	T1609	T1718	S1823		T1996	
					P1514		L1719		A1906	I1997	
	V1166	G1247		E1428	P1515	M1615			L1907	K1998	
	S1167		I1335	Y1431	T1526	V1616	G1722	E1825	D1908		
	M1168	S1262	I1338	Q1432	T1526	V1616		S1826	L1827	V2003	
	P1169	E1266	F1339	H1433	L1527	K1623	G1726	V1828	V1829	A2004	
	I1170	D1257	P1340	H1434	E1528	T1624	A1735	V1830	E1829	B2005	
	R1171	R1258	K1343	I1435	L1533	S1625	H1736	V1831	V1913	K2009	
	K1172	N1259	V1343	K1436	D1543	I1626	L1737	R1834	L1914	Y2010	
	V1173	Q1260	D1344	S1438	D1543	Q1627	F1738	G1835	I1917	T2011	
	F1174	I1262	L1347	I1441	P1547	G1630	E1739	M1836	K1918	P2012	
	K1175	K1263	L1348	A1442	S1548	M1631	T1740	T1837	L1919	N2013	
	P1176	K1264	K1349	V1443	T1549	I1632	L1741		L1920	L2014	
	S1177	M1265	L1350	V1443	M1550	L1637	V1742		K1921	T2015	
	M1180	Y1266	H1352	R1444	E1551	I1638	K1745	R1844	I1922	A2016	
		T1189	L1269	S1446	P1552	K1639	L1746	E1846	Q1928	K2017	

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.94Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.266 , 0.267 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	130.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 69.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 168120 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	88830	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

The worst 5 of 4773 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	18	75
1	B	1736/1887 (92%)	1619 (93%)	100 (6%)	17 (1%)	22	80
1	C	1736/1887 (92%)	1618 (93%)	96 (6%)	22 (1%)	18	75
2	G	2029/2051 (99%)	1825 (90%)	173 (8%)	31 (2%)	15	73
2	H	2029/2051 (99%)	1826 (90%)	173 (8%)	30 (2%)	15	73
2	I	2029/2051 (99%)	1829 (90%)	174 (9%)	26 (1%)	18	75
All	All	11295/11814 (96%)	10331 (92%)	816 (7%)	148 (1%)	18	75

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	PRO
1	A	504	ASP
1	A	538	GLU

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Mol	Chain	Res	Type
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%)	10	49
1	B	1460/1566 (93%)	1312 (90%)	148 (10%)	11	51
1	C	1460/1566 (93%)	1310 (90%)	150 (10%)	10	50
2	G	1772/1789 (99%)	1563 (88%)	209 (12%)	8	42
2	H	1772/1789 (99%)	1560 (88%)	212 (12%)	7	41
2	I	1772/1789 (99%)	1561 (88%)	211 (12%)	8	42
All	All	9696/10065 (96%)	8614 (89%)	1082 (11%)	9	45

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
1	C	1542	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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$
3	CER	A	2748	-	10,11,15	4.08	3 (30%)	12,13,17	3.10	5 (41%)
3	CER	B	2748	-	10,11,15	4.07	3 (30%)	12,13,17	2.99	5 (41%)
3	CER	C	2748	-	10,11,15	4.10	3 (30%)	12,13,17	3.09	5 (41%)
4	FMN	G	3051	-	33,33,33	6.19	21 (63%)	46,50,50	1.45	7 (15%)
4	FMN	H	3051	-	33,33,33	6.13	21 (63%)	46,50,50	1.45	8 (17%)
4	FMN	I	3051	-	33,33,33	6.16	22 (66%)	46,50,50	1.42	8 (17%)

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	-	-	0/12/12/16	0/0/0/0
3	CER	B	2748	-	-	0/12/12/16	0/0/0/0
3	CER	C	2748	-	-	0/12/12/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	G	3051	-	-	0/18/18/18	0/0/3/3
4	FMN	H	3051	-	-	0/18/18/18	0/0/3/3
4	FMN	I	3051	-	-	0/18/18/18	0/0/3/3

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3051	FMN	C6-C5A	14.48	1.59	1.41
4	G	3051	FMN	C6-C5A	14.11	1.58	1.41
4	H	3051	FMN	C6-C5A	13.85	1.58	1.41
3	C	2748	CER	O1-C4	11.36	1.41	1.21
3	A	2748	CER	O1-C4	11.34	1.41	1.21

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2748	CER	O1-C4-C3	-6.52	108.66	120.73
3	C	2748	CER	O1-C4-C3	-6.51	108.69	120.73
3	C	2748	CER	O1-C4-C5	-6.37	107.97	121.53
3	A	2748	CER	O1-C4-C5	-6.33	108.06	121.53
3	B	2748	CER	O1-C4-C3	-6.31	109.06	120.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	1750/1887 (92%)	0.12	59 (3%) 43 35	95, 134, 347, 457	0
1	B	1750/1887 (92%)	0.10	59 (3%) 43 35	96, 133, 302, 419	0
1	C	1750/1887 (92%)	0.17	90 (5%) 27 24	98, 135, 423, 568	0
2	G	2033/2051 (99%)	-0.01	11 (0%) 88 78	131, 169, 218, 267	0
2	H	2033/2051 (99%)	0.09	21 (1%) 79 65	130, 170, 215, 265	0
2	I	2033/2051 (99%)	0.02	11 (0%) 88 78	131, 171, 215, 261	0
All	All	11349/11814 (96%)	0.08	251 (2%) 59 46	95, 162, 239, 568	0

The worst 5 of 251 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1882	ALA	9.5
1	C	1838	GLU	8.1
1	C	1831	GLY	7.9
1	C	1832	ALA	7.5
1	C	1850	GLU	7.5

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CER	C	2748	12/16	0.33	2.30	67,131,249,250	0
3	CER	A	2748	12/16	0.28	1.63	67,131,240,249	0
4	FMN	I	3051	31/31	0.26	-0.07	129,161,178,201	0
4	FMN	H	3051	31/31	0.28	-0.20	131,157,181,186	0
4	FMN	G	3051	31/31	0.25	-0.31	135,158,184,203	0
3	CER	B	2748	12/16	0.20	-0.36	67,131,249,250	0

6.5 Other polymers

There are no such residues in this entry.