



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 10:06 PM UTC

PDB ID : 2PFF / pdb\_00002pff  
Title : Structural Insights of Yeast Fatty Acid Synthase  
Authors : Xiong, Y.; Lomakin, I.B.; Steitz, T.A.  
Deposited on : 2007-04-04  
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
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

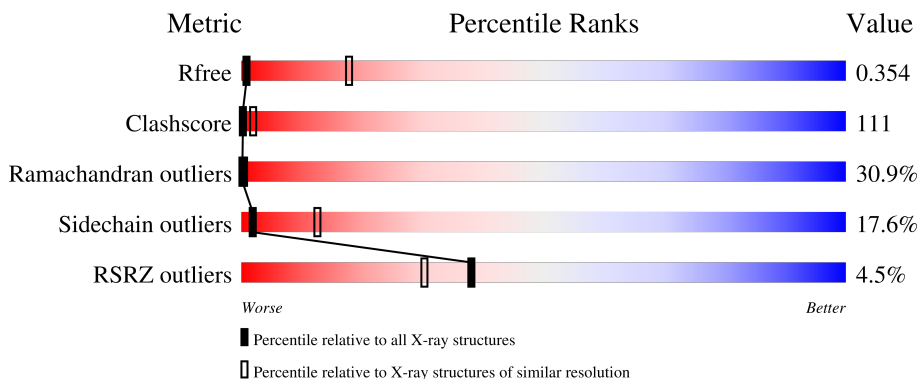
# 1 Overall quality at a glance

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.



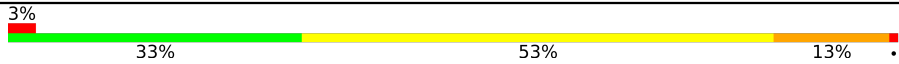

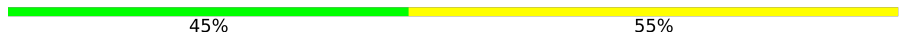

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1688	
1	D	1688	
1	G	1688	
2	B	2006	
2	E	2006	

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Mol	Chain	Length	Quality of chain
2	H	2006	 3% 33% 53% 13%
3	C	65	 46% 54%
3	F	65	 45% 55%
3	I	65	 42% 58%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 71862 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
			Total	C	N	O	S			
1	A	1683	11319	7070	2007	2205	37	0	0	0
1	D	1683	11319	7070	2007	2205	37	0	0	0
1	G	1683	11319	7070	2007	2205	37	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	2006	12310	7625	2253	2416	16	0	0	0
2	E	2006	12310	7625	2253	2416	16	0	0	0
2	H	2006	12310	7625	2253	2416	16	0	0	0

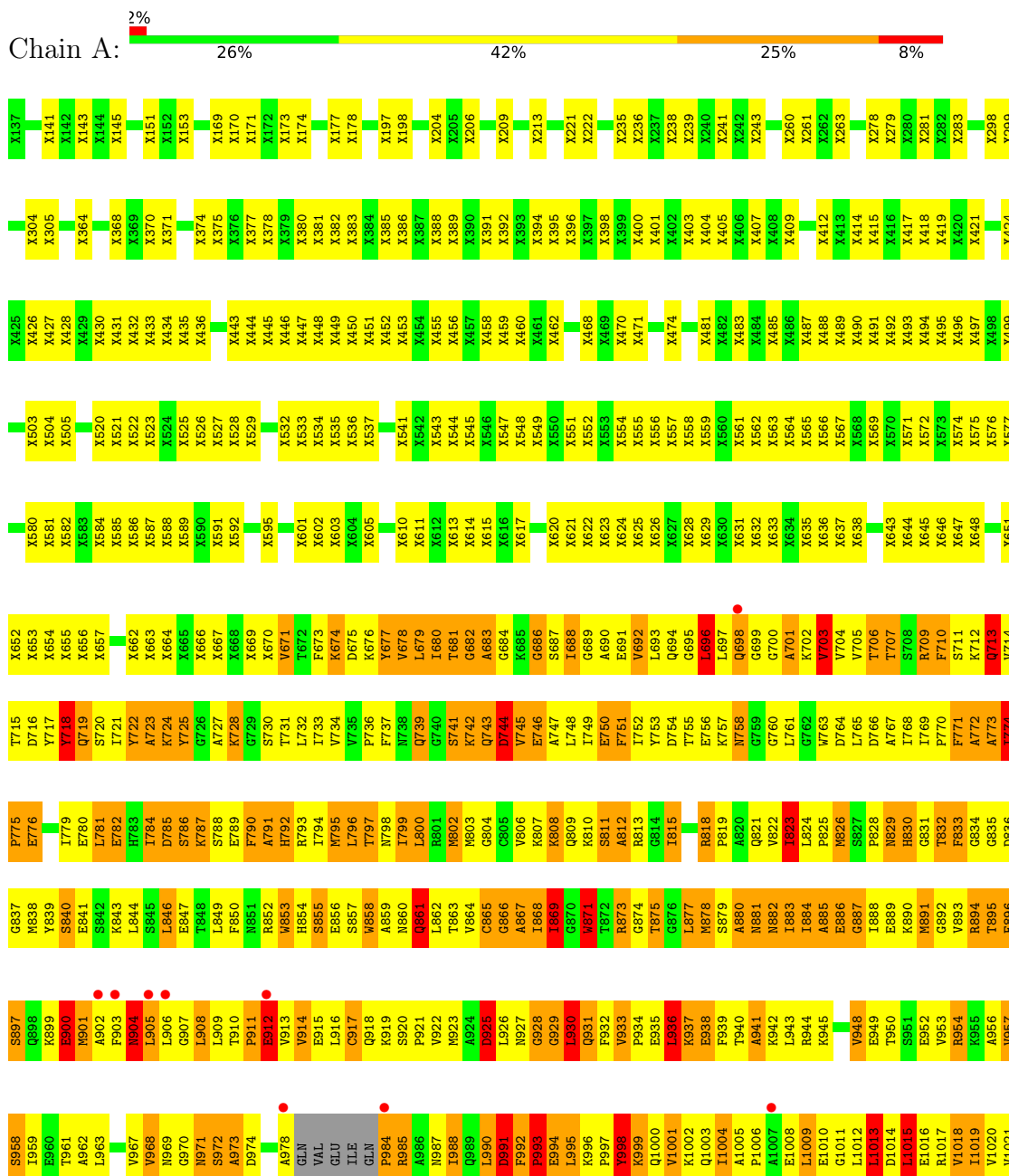
- Molecule 3 is a protein called Tail protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	65	325	195	65	65	0	0	0
3	F	65	325	195	65	65	0	0	0
3	I	65	325	195	65	65	0	0	0

### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Fatty acid synthase subunit alpha



X1749	K1686	Y1626	G1665	Q1505	N1444	I1384	K1323	D1263	D1203	Q1143	E1082	T1022
X1750	F1687	P1627	R1666	Q1506	N1445	Q1385	A1324	R1264	I1204	F1144	F1083	G1023
X1754	F1688	S1628	G1667	Q1507	K1446	I1386	I1325	F1265	I1205	H1145	F1084	A1024
N1690	H1689	K1629	G1668	Q1508	K1447	I1387	I1326	D1266	S1206	H1146	D1085	F1025
G1691	N1690	T1630	N1570	G1509	K1448	Q1388	I1327	D1267	Q1207	H1147	E1086	E1026
M1692	G1691	L1631	P1571	N1510	K1449	Q1389	I1328	E1268	H1208	H1148	K1087	E1027
Y1694	M1692	K1632	V1572	D1511	R1450	A1390	V1309	F1269	D1209	G1149	D1088	G1028
Y1694	L1693	T1633	I1573	F1512	Q1451	D1391	G1390	V1270	P1210	D1156	V1089	P1029
N1695	D1634	D1634	Y1513	Y1513	L1452	L1392	I1391	M1271	I1211	K1151	K1090	M1030
N1695	G1635	G1635	K1514	R1514	F1453	L1393	Y1392	M1272	T1212	V1152	A1091	G1031
N1696	V1636	V1636	R1515	K1515	T1454	L1394	I1393	D1273	L1213	H1153	K1092	S1032
L1697	Q1577	Q1577	D1516	R1516	R1455	L1395	I1395	I1274	F1214	I1154	Y1093	A1033
L1698	K1578	K1578	A1517	P1517	R1456	M1396	F1395	V1275	V1215	F1155	E1094	R1034
V1699	F1579	F1579	R1518	R1518	A1457	G1397	Q1386	Q1276	L1216	E1156	T1095	T1035
S1700	L1580	L1580	I1519	I1519	Q1458	P1398	E1337	E1277	V1217	I1157	S1096	R1036
K1701	T1581	T1581	A1520	A1520	L1459	P1399	E1338	S1278	S1218	P1157	I1097	M1037
E1702	G1582	G1582	P1521	P1521	K1460	I1400	G1399	F1279	V1219	P1158	E1098	E1038
H1703	H1583	H1583	D1461	D1461	Y1401	S1340	S1340	I1280	V1220	T1160	E1099	M1039
A1704	P1584	P1584	Y1462	Y1462	G1402	F1341	F1341	A1221	E1221	E1162	H1100	E1040
P1705	K1585	K1585	G1463	G1463	I1403	E1342	E1342	A1222	A1222	E1163	S1101	A1041
Y1706	G1586	G1586	E1464	E1464	V1404	F1343	F1343	F1223	F1223	Y1163	G1102	F1042
T1707	A1587	A1587	N1465	N1465	A1405	G1344	G1344	I1224	I1224	S1164	I1103	E1044
D1708	A1588	A1588	E1466	E1466	M1406	A1345	A1345	A1225	A1225	V1165	R1104	E1044
G1709	G1589	G1589	L1467	L1467	A1407	A1407	A1407	W1286	S1226	K1166	L1105	F1045
L1710	A1590	A1590	E1468	E1468	A1468	K1347	K1347	W1287	G1227	L1167	L1106	S1046
E1711	W1591	W1591	A1469	A1469	T1409	A1348	A1348	M1288	I1228	L1168	E1107	L1047
F1712	Q1592	Q1592	L1470	L1470	A1410	T1349	T1349	R1289	I1229	K1169	P1108	E1048
D1713	M1593	M1593	K1471	K1471	T1411	S1350	S1350	I1290	E1170	G1170	E1109	G1049
Y1714	I1594	I1594	L1472	L1472	D1412	N1351	N1351	L1291	A1171	L1110	F1111	C1050
Y1715	G1595	G1595	K1413	K1413	T1352	T1352	T1352	I1292	Y1232	T1172	F1111	F1051
L1716	A1596	A1596	A1474	A1474	I1414	L1353	L1353	S1293	E1233	L1173	M1112	E1052
L1717	L1597	L1597	E1475	E1475	G1445	E1354	E1354	S1294	M1234	Y1174	G1113	M1053
Q1718	Q1598	Q1598	R1416	R1416	R1416	E1355	E1355	S1295	Y1235	I1175	Y1114	A1094
L1719	D1659	D1659	L1477	L1477	V1417	F1356	F1356	P1296	K1236	P1176	M1115	W1055
A1720	Y1660	Y1660	P1478	P1478	V1418	E1357	E1357	P1297	Y1237	K1177	P1116	I1056
R1721	M1601	M1601	S1479	S1479	P1419	H1358	H1358	I1298	V1238	A1178	E1117	M1057
Y1722	S1602	S1602	E1480	E1480	A1420	G1359	G1359	K1299	H1239	L1179	K1118	G1058
G1663	G1603	G1603	D1481	D1481	P1421	R1360	R1360	T1300	V1240	R1180	K1119	F1059
A1664	I1604	I1604	Q1482	Q1482	G1422	T1361	T1361	P1301	S1241	F1181	E1120	I1060
T1665	T1605	T1605	F1485	F1485	K1423	P1362	P1362	V1302	E1242	D1182	M1121	S1061
E1666	G1607	G1607	L1486	L1486	G1424	A1363	A1363	G1303	V1243	R1183	I1122	Y1062
D1668	N1608	N1608	L1487	L1487	L1426	E1364	E1364	A1304	G1244	L1184	G1125	M1064
R1669	R1609	R1609	E1488	E1488	T1427	M1365	M1365	C1305	N1245	V1185	V1125	G1065
Y1670	M1610	M1610	R1489	R1489	T1428	S1366	S1366	A1306	S1246	A1186	L1127	G1066
M1671	A1611	A1611	T1490	T1490	A1429	P1367	P1367	S1307	S1247	G1187	E1128	L1067
E1672	D1612	D1612	K1551	K1551	R1430	P1368	P1368	S1308	G1248	Q1188	E1129	L1068
Y1673	N1613	N1613	N1551	N1551	A1431	A1369	A1369	V1309	S1249	I1189	D1130	G1069
V1674	V1614	V1614	E1492	E1492	H1432	T1370	T1370	S1131	M1251	T1191	L1131	R1070
A1675	K1615	K1615	H1494	H1494	H1433	T1372	T1372	V1312	G1252	G1192	E1132	P1071
K1676	K1616	K1616	N1495	N1495	S1434	R1373	R1373	D1313	G1253	M1193	F1133	Y1072
V1677	I1617	I1617	E1496	E1496	S1435	F1376	F1376	I1314	V1254	M1194	F1134	T1073
L1618	E1618	E1618	A1497	A1497	V1436	G1377	G1377	G1315	S1255	A1195	E1135	G1074
A1619	N1558	N1558	K1437	K1437	Y1438	E1378	E1378	S1316	A1256	A1196	A1136	W1075
R1680	Q1620	Q1620	Y1499	Y1499	Y1438	E1379	E1379	E1317	L1257	T1197	S1137	V1076
E1681	F1621	F1621	Q1500	Q1500	S1440	A1379	A1379	T1318	G1259	Y1198	D1077	D1077
K1682	E1622	E1622	L1501	L1501	S1440	Q1380	Q1380	I1319	G1259	G1199	E1139	S1078
S1683	Y1623	Y1623	R1502	R1502	P1441	G1381	G1381	L1520	M1260	I1200	T1140	K1079
A1684	V1624	V1624	H1503	H1503	N1442	A1382	A1382	S1321	F1261	S1201	A1141	T1099
Y1685	L1625	L1625	A1504	A1504	L1443	G1383	G1383	G1322	K1262	D1202	E1142	K1081

● Molecule 1: Fatty acid synthase subunit alpha



D1208	G1149	D1088	G1028	V968	L905	S845	I784	K724	M664	X587	E923	X435	X137
P1210	D1180	V1089	P1029	N969	L906	L846	D785	Y725	X665	X588	X594	X436	X374
I1211	K1151	K1090	M1030	G970	G907	T848	S786	G726	X666	X589	X595	X437	X141
I1212	V1152	A1091	G1031	N971	L908	T849	K787	A727	X667	X590	X526	X438	X376
L1213	D1153	K1092	S1032	S972	L909	L849	S788	G728	X668	X591	X527	X439	X143
F1214	K1154	Y1093	A1033	A973	T910	F850	E789	K729	X669	X592	X528	X440	X144
V1215	F1155	E1094	R1034	D974	P911	M851	F790	S730	X670	X595	X529	X441	X145
L1216	E1156	T1095	T1035	A975	E912	R852	A791	L731	X671	X596	X530	X442	X380
V1217	S1157	S1096	V1133	V913	V913	M853	H792	L732	X672	X597	X531	X443	X381
S1218	P1158	I1097	E1037	H914	V914	H854	A793	L733	F673	X601	X532	X444	X382
V1219	L1098	L1098	E1038	A978	E915	S855	I794	V734	K674	X602	X533	X445	X170
V1220	H1100	E1099	M1039	GLN	L916	E856	M795	V735	D675	X603	X534	X446	X171
G1221	G1161	H1100	E1040	VAL	C917	S857	V796	F736	K676	X604	X535	X447	X172
A1222	E1162	GLU	A1041	GLU	Q918	M858	T797	F737	X677	X605	X537	X448	X174
F1223	Y1163	I1102	F1042	ILE	R919	A859	N798	L738	X678	X610	X541	X449	X169
I1224	S1164	I1103	G1043	GLN	S920	N860	I799	Q739	X679	X611	X542	X450	X388
A1225	V1165	R1104	E1044	P984	P921	K861	L800	G740	X680	X612	X543	X451	X178
S1226	K1166	L1105	F1045	R985	V922	L862	R801	S741	T681	X613	X544	X452	X390
G1227	L1167	I1106	S1046	A986	M923	T863	M802	K742	G682	X614	X545	X453	X197
I1228	L1168	E1107	L1047	N987	A924	V864	M803	Q743	A683	X615	X546	X454	X198
I1229	K1169	P1108	E1048	I988	D925	G870	G804	D744	G684	X616	X547	X455	X204
D1230	G1170	E1109	G1049	Q989	L926	G866	C805	V745	K685	X617	X548	X456	X205
P1231	A1171	L1110	C1050	L990	N927	A867	R806	E746	G686	X618	X549	X457	X206
Y1232	T1172	F1111	V1051	D991	G928	I868	K807	A747	S687	X619	X550	X458	X396
E1233	L1173	N1112	E1052	F992	G929	I869	K808	L748	I688	X620	X551	X459	X397
M1234	Y1174	G1113	M1053	P993	L880	G870	Q809	I749	G689	X621	X552	X460	X209
Y1235	I1175	Y1114	A1054	E994	Q931	M871	R810	E750	A690	X622	X553	X461	X398
K1236	P1176	M1115	M1055	L995	F932	T872	S811	E751	E691	X623	X554	X462	X400
Y1237	K1177	P1116	L1056	K996	R933	R873	A812	I752	V692	X624	X555	X463	X213
I1238	A1178	E1117	M1057	P997	V934	G874	R813	L753	L693	X625	X556	X464	X235
H1239	L1179	K1118	G1058	Y998	E935	T875	G814	D754	O694	X626	X557	X465	X236
V1240	K1180	K1119	F1059	K999	L886	G876	I815	T755	G695	X627	X558	X466	X239
S1241	F1181	E1120	I1060	Q1000	K937	L877	E756	E756	L696	X628	X559	X467	X405
V1242	D1182	M1121	S1061	V1001	E938	M878	R818	K757	L697	X629	X560	X468	X240
G1243	L1183	I1122	Y1062	F939	R939	S879	P819	M758	G698	X630	X561	X469	X241
M1244	L1184	I1123	H1063	Q1003	T940	A880	A820	G759	G699	X631	X562	X470	X260
C1245	V1185	V1124	M1064	I1004	A941	M881	Q821	G760	G700	X632	X563	X471	X261
A1246	A1186	I1126	G1065	A1005	K942	M882	B822	L761	A701	X633	X564	X472	X262
G1247	G1187	V1127	M1066	P1006	L943	I853	L823	G762	K702	X634	X565	X473	X263
S1248	Q1188	E1128	L1067	P1006	R944	I894	L824	A763	W703	X635	X566	X474	X264
S1249	I1189	E1129	K1068	E1008	K945	A885	P825	D764	V704	X636	X567	X475	X278
G1250	P1190	D1130	G1069	L1009	K945	E886	M826	L765	W705	X637	X568	X476	X279
M1251	T1191	L1131	R1070	E1010	V948	G887	S827	D766	V706	X638	X569	X477	X281
G1252	G1192	E1132	P1071	G1011	E949	I888	P828	A767	T707	X639	X570	X478	X289
G1253	W1193	P1133	Y1072	L1012	T950	E889	N829	I768	S708	X640	X571	X479	X299
V1254	M1194	F1134	T1073	L1013	S951	K890	H830	I769	R709	X641	X572	X480	X304
S1255	A1195	E1135	G1074	M1014	E952	M891	G831	P770	F710	X642	X573	X481	X305
A1256	K1196	A1136	W1075	V953	R954	G892	T832	F771	S711	X643	X574	X482	X365
L1257	T1197	S1137	V1076	E1016	R954	V893	F833	A772	K712	X644	X575	X483	X368
R1258	Y1198	K1138	D1077	R1017	K955	R894	G834	A773	R713	X645	X576	X484	X369
G1259	G1199	E1139	S1078	V1018	A956	T895	G835	I774	V714	X646	X577	X485	X371
M1260	I1200	T1140	K1079	I1019	V957	F896	D836	I775	T715	X647	X578	X486	X424
F1261	S1201	A1141	T1080	V1020	S958	P897	D716	E776	T716	X648	X579	X487	X425
K1262	D1202	X1081	K1081	V1021	S958	G898	M838	Q777	Y717	X649	X580	X488	X426
D1263	L1203	Q1143	E1082	T1022	I959	K898	G788	G778	X718	X650	X581	X489	X427
R1264	L1204	F1144	P1083	G1023	T961	K899	R839	A779	Y719	X651	X582	X490	X428
F1265	I1205	K1145	V1084	F1024	A962	E900	S840	E780	W720	X652	X583	X491	X429
K1266	S1206	H1146	D1085	A1025	L963	M901	E841	E781	S720	X653	X584	X492	X430
V1267	Q1207	D1086	D1086	E1026	K943	F902	S942	L781	Y722	X654	X585	X493	X431
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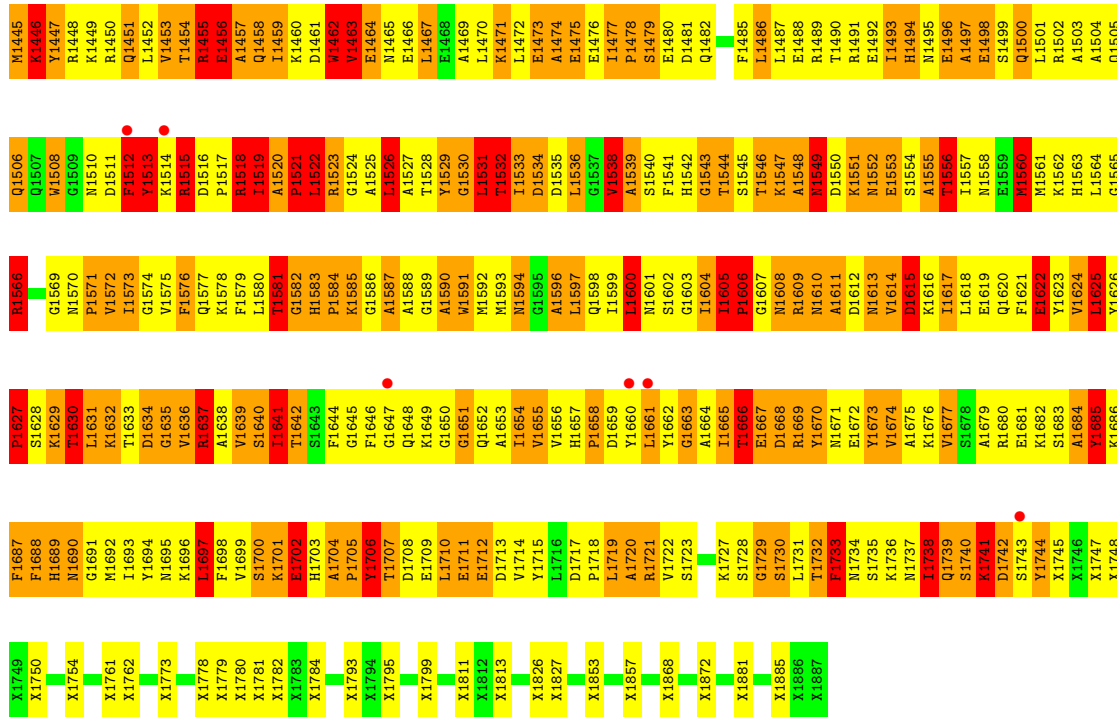
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• Molecule 1: Fatty acid synthase subunit alpha

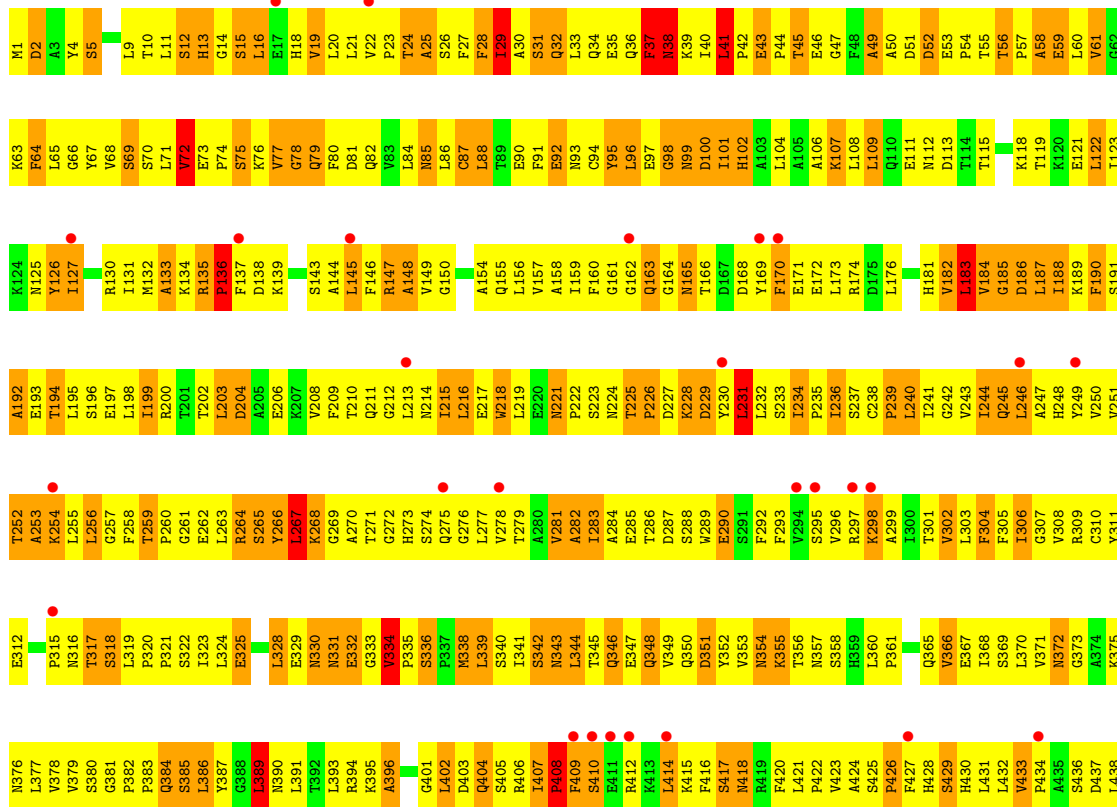


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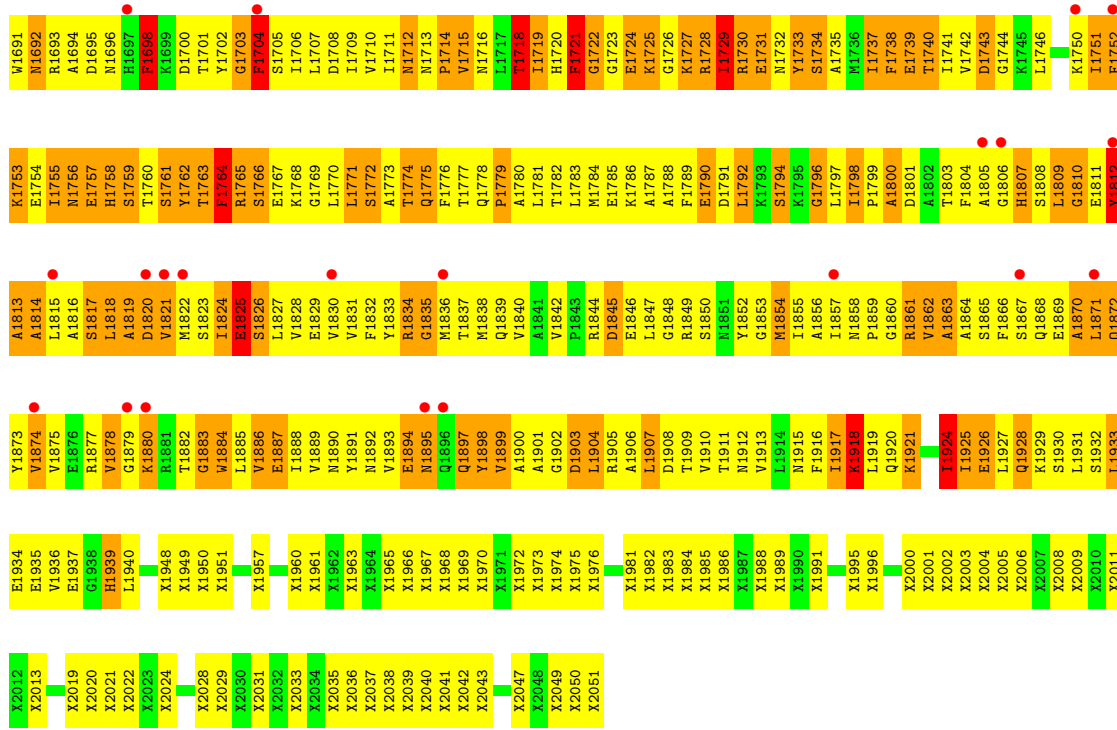




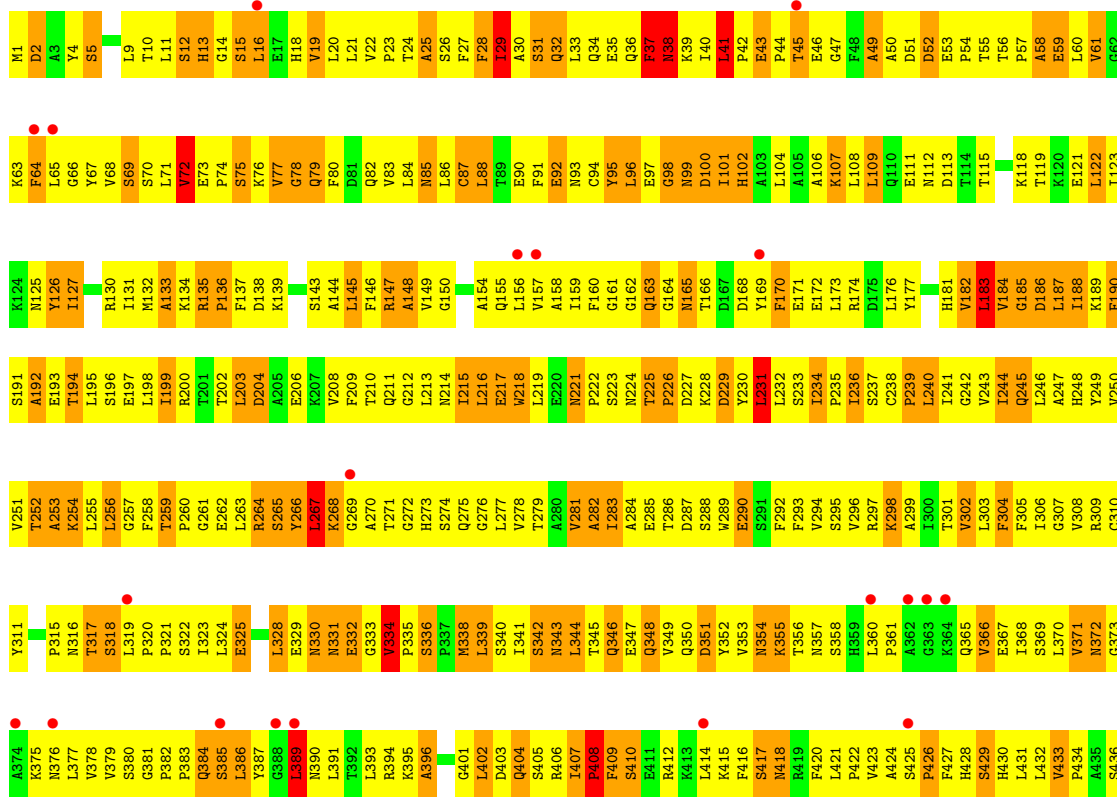
• Molecule 2: Fatty acid synthase subunit beta



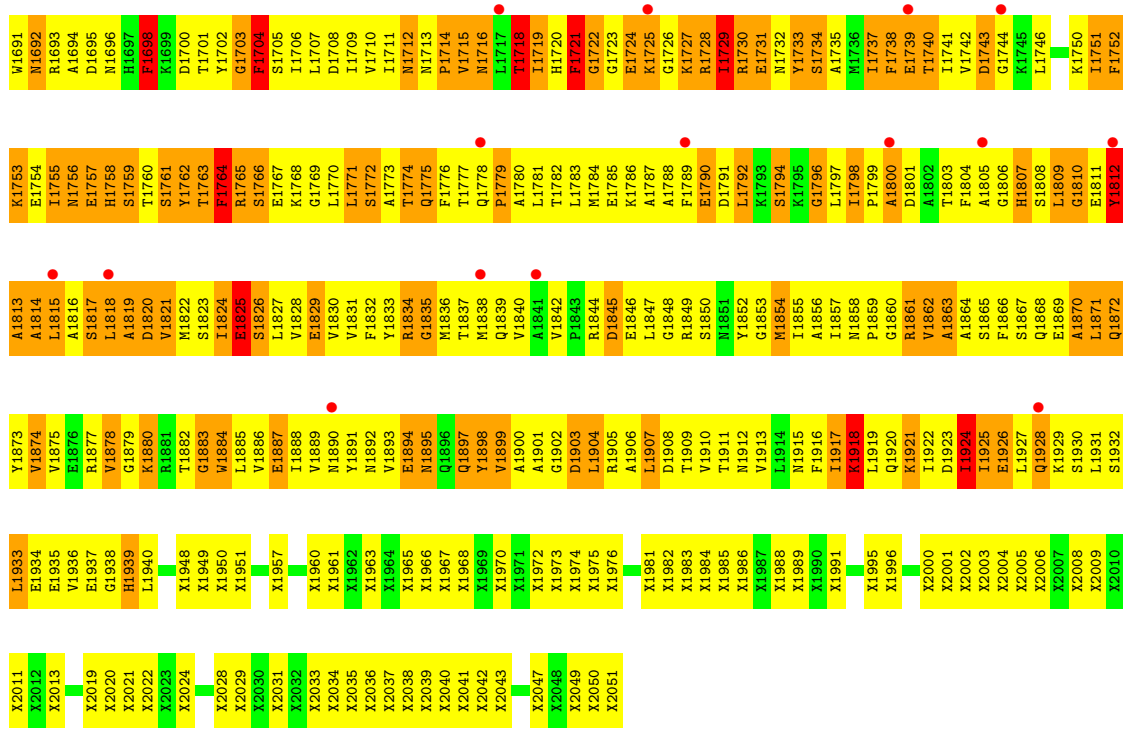
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X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1461	X1462	X1463	X1464	X1469	X1476	X1477	X1482	X1483	X1484	X1485	X1486	X1487	X1490	X1491	X1492	X1493	X1496	X1497	X1498	X1500	X1501	X1504	X1505	X1506	X1507	X1508	X1509	X1510	X1511	X1512	X1513	X1514						
X1519	X1520	X1521	X1531	X1532	X1533	X1534	X1535	X1536	X1537	X1538	X1539	X1540	X1541	X1542	X1543	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1558	X1559	X1560	X1561	X1562	X1563	X1564	X1573	X1574	X1575	X1581	X1582	X1583	X1584	X1585	X1586	X1587	X1588	X1589	X1590	X1591	X1592	X1593	X1594	X1595	X1596	X1602	X1603	X1604	X1605					
X1606	X1607	X1608	X1614	X1625	X1628	X1629	X1630	X1631	X1632	X1633	X1634	X1638	X1639	X1642	X1643	X1644	X1645	X1646	X1649	X1650	X1651	X1652	X1655	X1656	X1657	X1663	X1664	X1665	X1669	G1670	X1671	X1672	X1673	X1674	G1675	X1676	X1677	M1678	M1679	L1680	X1681	X1682	X1683	S1684	X1685	A1686	A1687	Q1688	D1689	X1690									



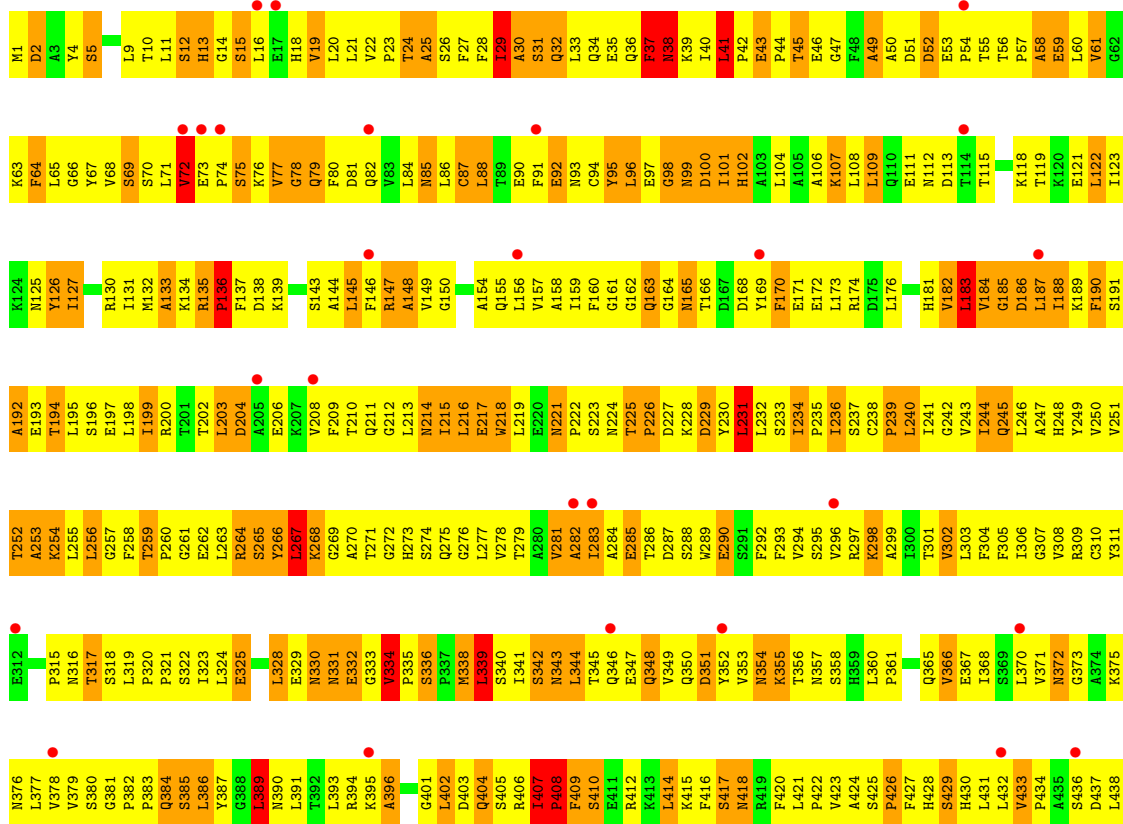
• Molecule 2: Fatty acid synthase subunit beta







• 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, $\alpha$ , $\beta$ , $\gamma$	231.34Å 231.34Å 754.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 4.00 60.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (60.00-4.00) 98.6 (60.00-4.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.88Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.319 , 0.346 0.320 , 0.354	Depositor DCC
$R_{free}$ test set	8857 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	152.3	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 279.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	71862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	151.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.80	9/8414 (0.1%)	1.35	156/11377 (1.4%)
1	D	0.80	9/8414 (0.1%)	1.35	149/11377 (1.3%)
1	G	0.82	9/8414 (0.1%)	1.36	157/11377 (1.4%)
2	B	0.49	0/6495	1.11	65/8812 (0.7%)
2	E	0.47	0/6495	1.11	66/8812 (0.7%)
2	H	0.49	0/6495	1.11	64/8812 (0.7%)
All	All	0.69	27/44727 (0.1%)	1.25	657/60567 (1.1%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1150	ASP	CB-CG	27.64	2.21	1.52
1	D	1150	ASP	CB-CG	27.30	2.20	1.52
1	A	1150	ASP	CB-CG	27.21	2.20	1.52
1	D	1181	PHE	CD2-CE2	14.26	1.81	1.38
1	G	1181	PHE	CD2-CE2	13.97	1.80	1.38

The worst 5 of 657 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1113	GLY	N-CA-C	-17.50	88.14	115.08
1	D	1113	GLY	N-CA-C	-17.39	88.30	115.08
1	A	1113	GLY	N-CA-C	-17.34	88.38	115.08
1	G	1065	GLY	N-CA-C	-16.33	92.57	112.33
1	D	1065	GLY	N-CA-C	-16.33	92.58	112.33

There are no chirality outliers.

There are no planarity outliers.

## 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	11319	0	8817	2644	24
1	D	11319	0	8818	2643	14
1	G	11319	0	8817	2655	24
2	B	12310	0	7819	1818	0
2	E	12310	0	7817	1840	0
2	H	12310	0	7816	1842	0
3	C	325	0	76	26	0
3	F	325	0	76	29	0
3	I	325	0	76	34	0
All	All	71862	0	50132	13492	38

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 111.

The worst 5 of 13492 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:G:1181:PHE:CE2	1:G:1181:PHE:CZ	1.76	1.71
1:A:1181:PHE:CZ	1:A:1181:PHE:CE2	1.75	1.69
1:D:1181:PHE:CE2	1:D:1181:PHE:CD2	1.81	1.68
1:G:1181:PHE:CZ	1:G:1181:PHE:CE1	1.75	1.68
1:D:1181:PHE:CD1	1:D:1181:PHE:CE1	1.78	1.66

The worst 5 of 38 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:D:1150:ASP:OD1	1:D:1181:PHE:CE2[7_555]	1.80	0.40
1:A:1150:ASP:OD1	1:G:1181:PHE:CE2[7_555]	1.85	0.35
1:A:1181:PHE:CE2	1:G:1150:ASP:OD1[7_555]	1.85	0.35
1:A:1150:ASP:CG	1:G:1181:PHE:CE2[7_555]	1.87	0.33
1:D:1150:ASP:CG	1:D:1181:PHE:CE2[7_555]	1.87	0.33

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1069/1688 (63%)	401 (38%)	298 (28%)	370 (35%)	0	0
1	D	1069/1688 (63%)	396 (37%)	307 (29%)	366 (34%)	0	0
1	G	1069/1688 (63%)	398 (37%)	307 (29%)	364 (34%)	0	0
2	B	817/2006 (41%)	356 (44%)	245 (30%)	216 (26%)	0	1
2	E	817/2006 (41%)	357 (44%)	244 (30%)	216 (26%)	0	1
2	H	817/2006 (41%)	352 (43%)	247 (30%)	218 (27%)	0	0
All	All	5658/11082 (51%)	2260 (40%)	1648 (29%)	1750 (31%)	0	0

5 of 1750 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	683	ALA
1	A	723	ALA
1	A	724	LYS
1	A	741	SER
1	A	742	LYS

### 5.3.2 Protein sidechains [i](#)

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	871/895 (97%)	675 (78%)	196 (22%)	1	6
1	D	871/895 (97%)	672 (77%)	199 (23%)	1	6
1	G	871/895 (97%)	677 (78%)	194 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	703/703 (100%)	623 (89%)	80 (11%)	5	22
2	E	703/703 (100%)	622 (88%)	81 (12%)	5	22
2	H	703/703 (100%)	622 (88%)	81 (12%)	5	22
All	All	4722/4794 (98%)	3891 (82%)	831 (18%)	2	12

5 of 831 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1677	VAL
1	G	796	LEU
2	H	528	ILE
2	E	29	ILE
1	D	1669	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 215 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	93	ASN
2	E	1912	ASN
2	H	346	GLN
2	E	221	ASN
2	E	376	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](#)

There are no ligands in this entry.

## 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
1	D	2
1	A	2
1	G	2

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	506:UNK	C	516:UNK	N	28.27
1	A	506:UNK	C	516:UNK	N	28.26
1	G	506:UNK	C	516:UNK	N	28.26
1	D	305:UNK	C	360:UNK	N	17.84
1	A	305:UNK	C	360:UNK	N	17.83

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	1069/1688 (63%)	0.29	38 (3%) 46 35	48, 122, 192, 203	0
1	D	1069/1688 (63%)	0.21	40 (3%) 45 34	53, 123, 194, 203	0
1	G	1069/1688 (63%)	0.18	31 (2%) 53 39	43, 112, 190, 203	0
2	B	818/2006 (40%)	0.55	52 (6%) 25 23	107, 177, 202, 203	0
2	E	818/2006 (40%)	0.45	41 (5%) 34 28	111, 190, 202, 203	0
2	H	818/2006 (40%)	0.51	53 (6%) 25 23	94, 183, 202, 203	0
3	C	0/65	-	-	-	-
3	F	0/65	-	-	-	-
3	I	0/65	-	-	-	-
All	All	5661/11277 (50%)	0.35	255 (4%) 38 30	43, 151, 201, 203	0

The worst 5 of 255 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	545	GLN	7.3
2	B	294	VAL	6.5
2	B	1895	ASN	6.2
2	B	1821	VAL	6.1
1	D	1354	GLU	6.0

### 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.