



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:55 PM BST

PDB ID : 3J96
EMDB ID: : EMD-6206
Title : Structure of 20S supercomplex determined by single particle cryoelectron microscopy (State I)
Authors : Zhao, M.; Wu, S.; Cheng, Y.; Brunger, A.T.
Deposited on : 2014-12-05
Resolution : 7.60 Å(reported)
Based on PDB ID : 1QCS, 1NSF, 1N7S

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

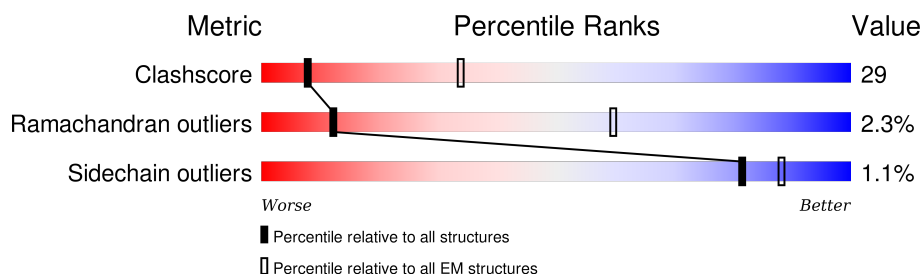
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	747	45% 42% . . 9%
1	B	747	46% 41% . 10%
1	C	747	47% 41% . 10%
1	D	747	45% 43% . 10%
1	E	747	45% 42% . 10%
1	F	747	44% 41% . 12%
2	G	297	49% 44% . .
2	H	297	54% 41% . .
2	I	297	57% 38% . .

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Mol	Chain	Length	Quality of chain
2	J	297	<div><div></div><div>52%42%</div><div></div></div>
3	K	63	<div><div></div><div>38%57%</div><div></div></div>
4	L	67	<div><div></div><div>51%43%</div><div></div></div>
5	M	188	<div><div></div><div>29%40%30%</div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41139 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	678	Total	C	N	O	S	0	0
			5048	3203	876	946	23		
1	B	672	Total	C	N	O	S	0	0
			5037	3197	872	944	24		
1	C	676	Total	C	N	O	S	0	0
			5039	3196	872	948	23		
1	D	673	Total	C	N	O	S	0	0
			4994	3174	857	939	24		
1	E	670	Total	C	N	O	S	0	0
			5012	3183	866	939	24		
1	F	654	Total	C	N	O	S	0	0
			4926	3130	849	923	24		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P18708
A	-1	ALA	-	EXPRESSION TAG	UNP P18708
A	0	HIS	-	EXPRESSION TAG	UNP P18708
B	-2	GLY	-	EXPRESSION TAG	UNP P18708
B	-1	ALA	-	EXPRESSION TAG	UNP P18708
B	0	HIS	-	EXPRESSION TAG	UNP P18708
C	-2	GLY	-	EXPRESSION TAG	UNP P18708
C	-1	ALA	-	EXPRESSION TAG	UNP P18708
C	0	HIS	-	EXPRESSION TAG	UNP P18708
D	-2	GLY	-	EXPRESSION TAG	UNP P18708
D	-1	ALA	-	EXPRESSION TAG	UNP P18708
D	0	HIS	-	EXPRESSION TAG	UNP P18708
E	-2	GLY	-	EXPRESSION TAG	UNP P18708
E	-1	ALA	-	EXPRESSION TAG	UNP P18708
E	0	HIS	-	EXPRESSION TAG	UNP P18708
F	-2	GLY	-	EXPRESSION TAG	UNP P18708
F	-1	ALA	-	EXPRESSION TAG	UNP P18708
F	0	HIS	-	EXPRESSION TAG	UNP P18708

- Molecule 2 is a protein called Alpha-soluble NSF attachment protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	286	Total	C	N	O	S	0	0
			2255	1424	373	441	17		
2	H	286	Total	C	N	O	S	0	0
			2255	1424	373	441	17		
2	I	286	Total	C	N	O	S	0	0
			2251	1421	372	441	17		
2	J	286	Total	C	N	O	S	0	0
			2255	1424	373	441	17		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	EXPRESSION TAG	UNP P54921
G	0	SER	-	EXPRESSION TAG	UNP P54921
H	-1	GLY	-	EXPRESSION TAG	UNP P54921
H	0	SER	-	EXPRESSION TAG	UNP P54921
I	-1	GLY	-	EXPRESSION TAG	UNP P54921
I	0	SER	-	EXPRESSION TAG	UNP P54921
J	-1	GLY	-	EXPRESSION TAG	UNP P54921
J	0	SER	-	EXPRESSION TAG	UNP P54921

- Molecule 3 is a protein called Vesicle-associated membrane protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	61	Total	C	N	O	S	0	0
			493	301	93	98	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	27	GLY	-	EXPRESSION TAG	UNP P63045

- Molecule 4 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	66	Total	C	N	O	S	0	0
			536	331	91	109	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	190	MET	-	EXPRESSION TAG	UNP P32851

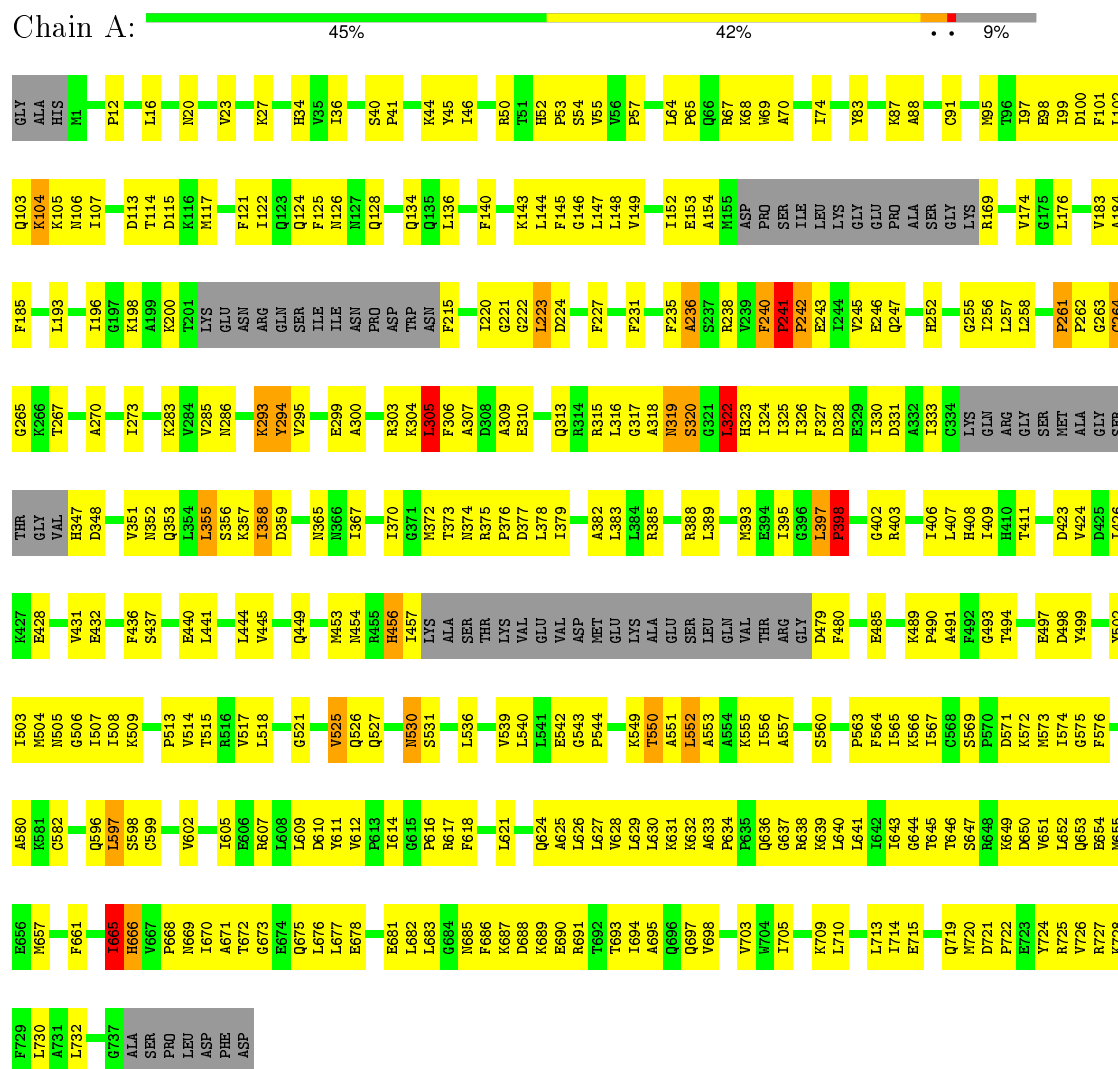
- Molecule 5 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	131	Total	C	N	O	S	0	0
			1038	614	194	221	9		

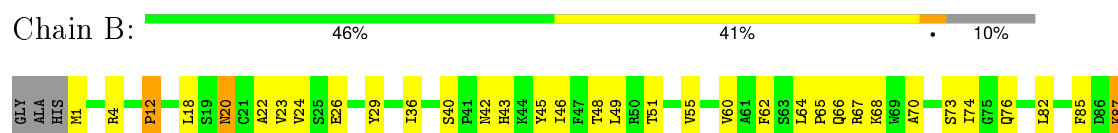
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Vesicle-fusing ATPase



• Molecule 1: Vesicle-fusing ATPase

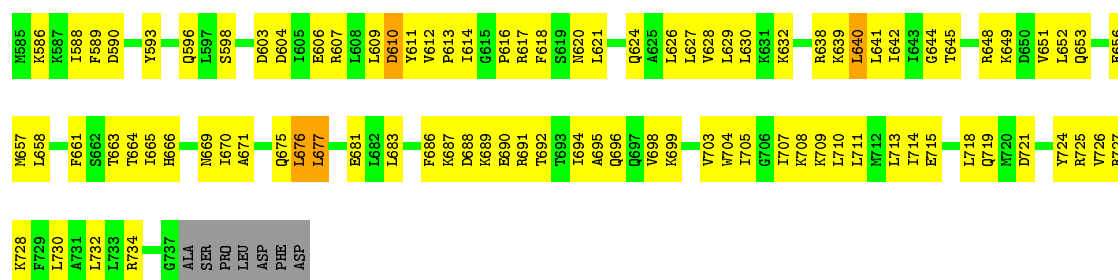


I707	K708	K709	L710	L711	M712	L713	L714	E715	M716	Q719	M720	D721	Y724	K728	F729	L732	ALA	SER	PRO	LEU	ASP	PHE	ASP	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960	L1961	L1962	L1963	L1964	L1965	L1966	L1967	L1968	L1969	L1970	L1971	L1972	L1973	L1974	L1975	L1976	L1977	L1978	L1979	L1980	L1981	L1982	L1983	L1984	L1985	L1986	L1987	L1988	L1989	L1990	L1991	L1992	L1993	L1994	L1995	L1996	L1997	L1998	L1999	L2000
L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						

• Molecule 1: Vesicle-fusing ATPase

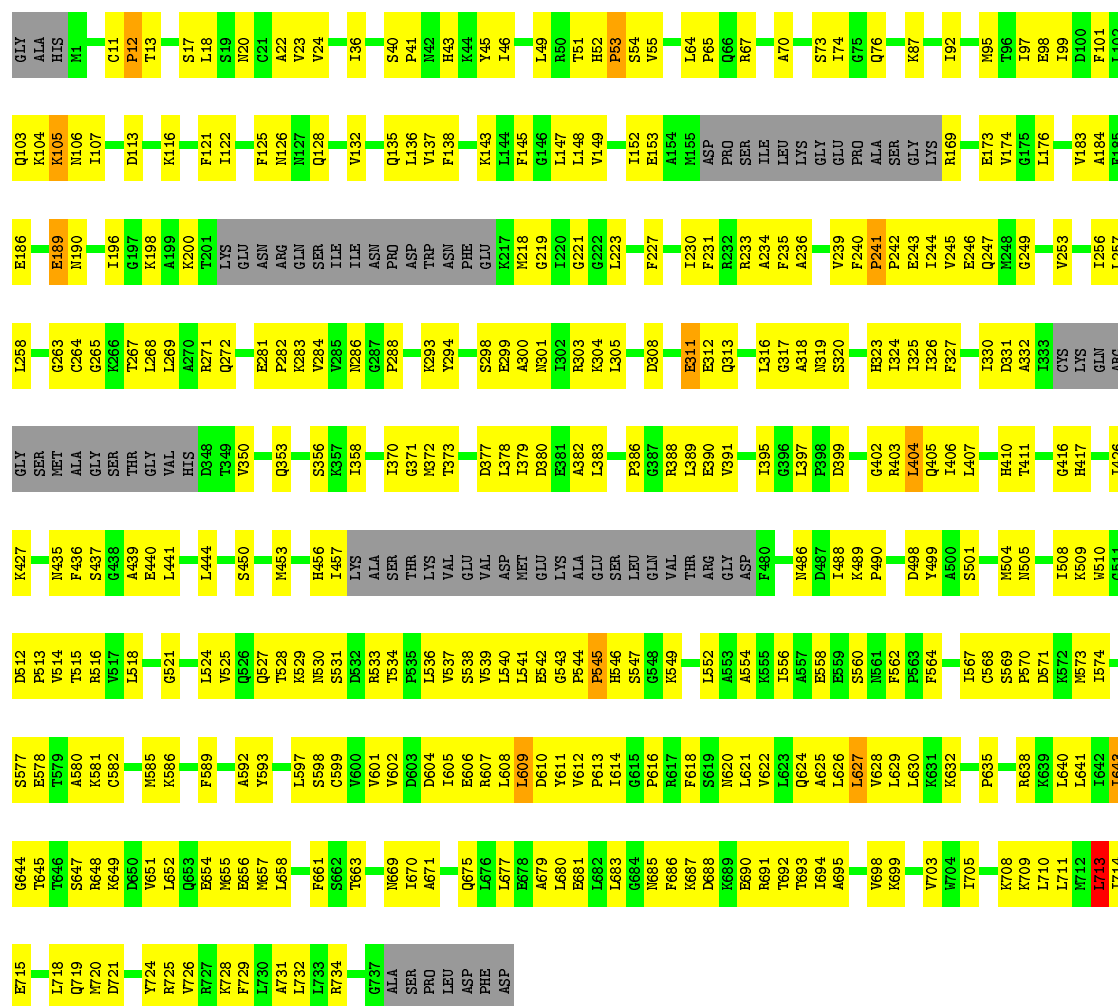
Chain C:

GLY	ALA	HIS	M1	P12	T13	D14	L18	S19	R20	V23	V24	K34	V35	I36	K44	Y45	I46	T48	L49	R50	T51	H52	P53	S54	L64	P65	Q66	R67	K68	H69	A70	I74	Y83	D86	A88	C91	N95	E98	F101	I107	T114	L122	F125	N126	I127	V132	G133	Q134	L136	Q135	V137	F138	S139	K143	L144	V145	G146	I152	E153	A154	M155	ASP	PRO	SER	ILE	LEU	L169	E173	V174	G175	L176	N180	V183	A184	N190	E198	L193	N194	L195	A199	K200
T201	LYS	GLU	ASN	ARG	GLN	SER	ILE	ILE	ASN	PRO	TRP	ASP	PHE	GLU	K217	R218	Q219	F227	F231	R232	R233	A234	F235	A236	S237	R238	G317	A318	N319	S320	E242	I244	V245	E246	Q247	P248	G249	R252	V253	K254	G255	L257	L258	G263	C264	G265	L268	A270	R271	G272	I273																														
E281	V284	V285	P288	E289	L291	K293	Q294	V295	G296	S298	E299	L305	D308	A309	E310	E311	E312	Q313	R314	R315	L316	G317	A318	N319	S320	G321	I322	I323	I325	I326	F327	I330	D331	A332	C334	LYS	GLN	ARG	GLY	SER	MET	ALA	GLY	THR	SER	GLY	THR	VAL	H347																																
D348	T349	V350	V351	N352	Q353	L354	L355	I358	N365	N366	I367	L368	V369	I370	G371	R375	P376	D377	L378	I379	L383	P386	G387	R388	L389	E390	V391	D399	K401	G402	R403	L404	L407	H408	T411	A412	N413	M414	L426	K427	E428	V431	E432	F436	S437	G438	A439	K440																																	
E440	L441	V445	R446	Q449	A452	M453	H456	L457	LYS	ALA	THR	LYS	VAL	GLU	VAL	ASP	MET	GLU	LYS	ALA	GLY	THR	VAL	THR	ARG	GLY	D479	P490	A491	F492	Q496	E497	D498	Y499	M505	G506	I507	I508	K509	M510	D512	P513	R516	V517	L518	G519	D520																																		
G521	E522	L523	L524	V525	Q526	G527	K529	N530	R533	L536	V537	S538	V539	L540	L541	E542	G543	P544	P545	H546	S547	G548	K549	T550	A551	L552	K555	L556	A557	E558	E559	S560	M561	F562	P563	F564	I565	K566	L567	S569	K572	M573	I574	Q575	F576	S577	E578	T579	A580	K581	Q582	L583	Q584																												



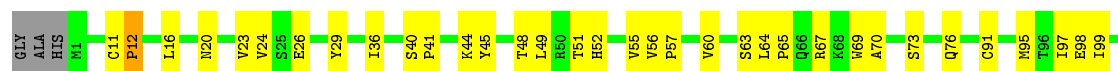
• Molecule 1: Vesicle-fusing ATPase

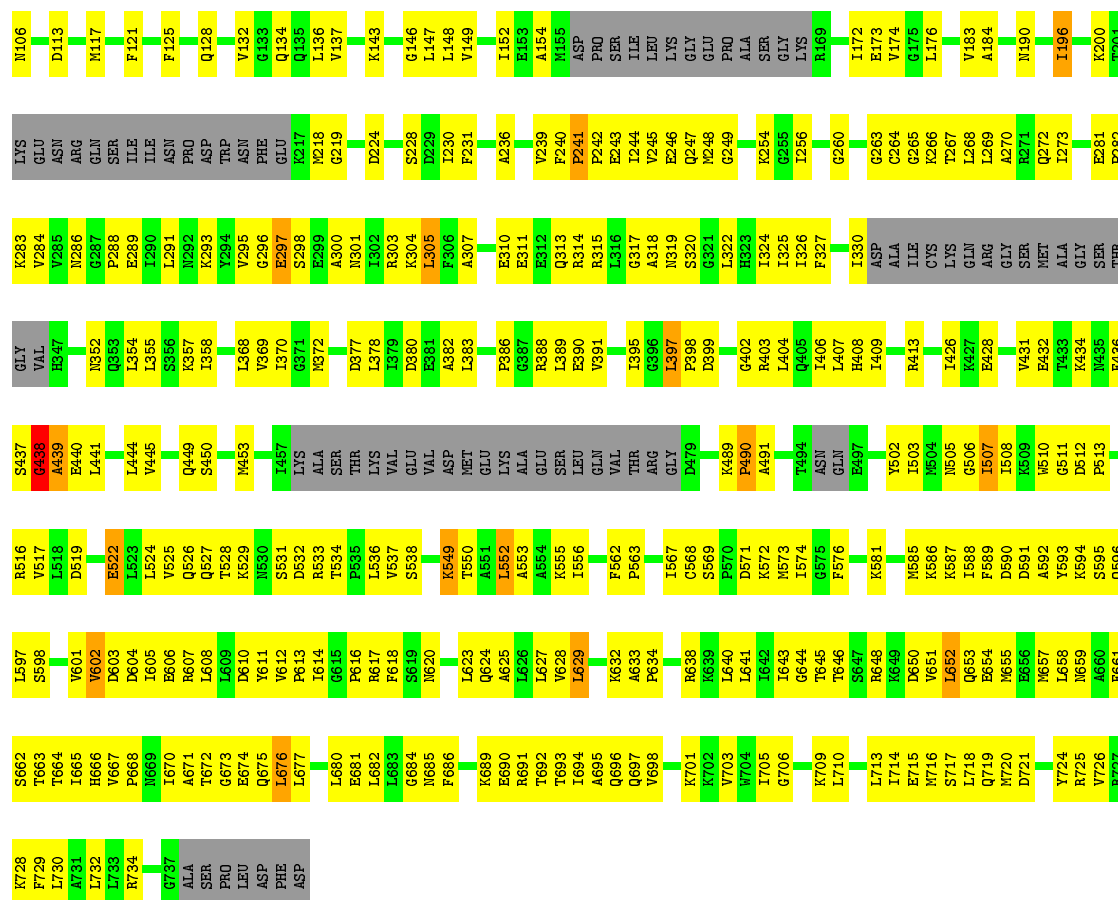
Chain D: 45% 43% 10%



• Molecule 1: Vesicle-fusing ATPase

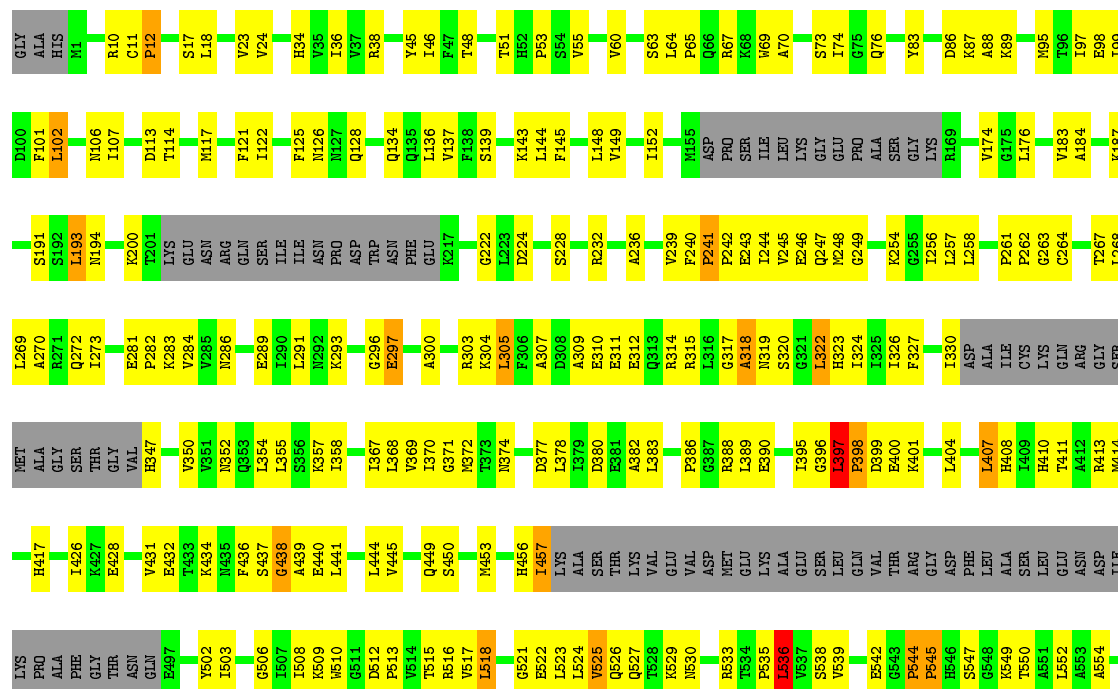
Chain E: 45% 42% 10%

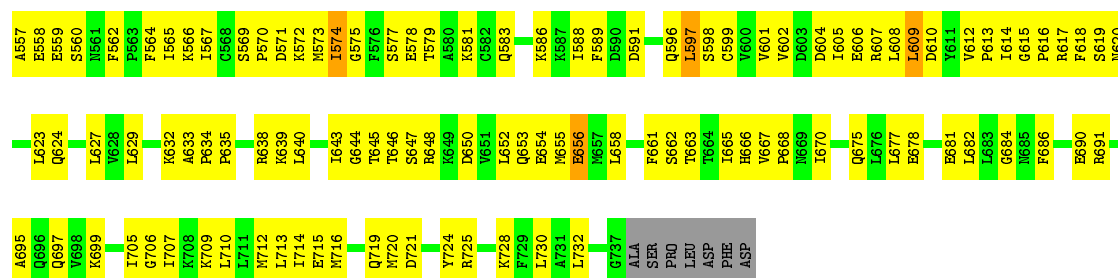




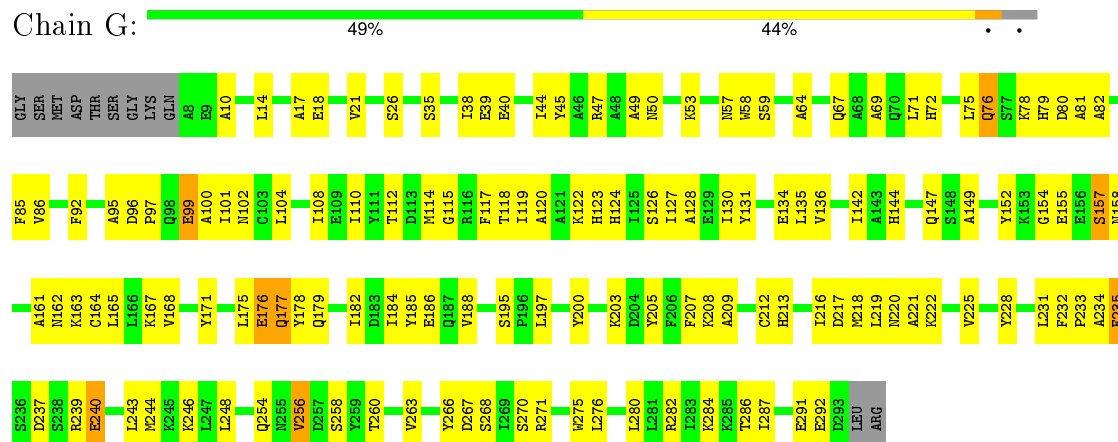
• Molecule 1: Vesicle-fusing ATPase

Chain F: 44% 41% 12%

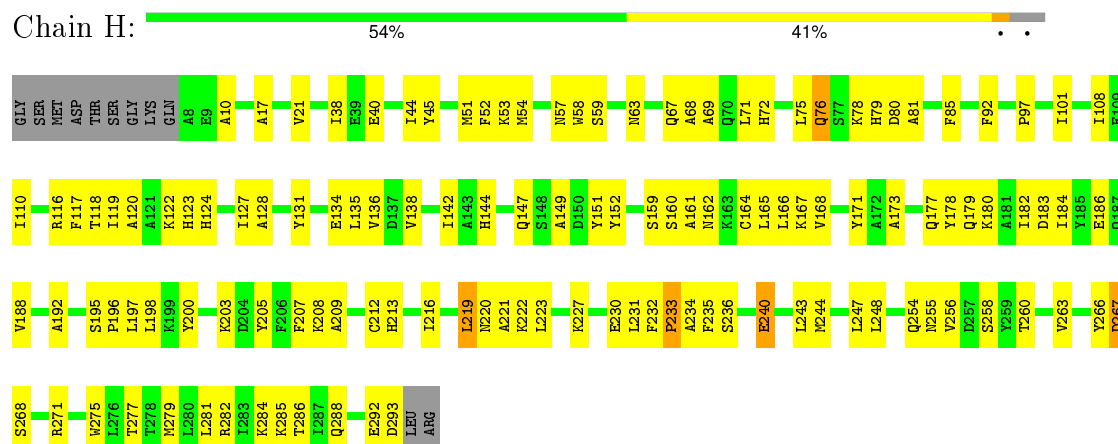




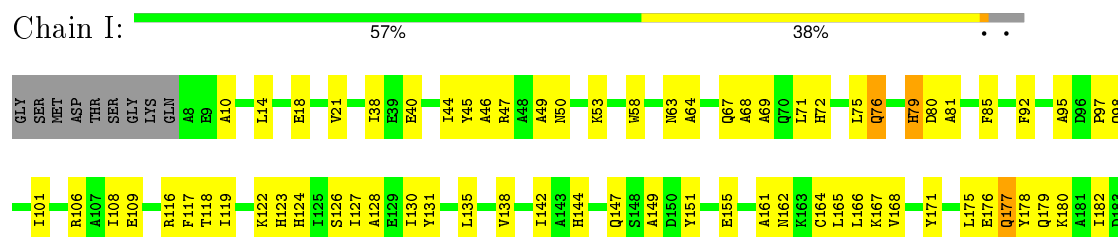
- Molecule 2: Alpha-soluble NSF attachment protein

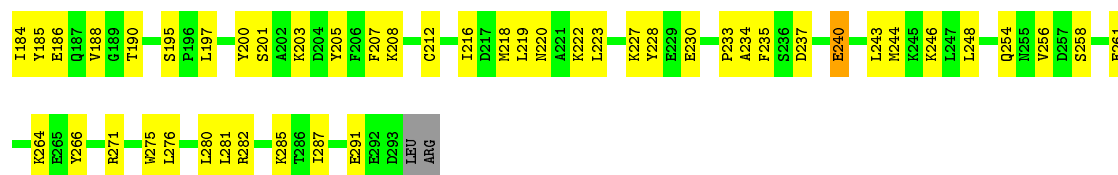


- Molecule 2: Alpha-soluble NSF attachment protein

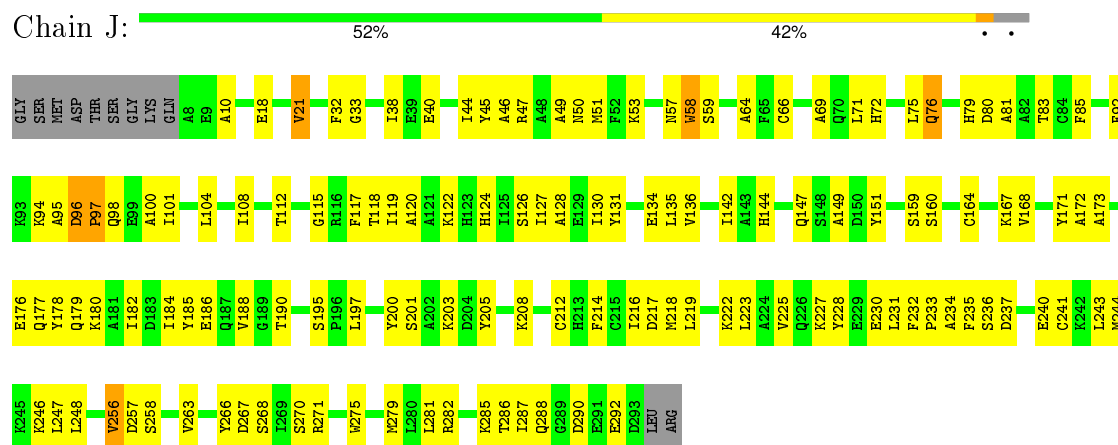


- Molecule 2: Alpha-soluble NSF attachment protein

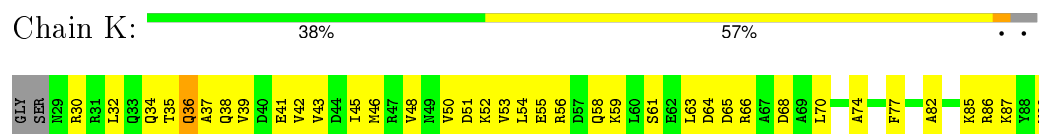




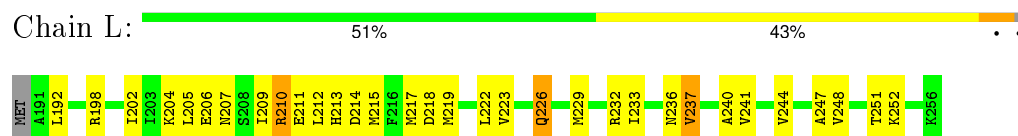
• Molecule 2: Alpha-soluble NSF attachment protein



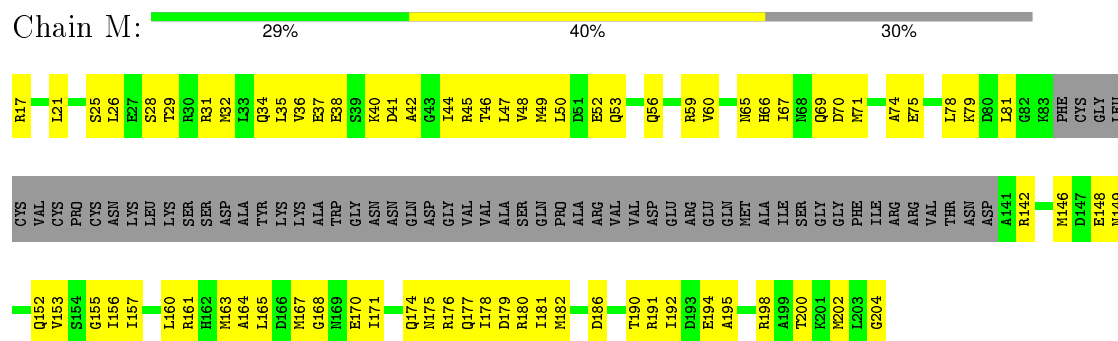
• Molecule 3: Vesicle-associated membrane protein 2



• Molecule 4: Syntaxin-1A



• Molecule 5: Synaptosomal-associated protein 25



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	29717	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	-1800	Depositor
Maximum defocus (nm)	-2800	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 >2	RMSZ	# Z >2
1	A	0.46	1/5124 (0.0%)	0.85	13/6935 (0.2%)
1	B	0.41	1/5113 (0.0%)	0.77	7/6915 (0.1%)
1	C	0.39	0/5115	0.75	6/6922 (0.1%)
1	D	0.43	0/5069	0.77	8/6864 (0.1%)
1	E	0.44	0/5088	0.83	14/6881 (0.2%)
1	F	0.44	1/5001 (0.0%)	0.81	14/6760 (0.2%)
2	G	0.36	0/2295	0.65	0/3086
2	H	0.36	0/2295	0.62	2/3086 (0.1%)
2	I	0.35	0/2291	0.61	0/3082
2	J	0.35	0/2295	0.62	1/3086 (0.0%)
3	K	0.24	0/496	0.41	0/664
4	L	0.24	0/541	0.43	0/723
5	M	0.22	0/1038	0.41	0/1381
All	All	0.41	3/41761 (0.0%)	0.75	65/56385 (0.1%)

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
1	A	0	1
1	B	0	1
1	E	0	1
1	F	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	SER	CB-OG	-6.72	1.33	1.42
1	B	708	LYS	CE-NZ	5.60	1.63	1.49
1	F	545	PRO	N-CD	5.21	1.55	1.47

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	708	LYS	CD-CE-NZ	14.61	145.29	111.70
1	F	518	LEU	CB-CG-CD1	-10.49	93.17	111.00
1	A	597	LEU	CB-CG-CD2	-10.05	93.91	111.00
1	F	397	LEU	CA-CB-CG	9.14	136.32	115.30
1	C	322	LEU	CA-CB-CG	8.22	134.21	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	PRO	Peptide
1	B	438	GLY	Peptide
1	E	438	GLY	Peptide
1	F	438	GLY	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	5048	0	4974	346	0
1	B	5037	0	4996	313	0
1	C	5039	0	4965	309	0
1	D	4994	0	4923	331	0
1	E	5012	0	4954	336	0
1	F	4926	0	4896	311	0
2	G	2255	0	2199	142	0
2	H	2255	0	2199	113	0
2	I	2251	0	2188	117	0
2	J	2255	0	2199	125	0
3	K	493	0	491	61	0
4	L	536	0	527	58	0
5	M	1038	0	1011	117	0
All	All	41139	0	40522	2385	0

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 29.

The worst 5 of 2385 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:F:263:GLY:HA3	1:F:437:SER:HB2	1.29	1.14
1:A:549:LYS:NZ	1:A:647:SER:OG	1.93	1.01
2:H:271:ARG:HH11	2:I:234:ALA:HB2	1.28	0.98
2:I:200:TYR:HB3	5:M:161:ARG:HD2	1.43	0.97
2:H:219:LEU:HB2	2:H:222:LYS:HB3	1.46	0.97

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	668/747 (89%)	610 (91%)	43 (6%)	15 (2%)	8	49
1	B	662/747 (89%)	592 (89%)	55 (8%)	15 (2%)	8	48
1	C	666/747 (89%)	616 (92%)	37 (6%)	13 (2%)	9	51
1	D	663/747 (89%)	607 (92%)	44 (7%)	12 (2%)	11	53
1	E	658/747 (88%)	604 (92%)	43 (6%)	11 (2%)	11	55
1	F	644/747 (86%)	583 (90%)	43 (7%)	18 (3%)	6	44
2	G	284/297 (96%)	238 (84%)	34 (12%)	12 (4%)	3	34
2	H	284/297 (96%)	232 (82%)	44 (16%)	8 (3%)	6	44
2	I	284/297 (96%)	233 (82%)	44 (16%)	7 (2%)	7	46
2	J	284/297 (96%)	234 (82%)	41 (14%)	9 (3%)	5	41
3	K	59/63 (94%)	55 (93%)	2 (3%)	2 (3%)	5	40
4	L	64/67 (96%)	60 (94%)	3 (5%)	1 (2%)	12	56
5	M	127/188 (68%)	125 (98%)	2 (2%)	0	100	100
All	All	5347/5988 (89%)	4789 (90%)	435 (8%)	123 (2%)	12	48

5 of 123 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	A	293	LYS
1	A	294	TYR
1	A	318	ALA
1	A	333	ILE

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 PDB entries followed by that with respect to all EM entries.

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	515/638 (81%)	503 (98%)	12 (2%)	58	83
1	B	521/638 (82%)	511 (98%)	10 (2%)	65	86
1	C	516/638 (81%)	511 (99%)	5 (1%)	82	92
1	D	511/638 (80%)	504 (99%)	7 (1%)	74	89
1	E	516/638 (81%)	511 (99%)	5 (1%)	82	92
1	F	512/638 (80%)	509 (99%)	3 (1%)	90	95
2	G	235/244 (96%)	235 (100%)	0	100	100
2	H	235/244 (96%)	234 (100%)	1 (0%)	93	96
2	I	234/244 (96%)	234 (100%)	0	100	100
2	J	235/244 (96%)	235 (100%)	0	100	100
3	K	52/54 (96%)	52 (100%)	0	100	100
4	L	60/61 (98%)	58 (97%)	2 (3%)	45	76
5	M	113/161 (70%)	112 (99%)	1 (1%)	84	93
All	All	4255/5080 (84%)	4209 (99%)	46 (1%)	81	91

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	610	ASP
1	C	537	VAL
2	H	183	ASP

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Mol	Chain	Res	Type
1	B	651	VAL
1	C	180	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	505	ASN
1	F	194	ASN
2	J	98	GLN
1	E	527	GLN
1	E	624	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 carbohydrates 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](#)

There are no chain breaks in this entry.