Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 03:09 PM JST

PDB ID	:	7WJI
EMDB ID	:	EMD-32544
Title	:	Architecture of the human NALCN channelosome
Authors	:	Wu, J.P.; Yan, Z.; Zhou, L.; Liu, H.; Zhao, Q.
Deposited on	:	2022-01-06
Resolution	:	4.50 Å(reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp
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:

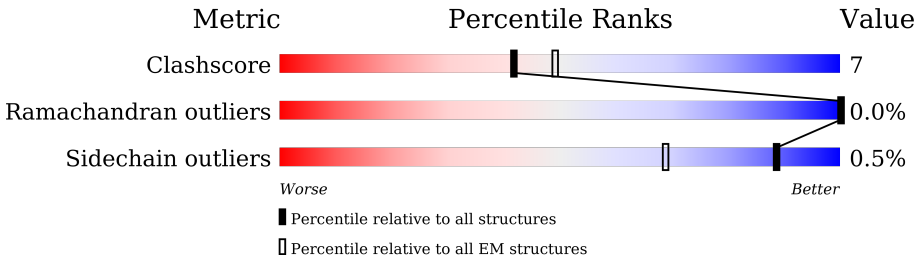
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3258	28% 44% 10% 46%
2	B	2658	35% 51% 12% 37%
3	E	149	83% 72% 13% 15%
4	C	1992	44% 59% 11% 30%
5	D	458	28% 29% 10% 60%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41173 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 Protein unc-80 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1763	14143	9070	2451	2525	97	0	0

- Molecule 2 is a protein called Protein unc-79 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1663	13146	8488	2188	2355	115	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2636	ASP	-	expression tag	UNP Q9P2D8
B	2637	GLU	-	expression tag	UNP Q9P2D8
B	2638	VAL	-	expression tag	UNP Q9P2D8
B	2639	ASP	-	expression tag	UNP Q9P2D8
B	2640	ALA	-	expression tag	UNP Q9P2D8
B	2641	GLY	-	expression tag	UNP Q9P2D8
B	2642	SER	-	expression tag	UNP Q9P2D8
B	2643	ASP	-	expression tag	UNP Q9P2D8
B	2644	TYR	-	expression tag	UNP Q9P2D8
B	2645	LYS	-	expression tag	UNP Q9P2D8
B	2646	ASP	-	expression tag	UNP Q9P2D8
B	2647	ASP	-	expression tag	UNP Q9P2D8
B	2648	ASP	-	expression tag	UNP Q9P2D8
B	2649	LYS	-	expression tag	UNP Q9P2D8
B	2650	GLY	-	expression tag	UNP Q9P2D8
B	2651	SER	-	expression tag	UNP Q9P2D8
B	2652	ASP	-	expression tag	UNP Q9P2D8
B	2653	TYR	-	expression tag	UNP Q9P2D8
B	2654	LYS	-	expression tag	UNP Q9P2D8
B	2655	ASP	-	expression tag	UNP Q9P2D8
B	2656	ASP	-	expression tag	UNP Q9P2D8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2657	ASP	-	expression tag	UNP Q9P2D8
B	2658	LYS	-	expression tag	UNP Q9P2D8

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	126	Total	C	N	O	S	0	0
			988	615	160	204	9		

- Molecule 4 is a protein called Sodium leak channel non-selective protein,Extended tegument protein pp150.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1394	Total	C	N	O	S	0	0
			11413	7523	1877	1926	87		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1739	LEU	-	linker	UNP Q8IZF0
C	1740	GLU	-	linker	UNP Q8IZF0
C	1741	GLY	-	linker	UNP Q8IZF0
C	1742	SER	-	linker	UNP Q8IZF0
C	1743	GLU	-	linker	UNP Q8IZF0
C	1744	ASN	-	linker	UNP Q8IZF0
C	1745	LEU	-	linker	UNP Q8IZF0
C	1746	TYR	-	linker	UNP Q8IZF0
C	1747	PHE	-	linker	UNP Q8IZF0
C	1748	GLN	-	linker	UNP Q8IZF0
C	1749	GLY	-	linker	UNP Q8IZF0
C	1750	GLY	-	linker	UNP Q8IZF0
C	1751	GLY	-	linker	UNP Q8IZF0
C	1752	GLY	-	linker	UNP Q8IZF0
C	1753	SER	-	linker	UNP Q8IZF0

- Molecule 5 is a protein called Transmembrane protein FAM155A.

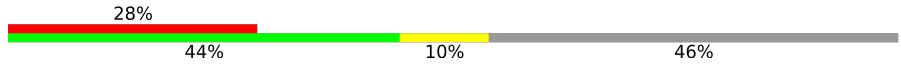
Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	182	Total	C	N	O	S	0	0
			1483	934	243	292	14		

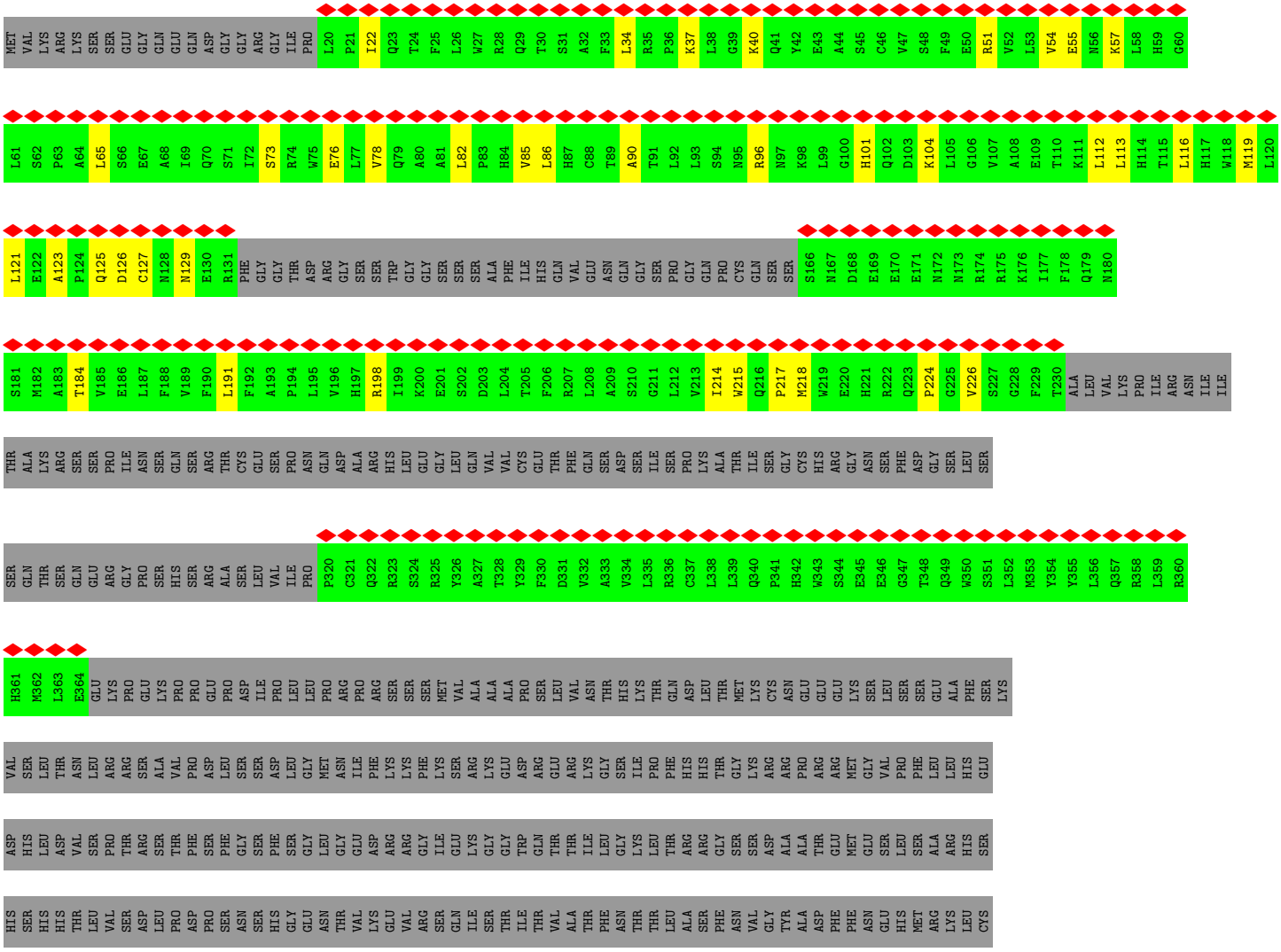
3 Residue-property plots (i)

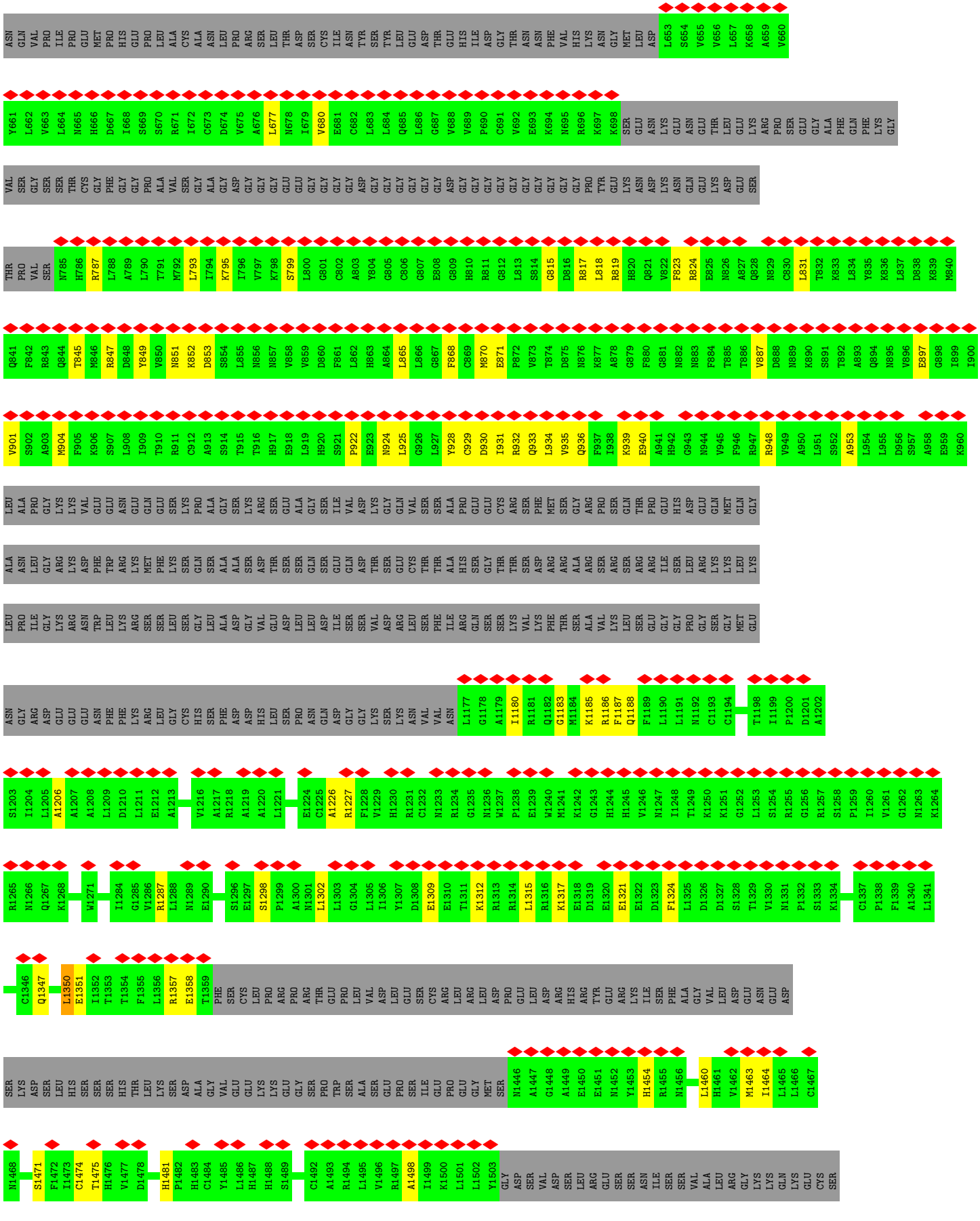
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

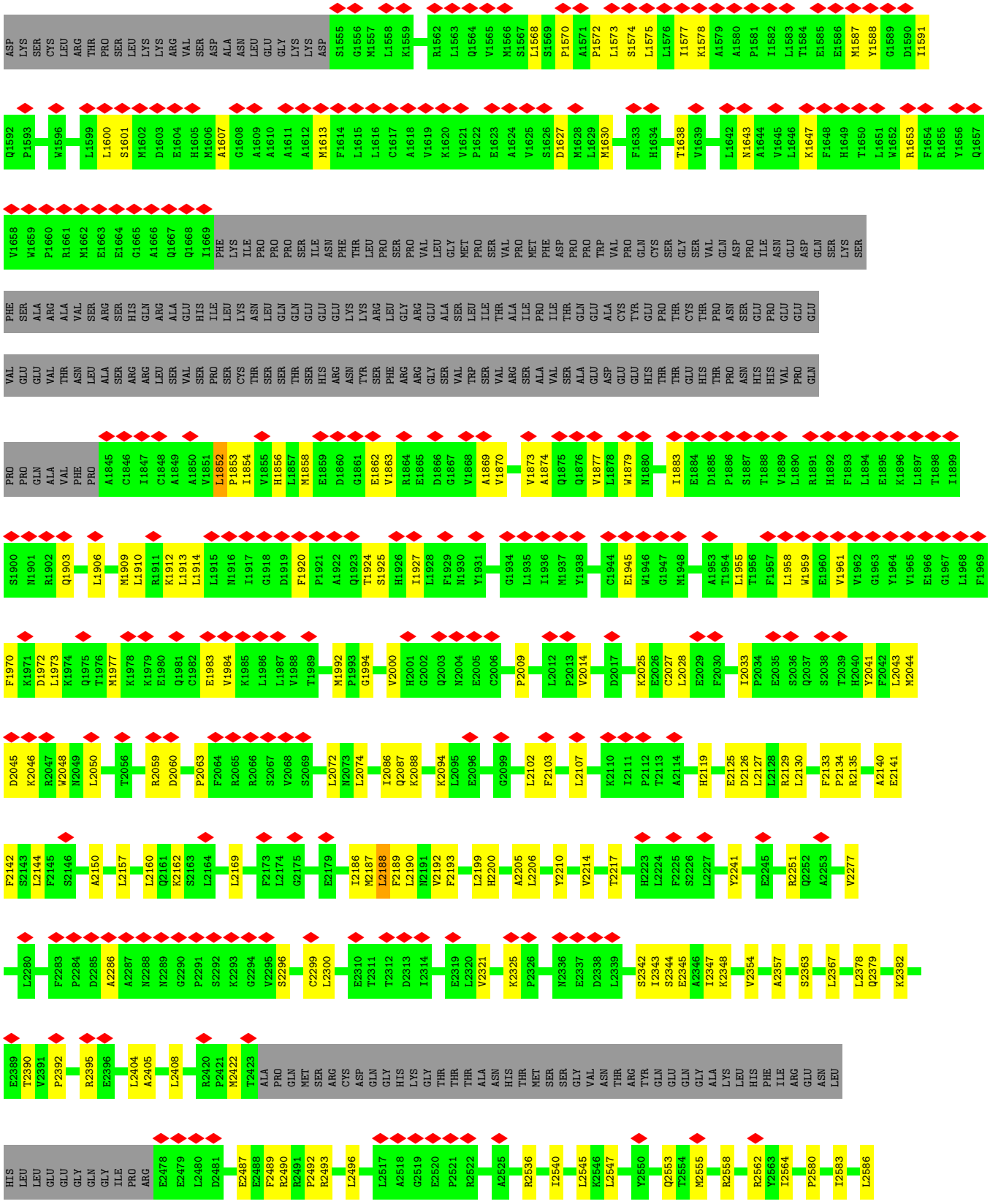
- Molecule 1: Protein unc-80 homolog

Chain A:






ASN GLN VAL PRO ILE PRO GLU MET PRO HIS GLU PRO LEU ALA CYS ALA ASN LEU PRO ARG SER LEU THR ASP SER CYS ILE ASN TYR SER TYR LEU GLU ASP THR GLU HIS ILE ASP GLY THR ASN ASN PHE VAL HIS LYS ASN GLY MET LEU ASP
L653 S654 V655 V656 L657 K658 A659 V660
Y661 L662 V663 L664 N665 H666 D667 I668 S669 S670 R671 I672 C673 D674 V675 A676 L677 N678 I679 V680 E681 C682 L683 L684 Q685 L686 G687 V688 V689 P690 C691 V692 E693 K694 N695 R696 K697 K698
SER GLU ASN LYS GLU ASN GLU THR LEU GLU GLY ALA PHE GLN PHE LYS GLY
VAL SER GLY SER SER THR CYS GLY PHE GLY GLY PRO ALA VAL SER GLY ALA GLY ASP GLY GLY GLY GLU GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY PRO TYR GLU LYS ASN ASP LYS ASN GLN GLU LYS ASP GLU SER
THR PRO VAL SER
N785 H786 R787 L788 A789 L790 T791 M792 L793 I794 K795 I796 V797 K798 S799 L800 G801 C802 A803 Y804 G805 C806 G807 E808 G809 H810 R811 G812 L813 S814 G815 D816 R817 L818 R819 H820 Q821 V822 F823 R824 E825 N826 A827 Q828 N829 C830 L831 T832 K833 L834 Y835 K836 L837 D838 K839 M840
Q841 F842 R843 Q844 T845 M846 R847 D848 Y849 V850 N851 K852 D853 S854 L855 N856 N857 V858 V859 D860 F861 L862 H863 A864 L865 L866 G867 F868 C869 M870 E871 P872 V873 T874 D875 N876 K877 A878 G879 F880 G881 N882 N883 F884 T885 T886 V887 D888 N889 K890 S891 T892 A893 Q894 N895 V896 E897 G898 I899 I900
V901 S902 A903 M904 F905 K906 S907 L908 I909 T910 R911 C912 A913 S914 T915 T916 H917 E918 L919 H920 S921 P922 E923 N924 L925 G926 L927 Y928 C929 D930 I931 R932 Q933 L934 V935 Q936 F937 I938 K939 E940 A941 H942 G943 N944 V945 F946 R947 R948 V949 A950 L951 S952 A953 L954 L955 D956 S957 A958 E959 K960
LEU ALA PRO GLY LYS LYS VAL GLU GLU GLN GLU ASN GLU GLN GLN GLU SER LYS PRO ALA ALA GLY SER LYS ARG SER GLU GLU ALA GLY SER ILE VAL ASP LYS GLY GLN VAL SER SER ALA PRO GLU GLU CYS ARG SER PHE MET SER GLY ARG PRO SER GLN THR PRO GLU HIS ASP GLU GLN MET GLN GLY
ALA ASN LEU GLY ARG LYS ASP PHE TRP ARG LYS MET PHE LYS SER GLN SER ALA ALA ASP SER ASP THR SER SER GLN SER GLU SER GLU ASP THR SER GLU GLN ASP ASP THR SER GLU CYS THR THR THR ALA HIS SER GLY THR THR SER ASP ARG ARG ALA ARG SER ARG SER ARG ARG ILE SER LEU ARG LYS LYS LEU LYS
LEU PRO ILE GLY LYS ARG ASN TRP LEU LYS ARG SER SER LEU SER GLY LEU ALA ASP GLY VAL GLU ASP LEU LEU ASP ILE SER SER VAL ASP ARG LEU SER PHE ILE ARG GLN SER SER LYS VAL LYS PHE THR SER ALA VAL LYS LEU SER GLU GLY GLY PRO GLY SER GLY MET GLU
ASN GLY ARG ASP GLU GLU GLU ASN PHE PHE LYS ARG LEU GLY CYS HIS SER PHE ASP ASP HIS LEU SER PRO ASN GLN ASP GLY GLY LYS SER LYS ASN VAL VAL ASN
L1177 G1178 A1179 I1180 R1181 Q1182 G1183 M1184 K1185 R1186 F1187 Q1188 F1189 L1190 L1191 N1192 C1193 C1194 T1198 I1199 P1200 D1201 A1202
S1203 I1204 L1205 A1206 A1207 A1208 L1209 D1210 L1211 E1212 A1213 V1216 A1217 R1218 A1219 A1220 L1221 E1224 C1225 A1226 R1227 F1228 V1229 H1230 R1231 C1232 N1233 R1234 G1235 N1236 W1237 P1238 E1239 W1240 M1241 K1242 G1243 H1244 H1245 V1246 N1247 I1248 T1249 K1250 K1251 G1252 L1253 S1254 R1255 G1256 R1257 S1258 P1259 I1260 V1261 G1262 N1263 K1264
R1265 N1266 Q1267 K1268 W1271 I1284 G1285 V1286 R1287 L1288 N1289 E1290 S1296 E1297 S1298 P1299 A1300 N1301 L1302 L1303 G1304 L1305 I1306 Y1307 D1308 E1309 E1310 T1311 K1312 R1313 R1314 L1315 R1316 K1317 E1318 D1319 E1320 E1321 E1322 D1323 F1324 L1325 D1326 D1327 S1328 T1329 V1330 N1331 P1332 S1333 K1334 C1337 P1338 F1339 A1340 L1341
C1346 Q1347 L1350 E1351 I1352 T1353 T1354 T1354 F1355 L1356 R1357 E1358 T1359
PHE SER CYS LEU PRO ARG PRO ARG THR GLU PRO LEU VAL ASP LEU GLU SER CYS ARG LEU ARG LEU ASP PRO GLU LEU ASP ARG HIS ARG TYR GLU ARG LYS ILE SER PHE ALA GLY VAL LEU ASP GLU ASN GLU ASP
SER LYS ASP SER LEU HIS SER SER HIS THR LEU LYS SER ASP ALA GLY VAL GLU GLU LYS LYS GLU GLY SER PRO TRP SER ALA SER GLU PRO SER ILE GLU PRO GLU GLY MET SER
N1446 A1447 G1448 A1449 E1450 E1451 N1452 Y1453 H1454 R1455 N1456 L1460 H1461 V1462 M1463 I1464 L1465 L1466 C1467
N1468 S1471 F1472 I1473 C1474 T1475 H1476 V1477 D1478 H1481 P1482 H1483 C1484 Y1485 L1486 H1487 H1488 S1489 C1492 A1493 R1494 L1495 V1496 R1497 A1498 I1499 K1500 L1501 L1502 Y1503
GLY ASP SER VAL ASP SER LEU ARG GLU SER SER ASN ILE SER SER VAL ALA LEU LEU ARG GLY LYS LYS GLN LYS GLU CYS SER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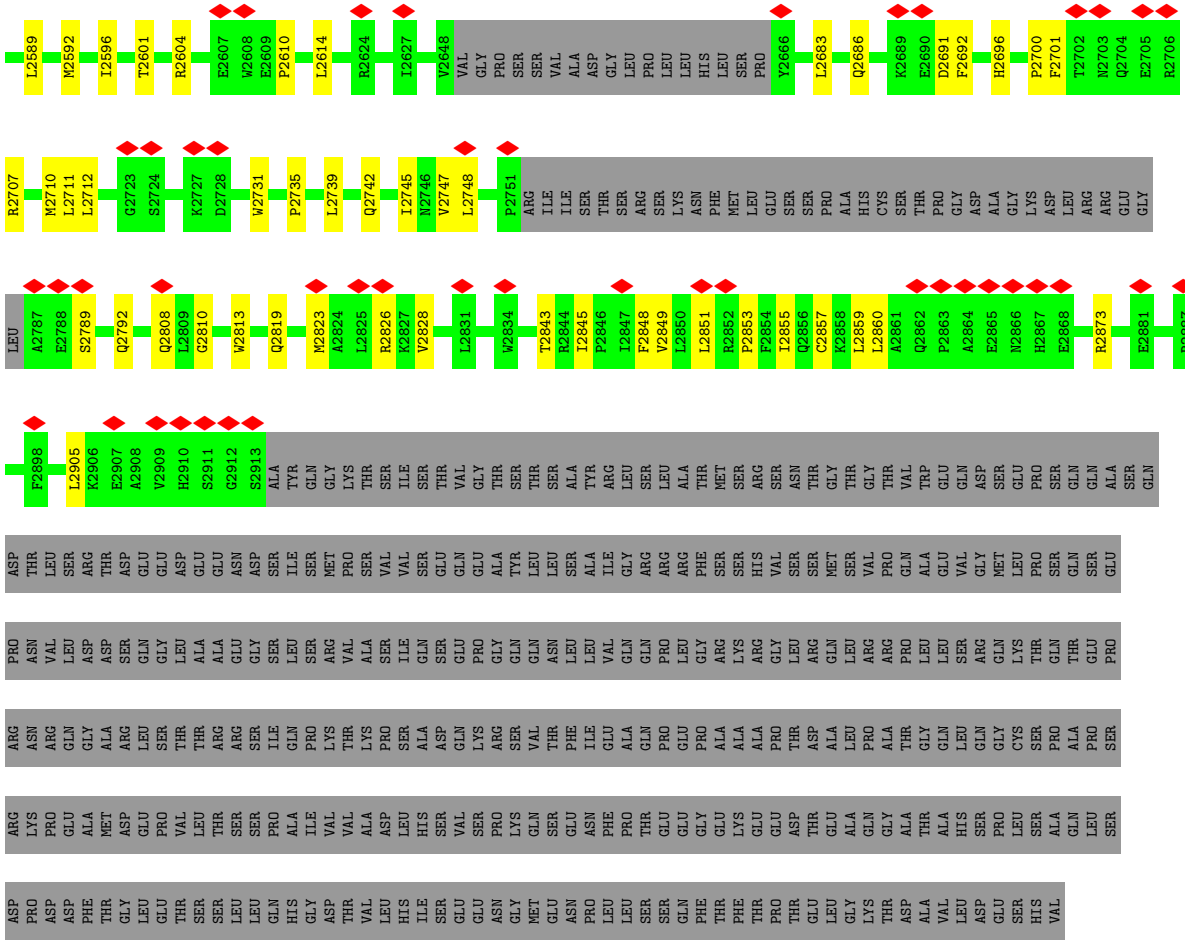
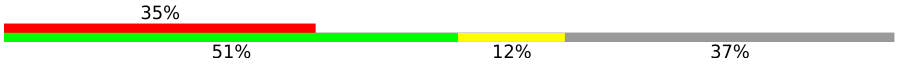
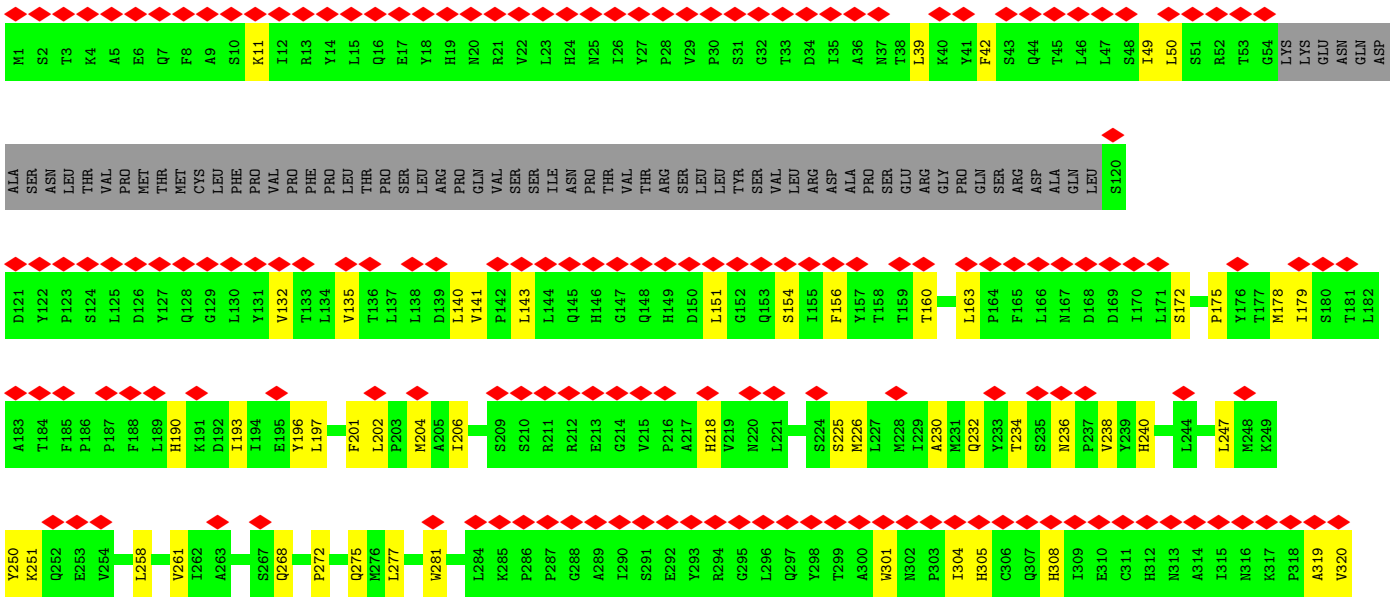
Q1592 P1593 W1596 L1599 L1600 S1601 M1602 D1603 E1604 H1605 M1606 A1607 G1608 A1609 A1610 A1611 A1612 M1613 F1614 L1615 L1616 C1617 A1618 V1619 K1620 V1621 P1622 E1623 A1624 V1625 S1626 D1627 M1628 L1629 M1630 F1633 H1634 T1638 V1639 L1642 N1643 A1644 V1645 L1646 K1647 F1648 H1649 T1650 L1651 W1652 R1653 F1654 R1655 Y1656 Q1657
V1658 W1659 P1660 R1661 M1662 E1663 E1664 G1665 A1666 Q1667 Q1668 I1669 PHE LYS ILE PRO PRO PRO SER ILE ASN PHE THR LEU PRO SER PRO VAL LEU GLY MET PRO SER VAL PRO MET PHE ASP PRO PRO TRP VAL PRO GLN CYS SER GLY SER VAL GLN ASP PRO ILE ASN GLU ASP GLN SER LYS SER
PHE SER ALA ARG ALA VAL SER ARG SER HIS GLN ARG ALA GLU HIS ILE LEU LYS ASN LEU GLN GLN GLU GLU GLU LYS LYS ARG LEU GLY ARG GLU GLU ALA SER LEU LEU ILE THR ALA ILE PRO ILE THR GLN GLU ALA CYS TYR GLU PRO THR CYS THR PRO PRO ASN SER GLU PRO ILE ASN GLU GLU GLU
VAL GLU GLU VAL THR ASN LEU ALA SER ARG ARG LEU SER VAL SER PRO SER CYS THR SER SER THR SER HIS ARG ASN TYR SER PHE ARG ARG GLY SER VAL TRP SER VAL ARG SER ALA VAL SER ALA GLU ASP GLU GLU HIS THR THR GLU HIS THR PRO ASN HIS HIS VAL PRO GLN
PRO PRO GLN ALA VAL PHE PRO A1845 C1846 I1847 C1848 A1849 A1850 V1851 L1852 P1853 I1854 V1855 H1856 L1857 M1858 E1859 D1860 G1861 E1862 V1863 R1864 E1865 D1866 G1867 V1868 A1869 V1870 V1873 A1874 Q1875 Q1876 V1877 L1878 W1879 N1880 I1883 E1884 D1885 P1886 S1887 T1888 V1889 L1890 R1891 H1892 F1893 L1894 E1895 K1896 L1897 T1898 I1899
S1900 N1901 R1902 Q1903 L1906 M1909 L1910 R1911 K1912 L1913 L1914 L1915 N1916 I1917 G1918 D1919 F1920 P1921 A1922 Q1923 T1924 S1925 H1926 I1927 L1928 F1929 N1930 Y1931 G1934 L1935 I1936 M1937 Y1938 C1944 E1945 W1946 G1947 M1948 A1953 T1954 L1955 T1956 F1957 L1958 W1959 E1960 V1961 V1962 G1963 Y1964 V1965 E1966 G1967 L1968 F1969
F1970 K1971 D1972 L1973 K1974 Q1975 T1976 M1977 K1978 K1979 E1980 Q1981 C1982 E1983 V1984 K1985 L1986 L1987 V1988 T1989 M1992 P1993 G1994 V2000 H2001 G2002 Q2003 N2004 E2005 C2006 P2009 L2012 P2013 V2014 D2017 K2025 E2026 C2027 L2028 E2029 F2030 I2033 P2034 E2035 S2036 Q2037 S2038 T2039 H2040 Y2041 F2042 L2043 M2044
D2045 K2046 R2047 W2048 N2049 L2050 T2056 R2059 D2060 P2063 F2064 R2065 R2066 S2067 V2068 S2069 L2072 N2073 L2074 I2086 Q2087 K2088 K2094 L2095 E2096 G2099 L2102 F2103 L2107 K2110 I2111 P2112 T2113 A2114 H2119 E2125 D2126 L2127 L2128 R2129 L2130 F2133 P2134 R2135 A2140 E2141
F2142 S2143 L2144 F2145 S2146 A2150 L2157 L2160 Q2161 K2162 S2163 L2164 L2169 F2173 L2174 G2175 E2179 I2186 M2187 L2188 F2189 L2190 N2191 V2192 F2193 L2199 H2200 A2205 L2206 Y2210 V2214 T2217 H2223 L2224 P2225 S2226 L2227 Y2241 E2245 R2251 Q2252 A2253 V2277
L2280 F2283 P2284 D2285 A2286 A2287 N2288 N2289 G2290 P2291 S2292 K2293 G2294 V2295 S2296 C2299 L2300 E2310 T2311 T2312 D2313 I2314 E2319 L2320 V2321 K2325 P2326 N2336 E2337 D2338 L2339 S2342 I2343 S2344 E2345 A2346 I2347 K2348 V2354 A2357 S2363 L2367 L2378 Q2379 K2382
E2389 T2390 V2391 P2392 R2395 E2396 L2404 A2405 L2408 R2420 P2421 M2422 T2423 ALA PRO GLN MET SER ARG CYS ASP GLN GLY HIS LYS GLY THR THR THR ALA ASN HIS THR MET SER SER GLY VAL ASN THR ARG TYR GLN GLU GLN GLY ALA LYS LEU HIS PHE ILE ARG GLU ASN LEU
HIS LEU LEU GLU GLU GLY GLN GLY ILE PRO ARG E2478 E2479 L2480 D2481 E2487 E2488 F2489 R2490 R2491 P2492 R2493 L2496 L2517 A2518 G2519 E2520 P2521 R2522 A2525 R2536 I2540 L2545 K2546 L2547 Y2550 Q2553 T2554 M2555 R2558 R2562 Y2563 I2564 P2580 I2583 L2586

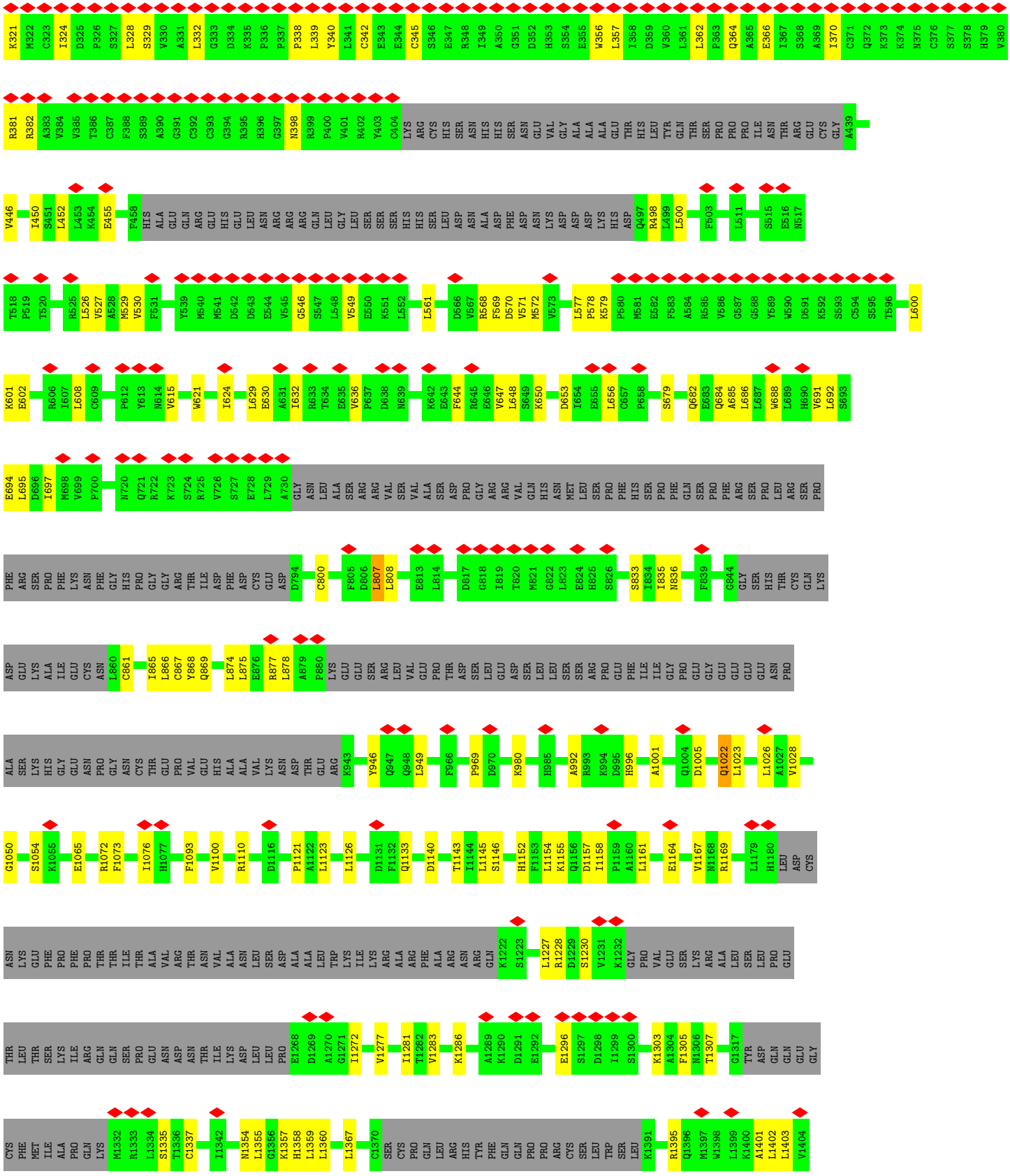


• Molecule 2: Protein unc-79 homolog

Chain B:



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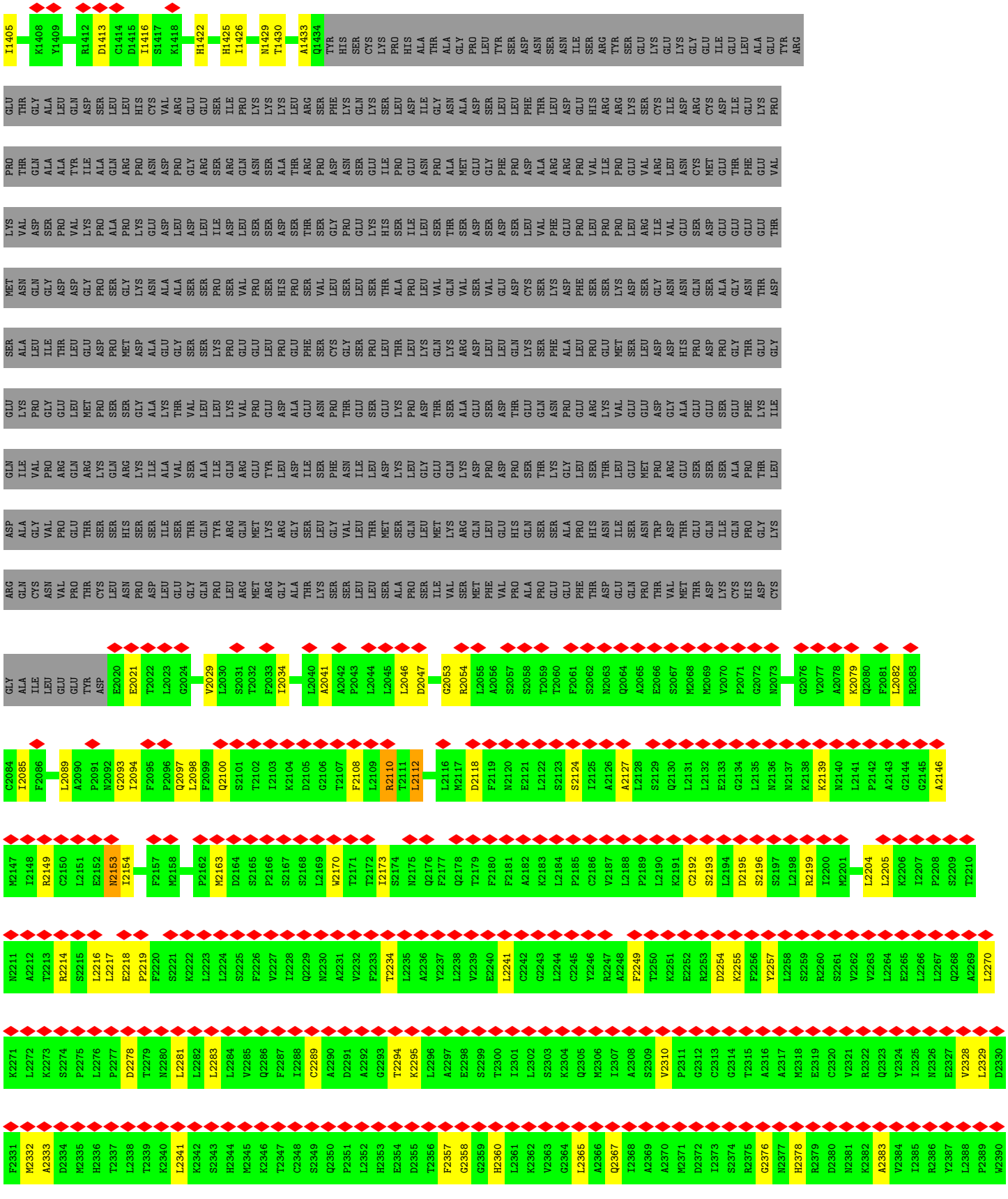
R381 R382 A383 V384 V385 T386 C387 F388 S389 A390 G391 C392 C393 G394 R395 H396 G397 N398 R399 P400 V401 R402 Y403 C404 LYS ARG CYS HIS SER ASN HIS HIS SER ASN GLU VAL GLY ALA ALA ALA GLU THR HIS LEU TYR GLN THR SER PRO PRO PRO ILE ASN THR ARG GLU CYS GLY A439
V446 I450 S451 L452 L453 K454 E455 F458 HIS ALA GLU GLN ARG GLU HIS GLU LEU ASN ARG ARG ARG GLN LEU GLY LEU SER SER SER HIS HIS SER LEU ASP ASN ALA ASP PHE ASP ASN LYS ASP ASP ASP LYS HIS ASP Q497 R498 L499 L500 F503 L511 S515 E516 N517
T518 P519 T520 R525 L526 V527 A528 M529 V530 F531 Y539 M540 M541 D542 D543 E544 V545 G546 S547 L548 V549 E550 K551 L552 L561 D566 V567 R568 F569 D570 V571 M572 V573 L577 P578 K579 P580 M581 E582 F583 A584 R585 V586 G587 G588 Y589 W590 D591 K592 S593 C594 S595 T596 L600
K601 E602 R606 I607 L608 C609 P612 Y613 N614 V615 W621 I624 L629 E630 A631 I632 R633 T634 E635 V636 P637 D638 N639 K642 E643 F644 R645 E646 V647 L648 S649 K650 D653 I654 E655 L656 C657 P658 S679 Q682 E683 Q684 A685 L686 L687 W688 L689 H690 V691 L692 S693
E694 L695 D696 I697 M698 V699 P700 N720 Q721 R722 K723 S724 R725 V726 S727 E728 L729 A730 GLY ASN LEU ALA SER ARG ARG VAL SER VAL ALA SER ASP PRO GLY ARG ARG VAL GLN HIS ASN MET LEU SER PRO PHE HIS SER PRO PHE GLN SER PRO PHE ARG SER PRO LEU ARG SER PRO
PHE ARG SER PRO PHE LYS ASN PHE GLY HIS PRO GLY GLY ARG THR ILE ASP PHE ASP CYS GLU ASP D794 C800 F805 D806 L807 L808 E813 L814 D817 G818 I819 T820 M821 G822 L823 E824 H825 S826 S833 I834 I835 N836 F839 G844 GLY SER HIS THR CYS GLN LYS
ASP GLU LYS ALA ILE GLU CYS ASN L860 C861 I865 L866 C867 Y868 Q869 L874 L875 E876 R877 L878 A879 P880 LYS GLU GLU SER ARG LEU VAL GLU PRO THR ASP SER LEU GLU ASP SER LEU LEU SER SER ARG PRO GLU PHE ILE ILE GLY PRO GLU GLY GLU GLU GLU GLU ASN PRO
ALA SER LYS HIS GLY GLU ASN PRO GLY ASN CYS THR GLU PRO VAL GLU HIS ALA ALA VAL LYS ASN ASP THR GLU ARG K943 Y946 Q947 Q948 L949 F966 P969 D970 K980 H985 A992 R993 K994 D995 H996 A1001 Q1004 D1005 Q1022 L1023 L1026 A1027 V1028
G1050 S1054 K1055 E1065 R1072 F1073 I1076 H1077 F1093 V1100 R1110 D1116 P1121 A1122 L1123 L1126 D1131 F1132 Q1133 D1140 T1143 I1144 L1145 S1146 H1152 F1153 L1154 K1155 Q1156 D1157 I1158 P1159 A1160 L1161 E1164 V1167 N1168 R1169 L1179 H1180 LEU ASP CYS
ASN LYS GLU PHE PRO PHE PRO THR THR ILE THR ALA VAL ARG THR ASN VAL ALA ASN LEU SER ASP ALA ALA LEU TRP LYS ILE LYS ARG ALA ARG PHE ALA ARG ASN ARG GLN K1222 S1223 L1227 R1228 D1229 S1230 V1231 K1232 GLY PRO VAL GLU SER LYS ARG ALA LEU SER LEU PRO GLU
THR LEU THR SER LYS ILE ARG GLN GLN SER PRO GLU ASN ASP ASN THR ILE LYS ASP LEU LEU PRO E1268 D1269 A1270 G1271 I1272 V1277 I1281 T1282 V1283 K1286 A1289 K1290 D1291 E1292 E1296 S1297 D1298 I1299 S1300 K1303 A1304 F1305 N1306 T1307 G1317 TYR ASP GLN GLN GLU GLY
CYS PHE MET ILE ALA PRO GLN LYS M1332 R1333 L1334 S1335 T1336 C1337 I1342 N1354 L1355 G1356 K1357 H1358 L1359 L1360 L1367 C1370 SER CYS PRO GLN LEU ARG HIS TYR PHE GLN GLN PRO PRO ARG CYS SER LEU TRP SER LEU K1391 R1395 Q1396 M1397 W1398 L1399 K1400 A1401 L1402 L1403 V1404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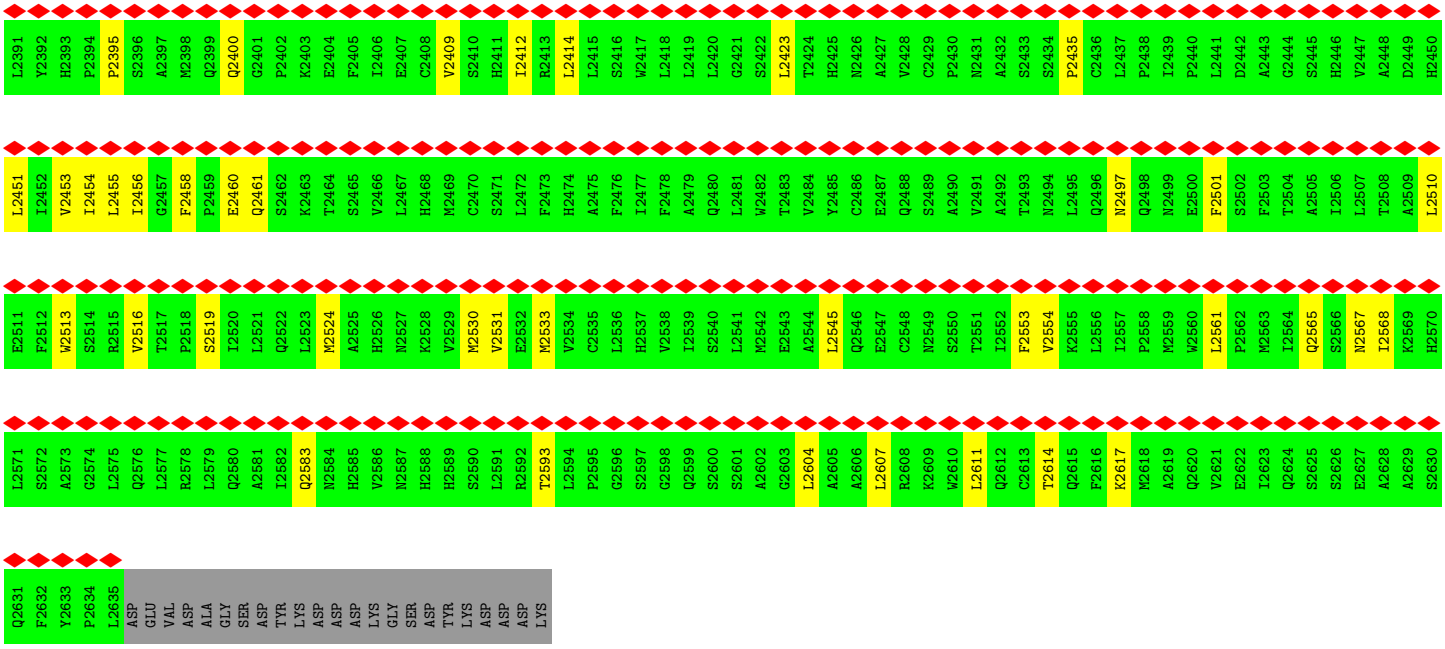
C2084 I2085 F2086 L2089 A2090 P2091 N2092 G2093 I2094 F2095 P2096 Q2097 L2098 F2099 Q2100 S2101 T2102 I2103 K2104 D2105 G2106 T2107 F2108 L2109 R2110 T2111 L2112 L2116 M2117 D2118 F2119 N2120 E2121 L2122 S2123 S2124 I2125 A2126 A2127 L2128 S2129 Q2130 L2131 L2132 E2133 G2134 L2135 N2136 N2137 K2138 K2139 N2140 L2141 P2142 A2143 G2144 G2145 A2146
M2147 I2148 R2149 C2150 L2151 E2152 N2153 I2154 F2157 M2158 P2162 M2163 D2164 S2165 P2166 S2167 S2168 L2169 W2170 T2171 T2172 I2173 S2174 N2175 Q2176 F2177 Q2178 T2179 F2180 F2181 A2182 K2183 L2184 P2185 C2186 V2187 L2188 P2189 L2190 K2191 C2192 S2193 L2194 D2195 S2196 S2197 L2198 R2199 I2200 M2201 L2204 L2205 K2206 I2207 P2208 S2209 T2210
N2211 A2212 T2213 R2214 S2215 L2216 L2217 E2218 P2219 F2220 S2221 K2222 L2223 L2224 S2225 F2226 V2227 I2228 Q2229 N2230 A2231 V2232 F2233 T2234 L2235 A2236 Y2237 L2238 V2239 E2240 L2241 C2242 G2243 L2244 C2245 Y2246 R2247 A2248 F2249 T2250 K2251 E2252 R2253 D2254 K2255 F2256 Y2257 L2258 S2259 R2260 S2261 V2262 V2263 L2264 E2265 L2266 L2267 Q2268 A2269 L2270
K2271 L2272 K2273 S2274 P2275 L2276 P2277 D2278 T2279 N2280 L2281 L2282 L2283 L2284 V2285 Q2286 F2287 I2288 C2289 A2290 D2291 A2292 G2293 T2294 K2295 L2296 A2297 E2298 S2299 T2300 I2301 L2302 S2303 K2304 Q2305 M2306 I2307 A2308 S2309 V2310 P2311 G2312 C2313 G2314 T2315 A2316 A2317 M2318 E2319 C2320 V2321 R2322 Q2323 Y2324 I2325 N2326 E2327 V2328 L2329 D2330
F2331 M2332 A2333 D2334 M2335 H2336 T2337 L2338 T2339 K2340 L2341 K2342 S2343 H2344 M2345 K2346 T2347 C2348 S2349 Q2350 P2351 L2352 H2353 E2354 D2355 T2356 F2357 G2358 G2359 H2360 L2361 K2362 V2363 G2364 L2365 A2366 Q2367 I2368 A2369 A2370 M2371 D2372 I2373 S2374 R2375 G2376 N2377 H2378 R2379 D2380 N2381 K2382 A2383 V2384 I2385 R2386 Y2387 L2388 P2389 W2390

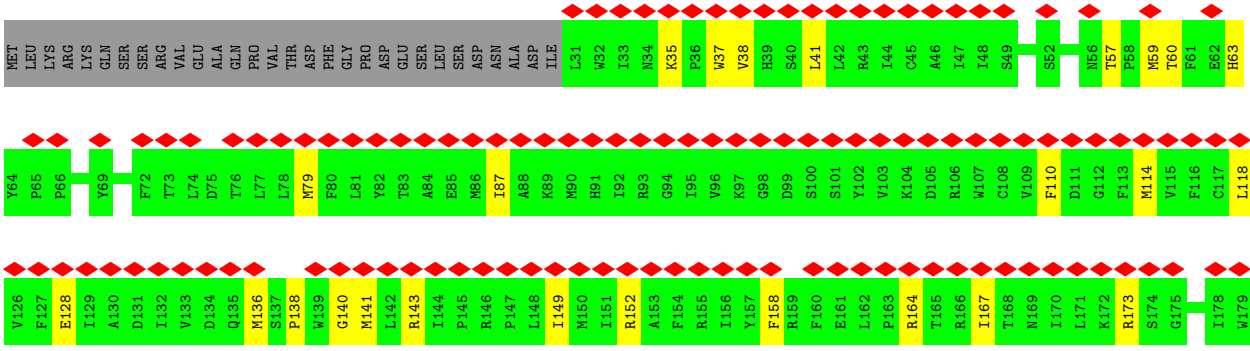


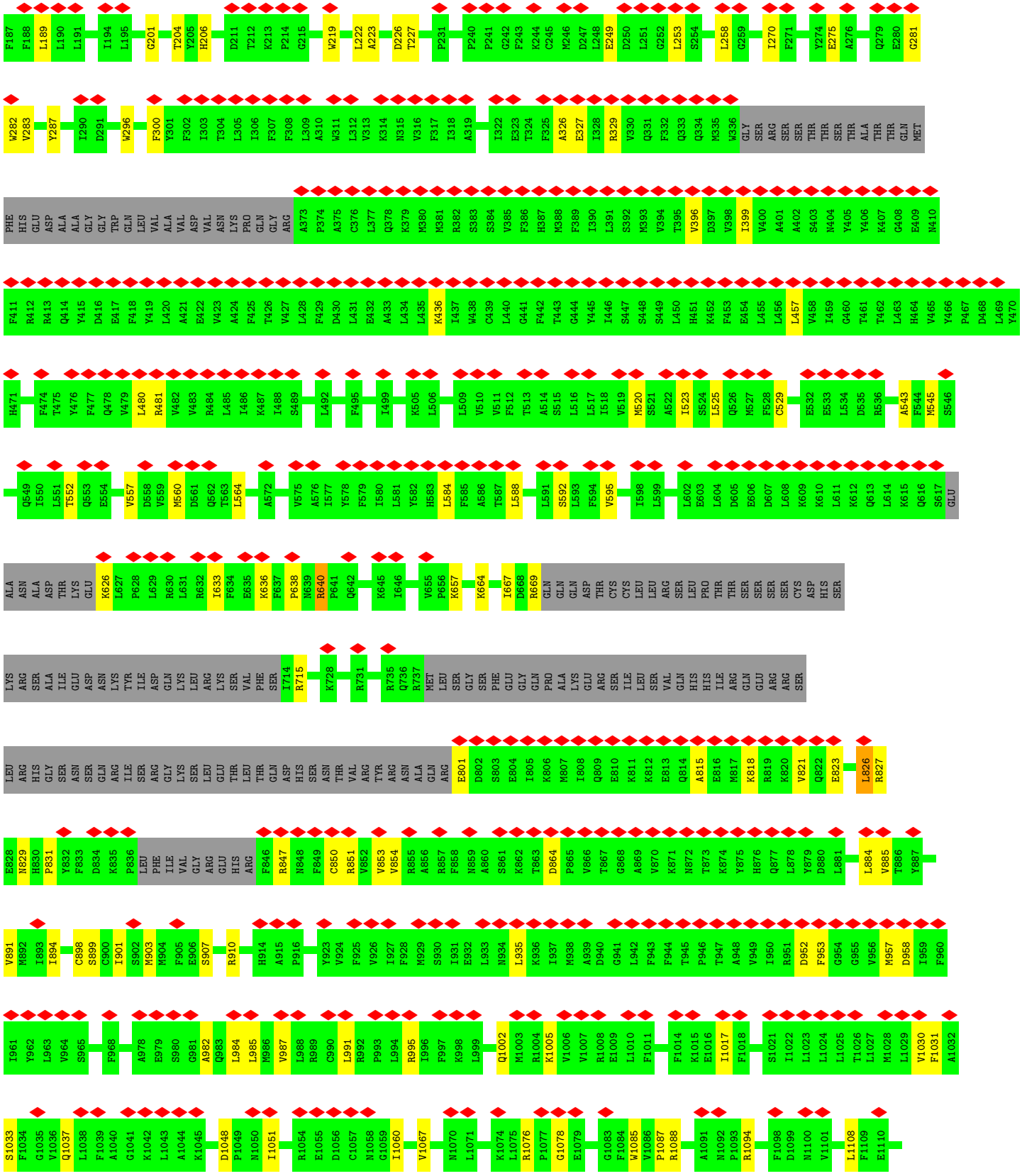
• Molecule 3: Calmodulin-1

Chain E:

• Molecule 4: Sodium leak channel non-selective protein,Extended tegument protein pp150

Chain C:

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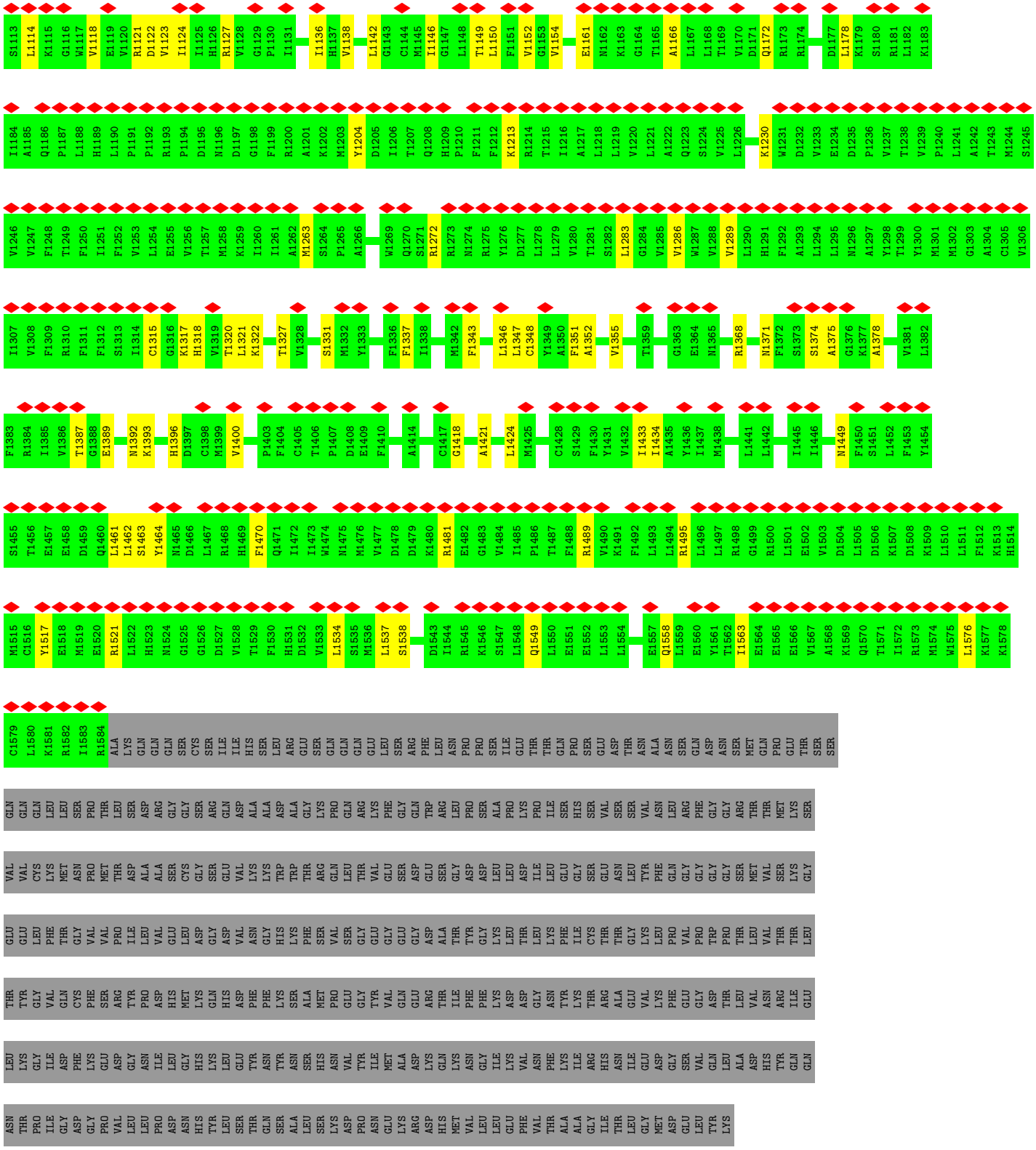
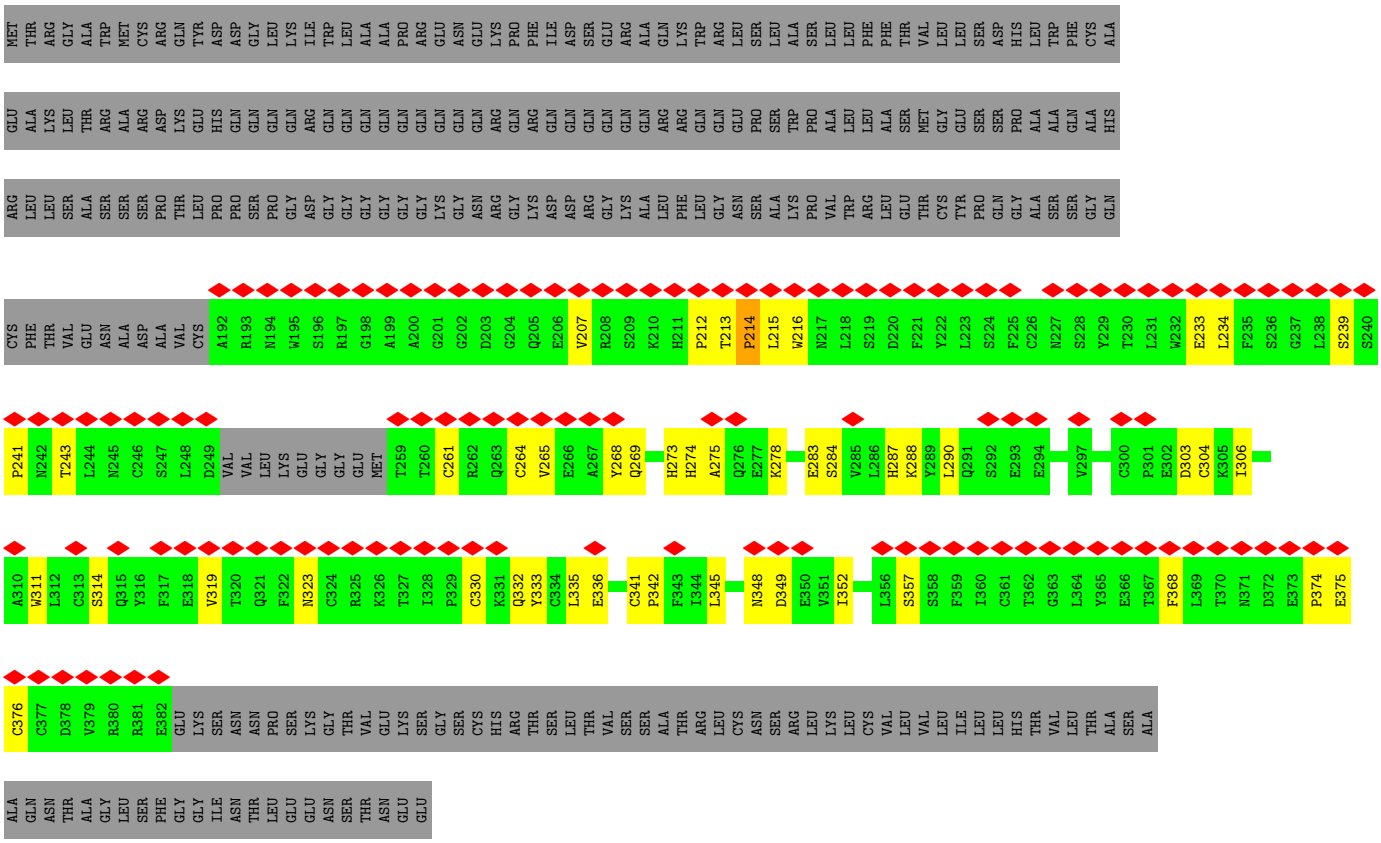
W282 V283 Y287 I290 D291 W296 F300 Y301 F302 I303 T304 L305 I306 F307 F308 L309 A310 W311 L312 V313 K314 N315 V316 F317 I318 A319 I322 E323 T324 F325 A326 E327 I328 R329 V330 Q331 F332 Q333 Q334 M335 W336 GLY SER ARG SER SER THR THR SER THR ALA THR THR GLN MET
PHE HIS GLU ASP ALA ALA GLY GLY TRP GLN LEU VAL ALA VAL ASP VAL ASN LYS PRO GLN GLY ARG A373 P374 A375 C376 L377 Q378 K379 M380 M381 R382 S383 S384 V385 F386 H387 M388 F389 I390 L391 S392 M393 V394 T395 V396 D397 V398 I399 V400 A401 A402 S403 N404 Y405 Y406 K407 G408 E409 N410
F411 R412 R413 Q414 Y415 D416 E417 F418 Y419 L420 A421 E422 V423 A424 F425 T426 V427 L428 F429 D430 L431 E432 A433 L434 L435 K436 I437 W438 C439 L440 G441 F442 T443 G444 Y445 I446 S447 S448 S449 L450 H451 K452 F453 E454 L455 L456 L457 V458 I459 G460 T461 T462 L463 H464 V465 Y466 P467 D468 L469 Y470
H471 F474 T475 Y476 F477 Q478 V479 L480 R481 V482 V483 R484 L485 I486 K487 I488 S489 L492 F495 I499 K505 L506 L509 V510 V511 F512 T513 A514 S515 L516 L517 I518 V519 M520 S521 A522 I523 S524 L525 Q526 M527 F528 C529 E532 E533 L534 D535 R536 A543 F544 M545 S546
Q549 I550 L551 T552 Q553 E554 V557 D558 V559 M560 D561 Q562 T563 L564 A572 V575 A576 I577 Y578 F579 I580 L581 Y582 H583 L584 F585 A586 T587 L588 L591 S592 L593 F594 V595 I598 L599 L602 E603 L604 D605 E606 D607 L608 K609 K610 L611 K612 Q613 L614 K615 Q616 S617 GLU
ALA ASN ALA ASP THR LYS GLU K626 L627 P628 L629 R630 L631 R632 I633 F634 E635 K636 F637 P638 N639 R640 P641 Q642 K645 I646 V655 P656 K657 K664 I667 D668 R669 GLN GLN GLN ASP THR CYS CYS LEU LEU ARG SER LEU PRO THR THR SER SER SER SER CYS ASP HIS SER
LYS ARG SER ALA ILE GLU ASP ASN LYS TYR ILE ASP GLN LYS LEU ARG LYS SER VAL PHE SER I714 R715 K728 R731 R735 Q736 R737 MET LEU SER GLY SER PHE GLU GLY GLN PRO ALA LYS GLU ARG SER ILE LEU SER VAL GLN HIS HIS ILE ARG GLN GLU ARG ARG SER
LEU ARG HIS GLY SER ASN SER GLN ARG ILE SER ARG GLY LYS SER LEU GLU THR LEU THR GLN ASP HIS SER ASN THR VAL ARG TYR ARG ASN ALA GLN ARG E801 D802 S803 E804 I805 K806 M807 I808 Q809 E810 K811 K812 E813 Q814 A815 E816 M817 K818 R819 K820 V821 Q822 E823 L826 R827
E828 N829 H830 P831 Y832 F833 D834 K835 P836 LEU PHE ILE VAL GLY ARG GLU HIS ARG F846 R847 N848 F849 C850 R851 V852 V853 V854 R855 A856 R857 F858 N859 A860 S861 K862 T863 D864 P865 V866 T867 G868 A869 V870 K871 N872 T873 K874 Y875 H876 Q877 L878 Y879 D880 L881 L884 V885 T886 Y887
V891 M892 I893 I894 C898 S899 C900 I901 S902 M903 M904 F905 E906 S907 R910 H914 A915 P916 Y923 V924 F925 V926 I927 F928 M929 S930 I931 E932 L933 N934 L935 K936 I937 M938 A939 D940 G941 L942 F943 F944 T945 P946 T947 A948 Y949 I950 R951 D952 F953 G954 G955 V956 M957 D958 I959 F960
I961 Y962 L963 V964 S965 F968 A978 E979 S980 G981 A982 Q983 L984 L985 M986 V987 L988 R989 C990 L991 R992 P993 L994 R995 I996 F997 K998 L999 Q1002 M1003 R1004 K1005 V1006 V1007 R1008 E1009 L1010 F1011 F1014 K1015 E1016 I1017 F1018 S1021 I1022 L1023 L1024 L1025 T1026 L1027 M1028 L1029 V1030 F1031 A1032
S1033 F1034 G1035 V1036 Q1037 L1038 F1039 A1040 G1041 K1042 L1043 A1044 K1045 D1048 P1049 N1050 I1051 R1054 E1055 D1056 C1057 N1058 G1059 I1060 V1067 N1070 L1071 K1074 L1075 R1076 P1077 G1078 E1079 G1083 F1084 W1085 V1086 P1087 R1088 A1091 N1092 P1093 R1094 F1098 D1099 N1100 V1101 L1108 F1109 E1110



• Molecule 5: Transmembrane protein FAM155A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GLU ALA LYS LEU THR ARG ALA ARG ASP LYS GLU HIS GLN GLN GLN GLN ARG GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN ARG GLN GLN GLN GLN GLN ARG ARG GLN GLN GLU PRO SER TRP PRO ALA LEU LEU ALA SER MET GLY GLU SER SER PRO ALA ALA ALA GLN ALA HIS
ARG LEU LEU SER ALA SER SER SER PRO THR LEU PRO PRO PRO SER PRO GLY ASP GLY GLY GLY GLY GLY LYS GLY GLY ASN ARG GLY LYS ASP ASP ARG GLY LYS ALA LEU PHE LEU GLY ASN SER ALA LYS PRO VAL TRP ARG LEU GLU THR CYS TYR PRO GLN GLY ALA SER SER GLY GLN
CYS PHE THR VAL GLU ASN ALA ASP ALA VAL CYS A192 R193 N194 W196 S196 R197 G198 A199 A200 G201 G202 D203 G204 Q205 E206 V207 R208 S209 K210 H211 P212 T213 P214 L215 W216 N217 L218 S219 D220 F221 Y222 L223 S224 F225 C226 N227 S228 Y229 T230 L231 W232 E233 L234 F235 S236 G237 L238 S239 S240
P241 N242 T243 L244 N245 C246 S247 L248 D249 VAL VAL LEU LYS GLU GLY GLY GLU MET T259 T260 C261 R262 Q263 C264 V265 E266 A267 Y268 Q269 H273 H274 A275 Q276 E277 K278 E283 S284 V285 L286 H287 K288 Y289 L290 Q291 S292 E293 E294 V297 C300 P301 E302 D303 C304 K305 I306
A310 W311 L312 C313 S314 Q315 Y316 F317 E318 V319 T320 Q321 F322 N323 C324 R325 K326 T327 I328 P329 C330 K331 Q332 Y333 C334 L335 E336 C341 P342 F343 I344 L345 N348 D349 E350 V351 I352 L356 S357 S358 F359 I360 C361 T362 G363 L364 Y365 E366 T367 F368 L369 T370 N371 D372 E373 P374 E375
C376 C377 D378 V379 R380 R381 E382 GLU LYS SER ASN ASN PRO SER LYS GLY THR VAL GLU LYS SER GLY SER CYS HIS ARG THR SER LEU THR VAL SER SER ALA THR ARG LEU CYS ASN SER ARG LEU LYS LEU CYS VAL LEU VAL LEU ILE LEU LEU HIS THR VAL LEU THR ALA SER ALA
ALA GLN ASN THR ALA GLY LEU SER PHE GLY GLY ILE ASN THR LEU GLU GLU ASN SER THR ASN GLU GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174294	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.947	Depositor
Minimum map value	-1.055	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	556.544, 556.544, 556.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.33	0/14450	0.69	0/19574
2	B	0.32	0/13441	0.68	0/18238
3	E	0.33	0/997	0.67	0/1335
4	C	0.34	0/11701	0.72	0/15843
5	D	0.38	0/1522	0.73	0/2065
All	All	0.33	0/42111	0.69	0/57055

There are no bond length outliers.

There are no bond angle outliers.

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	14143	0	14323	208	0
2	B	13146	0	13362	207	0
3	E	988	0	920	12	0
4	C	11413	0	11682	157	0
5	D	1483	0	1374	30	0
All	All	41173	0	41661	601	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 7.

All (601) 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)
2:B:178:MET:SD	2:B:197:LEU:HD22	1.47	1.53
1:A:1460:LEU:HD22	1:A:1463:MET:CE	1.47	1.40
2:B:178:MET:SD	2:B:197:LEU:CD2	2.34	1.15
1:A:1460:LEU:HD22	1:A:1463:MET:HE2	1.31	1.13
3:E:110:MET:HG3	4:C:1576:LEU:HD11	1.30	1.11
2:B:874:LEU:HG	2:B:877:ARG:HH21	1.16	1.09
1:A:2169:LEU:HD11	1:A:2192:VAL:HG21	1.34	1.05
1:A:1460:LEU:HD22	1:A:1463:MET:HE1	1.11	1.05
4:C:1318:HIS:CD2	4:C:1321:LEU:H	1.76	1.01
1:A:2169:LEU:CD1	1:A:2192:VAL:HG21	1.91	1.00
2:B:2054:ARG:HD3	2:B:2108:PHE:HB2	1.42	0.98
4:C:1347:LEU:CD2	4:C:1351:PHE:HE2	1.78	0.96
1:A:1460:LEU:CD2	1:A:1463:MET:CE	2.43	0.96
1:A:1463:MET:SD	1:A:1575:LEU:HD13	2.07	0.94
1:A:1460:LEU:CD2	1:A:1463:MET:HE1	1.99	0.93
4:C:1318:HIS:HD2	4:C:1321:LEU:H	1.14	0.91
1:A:1913:LEU:HD12	1:A:1914:LEU:N	1.89	0.88
2:B:197:LEU:HD23	2:B:201:PHE:HD2	1.39	0.88
5:D:261:CYS:O	5:D:265:VAL:HG23	1.72	0.88
4:C:1347:LEU:CD2	4:C:1351:PHE:CE2	2.58	0.87
2:B:304:ILE:CG2	2:B:340:TYR:CZ	2.58	0.86
2:B:1305:PHE:HZ	2:B:1359:LEU:HD21	1.38	0.86
4:C:457:LEU:HD11	4:C:481:ARG:HE	1.41	0.84
4:C:982:ALA:O	4:C:985:LEU:HB2	1.76	0.83
2:B:2053:GLY:HA3	2:B:2108:PHE:HE1	1.44	0.82
4:C:1347:LEU:HD21	4:C:1351:PHE:HE2	1.43	0.82
4:C:1347:LEU:HD23	4:C:1351:PHE:CE2	2.16	0.81
4:C:457:LEU:CD1	4:C:481:ARG:HE	1.92	0.81
2:B:874:LEU:HG	2:B:877:ARG:NH2	1.94	0.80
2:B:304:ILE:CG2	2:B:340:TYR:CE2	2.64	0.80
1:A:2363:SER:O	1:A:2367:LEU:HG	1.81	0.80
2:B:992:ALA:HA	2:B:996:HIS:HB2	1.64	0.80
4:C:136:MET:HG2	4:C:136:MET:O	1.81	0.80
1:A:1460:LEU:CD2	1:A:1463:MET:HE2	2.08	0.79
2:B:304:ILE:HG21	2:B:340:TYR:CZ	2.16	0.79
4:C:1347:LEU:HD21	4:C:1351:PHE:CE2	2.18	0.78
1:A:2000:VAL:O	1:A:2009:PRO:HA	1.83	0.78
2:B:450:ILE:HD11	2:B:526:LEU:HD23	1.66	0.78
2:B:197:LEU:HD23	2:B:201:PHE:CD2	2.20	0.77
2:B:304:ILE:HG22	2:B:340:TYR:CE2	2.20	0.77
4:C:1318:HIS:NE2	4:C:1320:THR:HB	2.00	0.77
1:A:2169:LEU:CD1	1:A:2192:VAL:CG2	2.63	0.77

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2748:LEU:HD22	1:A:2823:MET:CE	2.16	0.76
4:C:1114:LEU:HG	4:C:1114:LEU:O	1.84	0.76
4:C:1433:ILE:HG13	4:C:1434:ILE:HD12	1.69	0.75
1:A:922:PRO:O	1:A:925:LEU:HB2	1.86	0.74
2:B:450:ILE:HD11	2:B:526:LEU:CD2	2.17	0.74
2:B:193:ILE:O	2:B:197:LEU:HG	1.87	0.74
1:A:2748:LEU:HD22	1:A:2823:MET:HE1	1.68	0.73
4:C:1031:PHE:HD2	4:C:1108:LEU:HD21	1.52	0.73
1:A:2367:LEU:CD1	1:A:2492:PRO:HB3	2.19	0.72
2:B:835:ILE:HD11	2:B:874:LEU:HD22	1.71	0.72
1:A:1854:ILE:O	1:A:1858:MET:HG2	1.89	0.71
1:A:1350:LEU:HG	1:A:1575:LEU:HG	1.72	0.71
2:B:304:ILE:HG21	2:B:340:TYR:CE2	2.26	0.70
1:A:1910:LEU:HD13	1:A:1913:LEU:HD21	1.72	0.70
4:C:222:LEU:HD23	4:C:223:ALA:O	1.91	0.70
5:D:304:CYS:SG	5:D:341:CYS:HB2	2.31	0.69
1:A:1206:ALA:HB1	1:A:1287:ARG:HG3	1.74	0.69
4:C:552:THR:HG22	4:C:1114:LEU:HD11	1.75	0.68
2:B:304:ILE:HG22	2:B:340:TYR:CZ	2.28	0.68
2:B:304:ILE:CG2	2:B:340:TYR:OH	2.42	0.68
1:A:2378:LEU:HD21	1:A:2404:LEU:CD2	2.23	0.68
4:C:1352:ALA:HA	4:C:1355:VAL:HG12	1.75	0.68
2:B:2079:LYS:HE2	2:B:2112:LEU:HB3	1.75	0.67
2:B:833:SER:HA	2:B:836:ASN:HD22	1.60	0.67
2:B:2454:ILE:O	2:B:2458:PHE:HB2	1.94	0.67
2:B:324:ILE:HG22	2:B:338:PRO:HB3	1.77	0.67
4:C:1085:TRP:CD1	5:D:278:LYS:HG3	2.31	0.66
1:A:1852:LEU:HB3	1:A:1853:PRO:HD3	1.78	0.65
2:B:328:LEU:O	2:B:332:LEU:HB2	1.96	0.65
4:C:1213:LYS:HG2	4:C:1317:LYS:HE2	1.77	0.65
4:C:79:MET:HG3	4:C:122:LEU:HD11	1.76	0.65
1:A:2367:LEU:HD12	1:A:2492:PRO:HB3	1.79	0.64
1:A:2125:GLU:OE1	1:A:2129:ARG:NH1	2.30	0.64
2:B:2524:MET:HG2	2:B:2531:VAL:HG22	1.78	0.64
2:B:561:LEU:HD13	2:B:615:VAL:HG13	1.81	0.63
1:A:1463:MET:SD	1:A:1575:LEU:CD1	2.86	0.63
2:B:694:GLU:HG3	2:B:695:LEU:HD12	1.80	0.63
4:C:850:CYS:HB2	4:C:935:LEU:HG	1.81	0.61
5:D:239:SER:HB3	5:D:243:THR:HB	1.81	0.61
5:D:341:CYS:SG	5:D:342:PRO:HD2	2.41	0.61
2:B:232:GLN:OE1	2:B:268:GLN:NE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2367:LEU:CD1	1:A:2492:PRO:CB	2.79	0.60
1:A:819:ARG:HA	1:A:823:PHE:HB3	1.82	0.60
1:A:2379:GLN:OE1	1:A:2382:LYS:CE	2.50	0.60
4:C:884:LEU:HD12	4:C:885:VAL:HG13	1.82	0.60
1:A:123:ALA:O	1:A:127:CYS:HB3	2.02	0.60
3:E:64:ILE:HD11	3:E:69:PHE:HB2	1.83	0.60
2:B:630:GLU:HB3	2:B:688:TRP:HZ2	1.66	0.60
2:B:2046:LEU:HB3	2:B:2098:LEU:HD21	1.82	0.60
1:A:2580:PRO:HA	1:A:2583:ILE:HG12	1.83	0.59
4:C:1537:LEU:HD12	4:C:1538:SER:N	2.17	0.59
4:C:1002:GLN:HB3	4:C:1337:PHE:HE1	1.66	0.59
4:C:1400:VAL:H	4:C:1418:GLY:HA3	1.68	0.59
2:B:370:ILE:HG13	2:B:381:ARG:HB2	1.83	0.59
2:B:2205:LEU:HD11	2:B:2241:LEU:HD23	1.84	0.59
4:C:1343:PHE:O	4:C:1346:LEU:HG	2.02	0.59
4:C:1150:LEU:O	4:C:1154:VAL:HG12	2.02	0.59
1:A:2060:ASP:OD2	1:A:2135:ARG:NH1	2.35	0.59
2:B:2329:LEU:O	2:B:2333:ALA:HB2	2.02	0.59
2:B:304:ILE:HG22	2:B:340:TYR:OH	2.02	0.58
1:A:2558:ARG:HD2	1:A:2562:ARG:HH21	1.68	0.58
1:A:929:CYS:O	1:A:932:ARG:HB3	2.03	0.58
1:A:1973:LEU:O	1:A:1977:MET:HB2	2.03	0.58
1:A:2696:HIS:HA	1:A:2700:PRO:HD3	1.85	0.58
2:B:2192:CYS:SG	2:B:2193:SER:N	2.75	0.58
4:C:143:ARG:NH2	4:C:529:CYS:SG	2.76	0.58
2:B:202:LEU:HD11	2:B:247:LEU:HD13	1.85	0.58
1:A:2205:ALA:HB2	2:B:1072:ARG:HH12	1.69	0.58
4:C:227:THR:OG1	4:C:1368:ARG:NH2	2.37	0.58
2:B:577:LEU:HG	2:B:578:PRO:HD2	1.85	0.58
2:B:2234:THR:HA	2:B:2283:LEU:HD11	1.85	0.58
4:C:1393:LYS:HA	4:C:1396:HIS:HB2	1.86	0.58
1:A:1955:LEU:HA	1:A:1958:LEU:HB2	1.85	0.58
2:B:2524:MET:SD	2:B:2567:ASN:ND2	2.75	0.58
3:E:67:PRO:HA	3:E:70:LEU:HD12	1.86	0.58
2:B:450:ILE:HG23	2:B:529:MET:HG3	1.85	0.57
2:B:236:ASN:O	2:B:240:HIS:ND1	2.36	0.57
4:C:457:LEU:HD11	4:C:481:ARG:NE	2.14	0.57
2:B:2110:ARG:O	2:B:2110:ARG:HG2	2.04	0.57
2:B:1028:VAL:HG21	2:B:1073:PHE:HB3	1.84	0.57
4:C:520:MET:HA	4:C:523:ILE:HG12	1.85	0.57
2:B:608:LEU:HD22	2:B:647:VAL:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:621:TRP:HA	2:B:624:ILE:HG12	1.86	0.57
2:B:2079:LYS:CE	2:B:2112:LEU:HB3	2.34	0.57
1:A:933:GLN:O	1:A:936:GLN:HB3	2.04	0.57
5:D:330:CYS:HB2	5:D:374:PRO:HG2	1.85	0.57
4:C:326:ALA:HA	4:C:329:ARG:HD2	1.87	0.57
1:A:2127:LEU:HA	1:A:2130:LEU:HD12	1.86	0.57
2:B:2400:GLN:HE22	2:B:2456:ILE:HB	1.69	0.57
4:C:1318:HIS:HD2	4:C:1321:LEU:N	1.95	0.57
4:C:1033:SER:O	4:C:1037:GLN:HB2	2.05	0.57
5:D:233:GLU:OE2	5:D:323:ASN:ND2	2.38	0.56
2:B:320:VAL:HG13	2:B:321:LYS:HG2	1.86	0.56
1:A:1600:LEU:HD11	1:A:1643:ASN:HD21	1.69	0.56
1:A:2354:VAL:HG12	1:A:2363:SER:HA	1.85	0.56
1:A:2711:LEU:HD11	1:A:2747:VAL:HG11	1.87	0.56
2:B:2089:LEU:HG	2:B:2094:ILE:HG21	1.88	0.56
1:A:1464:ILE:HG21	1:A:1587:MET:SD	2.46	0.56
1:A:2589:LEU:HA	1:A:2592:MET:HG2	1.88	0.56
2:B:1395:ARG:NH2	2:B:1430:THR:O	2.38	0.56
1:A:2028:LEU:HD23	1:A:2033:ILE:HB	1.87	0.56
2:B:2332:MET:HG3	2:B:2414:LEU:HD23	1.88	0.56
2:B:160:THR:HA	2:B:163:LEU:HG	1.88	0.56
2:B:2530:MET:HA	2:B:2533:MET:HG2	1.88	0.55
4:C:87:ILE:HG22	4:C:87:ILE:O	2.06	0.55
1:A:932:ARG:O	1:A:932:ARG:NH1	2.39	0.55
1:A:54:VAL:HG12	1:A:55:GLU:HG2	1.88	0.55
2:B:2149:ARG:O	2:B:2153:ASN:HB2	2.06	0.55
4:C:664:LYS:HA	4:C:667:ILE:HG22	1.88	0.55
5:D:269:GLN:HG2	5:D:273:HIS:CE1	2.40	0.55
2:B:866:LEU:HD23	2:B:869:GLN:HE21	1.72	0.55
2:B:2218:GLU:HG2	2:B:2219:PRO:HD3	1.89	0.55
1:A:2855:ILE:HD13	1:A:2859:LEU:HD12	1.88	0.55
2:B:2561:LEU:HD22	2:B:2583:GLN:HE21	1.72	0.55
4:C:136:MET:O	4:C:136:MET:CG	2.51	0.55
4:C:957:MET:HE1	4:C:991:LEU:CD2	2.37	0.55
1:A:2748:LEU:HD22	1:A:2823:MET:HE2	1.88	0.54
2:B:1145:LEU:HD21	2:B:1169:ARG:HH22	1.71	0.54
1:A:1572:PRO:HA	1:A:1575:LEU:HB2	1.89	0.54
1:A:2044:MET:HG3	1:A:2050:LEU:O	2.08	0.54
2:B:2278:ASP:HA	2:B:2281:LEU:HB2	1.89	0.54
2:B:2395:PRO:HB2	2:B:2453:VAL:HG21	1.89	0.54
1:A:82:LEU:HD22	1:A:184:THR:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:LYS:NZ	2:B:602:GLU:OE2	2.40	0.54
4:C:57:THR:HB	4:C:60:THR:HG22	1.89	0.54
1:A:2379:GLN:OE1	1:A:2382:LYS:HE3	2.07	0.54
1:A:2169:LEU:HD13	1:A:2192:VAL:CG2	2.34	0.54
1:A:2277:VAL:HG21	1:A:2300:LEU:HD13	1.90	0.54
4:C:480:LEU:HD23	4:C:1030:VAL:HG21	1.89	0.54
1:A:2344:SER:HA	1:A:2347:ILE:HD12	1.90	0.54
1:A:1638:THR:HG21	1:A:1870:VAL:HG22	1.89	0.54
2:B:455:GLU:O	2:B:498:ARG:NH2	2.41	0.54
2:B:579:LYS:HE3	2:B:600:LEU:HD21	1.89	0.54
2:B:1227:LEU:O	2:B:1230:SER:HB3	2.07	0.54
5:D:333:TYR:O	5:D:336:GLU:HB2	2.07	0.54
1:A:2094:LYS:NZ	1:A:2141:GLU:OE1	2.37	0.54
2:B:319:ALA:HA	2:B:342:CYS:HA	1.89	0.53
4:C:891:VAL:HA	4:C:894:ILE:HG22	1.88	0.53
2:B:1360:LEU:HD11	2:B:1405:ILE:HG23	1.88	0.53
2:B:2254:ASP:HA	2:B:2257:TYR:HB2	1.91	0.53
1:A:1471:SER:HB2	1:A:1481:HIS:HE1	1.71	0.53
1:A:2169:LEU:HD13	1:A:2192:VAL:HG21	1.85	0.53
2:B:632:ILE:HD12	2:B:636:VAL:HG21	1.91	0.53
1:A:2027:CYS:HB2	1:A:2074:LEU:HD22	1.91	0.53
1:A:1653:ARG:NH2	2:B:2021:GLU:OE1	2.41	0.53
1:A:2087:GLN:HG3	1:A:2150:ALA:HB2	1.91	0.53
2:B:2124:SER:HA	2:B:2127:ALA:HB3	1.91	0.53
1:A:2321:VAL:O	1:A:2325:LYS:NZ	2.38	0.53
4:C:1118:VAL:HB	4:C:1121:ARG:HH21	1.72	0.53
5:D:234:LEU:HG	5:D:319:VAL:HG11	1.90	0.53
1:A:82:LEU:O	1:A:86:LEU:HB2	2.09	0.52
2:B:1022:GLN:H	2:B:1022:GLN:NE2	2.07	0.52
2:B:1076:ILE:HD11	2:B:1121:PRO:HB3	1.91	0.52
4:C:1318:HIS:HB3	4:C:1322:LYS:NZ	2.24	0.52
1:A:815:GLY:O	1:A:819:ARG:NH1	2.42	0.52
1:A:1570:PRO:HA	1:A:1573:LEU:HD13	1.91	0.52
1:A:1358:GLU:OE2	1:A:1578:LYS:NZ	2.41	0.52
1:A:2390:THR:HG22	1:A:2392:PRO:HD2	1.90	0.52
3:E:76:LYS:HG2	4:C:1495:ARG:HH11	1.73	0.52
4:C:1343:PHE:HA	4:C:1346:LEU:HD21	1.92	0.52
2:B:2341:LEU:HD12	2:B:2358:GLY:HA2	1.91	0.52
4:C:1318:HIS:HB3	4:C:1322:LYS:HZ3	1.74	0.52
4:C:991:LEU:O	4:C:991:LEU:HG	2.09	0.52
1:A:2043:LEU:HD12	1:A:2072:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2200:HIS:HB2	1:A:2206:LEU:HD13	1.91	0.52
2:B:2565:GLN:HG2	2:B:2568:ILE:HD12	1.92	0.52
1:A:2545:LEU:HB3	1:A:2592:MET:HE1	1.91	0.52
4:C:957:MET:CE	4:C:991:LEU:HD23	2.39	0.52
2:B:321:LYS:HB3	2:B:357:LEU:HB3	1.92	0.52
3:E:38:ARG:NH1	3:E:43:ASN:OD1	2.43	0.51
1:A:1324:PHE:HB2	1:A:1498:ALA:HB1	1.93	0.51
1:A:924:ASN:O	1:A:928:TYR:N	2.43	0.51
1:A:2490:ARG:NH1	1:A:2553:GLN:OE1	2.43	0.51
1:A:2586:LEU:HD23	1:A:2589:LEU:HD21	1.92	0.51
2:B:2118:ASP:OD1	2:B:2118:ASP:N	2.44	0.51
4:C:114:MET:O	4:C:118:LEU:HB2	2.11	0.51
4:C:173:ARG:NH1	4:C:327:GLU:OE2	2.42	0.51
4:C:640:ARG:HE	4:C:831:PRO:HD3	1.75	0.51
2:B:1426:ILE:HD13	2:B:1429:ASN:HB3	1.92	0.51
4:C:1161:GLU:HA	4:C:1166:ALA:HB2	1.92	0.51
2:B:946:TYR:HD1	2:B:949:LEU:HD12	1.76	0.51
1:A:1347:GLN:HA	1:A:1350:LEU:HB2	1.93	0.51
1:A:2134:PRO:HD3	1:A:2188:LEU:HD12	1.92	0.51
1:A:2296:SER:HG	1:A:2299:CYS:HG	1.58	0.51
2:B:653:ASP:HB3	2:B:656:LEU:HB2	1.92	0.51
4:C:396:VAL:HA	4:C:399:ILE:HG22	1.93	0.51
1:A:34:LEU:HD22	2:B:2510:LEU:HD13	1.92	0.51
1:A:847:ARG:O	1:A:851:ASN:ND2	2.44	0.51
1:A:2859:LEU:O	1:A:2873:ARG:NH1	2.42	0.51
2:B:452:LEU:HD11	2:B:500:LEU:HB2	1.93	0.51
2:B:644:PHE:HB3	2:B:648:LEU:HD12	1.93	0.51
2:B:1426:ILE:HA	2:B:1429:ASN:HB3	1.93	0.51
2:B:2328:VAL:HG13	2:B:2365:LEU:HB3	1.93	0.51
4:C:823:GLU:O	4:C:827:ARG:NH2	2.43	0.51
4:C:957:MET:HE1	4:C:991:LEU:HD21	1.93	0.51
1:A:86:LEU:HG	1:A:191:LEU:HD12	1.93	0.50
1:A:2193:PHE:HB3	1:A:2210:TYR:HE1	1.76	0.50
2:B:272:PRO:HA	2:B:275:GLN:HB3	1.93	0.50
2:B:1065:GLU:HB3	2:B:1110:ARG:HH12	1.76	0.50
5:D:275:ALA:HA	5:D:278:LYS:HE2	1.91	0.50
5:D:330:CYS:SG	5:D:376:CYS:SG	3.09	0.50
1:A:2848:PHE:HA	1:A:2851:LEU:HB2	1.93	0.50
2:B:2455:LEU:HD13	2:B:2519:SER:HB3	1.93	0.50
1:A:2558:ARG:O	1:A:2562:ARG:HB2	2.11	0.50
4:C:801:GLU:HG3	4:C:1558:GLN:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1076:ARG:HD2	4:C:1078:GLY:H	1.77	0.50
4:C:149:ILE:O	4:C:152:ARG:HB3	2.11	0.50
4:C:59:MET:O	4:C:63:HIS:ND1	2.44	0.50
4:C:592:SER:HA	4:C:595:VAL:HG22	1.93	0.50
4:C:1321:LEU:HB3	4:C:1322:LYS:NZ	2.27	0.49
1:A:101:HIS:ND1	1:A:104:LYS:O	2.45	0.49
3:E:37:MET:HG2	3:E:42:GLN:HB2	1.95	0.49
4:C:158:PHE:O	4:C:164:ARG:NH2	2.45	0.49
4:C:958:ASP:OD2	4:C:995:ARG:NH1	2.46	0.49
1:A:96:ARG:NH2	1:A:198:ARG:O	2.45	0.49
1:A:901:VAL:HA	1:A:904:MET:HG3	1.94	0.49
1:A:1183:GLY:O	1:A:1186:ARG:HB3	2.12	0.49
1:A:1920:PHE:HE1	1:A:1925:SER:HB3	1.77	0.49
2:B:324:ILE:HG12	2:B:356:TRP:HB3	1.94	0.49
1:A:1226:ALA:HB1	1:A:1351:GLU:HG3	1.95	0.49
1:A:2044:MET:HG2	1:A:2045:ASP:N	2.27	0.49
4:C:1517:TYR:HD2	4:C:1563:ILE:HG23	1.78	0.49
1:A:1958:LEU:HA	1:A:1961:VAL:HB	1.94	0.49
2:B:1155:LYS:HG3	2:B:1158:ILE:HG12	1.94	0.49
3:E:50:GLN:HA	3:E:53:ILE:HG22	1.93	0.49
4:C:1346:LEU:HD12	4:C:1347:LEU:N	2.28	0.49
4:C:1463:SER:OG	4:C:1464:TYR:N	2.44	0.49
2:B:2082:LEU:HA	2:B:2085:ILE:HG12	1.94	0.49
1:A:931:ILE:HA	1:A:934:LEU:HB3	1.95	0.49
1:A:2742:GLN:HA	1:A:2745:ILE:HG12	1.95	0.49
1:A:817:ARG:HG3	1:A:818:LEU:HD12	1.95	0.49
4:C:1178:LEU:HD13	4:C:1461:LEU:HD21	1.95	0.49
1:A:2810:GLY:HA2	1:A:2813:TRP:CH2	2.48	0.48
2:B:206:ILE:HG21	2:B:250:TYR:HB3	1.95	0.48
2:B:2451:LEU:HD23	2:B:2454:ILE:HD12	1.95	0.48
1:A:1627:ASP:HA	1:A:1630:MET:HG2	1.95	0.48
4:C:957:MET:CE	4:C:991:LEU:CD2	2.91	0.48
4:C:957:MET:HE3	4:C:991:LEU:HD23	1.95	0.48
1:A:1298:SER:O	1:A:1302:LEU:N	2.44	0.48
2:B:679:SER:HA	2:B:682:GLN:HB2	1.96	0.48
2:B:875:LEU:HD23	2:B:878:LEU:HD12	1.94	0.48
4:C:1315:CYS:HA	4:C:1322:LYS:HE3	1.94	0.48
1:A:2286:ALA:HB3	1:A:2558:ARG:HB2	1.96	0.48
3:E:104:ALA:O	3:E:108:HIS:ND1	2.40	0.48
2:B:1140:ASP:OD1	2:B:1228:ARG:NH1	2.46	0.48
2:B:2357:PHE:HA	2:B:2360:HIS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1017:ILE:HD11	4:C:1154:VAL:HG13	1.96	0.48
1:A:1909:MET:SD	1:A:1912:LYS:NZ	2.76	0.48
4:C:1343:PHE:HA	4:C:1346:LEU:CD2	2.44	0.48
1:A:2357:ALA:HB3	4:C:667:ILE:HD11	1.94	0.48
4:C:1048:ASP:OD2	4:C:1088:ARG:NE	2.47	0.48
1:A:22:ILE:HG12	1:A:65:LEU:HD12	1.95	0.48
1:A:2860:LEU:O	1:A:2873:ARG:NH2	2.46	0.47
2:B:364:GLN:NE2	2:B:366:GLU:O	2.47	0.47
2:B:569:PHE:HA	2:B:572:MET:HG2	1.95	0.47
1:A:2014:VAL:HG12	1:A:2059:ARG:HH21	1.78	0.47
4:C:907:SER:HB3	4:C:910:ARG:HB3	1.94	0.47
2:B:39:LEU:HA	2:B:42:PHE:HB2	1.96	0.47
2:B:132:VAL:HA	2:B:135:VAL:HG22	1.95	0.47
2:B:969:PRO:HB3	2:B:1023:LEU:HD11	1.97	0.47
4:C:1375:ALA:HA	4:C:1378:ALA:HB3	1.96	0.47
5:D:345:LEU:HA	5:D:357:SER:HA	1.94	0.47
1:A:1862:GLU:HB2	1:A:1870:VAL:HG21	1.96	0.47
2:B:2423:LEU:HD23	2:B:2611:LEU:HD13	1.97	0.47
4:C:1368:ARG:HH22	5:D:290:LEU:HD22	1.80	0.47
2:B:141:VAL:HG22	2:B:151:LEU:HD21	1.97	0.47
2:B:1100:VAL:HG11	2:B:1154:LEU:HD11	1.96	0.47
2:B:2545:LEU:HD22	2:B:2553:PHE:HB2	1.96	0.47
4:C:1031:PHE:HD2	4:C:1108:LEU:CD2	2.23	0.47
1:A:935:VAL:O	1:A:939:LYS:N	2.47	0.47
1:A:2745:ILE:HD12	1:A:2819:GLN:HG2	1.97	0.47
2:B:980:LYS:HE3	2:B:1026:LEU:HD22	1.97	0.47
4:C:864:ASP:OD1	4:C:864:ASP:N	2.47	0.47
4:C:899:SER:O	4:C:903:MET:HB3	2.15	0.47
1:A:2189:PHE:O	1:A:2192:VAL:HG22	2.15	0.47
1:A:2826:ARG:HB3	1:A:2828:VAL:HG23	1.97	0.47
2:B:807:LEU:HD23	2:B:808:LEU:HD23	1.97	0.47
1:A:871:GLU:OE2	1:A:933:GLN:NE2	2.47	0.47
2:B:686:LEU:HD21	2:B:800:CYS:HB3	1.97	0.47
2:B:2554:VAL:HG21	2:B:2593:THR:HG21	1.97	0.47
4:C:638:PRO:HG2	4:C:640:ARG:HH12	1.80	0.46
1:A:1869:ALA:HB3	1:A:1873:VAL:HG13	1.95	0.46
2:B:2460:GLU:HG3	2:B:2461:GLN:HG2	1.96	0.46
1:A:2241:TYR:O	1:A:2251:ARG:NH1	2.47	0.46
2:B:1403:LEU:CD1	2:B:2029:VAL:HB	2.46	0.46
4:C:899:SER:O	4:C:903:MET:CB	2.64	0.46
1:A:953:ALA:H	1:A:1187:PHE:HZ	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:SER:HB3	2:B:339:LEU:HG	1.96	0.46
2:B:1335:SER:OG	2:B:1337:CYS:SG	2.63	0.46
2:B:1403:LEU:HD12	2:B:2029:VAL:HG21	1.97	0.46
4:C:898:CYS:HA	4:C:901:ILE:HG12	1.96	0.46
4:C:1114:LEU:O	4:C:1114:LEU:CG	2.57	0.46
5:D:214:PRO:HD2	5:D:215:LEU:H	1.80	0.46
2:B:527:VAL:HA	2:B:530:VAL:HG12	1.97	0.46
2:B:1354:ASN:OD1	2:B:1355:LEU:N	2.45	0.46
4:C:110:PHE:O	4:C:114:MET:HG3	2.15	0.46
1:A:121:LEU:HD21	1:A:214:ILE:HB	1.97	0.46
1:A:126:ASP:HA	1:A:129:ASN:HB2	1.98	0.46
1:A:1474:CYS:SG	1:A:1475:THR:N	2.88	0.46
1:A:2186:ILE:O	1:A:2190:LEU:HG	2.15	0.46
2:B:2034:ILE:HG12	2:B:2041:ALA:HB3	1.97	0.46
4:C:184:PHE:HD1	4:C:1321:LEU:HG	1.81	0.46
4:C:201:GLY:HA2	4:C:1230:LYS:HD2	1.98	0.46
1:A:113:LEU:HD23	1:A:116:LEU:HD12	1.97	0.46
1:A:2126:ASP:O	1:A:2130:LEU:HG	2.16	0.46
4:C:189:LEU:HD21	4:C:270:ILE:HG23	1.97	0.46
2:B:172:SER:O	2:B:218:HIS:ND1	2.48	0.46
2:B:1296:GLU:OE2	2:B:1358:HIS:NE2	2.49	0.46
3:E:41:GLY:HA2	4:C:1489:ARG:HH21	1.81	0.46
4:C:815:ALA:HA	4:C:818:LYS:HE2	1.97	0.46
4:C:847:ARG:NH1	4:C:850:CYS:SG	2.83	0.46
4:C:1346:LEU:HD12	4:C:1346:LEU:C	2.35	0.46
4:C:1534:LEU:HA	4:C:1537:LEU:HG	1.97	0.46
1:A:215:TRP:HA	1:A:218:MET:HG2	1.97	0.46
1:A:1185:LYS:O	1:A:1188:GLN:HB3	2.16	0.46
1:A:1853:PRO:HA	1:A:1856:HIS:HB2	1.98	0.46
2:B:1001:ALA:O	2:B:1005:ASP:HB2	2.15	0.46
2:B:1157:ASP:OD1	2:B:1157:ASP:N	2.48	0.46
4:C:525:LEU:HD13	4:C:543:ALA:HB2	1.98	0.46
4:C:1149:THR:HA	4:C:1152:VAL:HG22	1.97	0.46
5:D:375:GLU:O	5:D:376:CYS:SG	2.74	0.46
1:A:1874:ALA:HA	1:A:1877:VAL:HG12	1.97	0.45
1:A:2025:LYS:HA	1:A:2025:LYS:HD3	1.83	0.45
1:A:2214:VAL:HA	1:A:2217:THR:HG22	1.97	0.45
1:A:2586:LEU:HA	1:A:2589:LEU:HG	1.98	0.45
2:B:2195:ASP:OD1	2:B:2195:ASP:N	2.49	0.45
1:A:2712:LEU:HD13	1:A:2905:LEU:HD13	1.97	0.45
5:D:335:LEU:HD11	5:D:368:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:282:TRP:HZ2	4:C:1387:THR:HG21	1.82	0.45
1:A:78:VAL:HG13	1:A:119:MET:HB2	1.97	0.45
1:A:1574:SER:HA	1:A:1577:ILE:HD12	1.99	0.45
2:B:2329:LEU:O	2:B:2333:ALA:CB	2.64	0.45
4:C:164:ARG:HH11	4:C:167:ILE:HG13	1.81	0.45
4:C:826:LEU:HD12	4:C:826:LEU:HA	1.79	0.45
1:A:2422:MET:HG2	1:A:2547:LEU:HD13	1.98	0.45
2:B:1335:SER:HG	2:B:1337:CYS:HG	1.59	0.45
2:B:2082:LEU:HD23	2:B:2085:ILE:HD11	1.98	0.45
1:A:2046:LYS:HA	1:A:2046:LYS:HD3	1.83	0.45
4:C:1392:ASN:OD1	4:C:1393:LYS:N	2.49	0.45
1:A:1959:TRP:HB2	1:A:2102:LEU:HG	1.98	0.45
1:A:2342:SER:OG	1:A:2343:ILE:N	2.49	0.45
4:C:640:ARG:HG3	4:C:829:ASN:HA	1.98	0.45
4:C:1286:VAL:HA	4:C:1289:VAL:HG22	1.99	0.45
1:A:953:ALA:HB1	1:A:1180:ILE:HG13	1.99	0.45
2:B:238:VAL:HG22	2:B:301:TRP:HA	1.98	0.45
2:B:446:VAL:O	2:B:450:ILE:HG12	2.16	0.45
2:B:692:LEU:CD1	2:B:697:ILE:HG13	2.47	0.45
4:C:984:LEU:HA	4:C:987:VAL:HG22	1.97	0.45
1:A:2405:ALA:HA	1:A:2408:LEU:HD12	1.99	0.45
2:B:2295:LYS:O	2:B:2367:GLN:NE2	2.48	0.45
5:D:274:HIS:O	5:D:278:LYS:HD3	2.17	0.45
2:B:629:LEU:HB3	2:B:688:TRP:CD1	2.52	0.45
2:B:650:LYS:HG3	2:B:656:LEU:HD23	1.98	0.45
4:C:545:MET:SD	4:C:1121:ARG:NH1	2.90	0.45
2:B:1143:THR:O	2:B:1146:SER:OG	2.30	0.44
2:B:1305:PHE:CZ	2:B:1359:LEU:HD21	2.31	0.44
2:B:2604:LEU:HA	2:B:2607:LEU:HB2	1.99	0.44
4:C:275:GLU:HG2	4:C:557:VAL:HG21	1.99	0.44
4:C:715:ARG:NH1	4:C:715:ARG:O	2.50	0.44
5:D:284:SER:HA	5:D:287:HIS:HD2	1.82	0.44
1:A:1588:TYR:HA	1:A:1591:ILE:HG22	1.99	0.44
1:A:1945:GLU:HG3	1:A:2048:TRP:HA	1.99	0.44
1:A:2701:PHE:O	1:A:2707:ARG:NE	2.42	0.44
2:B:2054:ARG:HA	2:B:2054:ARG:HD2	1.77	0.44
1:A:1994:GLY:HA2	1:A:2063:PRO:HA	1.99	0.44
2:B:251:LYS:HA	2:B:251:LYS:HD2	1.81	0.44
1:A:2691:ASP:CG	1:A:2692:PHE:H	2.21	0.44
1:A:2853:PRO:O	1:A:2857:CYS:HB2	2.17	0.44
2:B:342:CYS:H	2:B:345:CYS:HB3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1051:ILE:HD12	4:C:1051:ILE:HA	1.85	0.44
1:A:1315:LEU:HD23	1:A:1315:LEU:HA	1.88	0.44
1:A:2033:ILE:HD12	1:A:2041:TYR:HE2	1.82	0.44
2:B:179:ILE:HG21	2:B:226:MET:HG2	2.00	0.44
2:B:1422:HIS:O	2:B:1425:HIS:HB3	2.18	0.44
2:B:2093:GLY:O	2:B:2097:GLN:NE2	2.50	0.44
1:A:852:LYS:NZ	1:A:853:ASP:OD2	2.45	0.44
1:A:865:LEU:HD21	1:A:897:GLU:HA	2.00	0.44
1:A:2094:LYS:HG3	1:A:2157:LEU:HD13	2.00	0.44
2:B:1286:LYS:HE3	2:B:1286:LYS:HB2	1.82	0.44
4:C:283:VAL:O	4:C:287:TYR:HB3	2.17	0.44
4:C:952:ASP:HB3	4:C:953:PHE:H	1.54	0.44
2:B:1164:GLU:HA	2:B:1167:VAL:HG12	2.00	0.44
4:C:1142:LEU:O	4:C:1146:ILE:HG22	2.17	0.44
2:B:2214:ARG:HA	2:B:2217:LEU:HD13	2.00	0.43
4:C:138:PRO:O	4:C:141:MET:HG2	2.18	0.43
1:A:887:VAL:HB	1:A:948:ARG:HH22	1.82	0.43
2:B:1429:ASN:O	2:B:1433:ALA:N	2.51	0.43
2:B:2196:SER:N	2:B:2199:ARG:HH21	2.16	0.43
2:B:2270:LEU:HD13	2:B:2365:LEU:HD11	1.98	0.43
2:B:2614:THR:HA	2:B:2617:LYS:HB2	2.00	0.43
3:E:132:ASP:N	3:E:132:ASP:OD1	2.50	0.43
4:C:204:THR:HG21	4:C:249:GLU:HB2	1.99	0.43
4:C:633:ILE:HA	4:C:636:LYS:HE2	1.99	0.43
1:A:2564:ILE:HG21	1:A:2614:LEU:HA	2.01	0.43
2:B:2617:LYS:HD3	2:B:2617:LYS:HA	1.79	0.43
3:E:87:ARG:HG2	3:E:143:VAL:HG21	1.99	0.43
5:D:303:ASP:HA	5:D:306:ILE:HG12	2.01	0.43
2:B:1152:HIS:HB2	2:B:1161:LEU:HD13	2.00	0.43
4:C:1060:ILE:HA	4:C:1087:PRO:HA	2.01	0.43
1:A:1600:LEU:HG	1:A:1647:LYS:HE3	2.00	0.43
2:B:1145:LEU:HD22	2:B:1283:VAL:HG21	2.00	0.43
4:C:38:VAL:HA	4:C:41:LEU:HG	2.00	0.43
5:D:332:GLN:HA	5:D:335:LEU:HD13	2.01	0.43
1:A:1972:ASP:OD1	1:A:1972:ASP:N	2.49	0.43
2:B:2100:GLN:NE2	2:B:2146:ALA:O	2.46	0.43
2:B:2170:TRP:HA	2:B:2173:ILE:HD13	2.01	0.43
4:C:1348:CYS:HA	4:C:1351:PHE:HD2	1.84	0.43
1:A:868:PHE:HE2	1:A:930:ASP:HB3	1.82	0.43
2:B:2328:VAL:HA	2:B:2365:LEU:HD13	2.00	0.43
4:C:669:ARG:HD2	4:C:669:ARG:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1537:LEU:HD12	4:C:1537:LEU:C	2.39	0.43
5:D:348:ASN:HB3	5:D:352:ILE:HA	2.00	0.43
1:A:1879:TRP:O	1:A:1883:ILE:N	2.52	0.43
1:A:2345:GLU:HA	1:A:2348:LYS:HB3	2.01	0.43
2:B:2289:CYS:O	2:B:2294:THR:OG1	2.31	0.43
4:C:584:LEU:HD12	4:C:588:LEU:HB2	2.00	0.43
4:C:1094:ARG:NH2	4:C:1396:HIS:O	2.52	0.43
5:D:207:VAL:HG23	5:D:212:PRO:HG3	1.99	0.43
1:A:2843:THR:HG23	1:A:2845:ILE:HG23	2.01	0.43
5:D:283:GLU:OE1	5:D:287:HIS:NE2	2.52	0.43
1:A:2735:PRO:O	1:A:2739:LEU:HG	2.18	0.43
2:B:861:CYS:O	2:B:865:ILE:HD12	2.19	0.43
2:B:1050:GLY:O	2:B:1054:SER:OG	2.37	0.43
4:C:120:VAL:HA	4:C:123:VAL:HG12	2.00	0.43
1:A:90:ALA:HB2	1:A:191:LEU:HB3	2.00	0.42
1:A:677:LEU:HA	1:A:680:VAL:HG22	2.01	0.42
1:A:1317:LYS:NZ	1:A:1321:GLU:OE1	2.47	0.42
1:A:2489:PHE:O	1:A:2493:ARG:NH1	2.41	0.42
1:A:2683:LEU:HA	1:A:2686:GLN:HE21	1.83	0.42
2:B:362:LEU:HB2	2:B:398:ASN:HB2	2.01	0.42
4:C:850:CYS:HA	4:C:853:VAL:HG12	2.00	0.42
5:D:241:PRO:HB2	5:D:264:CYS:HB2	2.01	0.42
5:D:349:ASP:N	5:D:349:ASP:OD1	2.49	0.42
1:A:1357:ARG:HD2	1:A:1454:HIS:HB2	2.00	0.42
1:A:2140:ALA:HB3	1:A:2142:PHE:CE1	2.54	0.42
4:C:1462:LEU:HD13	4:C:1470:PHE:HE1	1.84	0.42
2:B:39:LEU:HD23	2:B:154:SER:HB2	2.01	0.42
2:B:1093:PHE:HB2	2:B:1126:LEU:HD22	2.01	0.42
4:C:281:GLY:N	4:C:1389:GLU:OE1	2.52	0.42
1:A:787:ARG:NH1	1:A:845:THR:O	2.53	0.42
1:A:1984:VAL:HG13	1:A:1992:MET:HB3	2.02	0.42
1:A:2395:ARG:HA	1:A:2395:ARG:HD3	1.82	0.42
2:B:319:ALA:HB2	2:B:340:TYR:HD2	1.84	0.42
4:C:206:HIS:CD2	4:C:226:ASP:OD2	2.72	0.42
4:C:818:LYS:HA	4:C:821:VAL:HG12	2.00	0.42
4:C:1138:VAL:O	4:C:1142:LEU:HG	2.19	0.42
1:A:824:ARG:HD2	1:A:824:ARG:HA	1.88	0.42
1:A:1601:SER:HB2	1:A:1607:ALA:HB2	2.01	0.42
1:A:1903:GLN:HA	1:A:1906:LEU:HB2	2.00	0.42
1:A:1913:LEU:HD12	1:A:1913:LEU:C	2.38	0.42
2:B:308:HIS:HE2	2:B:332:LEU:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1283:LEU:HA	4:C:1286:VAL:HG12	2.02	0.42
1:A:214:ILE:HD13	1:A:226:VAL:HG21	2.01	0.42
1:A:2088:LYS:HD2	1:A:2088:LYS:HA	1.81	0.42
2:B:1133:GLN:HE22	2:B:1227:LEU:HD22	1.85	0.42
2:B:1360:LEU:HD11	2:B:1405:ILE:HD12	2.01	0.42
2:B:2217:LEU:O	2:B:2257:TYR:OH	2.36	0.42
4:C:125:GLN:HA	4:C:128:GLU:HB2	2.01	0.42
4:C:1121:ARG:NH1	4:C:1122:ASP:OD1	2.52	0.42
1:A:2160:LEU:HD11	2:B:1110:ARG:HG3	2.01	0.42
2:B:258:LEU:HA	2:B:261:VAL:HG12	2.01	0.42
4:C:436:LYS:HA	4:C:436:LYS:HD3	1.90	0.42
4:C:1005:LYS:HB2	4:C:1005:LYS:HE2	1.81	0.42
4:C:1327:THR:O	4:C:1331:SER:OG	2.38	0.42
4:C:1421:ALA:HA	4:C:1424:LEU:HG	2.02	0.42
5:D:213:THR:HG23	5:D:216:TRP:HB2	2.02	0.42
1:A:51:ARG:O	1:A:57:LYS:N	2.52	0.42
3:E:5:LEU:HD22	3:E:70:LEU:HD22	2.01	0.42
1:A:73:SER:HB3	1:A:76:GLU:HG3	2.00	0.42
2:B:156:PHE:HB3	2:B:196:TYR:CE2	2.55	0.42
2:B:175:PRO:O	2:B:178:MET:HB3	2.20	0.42
2:B:526:LEU:HD23	2:B:526:LEU:HA	1.92	0.42
2:B:685:ALA:HA	2:B:688:TRP:HE3	1.85	0.42
4:C:296:TRP:O	4:C:300:PHE:HB2	2.20	0.42
4:C:1123:VAL:HG22	4:C:1127:ARG:HH21	1.85	0.42
4:C:1204:TYR:HE1	4:C:1263:MET:HB3	1.85	0.42
1:A:125:GLN:O	1:A:129:ASN:ND2	2.46	0.42
2:B:230:ALA:O	2:B:234:THR:OG1	2.38	0.42
2:B:1303:LYS:O	2:B:1307:THR:OG1	2.28	0.42
2:B:2376:GLY:HA3	2:B:2383:ALA:HB2	2.02	0.42
2:B:11:LYS:HD2	2:B:11:LYS:HA	1.92	0.41
2:B:1413:ASP:HB2	2:B:1416:ILE:HD11	2.02	0.41
4:C:560:MET:HB2	4:C:564:LEU:HD23	2.02	0.41
4:C:1321:LEU:HD22	4:C:1322:LYS:HZ2	1.84	0.41
1:A:1309:GLU:HA	1:A:1312:LYS:HD3	2.02	0.41
1:A:1347:GLN:HG2	1:A:1568:LEU:HD22	2.01	0.41
1:A:2731:TRP:HE1	1:A:2808:GLN:HG3	1.84	0.41
2:B:305:HIS:O	2:B:340:TYR:OH	2.33	0.41
2:B:2163:MET:SD	2:B:2163:MET:N	2.93	0.41
4:C:626:LYS:HB3	4:C:626:LYS:HE2	1.86	0.41
4:C:657:LYS:HE3	4:C:657:LYS:HB3	1.84	0.41
4:C:1322:LYS:H	4:C:1322:LYS:HG2	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:867:CYS:SG	2:B:868:TYR:N	2.94	0.41
4:C:119:TRP:HA	4:C:122:LEU:HD12	2.02	0.41
1:A:217:PRO:HG2	1:A:224:PRO:HB3	2.03	0.41
1:A:870:MET:SD	1:A:870:MET:N	2.88	0.41
1:A:2496:LEU:HD12	1:A:2540:ILE:HD13	2.02	0.41
2:B:1401:ALA:O	2:B:1405:ILE:HG12	2.19	0.41
1:A:1909:MET:HA	1:A:1912:LYS:HZ3	1.85	0.41
2:B:163:LEU:HD13	2:B:204:MET:HG2	2.03	0.41
4:C:457:LEU:CD1	4:C:481:ARG:NE	2.72	0.41
1:A:85:VAL:HB	1:A:112:LEU:HD11	2.01	0.41
1:A:1970:PHE:HD1	1:A:2119:HIS:HD1	1.68	0.41
1:A:2536:ARG:O	1:A:2540:ILE:HG13	2.20	0.41
1:A:2601:THR:HG22	1:A:2604:ARG:HH21	1.86	0.41
2:B:49:ILE:HG22	2:B:50:LEU:HD12	2.02	0.41
2:B:2513:TRP:HA	2:B:2516:VAL:HG12	2.01	0.41
4:C:1318:HIS:CD2	4:C:1321:LEU:N	2.61	0.41
2:B:1123:LEU:HB3	2:B:1158:ILE:HD13	2.02	0.41
4:C:219:TRP:HB2	4:C:1067:VAL:HG21	2.03	0.41
4:C:1327:THR:HG23	4:C:1449:ASN:HB2	2.01	0.41
1:A:1977:MET:HG2	1:A:1983:GLU:HA	2.02	0.41
1:A:2789:SER:HA	1:A:2792:GLN:HG3	2.03	0.41
2:B:568:ARG:HB3	2:B:571:VAL:HG22	2.03	0.41
2:B:2154:ILE:HD12	2:B:2154:ILE:HA	1.94	0.41
2:B:2295:LYS:HE3	2:B:2310:VAL:HG23	2.02	0.41
2:B:2497:ASN:OD1	2:B:2501:PHE:N	2.52	0.41
1:A:2086:ILE:HG22	1:A:2144:LEU:HD11	2.01	0.41
1:A:2133:PHE:HA	1:A:2134:PRO:HA	1.75	0.41
1:A:2710:MET:HE3	1:A:2710:MET:HB2	1.85	0.41
2:B:140:LEU:HG	2:B:143:LEU:HD12	2.02	0.41
2:B:688:TRP:HA	2:B:691:VAL:HG22	2.03	0.41
2:B:2047:ASP:OD1	2:B:2047:ASP:N	2.53	0.41
2:B:2204:LEU:HD21	2:B:2216:LEU:HD12	2.02	0.41
2:B:2328:VAL:HG22	2:B:2365:LEU:HD22	2.03	0.41
4:C:35:LYS:HG3	4:C:37:TRP:H	1.86	0.41
4:C:223:ALA:HA	5:D:288:LYS:HB3	2.03	0.41
4:C:851:ARG:HA	4:C:854:VAL:HG12	2.02	0.41
1:A:2487:GLU:HG2	1:A:2490:ARG:HH21	1.85	0.41
2:B:277:LEU:O	2:B:281:TRP:N	2.53	0.41
2:B:546:GLY:HA2	2:B:549:VAL:HG12	2.03	0.41
4:C:1374:SER:O	4:C:1378:ALA:N	2.54	0.41
1:A:214:ILE:HG23	1:A:215:TRP:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:LEU:HD13	1:A:831:LEU:HD21	2.04	0.40
1:A:831:LEU:HA	1:A:831:LEU:HD23	1.88	0.40
1:A:936:GLN:O	1:A:940:GLU:N	2.52	0.40
2:B:570:ASP:N	2:B:570:ASP:OD1	2.53	0.40
2:B:577:LEU:HD23	2:B:579:LYS:H	1.85	0.40
1:A:2555:MET:HB3	1:A:2610:PRO:HB2	2.03	0.40
2:B:190:HIS:HD2	2:B:193:ILE:HD12	1.86	0.40
2:B:1367:LEU:HD21	2:B:1402:LEU:HD21	2.02	0.40
2:B:2249:PHE:O	2:B:2255:LYS:NZ	2.54	0.40
5:D:311:TRP:HA	5:D:314:SER:HB3	2.03	0.40
1:A:849:TYR:HA	1:A:852:LYS:HE3	2.04	0.40
1:A:2103:PHE:O	1:A:2107:LEU:HB2	2.22	0.40
1:A:2849:VAL:O	2:B:225:SER:OG	2.29	0.40
4:C:253:LEU:HD13	4:C:258:LEU:HD21	2.04	0.40
1:A:795:LYS:O	1:A:799:SER:OG	2.31	0.40
1:A:1863:VAL:HG11	2:B:1272:ILE:HG23	2.04	0.40
2:B:1277:VAL:O	2:B:1281:ILE:HG12	2.22	0.40
2:B:2378:HIS:CE1	2:B:2435:PRO:HD2	2.57	0.40
2:B:2409:VAL:HA	2:B:2412:ILE:HG22	2.04	0.40
4:C:1124:ILE:HG21	4:C:1136:ILE:HD13	2.04	0.40
4:C:1172:GLN:NE2	4:C:1549:GLN:HB3	2.37	0.40
5:D:239:SER:OG	5:D:268:TYR:OH	2.36	0.40
1:A:1924:THR:HA	1:A:1927:ILE:HG22	2.03	0.40
1:A:2162:LYS:HE2	1:A:2199:LEU:HD22	2.03	0.40
1:A:2367:LEU:HD13	1:A:2492:PRO:HA	2.04	0.40
4:C:140:GLY:O	4:C:143:ARG:HB2	2.20	0.40

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	1739/3258 (53%)	1635 (94%)	104 (6%)	0	100	100
2	B	1639/2658 (62%)	1527 (93%)	112 (7%)	0	100	100
3	E	118/149 (79%)	111 (94%)	7 (6%)	0	100	100
4	C	1382/1992 (69%)	1311 (95%)	71 (5%)	0	100	100
5	D	178/458 (39%)	162 (91%)	15 (8%)	1 (1%)	25	65
All	All	5056/8515 (59%)	4746 (94%)	309 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	214	PRO

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 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	1563/2853 (55%)	1554 (99%)	9 (1%)	86	92
2	B	1486/2380 (62%)	1477 (99%)	9 (1%)	86	92
3	E	103/127 (81%)	103 (100%)	0	100	100
4	C	1261/1787 (71%)	1255 (100%)	6 (0%)	88	93
5	D	168/397 (42%)	168 (100%)	0	100	100
All	All	4581/7544 (61%)	4557 (100%)	24 (0%)	89	93

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	40	LYS
1	A	1227	ARG
1	A	1350	LEU
1	A	1613	MET
1	A	1852	LEU
1	A	2187	MET

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Mol	Chain	Res	Type
1	A	2188	LEU
1	A	2596	ILE
2	B	382	ARG
2	B	684	GLN
2	B	807	LEU
2	B	1022	GLN
2	B	1357	LYS
2	B	2110	ARG
2	B	2112	LEU
2	B	2139	LYS
2	B	2153	ASN
4	C	640	ARG
4	C	826	LEU
4	C	1272	ARG
4	C	1371	ASN
4	C	1481	ARG
4	C	1521	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	684	GLN
2	B	836	ASN
2	B	996	HIS
2	B	1022	GLN
2	B	2425	HIS
4	C	1274	ASN
4	C	1318	HIS
5	D	269	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 monosaccharides 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.

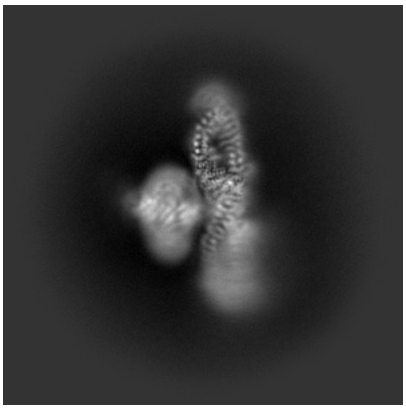
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32544. These allow visual inspection of the internal detail of the map and identification of artifacts.

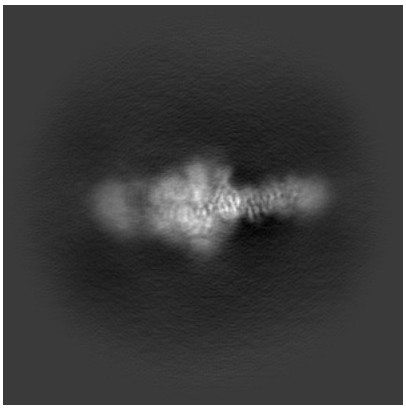
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

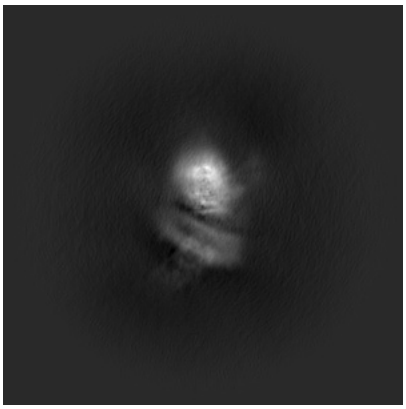
6.1.1 Primary map



X

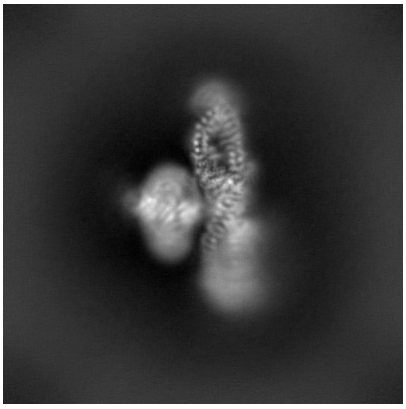


Y

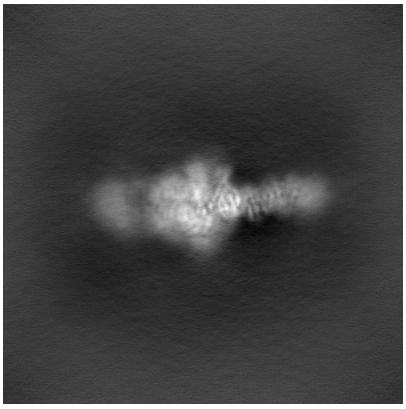


Z

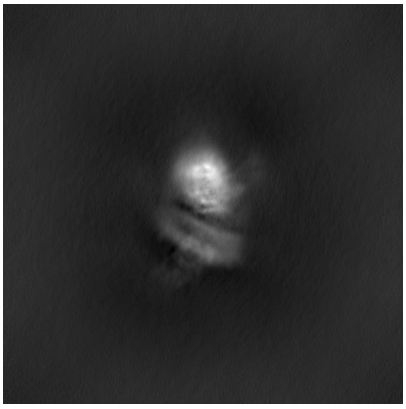
6.1.2 Raw map



X



Y

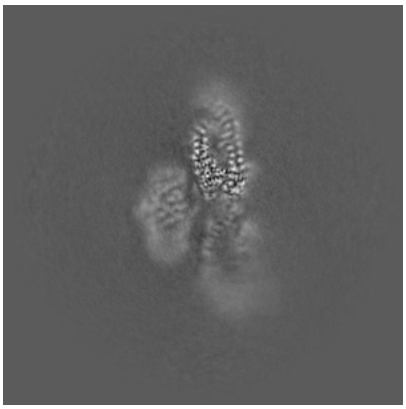


Z

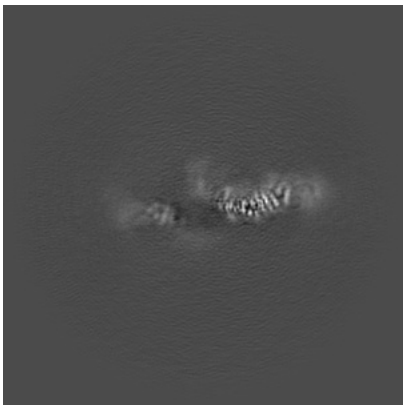
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

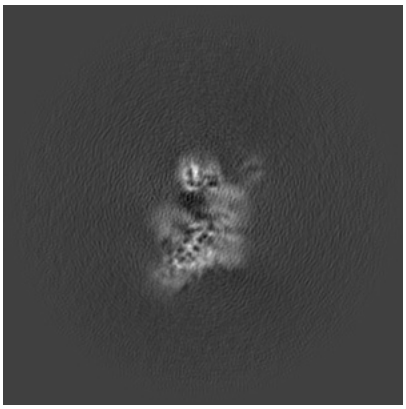
6.2.1 Primary map



X Index: 256

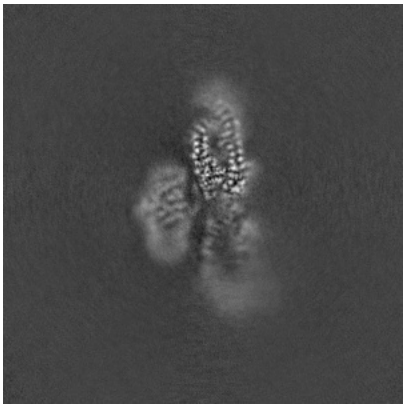


Y Index: 256

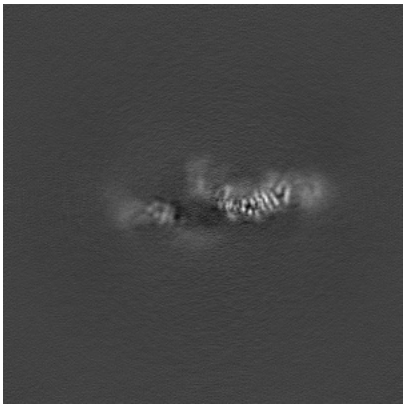


Z Index: 256

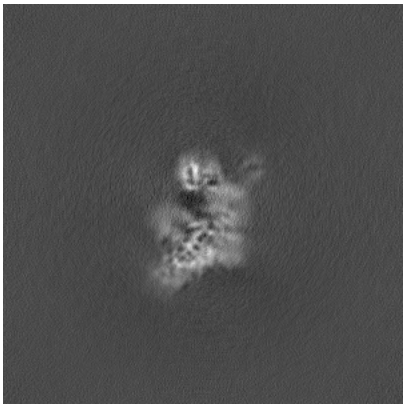
6.2.2 Raw map



X Index: 256



Y Index: 256

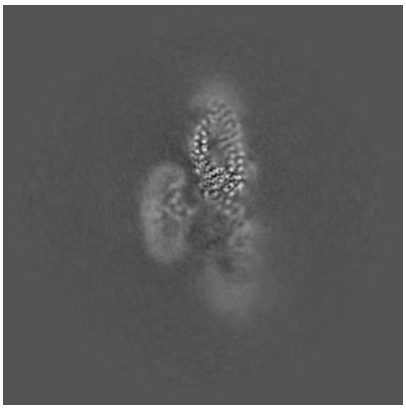


Z Index: 256

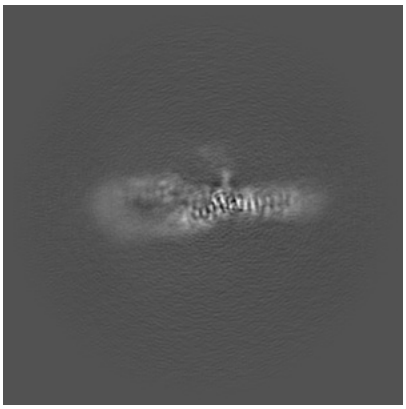
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

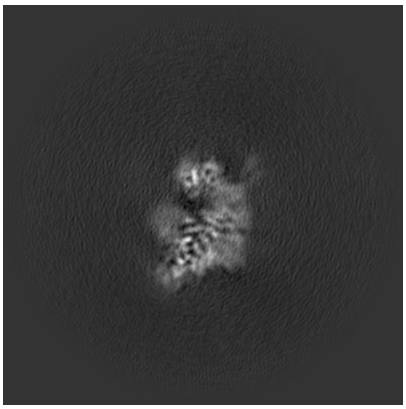
6.3.1 Primary map



X Index: 261

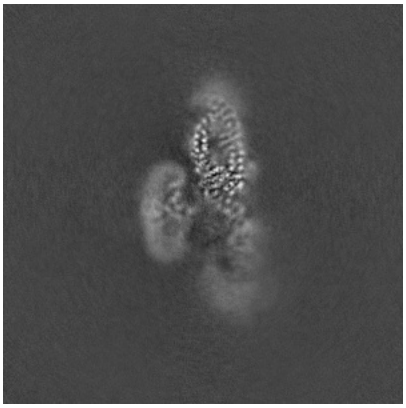


Y Index: 293

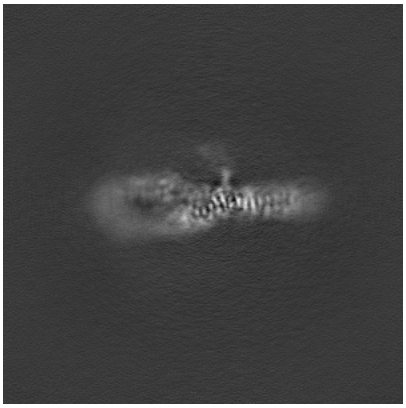


Z Index: 249

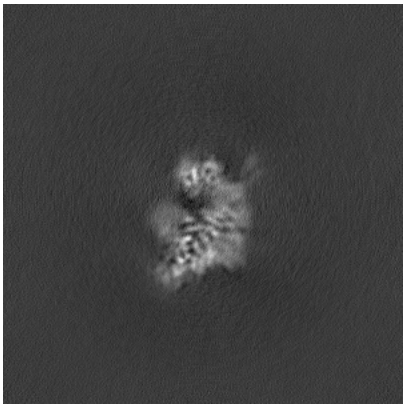
6.3.2 Raw map



X Index: 261



Y Index: 293



Z Index: 249

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

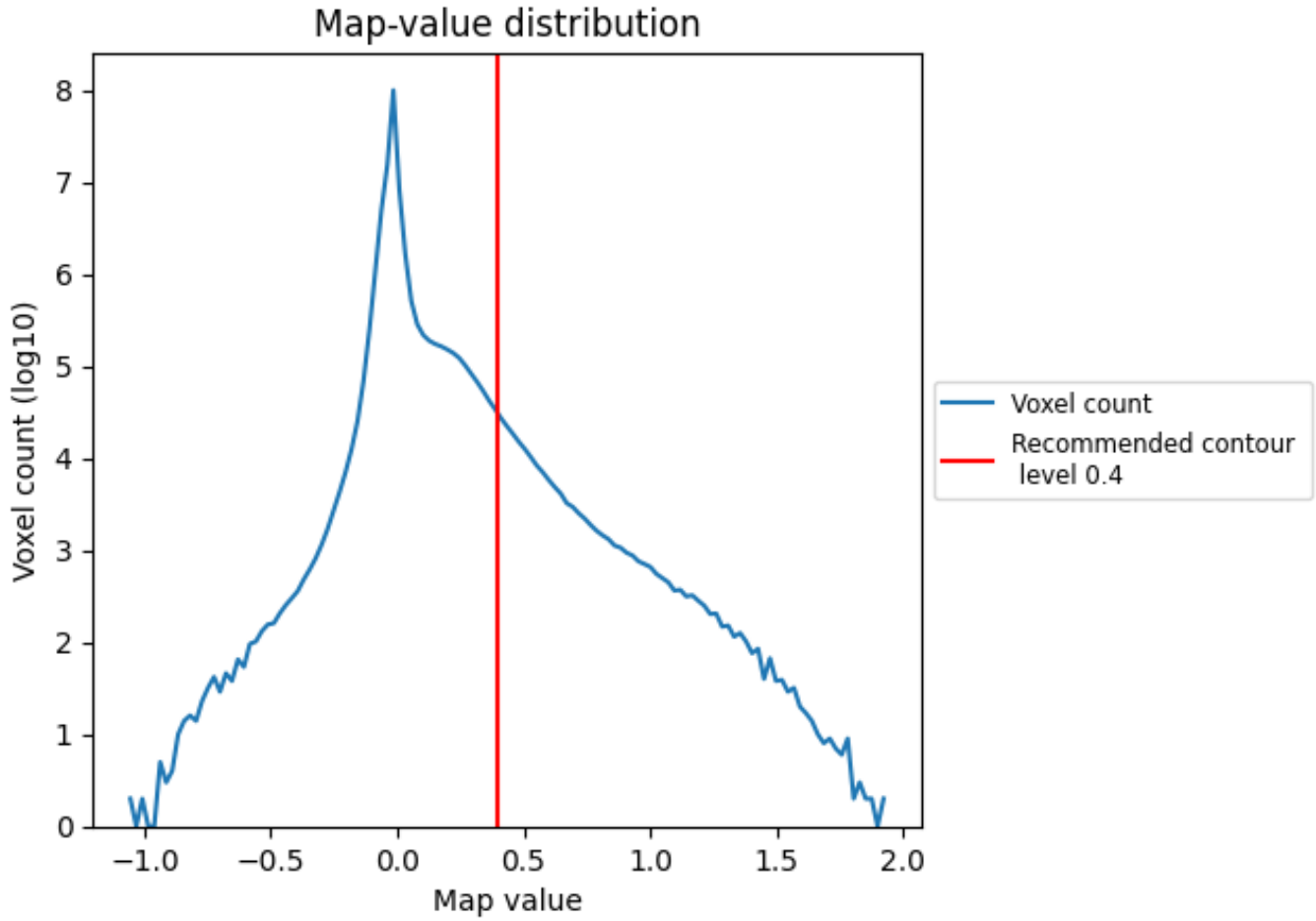
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

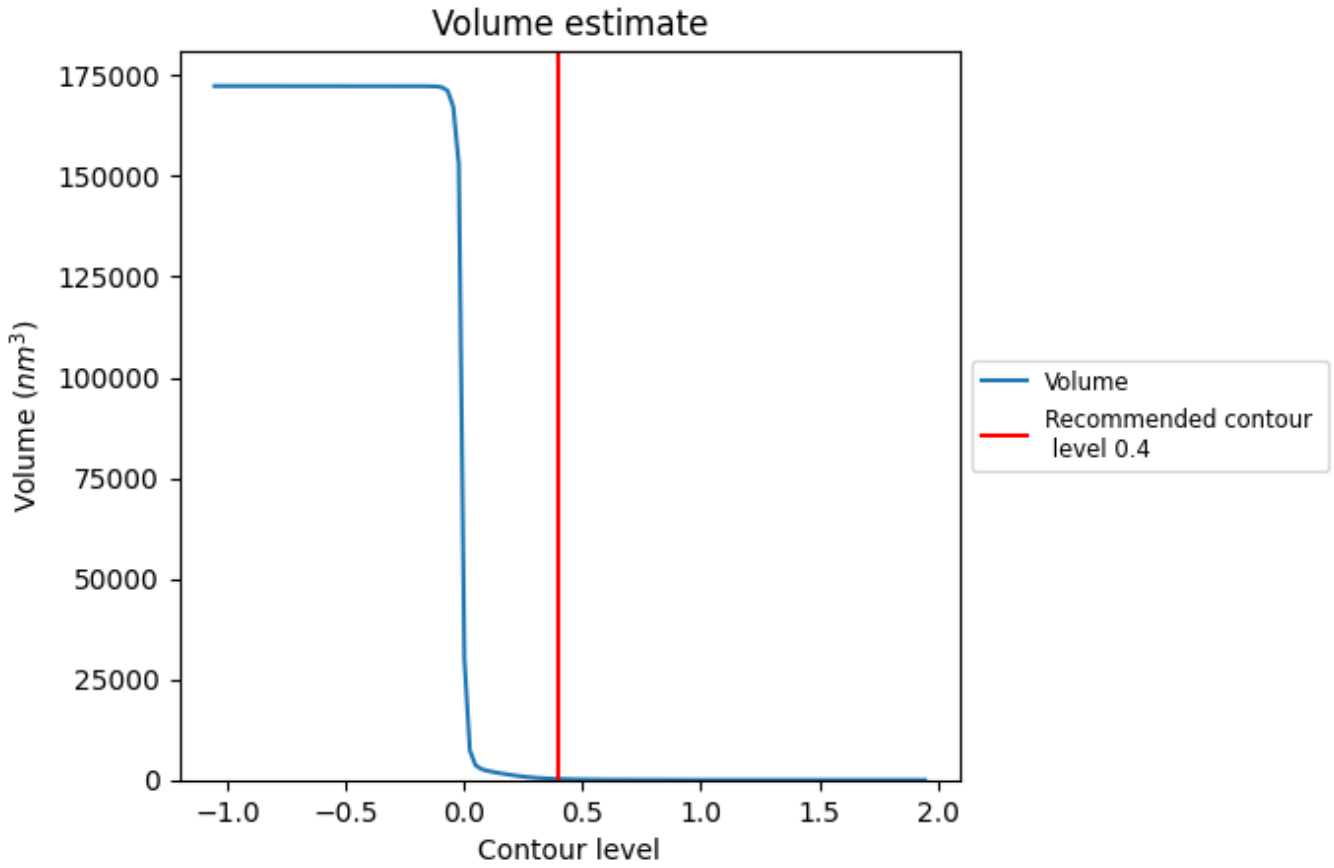
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

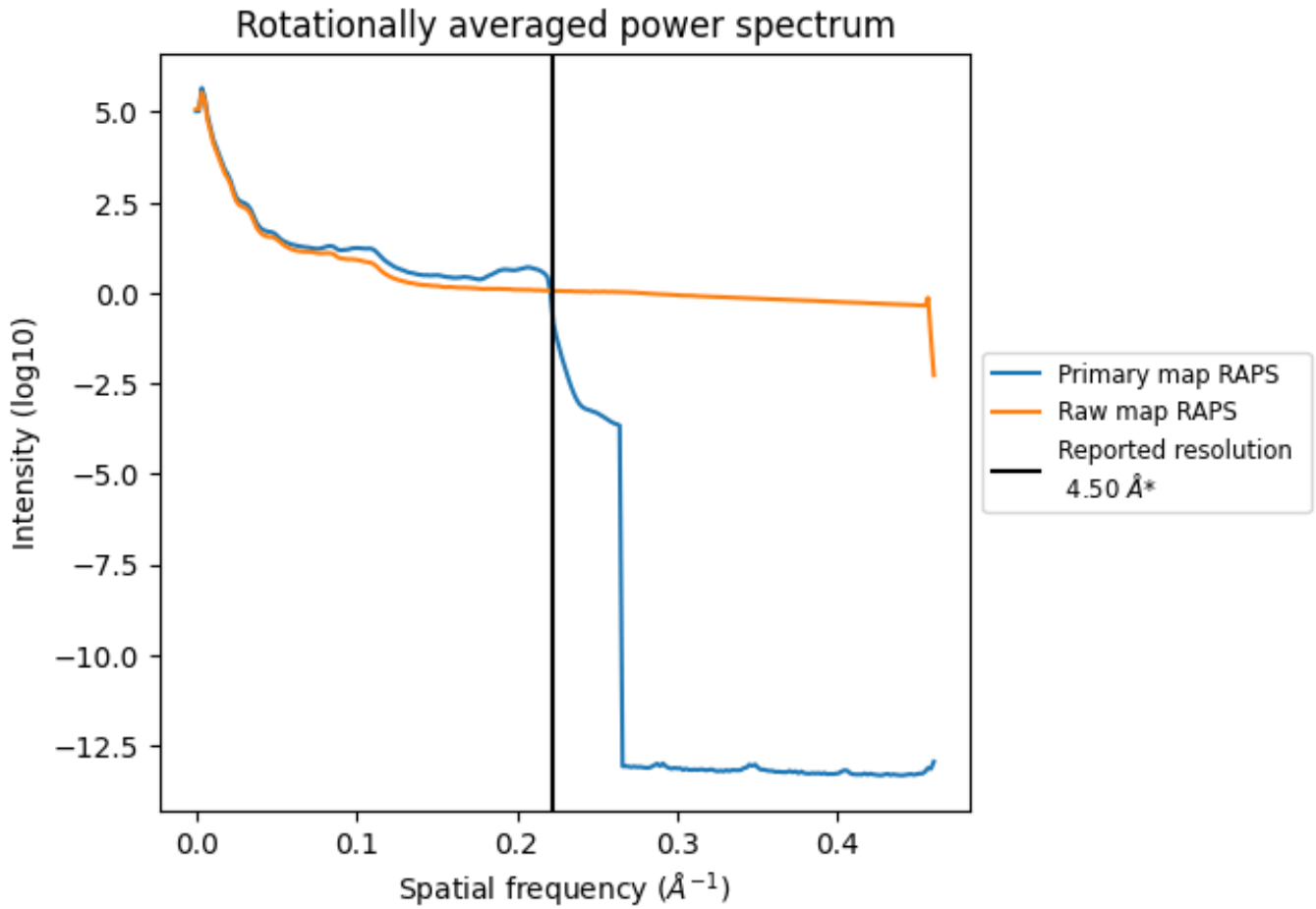
7.2 Volume estimate



The volume at the recommended contour level is 230 nm^3; this corresponds to an approximate mass of 207 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

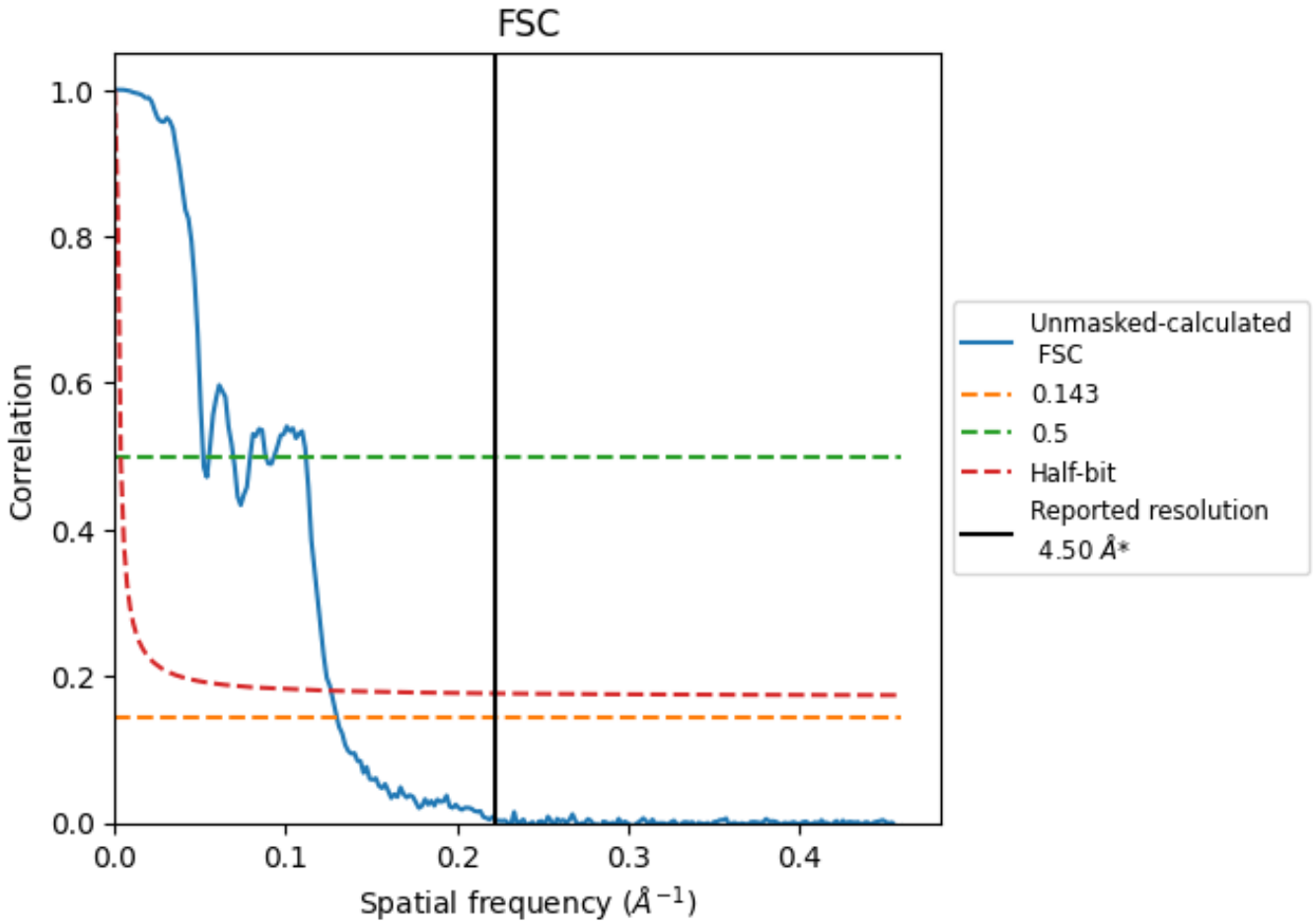


*Reported resolution corresponds to spatial frequency of 0.222 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8.2 Resolution estimates (i)

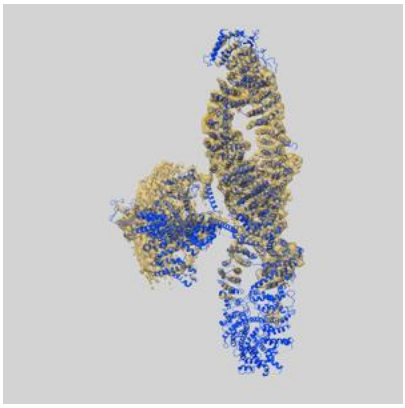
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.70	19.31	7.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.70 differs from the reported value 4.5 by more than 10 %

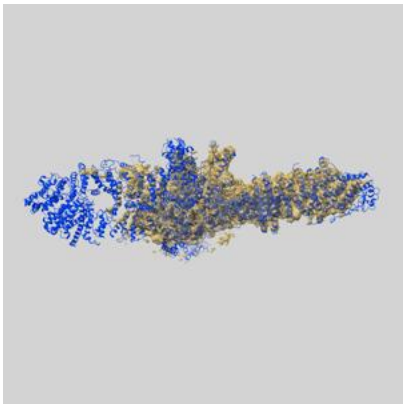
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32544 and PDB model 7WJI. Per-residue inclusion information can be found in section 3 on page 5.

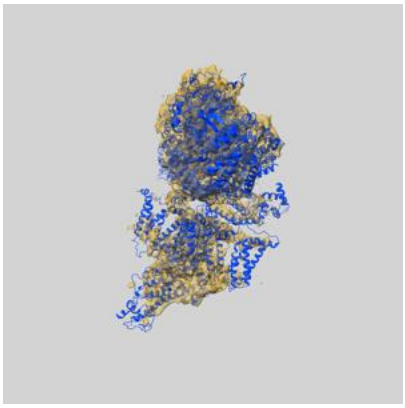
9.1 Map-model overlay



X



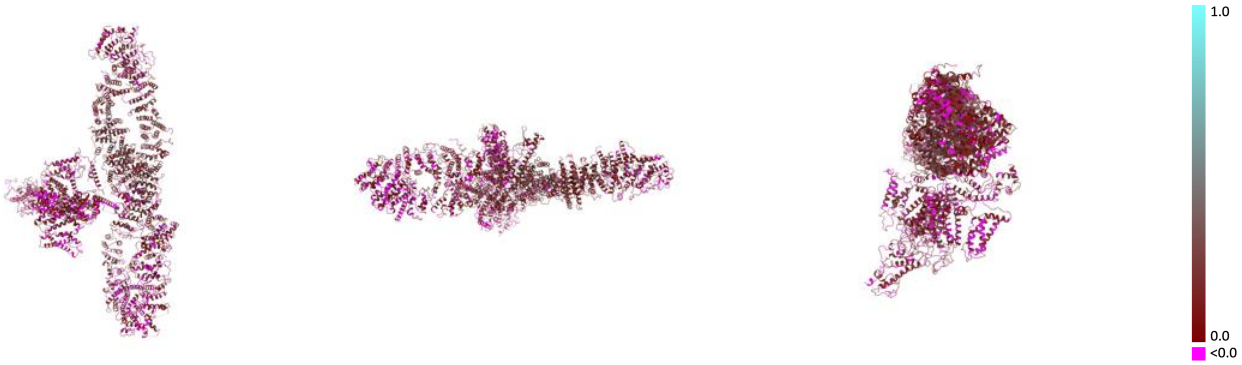
Y



Z

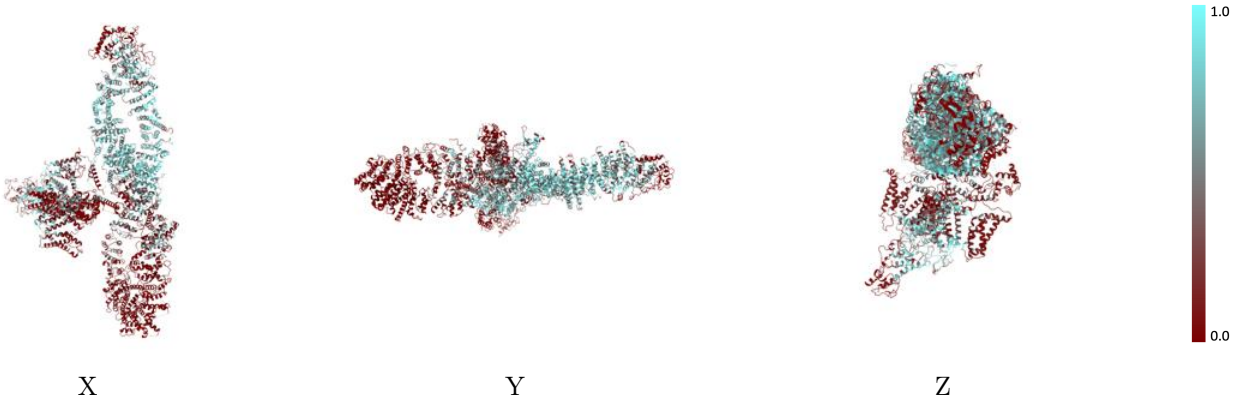
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



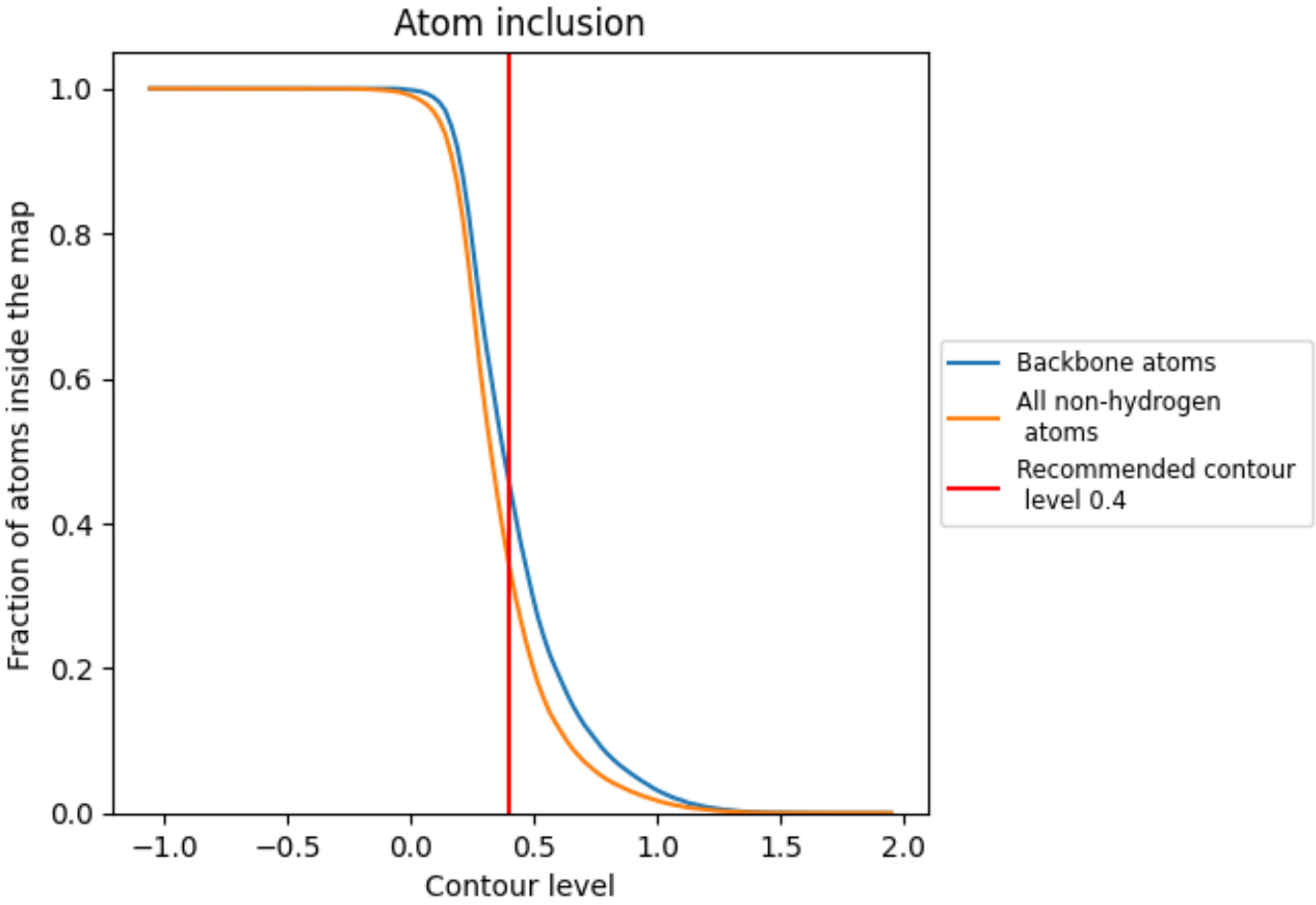
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 34% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3406	0.1390
A	0.3790	0.1700
B	0.3525	0.1440
C	0.3141	0.0990
D	0.2646	0.1070
E	0.0534	0.1160