Full wwPDB EM Validation Report ⓘ

Feb 4, 2024 – 10:45 AM EST

PDB ID	:	8DGC
EMDB ID	:	EMD-27421
Title	:	Avs3 bound to phage PhiV-1 terminase
Authors	:	Wilkinson, M.E.; Gao, L.; Strecker, J.; Makarova, K.S.; Macrae, R.K.; Koonin, E.V.; Zhang, F.
Deposited on	:	2022-06-23
Resolution	:	3.40 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:

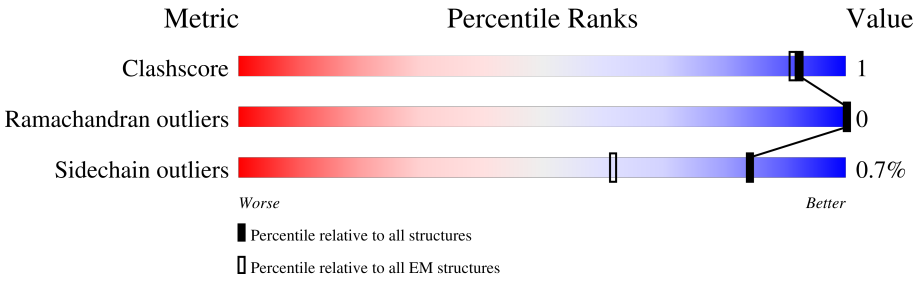
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	2092	66% 93%
1	B	2092	65% 91% 5%
1	C	2092	66% 93%
1	D	2092	65% 91% 5%
2	E	586	92% 87% 8%
2	F	586	92% 87% 5% 8%
2	G	586	92% 87% 5% 8%
2	H	586	92% 86% 5% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 81600 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.

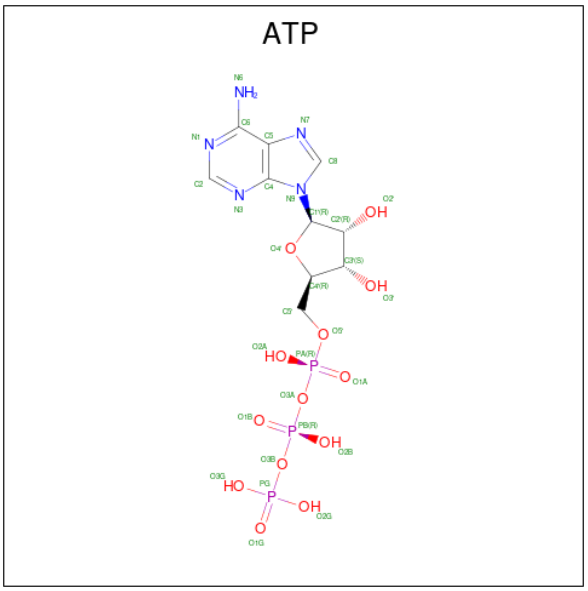
- Molecule 1 is a protein called SeAvs3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2028	Total	C	N	O	S	0	0
			16152	10199	2840	3056	57		
1	B	2004	Total	C	N	O	S	0	0
			15974	10095	2809	3014	56		
1	C	2028	Total	C	N	O	S	0	0
			16152	10199	2840	3056	57		
1	D	2004	Total	C	N	O	S	0	0
			15974	10095	2809	3014	56		

- Molecule 2 is a protein called Terminase, large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	538	Total	C	N	O	S	0	0
			4273	2717	741	796	19		
2	F	538	Total	C	N	O	S	0	0
			4273	2717	741	796	19		
2	G	538	Total	C	N	O	S	0	0
			4273	2717	741	796	19		
2	H	538	Total	C	N	O	S	0	0
			4273	2717	741	796	19		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	

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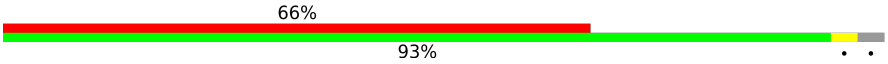
Mol	Chain	Residues	Atoms	AltConf
4	D	1	Total Mg 1 1	0
4	E	1	Total Mg 1 1	0
4	F	1	Total Mg 1 1	0
4	G	1	Total Mg 1 1	0
4	H	1	Total Mg 1 1	0

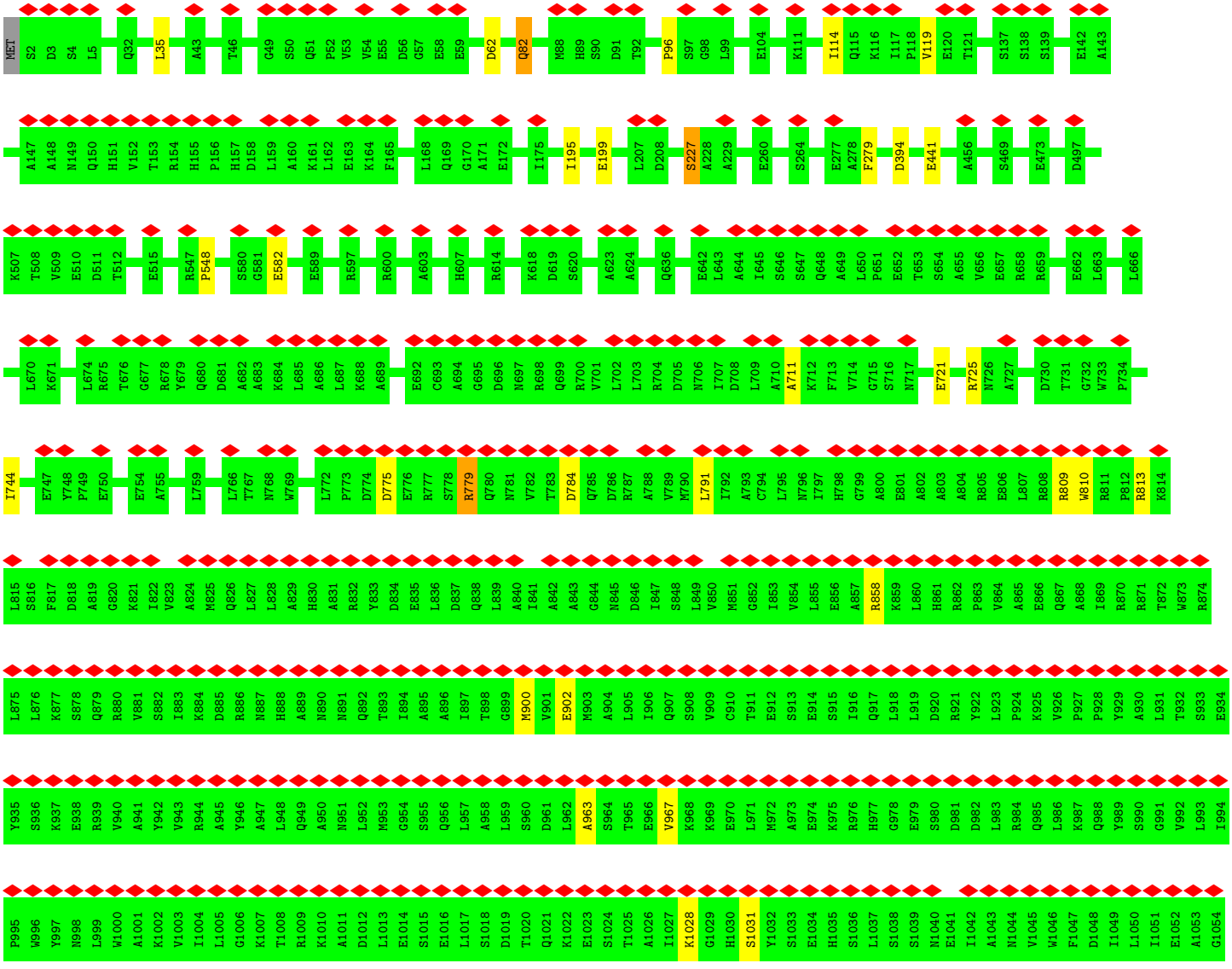
3 Residue-property plots (i)

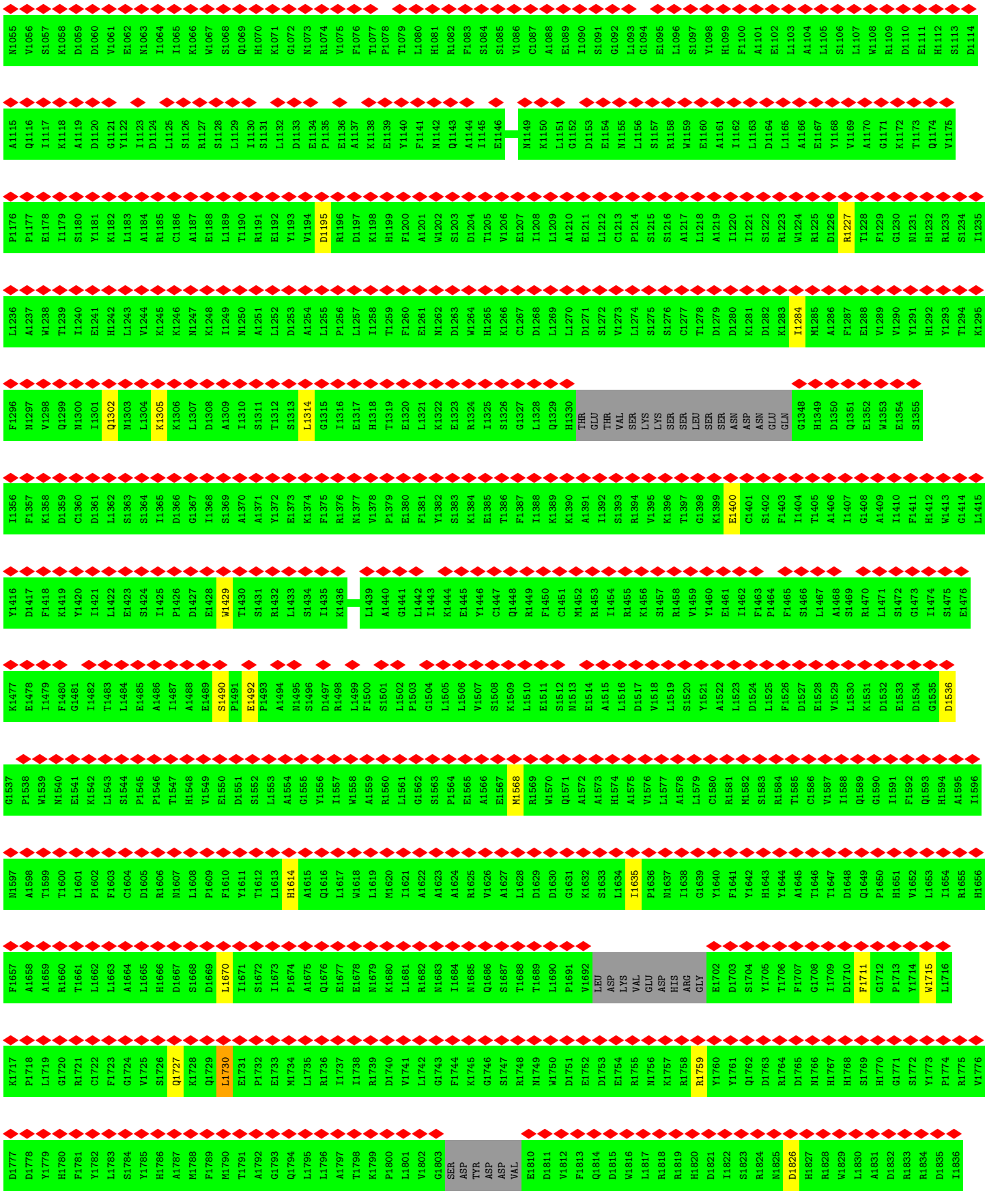
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: SeAvs3

Chain A:



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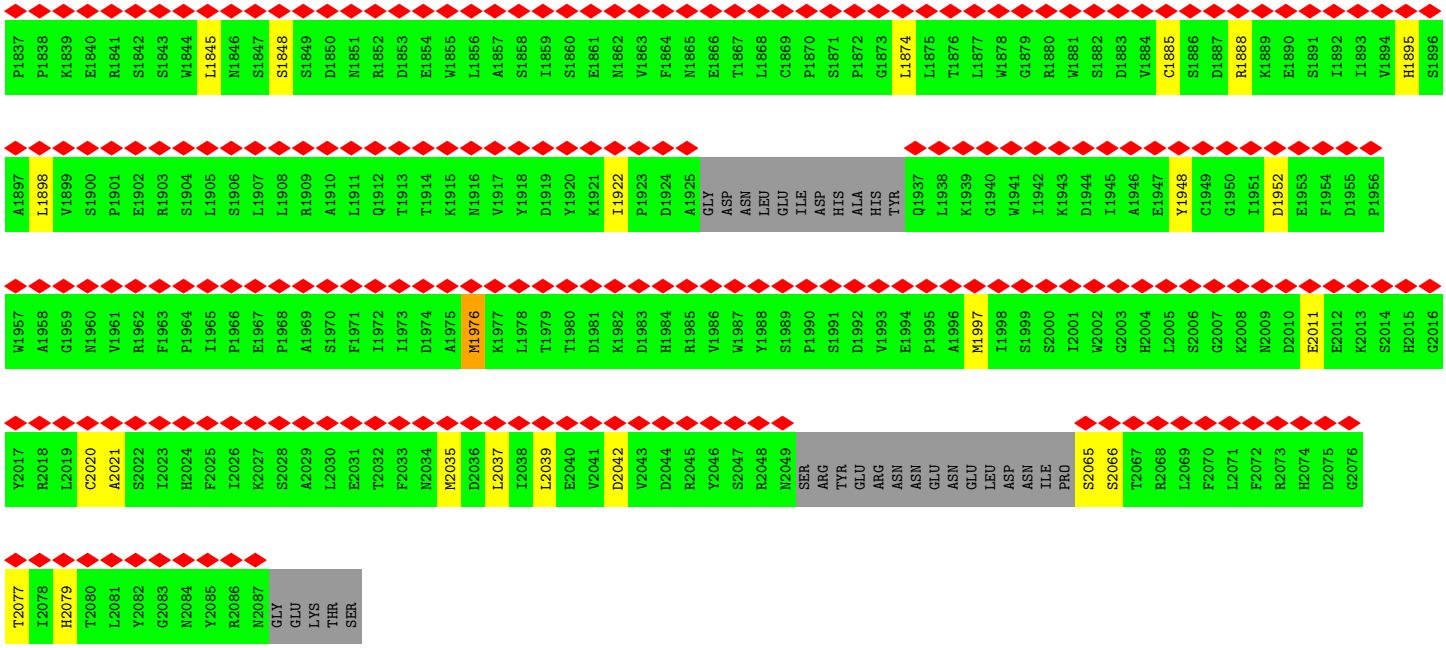
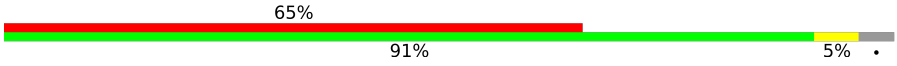
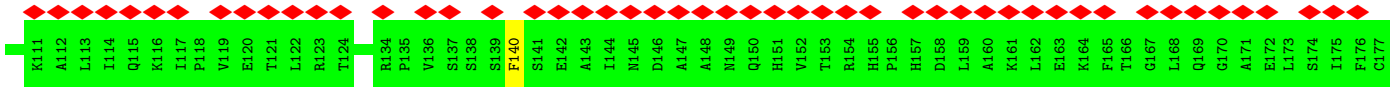
A1115 Q1116 I1117 K1118 A1119 D1120 G1121 Y1122 I1123 D1124 L1125 S1126 R1127 S1128 L1129 I1130 S1131 L1132 D1133 E1134 P1135 E1136 A1137 K1138 E1139 Y1140 F1141 N1142 Q1143 A1144 I1145 E1146 N1149 K1150 L1151 G1152 D1153 E1154 N1155 L1156 S1157 R1158 W1159 E1160 A1161 I1162 L1163 D1164 L1165 A1166 E1167 Y1168 V1169 A1170 G1171 K1172 T1173 Q1174 V1175
P1176 P1177 E1178 I1179 S1180 Y1181 K1182 L1183 A1184 R1185 C1186 A1187 E1188 L1189 T1190 R1191 E1192 Y1193 V1194 D1195 R1196 D1197 K1198 H1199 F1200 A1201 W1202 S1203 D1204 T1205 V1206 E1207 I1208 L1209 A1210 E1211 L1212 C1213 P1214 S1215 S1216 A1217 L1218 A1219 I1220 I1221 S1222 R1223 W1224 R1225 D1226 R1227 T1228 F1229 G1230 N1231 H1232 R1233 S1234 I1235
L1236 A1237 W1238 T1239 I1240 E1241 H1242 L1243 V1244 K1245 K1246 N1247 K1248 I1249 N1250 A1251 L1252 D1253 A1254 L1255 P1256 L1257 I1258 T1259 F1260 E1261 N1262 D1263 W1264 H1265 K1266 C1267 D1268 L1269 L1270 D1271 S1272 V1273 L1274 S1275 S1276 C1277 T1278 D1279 D1280 K1281 D1282 K1283 I1284 M1285 A1286 F1287 E1288 V1289 V1290 Y1291 H1292 Y1293 T1294 K1295
F1296 N1297 V1298 Q1299 N1300 I1301 Q1302 N1303 L1304 K1305 K1306 L1307 D1308 A1309 I1310 S1311 T1312 S1313 L1314 G1315 I1316 E1317 H1318 T1319 E1320 L1321 K1322 E1323 R1324 I1325 S1326 G1327 L1328 Q1329 H1330 THR GLU THR VAL SER LYS LYS SER SER LEU SER SER ASN ASP ASN GLU GLN G1348 H1349 D1350 Q1351 E1352 W1353 E1354 S1355
I1356 F1357 K1358 D1359 C1360 D1361 L1362 S1363 S1364 I1365 D1366 G1367 I1368 S1369 A1370 A1371 Y1372 E1373 K1374 F1375 R1376 N1377 V1378 P1379 E1380 F1381 Y1382 S1383 K1384 E1385 T1386 F1387 I1388 K1389 K1390 A1391 I1392 S1393 R1394 V1395 K1396 T1397 G1398 K1399 E1400 C1401 S1402 F1403 I1404 T1405 A1406 I1407 G1408 A1409 I1410 F1411 H1412 W1413 G1414 L1415
Y1416 D1417 F1418 K1419 Y1420 I1421 L1422 E1423 S1424 I1425 P1426 D1427 E1428 W1429 T1430 S1431 R1432 L1433 S1434 I1435 K1436 L1439 A1440 G1441 L1442 I1443 K1444 E1445 Y1446 C1447 Q1448 R1449 F1450 C1451 M1452 R1453 I1454 R1455 K1456 S1457 R1458 V1459 Y1460 E1461 I1462 F1463 P1464 F1465 S1466 L1467 A1468 S1469 R1470 L1471 S1472 G1473 I1474 S1475 E1476
K1477 E1478 I1479 F1480 G1481 I1482 T1483 L1484 E1485 A1486 I1487 A1488 E1489 S1490 P1491 E1492 P1493 A1494 N1495 S1496 D1497 R1498 L1499 F1500 S1501 L1502 P1503 G1504 L1505 L1506 V1507 S1508 K1509 L1510 E1511 S1512 N1513 E1514 A1515 L1516 D1517 V1518 L1519 S1520 Y1521 A1522 L1523 D1524 L1525 F1526 D1527 E1528 V1529 L1530 K1531 D1532 E1533 D1534 G1535 D1536
G1537 P1538 W1539 N1540 E1541 K1542 L1543 S1544 P1545 P1546 T1547 H1548 V1549 E1550 D1551 S1552 L1553 A1554 G1555 Y1556 I1557 W1558 A1559 R1560 L1561 G1562 S1563 P1564 E1565 A1566 E1567 M1568 R1569 W1570 Q1571 A1572 A1573 H1574 A1575 V1576 L1577 A1578 L1579 C1580 R1581 M1582 S1583 R1584 T1585 C1586 V1587 I1588 Q1589 G1590 I1591 F1592 Q1593 H1594 A1595 I1596
N1597 A1598 T1599 T1600 L1601 P1602 F1603 C1604 D1605 R1606 N1607 L1608 P1609 F1610 Y1611 T1612 L1613 H1614 A1615 Q1616 L1617 W1618 L1619 M1620 I1621 A1622 A1623 A1624 R1625 V1626 A1627 L1628 D1629 D1630 G1631 K1632 S1633 L1634 I1635 P1636 N1637 I1638 G1639 Y1640 F1641 Y1642 H1643 Y1644 A1645 T1646 T1647 D1648 Q1649 P1650 H1651 V1652 L1653 I1654 R1655 H1656
F1657 A1658 A1659 R1660 T1661 L1662 L1663 A1664 L1665 H1666 D1667 S1668 D1669 L1670 I1671 S1672 I1673 P1674 A1675 Q1676 E1677 E1678 N1679 K1680 L1681 R1682 N1683 I1684 N1685 Q1686 S1687 T1688 T1689 L1690 P1691 V1692 LEU ASP LYS VAL GLU ASP HIS ARG GLY E1702 D1703 S1704 Y1705 T1706 F1707 G1708 I1709 D1710 F1711 G1712 P1713 Y1714 W1715 L1716
K1717 P1718 L1719 G1720 R1721 C1722 F1723 G1724 V1725 S1726 Q1727 K1728 Q1729 L1730 E1731 P1732 E1733 M1734 L1735 R1736 I1737 I1738 R1739 D1740 V1741 L1742 G1743 F1744 K1745 G1746 S1747 R1748 N1749 W1750 D1751 E1752 D1763 E1754 R1755 N1756 K1757 R1758 R1759 Y1760 Y1761 Q1762 D1763 R1764 D1765 N1766 H1767 H1768 S1769 H1770 G1771 S1772 Y1773 P1774 R1775 V1776
D1777 D1778 Y1779 H1780 F1781 Y1782 L1783 S1784 Y1785 H1786 A1787 M1788 F1789 M1790 T1791 A1792 G1793 Q1794 L1795 L1796 A1797 T1798 K1799 P1800 L1801 V1802 G1803 SER ASP TYR ASP ASP VAL E1810 D1811 V1812 F1813 Q1814 D1815 W1816 L1817 R1818 R1819 H1820 D1821 I1822 S1823 R1824 N1825 D1826 H1827 R1828 W1829 L1830 A1831 D1832 R1833 R1834 D1835 I1836

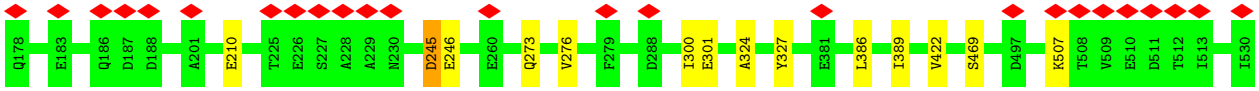


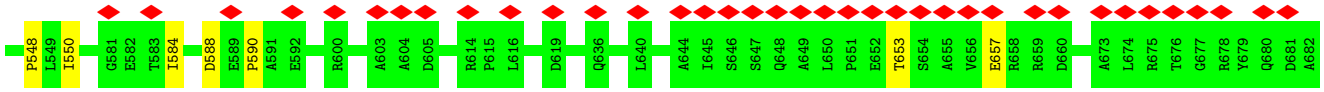
- Molecule 1: SeAvs3

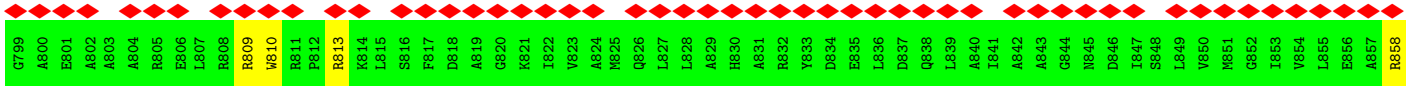
Chain B:

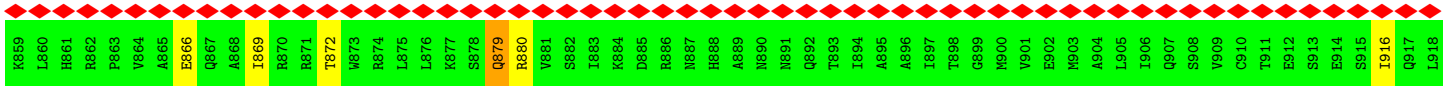


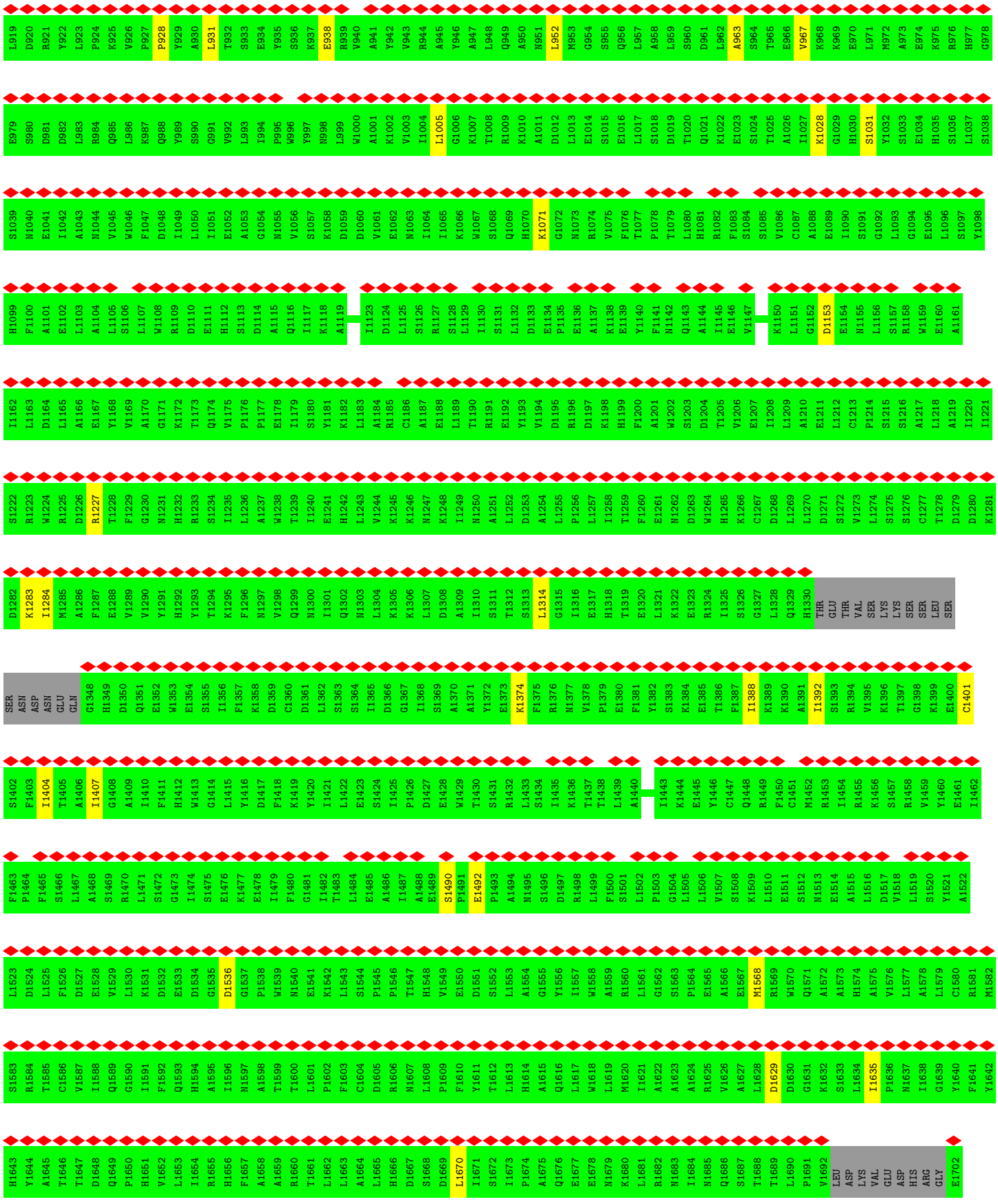








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E979 S980 D981 D982 L983 R984 Q985 L986 K987 Q988 Y989 S990 G991 V992 L993 I994 P995 W996 Y997 N998 L999 W1000 A1001 K1002 V1003 I1004 L1005 G1006 K1007 T1008 R1009 K1010 A1011 D1012 L1013 E1014 S1015 E1016 L1017 S1018 D1019 T1020 Q1021 K1022 E1023 S1024 T1025 A1026 I1027 K1028 G1029 H1030 S1031 Y1032 S1033 E1034 H1035 S1036 L1037 S1038
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SER ASN ASP ASN GLU GLN G1348 H1349 D1350 Q1351 E1352 W1353 E1354 S1355 I1356 F1357 K1358 D1359 C1360 D1361 L1362 S1363 S1364 I1365 D1366 G1367 I1368 S1369 A1370 A1371 Y1372 E1373 K1374 F1375 R1376 N1377 V1378 P1379 E1380 F1381 Y1382 S1383 K1384 E1385 T1386 F1387 I1388 K1389 K1390 A1391 I1392 S1393 R1394 V1395 K1396 T1397 G1398 K1399 E1400 C1401
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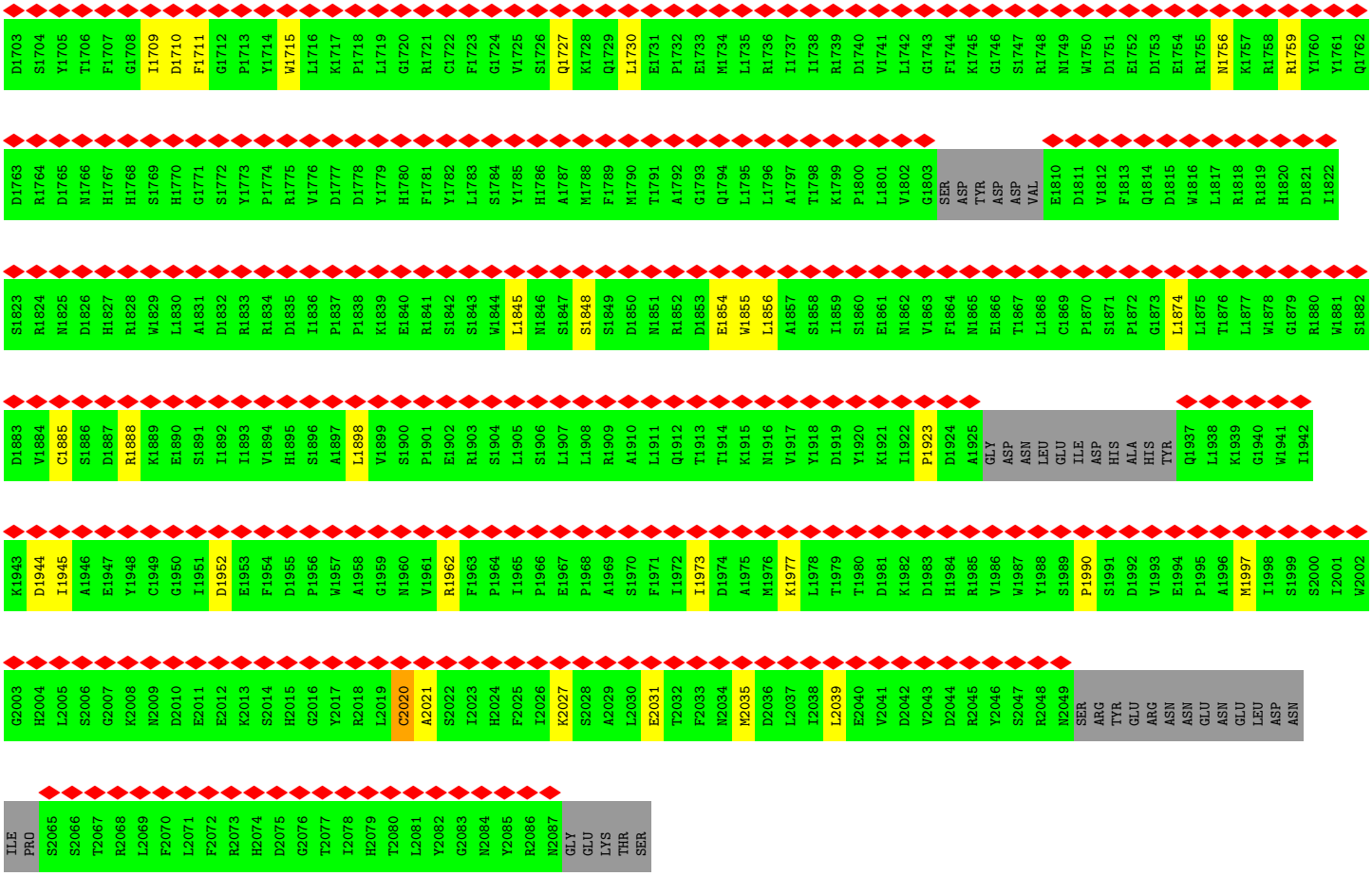
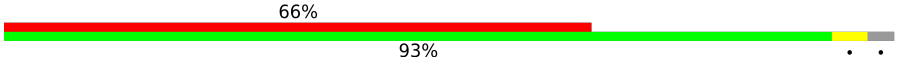
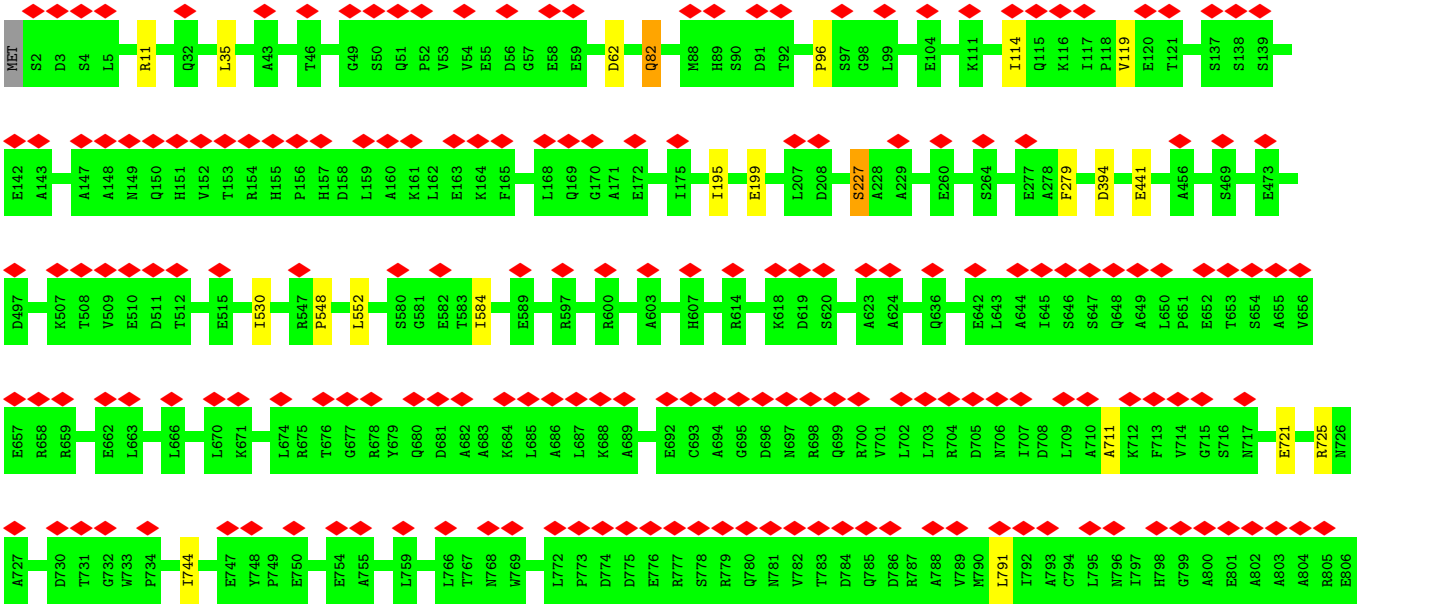
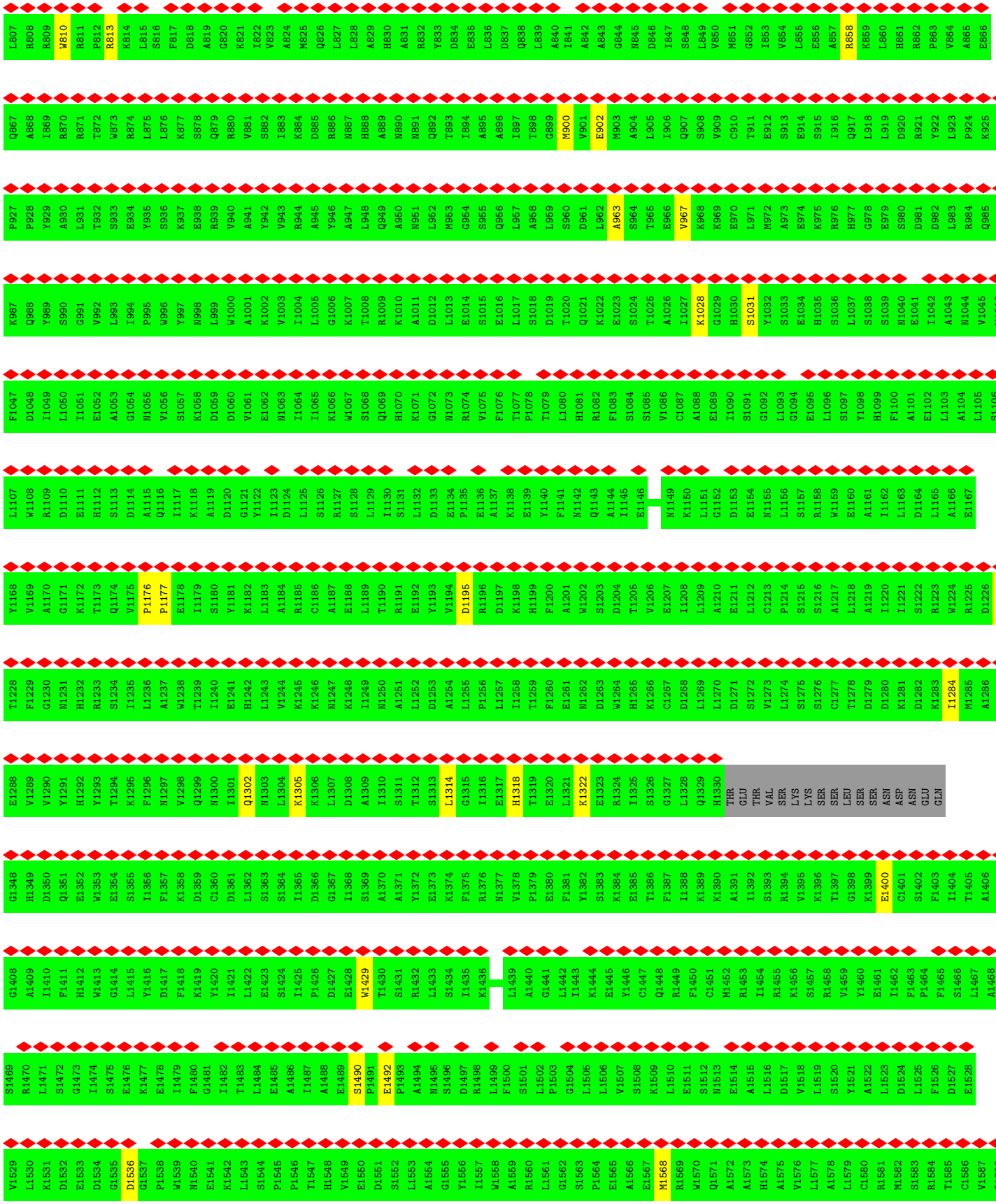


- Molecule 1: SeAvs3

Chain C:



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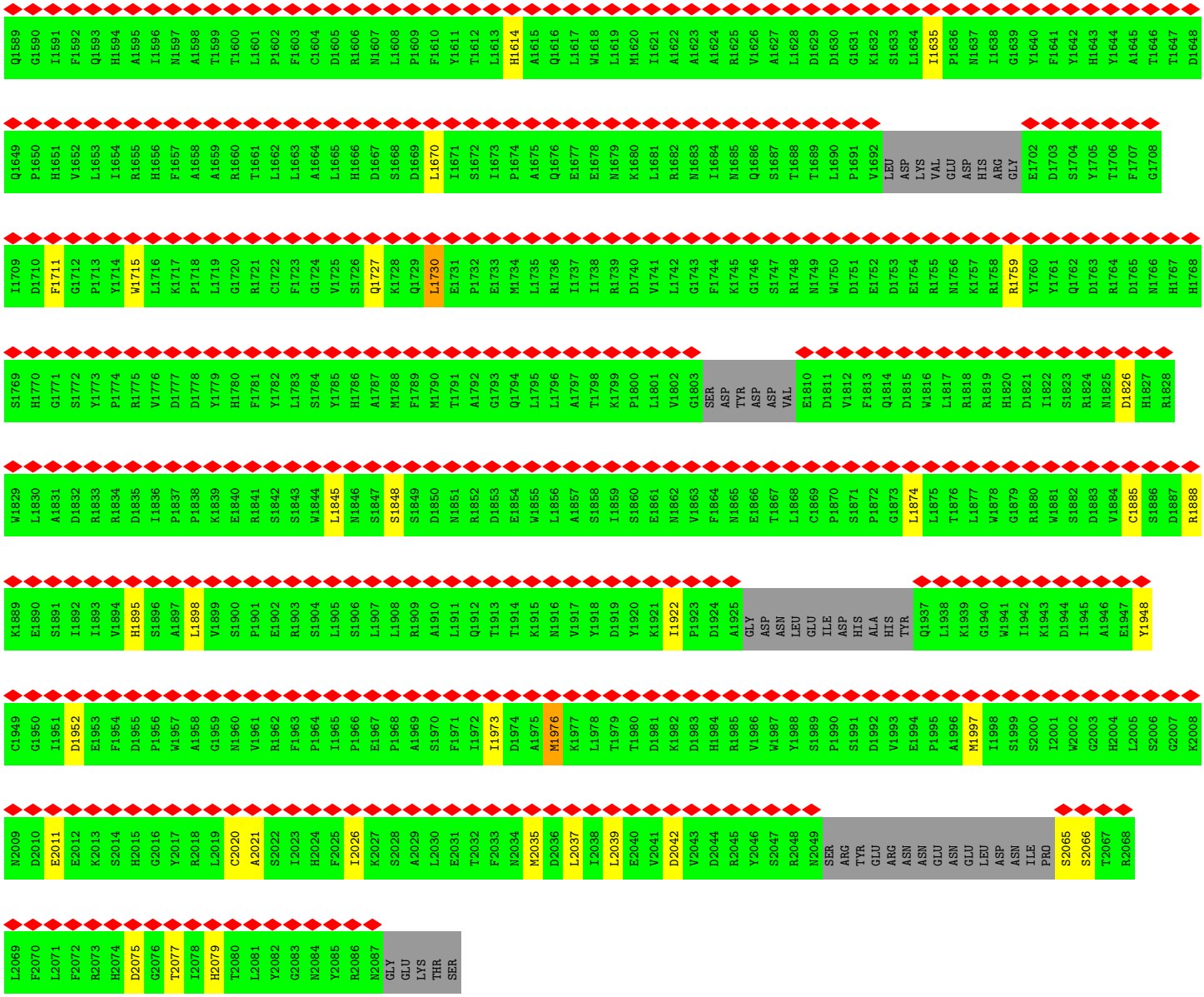
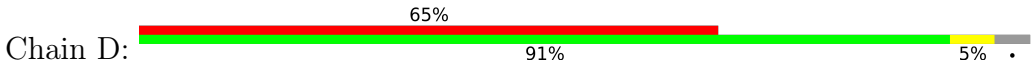
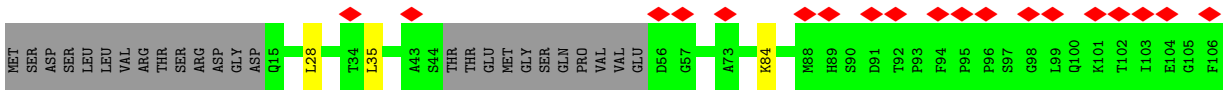
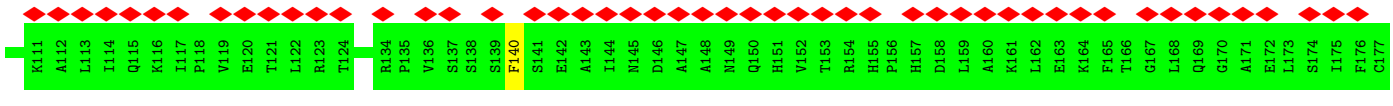


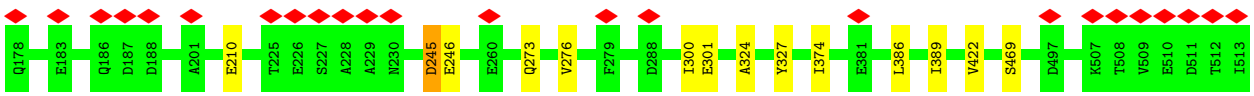
- Molecule 1: SeAvs3

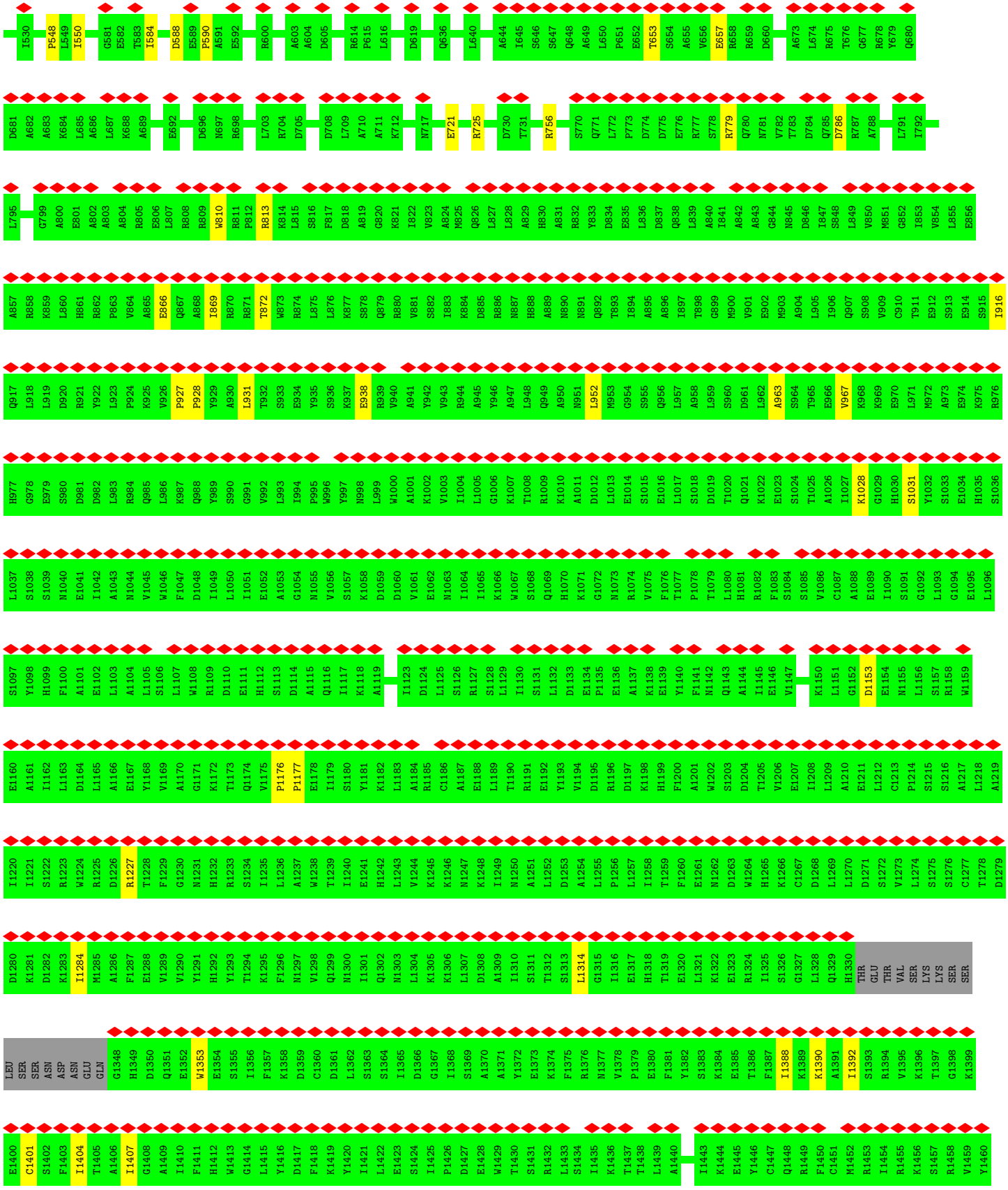
Chain D:







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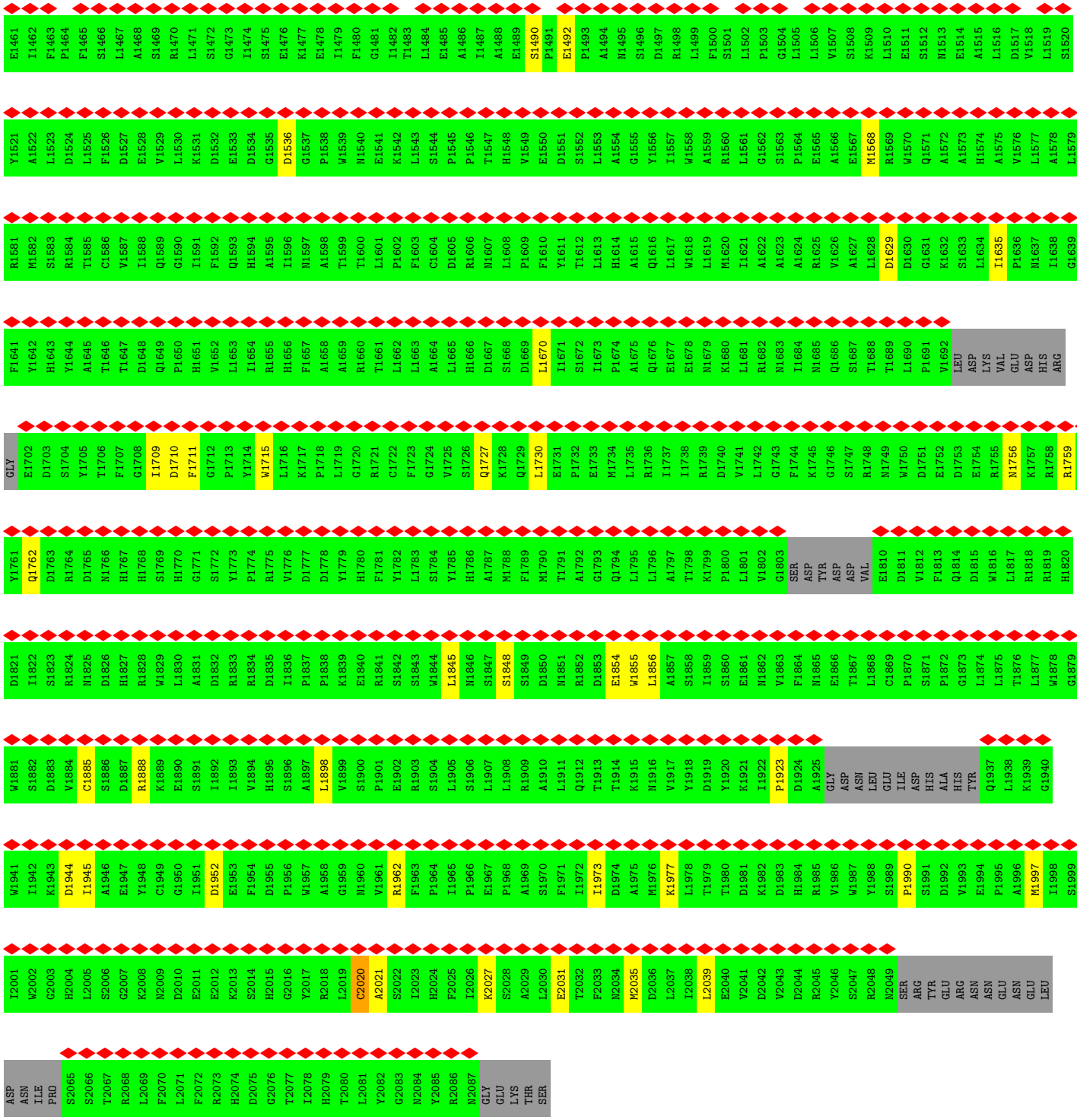
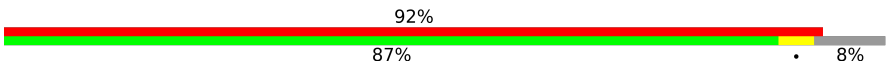
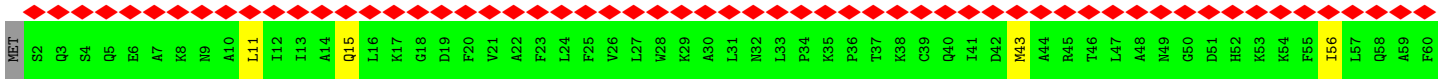
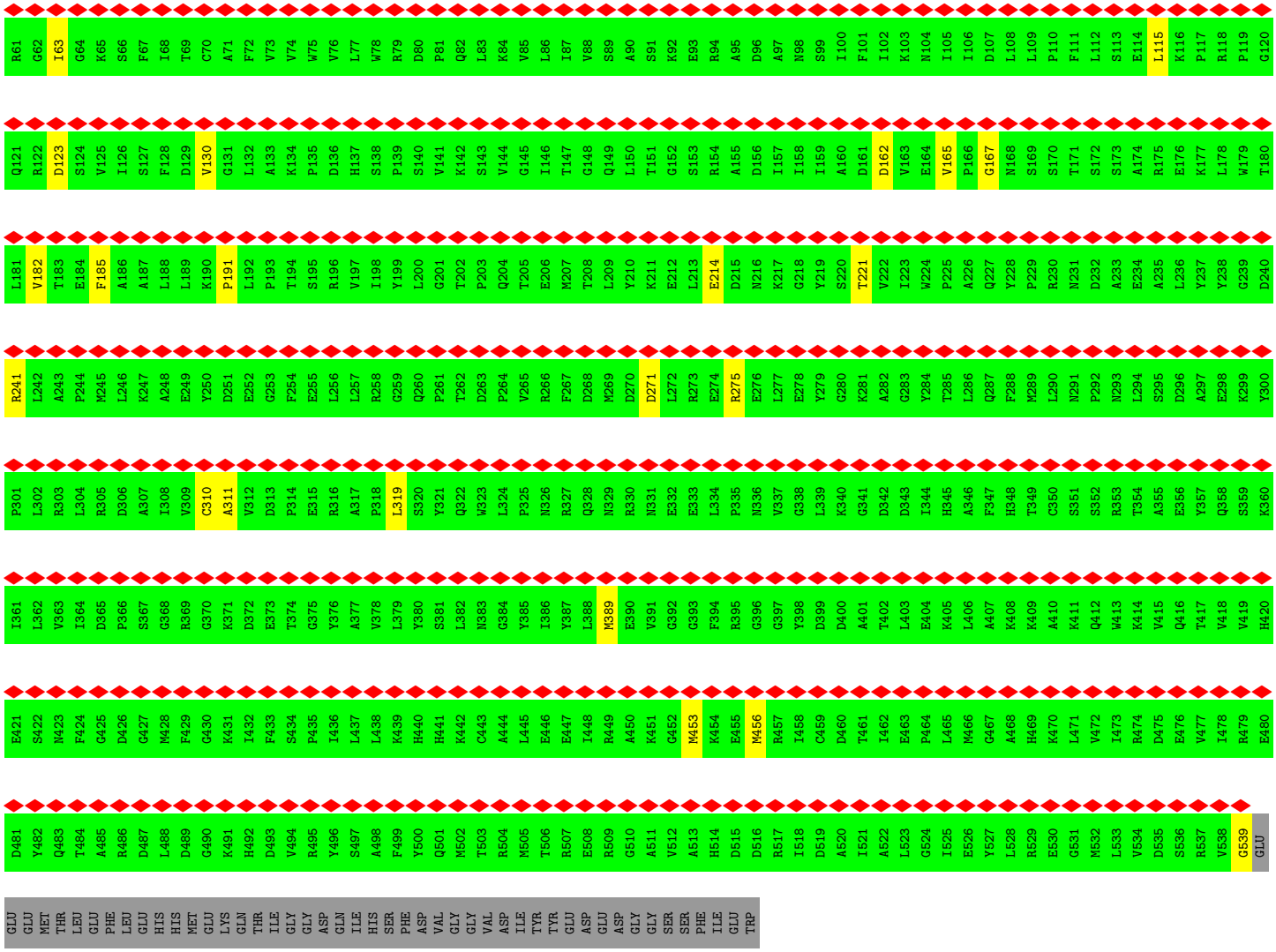


• Molecule 2: Terminase, large subunit

Chain E:

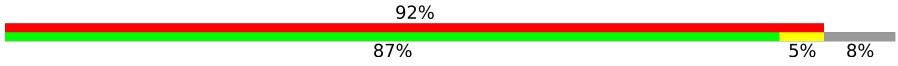


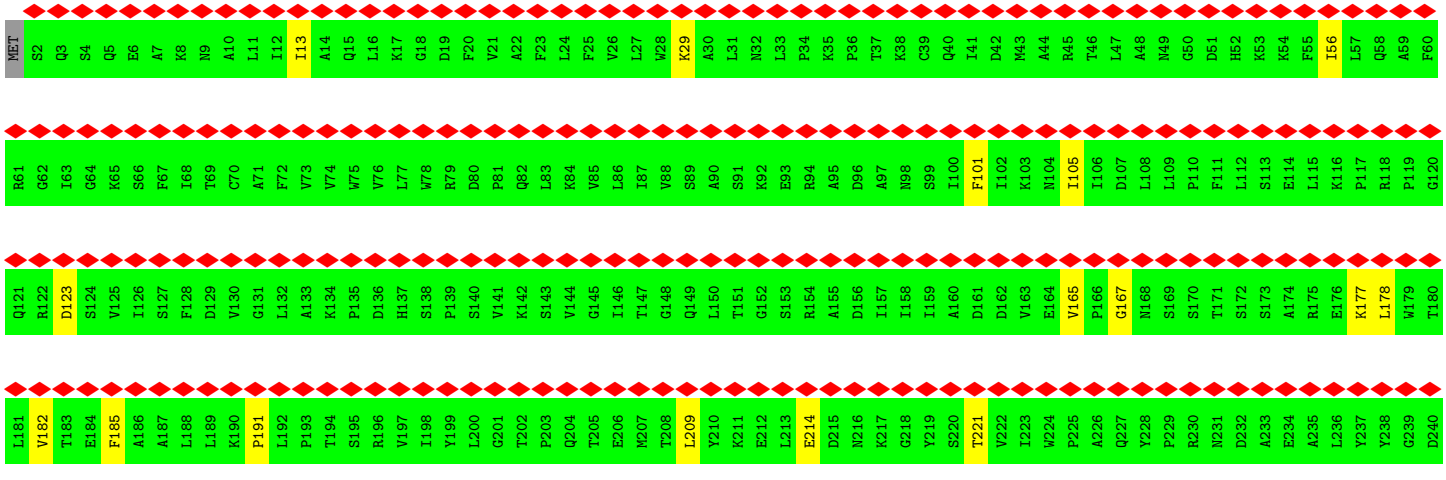


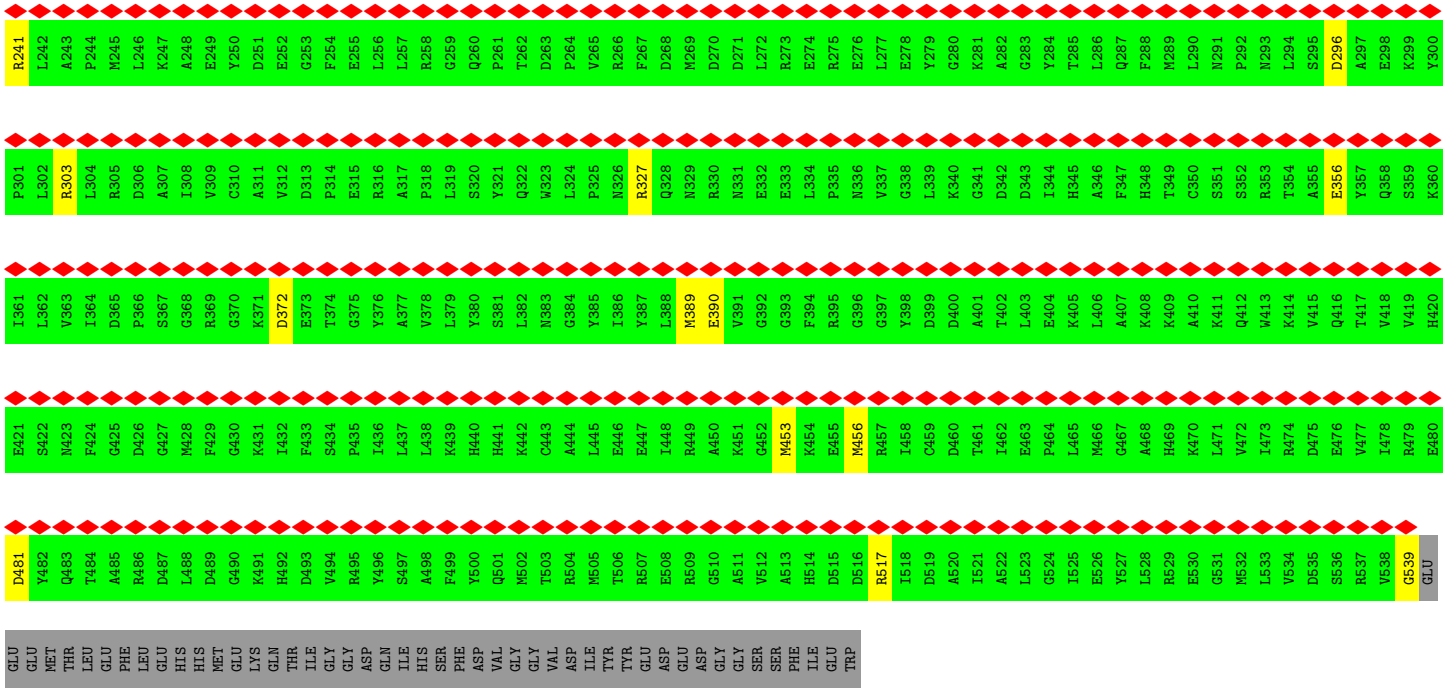


• Molecule 2: Terminase, large subunit

Chain F:

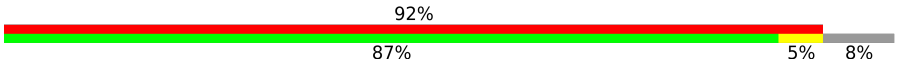


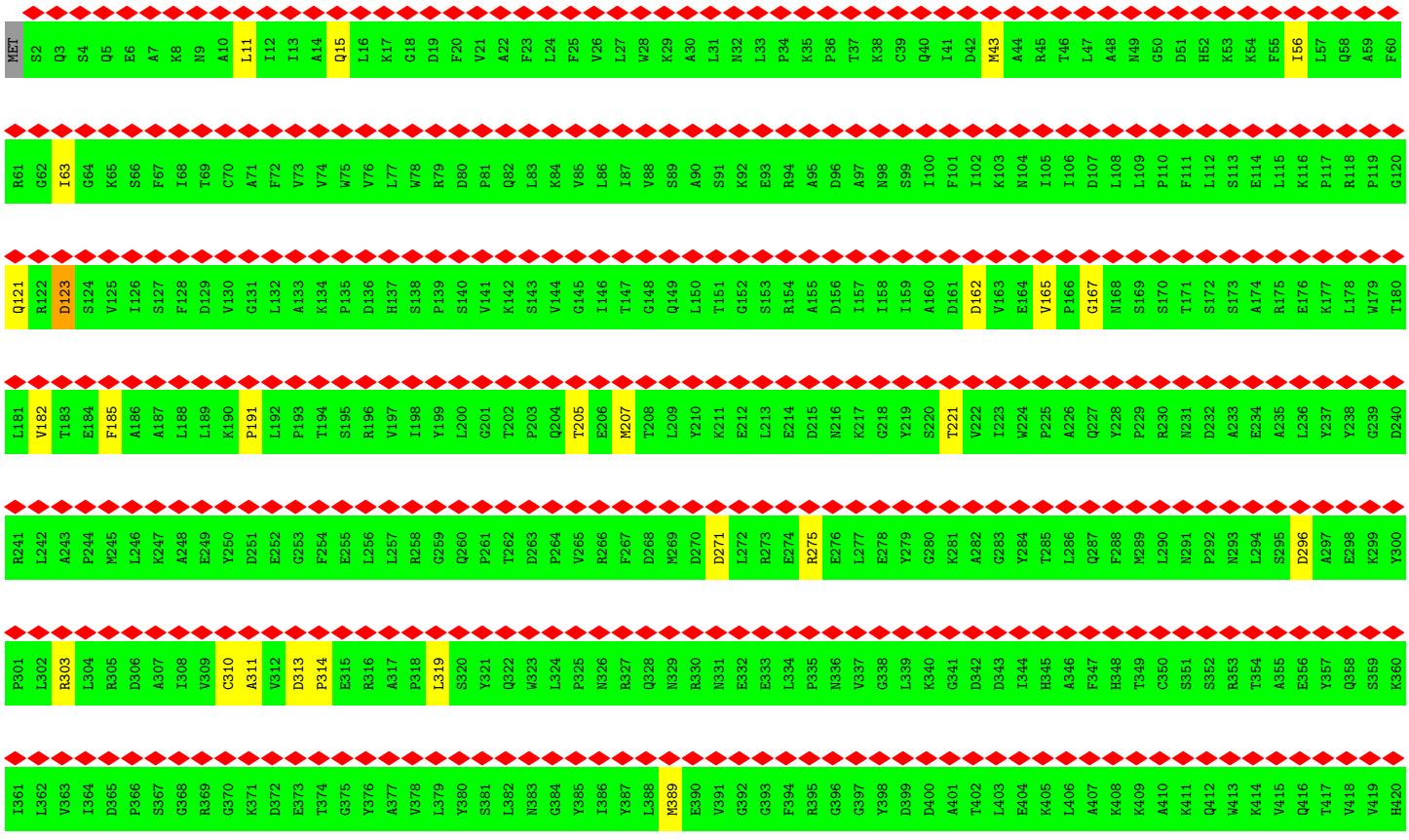


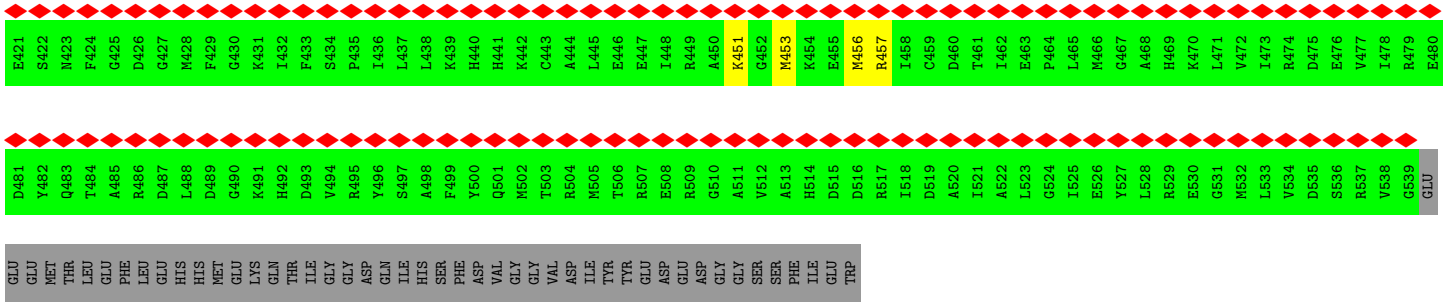


• Molecule 2: Terminase, large subunit

Chain G:

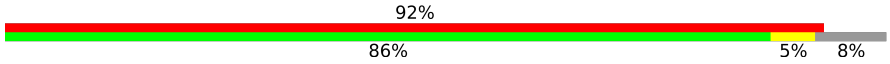


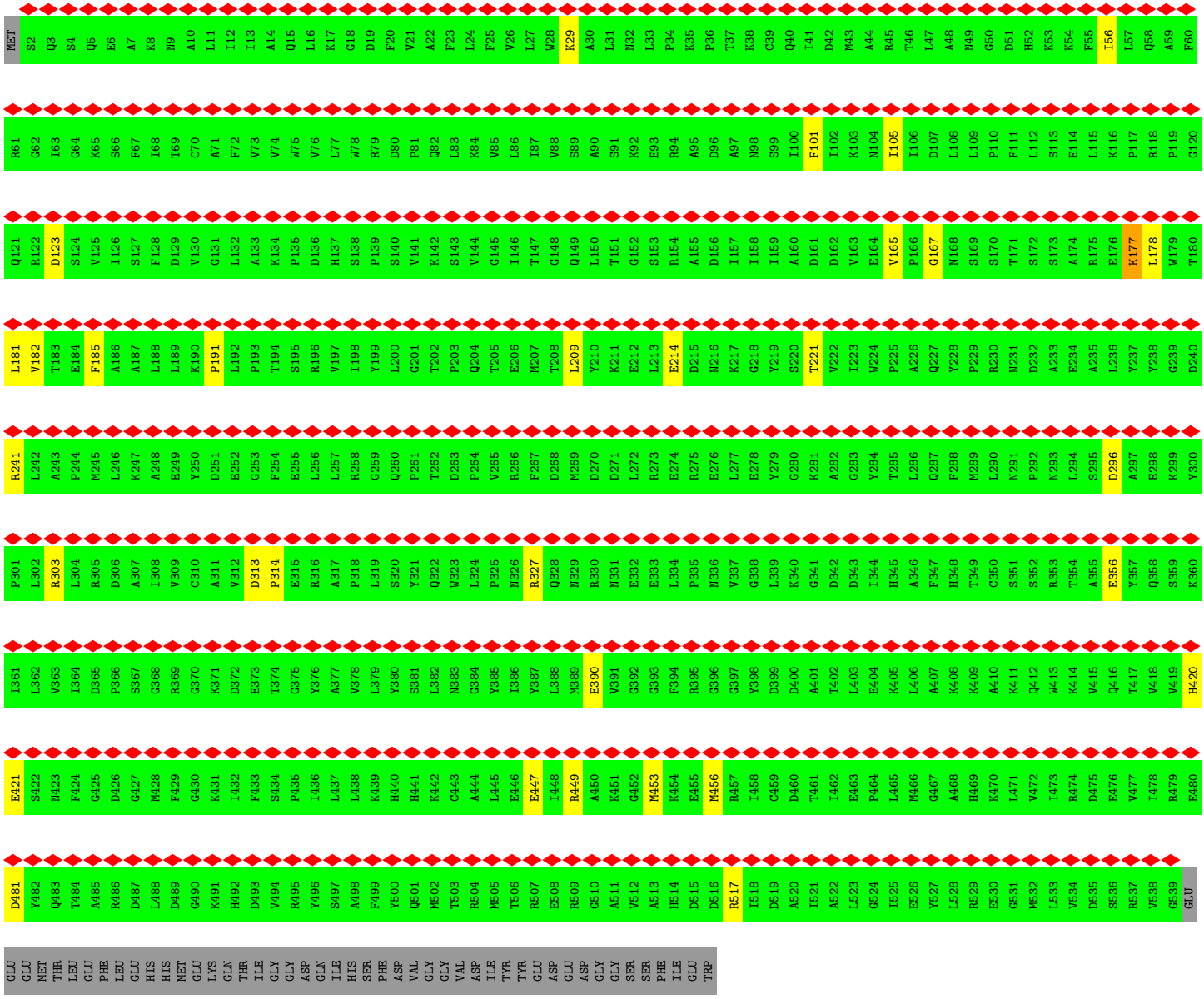




• Molecule 2: Terminase, large subunit

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	44479	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	313.092, 313.092, 313.092	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8697, 0.8697, 0.8697	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG

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	0.31	0/16499	0.62	6/22369 (0.0%)
1	B	0.31	0/16319	0.62	5/22123 (0.0%)
1	C	0.31	0/16499	0.61	6/22369 (0.0%)
1	D	0.31	0/16319	0.62	5/22123 (0.0%)
2	E	0.30	0/4363	0.66	6/5899 (0.1%)
2	F	0.31	0/4363	0.65	3/5899 (0.1%)
2	G	0.30	0/4363	0.66	5/5899 (0.1%)
2	H	0.30	0/4363	0.64	2/5899 (0.0%)
All	All	0.31	0/83088	0.63	38/112580 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1923	PRO	CA-N-CD	-11.88	94.87	111.50
1	B	1923	PRO	CA-N-CD	-11.86	94.90	111.50
1	B	1153	ASP	CB-CG-OD2	8.68	126.12	118.30
1	D	1153	ASP	CB-CG-OD2	8.47	125.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	191	PRO	CA-N-CD	-8.29	99.89	111.50
2	H	191	PRO	CA-N-CD	-8.27	99.93	111.50
2	G	191	PRO	CA-N-CD	-8.26	99.94	111.50
2	E	191	PRO	CA-N-CD	-8.23	99.98	111.50
2	F	123	ASP	CB-CG-OD2	8.07	125.56	118.30
2	H	123	ASP	CB-CG-OD2	8.04	125.54	118.30
1	A	96	PRO	N-CD-CG	-7.22	92.38	103.20
1	C	96	PRO	N-CD-CG	-7.20	92.41	103.20
2	E	123	ASP	CB-CG-OD2	6.98	124.58	118.30
2	E	162	ASP	CB-CG-OD1	6.94	124.55	118.30
2	G	389	MET	CG-SD-CE	-6.91	89.15	100.20
2	G	162	ASP	CB-CG-OD1	6.89	124.50	118.30
2	E	389	MET	CG-SD-CE	-6.87	89.20	100.20
2	F	389	MET	CG-SD-CE	-6.87	89.21	100.20
1	D	1845	LEU	CA-CB-CG	6.62	130.53	115.30
1	B	1845	LEU	CA-CB-CG	6.61	130.49	115.30
1	D	245	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	245	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	1845	LEU	CA-CB-CG	5.37	127.64	115.30
1	D	1923	PRO	N-CD-CG	-5.35	95.17	103.20
1	B	1923	PRO	N-CD-CG	-5.34	95.19	103.20
1	C	35	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	35	LEU	CA-CB-CG	5.34	127.57	115.30
1	C	1730	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	1845	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	1730	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	791	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	791	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	1976	MET	CB-CG-SD	5.09	127.67	112.40
1	C	1976	MET	CB-CG-SD	5.08	127.64	112.40
2	E	319	LEU	CA-CB-CG	5.05	126.92	115.30
2	E	191	PRO	N-CD-CG	-5.05	95.63	103.20
2	G	319	LEU	CA-CB-CG	5.04	126.89	115.30
2	G	191	PRO	N-CD-CG	-5.02	95.67	103.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	548	PRO	Peptide
1	B	548	PRO	Peptide
1	C	548	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	D	548	PRO	Peptide

5.2 Too-close contacts (i)

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	16152	0	15975	34	0
1	B	15974	0	15804	49	0
1	C	16152	0	15975	37	0
1	D	15974	0	15804	49	0
2	E	4273	0	4283	11	0
2	F	4273	0	4283	14	0
2	G	4273	0	4283	13	0
2	H	4273	0	4283	16	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
3	E	31	0	12	0	0
3	F	31	0	12	0	0
3	G	31	0	12	0	0
3	H	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
All	All	81600	0	80786	221	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 1.

All (221) 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:F:165:VAL:HG12	2:F:167:GLY:H	1.55	0.72
2:H:165:VAL:HG12	2:H:167:GLY:H	1.55	0.70
2:G:165:VAL:HG12	2:G:167:GLY:H	1.61	0.65
1:B:1944:ASP:OD2	1:B:1945:ILE:N	2.30	0.65
2:E:165:VAL:HG12	2:E:167:GLY:H	1.61	0.64
1:D:1944:ASP:OD2	1:D:1945:ILE:N	2.30	0.64
1:B:245:ASP:OD2	1:B:246:GLU:N	2.32	0.63
1:D:245:ASP:OD2	1:D:246:GLU:N	2.32	0.63
1:B:1898:LEU:HB3	1:B:2035:MET:HG2	1.81	0.63
1:D:1898:LEU:HB3	1:D:2035:MET:HG2	1.81	0.62
1:A:1028:LYS:HE3	1:A:1031:SER:HB2	1.81	0.62
1:C:1028:LYS:HE3	1:C:1031:SER:HB2	1.82	0.62
1:C:62:ASP:OD2	1:C:82:GLN:NE2	2.33	0.61
1:B:469:SER:OG	1:B:756:ARG:NH1	2.33	0.61
1:C:1635:ILE:HD11	1:C:1670:LEU:HD12	1.82	0.61
1:D:1635:ILE:HD11	1:D:1670:LEU:HD12	1.83	0.61
1:D:469:SER:OG	1:D:756:ARG:NH1	2.33	0.61
1:A:62:ASP:OD2	1:A:82:GLN:NE2	2.33	0.60
1:B:1635:ILE:HD11	1:B:1670:LEU:HD12	1.83	0.60
1:A:1635:ILE:HD11	1:A:1670:LEU:HD12	1.83	0.60
1:D:963:ALA:HB1	1:D:967:VAL:HG23	1.83	0.60
2:G:43:MET:HE1	2:G:63:ILE:HD13	1.83	0.59
1:C:1848:SER:O	1:C:1888:ARG:NH2	2.35	0.59
1:B:963:ALA:HB1	1:B:967:VAL:HG23	1.83	0.59
2:E:43:MET:HE1	2:E:63:ILE:HD13	1.83	0.59
1:A:1490:SER:OG	1:A:1492:GLU:OE1	2.21	0.58
1:A:1848:SER:O	1:A:1888:ARG:NH2	2.35	0.58
1:C:1490:SER:OG	1:C:1492:GLU:OE1	2.21	0.58
1:D:1490:SER:OG	1:D:1492:GLU:OE1	2.22	0.56
1:B:1490:SER:OG	1:B:1492:GLU:OE1	2.22	0.56
1:B:1388:ILE:HD12	1:B:1407:ILE:HD11	1.88	0.56
1:A:809:ARG:NH2	2:E:539:GLY:O	2.38	0.56
1:D:1388:ILE:HD12	1:D:1407:ILE:HD11	1.87	0.55
1:B:879:GLN:NE2	1:B:880:ARG:O	2.40	0.55
1:D:1388:ILE:O	1:D:1392:ILE:HG13	2.07	0.55
1:D:210:GLU:N	1:D:210:GLU:OE2	2.39	0.54
1:B:210:GLU:N	1:B:210:GLU:OE2	2.39	0.54
1:B:1227:ARG:NH1	1:B:1536:ASP:OD1	2.36	0.54
1:A:2077:THR:OG1	1:A:2079:HIS:NE2	2.41	0.54
1:C:1302:GLN:HA	1:C:1305:LYS:HE3	1.90	0.53
1:D:928:PRO:HD2	1:D:931:LEU:HD23	1.90	0.53
1:D:810:TRP:O	1:D:813:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1388:ILE:O	1:B:1392:ILE:HG13	2.09	0.53
1:A:227:SER:OG	1:A:227:SER:O	2.28	0.53
1:C:1227:ARG:NH1	1:C:1536:ASP:OD1	2.36	0.52
2:F:182:VAL:HG11	2:F:209:LEU:HD13	1.90	0.52
2:H:182:VAL:HG11	2:H:209:LEU:HD13	1.90	0.52
1:B:1028:LYS:HE3	1:B:1031:SER:HB2	1.92	0.52
1:A:1227:ARG:NH1	1:A:1536:ASP:OD1	2.35	0.52
1:A:1302:GLN:HA	1:A:1305:LYS:HE3	1.90	0.52
1:B:810:TRP:O	1:B:813:ARG:NH1	2.43	0.52
1:D:1762:GLN:N	1:D:1762:GLN:OE1	2.42	0.52
2:F:56:ILE:HB	2:F:221:THR:HG22	1.91	0.51
2:H:56:ILE:HB	2:H:221:THR:HG22	1.92	0.51
1:A:1997:MET:HG2	1:A:2021:ALA:HB2	1.93	0.51
2:E:56:ILE:HB	2:E:221:THR:HG22	1.92	0.51
1:A:1826:ASP:OD1	1:A:1826:ASP:N	2.35	0.51
1:C:711:ALA:HB2	1:C:744:ILE:HG13	1.92	0.51
1:D:1028:LYS:HE3	1:D:1031:SER:HB2	1.92	0.51
1:B:1952:ASP:OD1	1:B:1952:ASP:N	2.43	0.50
1:C:1997:MET:HG2	1:C:2021:ALA:HB2	1.93	0.50
1:B:809:ARG:NH2	2:F:539:GLY:O	2.44	0.50
1:A:711:ALA:HB2	1:A:744:ILE:HG13	1.93	0.50
2:G:121:GLN:HB3	2:G:123:ASP:HB3	1.93	0.50
1:A:2042:ASP:OD2	1:A:2065:SER:OG	2.23	0.50
1:A:1898:LEU:HD23	1:A:2037:LEU:HD13	1.94	0.50
1:C:1400:GLU:HB3	1:C:1429:TRP:CZ3	2.47	0.50
1:C:1898:LEU:HD23	1:C:2037:LEU:HD13	1.93	0.50
2:F:101:PHE:O	2:F:105:ILE:HG12	2.11	0.50
1:A:1400:GLU:HB3	1:A:1429:TRP:CZ3	2.47	0.50
2:F:296:ASP:O	2:F:303:ARG:NH2	2.41	0.50
2:H:101:PHE:O	2:H:105:ILE:HG12	2.12	0.50
1:C:1874:LEU:HB3	1:C:2020:CYS:SG	2.52	0.49
1:C:2042:ASP:OD2	1:C:2065:SER:OG	2.24	0.49
2:H:296:ASP:O	2:H:303:ARG:NH2	2.42	0.49
1:A:1874:LEU:HB3	1:A:2020:CYS:SG	2.52	0.49
1:A:1284:ILE:HD13	1:A:1314:LEU:HD23	1.94	0.49
1:A:1727:GLN:HA	1:A:1730:LEU:HG	1.94	0.49
1:D:653:THR:OG1	1:D:657:GLU:OE1	2.30	0.49
1:B:916:ILE:HD11	1:B:952:LEU:HB3	1.94	0.49
1:C:1284:ILE:HD13	1:C:1314:LEU:HD23	1.94	0.49
1:B:550:ILE:HB	1:B:584:ILE:HG22	1.94	0.49
1:B:653:THR:OG1	1:B:657:GLU:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:963:ALA:HB1	1:C:967:VAL:HG23	1.95	0.49
1:C:1727:GLN:HA	1:C:1730:LEU:HG	1.94	0.49
1:D:550:ILE:HB	1:D:584:ILE:HG22	1.94	0.49
1:C:227:SER:O	1:C:227:SER:OG	2.28	0.49
1:D:1952:ASP:OD1	1:D:1952:ASP:N	2.43	0.49
2:G:205:THR:OG1	2:G:207:MET:O	2.28	0.48
1:D:1227:ARG:NH1	1:D:1536:ASP:OD1	2.36	0.48
1:A:775:ASP:O	1:A:779:ARG:NE	2.42	0.48
1:B:721:GLU:OE2	1:B:725:ARG:NH2	2.46	0.48
1:D:386:LEU:HB3	1:D:422:VAL:HG12	1.96	0.48
1:D:1284:ILE:HD13	1:D:1314:LEU:HD23	1.95	0.48
2:G:56:ILE:HB	2:G:221:THR:HG22	1.95	0.48
1:D:721:GLU:OE2	1:D:725:ARG:NH2	2.46	0.48
2:F:481:ASP:OD1	2:F:517:ARG:NH1	2.47	0.48
2:G:11:LEU:O	2:G:15:GLN:HG3	2.14	0.48
2:H:453:MET:HG2	2:H:456:MET:H	1.79	0.48
1:A:721:GLU:OE2	1:A:725:ARG:NH2	2.46	0.47
1:D:916:ILE:HD11	1:D:952:LEU:HB3	1.97	0.47
1:A:963:ALA:HB1	1:A:967:VAL:HG23	1.95	0.47
1:B:1848:SER:O	1:B:1888:ARG:NH2	2.40	0.47
1:A:2011:GLU:OE1	1:A:2011:GLU:N	2.43	0.47
1:B:386:LEU:HB3	1:B:422:VAL:HG12	1.96	0.47
1:D:1401:CYS:HA	1:D:1404:ILE:HD12	1.97	0.47
1:A:195:ILE:O	1:A:199:GLU:HG2	2.15	0.47
1:B:1284:ILE:HD13	1:B:1314:LEU:HD23	1.95	0.47
1:B:1401:CYS:HA	1:B:1404:ILE:HD12	1.97	0.47
1:D:273:GLN:HA	1:D:276:VAL:HG12	1.98	0.46
1:C:195:ILE:O	1:C:199:GLU:HG2	2.15	0.46
1:B:938:GLU:N	1:B:938:GLU:OE2	2.49	0.46
1:C:721:GLU:OE2	1:C:725:ARG:NH2	2.47	0.46
2:H:178:LEU:O	2:H:182:VAL:HG12	2.16	0.46
1:C:810:TRP:O	1:C:813:ARG:NH1	2.49	0.46
2:E:11:LEU:O	2:E:15:GLN:HG3	2.14	0.46
2:F:453:MET:HG2	2:F:456:MET:H	1.80	0.46
1:A:810:TRP:O	1:A:813:ARG:NH1	2.49	0.45
1:B:273:GLN:HA	1:B:276:VAL:HG12	1.98	0.45
2:H:481:ASP:OD1	2:H:517:ARG:NH1	2.49	0.45
1:A:858:ARG:NH1	1:A:902:GLU:OE2	2.49	0.45
1:B:2027:LYS:O	1:B:2031:GLU:HG2	2.16	0.45
2:E:453:MET:HG2	2:E:456:MET:H	1.80	0.45
1:A:1711:PHE:O	1:A:1715:TRP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1711:PHE:O	1:C:1715:TRP:HB2	2.17	0.45
1:D:938:GLU:N	1:D:938:GLU:OE2	2.50	0.45
2:F:178:LEU:O	2:F:182:VAL:HG12	2.16	0.45
1:A:1952:ASP:OD1	1:A:1952:ASP:N	2.43	0.45
1:D:1727:GLN:HA	1:D:1730:LEU:HG	1.99	0.45
2:G:453:MET:HG2	2:G:456:MET:H	1.82	0.44
1:B:588:ASP:OD2	1:B:590:PRO:HD2	2.17	0.44
1:A:394:ASP:OD1	1:A:394:ASP:N	2.51	0.44
1:B:928:PRO:HD2	1:B:931:LEU:HD23	1.99	0.44
1:D:1848:SER:O	1:D:1888:ARG:NH2	2.40	0.44
1:B:1727:GLN:HA	1:B:1730:LEU:HG	1.98	0.44
1:D:1973:ILE:H	1:D:1973:ILE:HG13	1.58	0.44
2:H:29:LYS:HA	2:H:29:LYS:HD3	1.80	0.44
2:H:182:VAL:HA	2:H:185:PHE:CE1	2.53	0.44
1:A:114:ILE:HD12	1:A:119:VAL:HG22	1.99	0.44
1:C:858:ARG:NH1	1:C:902:GLU:OE2	2.50	0.44
1:A:441:GLU:N	1:A:441:GLU:OE2	2.51	0.44
1:A:582:GLU:N	1:A:582:GLU:OE1	2.50	0.43
1:B:1071:LYS:HE3	1:B:1071:LYS:HB3	1.86	0.43
1:D:588:ASP:OD2	1:D:590:PRO:HD2	2.17	0.43
1:B:1854:GLU:H	1:B:1854:GLU:CD	2.21	0.43
1:B:1855:TRP:HE3	1:B:1856:LEU:HD23	1.83	0.43
1:D:1854:GLU:H	1:D:1854:GLU:CD	2.21	0.43
2:F:182:VAL:HA	2:F:185:PHE:CE1	2.53	0.43
1:D:1711:PHE:O	1:D:1715:TRP:HB2	2.19	0.43
1:C:114:ILE:HD12	1:C:119:VAL:HG22	1.99	0.43
1:D:866:GLU:HA	1:D:869:ILE:HG22	2.01	0.43
1:D:2027:LYS:O	1:D:2031:GLU:HG2	2.18	0.43
1:C:441:GLU:OE2	1:C:441:GLU:N	2.52	0.43
1:B:1977:LYS:HB3	1:B:1990:PRO:HG3	2.01	0.43
1:B:1374:LYS:HD3	1:B:1374:LYS:HA	1.81	0.42
1:D:1977:LYS:HB3	1:D:1990:PRO:HG3	2.01	0.42
2:H:420:HIS:NE2	2:H:447:GLU:OE2	2.44	0.42
1:B:1973:ILE:H	1:B:1973:ILE:HG13	1.58	0.42
1:A:784:ASP:OD1	1:A:784:ASP:N	2.50	0.42
1:D:1855:TRP:HE3	1:D:1856:LEU:HD23	1.83	0.42
1:B:866:GLU:HA	1:B:869:ILE:HG22	2.01	0.42
1:B:1711:PHE:O	1:B:1715:TRP:HB2	2.19	0.42
1:D:869:ILE:HA	1:D:872:THR:HG22	2.02	0.42
1:C:2011:GLU:OE1	1:C:2011:GLU:N	2.43	0.42
2:E:271:ASP:O	2:E:275:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:LEU:HD23	1:B:1005:LEU:HD11	2.00	0.42
2:F:13:ILE:HD12	2:F:13:ILE:HA	1.97	0.42
2:G:182:VAL:HA	2:G:185:PHE:CE1	2.55	0.42
1:D:1709:ILE:HG23	1:D:1710:ASP:OD1	2.20	0.41
1:D:1756:ASN:O	1:D:1759:ARG:NH1	2.53	0.41
1:B:300:ILE:HG21	1:B:389:ILE:HD11	2.02	0.41
1:B:869:ILE:HA	1:B:872:THR:HG22	2.02	0.41
1:B:1874:LEU:HB3	1:B:2020:CYS:SG	2.60	0.41
1:B:324:ALA:HA	1:B:327:TYR:CZ	2.55	0.41
1:B:1709:ILE:HG23	1:B:1710:ASP:OD1	2.20	0.41
1:C:1895:HIS:HB2	1:C:1922:ILE:HD13	2.02	0.41
2:E:115:LEU:HD12	2:E:130:VAL:HG11	2.03	0.41
1:D:28:LEU:HD23	1:D:35:LEU:HG	2.01	0.41
1:D:300:ILE:HG21	1:D:389:ILE:HD11	2.02	0.41
1:D:324:ALA:HA	1:D:327:TYR:CZ	2.55	0.41
2:G:271:ASP:O	2:G:275:ARG:HG2	2.20	0.41
1:A:1895:HIS:HB2	1:A:1922:ILE:HD13	2.02	0.41
1:D:927:PRO:HA	1:D:928:PRO:HD3	1.96	0.41
1:C:1826:ASP:OD1	1:C:1826:ASP:N	2.35	0.41
2:E:182:VAL:HA	2:E:185:PHE:CE1	2.55	0.41
1:B:1283:LYS:H	1:B:1283:LYS:HG3	1.68	0.41
1:B:1756:ASN:O	1:B:1759:ARG:NH1	2.53	0.41
1:C:2077:THR:HG1	1:C:2079:HIS:CE1	2.38	0.41
2:E:214:GLU:CD	2:E:241:ARG:HH12	2.24	0.41
2:H:101:PHE:CZ	2:H:105:ILE:HD11	2.56	0.41
2:G:296:ASP:O	2:G:303:ARG:NH2	2.51	0.41
2:H:214:GLU:CD	2:H:241:ARG:HH12	2.24	0.41
1:C:552:LEU:HD21	1:C:584:ILE:HD11	2.02	0.41
1:D:84:LYS:HE2	1:D:84:LYS:HB3	1.94	0.41
1:D:1353:TRP:CD2	1:D:1390:LYS:HE2	2.56	0.41
2:G:451:LYS:O	2:G:457:ARG:NH1	2.54	0.41
2:H:177:LYS:O	2:H:181:LEU:HG	2.21	0.41
2:H:313:ASP:HA	2:H:314:PRO:HD3	1.95	0.41
1:C:1952:ASP:OD1	1:C:1952:ASP:N	2.43	0.41
2:F:29:LYS:HD3	2:F:29:LYS:HA	1.79	0.41
2:F:101:PHE:CZ	2:F:105:ILE:HD11	2.56	0.41
2:G:310:CYS:SG	2:G:311:ALA:N	2.94	0.41
1:C:530:ILE:H	1:C:530:ILE:HG12	1.74	0.40
1:C:2026:ILE:HD11	1:C:2037:LEU:HD23	2.03	0.40
1:D:374:ILE:HD12	1:D:374:ILE:HA	1.95	0.40
1:C:2075:ASP:OD1	1:C:2075:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1176:PRO:HA	1:D:1177:PRO:HD3	1.96	0.40
1:D:2020:CYS:SG	1:D:2021:ALA:N	2.94	0.40
1:C:394:ASP:OD1	1:C:394:ASP:N	2.51	0.40
1:C:1973:ILE:H	1:C:1973:ILE:HG13	1.61	0.40
2:E:310:CYS:SG	2:E:311:ALA:N	2.95	0.40
2:G:313:ASP:HA	2:G:314:PRO:HD3	1.90	0.40
1:B:28:LEU:HD23	1:B:35:LEU:HG	2.01	0.40
1:D:1388:ILE:HG22	1:D:1392:ILE:HD11	2.03	0.40
2:H:421:GLU:OE1	2:H:449:ARG:HA	2.22	0.40
1:B:1997:MET:HG2	1:B:2021:ALA:HB2	2.04	0.40
1:B:2020:CYS:SG	1:B:2021:ALA:N	2.94	0.40
1:C:1176:PRO:HA	1:C:1177:PRO:HD3	1.96	0.40
1:C:1318:HIS:O	1:C:1322:LYS:HG2	2.22	0.40
1:D:1997:MET:HG2	1:D:2021:ALA:HB2	2.04	0.40
2:F:214:GLU:CD	2:F:241:ARG:HH12	2.24	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	2016/2092 (96%)	1980 (98%)	36 (2%)	0	100	100
1	B	1990/2092 (95%)	1953 (98%)	37 (2%)	0	100	100
1	C	2016/2092 (96%)	1980 (98%)	36 (2%)	0	100	100
1	D	1990/2092 (95%)	1953 (98%)	37 (2%)	0	100	100
2	E	536/586 (92%)	526 (98%)	10 (2%)	0	100	100
2	F	536/586 (92%)	523 (98%)	13 (2%)	0	100	100
2	G	536/586 (92%)	526 (98%)	10 (2%)	0	100	100
2	H	536/586 (92%)	524 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	10156/10712 (95%)	9965 (98%)	191 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	1754/1814 (97%)	1739 (99%)	15 (1%)	78 90
1	B	1732/1814 (96%)	1719 (99%)	13 (1%)	81 91
1	C	1754/1814 (97%)	1739 (99%)	15 (1%)	78 90
1	D	1732/1814 (96%)	1722 (99%)	10 (1%)	86 94
2	E	458/500 (92%)	458 (100%)	0	100 100
2	F	458/500 (92%)	453 (99%)	5 (1%)	73 86
2	G	458/500 (92%)	457 (100%)	1 (0%)	93 98
2	H	458/500 (92%)	454 (99%)	4 (1%)	78 90
All	All	8804/9256 (95%)	8741 (99%)	63 (1%)	84 92

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	227	SER
1	A	279	PHE
1	A	779	ARG
1	A	900	MET
1	A	1195	ASP
1	A	1568	MET
1	A	1614	HIS
1	A	1759	ARG
1	A	1885	CYS
1	A	1948	TYR
1	A	1976	MET

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Mol	Chain	Res	Type
1	A	2035	MET
1	A	2039	LEU
1	A	2066	SER
1	B	140	PHE
1	B	301	GLU
1	B	507	LYS
1	B	779	ARG
1	B	786	ASP
1	B	858	ARG
1	B	879	GLN
1	B	1568	MET
1	B	1629	ASP
1	B	1885	CYS
1	B	1962	ARG
1	B	2020	CYS
1	B	2039	LEU
1	C	11	ARG
1	C	82	GLN
1	C	227	SER
1	C	279	PHE
1	C	900	MET
1	C	1195	ASP
1	C	1568	MET
1	C	1614	HIS
1	C	1759	ARG
1	C	1885	CYS
1	C	1948	TYR
1	C	1976	MET
1	C	2035	MET
1	C	2039	LEU
1	C	2066	SER
1	D	140	PHE
1	D	301	GLU
1	D	779	ARG
1	D	786	ASP
1	D	1568	MET
1	D	1629	ASP
1	D	1885	CYS
1	D	1962	ARG
1	D	2020	CYS
1	D	2039	LEU
2	F	177	LYS

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Mol	Chain	Res	Type
2	F	327	ARG
2	F	356	GLU
2	F	372	ASP
2	F	390	GLU
2	G	123	ASP
2	H	177	LYS
2	H	327	ARG
2	H	356	GLU
2	H	390	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	C	2101	4	26,33,33	0.66	0	31,52,52	0.73	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ATP	G	601	4	26,33,33	0.67	0	31,52,52	0.74	2 (6%)
3	ATP	A	2101	4	26,33,33	0.66	0	31,52,52	0.73	1 (3%)
3	ATP	H	601	4	26,33,33	0.67	0	31,52,52	0.75	2 (6%)
3	ATP	D	2101	4	26,33,33	0.67	0	31,52,52	0.82	1 (3%)
3	ATP	E	601	4	26,33,33	0.68	0	31,52,52	0.74	2 (6%)
3	ATP	B	2101	4	26,33,33	0.66	0	31,52,52	0.81	1 (3%)
3	ATP	F	601	4	26,33,33	0.67	0	31,52,52	0.75	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	C	2101	4	-	2/18/38/38	0/3/3/3
3	ATP	G	601	4	-	3/18/38/38	0/3/3/3
3	ATP	A	2101	4	-	2/18/38/38	0/3/3/3
3	ATP	H	601	4	-	2/18/38/38	0/3/3/3
3	ATP	D	2101	4	-	4/18/38/38	0/3/3/3
3	ATP	E	601	4	-	2/18/38/38	0/3/3/3
3	ATP	B	2101	4	-	4/18/38/38	0/3/3/3
3	ATP	F	601	4	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2101	ATP	C5-C6-N6	2.28	123.82	120.35
3	C	2101	ATP	C5-C6-N6	2.27	123.80	120.35
3	B	2101	ATP	C5-C6-N6	2.19	123.67	120.35
3	D	2101	ATP	C5-C6-N6	2.18	123.66	120.35
3	F	601	ATP	C5-C6-N6	2.13	123.59	120.35
3	H	601	ATP	C5-C6-N6	2.11	123.56	120.35
3	E	601	ATP	C5-C6-N6	2.11	123.55	120.35
3	G	601	ATP	C5-C6-N6	2.07	123.49	120.35
3	H	601	ATP	PB-O3B-PG	2.05	139.87	132.83
3	E	601	ATP	PB-O3B-PG	2.04	139.84	132.83
3	F	601	ATP	PB-O3B-PG	2.02	139.76	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	601	ATP	PB-O3B-PG	2.01	139.73	132.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	ATP	O4'-C4'-C5'-O5'
3	H	601	ATP	O4'-C4'-C5'-O5'
3	B	2101	ATP	O4'-C4'-C5'-O5'
3	B	2101	ATP	C3'-C4'-C5'-O5'
3	D	2101	ATP	O4'-C4'-C5'-O5'
3	D	2101	ATP	C3'-C4'-C5'-O5'
3	F	601	ATP	O4'-C4'-C5'-O5'
3	G	601	ATP	O4'-C4'-C5'-O5'
3	A	2101	ATP	PA-O3A-PB-O1B
3	C	2101	ATP	PA-O3A-PB-O1B
3	F	601	ATP	C3'-C4'-C5'-O5'
3	G	601	ATP	C3'-C4'-C5'-O5'
3	F	601	ATP	C4'-C5'-O5'-PA
3	H	601	ATP	C4'-C5'-O5'-PA
3	B	2101	ATP	C5'-O5'-PA-O3A
3	D	2101	ATP	C5'-O5'-PA-O3A
3	B	2101	ATP	PA-O3A-PB-O2B
3	D	2101	ATP	PA-O3A-PB-O2B
3	E	601	ATP	C4'-C5'-O5'-PA
3	G	601	ATP	C4'-C5'-O5'-PA
3	A	2101	ATP	PA-O3A-PB-O2B
3	C	2101	ATP	PA-O3A-PB-O2B

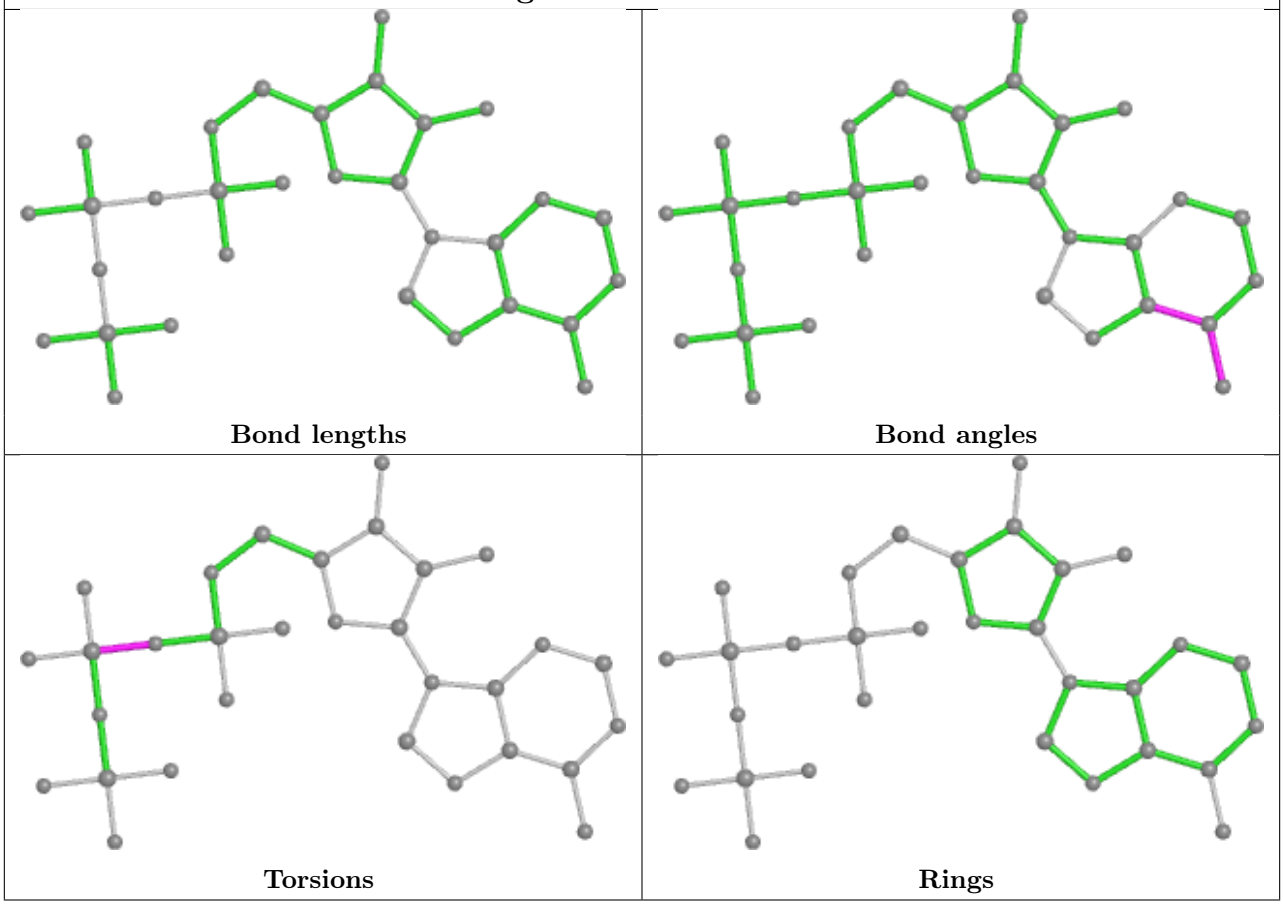
There are no ring outliers.

No monomer is involved in short contacts.

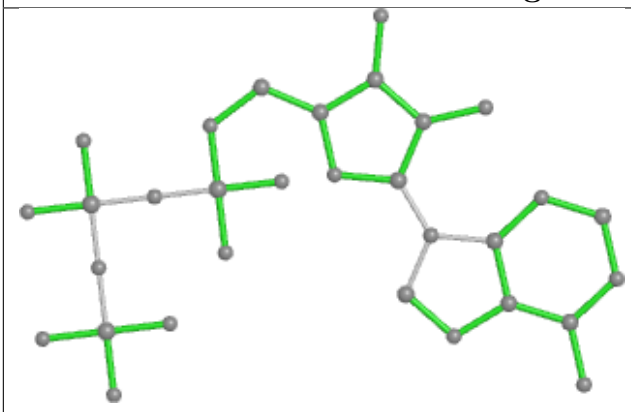
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

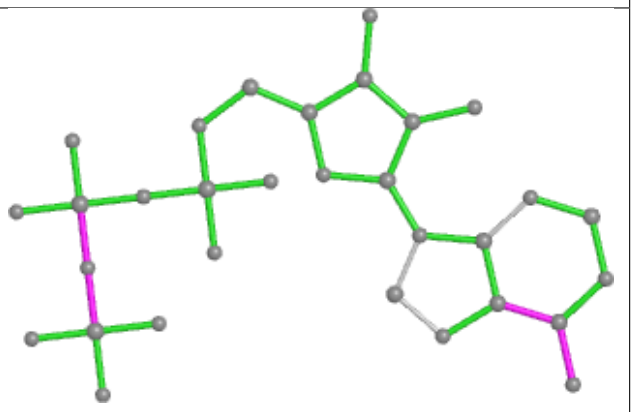
Ligand ATP C 2101



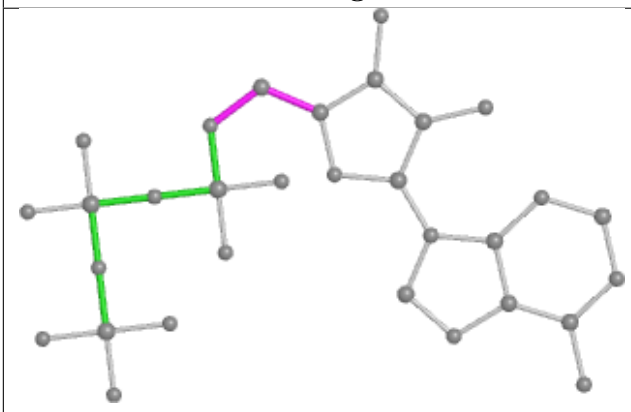
Ligand ATP G 601



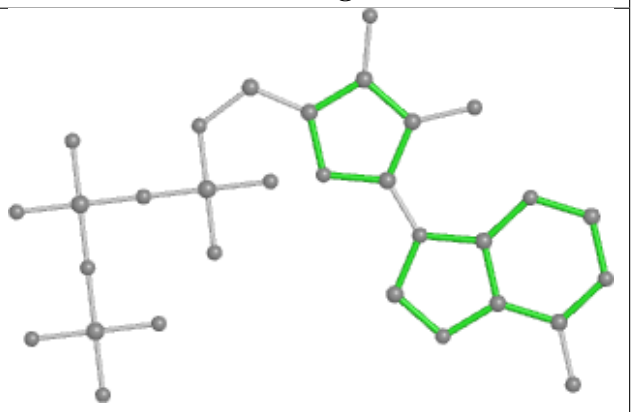
Bond lengths



Bond angles

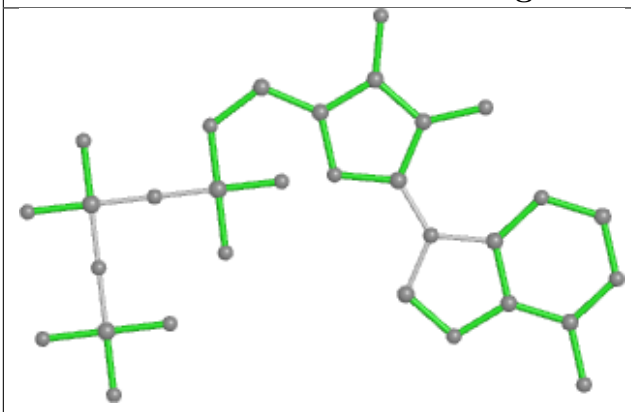


Torsions

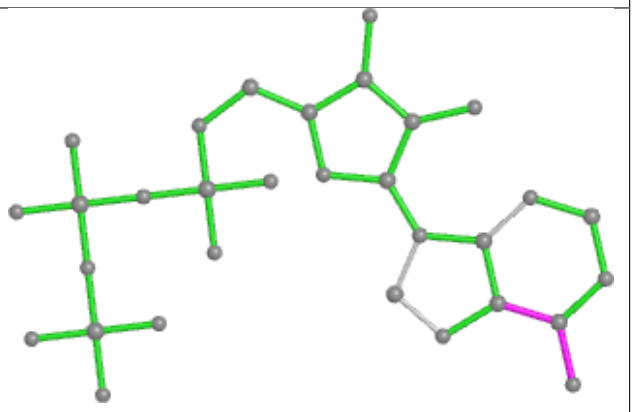


Rings

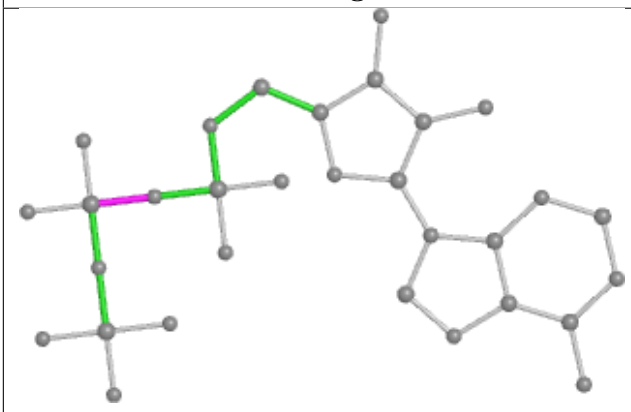
Ligand ATP A 2101



Bond lengths



Bond angles



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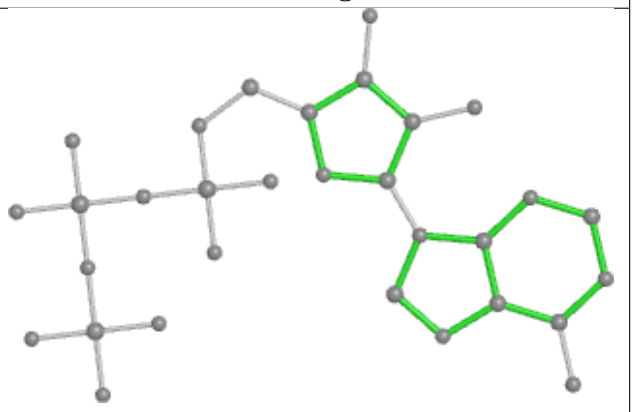
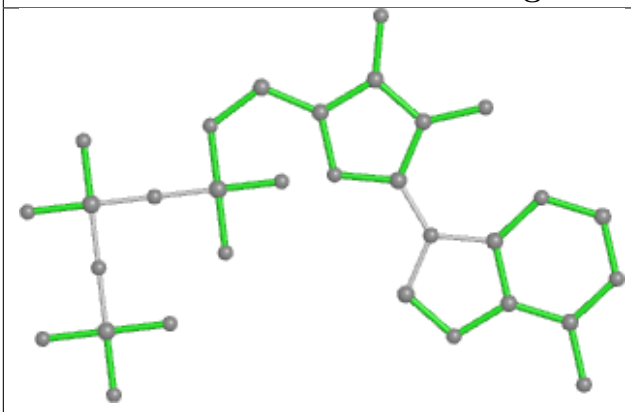
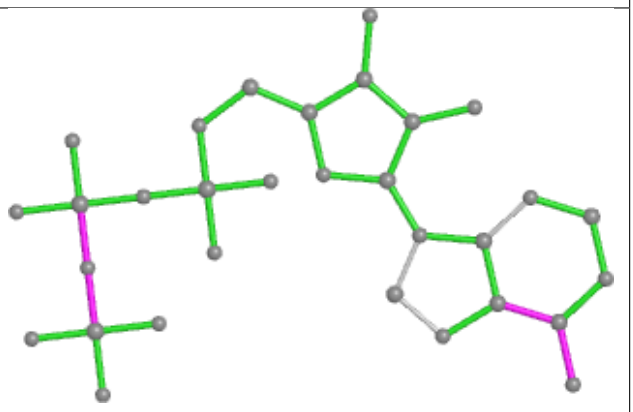


Rings

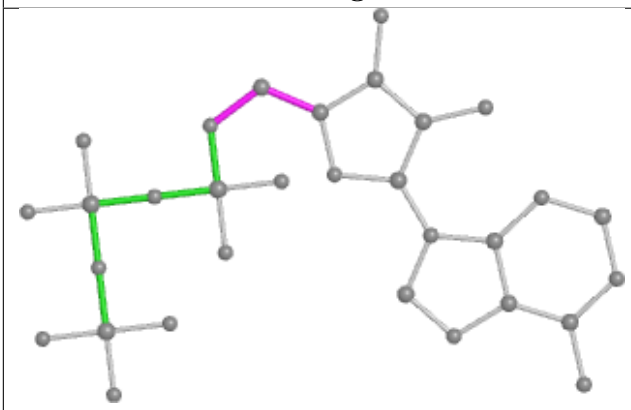
Ligand ATP H 601



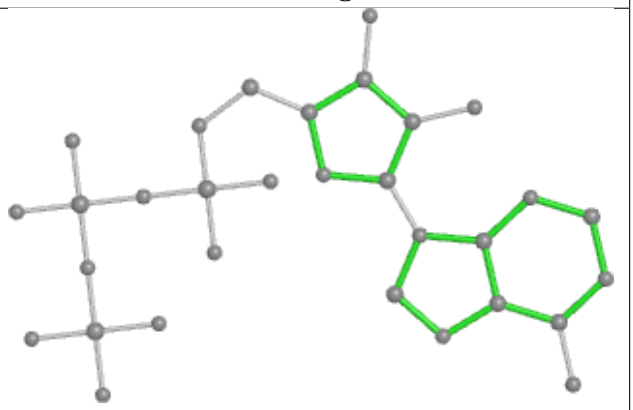
Bond lengths



Bond angles

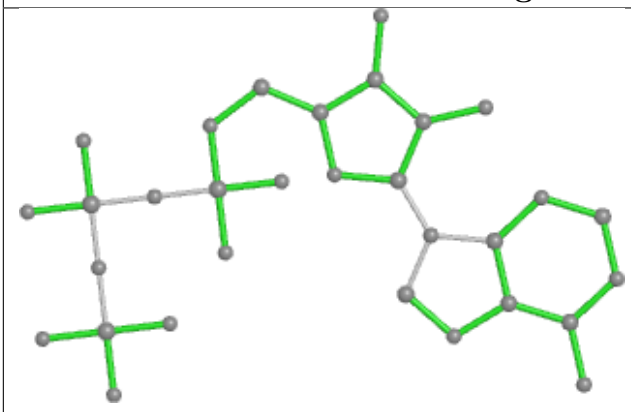


Torsions

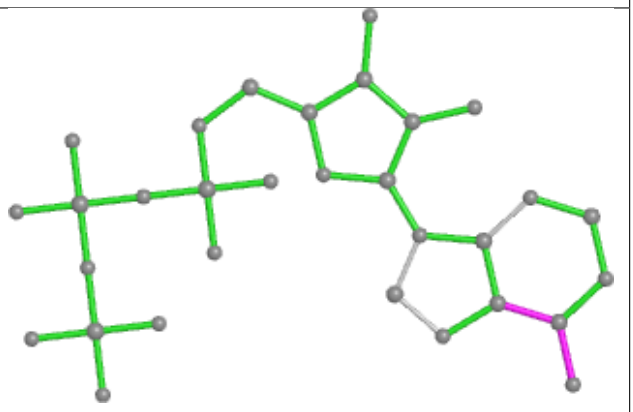


Rings

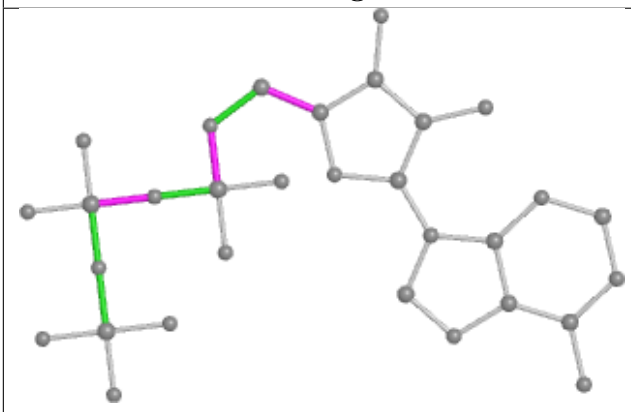
Ligand ATP D 2101



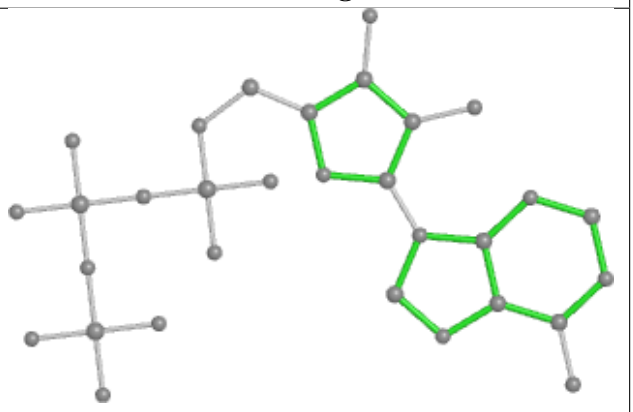
Bond lengths



Bond angles

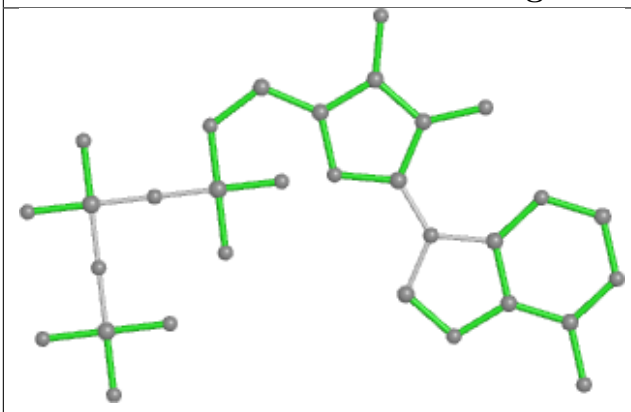


Torsions

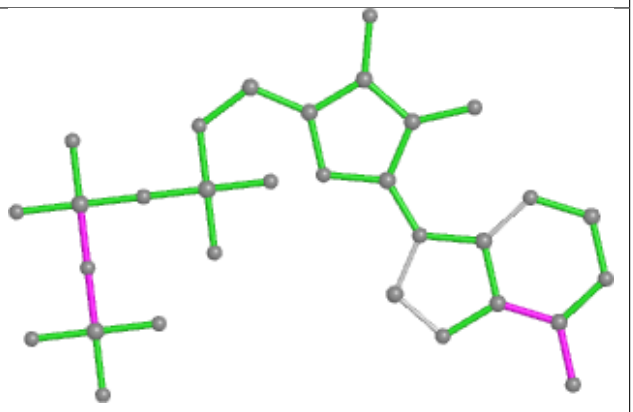


Rings

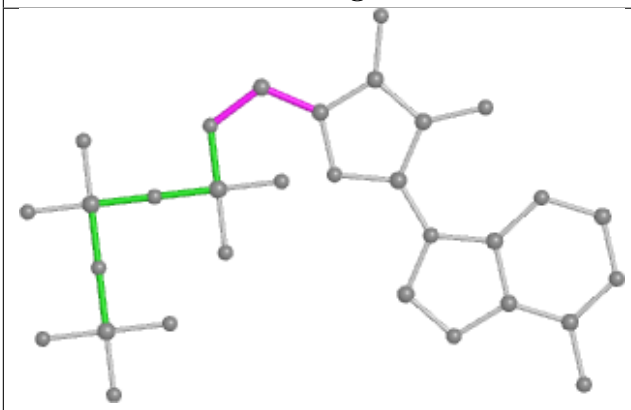
Ligand ATP E 601



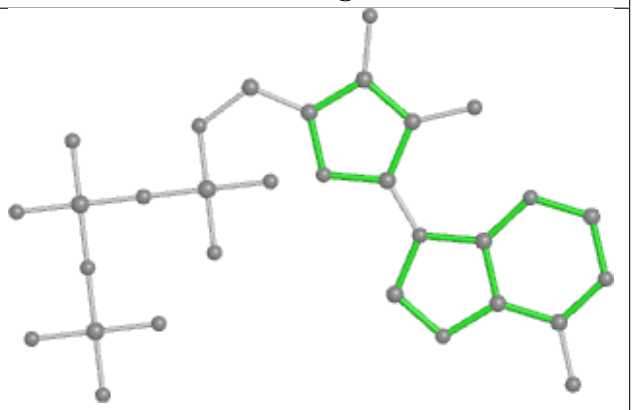
Bond lengths



Bond angles

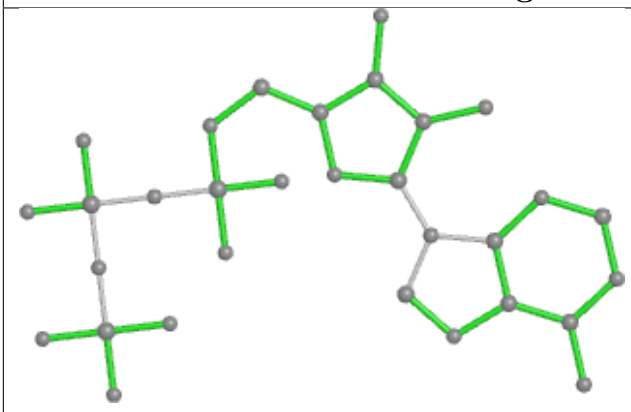


Torsions

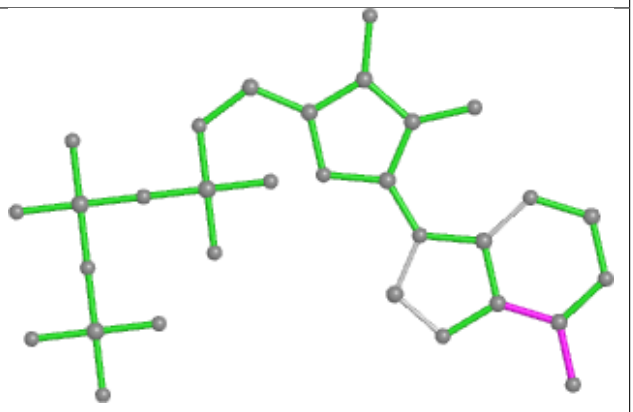


Rings

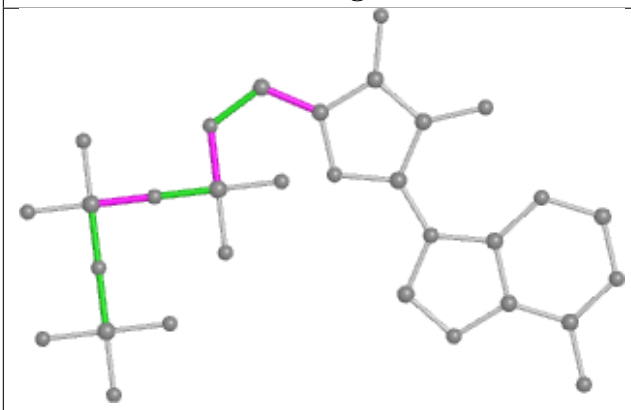
Ligand ATP B 2101



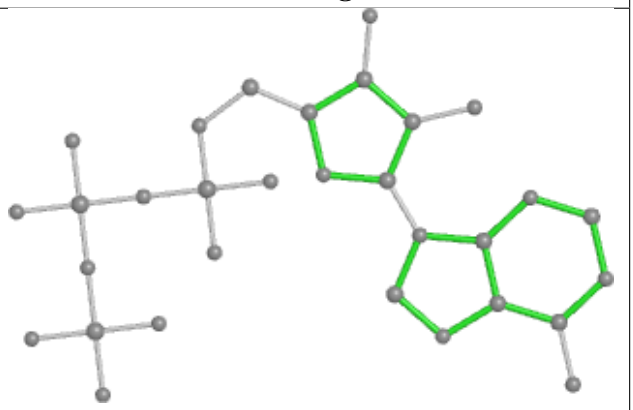
Bond lengths



Bond angles

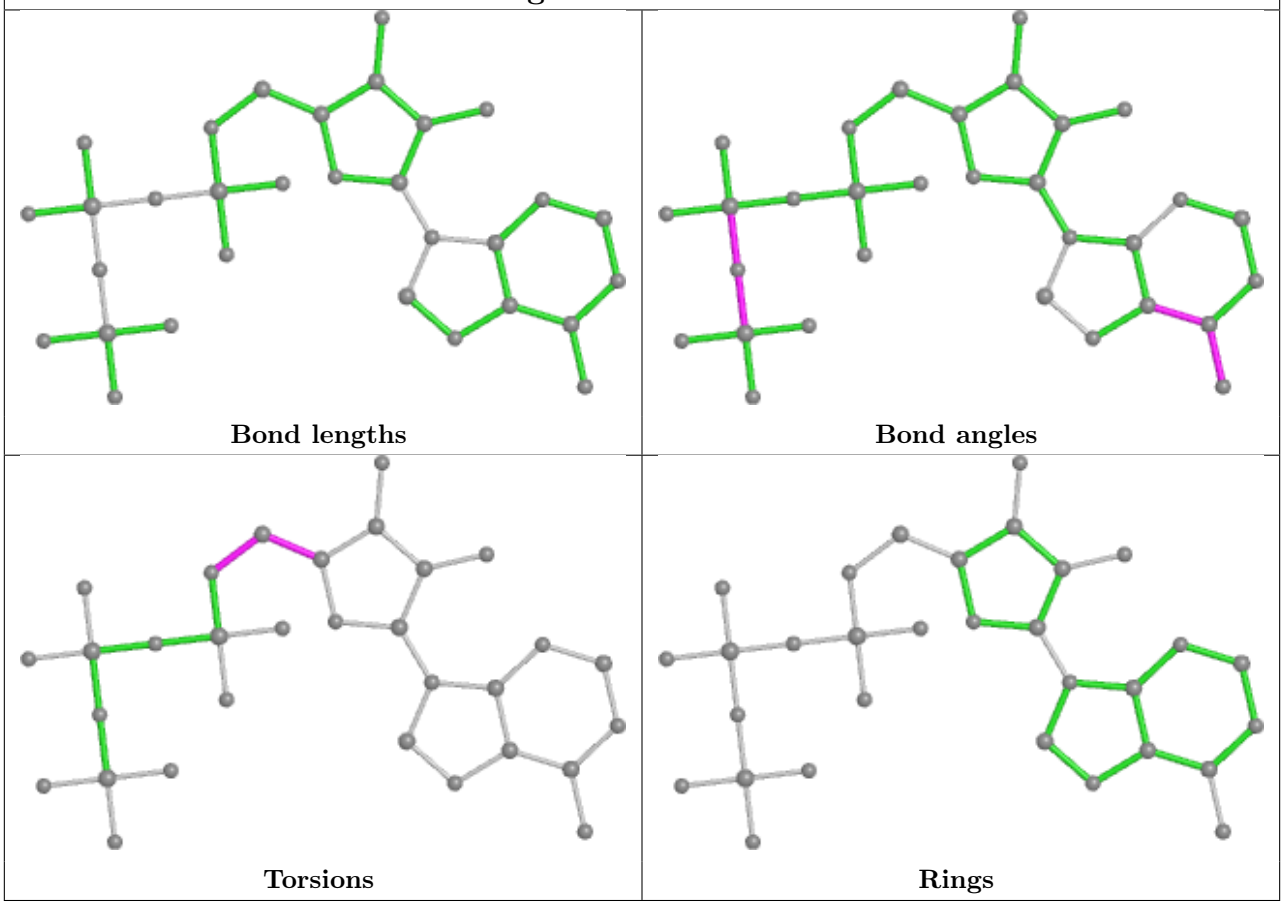


Torsions



Rings

Ligand ATP F 601



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.

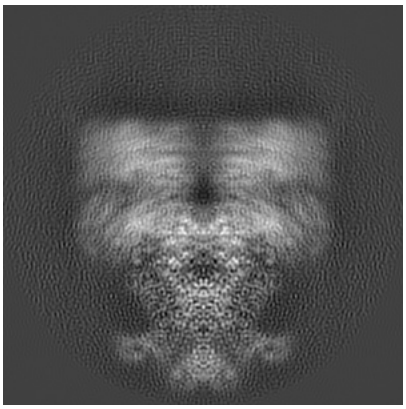
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27421. These allow visual inspection of the internal detail of the map and identification of artifacts.

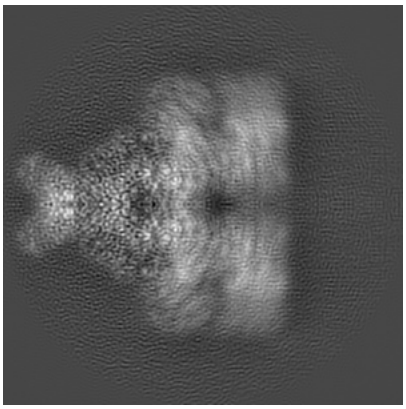
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

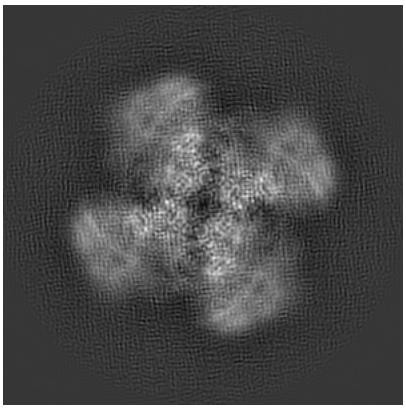
6.1.1 Primary map



X

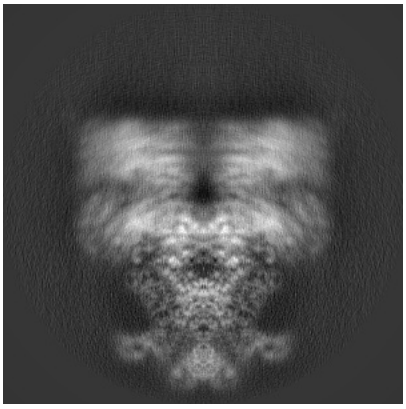


Y

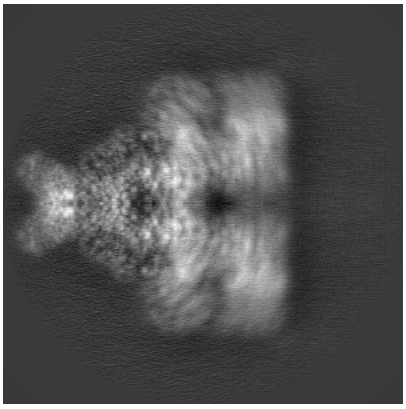


Z

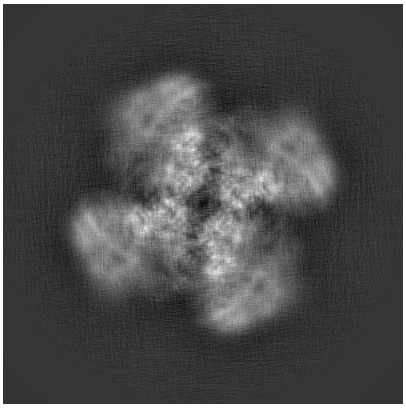
6.1.2 Raw map



X



Y

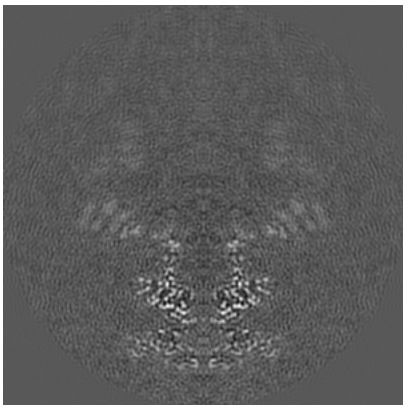


Z

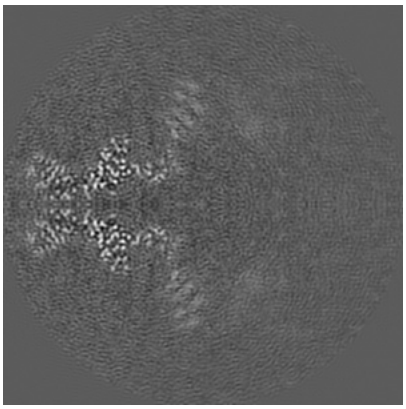
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

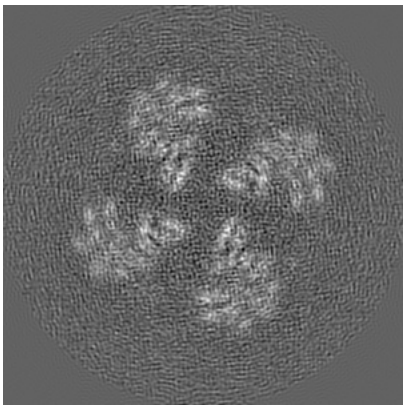
6.2.1 Primary map



X Index: 180

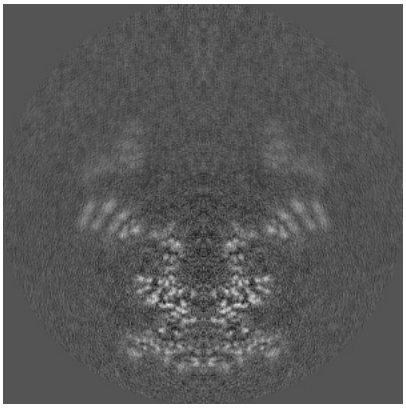


Y Index: 180

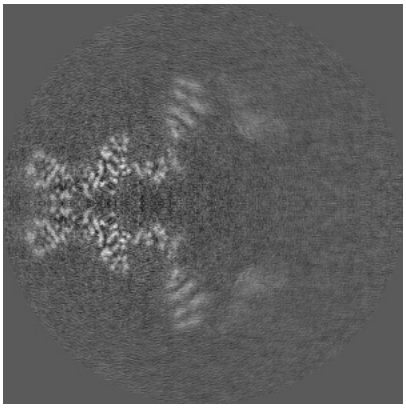


Z Index: 180

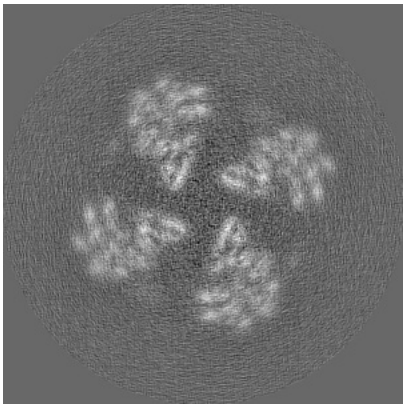
6.2.2 Raw map



X Index: 180



Y Index: 180

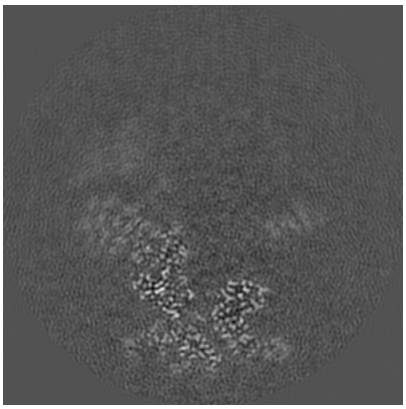


Z Index: 180

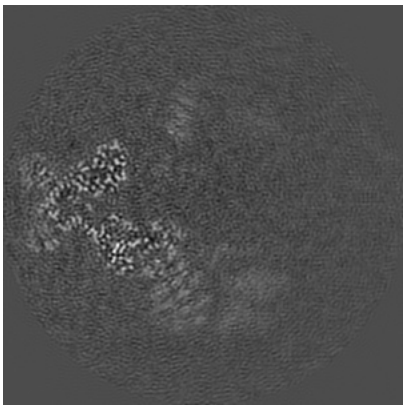
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

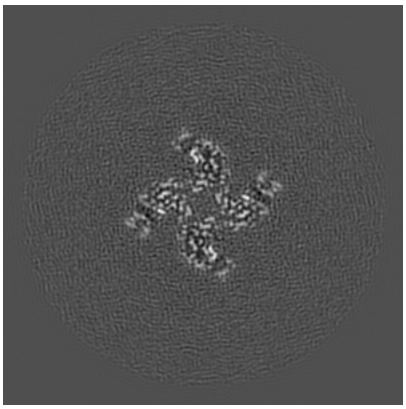
6.3.1 Primary map



X Index: 187

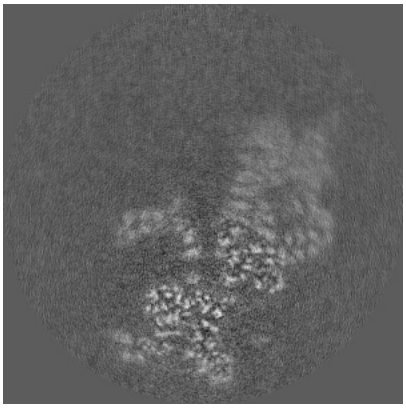


Y Index: 173

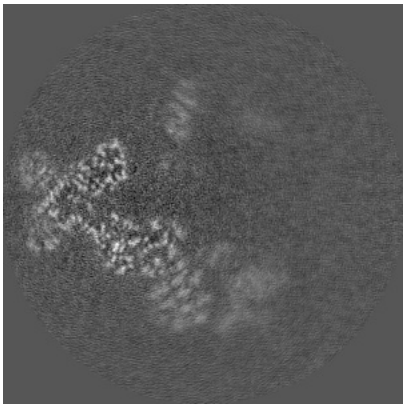


Z Index: 102

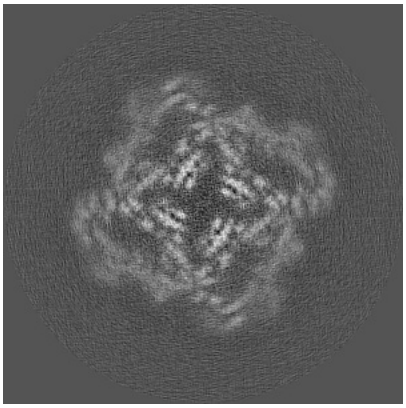
6.3.2 Raw map



X Index: 163



Y Index: 173

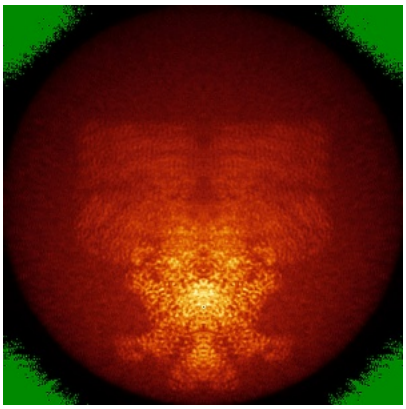


Z Index: 155

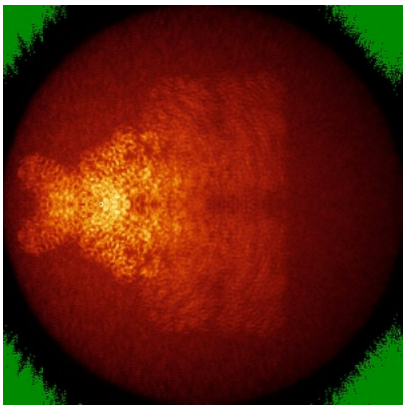
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

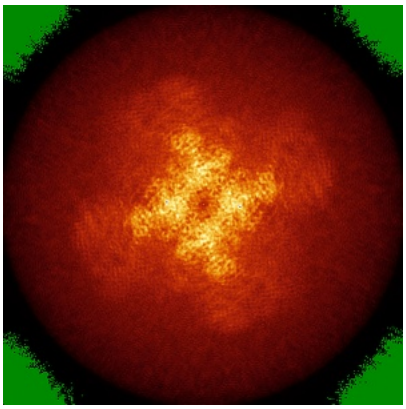
6.4.1 Primary map



X

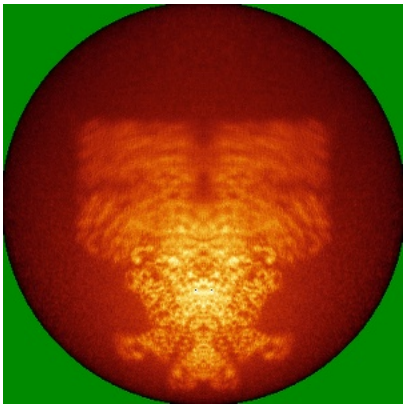


Y

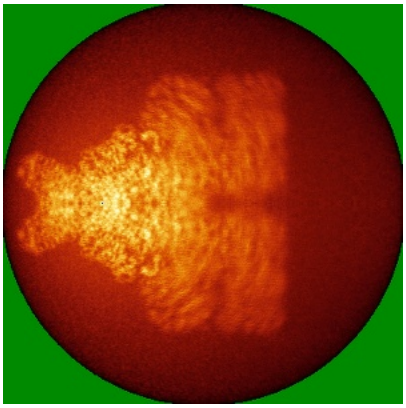


Z

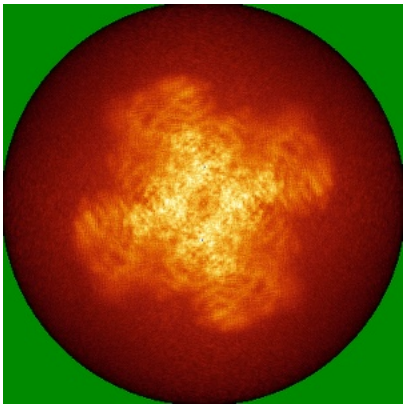
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

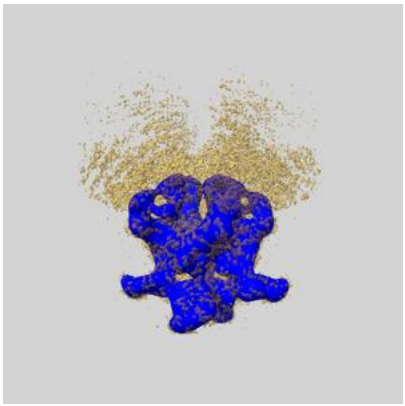
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

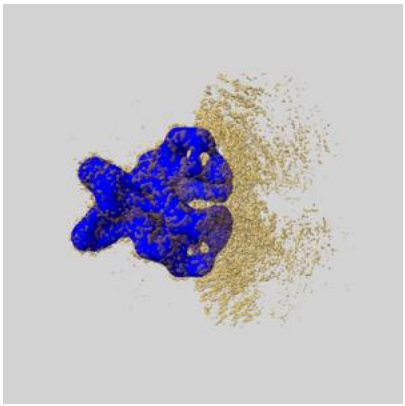
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

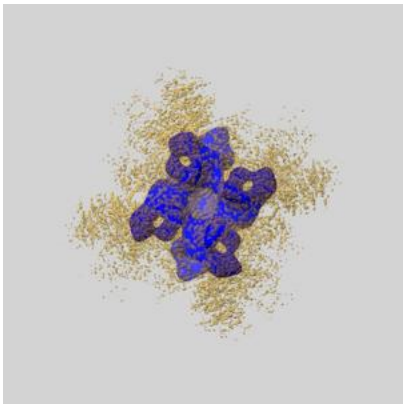
6.6.1 emd_27421_msk_1.map (i)



X



Y

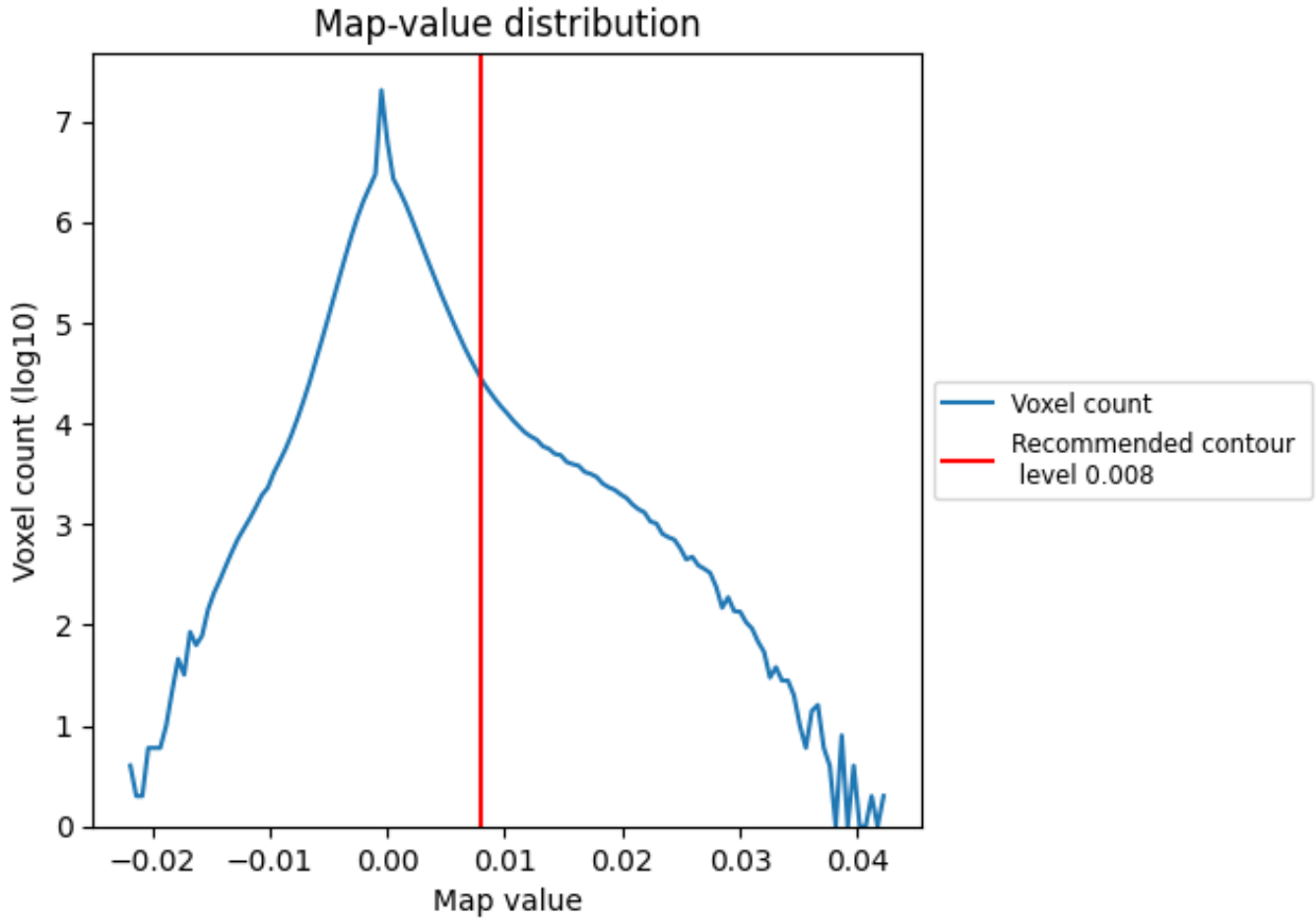


Z

7 Map analysis

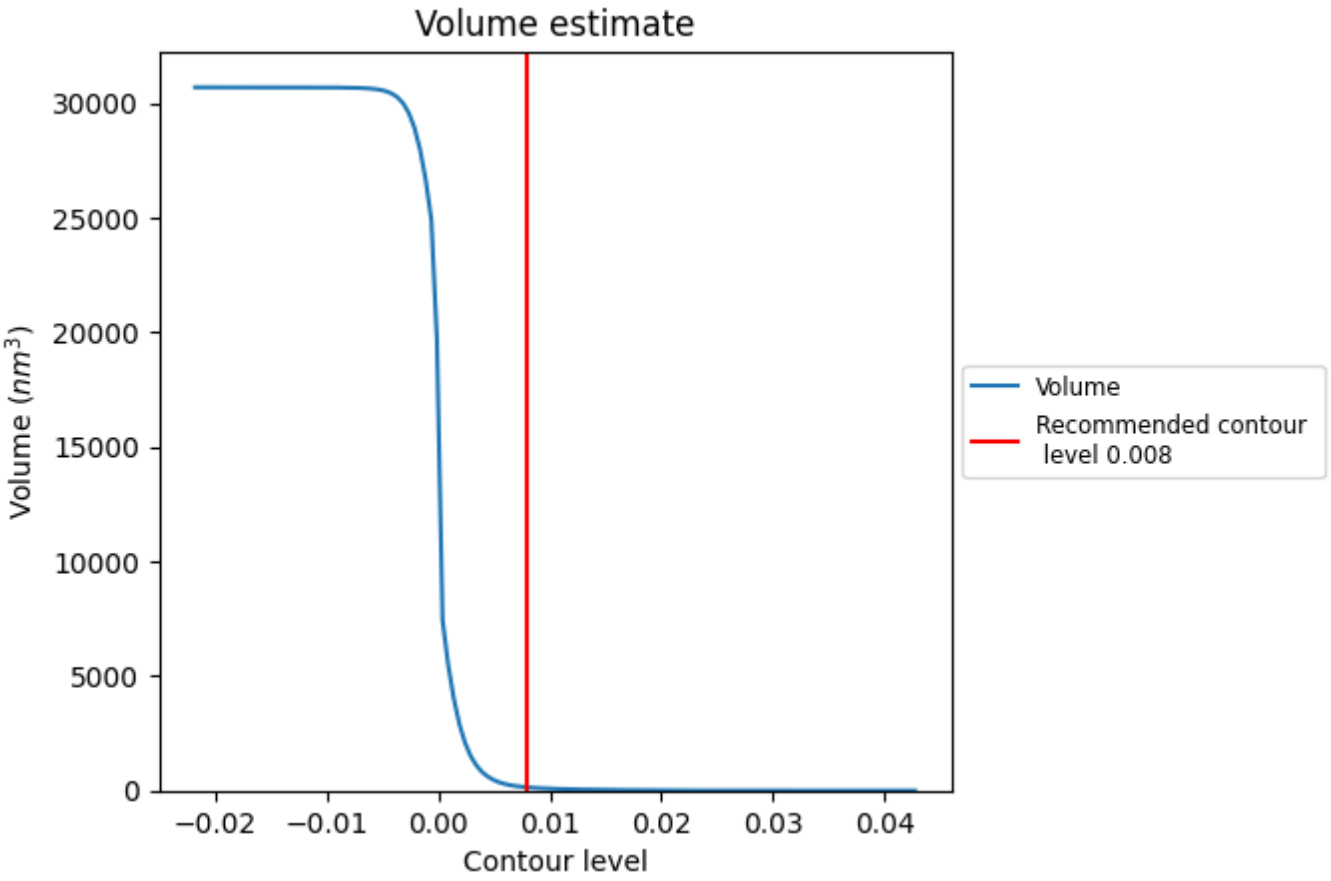
This section contains the results of statistical analysis of the map.

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.

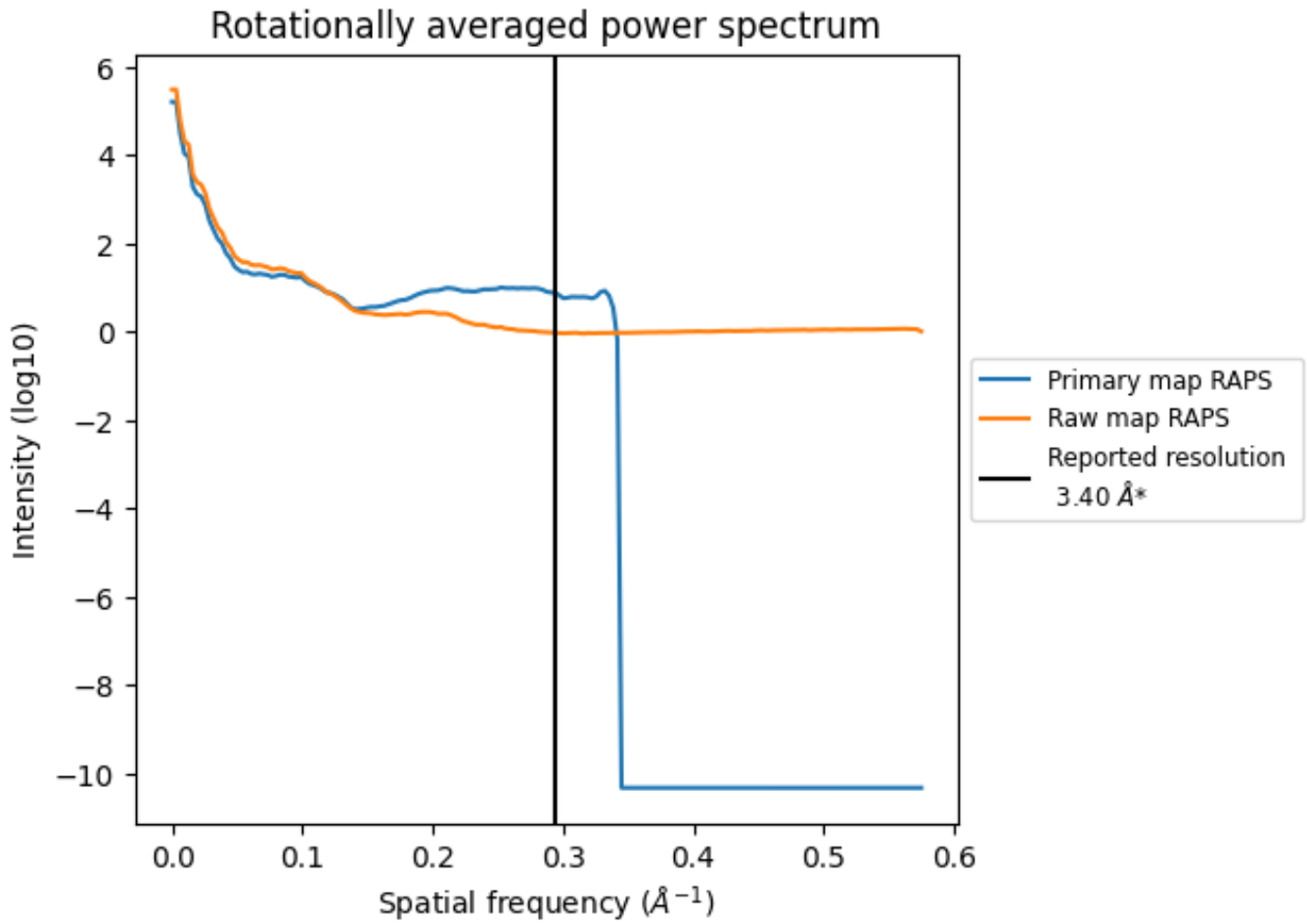
7.2 Volume estimate



The volume at the recommended contour level is 138 nm^3; this corresponds to an approximate mass of 125 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)

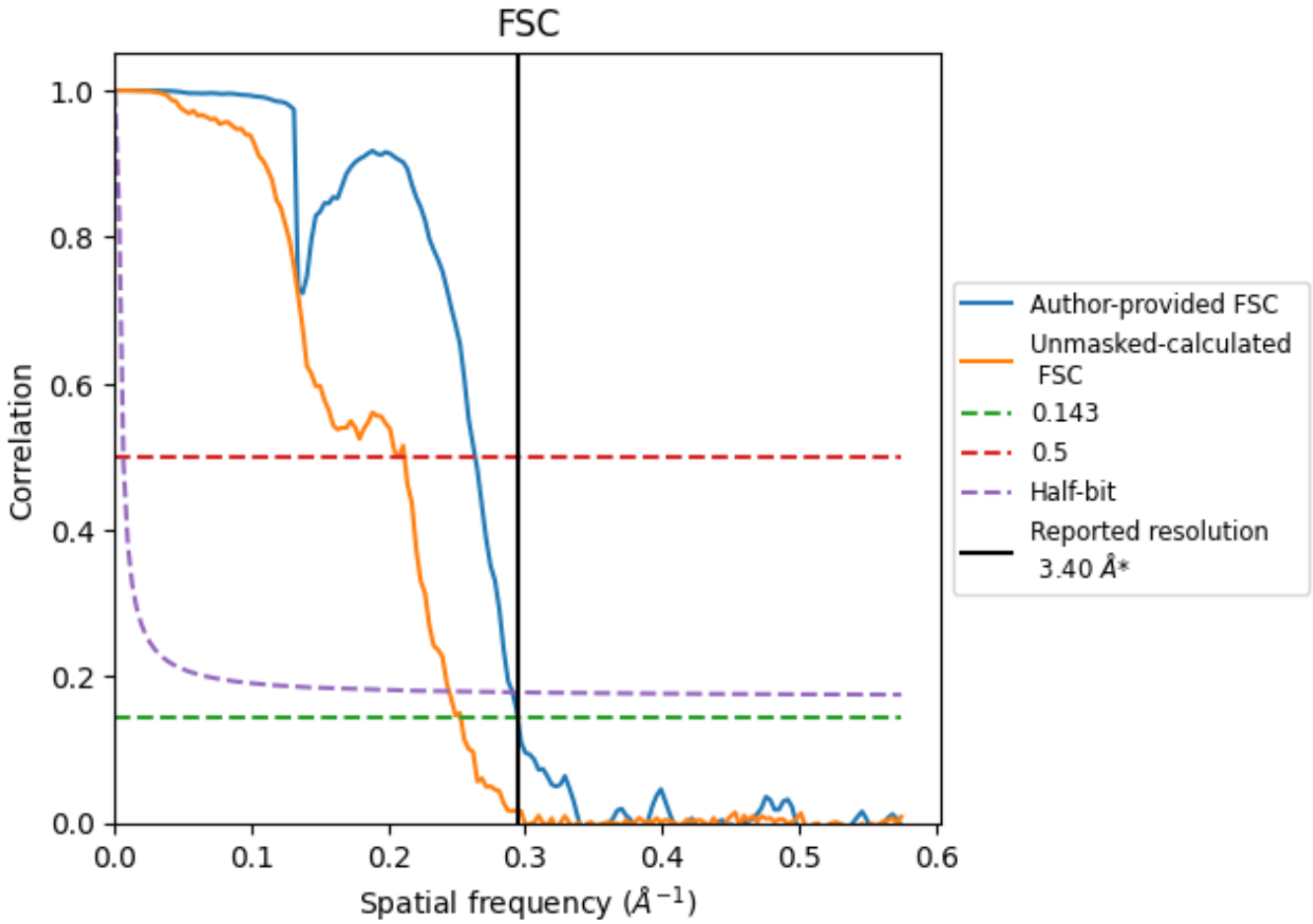


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

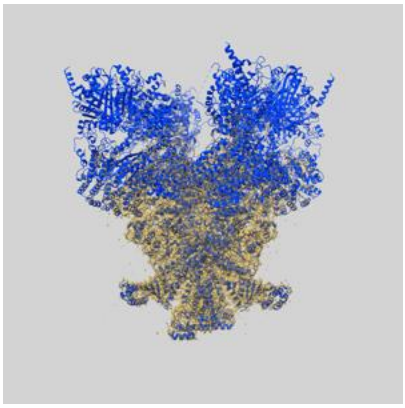
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.80	3.44
Unmasked-calculated*	3.95	4.83	4.09

*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 3.95 differs from the reported value 3.4 by more than 10 %

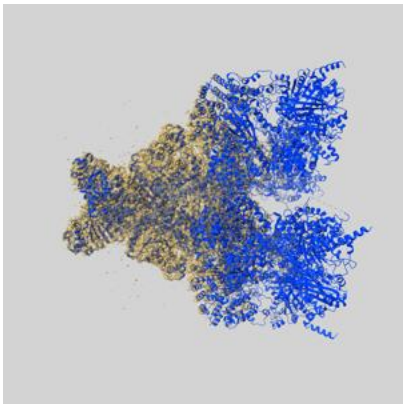
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27421 and PDB model 8DGC. Per-residue inclusion information can be found in section 3 on page 6.

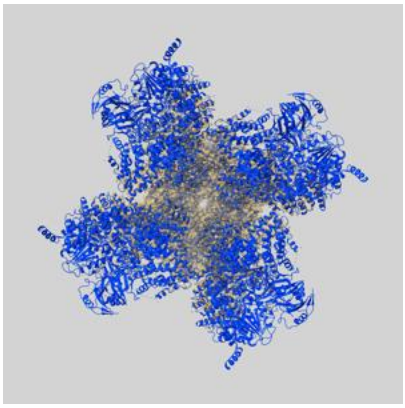
9.1 Map-model overlay



X



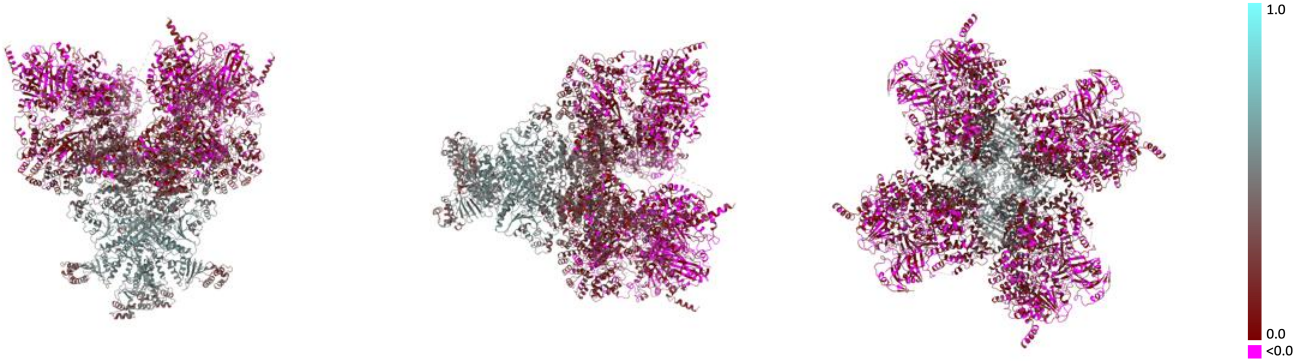
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

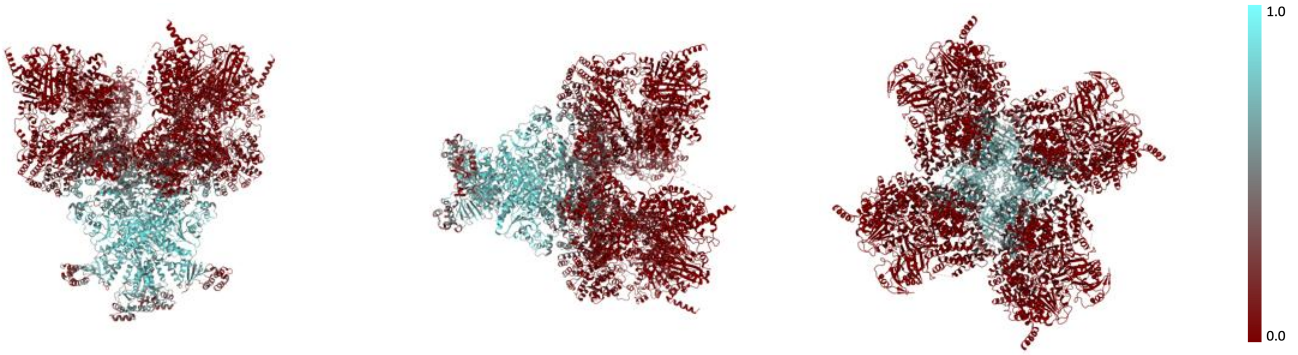
9.2 Q-score mapped to coordinate model



X Y Z

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.

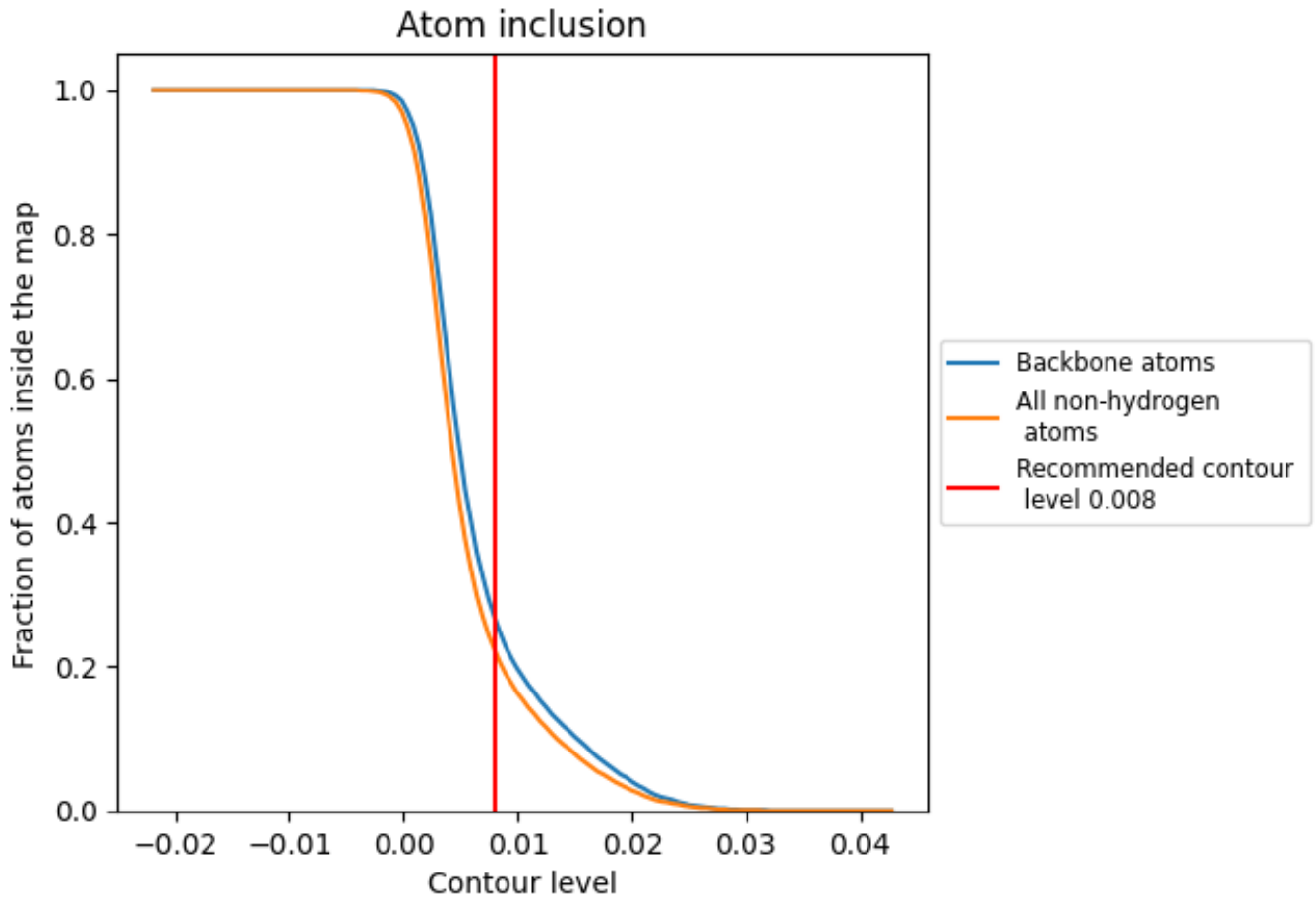
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 27% of all backbone atoms, 22% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2220	0.2180
A	0.2790	0.2510
B	0.2790	0.2580
C	0.2800	0.2470
D	0.2790	0.2600
E	0.0070	0.0760
F	0.0090	0.0900
G	0.0070	0.0720
H	0.0090	0.0900