wwPDB EM Validation Summary Report

Oct 30, 2023 – 02:01 PM EDT

PDB ID	:	8TKI
EMDB ID	:	EMD-41352
Title	:	Human Type 3 IP3 Receptor - Labile Resting State 2 (+IP3/ATP)
Authors	:	Paknejad, N.; Sapuru, V.; Hite, R.K.
Deposited on	:	2023-07-25
Resolution	:	3.60 Å(reported)

This is a wwPDB EM Validation Summary 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:

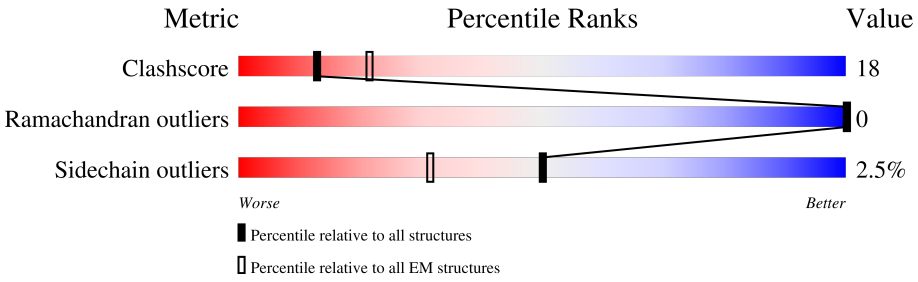
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	2671	71% 13% • 15%
1	B	2671	5% 60% 23% • 15%
1	C	2671	5% 64% 20% • 15%
1	D	2671	5% 61% 23% • 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 145900 atoms, of which 72928 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.

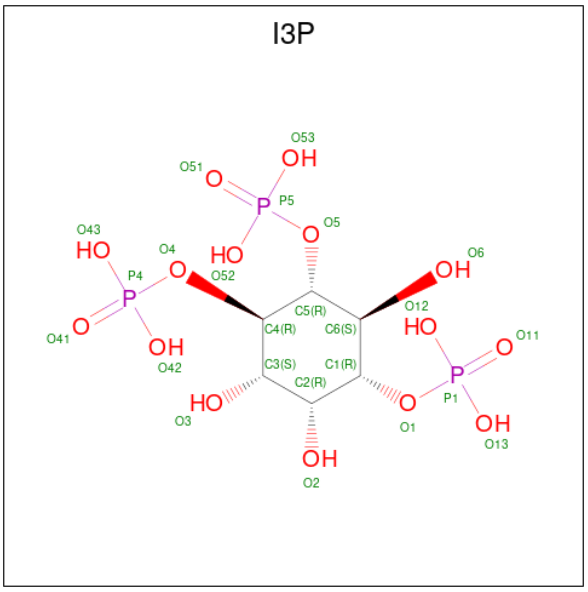
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2268	Total 36398	C 11601	H 18211	N 3116	O 3355	S 115	0	0
1	B	2268	Total 36398	C 11601	H 18211	N 3116	O 3355	S 115	0	0
1	C	2268	Total 36398	C 11601	H 18211	N 3116	O 3355	S 115	0	0
1	D	2268	Total 36398	C 11601	H 18211	N 3116	O 3355	S 115	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

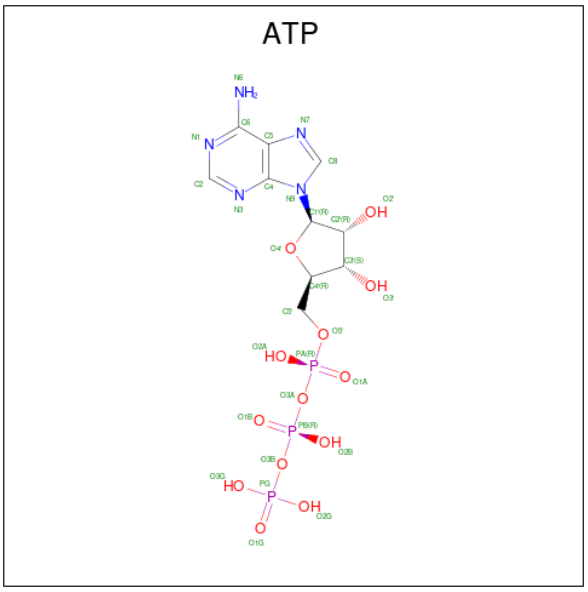
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

- Molecule 4 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).



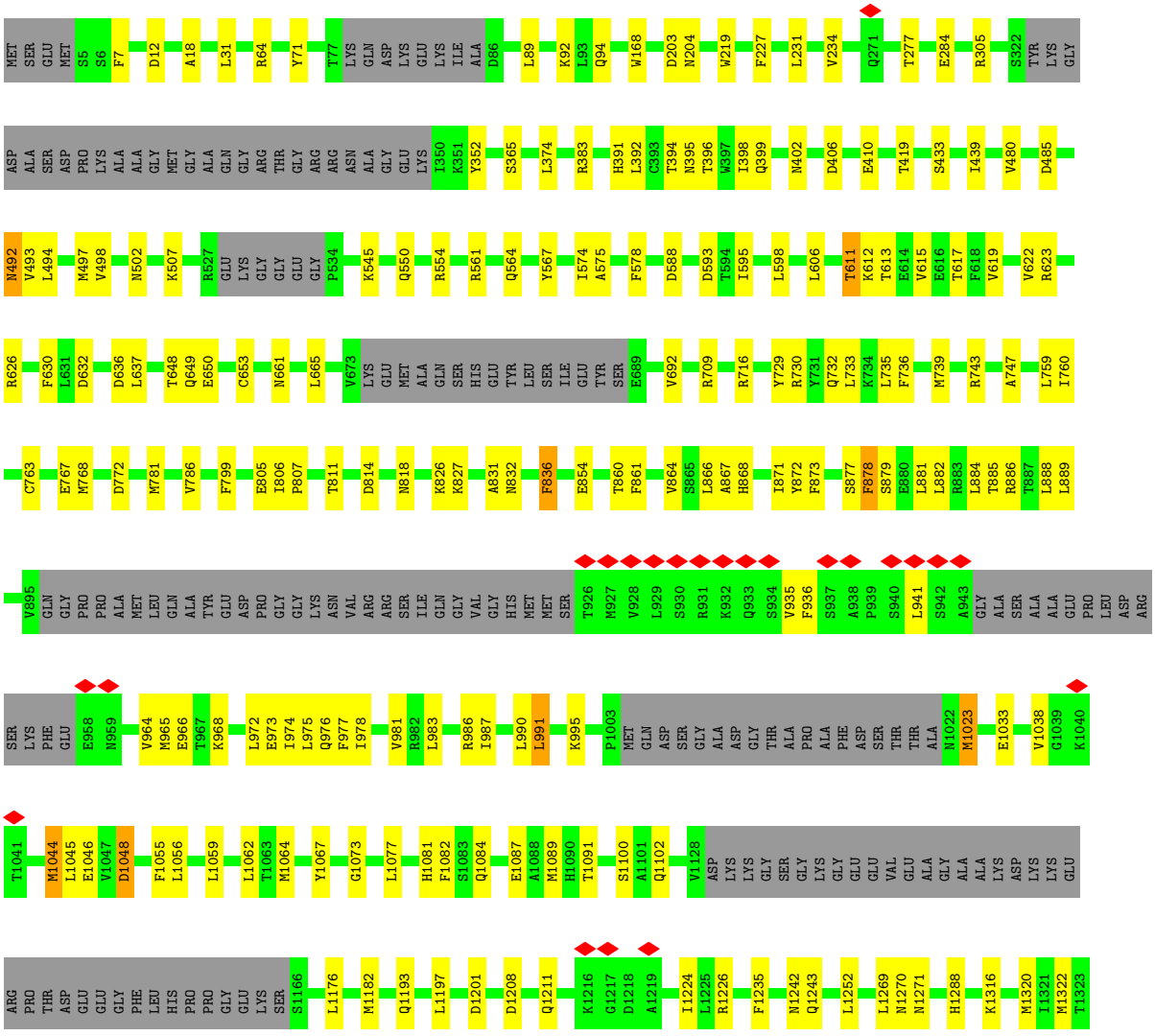
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

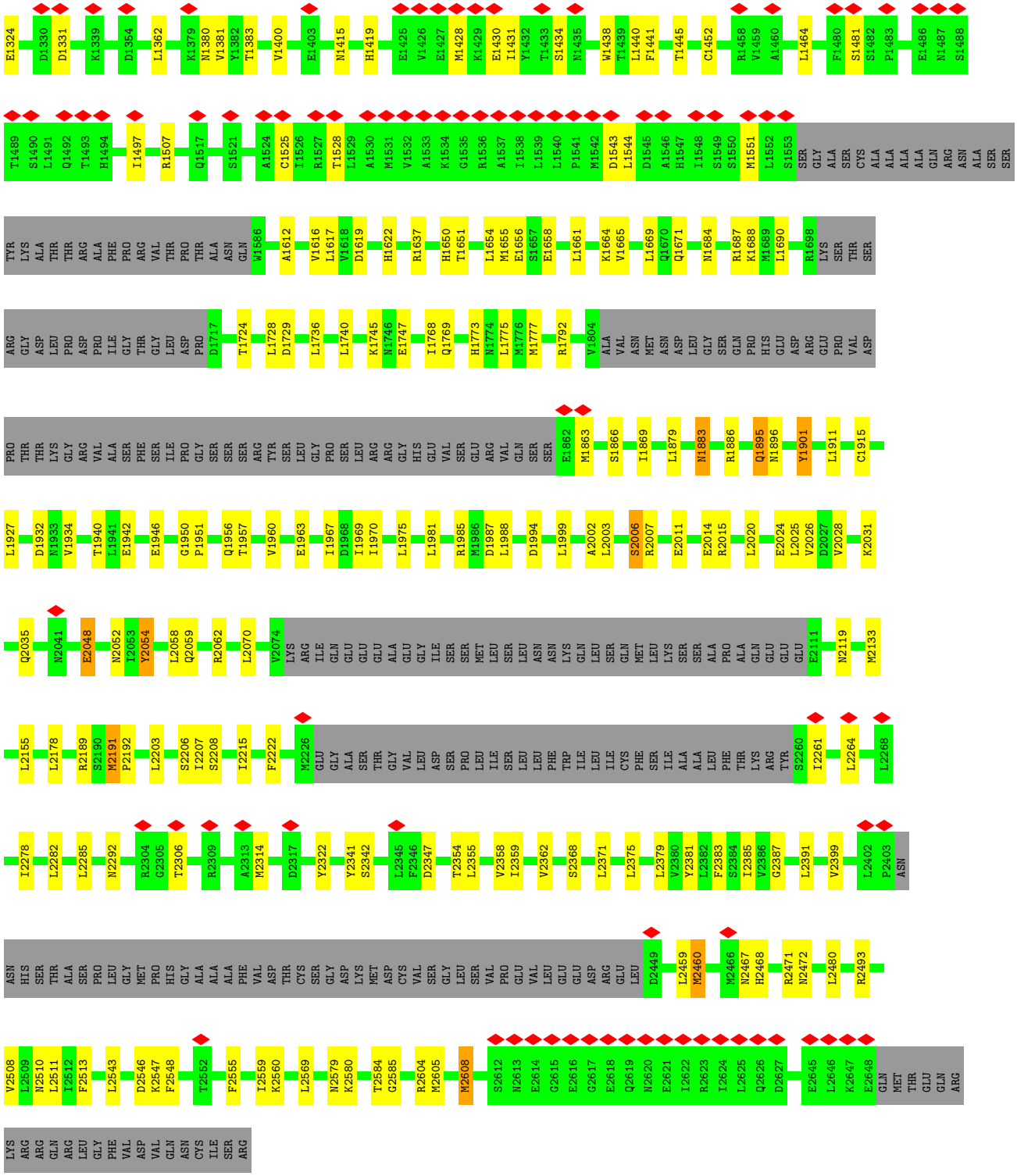
3 Residue-property plots (i)

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: Inositol 1,4,5-trisphosphate receptor type 3

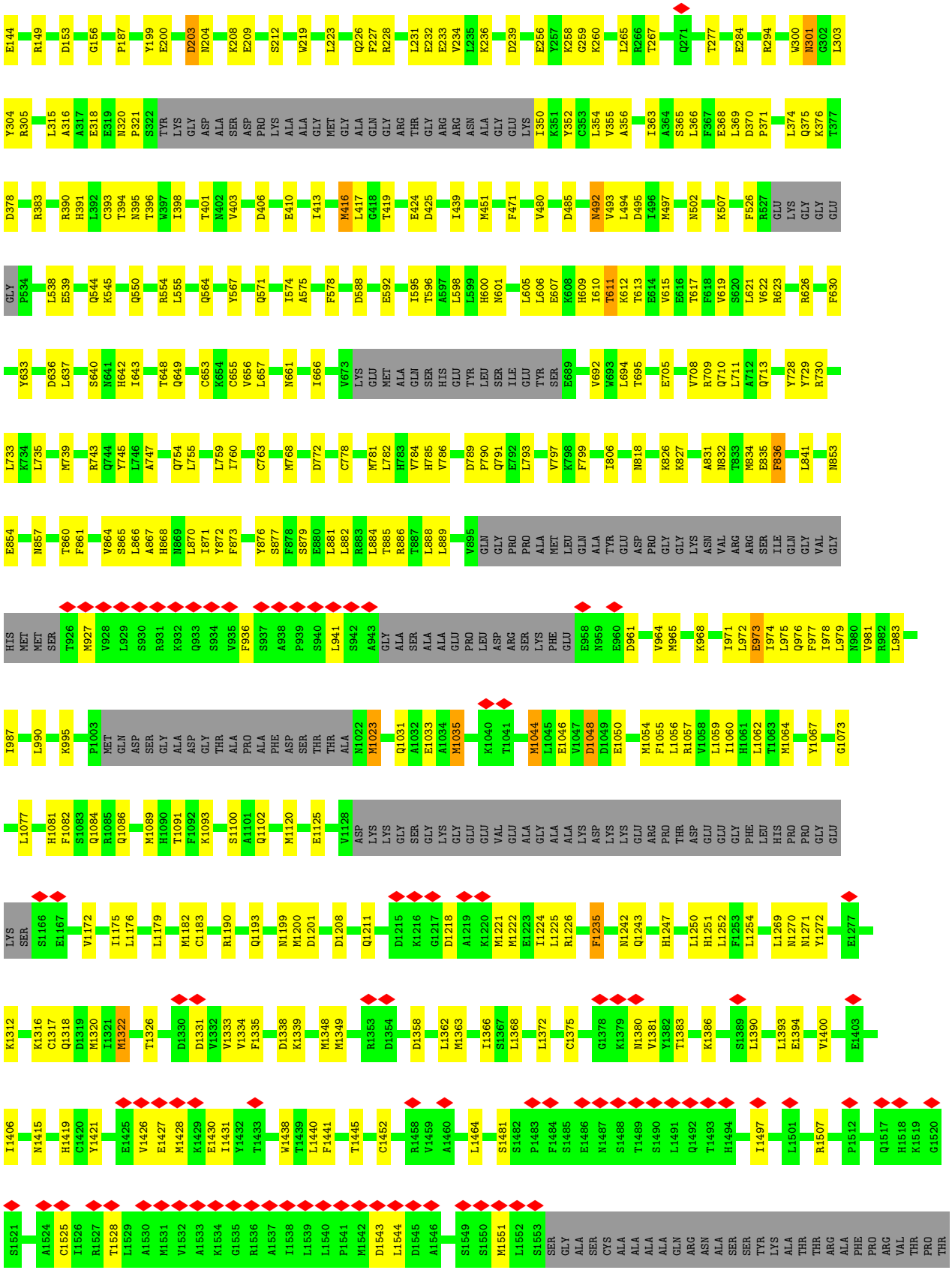
Chain A:

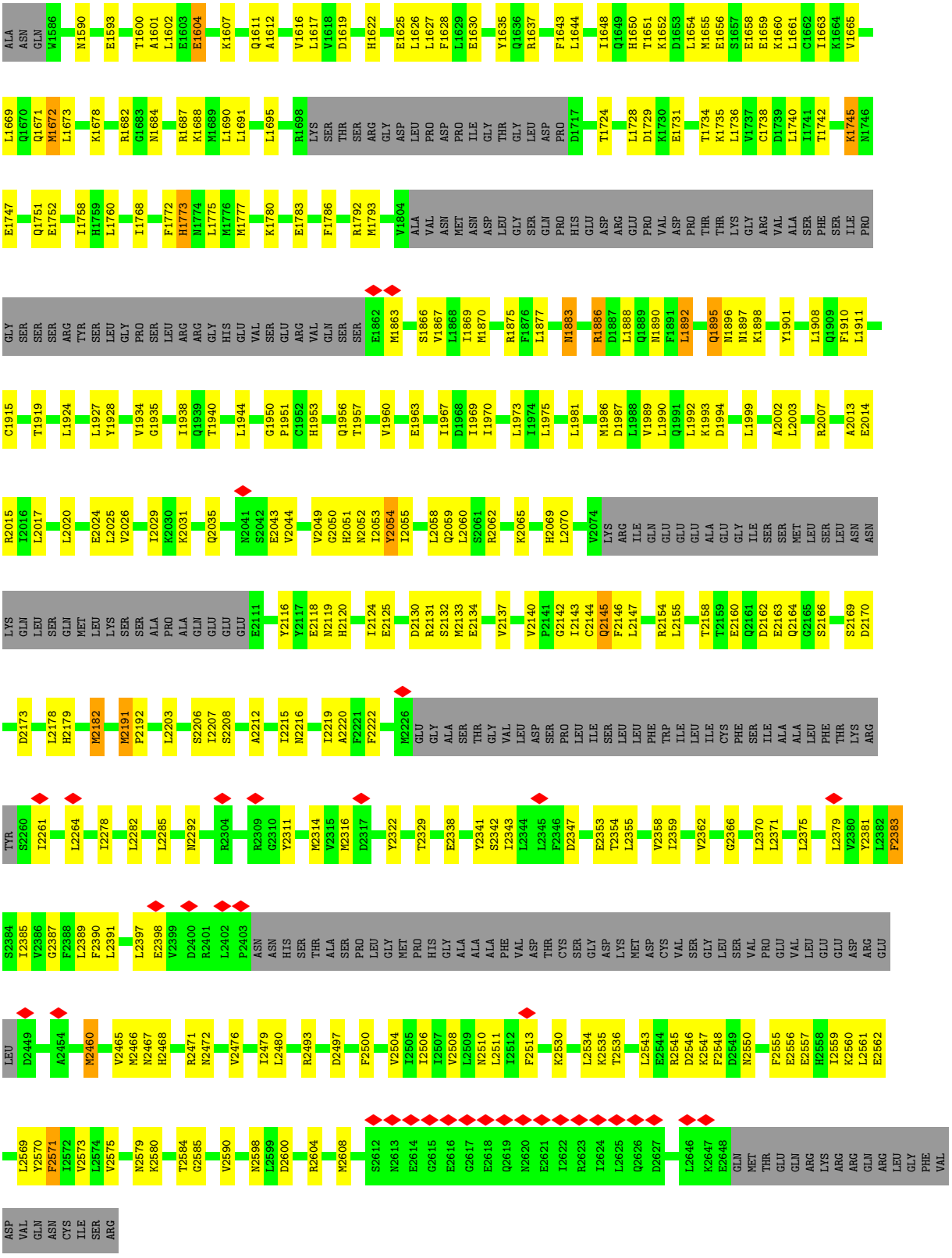




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

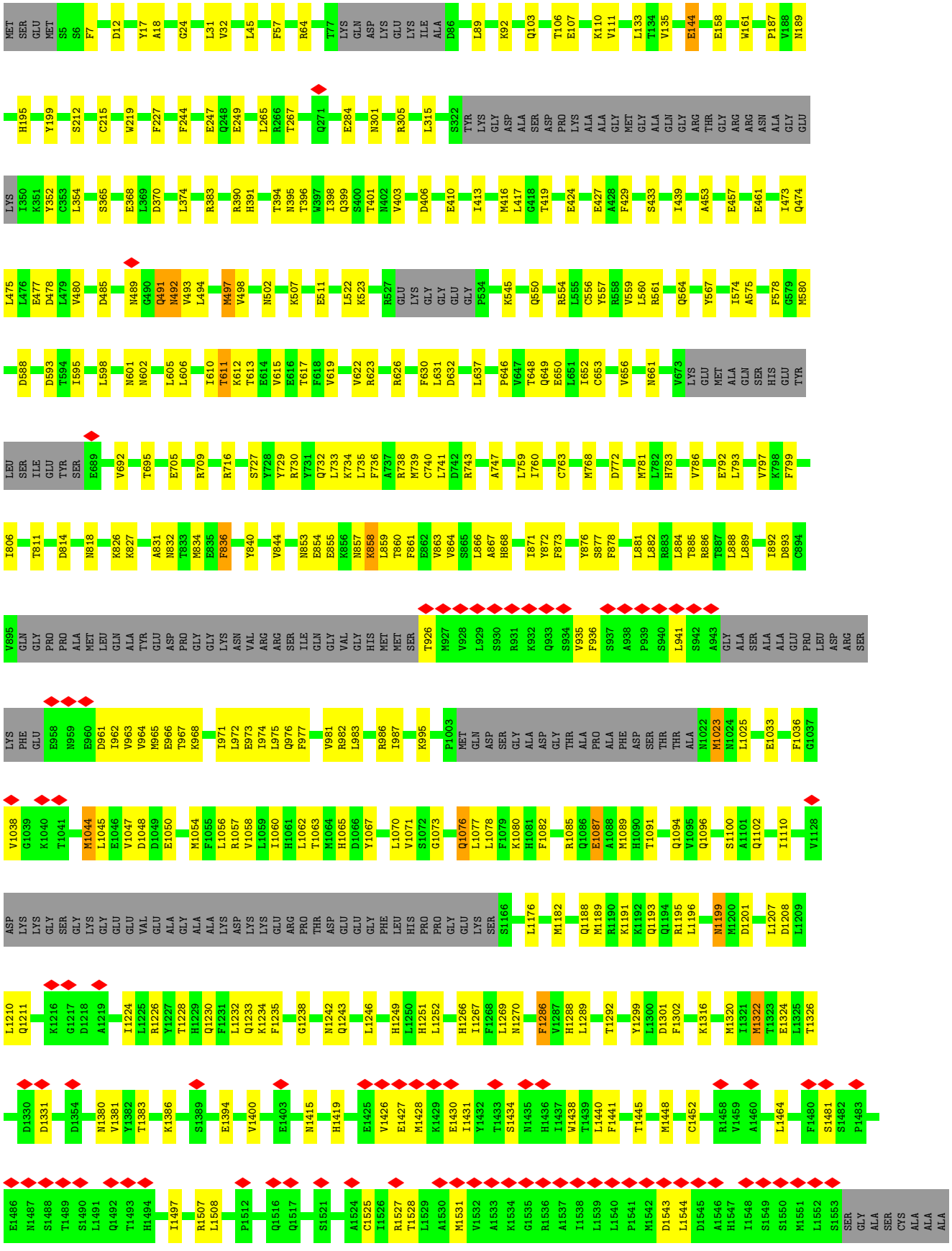
Chain B:

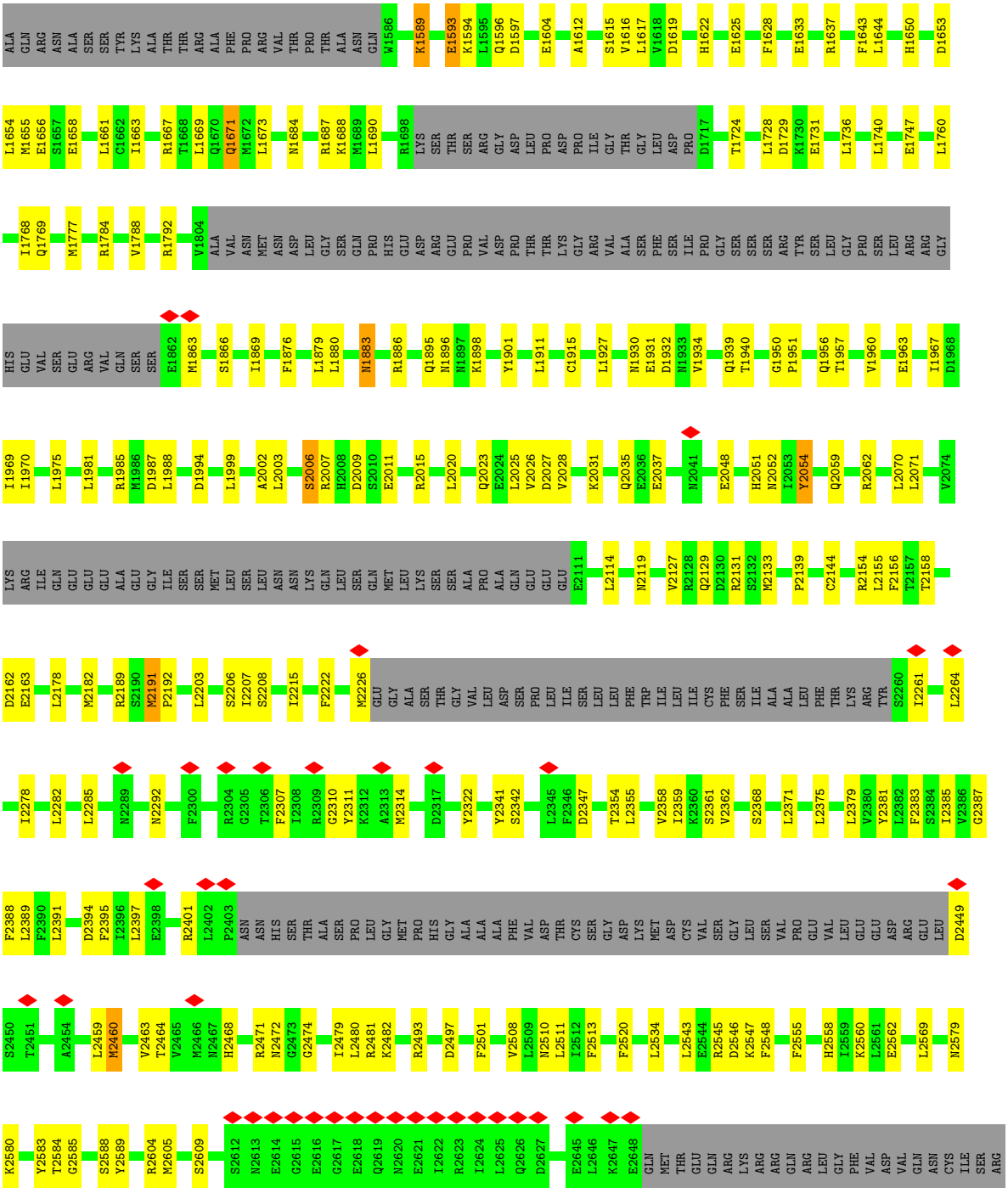




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

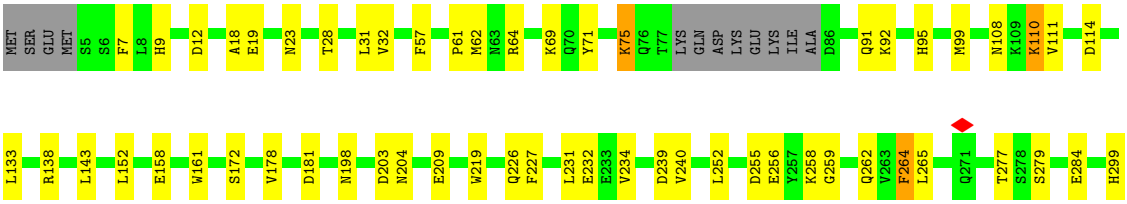
Chain C:

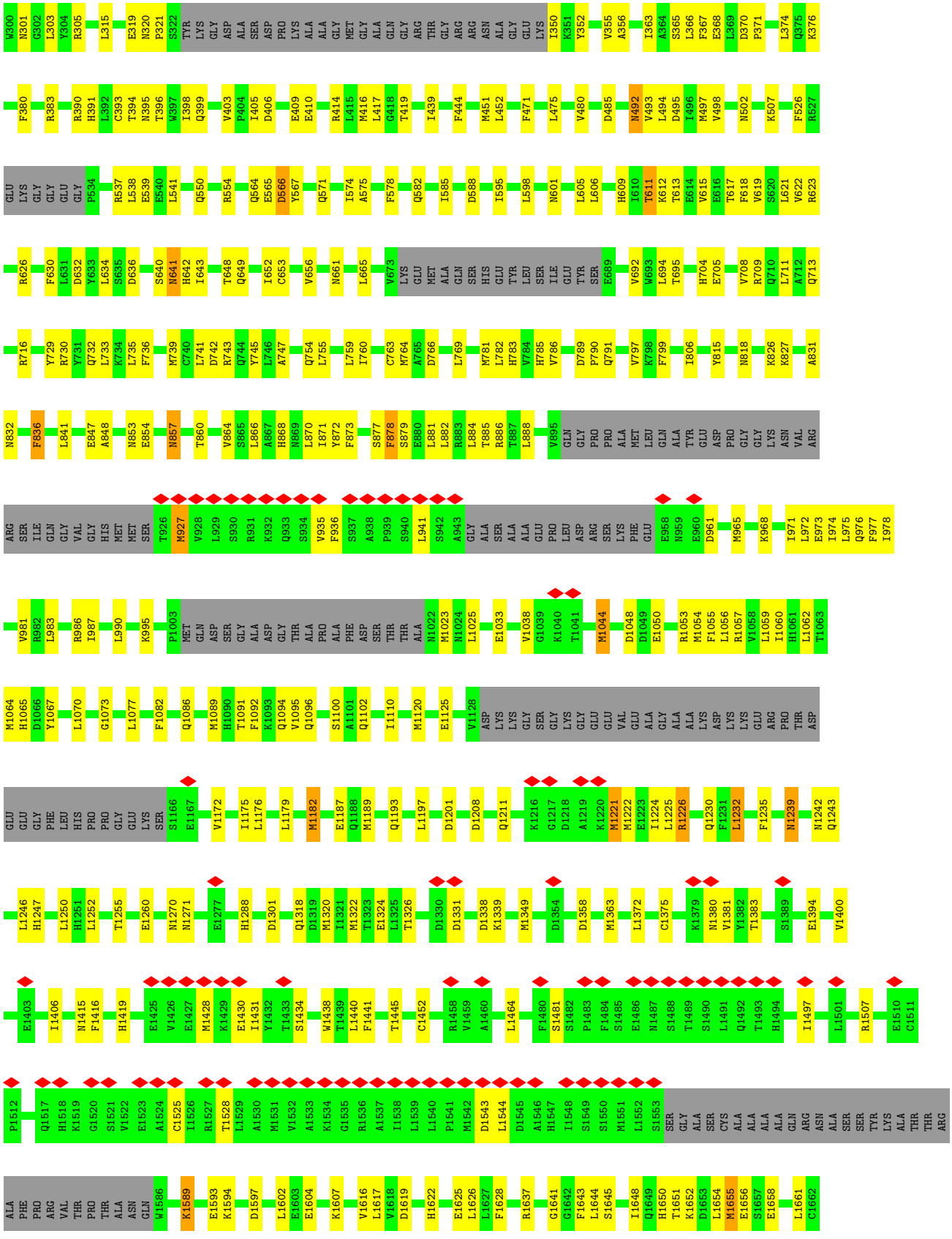


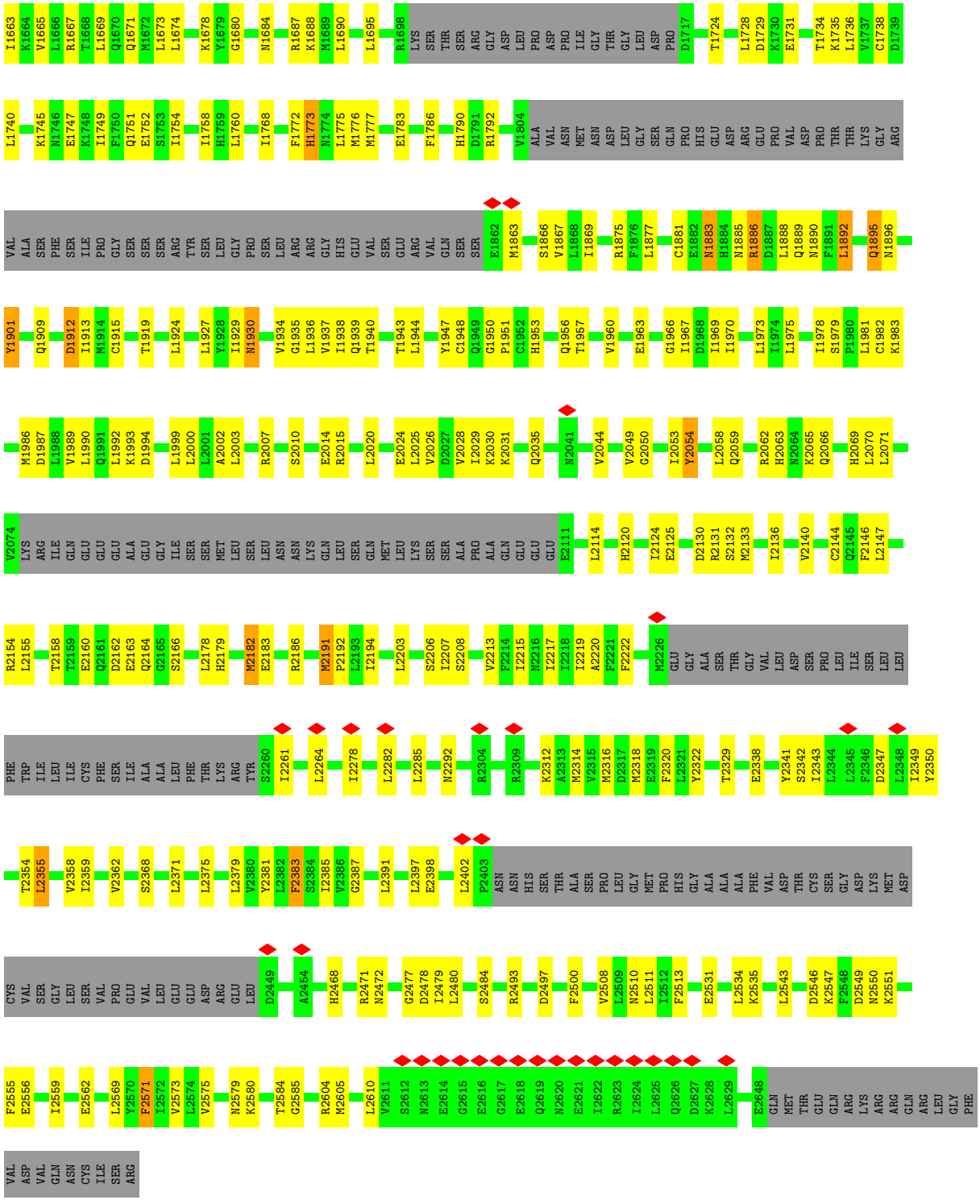


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain D:




W300 N301 G302 L303 Y304 R305 L315 E319 N320 P321 S322 TYR LYS GLY ASP ALA SER ASP PRO LYS ALA ALA GLY MET GLY ALA GLN GLY ARG THR GLY ARG ARG ASN ALA ALA GLY GLU LYS I350 K351 Y352 V355 A356 I363 A364 S365 L366 F367 E368 L369 D370 P371 L374 Q375 K376
F380 R383 R390 H391 L392 C393 T394 N395 T396 W397 I398 Q399 V403 P404 I405 D406 E409 E410 R414 L415 M416 L417 G418 T419 I439 F444 M451 L452 F471 L475 V480 D485 N492 V493 L494 D495 I496 M497 V498 N502 K507 F526 R527
GLU LYS GLY GLY GLU GLY P534 R537 L538 E539 E540 L541 Q550 R554 Q564 E565 D566 Y567 Q571 I574 A575 F578 Q582 I585 D588 I595 L598 N601 L605 L606 H609 I610 T611 K612 T613 E614 V615 E616 T617 F618 V619 S620 L621 V622 R623
R626 F630 L631 D632 Y633 L634 S635 D636 S640 N641 H642 I643 T648 Q649 I652 C653 V656 N661 L665 V673 LYS GLU MET ALA GLN SER HIS GLU TYR LEU SER ILE GLU TYR SER E689 V692 W693 L694 T695 H704 E705 V708 R709 Q710 L711 A712 Q713
R716 Y729 R730 Y731 Q732 L733 K734 L735 F736 M739 C740 L741 D742 R743 Q744 Y745 L746 A747 Q754 L755 L759 I760 C763 M764 A765 D766 L769 M781 L782 H783 V784 H785 V786 D789 P790 Q791 V797 K798 F799 I806 Y815 N818 K826 K827 A831
N832 F836 L841 E847 A848 N853 E854 N857 T860 V864 S865 L866 A867 H868 N869 L870 I871 Y872 F873 S877 F878 S879 E880 L881 L882 R883 L884 T885 R886 T887 L888 V895 GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG
ARG SER ILE GLN GLY VAL GLY HIS MET MET SER T926 M927 V928 L929 S930 R931 K932 Q933 S934 V935 F936 S937 A938 P939 S940 L941 S942 A943 GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU E958 N959 E960 D961 M965 K968 I971 L972 E973 I974 L975 Q976 F977 I978
V981 R982 L983 R986 I987 L990 K995 P1003 MET GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA N1022 M1023 N1024 L1025 E1033 V1038 G1039 K1040 T1041 M1044 D1048 D1049 E1050 R1053 M1054 F1055 L1056 R1057 V1058 L1059 I1060 H1061 L1062 T1063
M1064 H1065 D1066 Y1067 L1070 G1073 L1077 F1082 Q1086 M1089 H1090 T1091 F1092 K1093 Q1094 V1095 Q1096 S1100 A1101 Q1102 I1110 M1120 E1125 V1128 ASP LYS LYS GLY SER GLY LYS GLY GLU GLU VAL GLU ALA GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP
GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER S1166 E1167 V1172 I1175 L1176 L1179 M1182 E1187 Q1188 M1189 Q1193 L1197 D1201 D1208 Q1211 K1216 G1217 D1218 A1219 K1220 M1221 M1222 E1223 I1224 L1225 R1226 Q1230 F1231 L1232 F1235 N1239 N1242 Q1243
L1246 H1247 L1250 H1251 L1252 T1255 E1260 N1270 N1271 E1277 H1288 D1301 Q1318 D1319 M1320 I1321 M1322 T1323 E1324 L1325 T1326 D1330 D1331 D1338 K1339 M1349 D1354 D1358 M1363 L1372 C1375 K1379 N1380 V1381 Y1382 T1383 S1389 E1394 V1400
E1403 I1406 N1415 F1416 H1419 E1425 V1426 E1427 M1428 K1429 E1430 I1431 Y1432 T1433 S1434 W1438 T1439 L1440 F1441 T1445 C1452 R1458 V1459 A1460 L1464 F1480 S1481 S1482 P1483 F1484 S1485 E1486 N1487 S1488 T1489 S1490 L1491 Q1492 T1493 H1494 I1497 L1501 R1507 E1510 C1511
P1512 Q1517 H1518 K1519 G1520 S1521 V1522 E1523 A1524 C1525 T1526 R1527 T1528 L1529 A1530 M1531 V1532 A1533 K1534 G1535 R1536 A1537 I1538 L1539 L1540 P1541 M1542 D1543 L1544 D1545 A1546 H1547 I1548 S1549 S1550 M1551 L1552 S1553 SER GLY ALA SER CYS ALA ALA ALA ALA GLN ARG ASN ALA SER SER TYR LYS ALA THR THR ARG
ALA PHE PRO ARG VAL THR PRO THR ALA ASN GLN W1586 K1589 E1593 K1594 D1597 L1602 E1603 E1604 K1607 V1616 L1617 V1618 D1619 H1622 E1625 L1626 L1627 F1628 R1637 G1641 G1642 F1643 L1644 S1645 I1648 Q1649 H1650 T1651 K1652 D1653 L1654 M1655 E1656 S1657 E1658 L1661 C1662


I1663 K1664 V1665 L1666 R1667 T1668 L1669 Q1670 Q1671 M1672 L1673 L1674 K1678 Y1679 G1680 N1684 R1687 K1688 M1689 L1690 L1695 R1698 D1717 T1724 L1728 D1729 K1730 E1731 T1734 K1735 L1736 V1737 C1738 D1739
L1740 K1745 N1746 E1747 K1748 I1749 F1750 Q1751 E1752 S1753 I1754 I1758 H1759 L1760 I1768 F1772 H1773 N1774 L1775 M1776 M1777 E1783 F1786 H1790 D1791 R1792 V1804
VAL ALA SER PHE SER ILE PRO GLY SER SER SER ARG TYR SER LEU GLY PRO SER LEU ARG ARG GLY HIS GLU VAL SER GLU ARG VAL GLN SER SER E1862 M1863 S1866 V1867 L1868 I1869 R1875 F1876 L1877 C1881 E1882 N1883 H1884 N1885 R1886 D1887 L1888 Q1889 N1890 F1891 L1892 Q1895 N1896
Y1901 Q1909 D1912 I1913 M1914 C1915 T1919 L1924 L1927 Y1928 I1929 N1930 V1934 G1935 L1936 V1937 I1938 Q1939 T1940 T1943 L1944 Y1947 C1948 Q1949 G1950 P1951 C1952 H1953 Q1956 T1957 V1960 E1963 G1966 I1967 D1968 I1969 I1970 L1973 I1974 L1975 I1978 S1979 P1980 L1981 C1982 K1983
M1986 D1987 L1988 V1989 L1990 Q1991 L1992 K1993 D1994 L1999 L2000 L2001 A2002 L2003 R2007 S2010 E2014 R2015 L2020 E2024 L2025 V2026 D2027 V2028 I2029 K2030 K2031 Q2035 N2041 V2044 V2049 G2050 I2053 Y2064 L2058 Q2059 R2062 H2063 N2064 K2065 Q2066 H2069 L2070 L2071
V2074 LYS ARG ILE GLN GLU GLU GLU ALA GLU GLY ILE SER SER MET LEU SER LEU ASN ASN LYS GLN LEU SER GLN MET LEU LYS SER SER ALA PRO ALA GLN GLU GLU GLU E2111 L2114 H2120 I2124 E2125 D2130 R2131 S2132 M2133 I2136 V2140 C2144 Q2145 F2146 L2147
R2154 L2155 T2158 T2159 E2160 Q2161 D2162 E2163 Q2164 G2165 S2166 L2178 H2179 M2182 E2183 R2186 M2191 P2192 L2193 I2194 L2203 S2206 I2207 S2208 V2213 F2214 I2215 N2216 I2217 I2218 I2219 A2220 F2221 F2222 M2226 GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO LEU ILE SER LEU LEU
PHE TRP ILE LEU ILE CYS PHE SER ILE ALA ALA LEU PHE THR LYS ARG TYR S2260 I2261 L2264 I2278 L2282 L2286 N2292 R2304 R2309 K2312 A2313 M2314 V2315 M2316 D2317 M2318 E2319 F2320 L2321 Y2322 T2329 E2338 Y2341 S2342 I2343 L2344 L2345 F2346 D2347 L2348 I2349 Y2350
T2354 L2355 V2358 I2359 V2362 S2368 L2371 L2375 L2379 V2380 Y2381 L2382 F2383 S2384 I2385 V2386 G2387 L2391 L2397 E2398 L2402 P2403 ASN ASN HIS SER THR ALA SER PRO LEU GLY MET PRO HIS GLY ALA ALA ALA PHE VAL ASP THR CYS SER GLY ASP LYS MET ASP
CYS VAL SER GLY LEU SER VAL PRO GLU VAL LEU LEU GLU GLU ASP ARG GLU LEU D2449 A2454 H2468 R2471 N2472 G2477 D2478 I2479 L2480 S2484 R2493 D2497 F2500 V2508 L2509 N2510 L2511 I2512 F2513 E2531 L2534 K2535 L2543 D2546 K2547 F2548 D2549 N2550 K2551
F2555 E2556 I2559 E2562 L2569 Y2570 F2571 I2572 V2573 L2574 V2575 N2579 K2580 T2584 G2585 R2604 M2605 L2610 V2611 S2612 N2613 E2614 G2615 E2616 G2617 E2618 Q2619 N2620 E2621 I2622 R2623 I2624 L2625 Q2626 D2627 K2628 L2629 E2648 GLN MET THR GLU GLN ARG LYS ARG ARG GLN ARG LEU GLY PHE
VAL ASP VAL GLN ASN CYS ILE SER ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155671	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 ($e^-/Å^2$)	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.933	Depositor
Minimum map value	-0.374	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I3P, ATP, ZN

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	0.24	0/18521	0.46	0/25031
1	B	0.24	0/18521	0.46	0/25031
1	C	0.24	0/18521	0.46	0/25031
1	D	0.24	0/18521	0.46	0/25031
All	All	0.24	0/74084	0.46	0/100124

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	18187	18211	18206	363	0
1	B	18187	18211	18209	859	0
1	C	18187	18211	18208	741	0
1	D	18187	18211	18207	917	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	9	9	0	0
3	C	24	9	9	0	0
3	D	24	9	9	0	0
4	A	31	12	12	1	0
4	B	31	12	12	0	0
4	C	31	12	12	1	0
4	D	31	12	12	0	0
All	All	72972	72928	72914	2691	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 18.

The worst 5 of 2691 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2355:LEU:CB	1:D:2371:LEU:HD21	1.21	1.64
1:B:138:ARG:NH1	1:C:1288:HIS:CE1	1.70	1.59
1:A:1288:HIS:CE1	1:D:138:ARG:NH1	1.70	1.57
1:B:2497:ASP:CA	1:C:2471:ARG:NH2	1.71	1.53
1:A:1288:HIS:CE1	1:D:138:ARG:CZ	1.89	1.52

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	2238/2671 (84%)	2202 (98%)	36 (2%)	0	100	100
1	B	2238/2671 (84%)	2202 (98%)	36 (2%)	0	100	100
1	C	2238/2671 (84%)	2203 (98%)	35 (2%)	0	100	100
1	D	2238/2671 (84%)	2203 (98%)	35 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8952/10684 (84%)	8810 (98%)	142 (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	2021/2385 (85%)	1977 (98%)	44 (2%)	52 77
1	B	2021/2385 (85%)	1966 (97%)	55 (3%)	44 73
1	C	2021/2385 (85%)	1974 (98%)	47 (2%)	50 76
1	D	2021/2385 (85%)	1963 (97%)	58 (3%)	42 72
All	All	8084/9540 (85%)	7880 (98%)	204 (2%)	50 75

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1044	MET
1	C	2383	PHE
1	D	2191	MET
1	C	1087	GLU
1	C	1622	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1271	ASN
1	D	1953	HIS
1	B	2510	ASN
1	B	2120	HIS
1	D	2035	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 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	I3P	A	3002	-	24,24,24	2.07	3 (12%)	36,39,39	0.84	0
4	ATP	B	3003	-	26,33,33	0.61	0	31,52,52	1.05	2 (6%)
4	ATP	A	3003	-	26,33,33	0.60	0	31,52,52	1.05	2 (6%)
3	I3P	C	3002	-	24,24,24	2.06	3 (12%)	36,39,39	0.84	0
3	I3P	B	3002	-	24,24,24	2.07	3 (12%)	36,39,39	0.84	0
4	ATP	D	3003	-	26,33,33	0.60	0	31,52,52	1.05	2 (6%)
3	I3P	D	3002	-	24,24,24	2.06	3 (12%)	36,39,39	0.85	0
4	ATP	C	3003	-	26,33,33	0.60	0	31,52,52	1.05	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	I3P	A	3002	-	-	1/15/39/39	0/1/1/1
4	ATP	B	3003	-	-	9/18/38/38	0/3/3/3
4	ATP	A	3003	-	-	9/18/38/38	0/3/3/3
3	I3P	C	3002	-	-	1/15/39/39	0/1/1/1
3	I3P	B	3002	-	-	1/15/39/39	0/1/1/1
4	ATP	D	3003	-	-	9/18/38/38	0/3/3/3
3	I3P	D	3002	-	-	1/15/39/39	0/1/1/1
4	ATP	C	3003	-	-	9/18/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3002	I3P	P4-O4	5.74	1.70	1.59
3	A	3002	I3P	P4-O4	5.72	1.70	1.59
3	C	3002	I3P	P4-O4	5.70	1.70	1.59
3	D	3002	I3P	P4-O4	5.69	1.70	1.59
3	B	3002	I3P	P5-O5	5.58	1.69	1.59

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3003	ATP	C5-C6-N6	2.30	123.84	120.35
4	D	3003	ATP	C5-C6-N6	2.29	123.84	120.35
4	C	3003	ATP	C5-C6-N6	2.28	123.82	120.35
4	B	3003	ATP	C5-C6-N6	2.28	123.82	120.35
4	C	3003	ATP	PB-O3B-PG	2.07	139.92	132.83

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3003	ATP	PB-O3B-PG-O3G
4	A	3003	ATP	C5'-O5'-PA-O2A
4	B	3003	ATP	PB-O3B-PG-O3G
4	B	3003	ATP	C5'-O5'-PA-O2A
4	C	3003	ATP	PB-O3B-PG-O3G

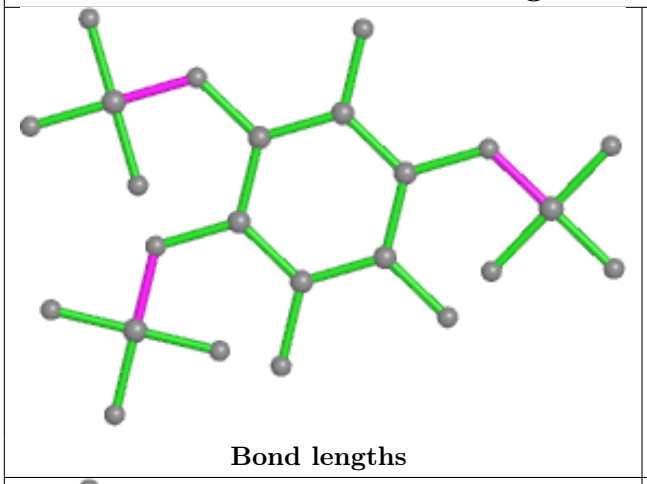
There are no ring outliers.

2 monomers are involved in 2 short contacts:

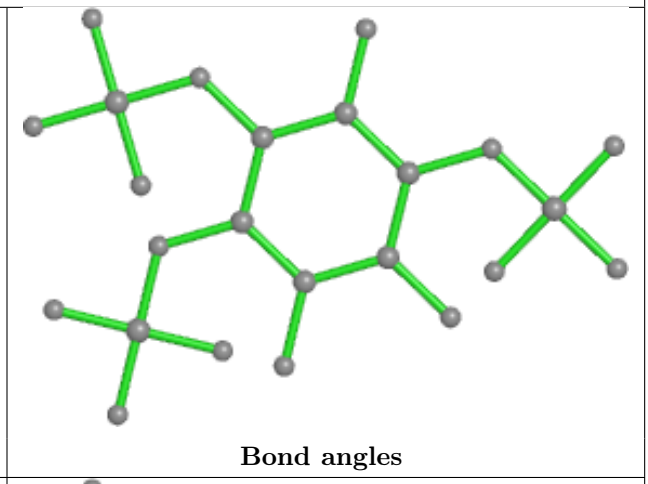
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3003	ATP	1	0
4	C	3003	ATP	1	0

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.

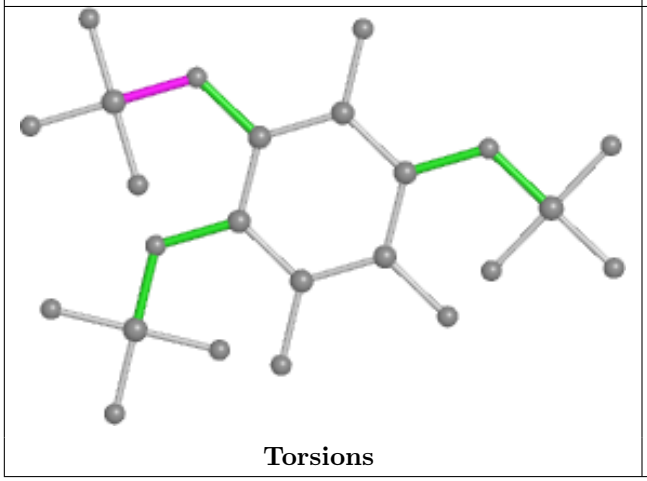
Ligand I3P A 3002



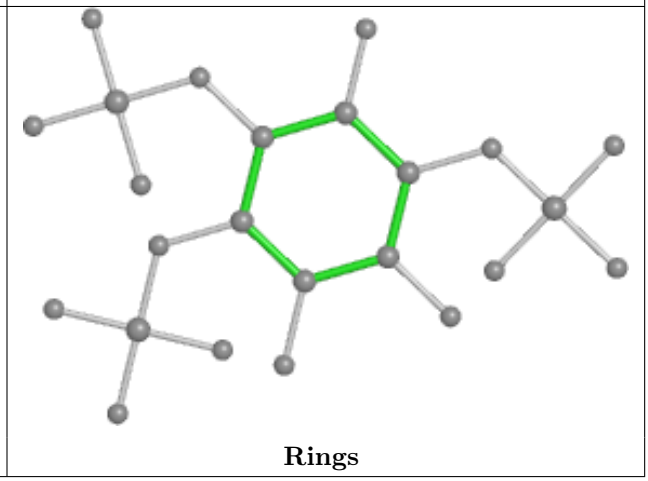
Bond lengths



Bond angles

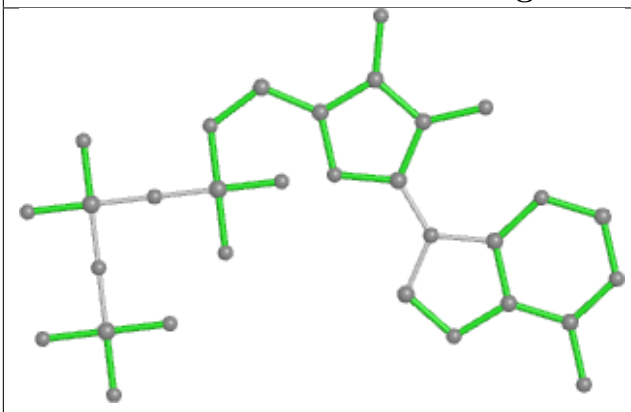


Torsions

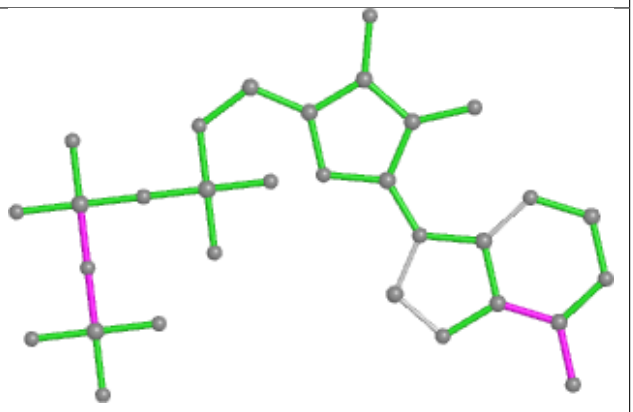


Rings

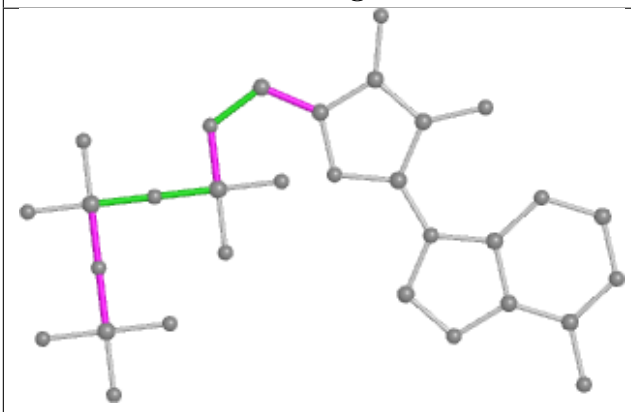
Ligand ATP B 3003



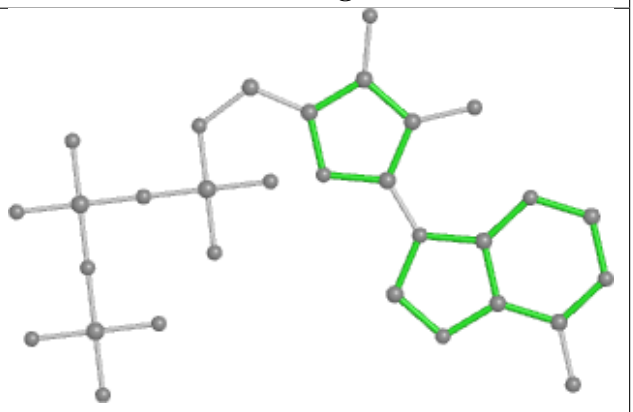
Bond lengths



Bond angles

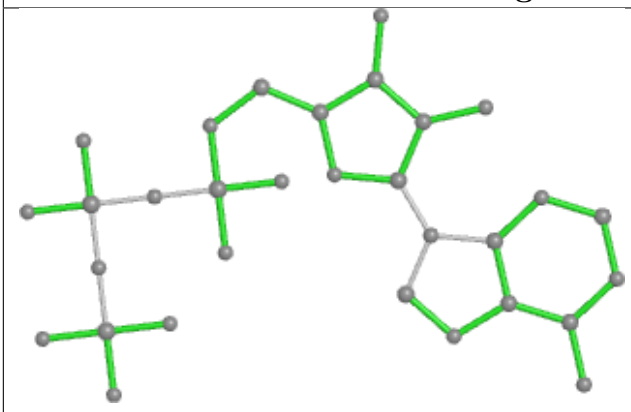


Torsions

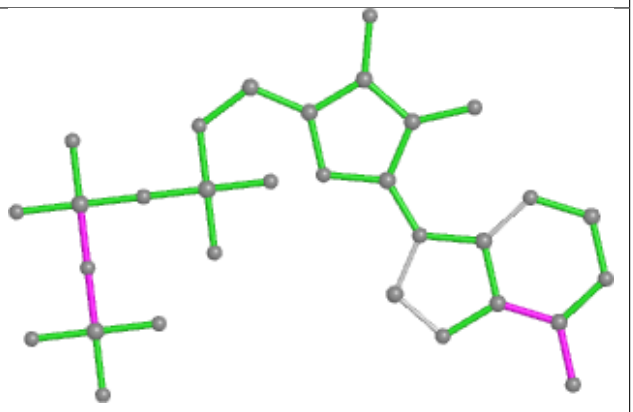


Rings

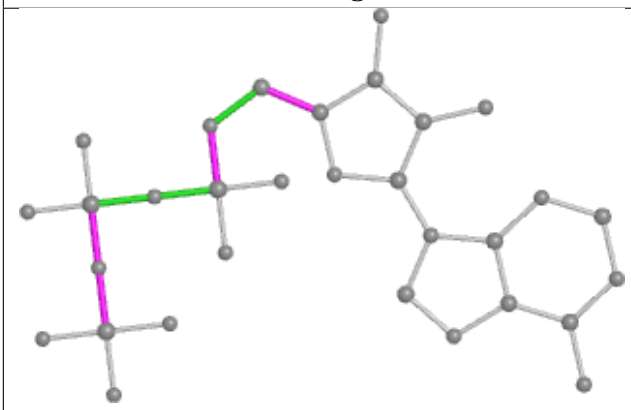
Ligand ATP A 3003



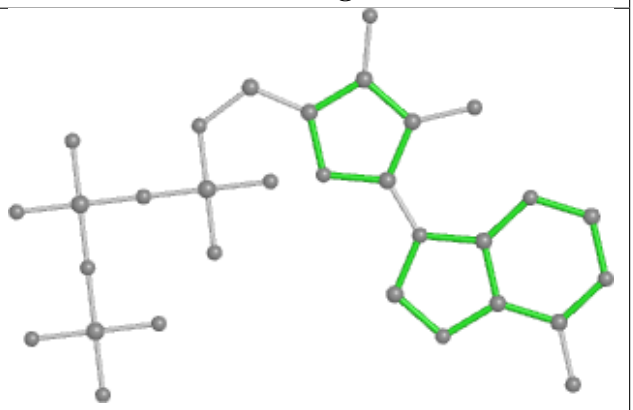
Bond lengths



Bond angles

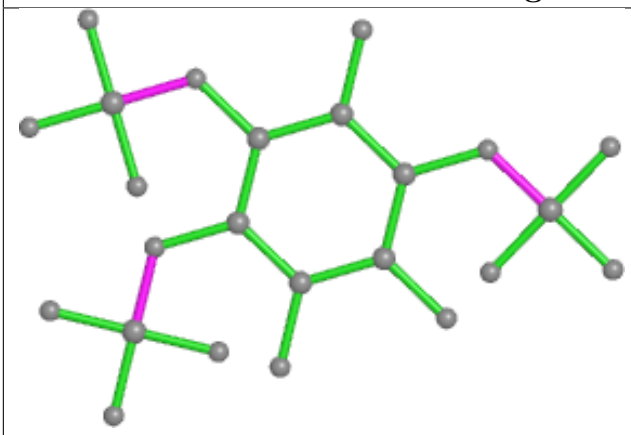


Torsions

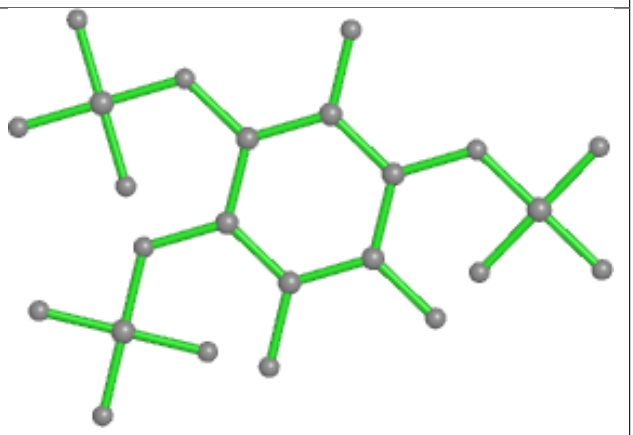


Rings

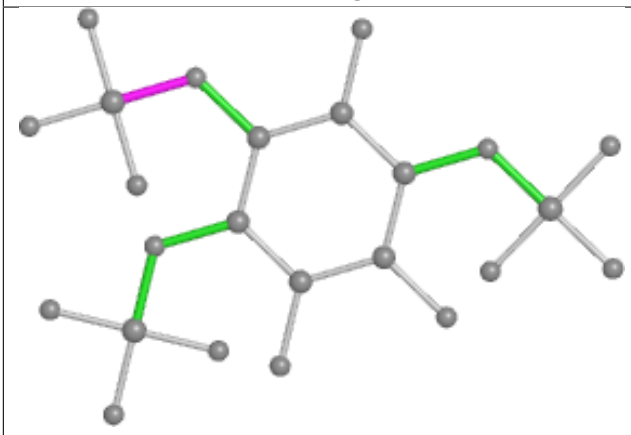
Ligand I3P C 3002



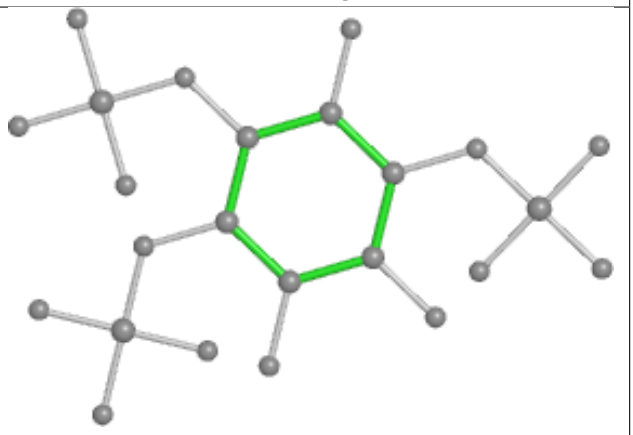
Bond lengths



Bond angles

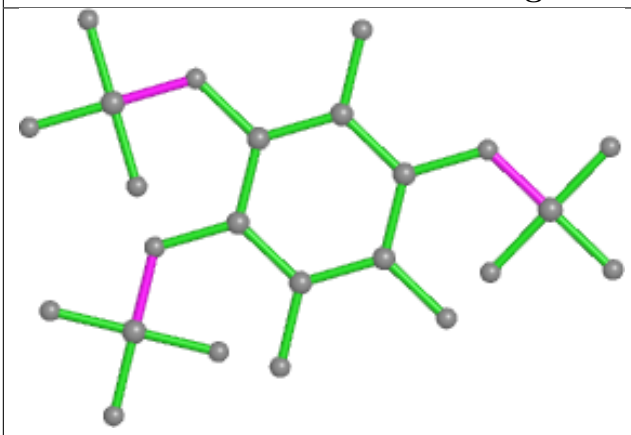


Torsions

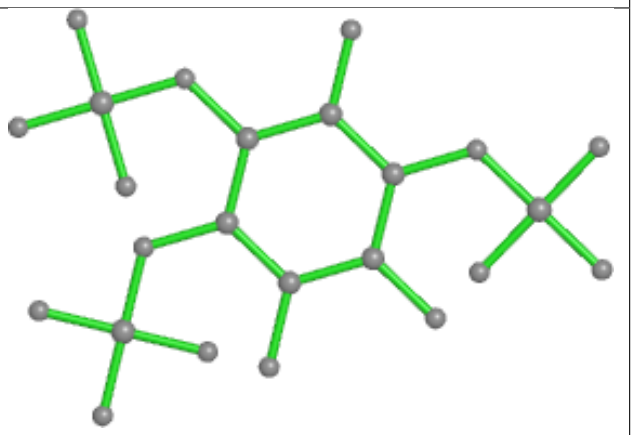


Rings

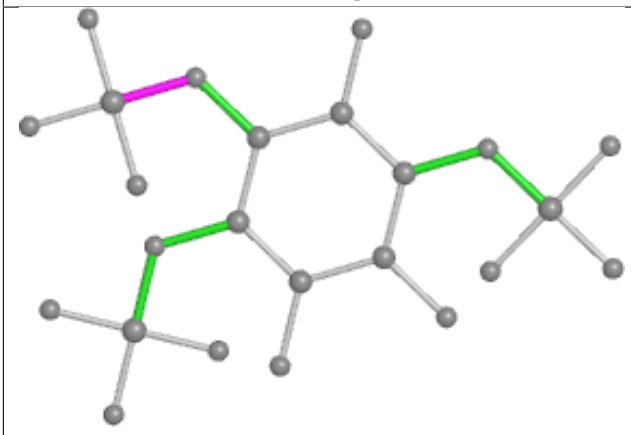
Ligand I3P B 3002



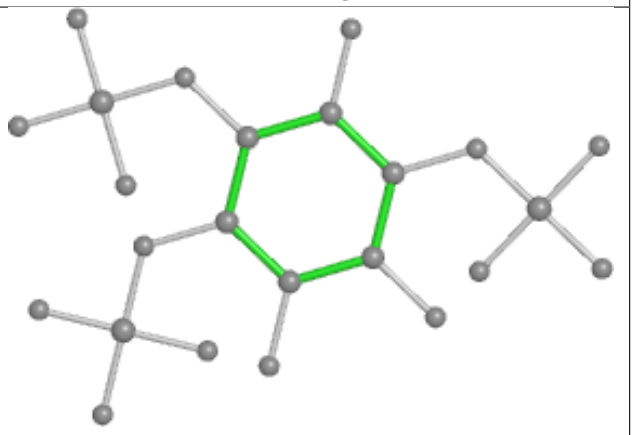
Bond lengths



Bond angles

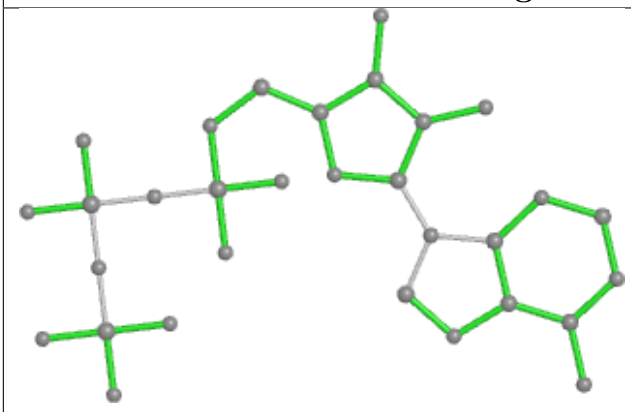


Torsions

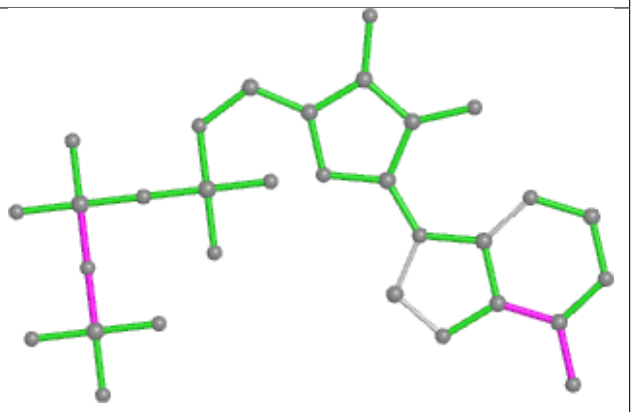


Rings

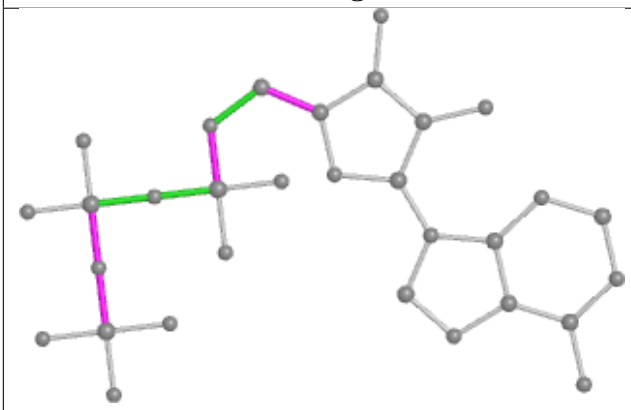
Ligand ATP D 3003



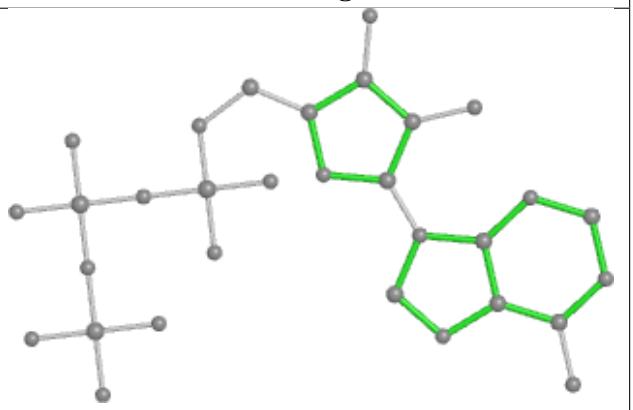
Bond lengths



Bond angles

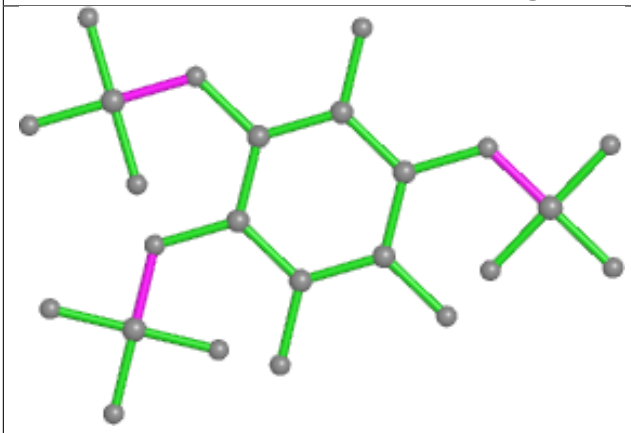


Torsions

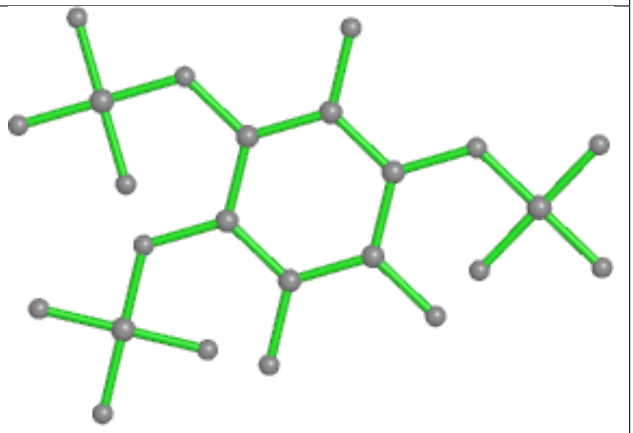


Rings

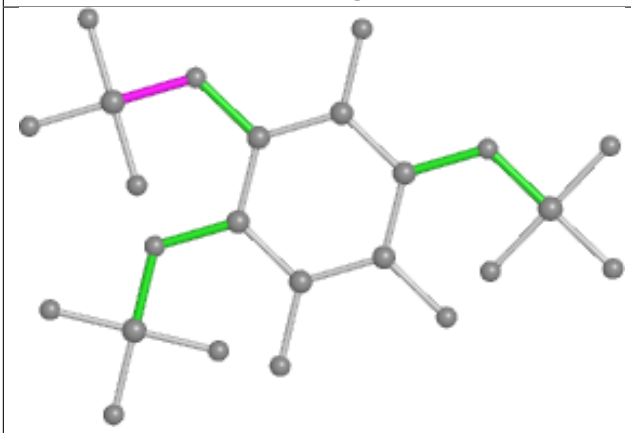
Ligand I3P D 3002



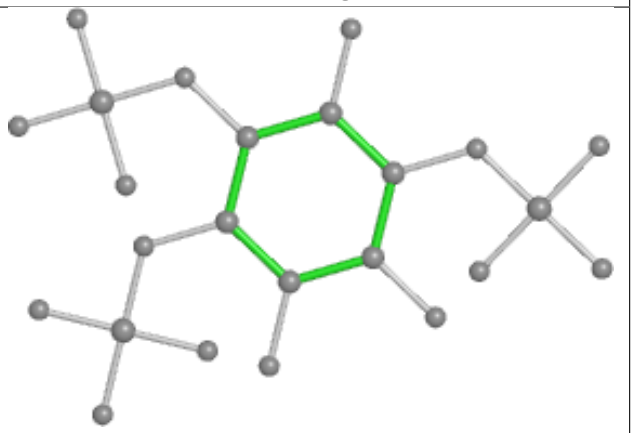
Bond lengths



Bond angles

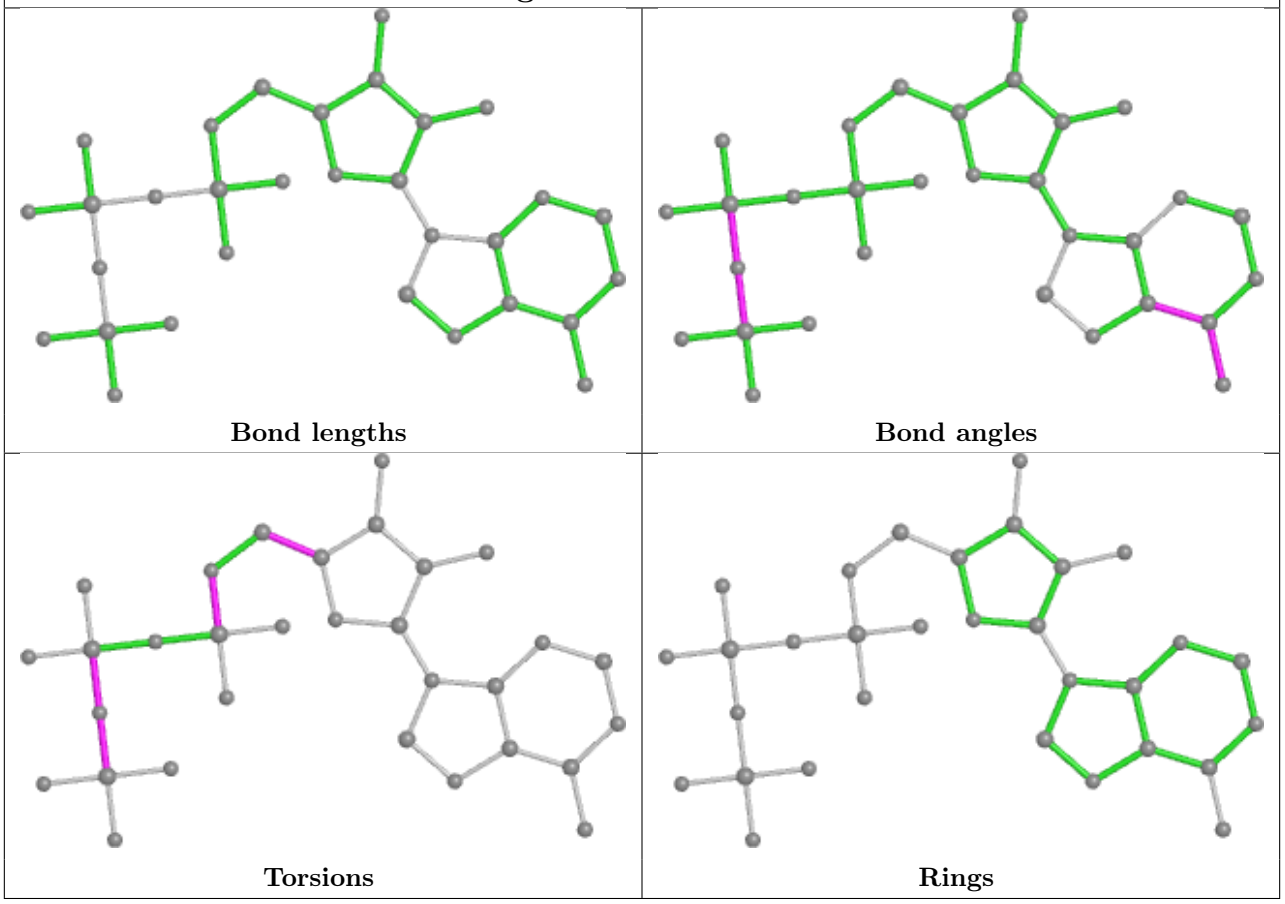


Torsions



Rings

Ligand ATP C 3003



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.

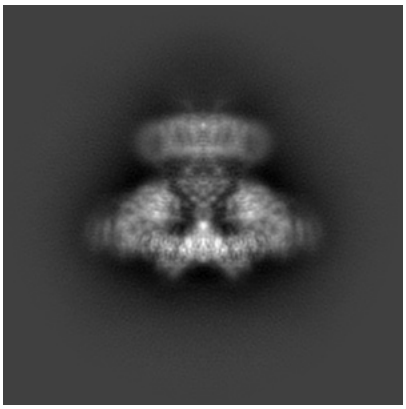
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41352. These allow visual inspection of the internal detail of the map and identification of artifacts.

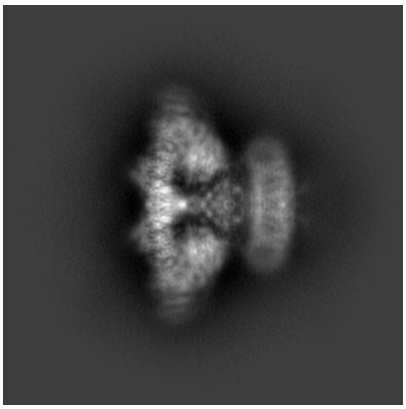
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

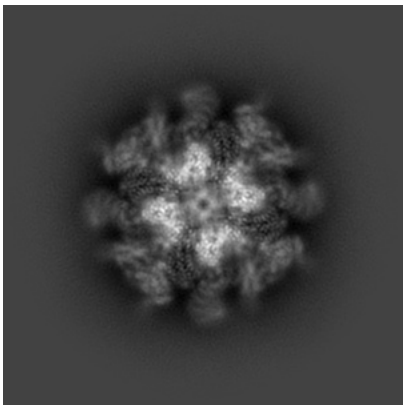
6.1.1 Primary map



X

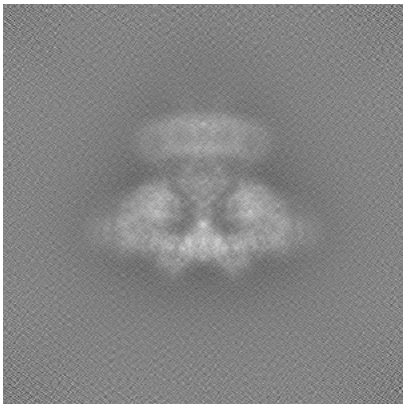


Y

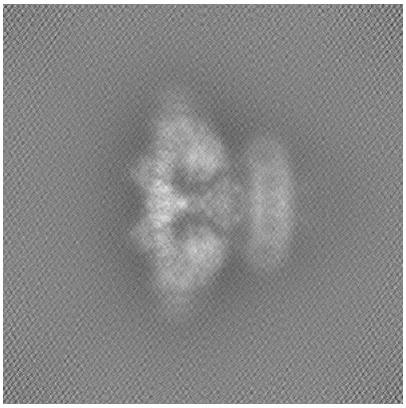


Z

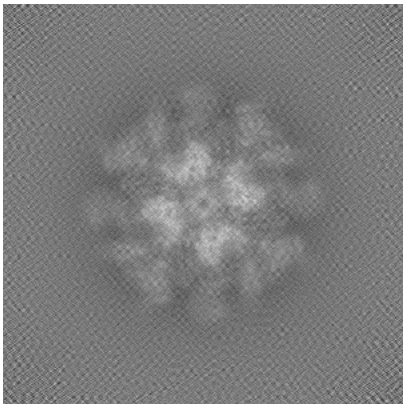
6.1.2 Raw map



X



Y

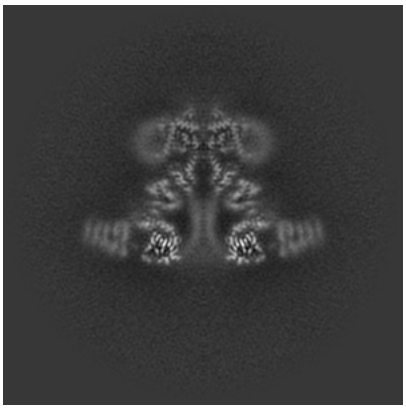


Z

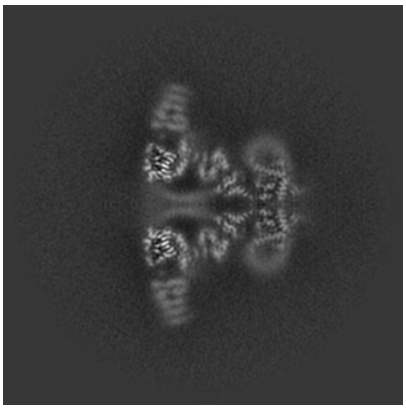
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

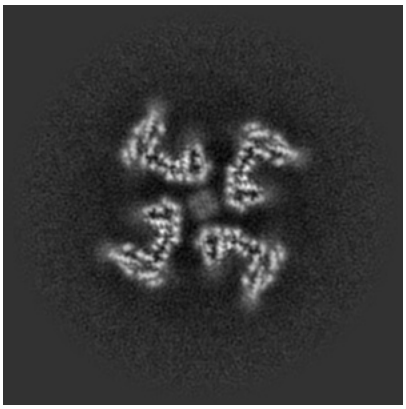
6.2.1 Primary map



X Index: 256

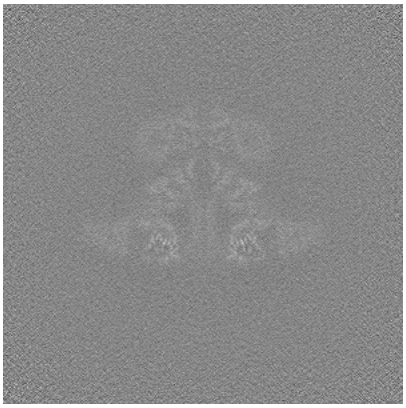


Y Index: 256

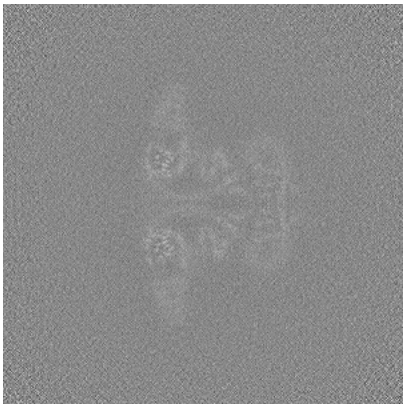


Z Index: 256

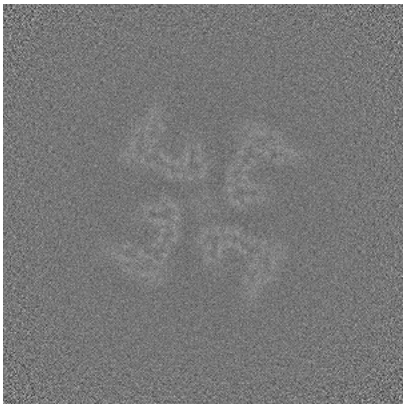
6.2.2 Raw map



X Index: 256



Y Index: 256

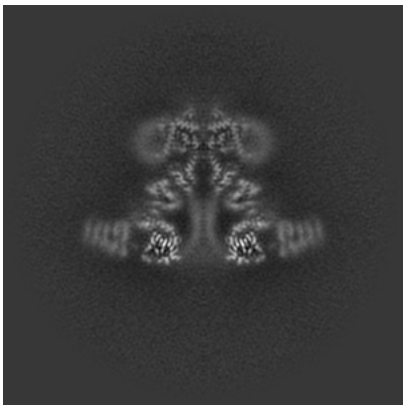


Z Index: 256

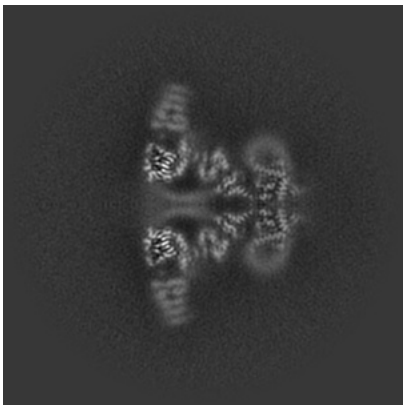
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

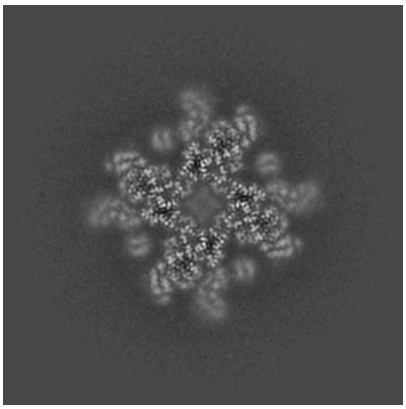
6.3.1 Primary map



X Index: 256

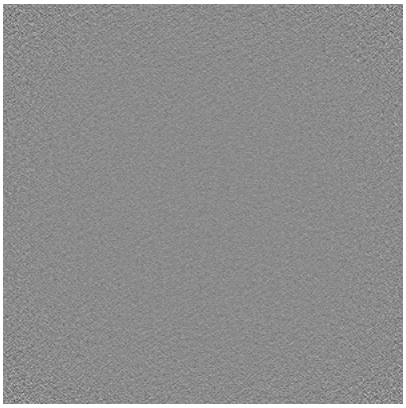


Y Index: 256

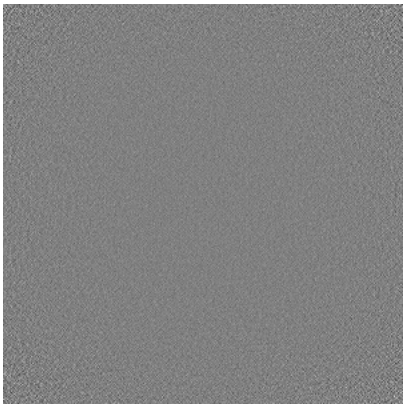


Z Index: 205

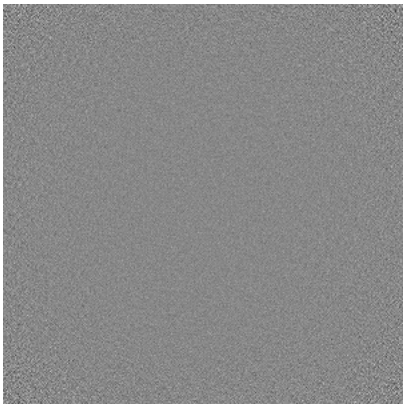
6.3.2 Raw map



X Index: 0



Y Index: 0

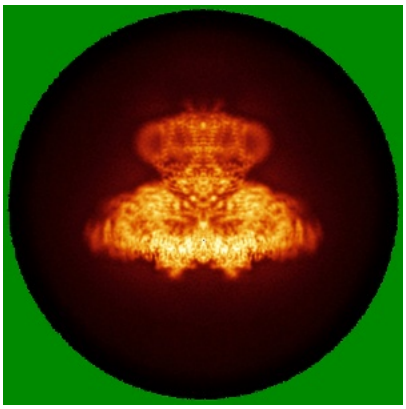


Z Index: 0

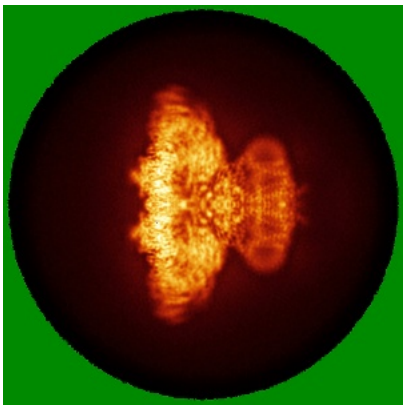
The images above show the largest variance slices of the map in three orthogonal directions.

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

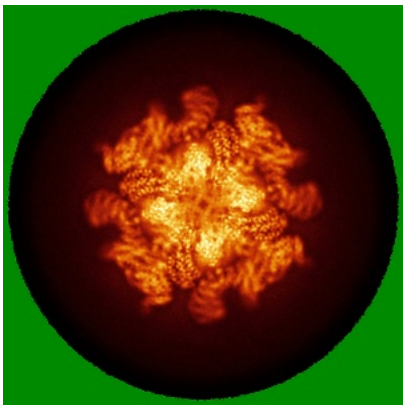
6.4.1 Primary map



X

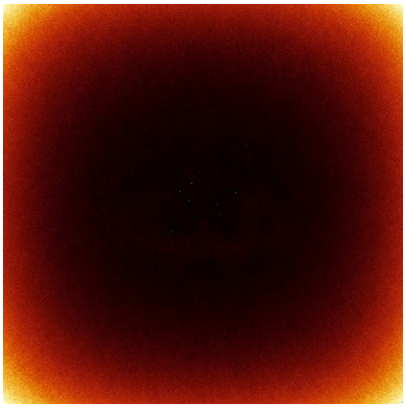


Y

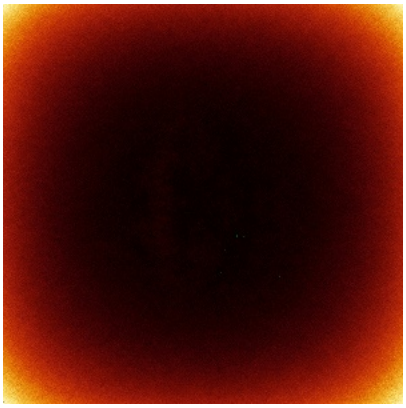


Z

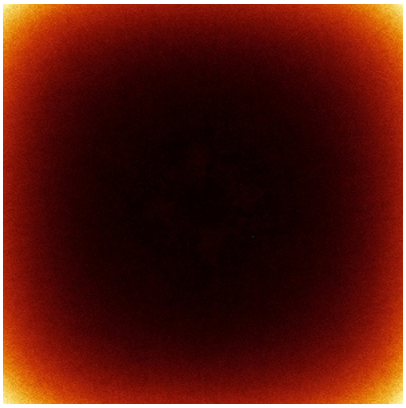
6.4.2 Raw map



X



Y

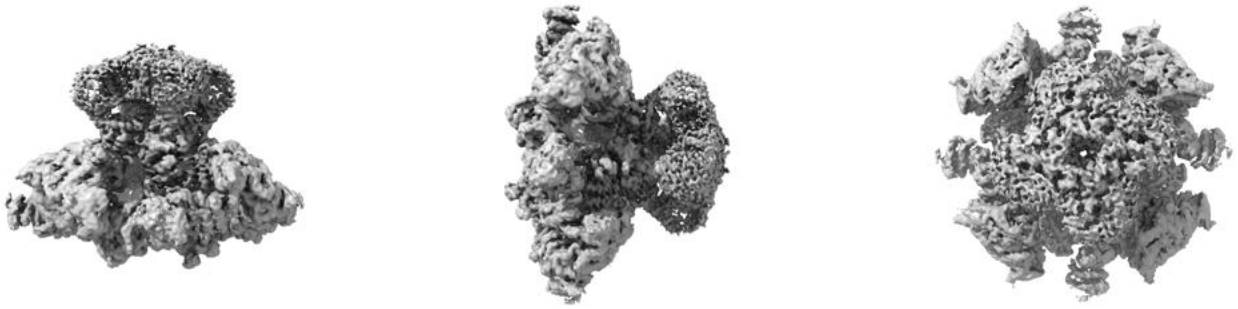


Z

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)

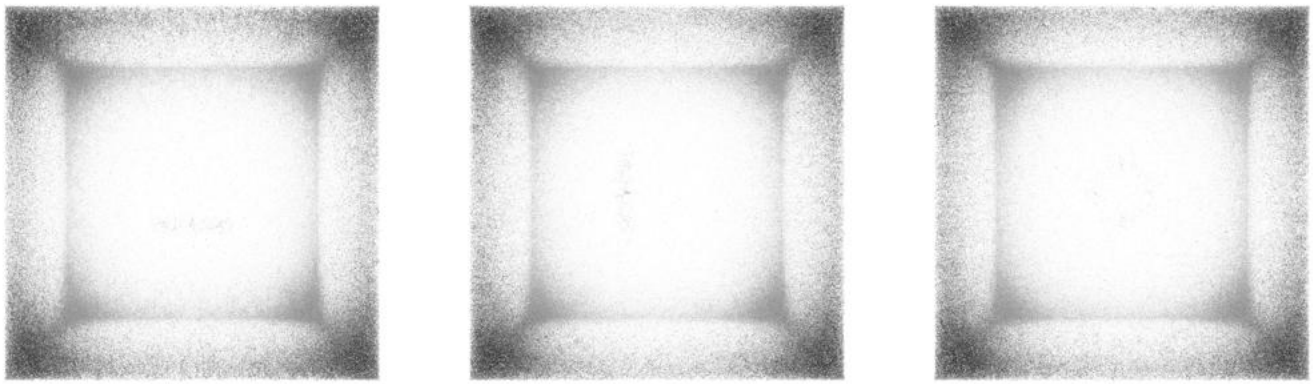
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

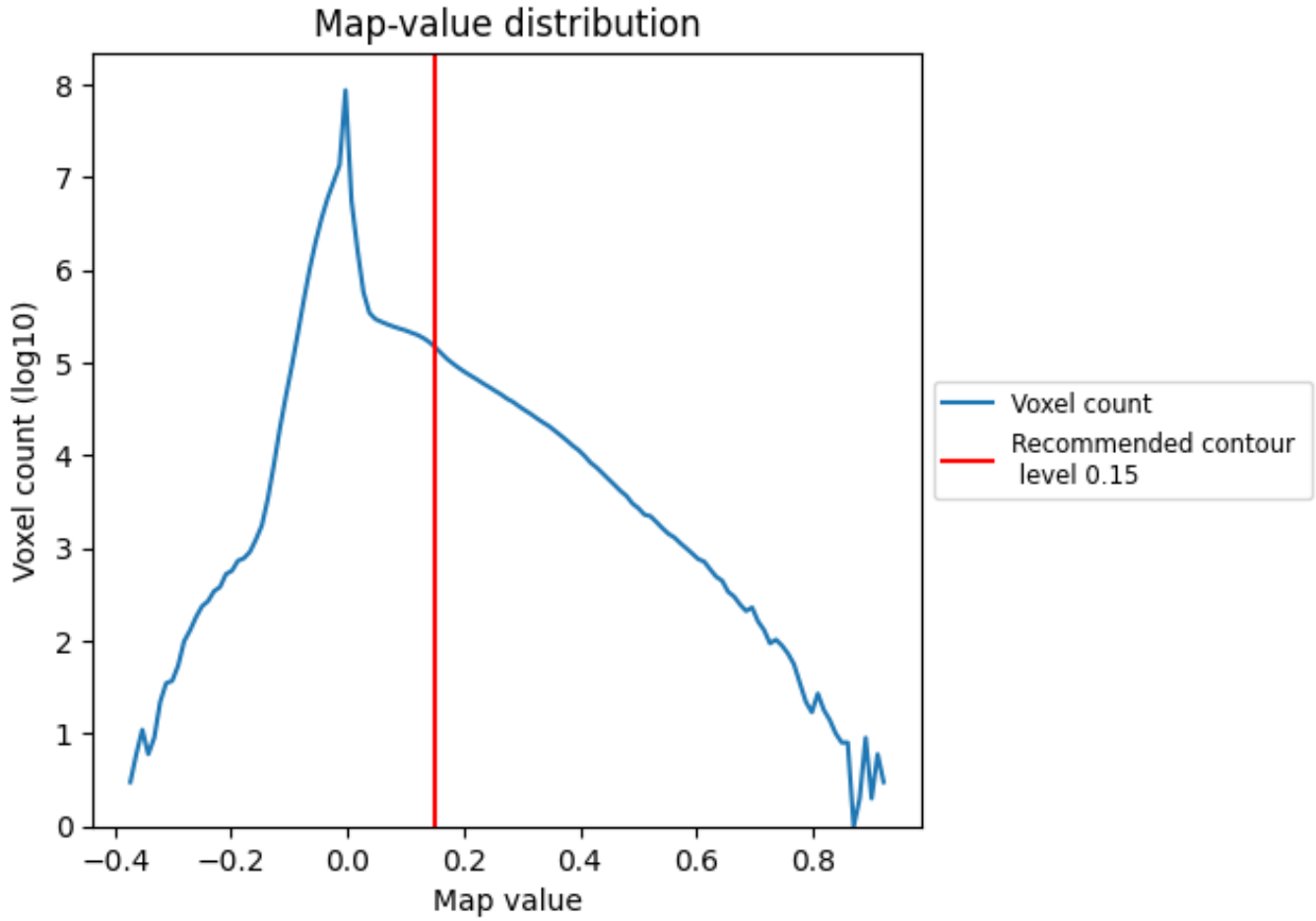
6.6 Mask visualisation (i)

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

7 Map analysis

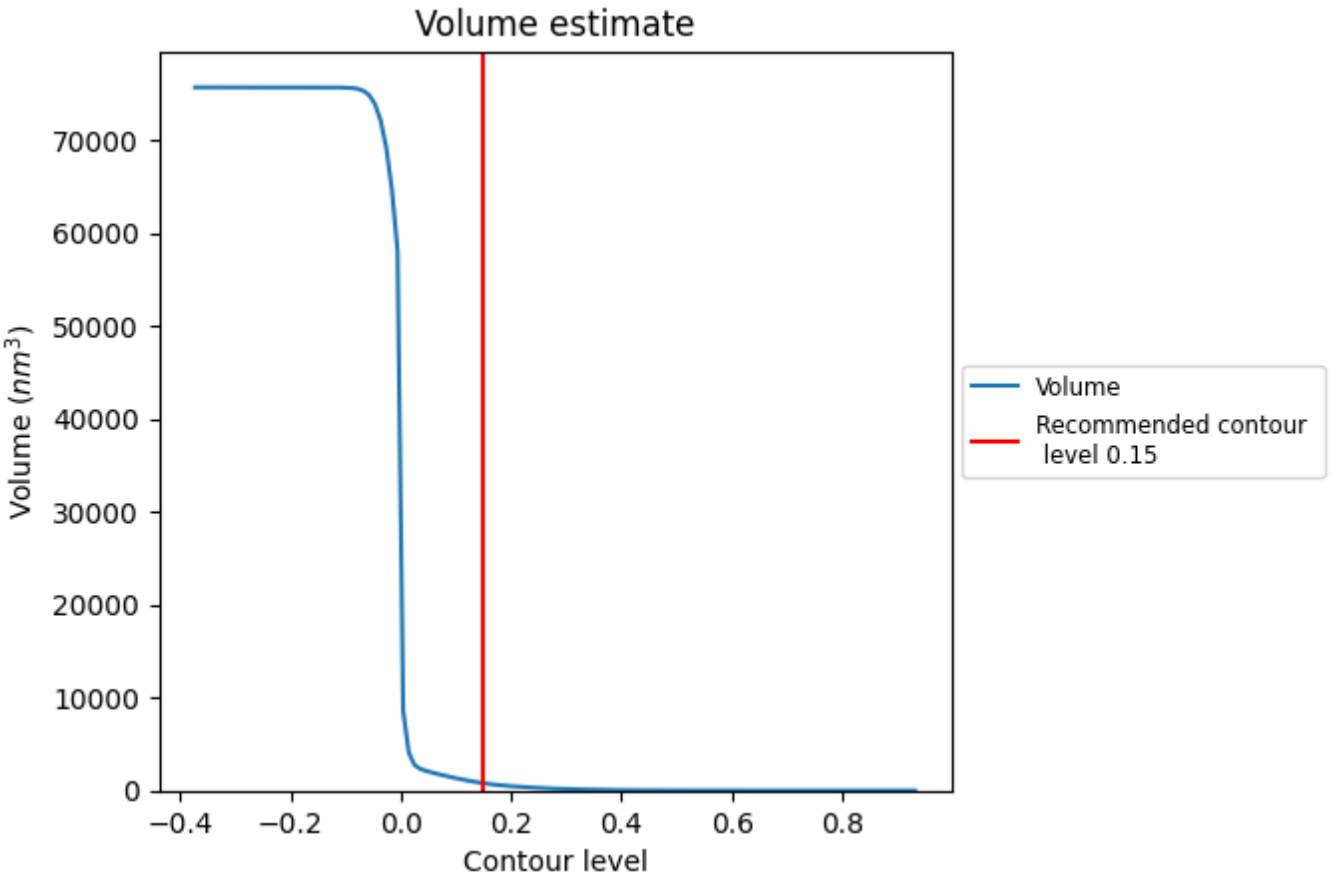
This section contains the results of statistical analysis of the map.

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.

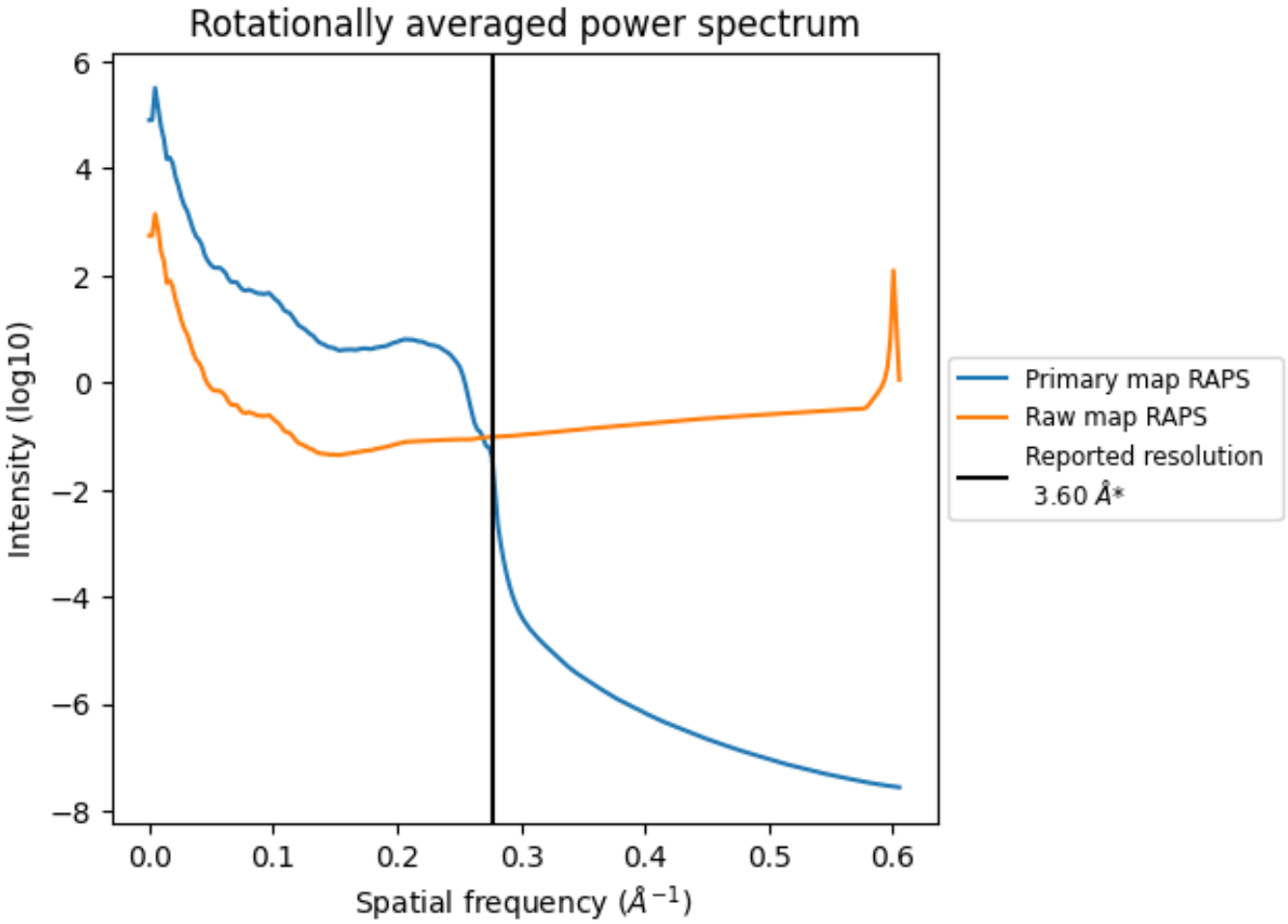
7.2 Volume estimate (i)



The volume at the recommended contour level is 788 nm^3; this corresponds to an approximate mass of 711 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)

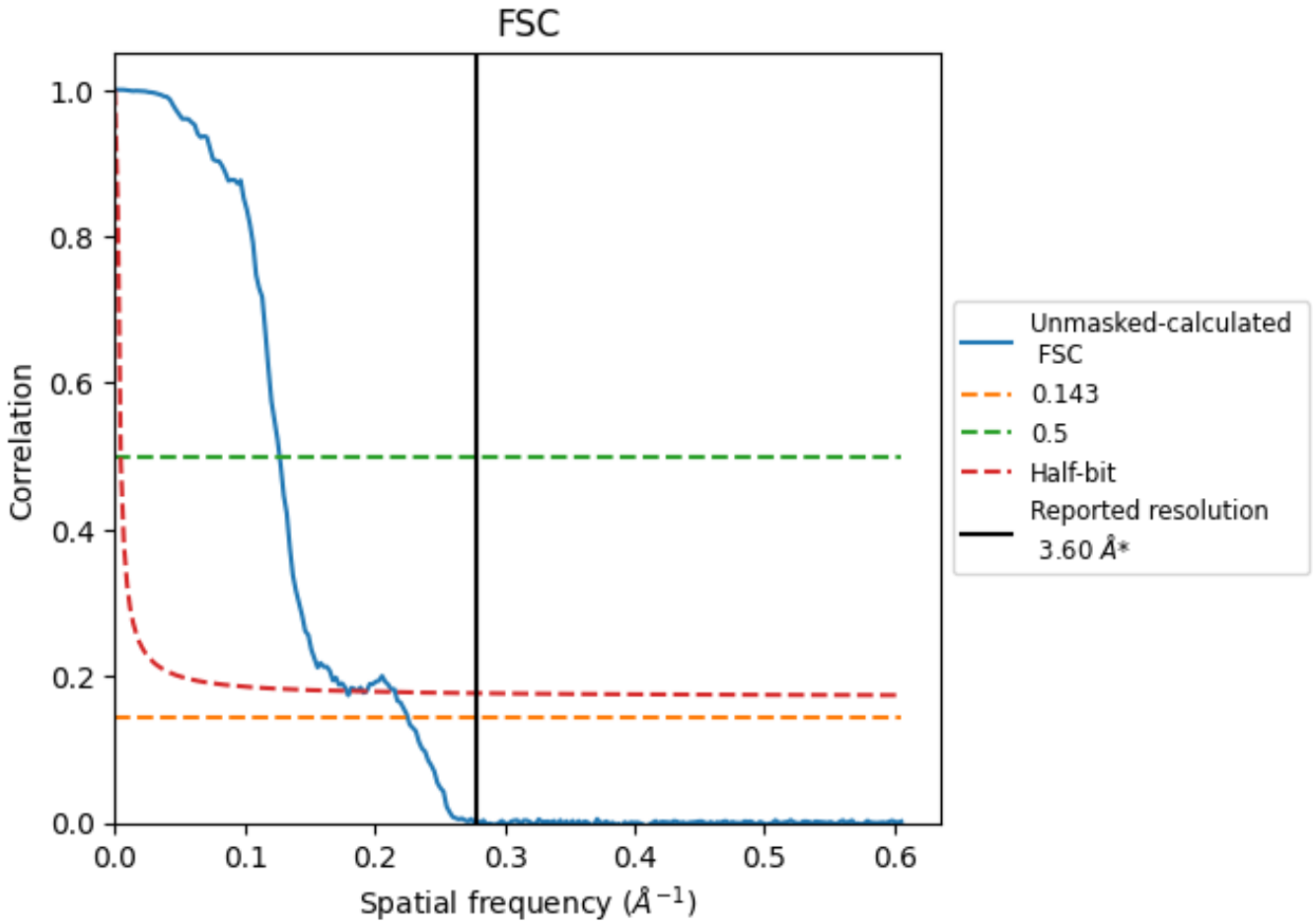


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

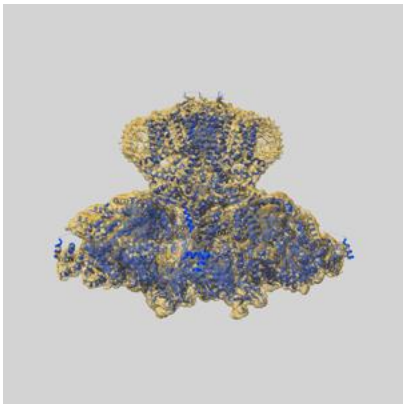
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.43	7.89	5.61

*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 4.43 differs from the reported value 3.6 by more than 10 %

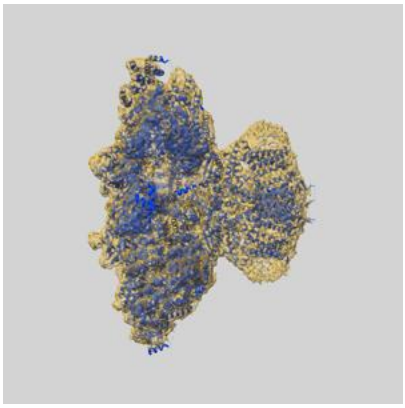
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41352 and PDB model 8TKI. Per-residue inclusion information can be found in section 3 on page 6.

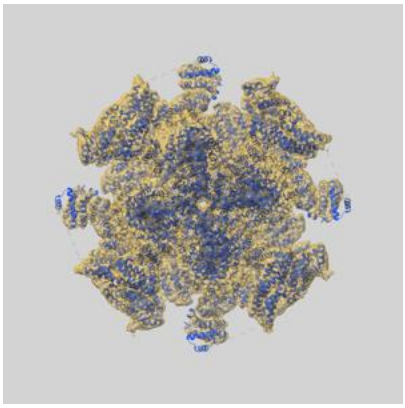
9.1 Map-model overlay



X



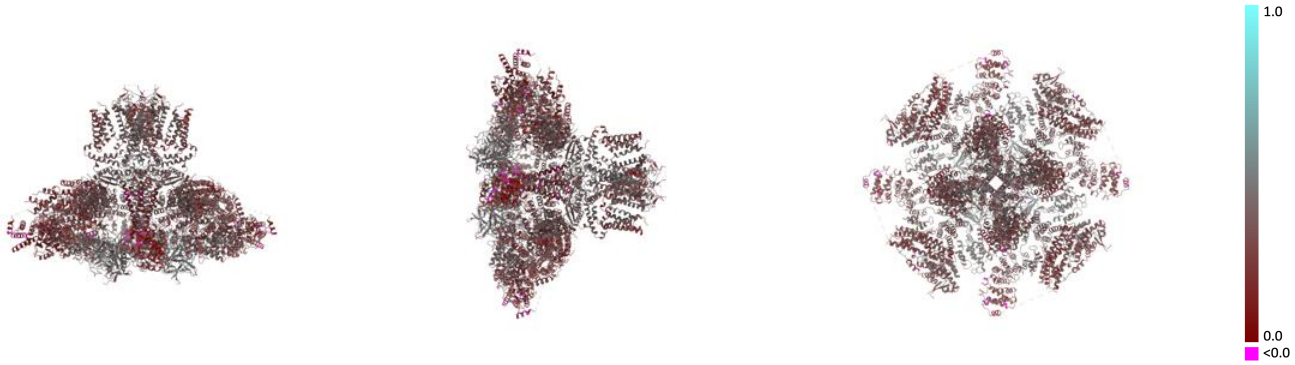
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

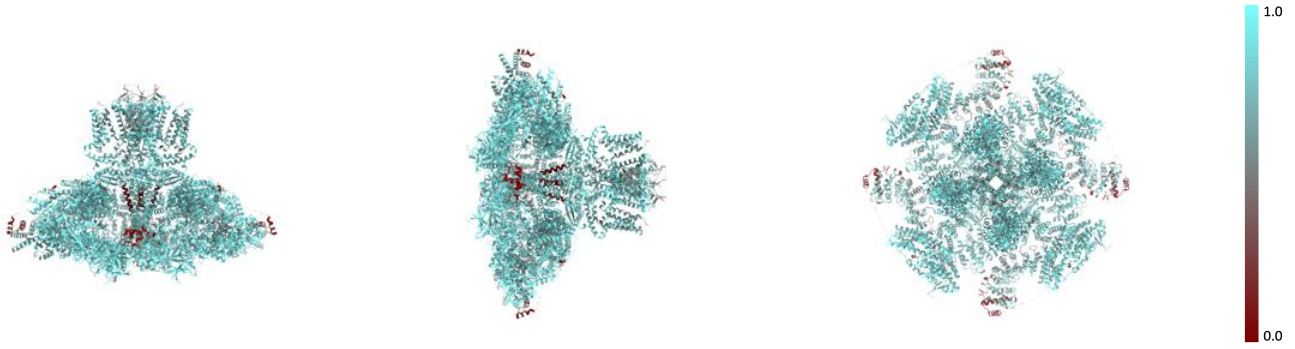
9.2 Q-score mapped to coordinate model



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.

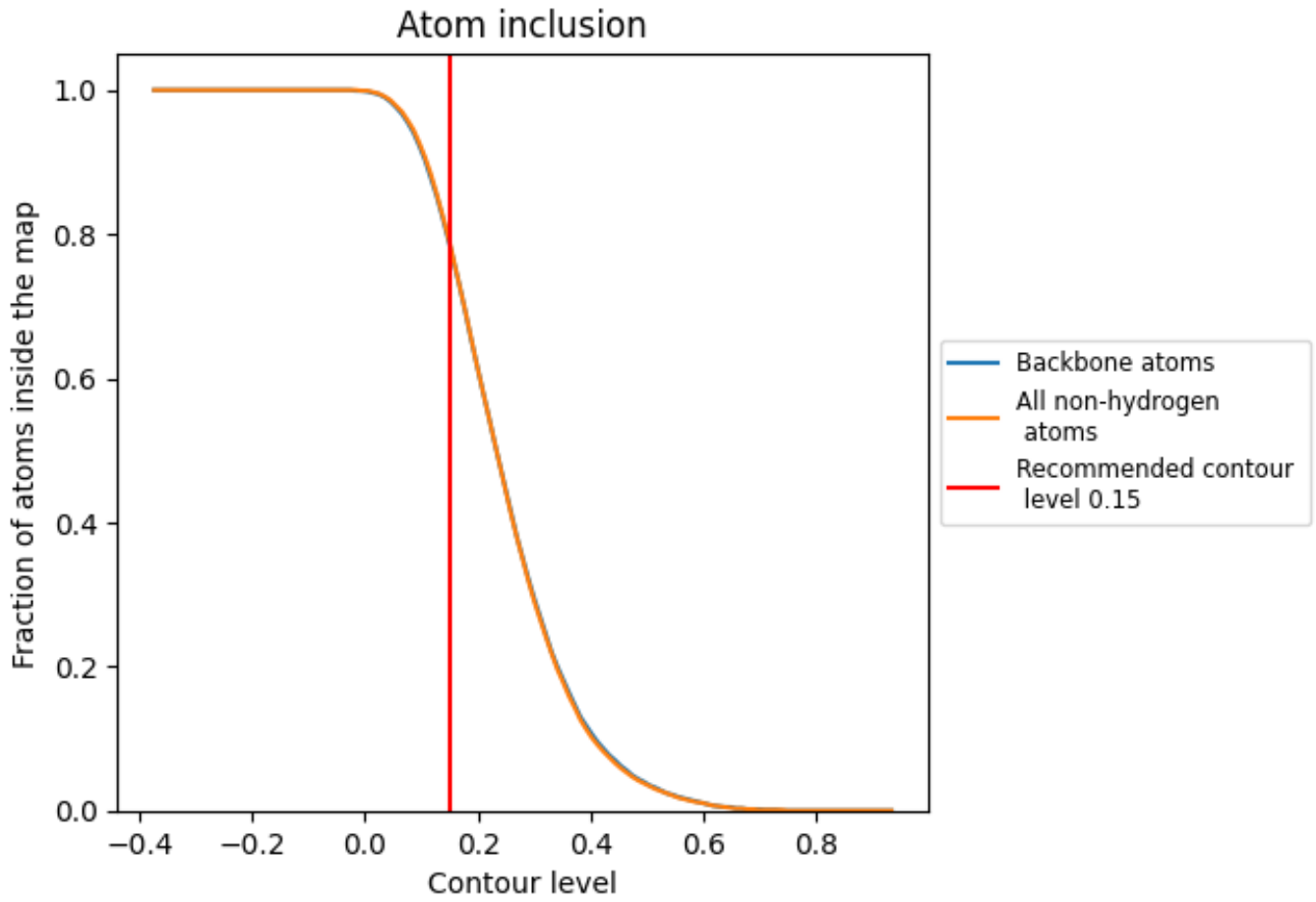
9.3 Atom inclusion mapped to coordinate model



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 79% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7880	0.3370
A	0.7970	0.3410
B	0.7900	0.3330
C	0.7970	0.3410
D	0.7890	0.3340