wwPDB EM Validation Summary Report ⓘ

Oct 20, 2024 – 06:18 PM EDT

PDB ID	:	7T3T
EMDB ID	:	EMD-25670
Title	:	IP3, ATP, and Ca2+ bound type 3 IP3 receptor in the active state
Authors	:	Schmitz, E.A.; Takahashi, H.; Karakas, E.
Deposited on	:	2021-12-08
Resolution	:	3.80 Å(reported)
Based on initial model	:	6UQK

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:

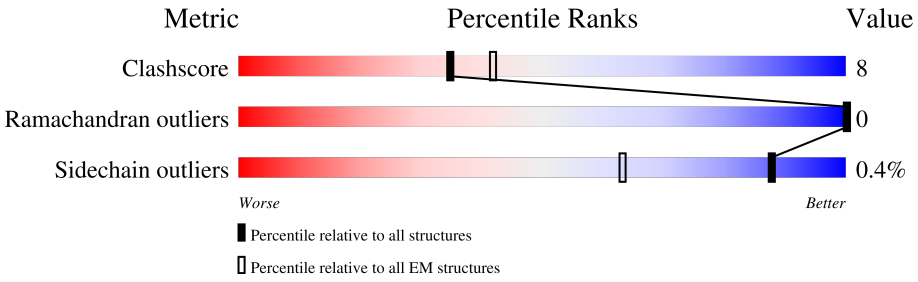
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2633	65% 15% 19%
1	B	2633	66% 15% 19%
1	C	2633	65% 15% 19%
1	D	2633	65% 15% 19%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 68516 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.

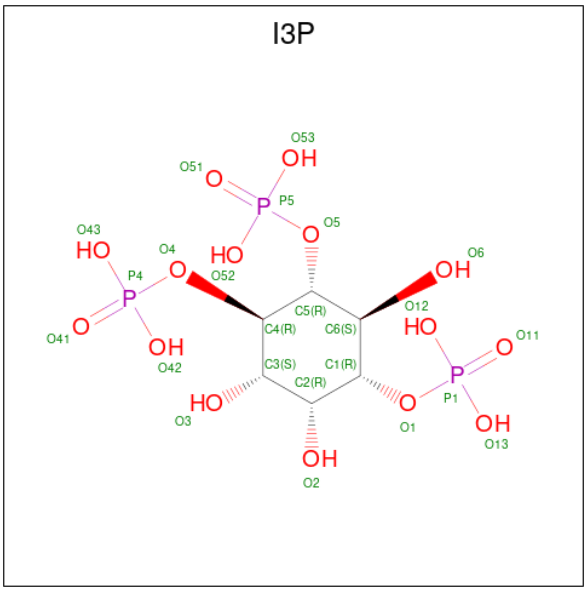
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2121	Total 17072	C 10908	N 2923	O 3138	S 103	0	0
1	B	2121	Total 17072	C 10908	N 2923	O 3138	S 103	0	0
1	C	2121	Total 17072	C 10908	N 2923	O 3138	S 103	0	0
1	D	2121	Total 17072	C 10908	N 2923	O 3138	S 103	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

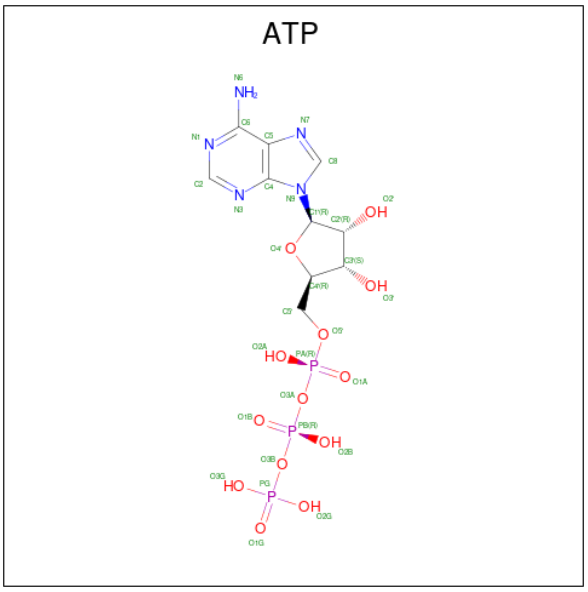
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0

- 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	O	P	0
			24	6	15	3	
3	B	1	Total	C	O	P	0
			24	6	15	3	
3	C	1	Total	C	O	P	0
			24	6	15	3	
3	D	1	Total	C	O	P	0
			24	6	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	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

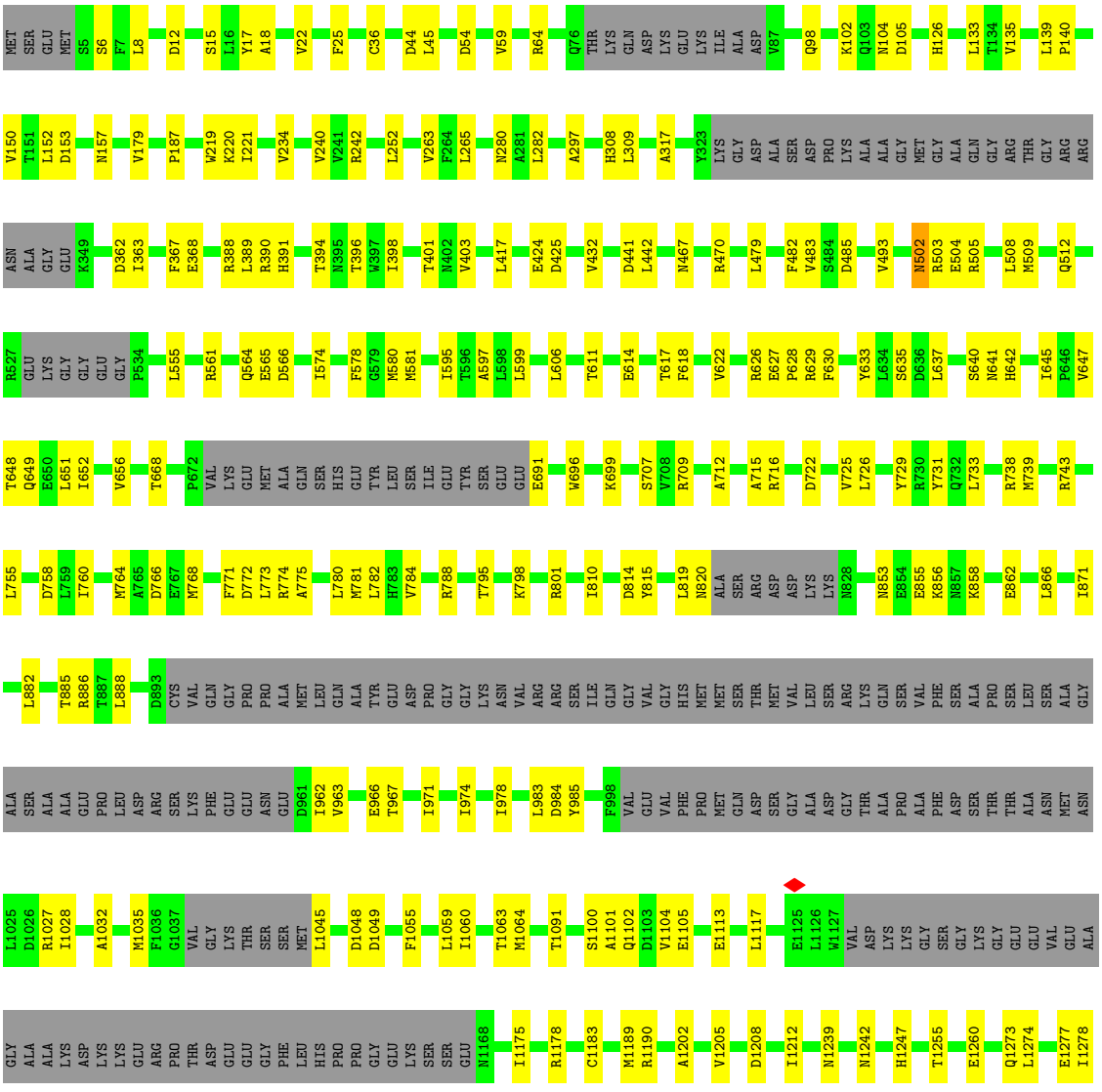
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

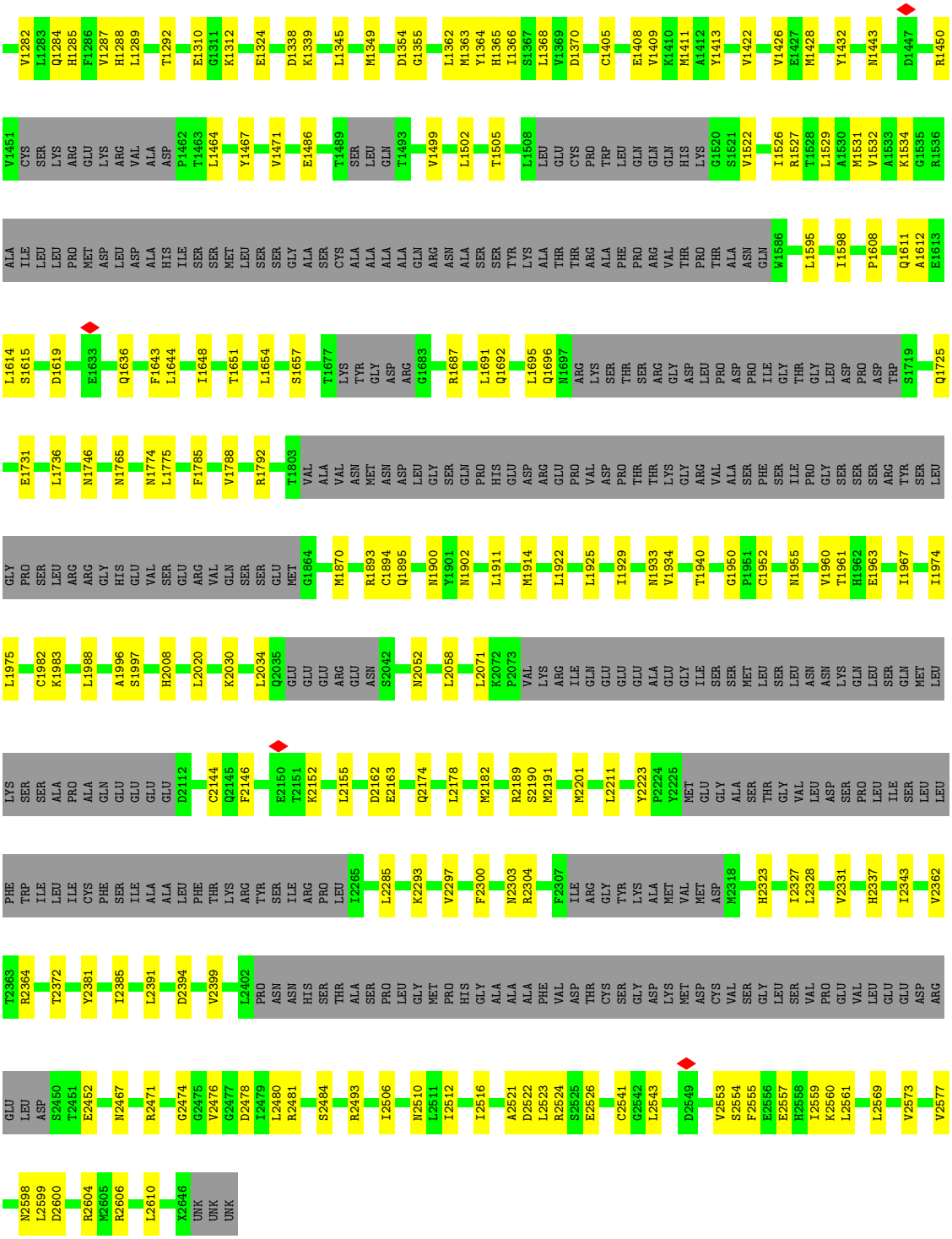
3 Residue-property plots (i)

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

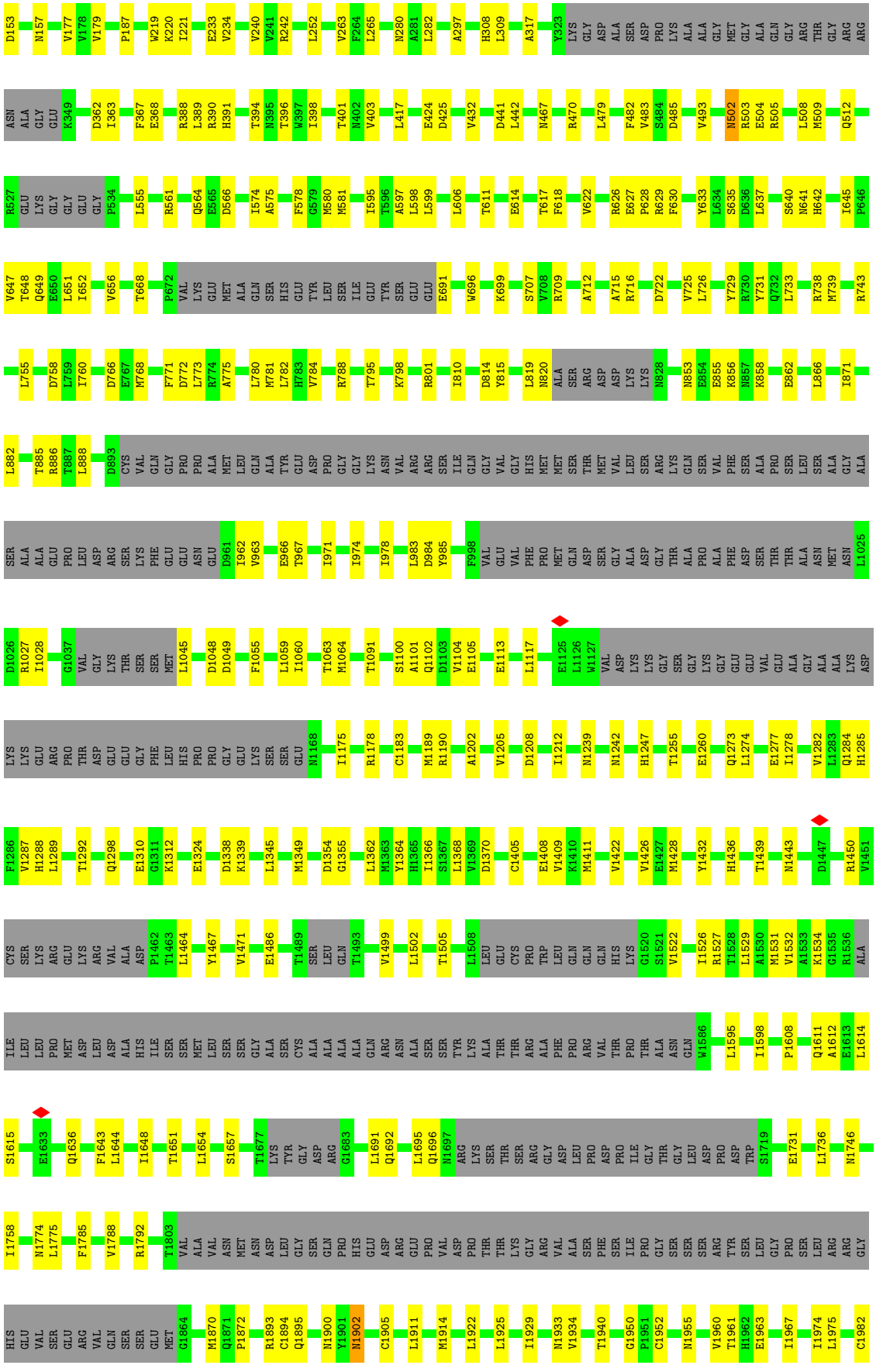
Chain A:

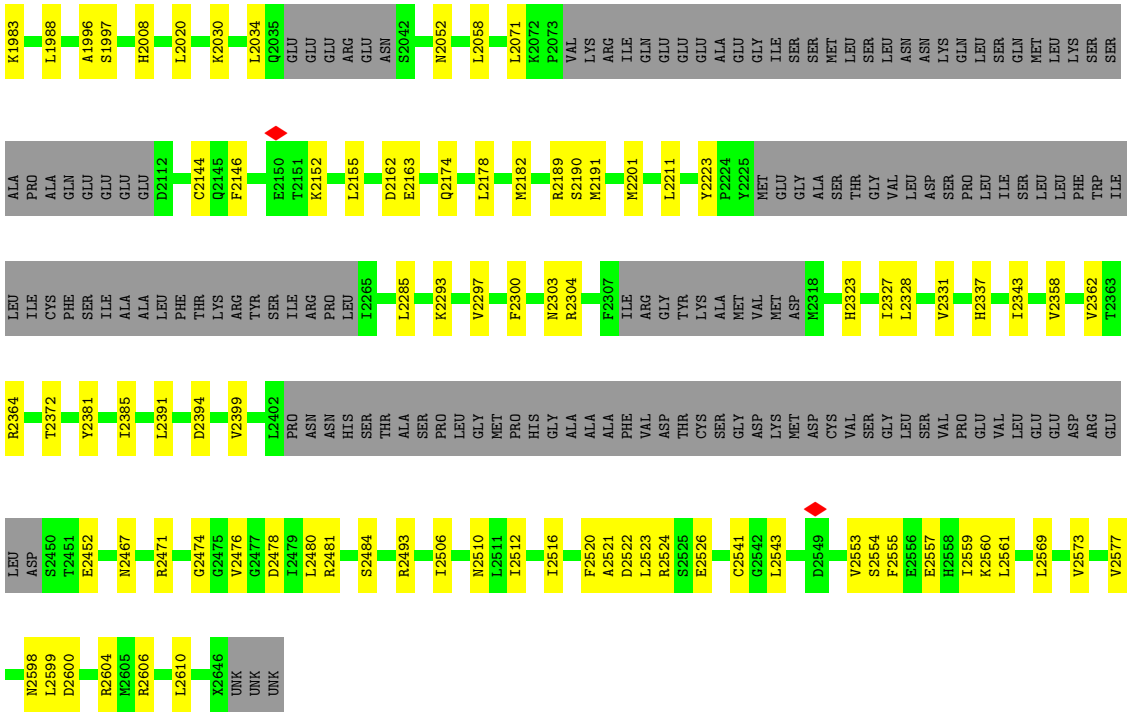




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

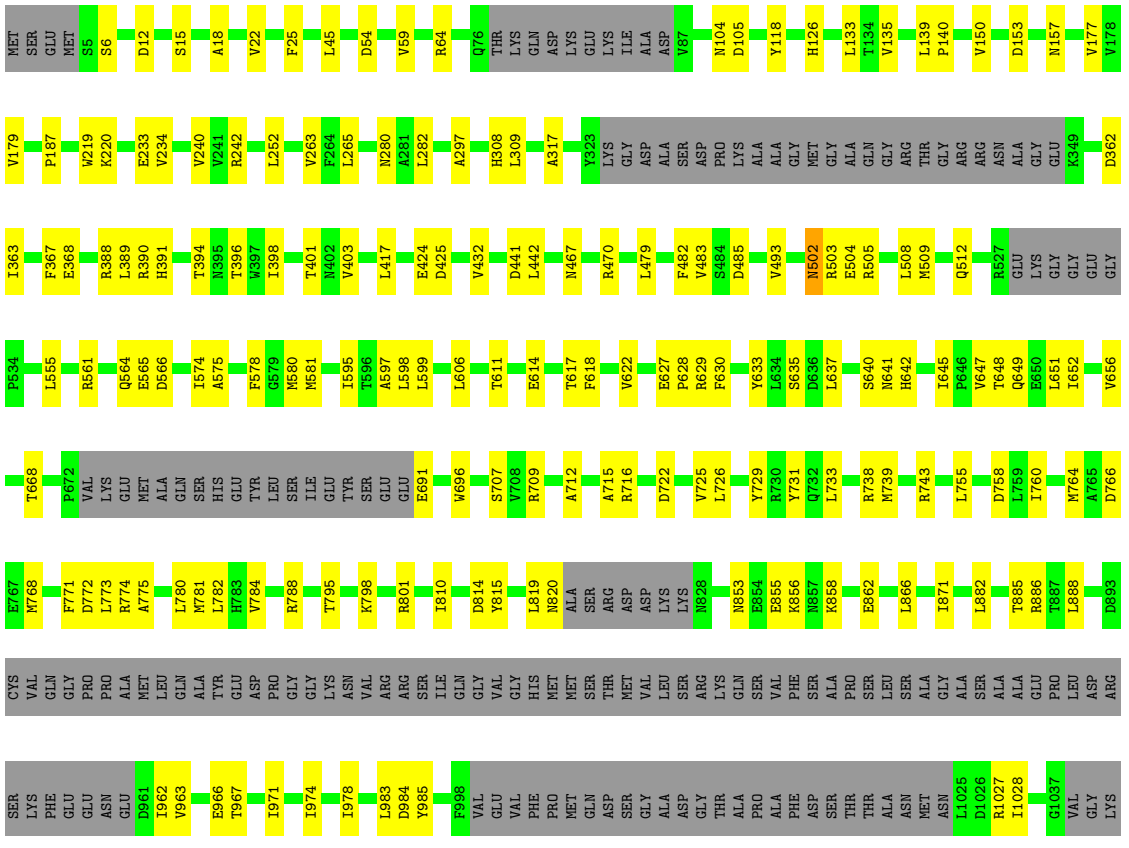
Chain B:

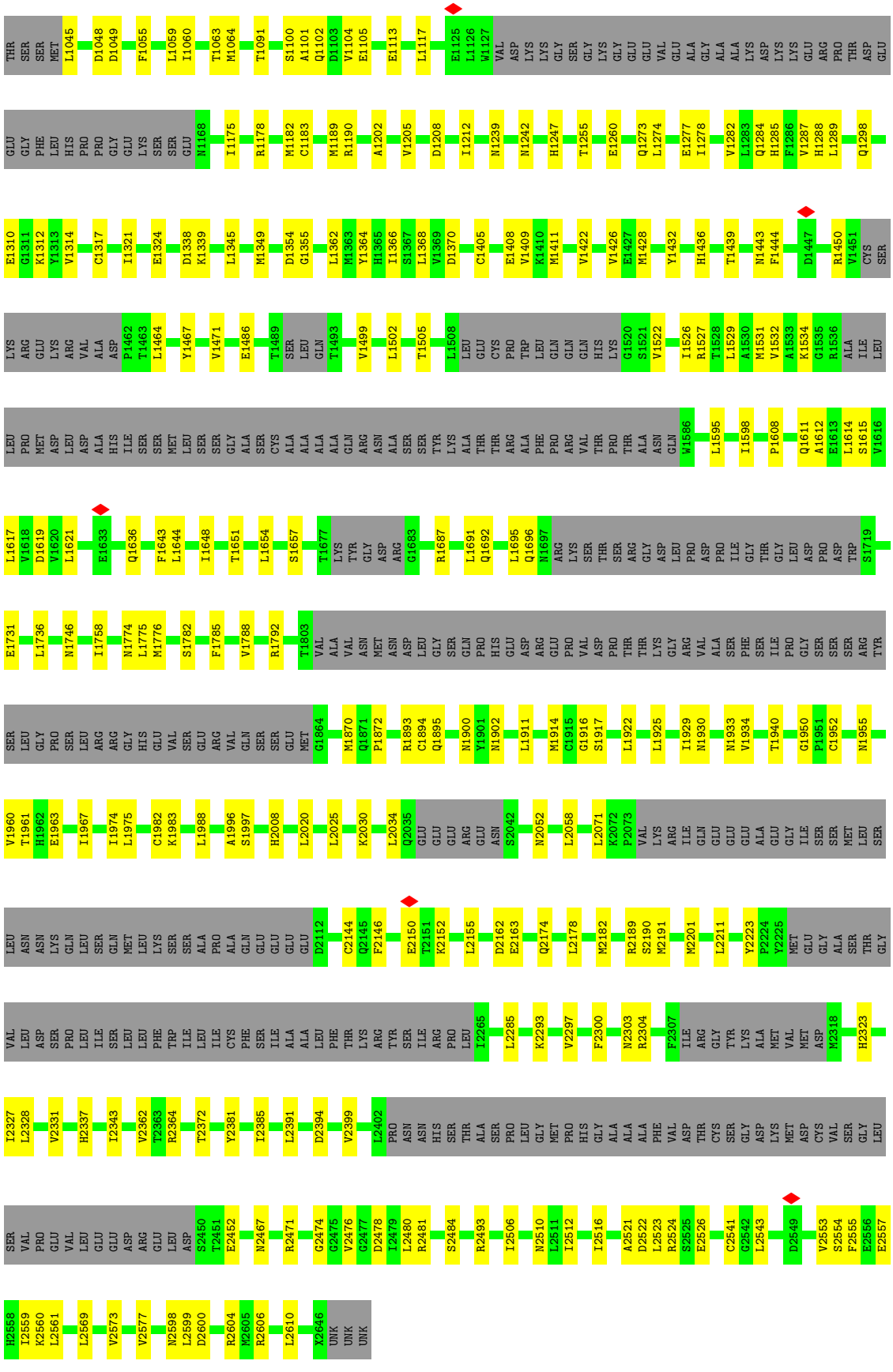

D153 N157 V177 V178 V179 P187 W219 K220 I221 E233 V234 V240 V241 R242 L252 V263 F264 L265 N280 A281 L282 A297 H308 L309 A317 Y323
ASN ALA GLY GLU K349 D362 I363 F367 E368 R388 L389 R390 H391 T394 N395 T396 W397 I398 T401 N402 V403 L417 L598 L599 E424 D425 V432 D441 L442 N467 R470 L479 F482 V483 S484 D485 V493 N502 R503 E504 R505 L508 M509 Q512
R527 GLU LYS GLY GLU GLY P534 L555 R561 Q564 E565 D566 I574 A575 F578 G579 M580 M581 I595 T596 A597 L606 T611 E614 T617 F618 V622 R626 E627 P628 R629 F630 Y633 L634 S635 D636 L637 S640 N641 H642 I645 P646
V647 T648 Q649 E650 L651 I652 V656 T668 P672 VAL LYS GLU MET ALA GLN SER HIS GLU TYR LEU SER ILE GLU TYR SER GLU GLU E691 W696 K699 S707 V708 R709 A712 A715 R716 D722 V725 L726 Y729 R730 Y731 Q732 L733 R738 M739 R743
L755 D758 L759 I760 D766 E767 M768 F771 D772 L773 R774 A775 L780 M781 L782 H783 V784 R788 T795 K798 R801 I810 D814 Y815 L819 N820 ALA SER ARG ASP ASP LYS LYS N828 N853 E854 E855 K856 N857 K858 E862 L866 I871
L882 T885 R886 T887 L888 D893 CYS VAL 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 THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA
SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 I962 V963 E966 T967 I971 I974 I978 L983 D984 Y985 F998 VAL GLU GLU VAL PHE PRO MET GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA ALA ASN MET ASN L1025
D1026 R1027 I1028 G1037 VAL GLY LYS THR SER SER MET L1045 D1048 D1049 F1055 L1059 I1060 T1063 M1064 T1091 S1100 A1101 Q1102 D1103 V1104 E1105 E1113 L1117 E1125 L1126 W1127 VAL 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 SER GLU N1168 I1175 R1178 C1183 M1189 R1190 A1202 V1205 D1208 I1212 N1239 N1242 H1247 T1255 E1260 Q1273 L1274 E1277 I1278 V1282 L1283 Q1284 H1285
F1286 V1287 H1288 L1289 T1292 Q1298 E1310 G1311 K1312 E1324 D1338 K1339 L1345 M1349 D1354 G1355 L1362 M1363 Y1364 H1365 I1366 S1367 L1368 V1369 D1370 C1405 E1408 V1409 K1410 M1411 V1422 V1426 E1427 M1428 Y1432 H1436 T1439 N1443 D1447 R1450 V1451
CYS SER LYS ARG GLU LYS ARG VAL ALA ASP P1462 T1463 L1464 Y1467 V1471 E1486 T1489 SER LEU GLN T1493 V1499 L1502 T1505 L1508 LEU GLU CYS PRO TRP LEU GLN GLN GLN HIS LYS G1520 S1521 V1522 I1526 R1527 T1528 L1529 A1530 M1531 V1532 A1533 K1534 G1535 R1536 ALA
ILE LEU LEU PRO MET ASP LEU ASP ALA HIS ILE SER SER MET LEU SER 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 L1595 I1598 P1608 Q1611 A1612 E1613 L1614
S1615 E1633 Q1636 F1643 L1644 I1648 T1651 L1654 S1657 T1677 LYS TYR GLY ASP ARG G1683 L1691 Q1692 L1695 Q1696 N1697 ARG LYS SER THR THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO ASP TRP S1719 E1731 L1736 N1746
I1758 N1774 L1775 F1785 V1788 R1792 T1803 VAL ALA VAL ASN MET ASN ASP LEU GLY SER GLN PRO HIS GLU ASP ARG GLU PRO VAL ASP PRO THR THR LYS GLY ARG 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 GLU MET G1864 M1870 Q1871 P1872 R1893 C1894 Q1895 N1900 Y1901 N1902 C1905 L1911 M1914 L1922 L1925 I1929 N1933 V1934 T1940 G1950 P1951 C1952 N1955 V1960 T1961 H1962 E1963 I1967 I1974 L1975 C1982



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

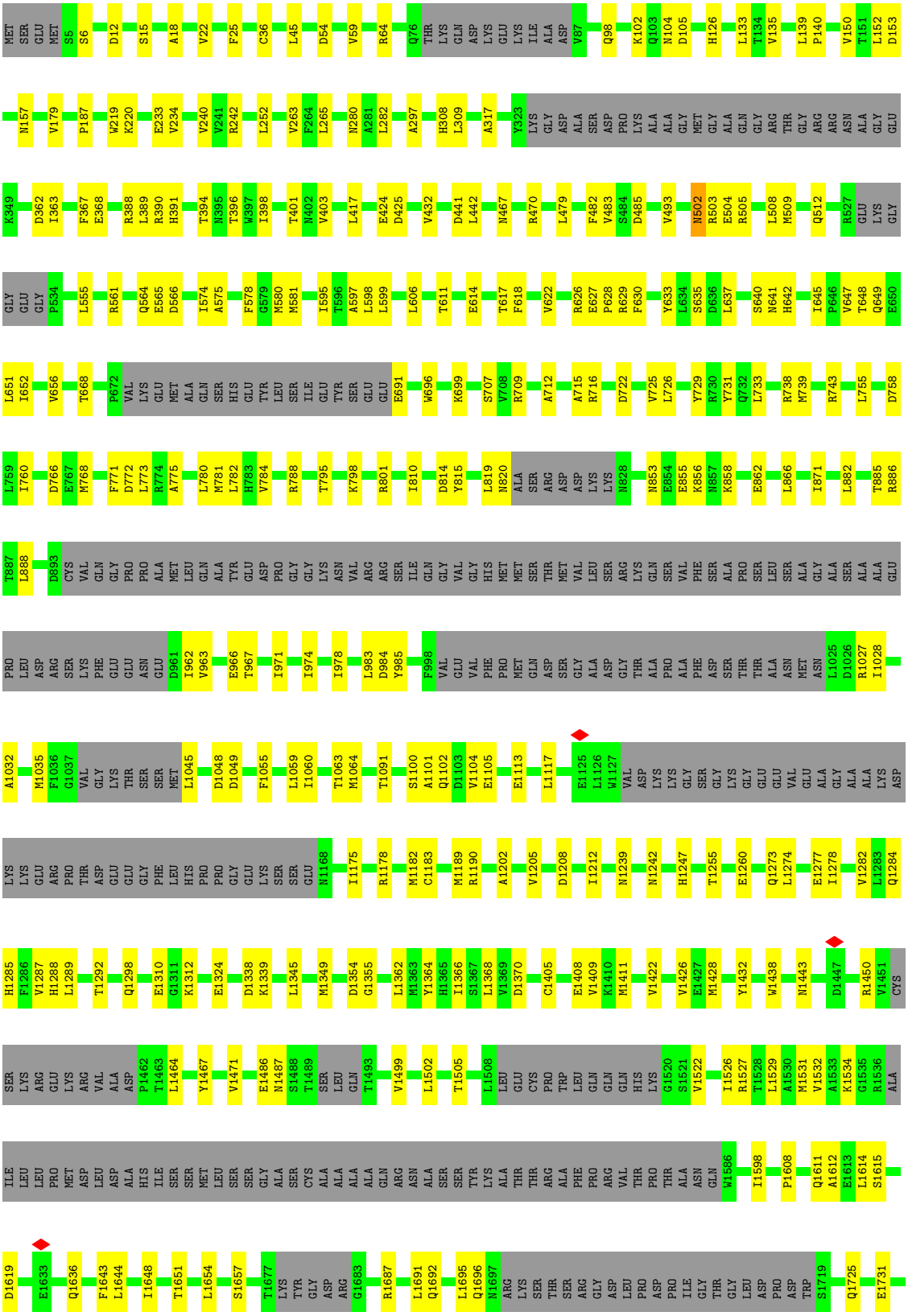
Chain C:

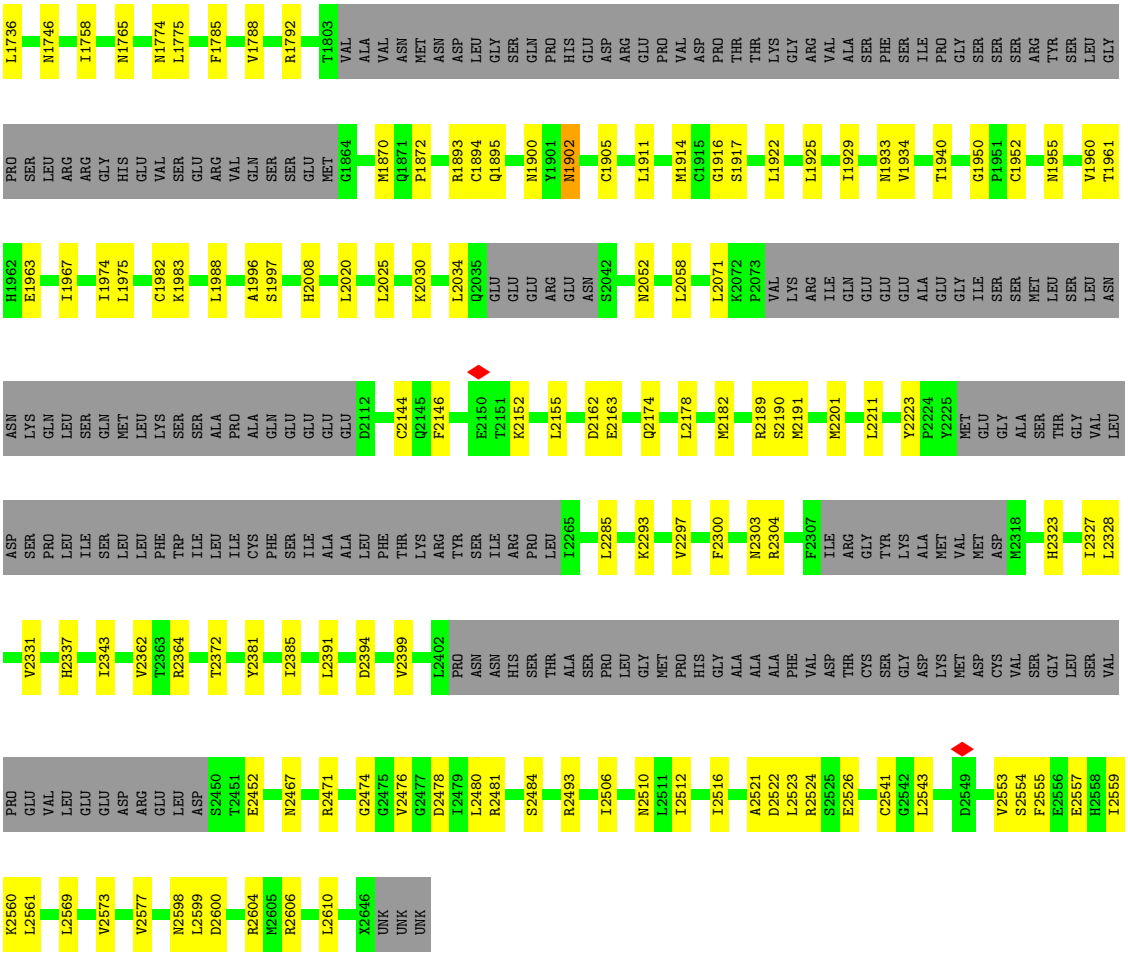




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain D:




L1736 N1746 I1758 N1765 N1774 L1775 F1785 V1788 R1792 T1803 VAL ALA VAL ASN MET ASN ASP LEU GLY SER GLN PRO HIS GLU ASP ARG GLU PRO VAL ASP PRO THR THR LYS GLY ARG 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 GLU MET G1864 M1870 Q1871 P1872 R1893 C1894 Q1895 N1900 Y1901 N1902 C1905 L1911 M1914 C1915 G1916 S1917 L1922 L1925 I1929 N1933 V1934 T1940 G1950 P1951 C1952 N1955 V1960 T1961
H1962 E1963 I1967 I1974 L1975 C1982 K1983 L1988 A1996 S1997 H2008 L2020 L2025 K2030 L2034 Q2035 GLU GLU GLU ARG GLU ASN S2042 N2052 L2058 L2071 K2072 P2073 VAL 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 GLU D2112 C2144 Q2145 F2146 E2150 T2151 K2152 L2155 D2162 E2163 Q2174 L2178 M2182 R2189 S2190 M2191 M2201 L2211 Y2223 P2224 Y2225 MET 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 SER ILE ARG PRO LEU I2265 L2285 K2293 V2297 F2300 N2303 R2304 F2307 ILE ARG GLY TYR LYS ALA MET VAL MET ASP M2318 H2323 I2327 L2328
V2331 H2337 I2343 V2362 T2363 R2364 T2372 Y2381 I2385 L2391 D2394 V2399 L2402 PRO 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 GLU GLU ASP ARG GLU LEU ASP S2450 T2451 E2452 N2467 R2471 G2474 C2475 V2476 G2477 D2478 I2479 L2480 R2481 S2484 R2493 I2506 N2510 L2511 I2512 I2516 A2521 D2522 L2523 R2524 S2525 E2526 C2541 G2542 L2543 D2549 V2553 S2554 F2555 E2556 E2557 H2558 I2559
K2560 L2561 L2569 V2573 V2577 N2598 L2599 D2600 R2604 M2605 R2606 L2610 X2646 UNK UNK UNK

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20039	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.560	Depositor
Minimum map value	-0.794	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	397.44, 397.44, 397.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/17287	0.47	1/23345 (0.0%)
1	B	0.26	0/17287	0.47	1/23345 (0.0%)
1	C	0.26	0/17287	0.47	1/23345 (0.0%)
1	D	0.26	0/17287	0.47	1/23345 (0.0%)
All	All	0.26	0/69148	0.47	4/93380 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1370	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	1370	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	1370	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	1370	ASP	CB-CG-OD2	5.19	122.97	118.30

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	17072	0	17103	269	0
1	B	17072	0	17103	269	0
1	C	17072	0	17103	274	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	17072	0	17103	269	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	0	9	0	0
3	B	24	0	9	0	0
3	C	24	0	9	0	0
3	D	24	0	9	0	0
4	A	31	0	12	3	0
4	B	31	0	12	3	0
4	C	31	0	12	3	0
4	D	31	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	68516	0	68496	1065	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 8.

The worst 5 of 1065 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:B:240:VAL:HG11	1:B:309:LEU:HD11	1.51	0.91
1:D:240:VAL:HG11	1:D:309:LEU:HD11	1.51	0.91
1:C:240:VAL:HG11	1:C:309:LEU:HD11	1.51	0.90
1:A:240:VAL:HG11	1:A:309:LEU:HD11	1.51	0.88
1:C:712:ALA:HB1	1:C:716:ARG:HH12	1.42	0.85

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	2058/2633 (78%)	1969 (96%)	89 (4%)	0	100	100
1	B	2058/2633 (78%)	1969 (96%)	89 (4%)	0	100	100
1	C	2058/2633 (78%)	1969 (96%)	89 (4%)	0	100	100
1	D	2058/2633 (78%)	1969 (96%)	89 (4%)	0	100	100
All	All	8232/10532 (78%)	7876 (96%)	356 (4%)	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	1899/2329 (82%)	1892 (100%)	7 (0%)	89	91
1	B	1899/2329 (82%)	1892 (100%)	7 (0%)	89	91
1	C	1899/2329 (82%)	1892 (100%)	7 (0%)	89	91
1	D	1899/2329 (82%)	1892 (100%)	7 (0%)	89	91
All	All	7596/9316 (82%)	7568 (100%)	28 (0%)	88	91

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	502	ASN
1	D	1902	ASN
1	C	1450	ARG
1	D	1450	ARG
1	C	1443	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1933	ASN
1	C	1746	ASN
1	D	1933	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	I3P	D	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.81	3 (7%)
4	ATP	C	2703	-	28,33,33	0.67	0	34,52,52	0.92	1 (2%)
3	I3P	A	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.81	2 (5%)
3	I3P	B	2702	-	24,24,24	1.29	3 (12%)	39,39,39	0.81	2 (5%)
3	I3P	C	2702	-	24,24,24	1.29	3 (12%)	39,39,39	0.81	2 (5%)
4	ATP	D	2703	-	28,33,33	0.67	0	34,52,52	0.92	1 (2%)
4	ATP	A	2703	-	28,33,33	0.67	0	34,52,52	0.92	1 (2%)
4	ATP	B	2703	-	28,33,33	0.66	0	34,52,52	0.92	1 (2%)

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	D	2702	-	-	4/15/39/39	0/1/1/1
4	ATP	C	2703	-	-	5/18/38/38	0/3/3/3
3	I3P	A	2702	-	-	4/15/39/39	0/1/1/1
3	I3P	B	2702	-	-	4/15/39/39	0/1/1/1
3	I3P	C	2702	-	-	4/15/39/39	0/1/1/1
4	ATP	D	2703	-	-	5/18/38/38	0/3/3/3
4	ATP	A	2703	-	-	5/18/38/38	0/3/3/3
4	ATP	B	2703	-	-	5/18/38/38	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	2702	I3P	P1-O1	3.15	1.65	1.59
3	A	2702	I3P	P1-O1	3.11	1.65	1.59
3	C	2702	I3P	P1-O1	3.11	1.65	1.59
3	D	2702	I3P	P1-O1	3.08	1.64	1.59
3	C	2702	I3P	P4-O4	3.07	1.64	1.59

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2703	ATP	C5-C6-N6	2.25	123.74	120.31
4	B	2703	ATP	C5-C6-N6	2.25	123.74	120.31
4	C	2703	ATP	C5-C6-N6	2.25	123.74	120.31
4	D	2703	ATP	C5-C6-N6	2.25	123.74	120.31
3	D	2702	I3P	P5-O5-C5	-2.08	117.88	123.43

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2703	ATP	C5'-O5'-PA-O3A
4	B	2703	ATP	C5'-O5'-PA-O3A
4	C	2703	ATP	C5'-O5'-PA-O3A
4	D	2703	ATP	C5'-O5'-PA-O3A
4	A	2703	ATP	O4'-C4'-C5'-O5'

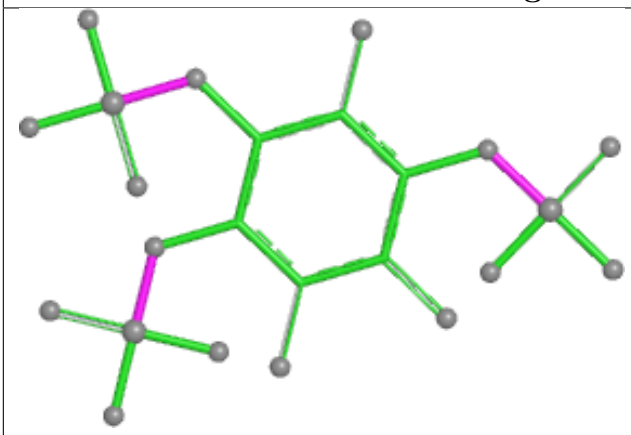
There are no ring outliers.

4 monomers are involved in 11 short contacts:

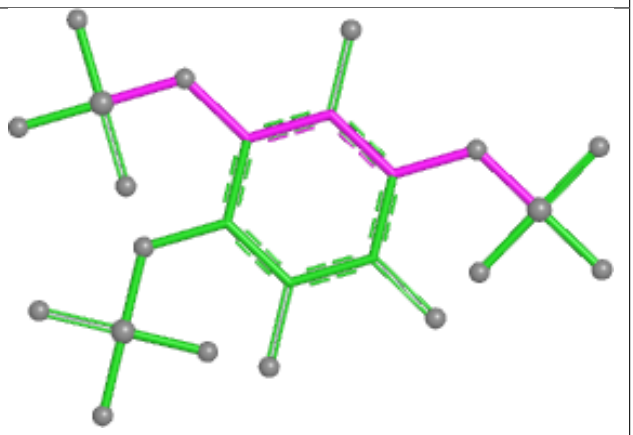
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2703	ATP	3	0
4	D	2703	ATP	2	0
4	A	2703	ATP	3	0
4	B	2703	ATP	3	0

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.

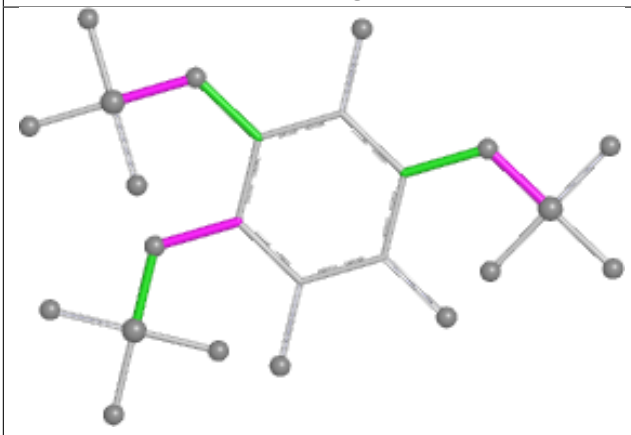
Ligand I3P D 2702



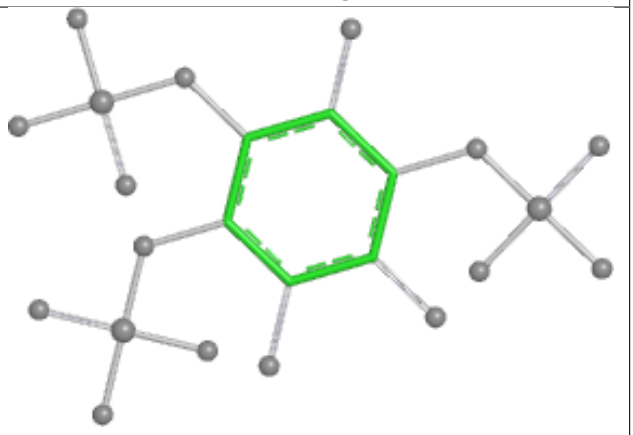
Bond lengths



Bond angles

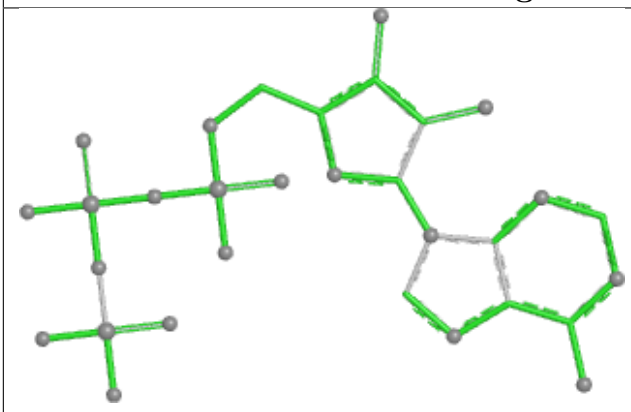


Torsions

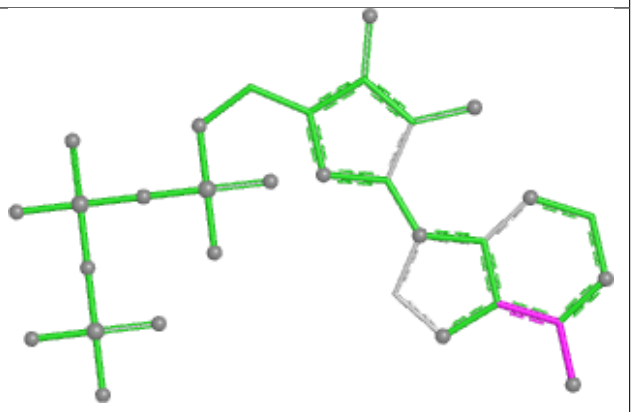


Rings

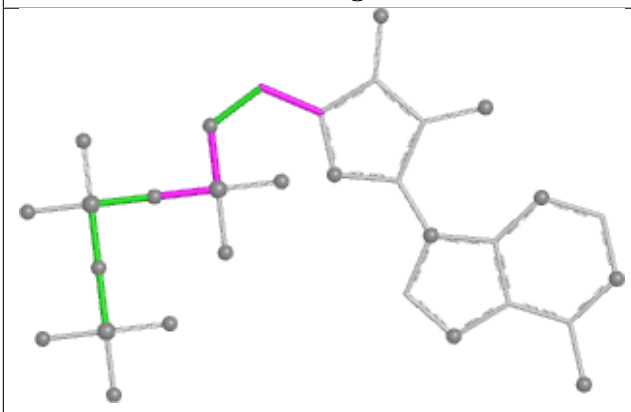
Ligand ATP C 2703



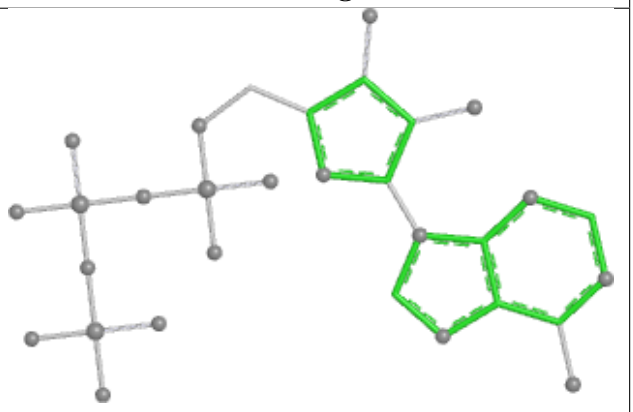
Bond lengths



Bond angles

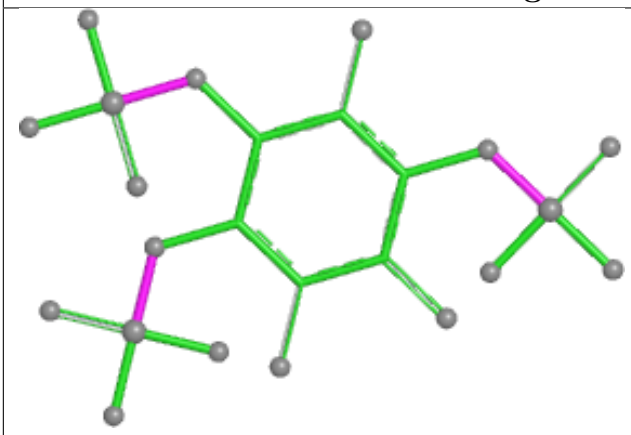


Torsions

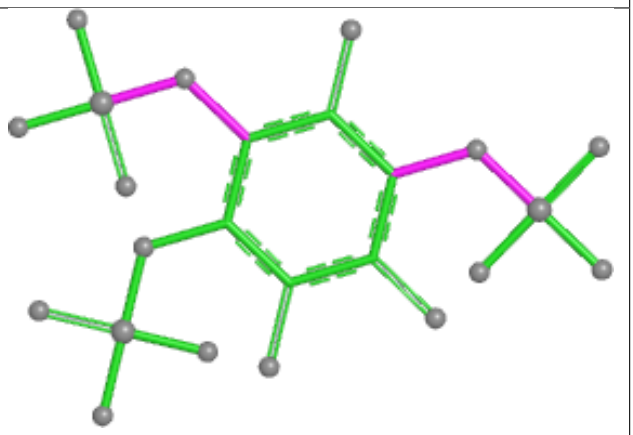


Rings

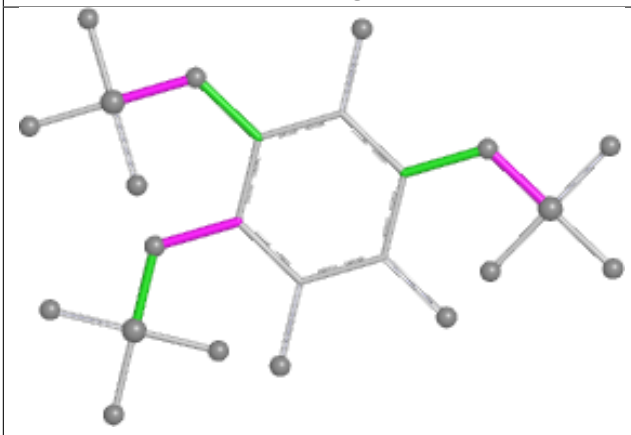
Ligand I3P A 2702



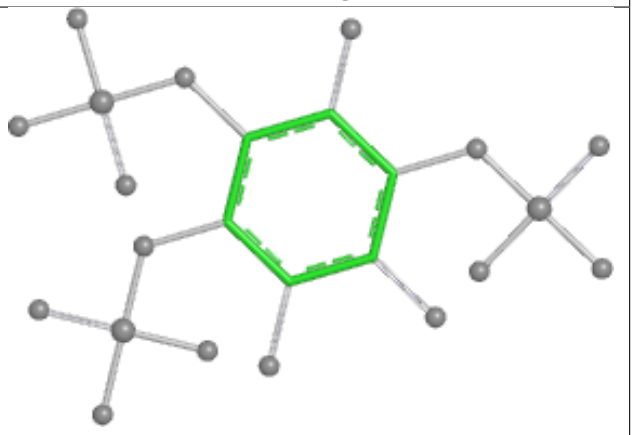
Bond lengths



Bond angles

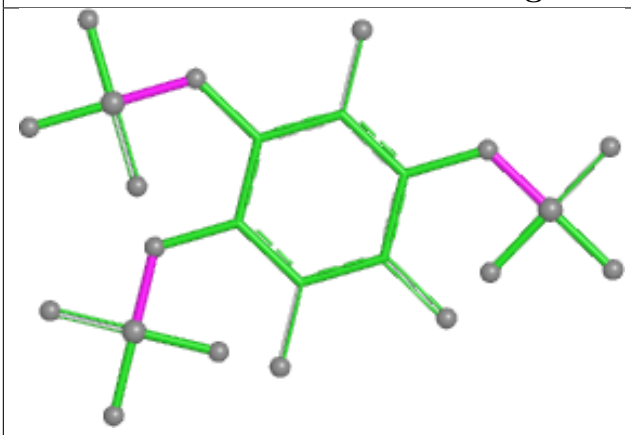


Torsions



Rings

Ligand I3P B 2702



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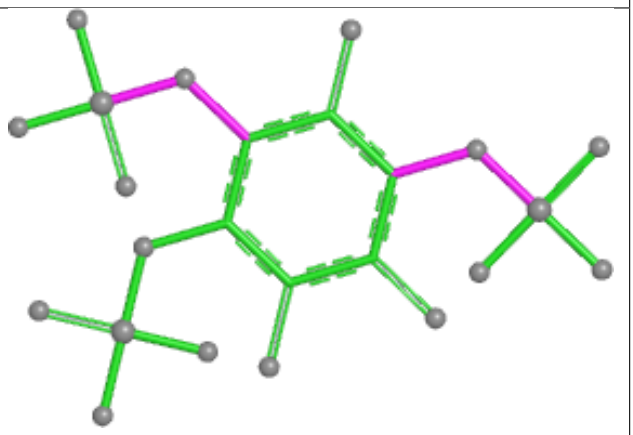
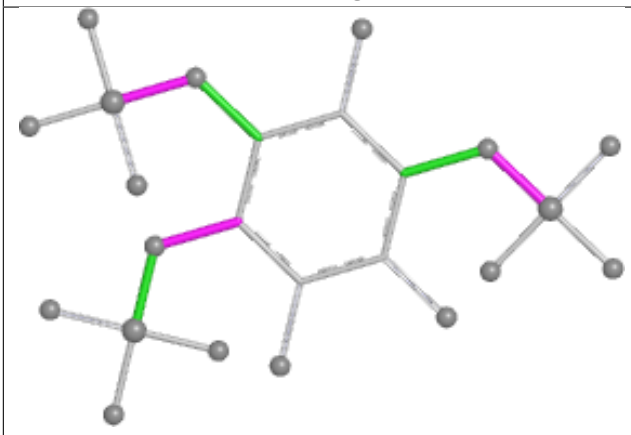
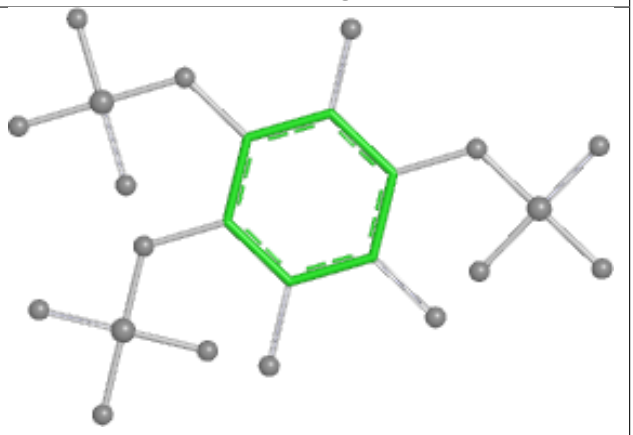


Bond angles

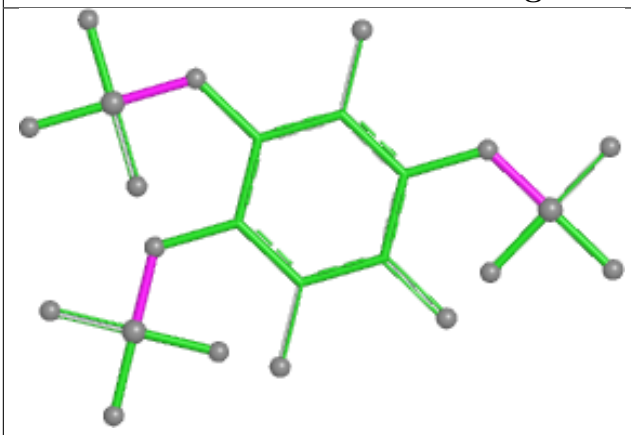


Torsions



Rings

Ligand I3P C 2702



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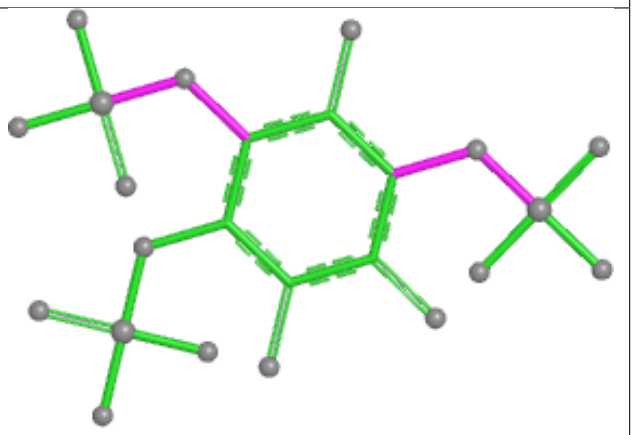
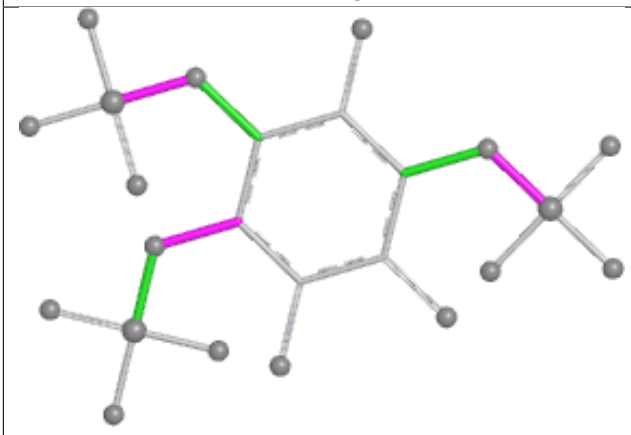


Bond angles



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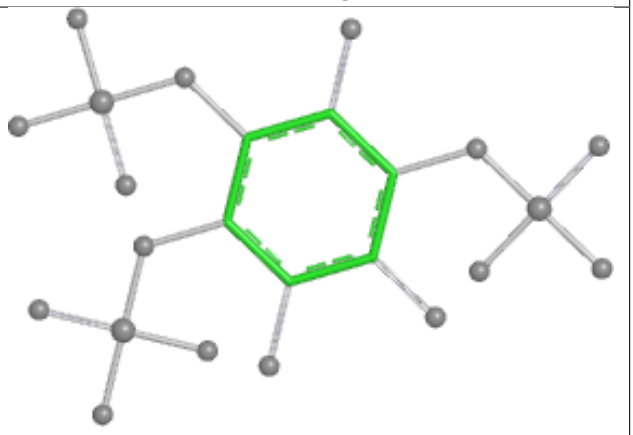
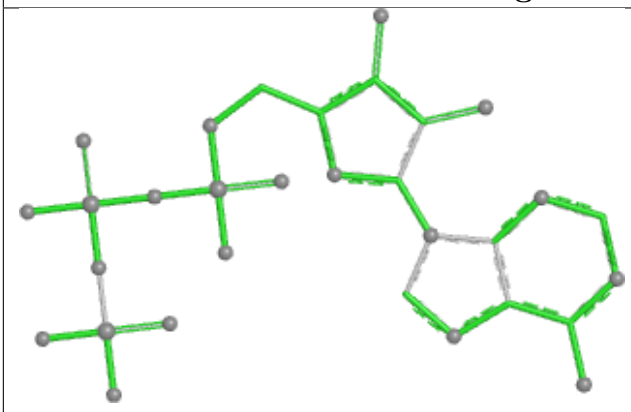
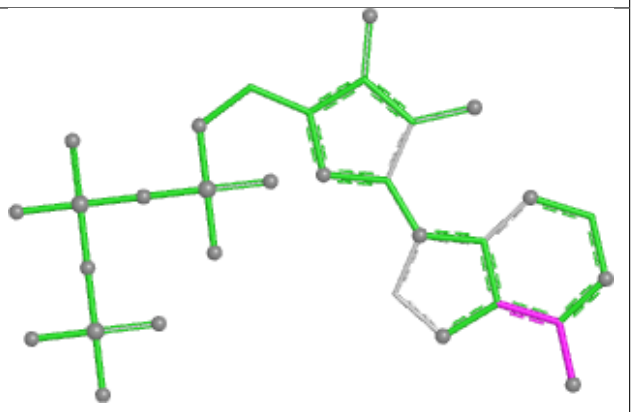


Rings

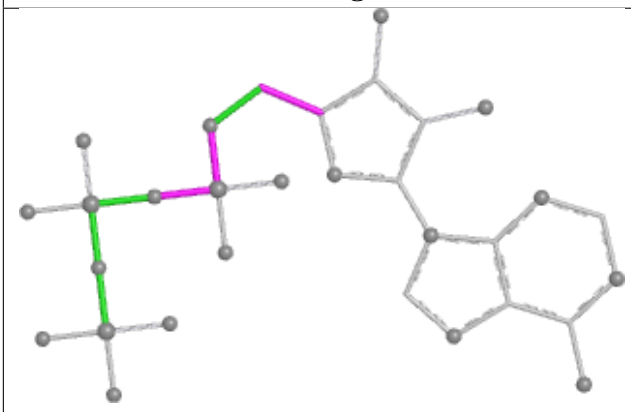
Ligand ATP D 2703



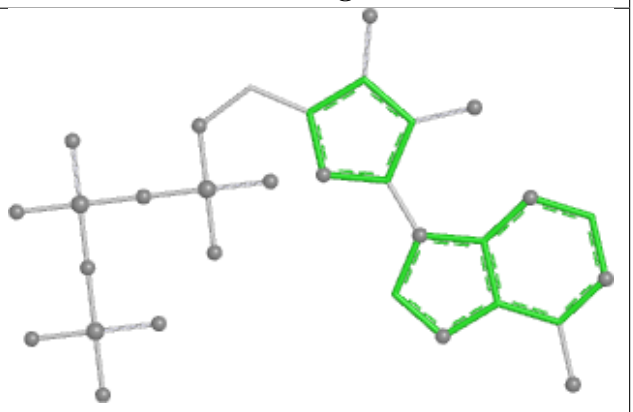
Bond lengths



Bond angles

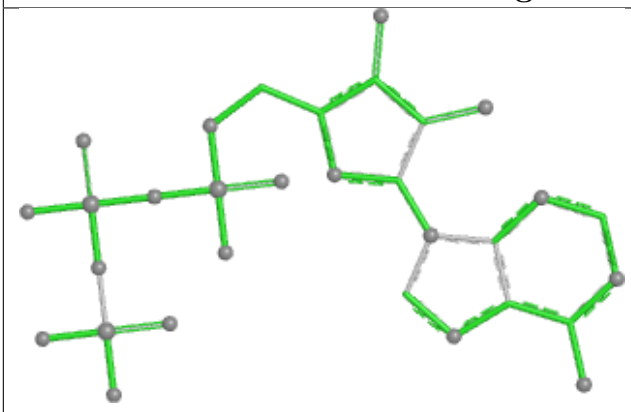


Torsions



Rings

Ligand ATP A 2703



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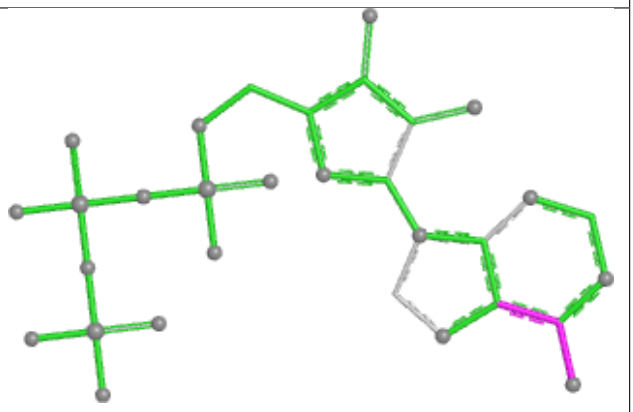
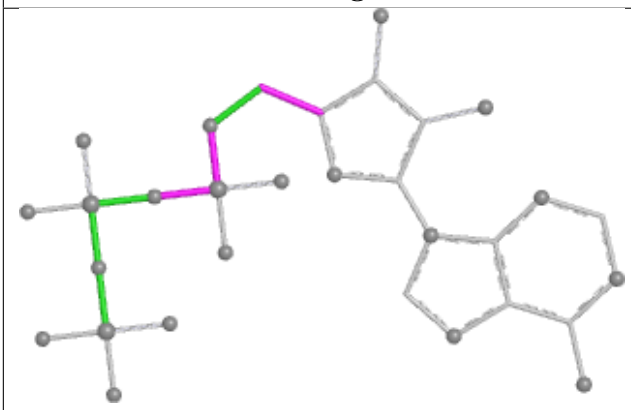
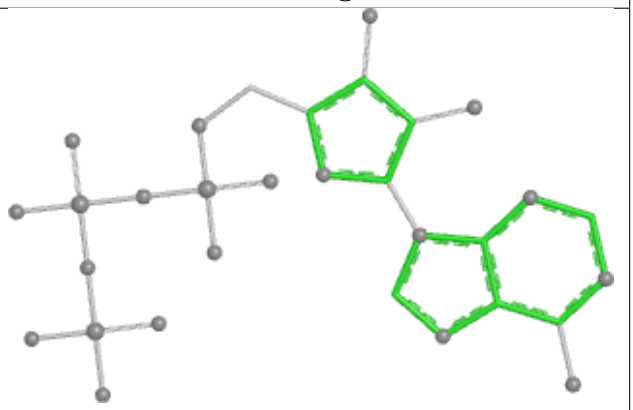


Bond angles

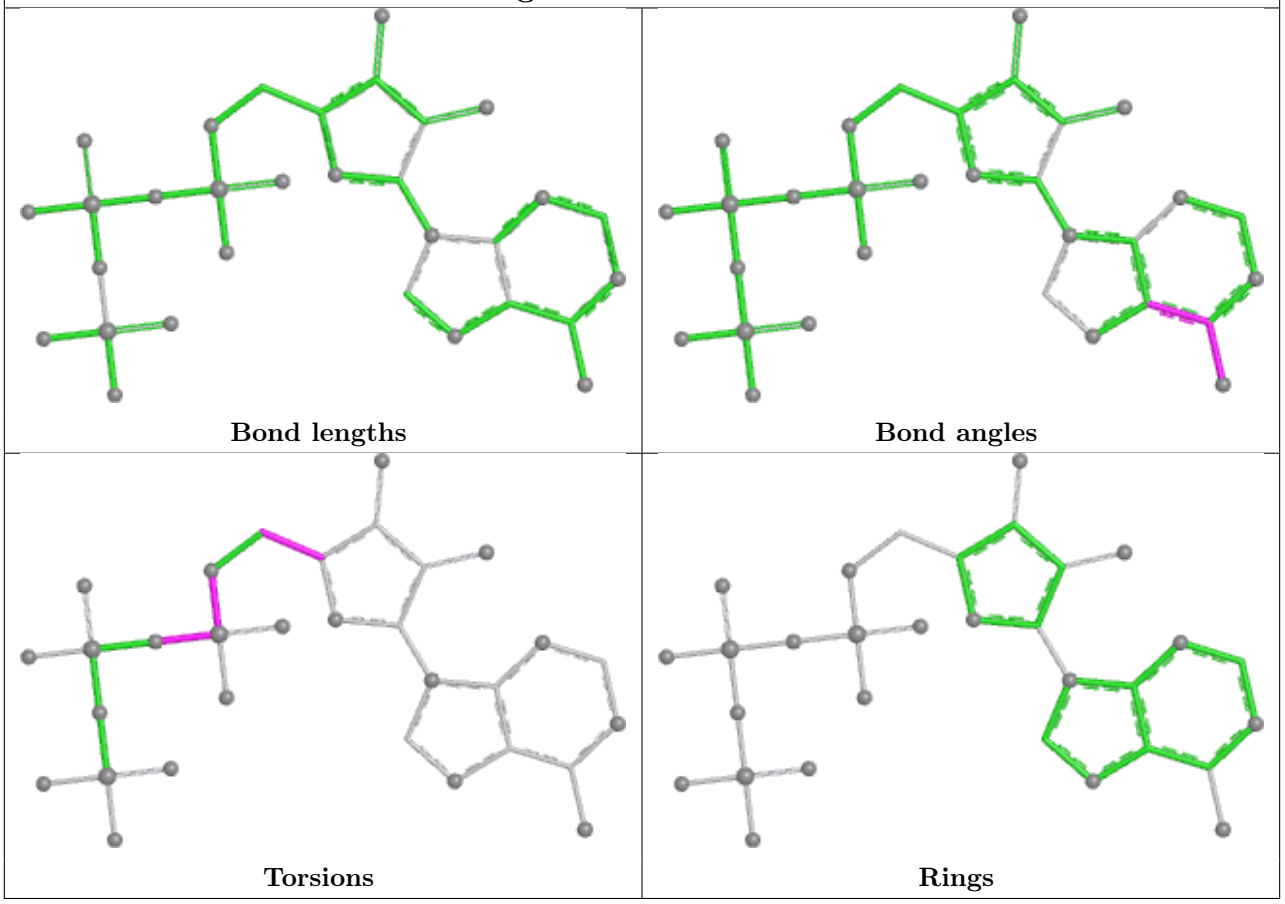


Torsions



Rings

Ligand ATP B 2703



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2611:VAL	C	2628:UNK	N	28.89
1	B	2611:VAL	C	2628:UNK	N	28.89

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2611:VAL	C	2628:UNK	N	28.89
1	D	2611:VAL	C	2628:UNK	N	28.89

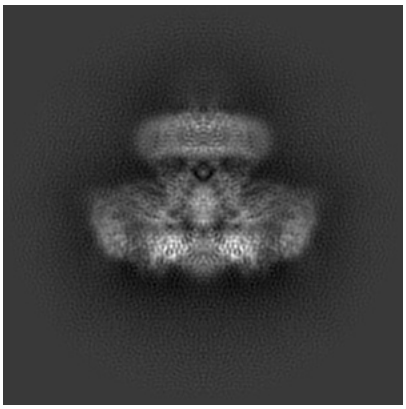
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25670. These allow visual inspection of the internal detail of the map and identification of artifacts.

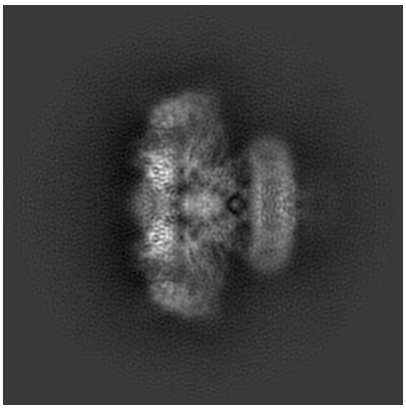
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

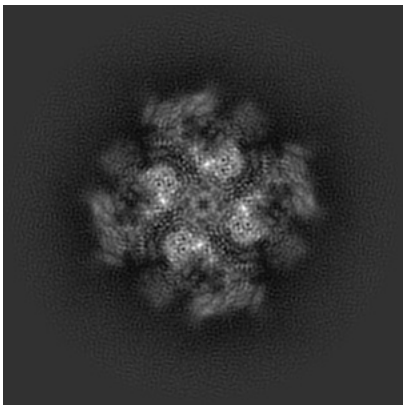
6.1.1 Primary map



X

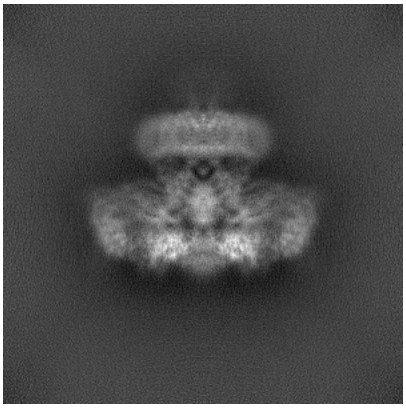


Y

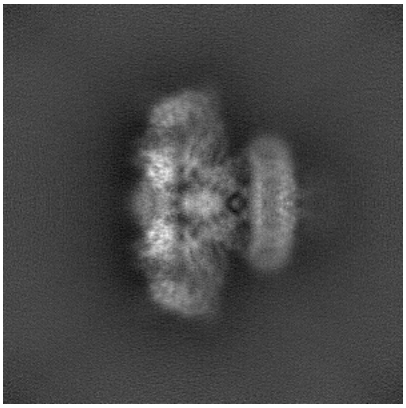


Z

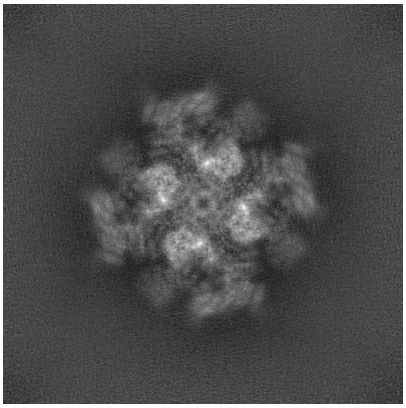
6.1.2 Raw map



X



Y

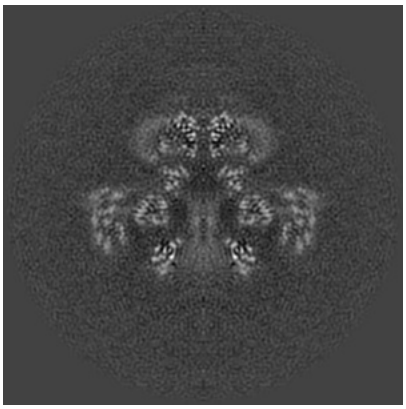


Z

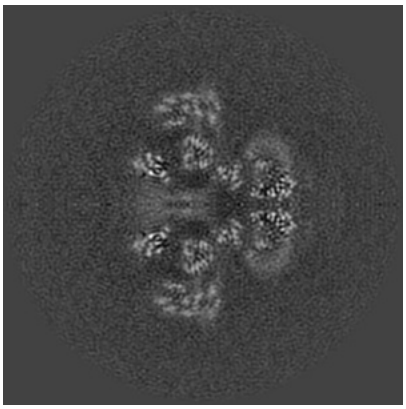
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 240



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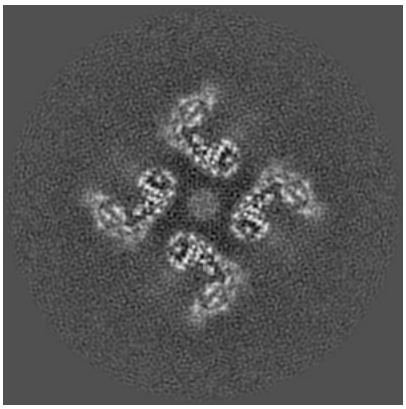
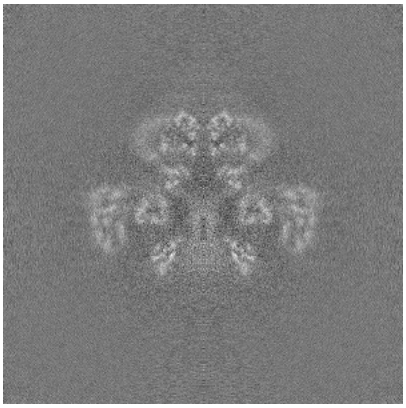


Z Index: 240

6.2.2 Raw map



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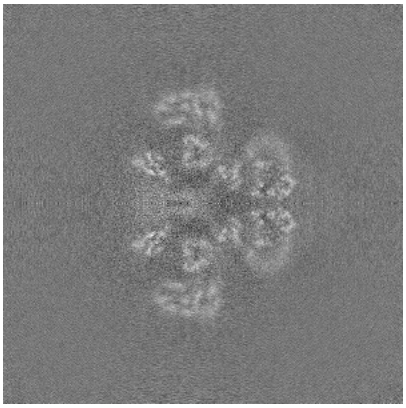

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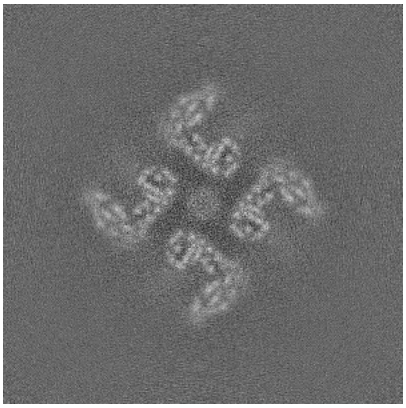
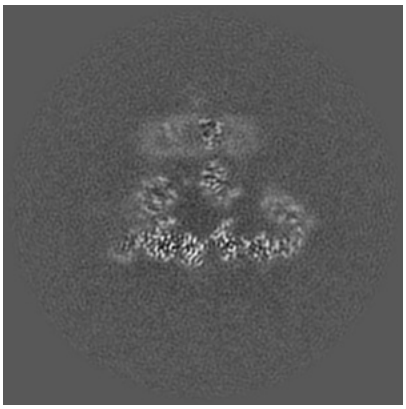


Z Index: 240

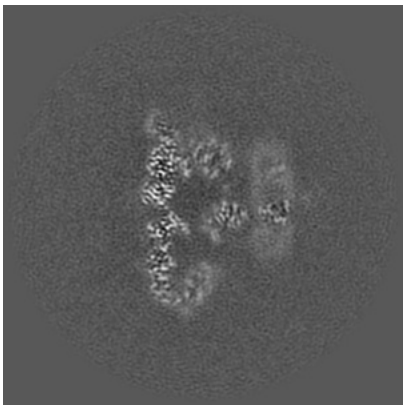
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

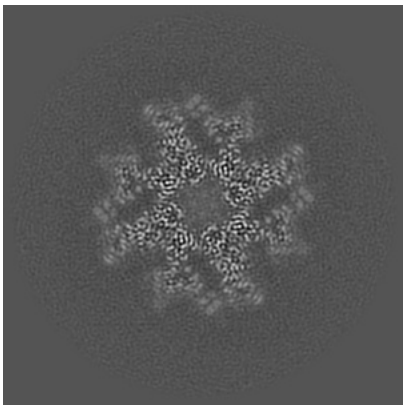
6.3.1 Primary map



X Index: 206

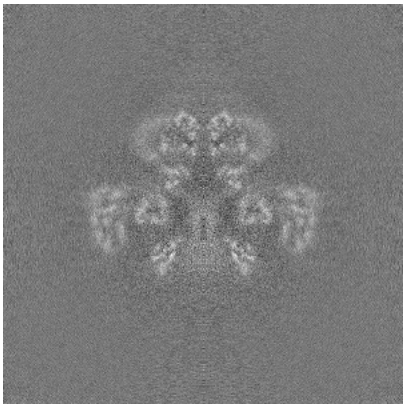


Y Index: 206

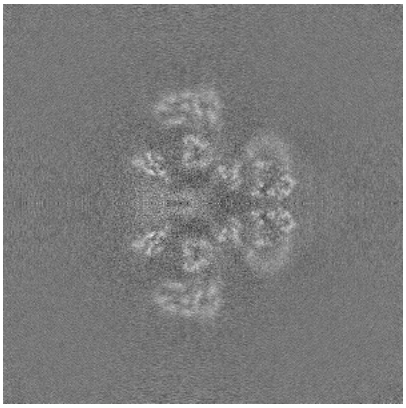


Z Index: 191

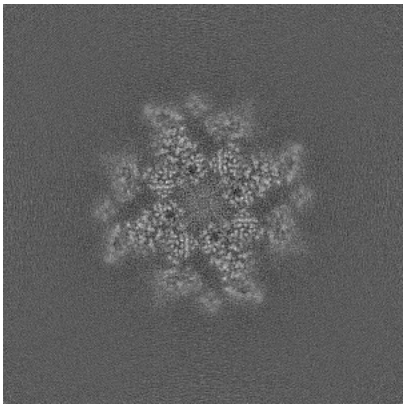
6.3.2 Raw map



X Index: 240



Y Index: 240

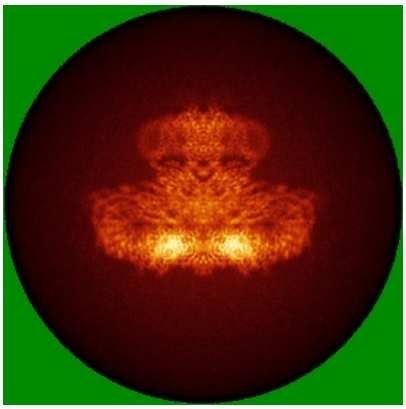


Z Index: 189

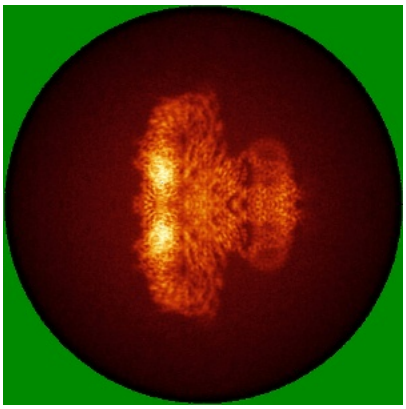
The images above show the largest variance slices of the map in three orthogonal directions.

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

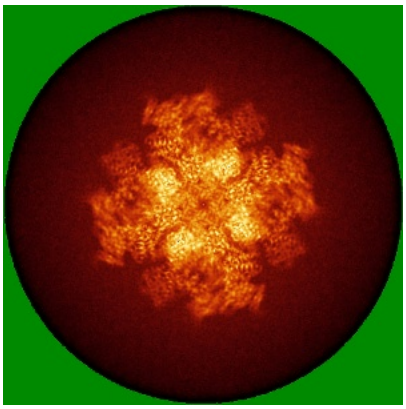
6.4.1 Primary map



X

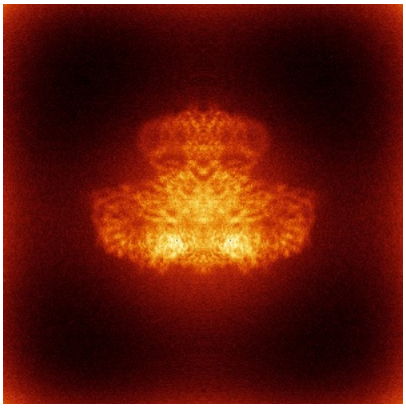


Y

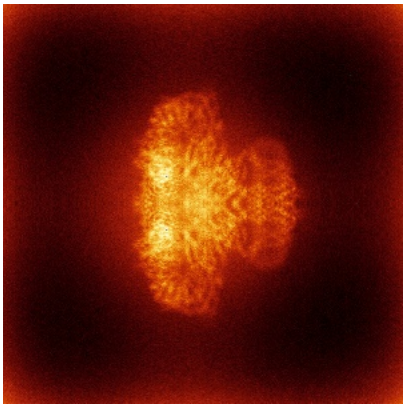


Z

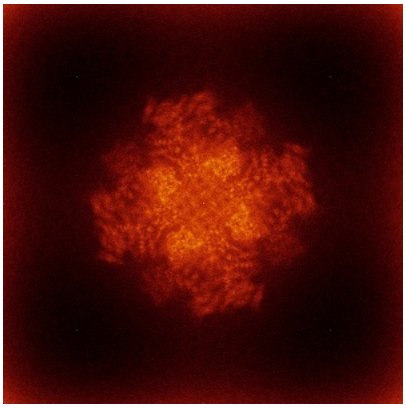
6.4.2 Raw map



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.

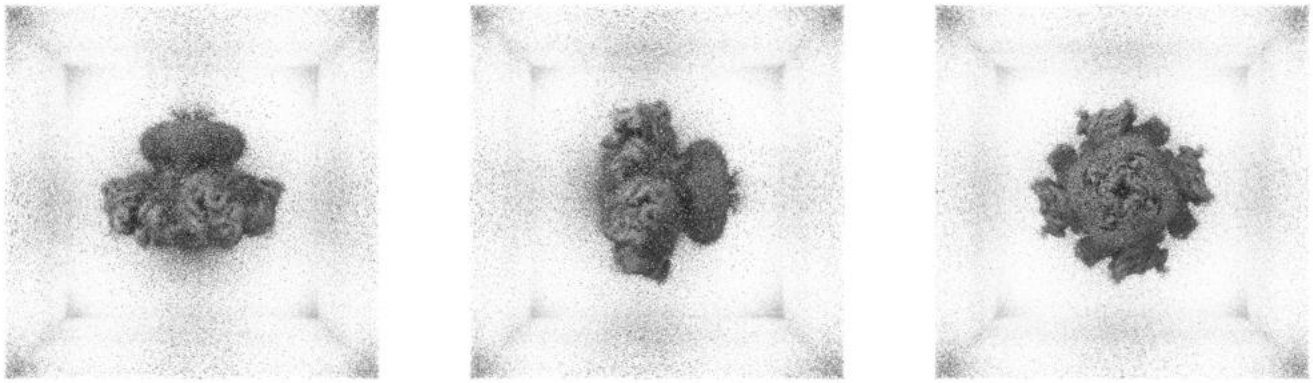
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

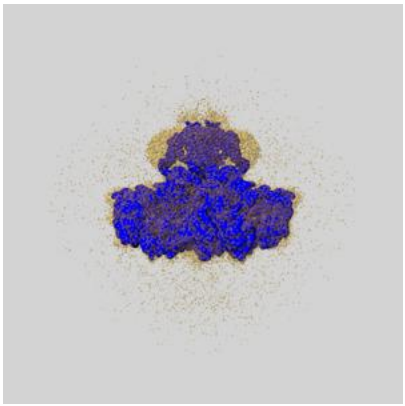
6.6 Mask visualisation (i)

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

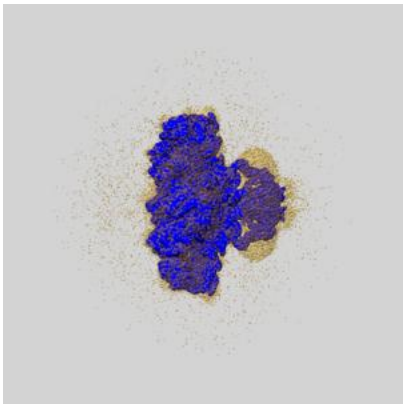
A mask typically either:

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

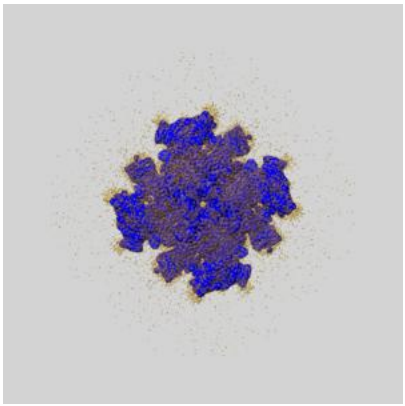
6.6.1 emd_25670_msk_1.map (i)



X



Y

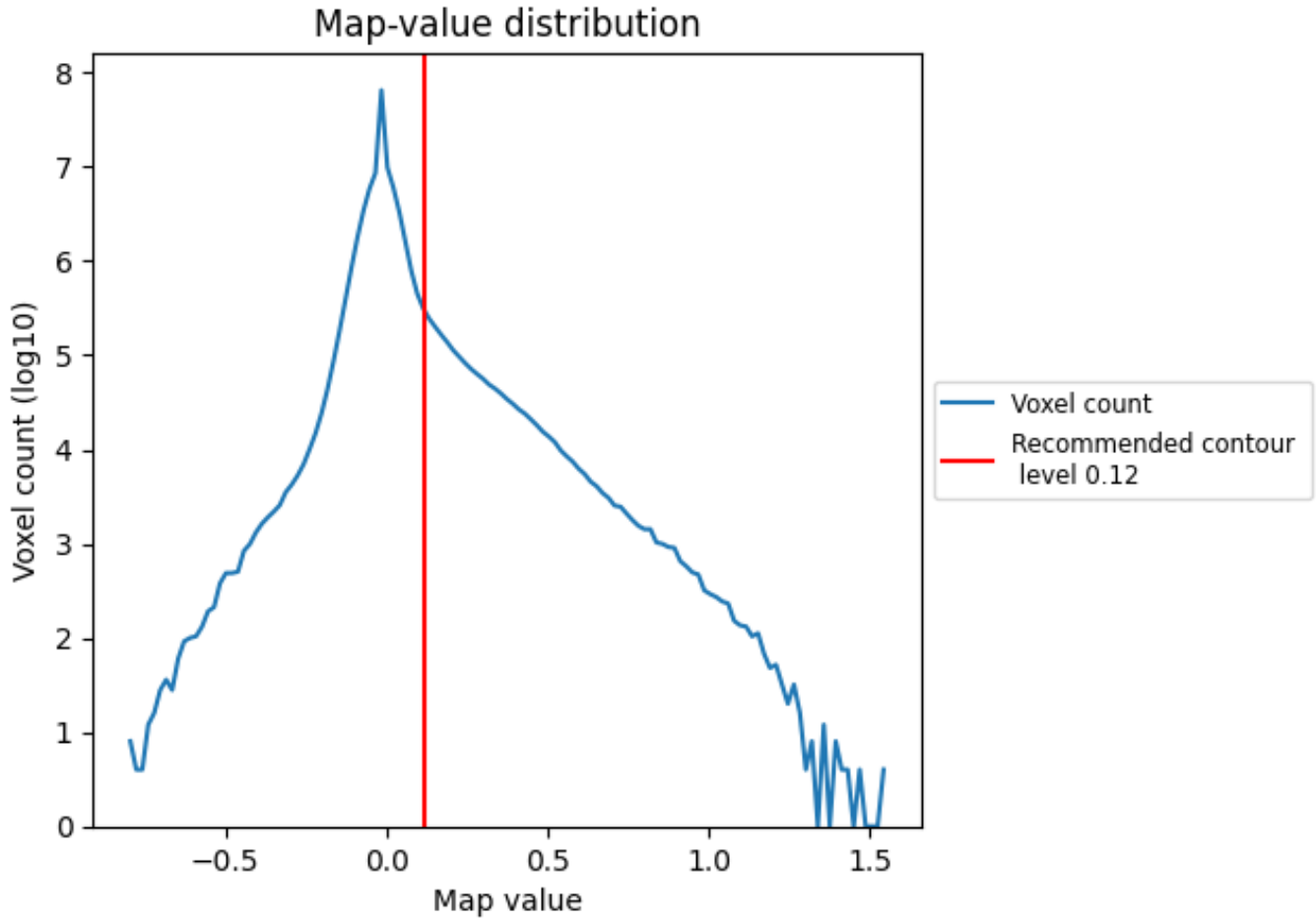


Z

7 Map analysis

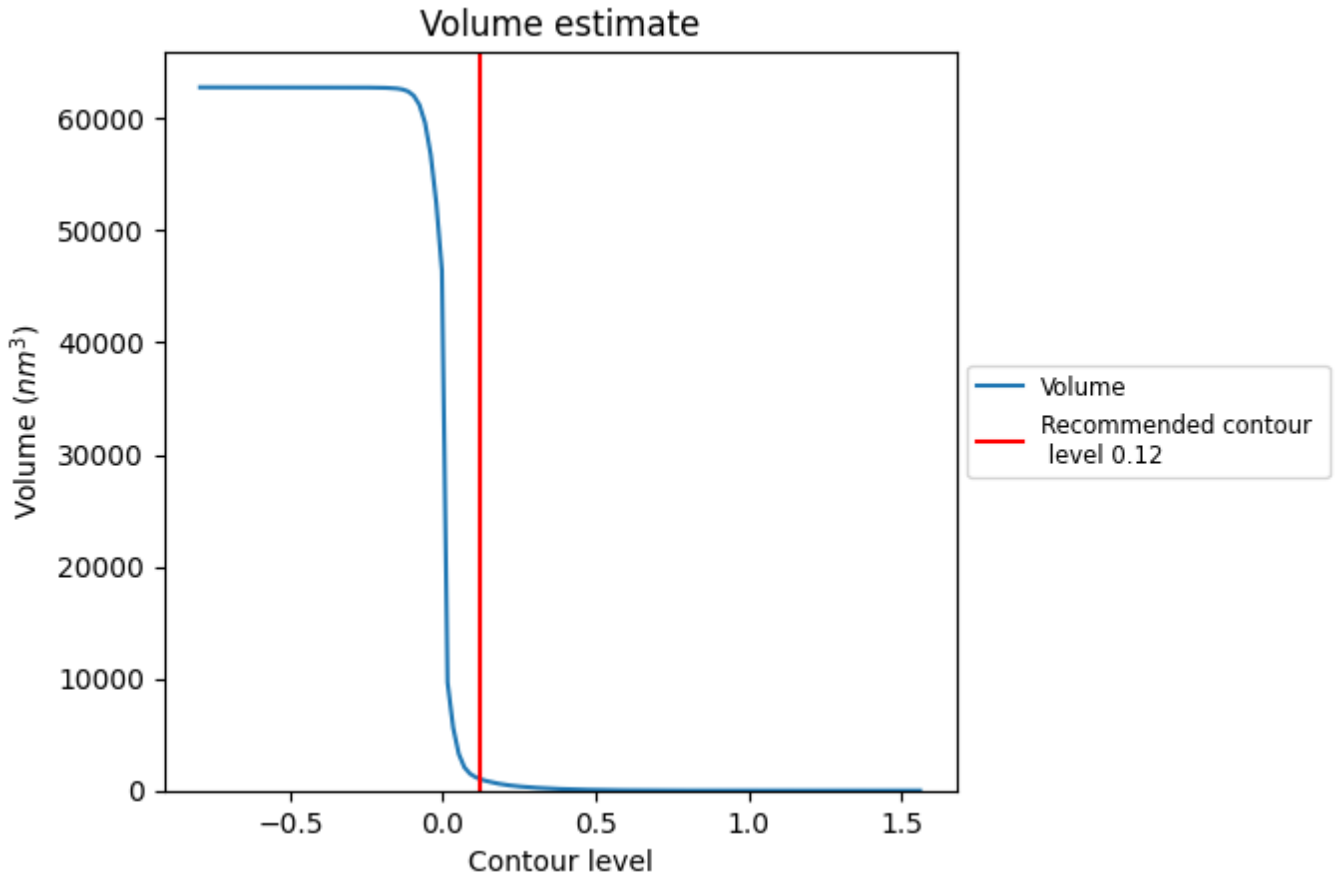
This section contains the results of statistical analysis of the map.

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.

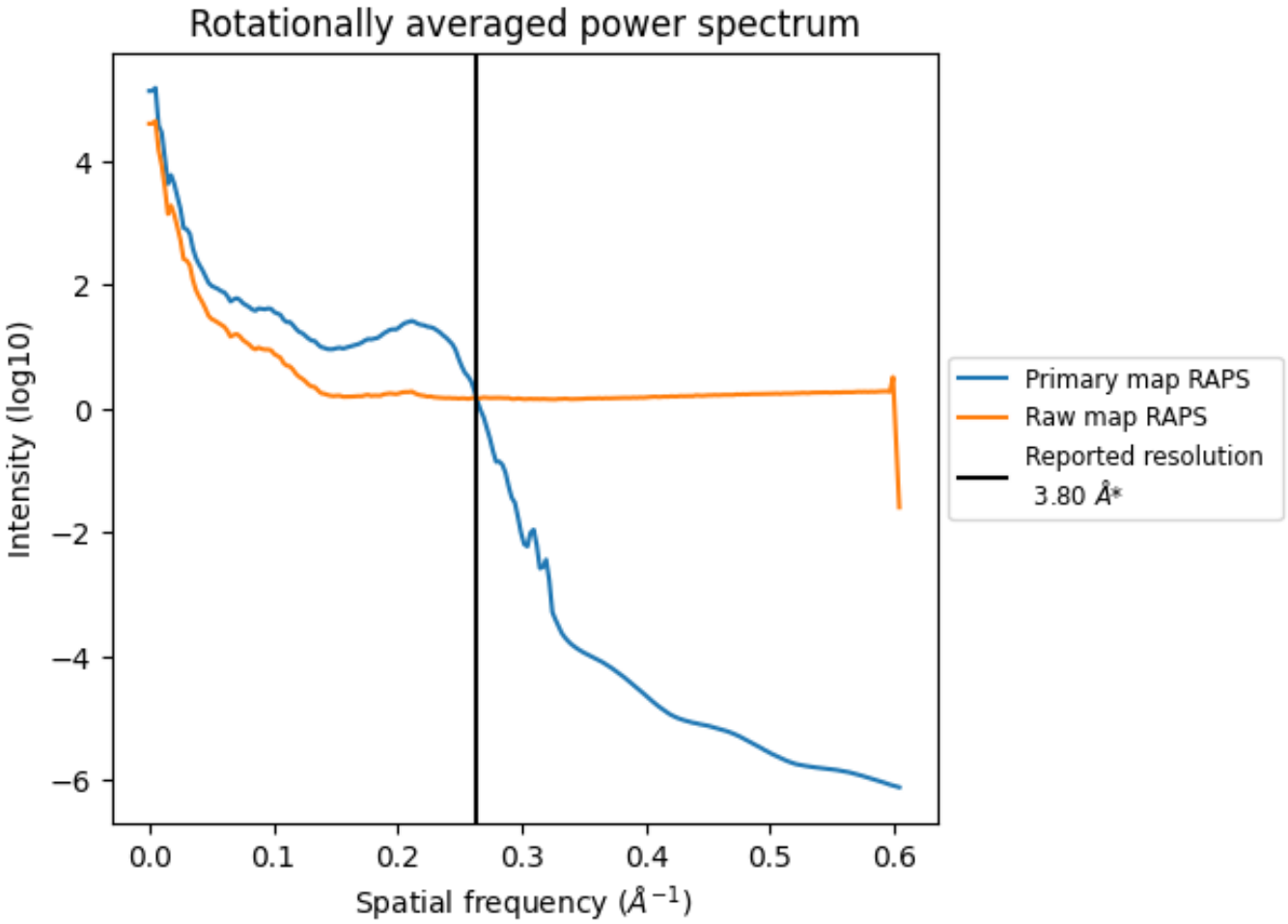
7.2 Volume estimate (i)



The volume at the recommended contour level is 1054 nm^3; this corresponds to an approximate mass of 952 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)

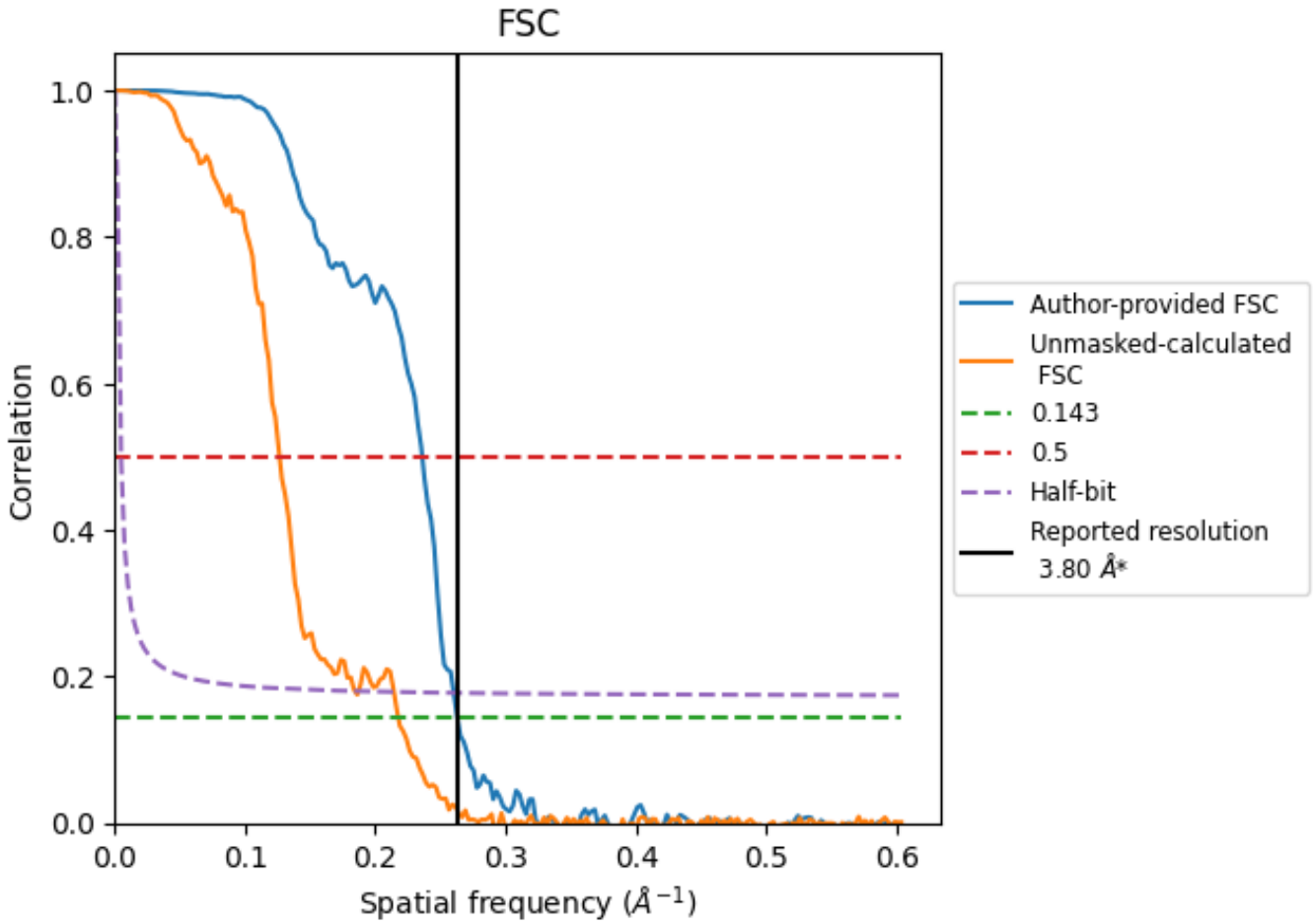


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

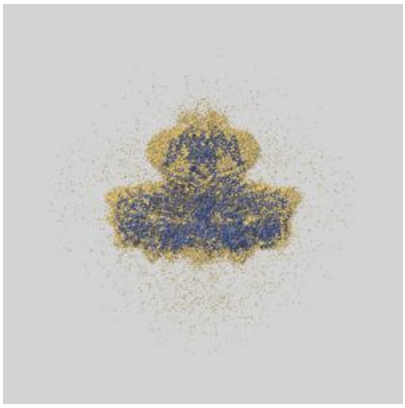
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.24	3.84
Unmasked-calculated*	4.59	7.90	5.42

*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 4.59 differs from the reported value 3.8 by more than 10 %

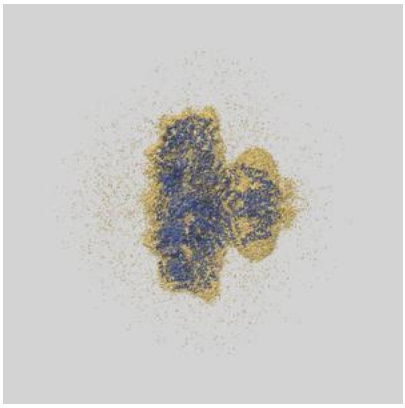
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25670 and PDB model 7T3T. Per-residue inclusion information can be found in section 3 on page 6.

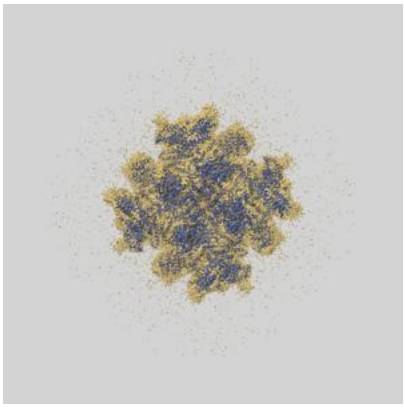
9.1 Map-model overlay



X



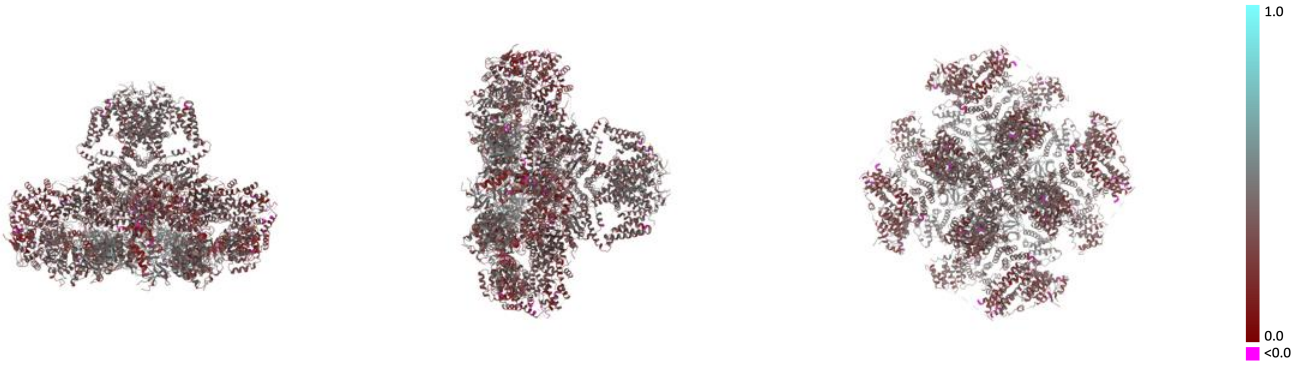
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

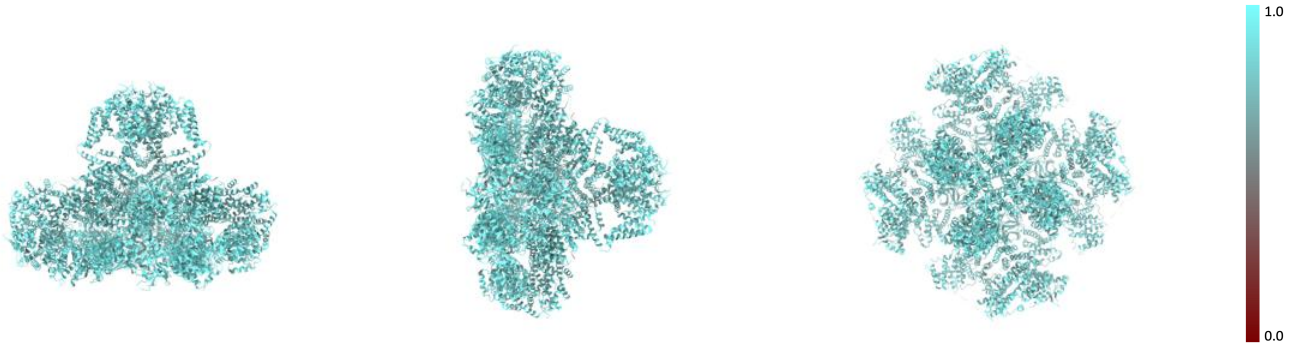
9.2 Q-score mapped to coordinate model (i)



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.

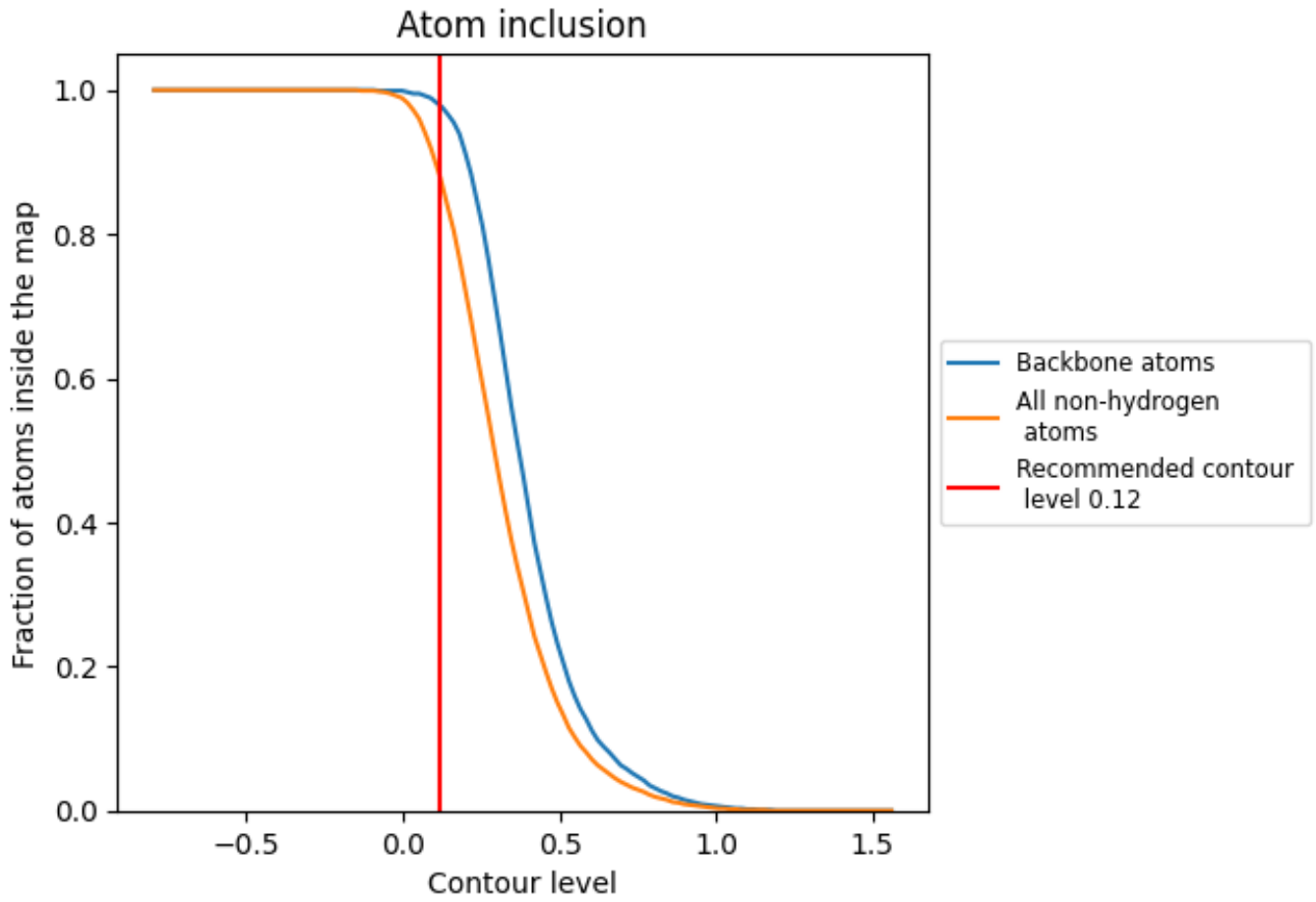
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 88% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.3570
A	0.8780	0.3570
B	0.8780	0.3570
C	0.8780	0.3570
D	0.8780	0.3570