wwPDB EM Validation Summary Report ⓘ

Nov 28, 2022 – 05:03 PM EST

PDB ID	:	7T3P
EMDB ID	:	EMD-25667
Title	:	IP3 and ATP bound type 3 IP3 receptor in the pre-active A state
Authors	:	Schmitz, E.A.; Takahashi, H.; Karakas, E.
Deposited on	:	2021-12-08
Resolution	:	3.20 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:

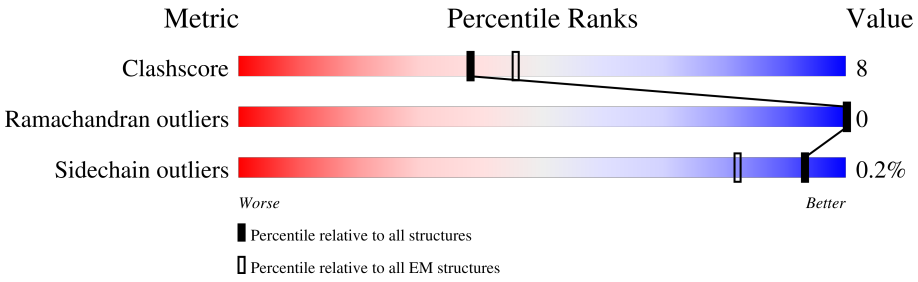
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.20 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	2633	6% 64% 14% 22%
1	B	2633	7% 64% 14% 22%
1	C	2633	6% 64% 14% 22%
1	D	2633	6% 64% 14% 22%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 66992 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.

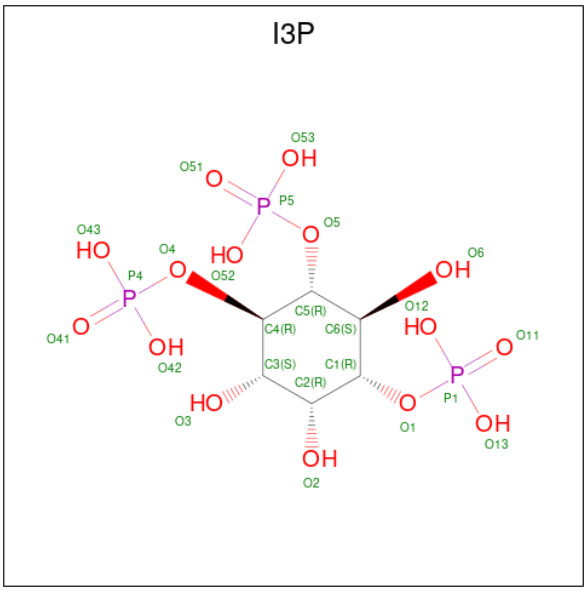
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		
1	B	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		
1	C	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		
1	D	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		

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

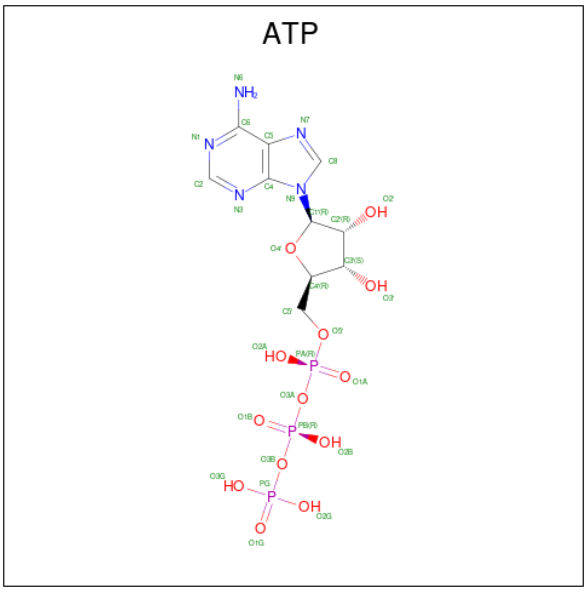
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- 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).



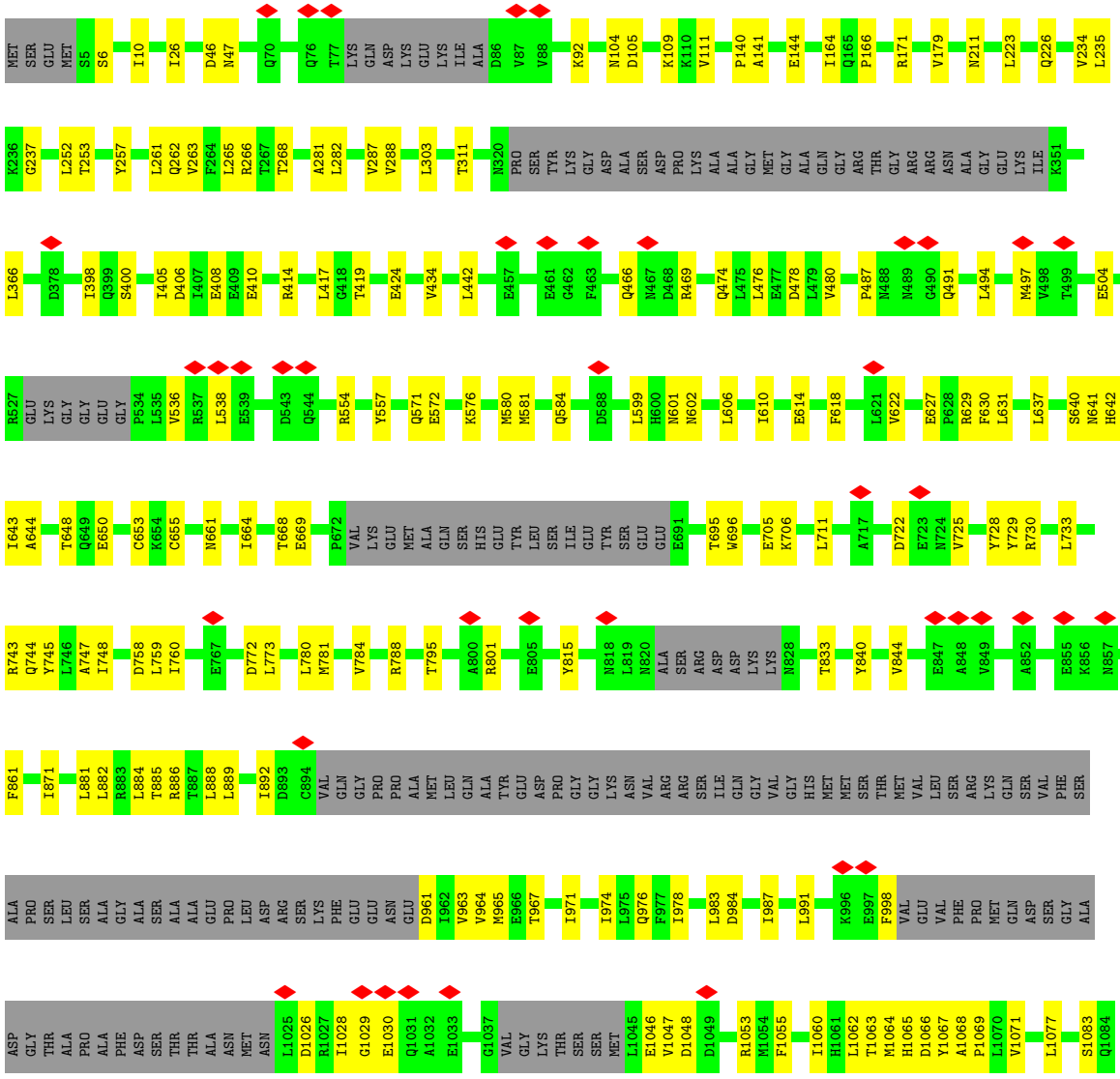
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

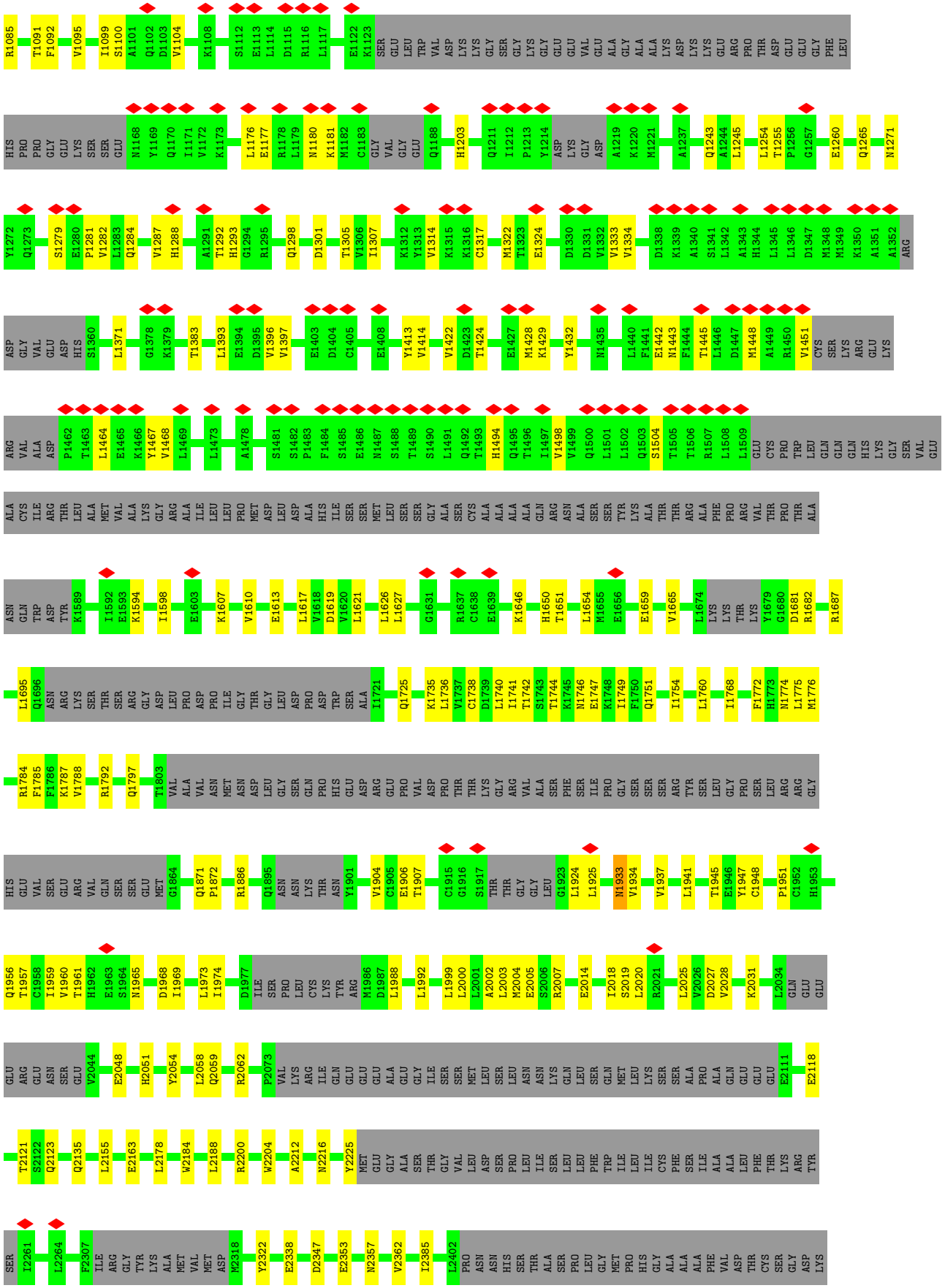
3 Residue-property plots (i)

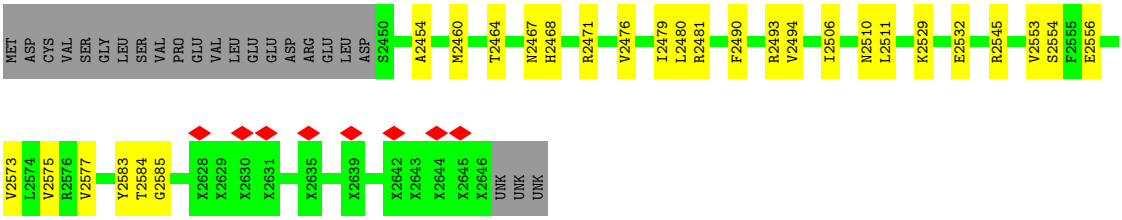
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

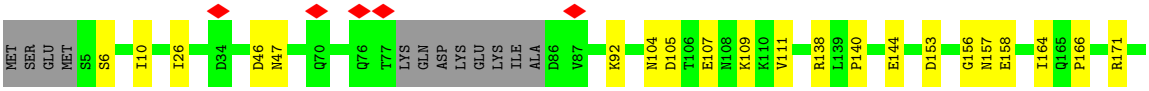


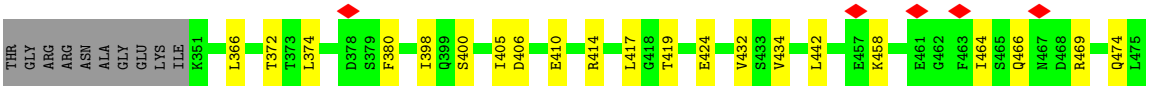


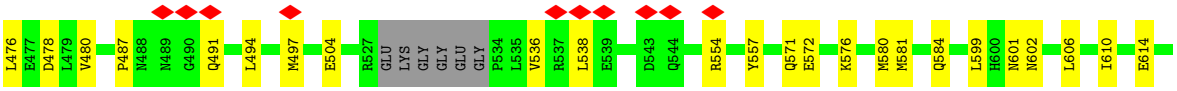


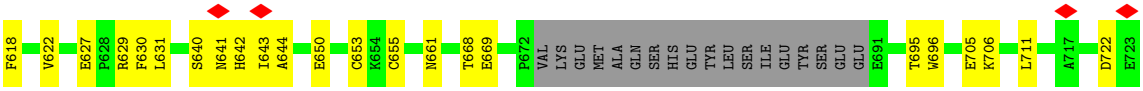
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

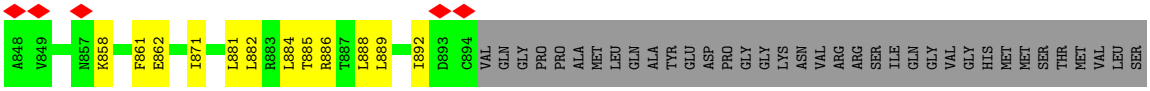
Chain B:

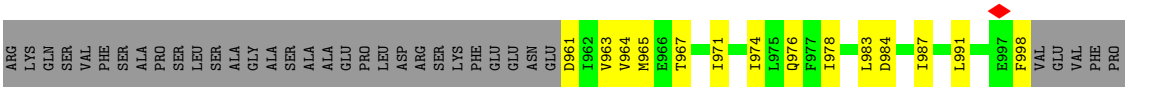


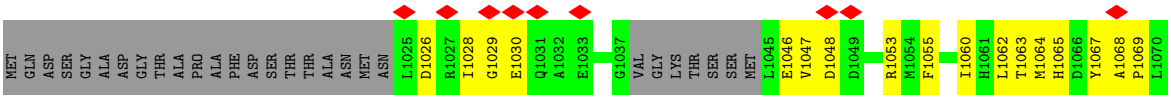


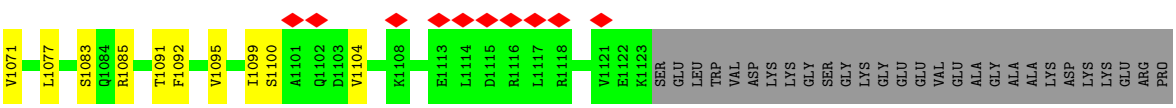


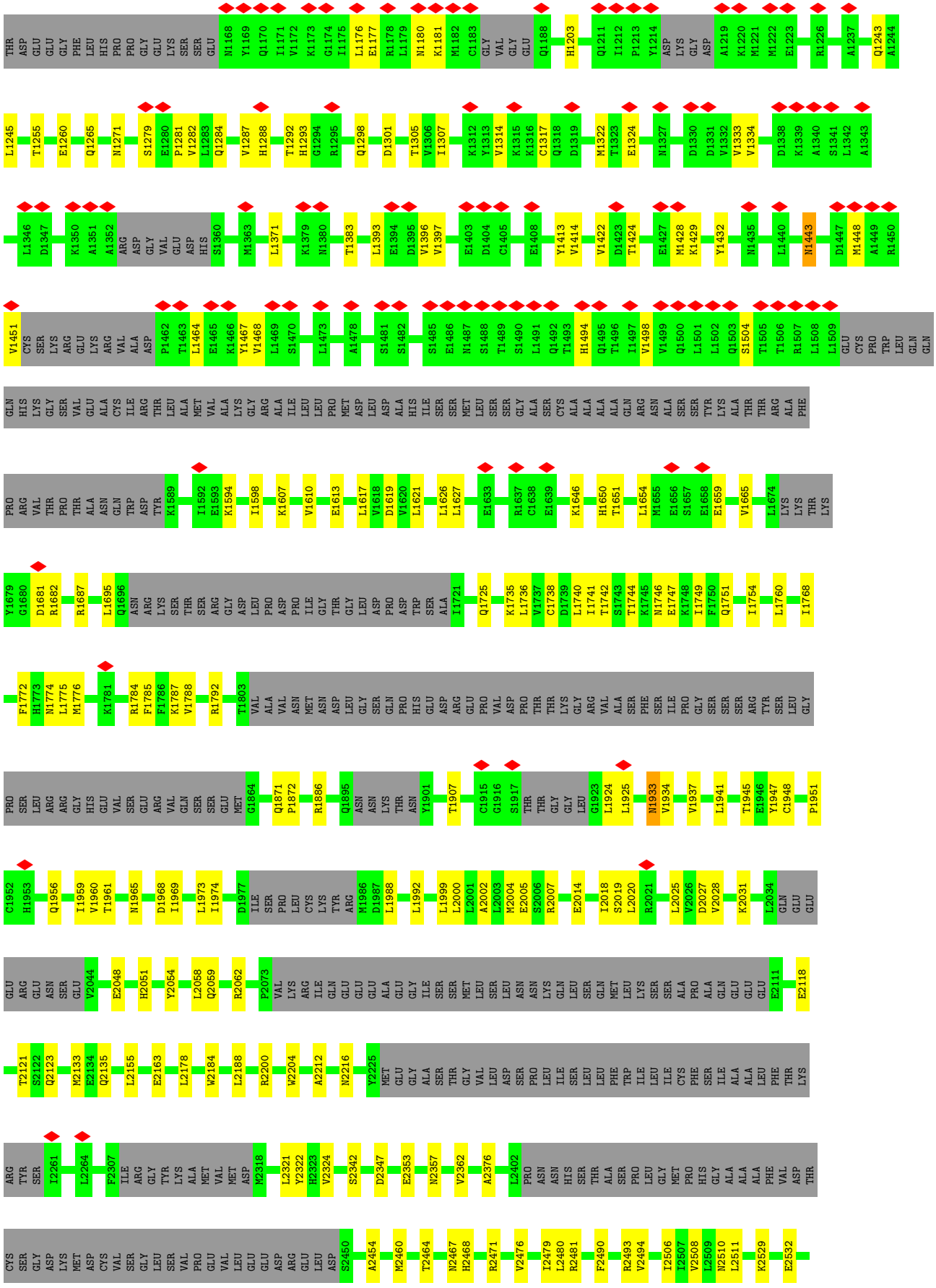


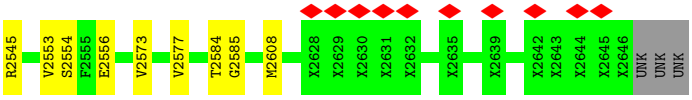






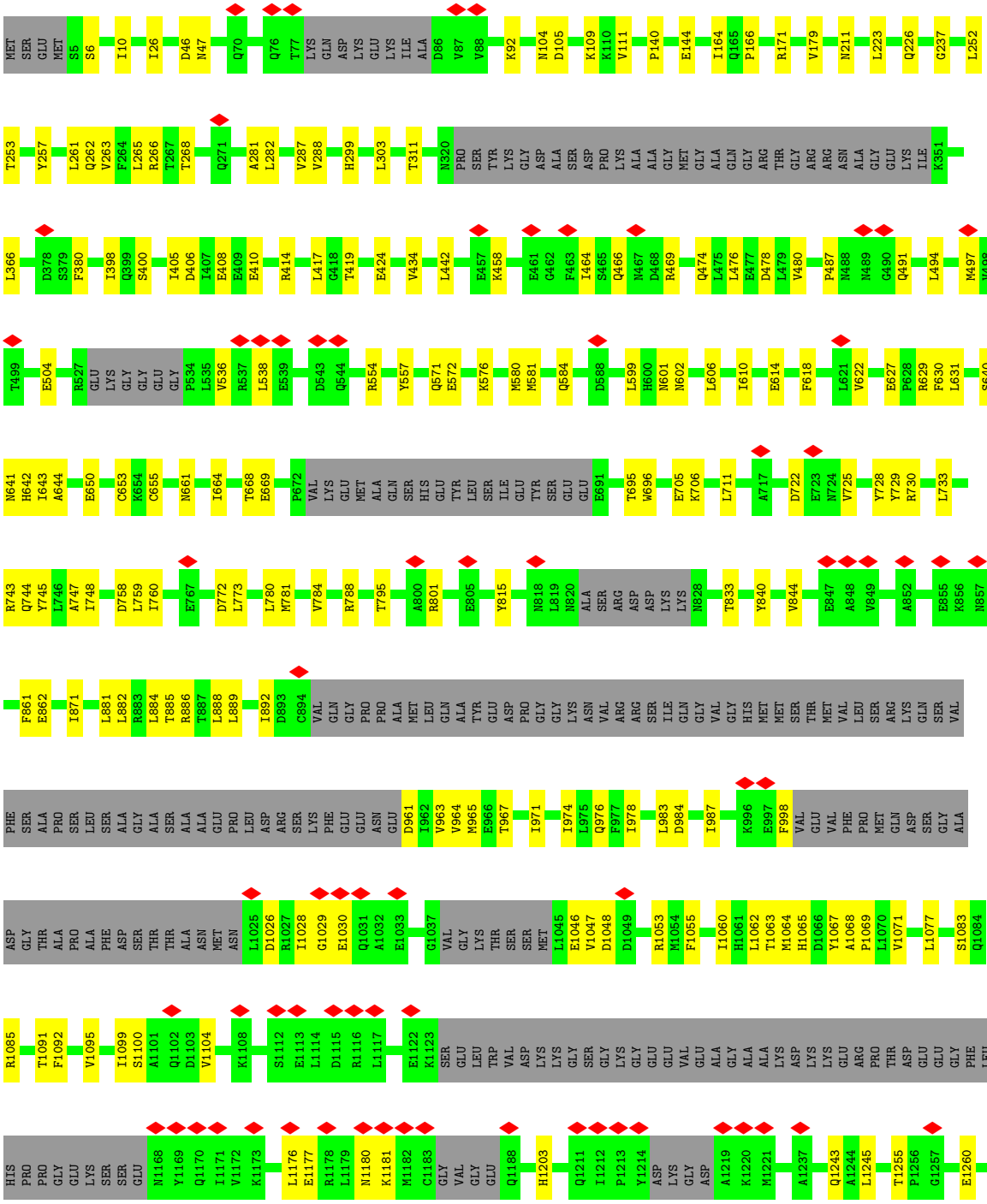


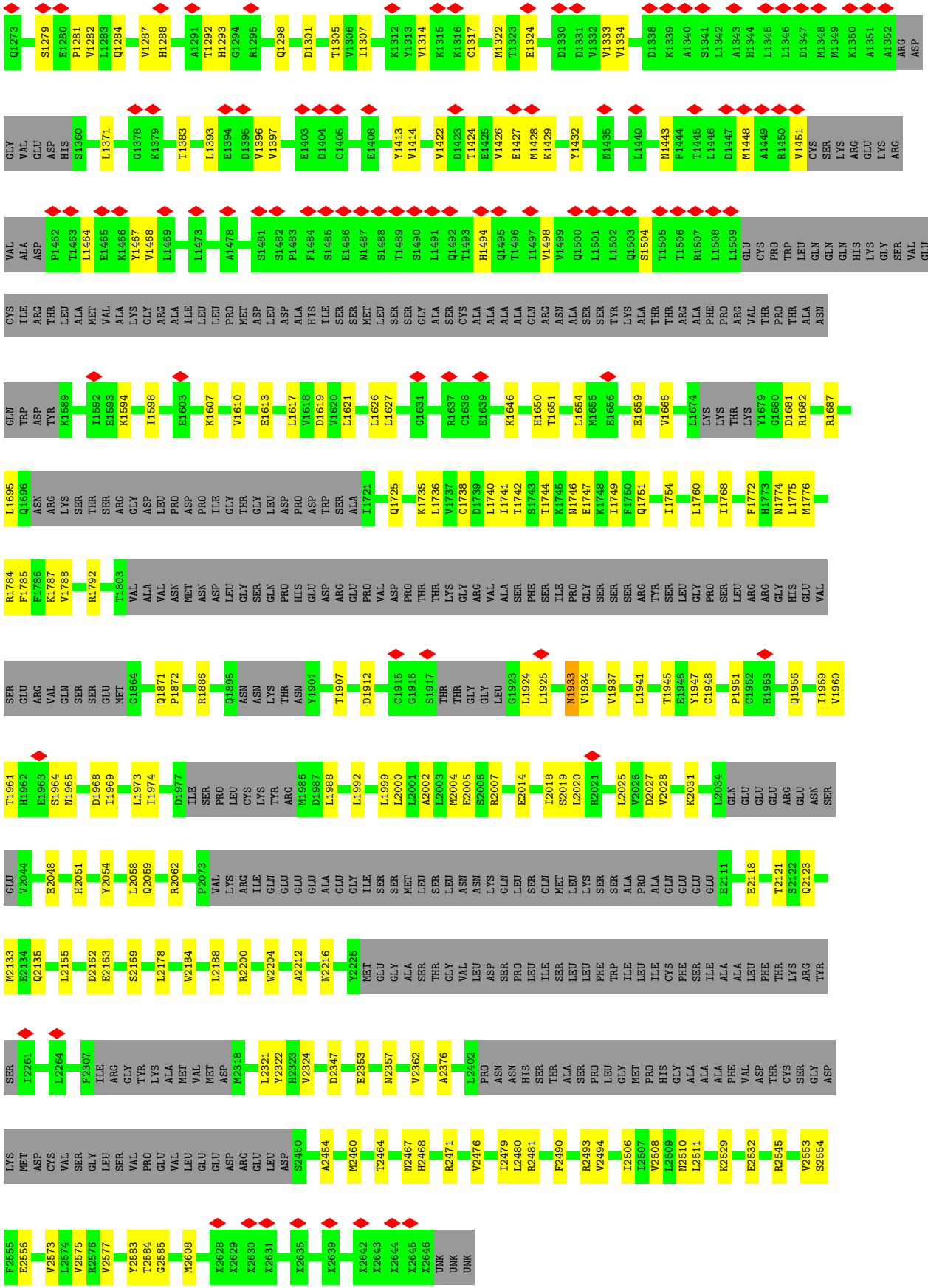




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

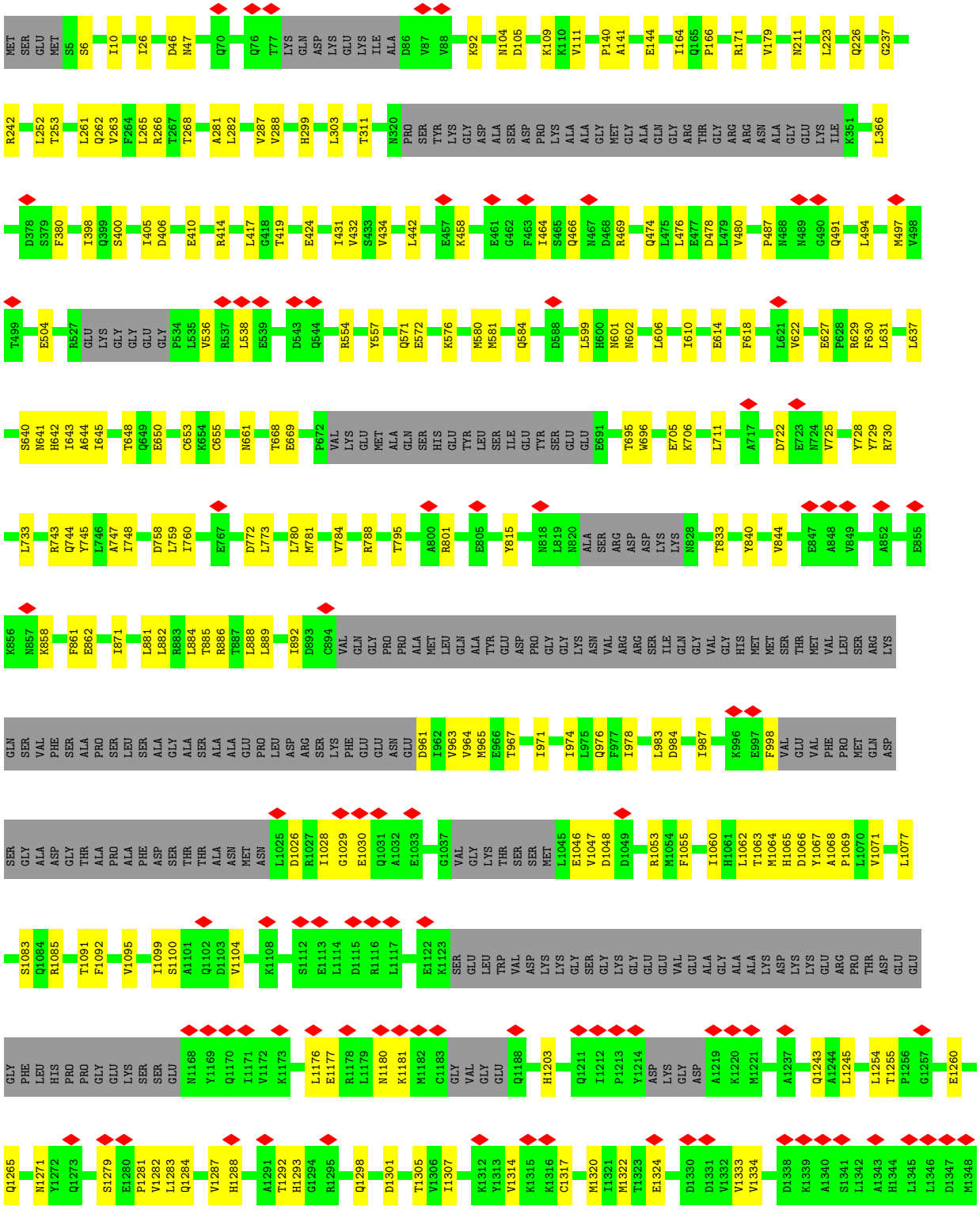
Chain C:

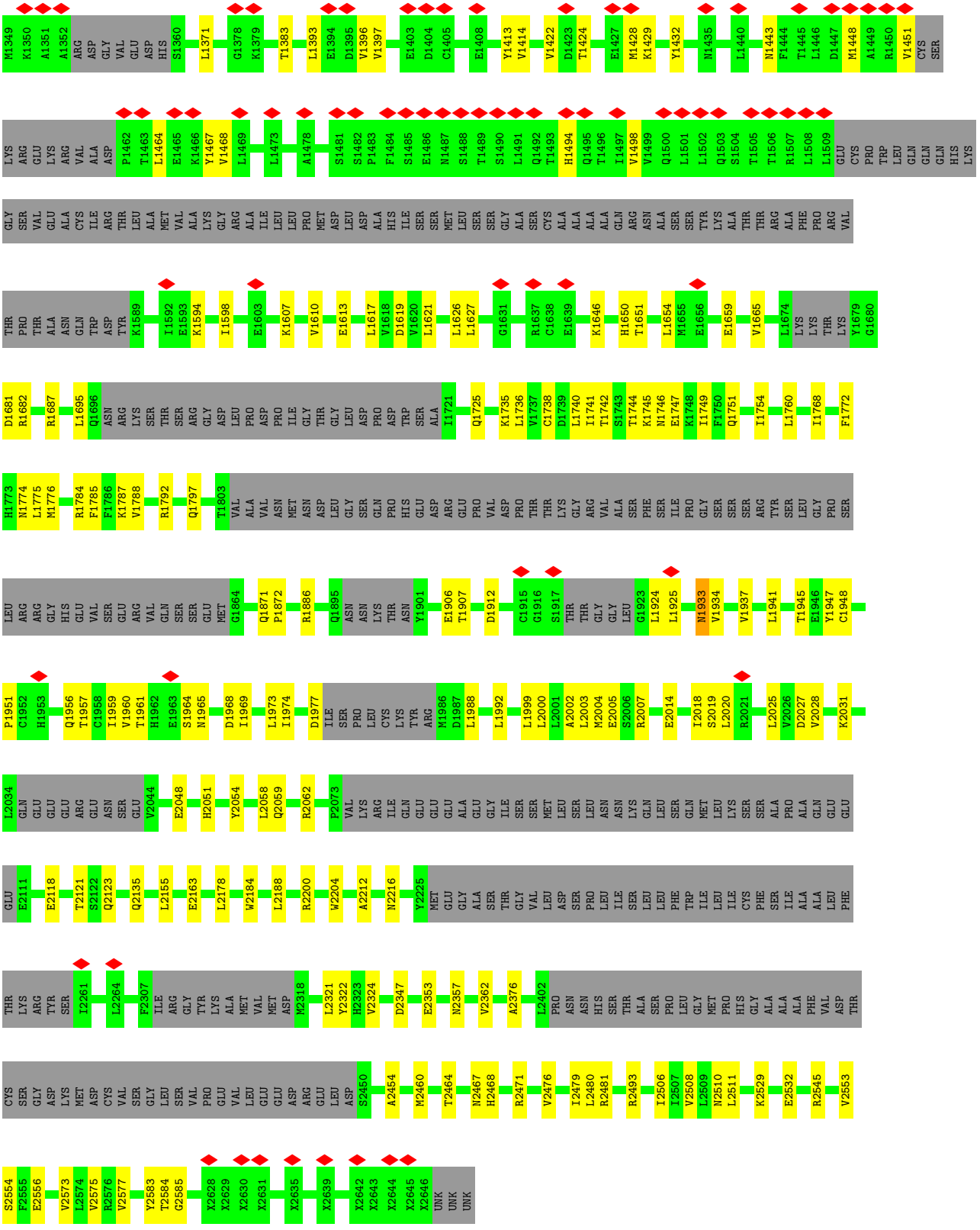




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain D:




M1349 K1350 A1351 A1352 ARG ASP GLY VAL GLU ASP HIS S1360 L1371 G1378 K1379 T1383 L1393 E1394 D1395 V1396 V1397 E1403 D1404 C1405 E1408 Y1413 V1414 V1422 D1423 T1424 E1427 M1428 K1429 Y1432 N1435 L1440 N1443 F1444 T1445 L1446 D1447 M1448 A1449 R1450 V1451 CYS SER
LYS ARG GLU LYS ARG VAL ALA ASP P1462 T1463 L1464 E1465 K1466 Y1467 V1468 L1469 L1473 A1478 S1481 S1482 P1483 F1484 S1485 E1486 N1487 S1488 T1489 S1490 L1491 Q1492 T1493 H1494 Q1495 T1496 I1497 V1498 V1499 Q1500 L1501 L1502 Q1503 S1504 T1505 T1506 R1507 L1508 L1509 GLU CYS PRO TRP LEU GLN GLN GLN HIS LYS
GLY SER VAL GLU ALA CYS ILE ARG THR LEU ALA MET VAL ALA LYS GLY ARG 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 TRP ASP TYR K1589 I1592 E1593 K1594 I1598 E1603 K1607 V1610 E1613 L1617 V1618 D1619 V1620 L1621 L1626 L1627 G1631 R1637 C1638 E1639 K1646 H1650 T1651 L1654 M1655 E1656 E1659 V1665 L1674 LYS LYS THR LYS Y1679 G1680
D1681 R1682 R1687 L1695 Q1696 ASN ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO ASP TRP SER ALA I1721 Q1725 K1735 L1736 V1737 C1738 D1739 L1740 I1741 T1742 S1743 T1744 K1745 N1746 E1747 K1748 I1749 F1750 Q1751 I1754 L1760 I1768 F1772
H1773 N1774 L1775 M1776 R1784 F1785 F1786 K1787 V1788 R1792 Q1797 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 Q1871 P1872 R1886 Q1895 ASN ASN LYS THR ASN Y1901 E1906 T1907 D1912 C1915 G1916 S1917 THR THR GLY GLY LEU G1923 L1924 L1925 N1933 V1934 V1937 L1941 T1945 E1946 Y1947 C1948
P1951 C1952 H1953 Q1956 T1957 C1958 I1959 V1960 T1961 H1962 E1963 S1964 N1965 D1968 I1969 L1973 I1974 D1977 ILE SER PRO LEU CYS LYS TYR ARG M1986 D1987 L1988 L1992 L1999 L2000 L2001 A2002 L2003 M2004 E2005 S2006 R2007 E2014 I2018 S2019 L2020 R2021 L2025 V2026 D2027 V2028 K2031
L2034 GLN GLU GLU GLU ARG GLU ASN SER GLU V2044 E2048 H2051 Y2054 L2058 Q2059 R2062 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 E2111 E2118 T2121 S2122 Q2123 Q2135 L2155 E2163 L2178 W2184 L2188 R2200 W2204 A2212 N2216 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 I2261 L2264 F2307 ILE ARG GLY TYR LYS ALA MET VAL MET ASP M2318 L2321 Y2322 H2323 V2324 D2347 E2353 N2357 V2362 A2376 L2402 PRO ASN ASN HIS SER THR ALA SER PRO LEU 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 A2454 M2460 T2464 N2467 H2468 R2471 V2476 I2479 L2480 R2481 R2493 I2506 I2507 V2508 L2509 N2510 L2511 K2529 E2532 R2545 V2553
S2554 F2555 E2556 V2573 L2574 V2575 R2576 V2577 Y2583 T2584 G2585 X2628 X2629 X2630 X2631 X2635 X2639 X2642 X2643 X2644 X2645 X2646 UNK UNK UNK

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	116925	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	2.847	Depositor
Minimum map value	-1.846	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.2	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: 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	0.29	0/16897	0.47	0/22813
1	B	0.29	0/16897	0.47	0/22813
1	C	0.29	0/16897	0.47	0/22813
1	D	0.29	0/16897	0.47	0/22813
All	All	0.29	0/67588	0.47	0/91252

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	16692	0	16773	272	0
1	B	16692	0	16773	281	0
1	C	16692	0	16773	281	0
1	D	16692	0	16773	274	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	9	2	0
3	C	24	0	9	2	0
3	D	24	0	9	2	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
All	All	66992	0	67176	1071	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 1071 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:C:801:ARG:NH2	1:C:984:ASP:OD1	2.09	0.86
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.09	0.86
1:D:801:ARG:NH2	1:D:984:ASP:OD1	2.09	0.85
1:A:627:GLU:OE1	1:A:629:ARG:NH1	2.10	0.84
1:A:801:ARG:NH2	1:A:984:ASP:OD1	2.09	0.84

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	1995/2633 (76%)	1913 (96%)	82 (4%)	0	100	100
1	B	1995/2633 (76%)	1912 (96%)	83 (4%)	0	100	100
1	C	1995/2633 (76%)	1913 (96%)	82 (4%)	0	100	100
1	D	1995/2633 (76%)	1913 (96%)	82 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	7980/10532 (76%)	7651 (96%)	329 (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	1865/2329 (80%)	1861 (100%)	4 (0%)	93 98
1	B	1865/2329 (80%)	1861 (100%)	4 (0%)	93 98
1	C	1865/2329 (80%)	1861 (100%)	4 (0%)	93 98
1	D	1865/2329 (80%)	1861 (100%)	4 (0%)	93 98
All	All	7460/9316 (80%)	7444 (100%)	16 (0%)	93 98

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1735	LYS
1	D	1682	ARG
1	C	1443	ASN
1	D	1443	ASN
1	B	1933	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1243	GLN
1	B	1243	GLN
1	C	1243	GLN
1	D	1243	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	$\#\|Z\| > 2$
4	ATP	B	2703	-	26,33,33	0.64	0	31,52,52	1.08	3 (9%)
3	I3P	C	2702	-	24,24,24	1.25	3 (12%)	36,39,39	0.55	0
4	ATP	C	2703	-	26,33,33	0.64	0	31,52,52	1.08	3 (9%)
3	I3P	B	2702	-	24,24,24	1.25	3 (12%)	36,39,39	0.55	0
3	I3P	D	2702	-	24,24,24	1.25	3 (12%)	36,39,39	0.55	0
4	ATP	D	2703	-	26,33,33	0.65	0	31,52,52	1.08	3 (9%)
3	I3P	A	2702	-	24,24,24	1.25	3 (12%)	36,39,39	0.55	0
4	ATP	A	2703	-	26,33,33	0.65	0	31,52,52	1.08	3 (9%)

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
4	ATP	B	2703	-	-	3/18/38/38	0/3/3/3
3	I3P	C	2702	-	-	3/15/39/39	0/1/1/1
4	ATP	C	2703	-	-	3/18/38/38	0/3/3/3
3	I3P	B	2702	-	-	3/15/39/39	0/1/1/1
3	I3P	D	2702	-	-	3/15/39/39	0/1/1/1
4	ATP	D	2703	-	-	3/18/38/38	0/3/3/3
3	I3P	A	2702	-	-	3/15/39/39	0/1/1/1
4	ATP	A	2703	-	-	3/18/38/38	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	P4-O4	2.99	1.65	1.59
3	A	2702	I3P	P4-O4	2.96	1.64	1.59
3	C	2702	I3P	P4-O4	2.96	1.64	1.59
3	D	2702	I3P	P4-O4	2.96	1.64	1.59
3	A	2702	I3P	P5-O5	2.89	1.64	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2703	ATP	C5-C6-N6	2.31	123.86	120.35
4	B	2703	ATP	C5-C6-N6	2.31	123.86	120.35
4	C	2703	ATP	C5-C6-N6	2.31	123.86	120.35
4	D	2703	ATP	C5-C6-N6	2.31	123.86	120.35
4	B	2703	ATP	PB-O3B-PG	2.05	139.86	132.83

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2702	I3P	C1-O1-P1-O12
3	A	2702	I3P	C5-O5-P5-O53
3	B	2702	I3P	C1-O1-P1-O12
3	B	2702	I3P	C5-O5-P5-O53
3	C	2702	I3P	C1-O1-P1-O12

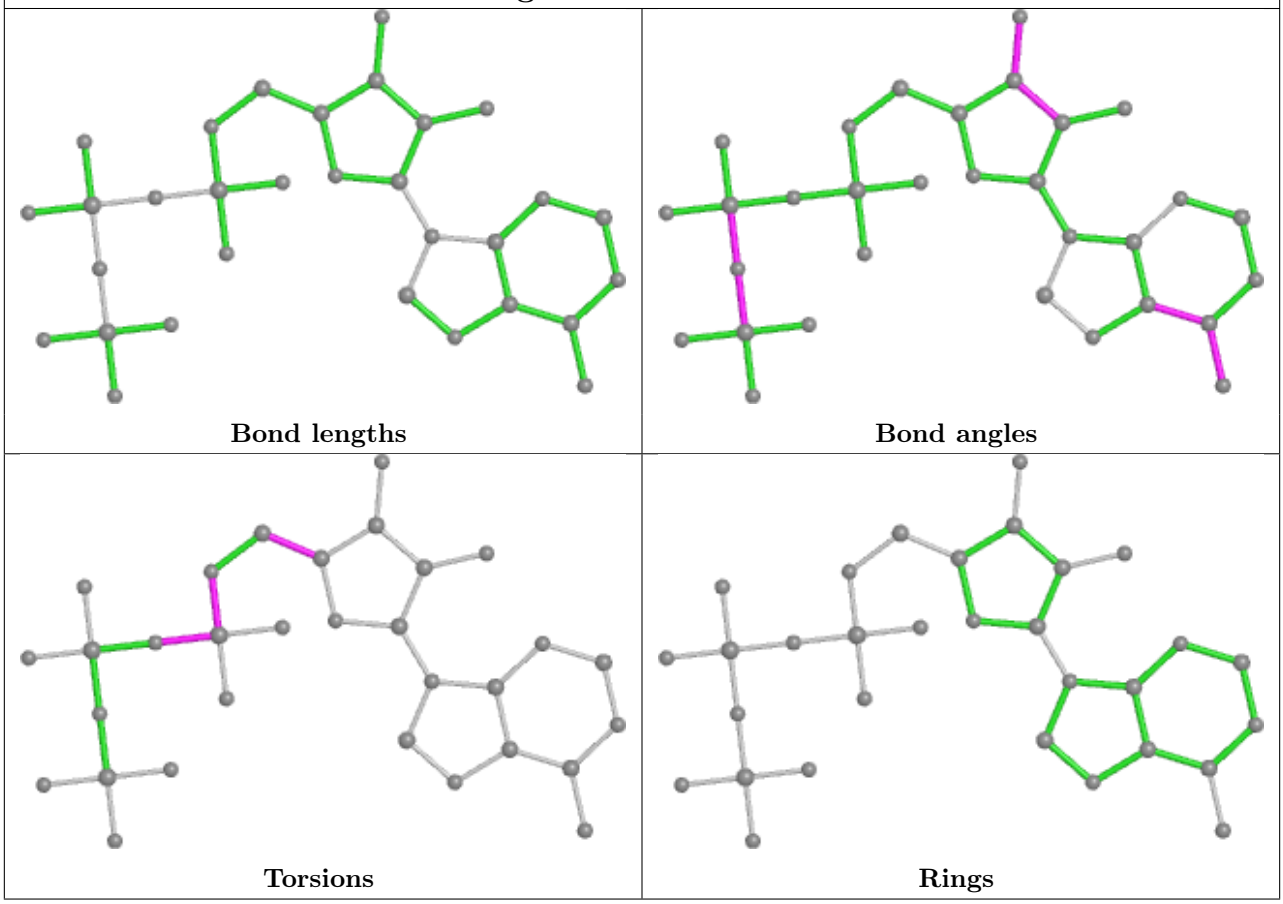
There are no ring outliers.

4 monomers are involved in 8 short contacts:

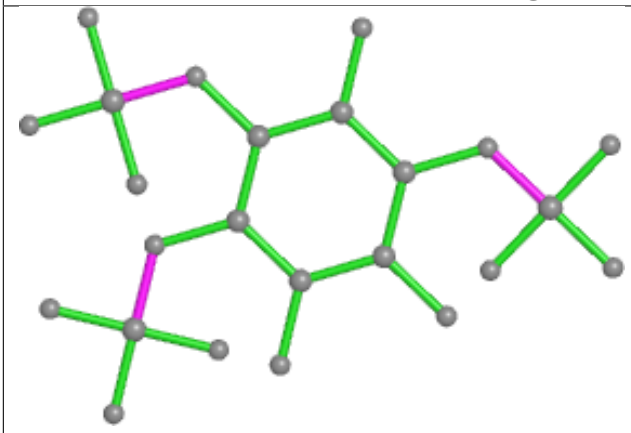
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2702	I3P	2	0
3	B	2702	I3P	2	0
3	D	2702	I3P	2	0
3	A	2702	I3P	2	0

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.

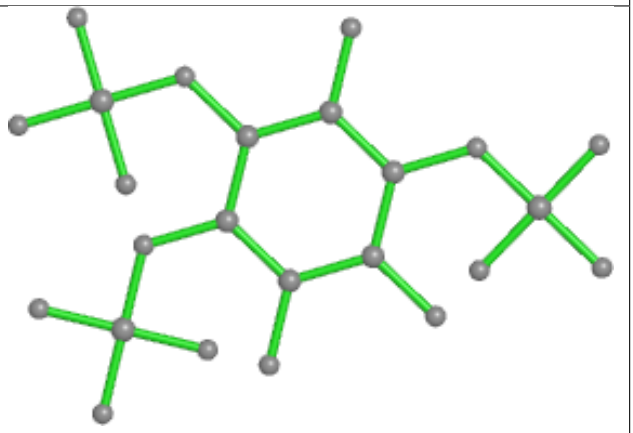
Ligand ATP B 2703



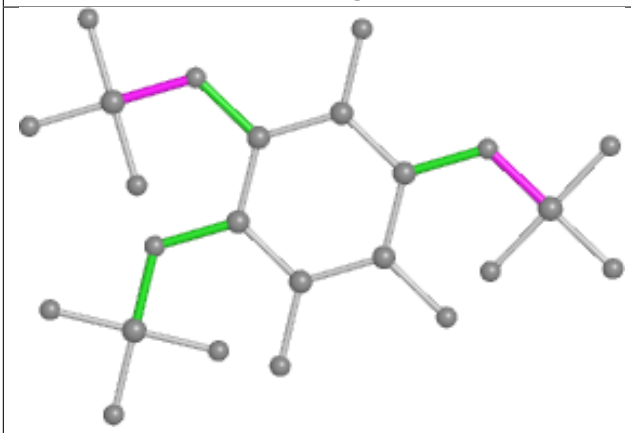
Ligand I3P C 2702



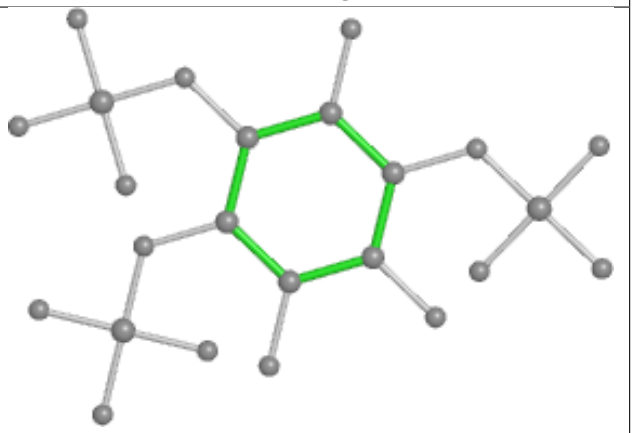
Bond lengths



Bond angles

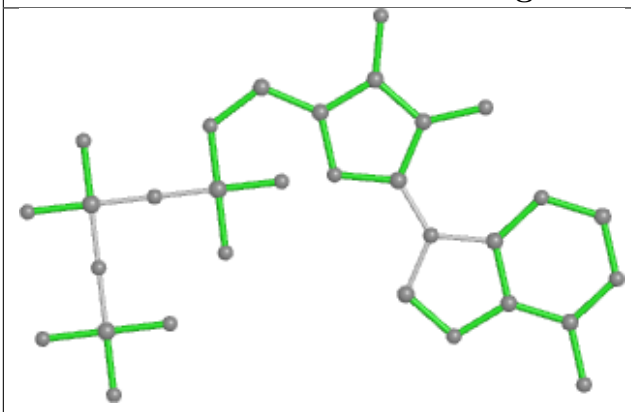


Torsions

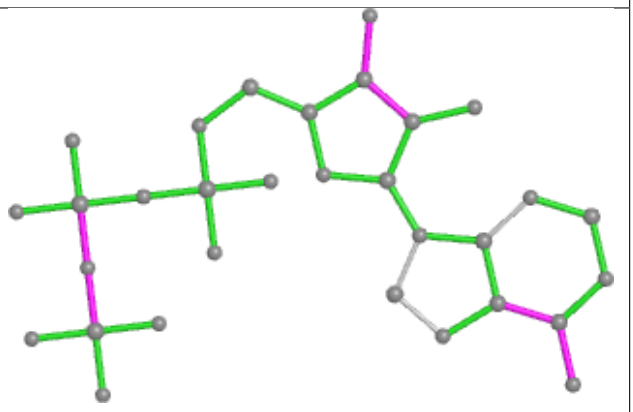


Rings

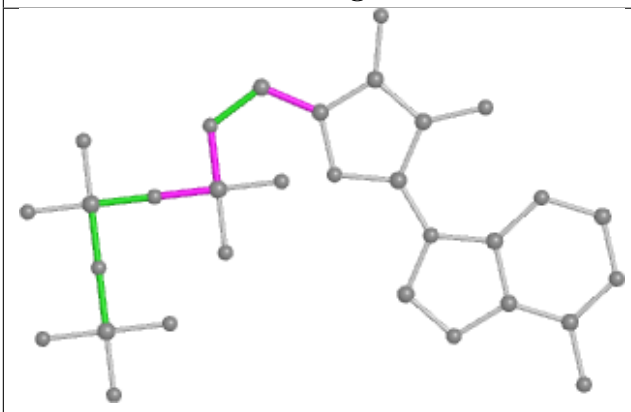
Ligand ATP C 2703



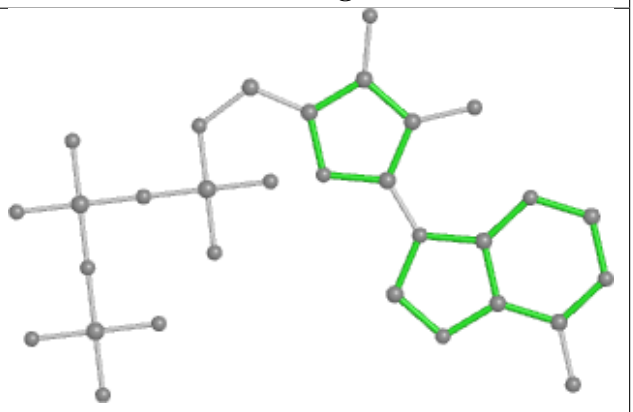
Bond lengths



Bond angles

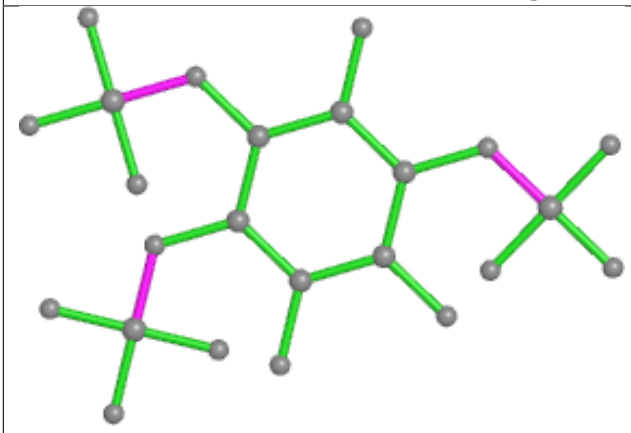


Torsions

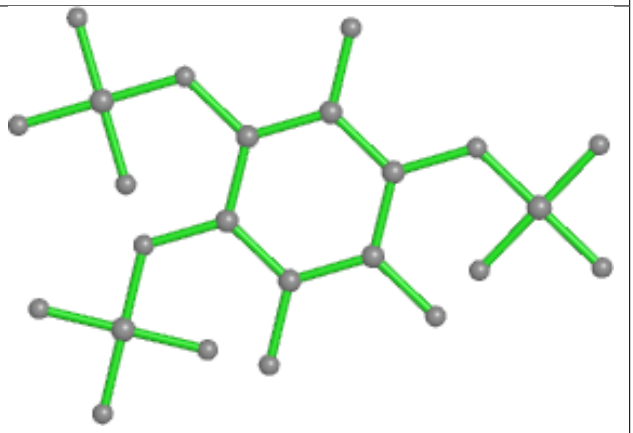


Rings

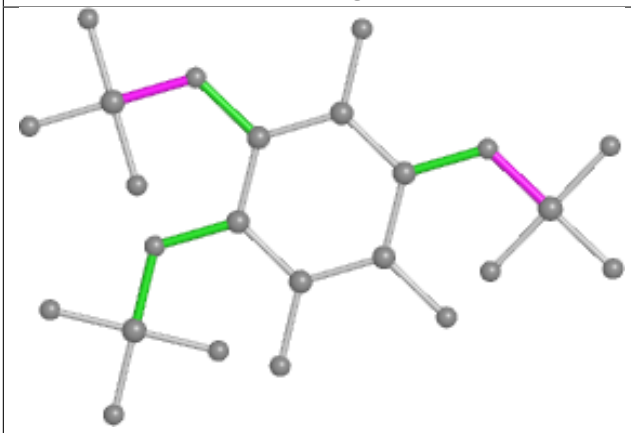
Ligand I3P B 2702



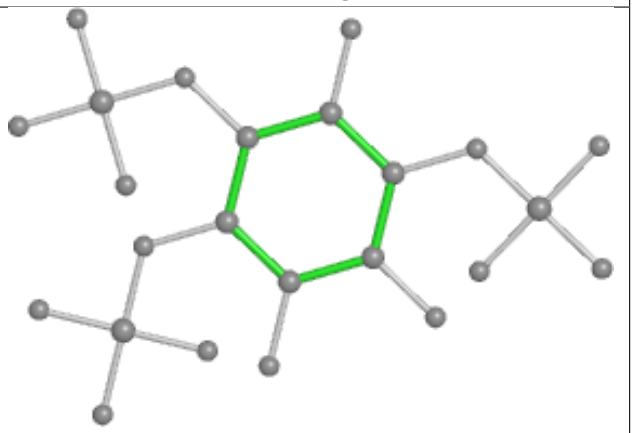
Bond lengths



Bond angles

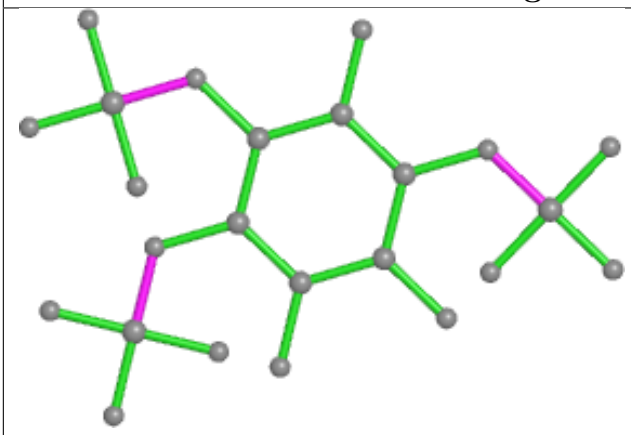


Torsions

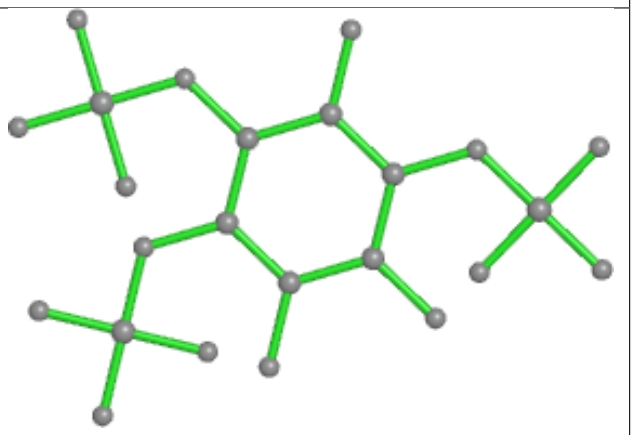


Rings

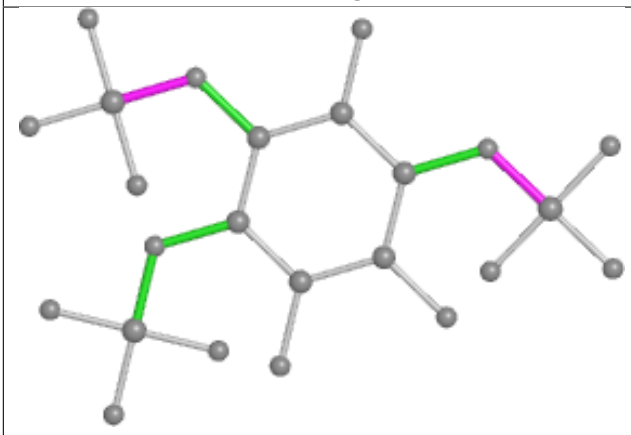
Ligand I3P D 2702



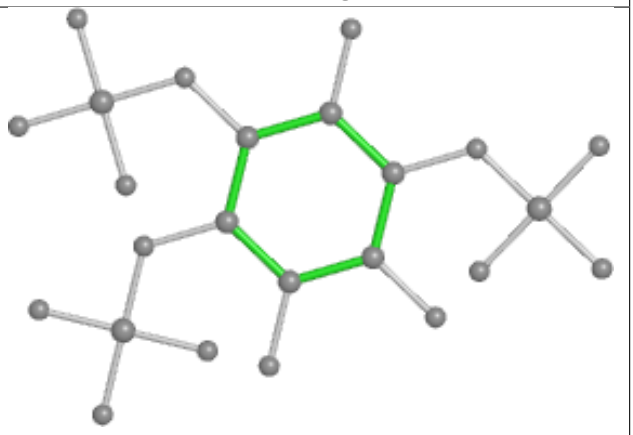
Bond lengths



Bond angles

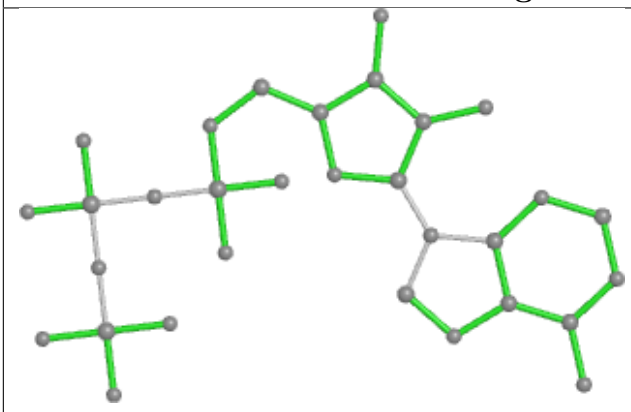


Torsions

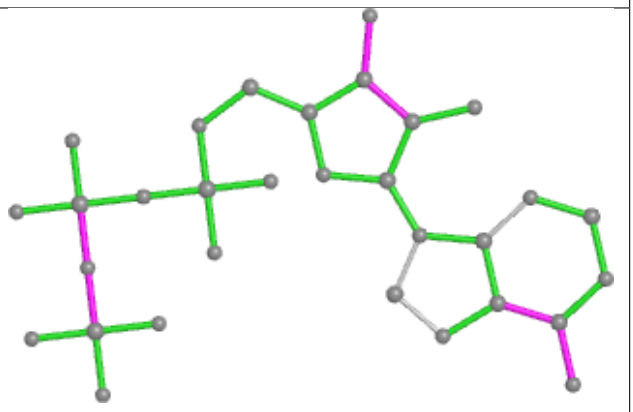


Rings

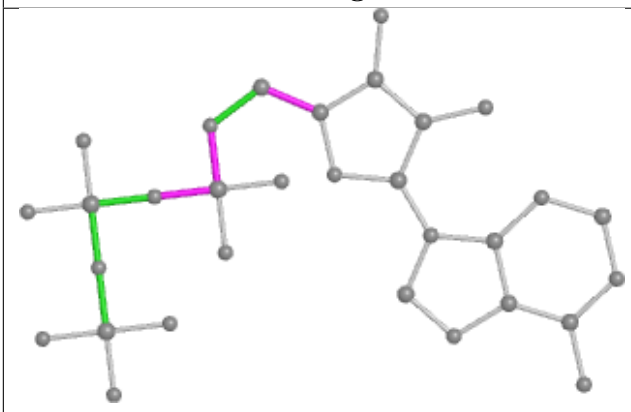
Ligand ATP D 2703



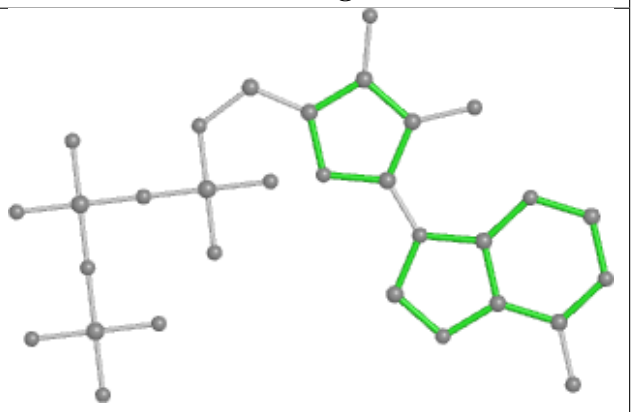
Bond lengths



Bond angles

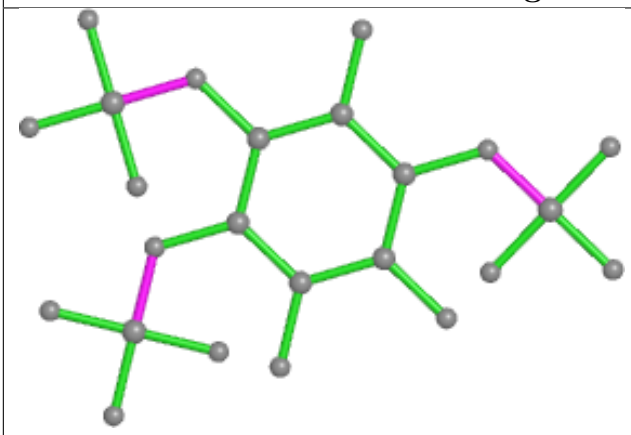


Torsions

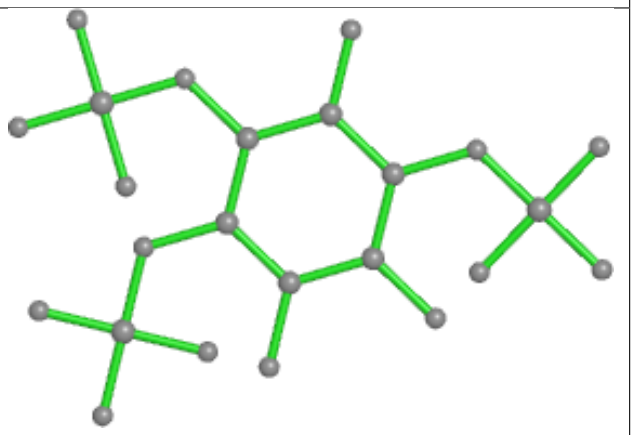


Rings

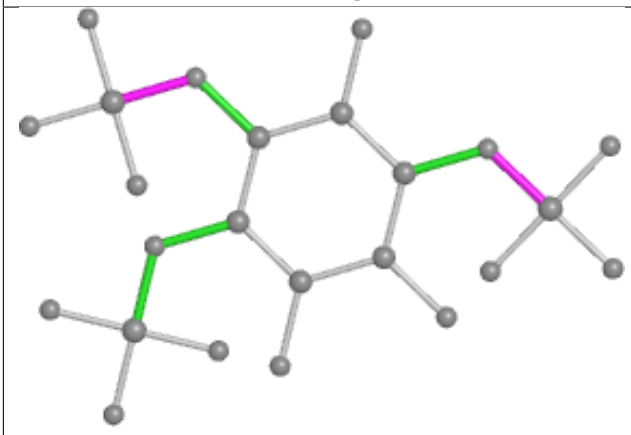
Ligand I3P A 2702



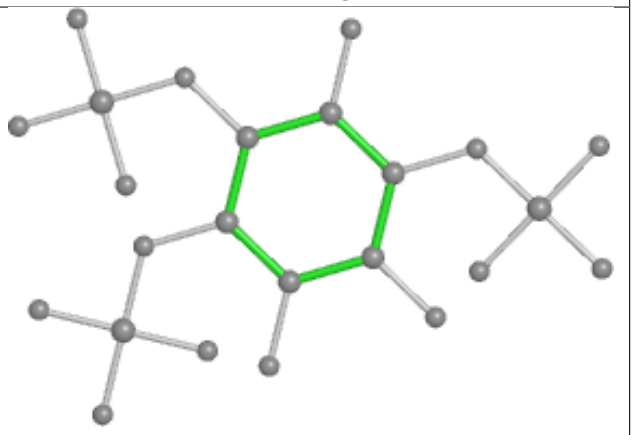
Bond lengths



Bond angles

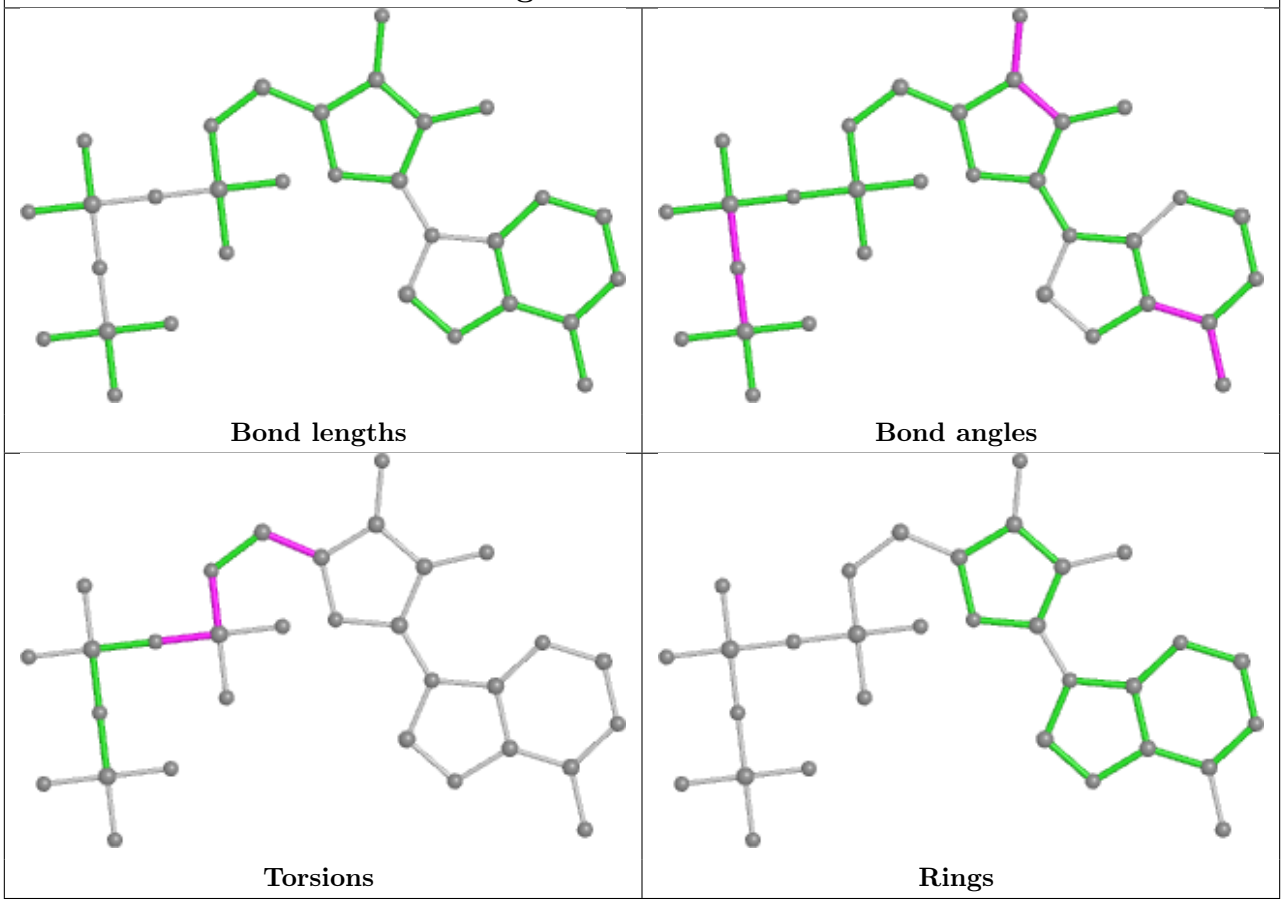


Torsions



Rings

Ligand ATP A 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	25.33
1	B	2611:VAL	C	2628:UNK	N	25.33

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	25.33
1	D	2611:VAL	C	2628:UNK	N	25.33

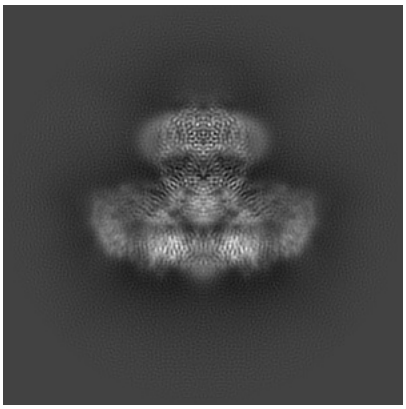
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25667. These allow visual inspection of the internal detail of the map and identification of artifacts.

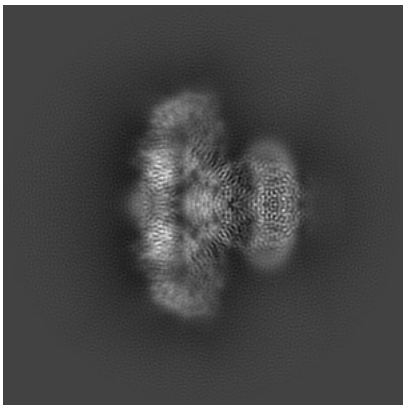
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

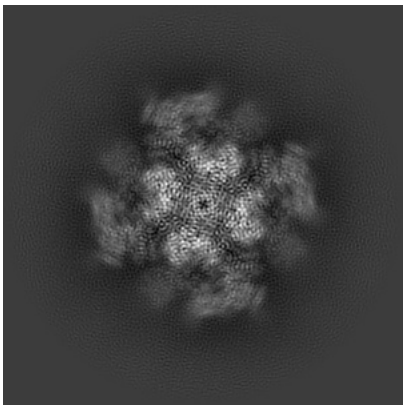
6.1.1 Primary map



X

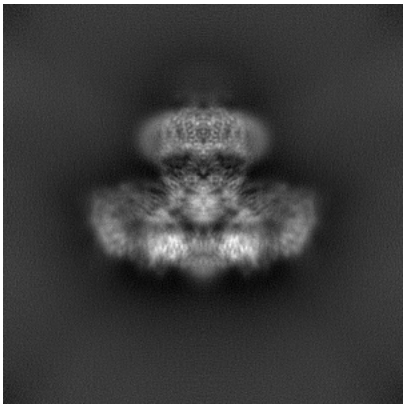


Y

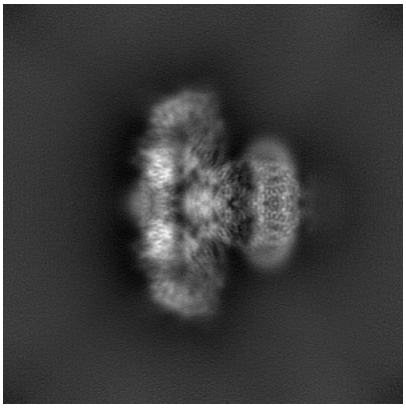


Z

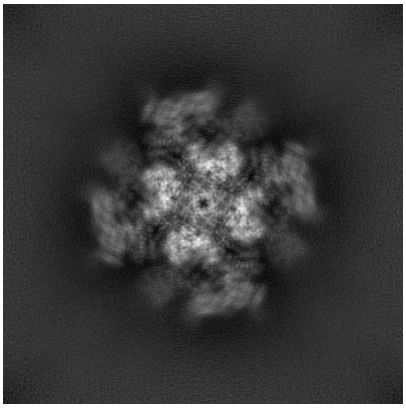
6.1.2 Raw map



X



Y

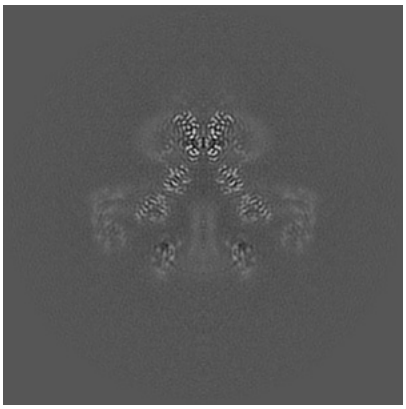


Z

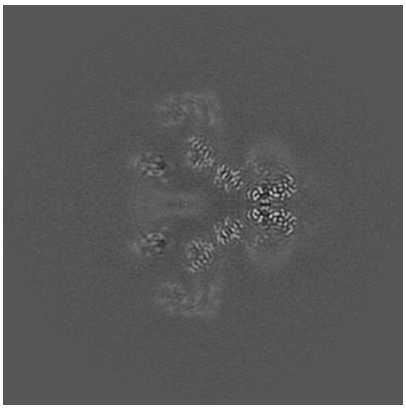
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

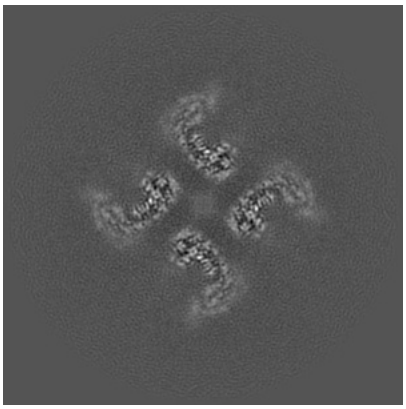
6.2.1 Primary map



X Index: 240

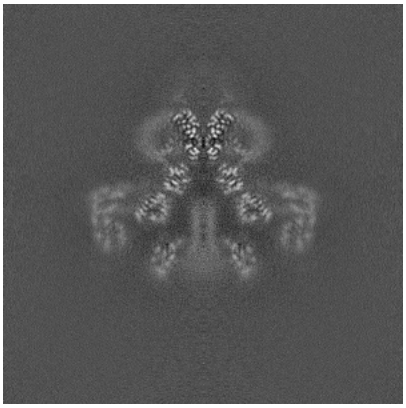


Y Index: 240

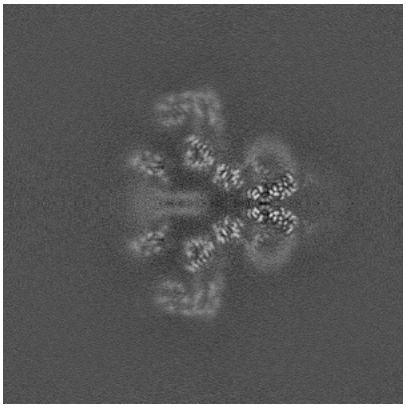


Z Index: 240

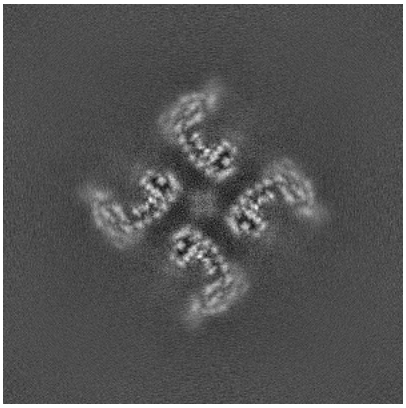
6.2.2 Raw map



X Index: 240



Y Index: 240

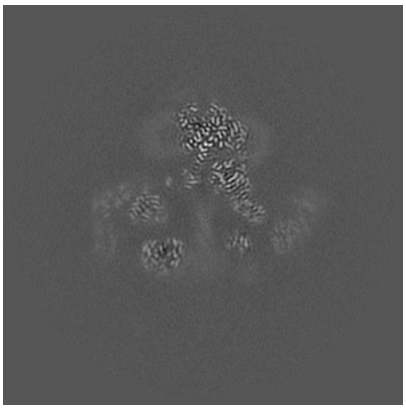


Z Index: 240

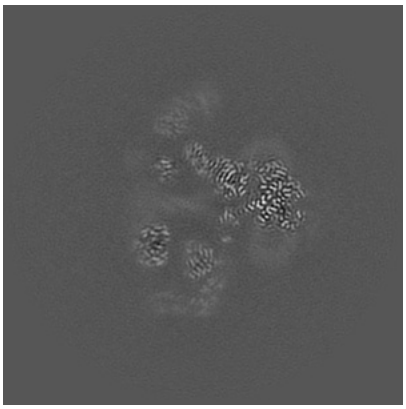
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

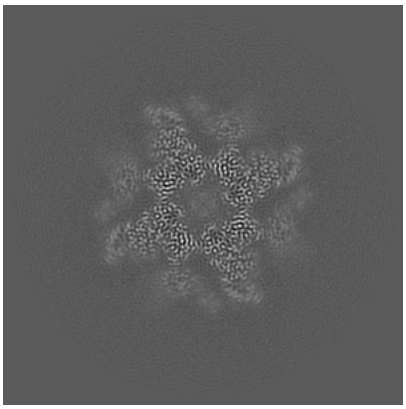
6.3.1 Primary map



X Index: 250

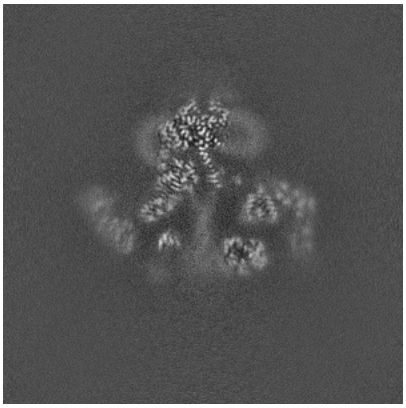


Y Index: 230

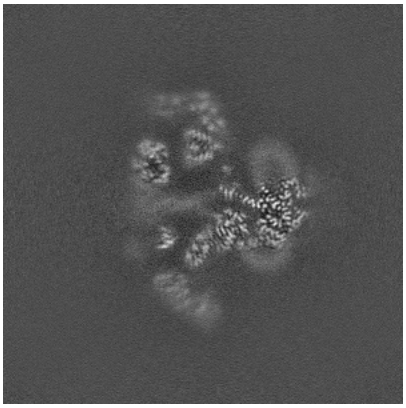


Z Index: 188

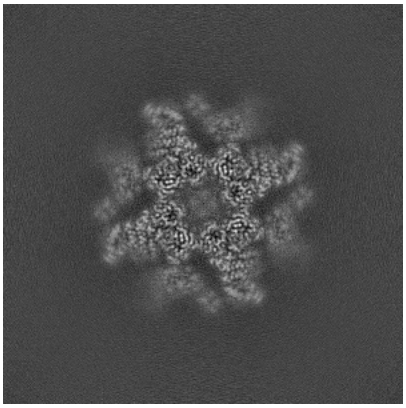
6.3.2 Raw map



X Index: 229



Y Index: 251

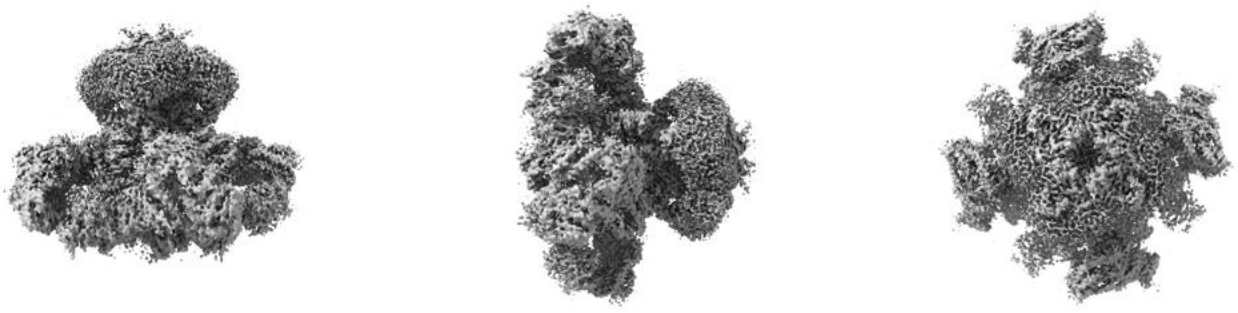


Z Index: 189

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

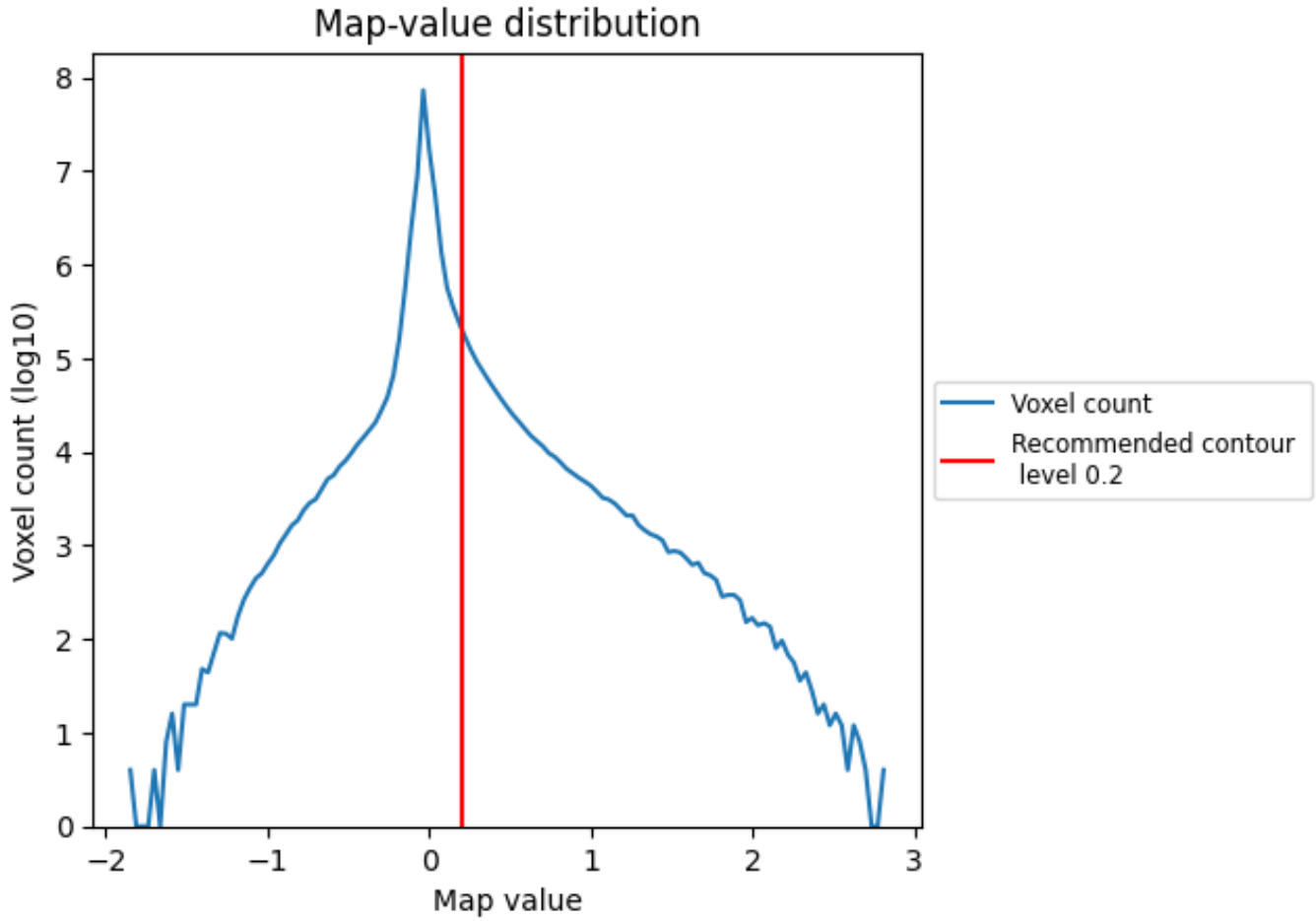
6.5 Mask visualisation (i)

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

7 Map analysis

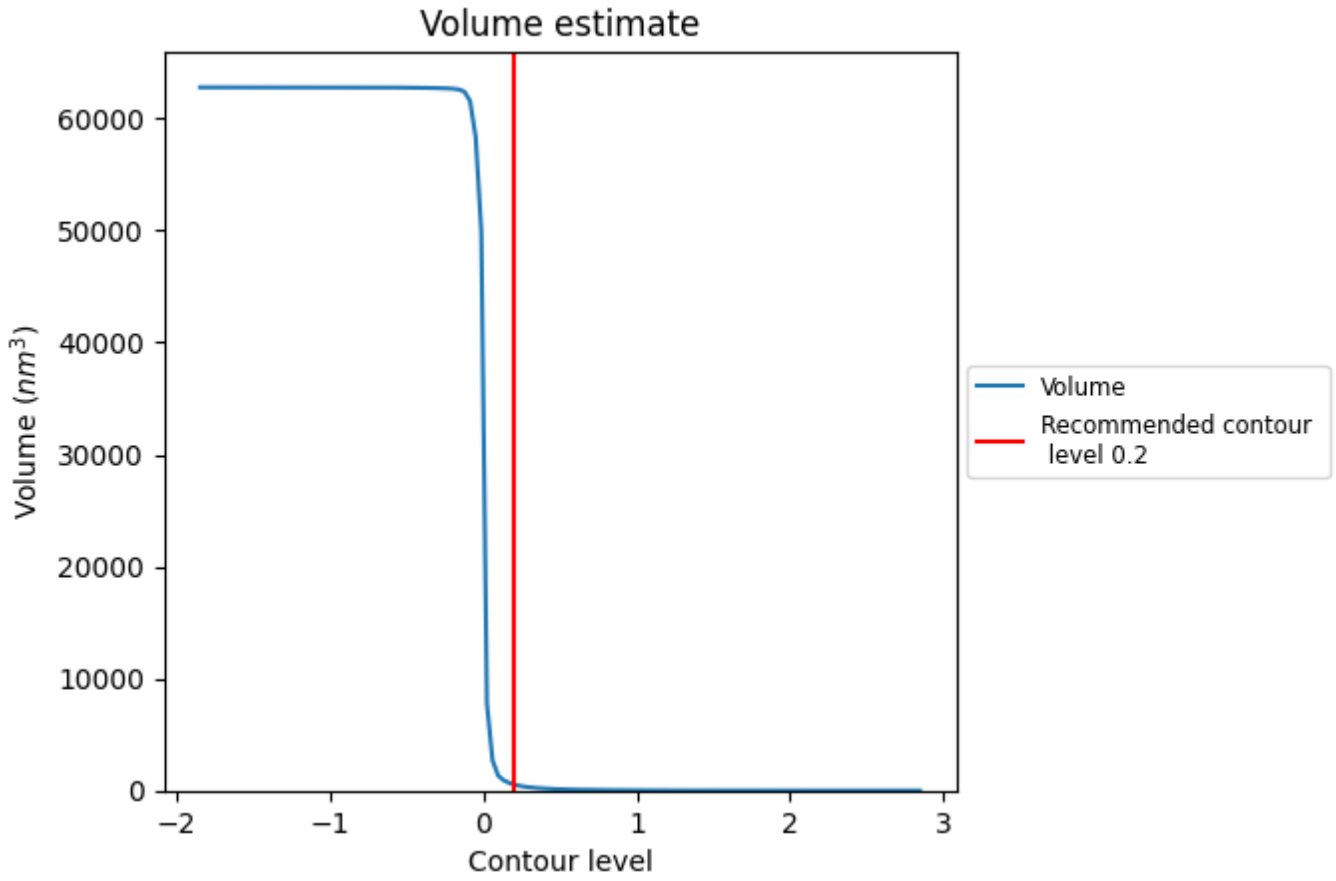
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

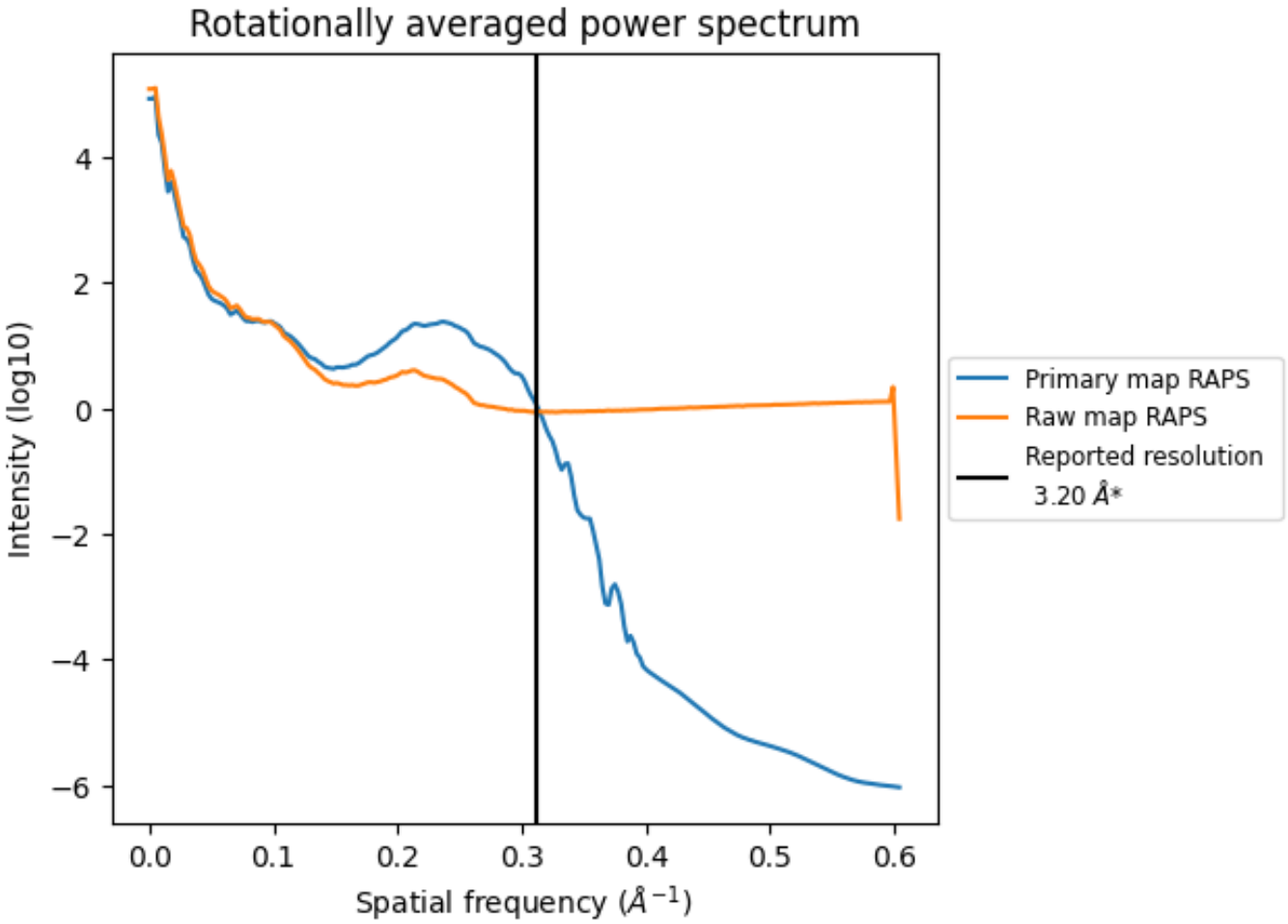
7.2 Volume estimate (i)



The volume at the recommended contour level is 544 nm^3; this corresponds to an approximate mass of 491 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)

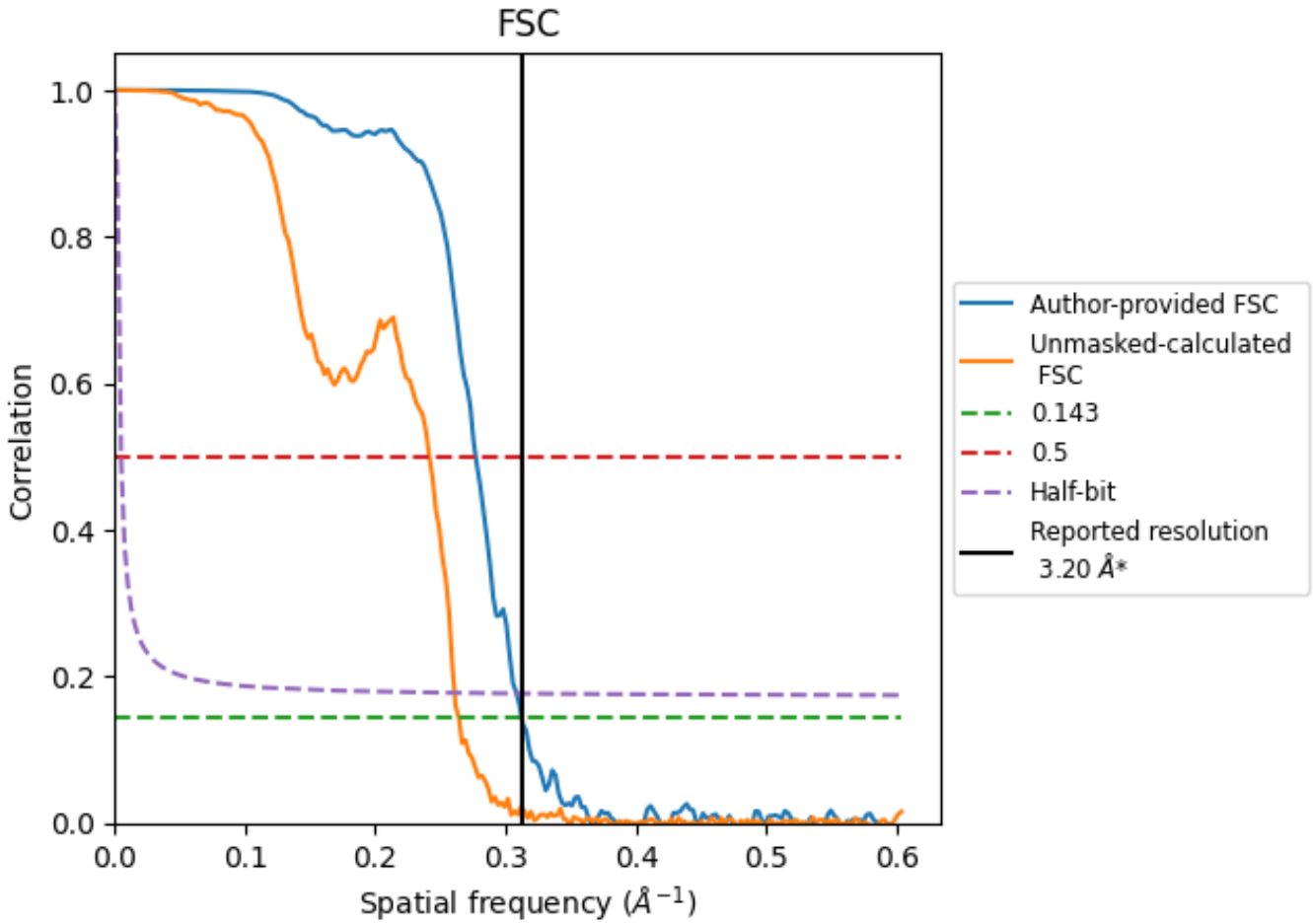


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

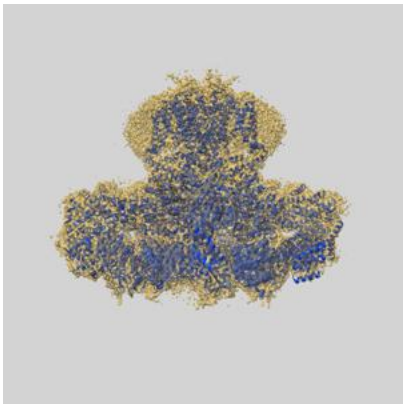
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.61	3.24
Unmasked-calculated*	3.79	4.14	3.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 3.2 by more than 10 %

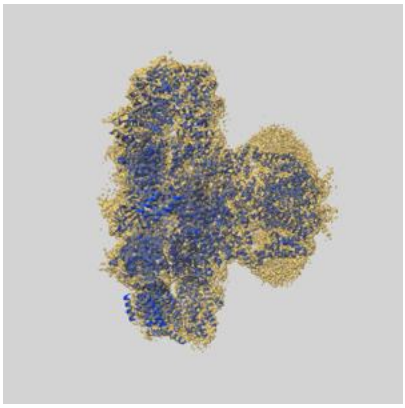
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25667 and PDB model 7T3P. Per-residue inclusion information can be found in section 3 on page 6.

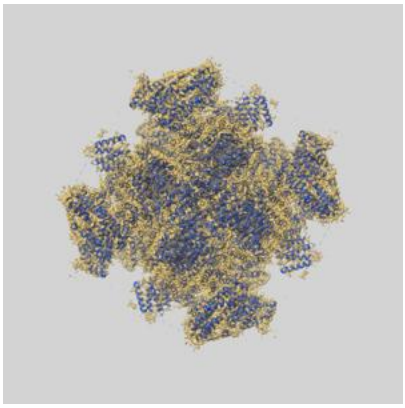
9.1 Map-model overlay



X



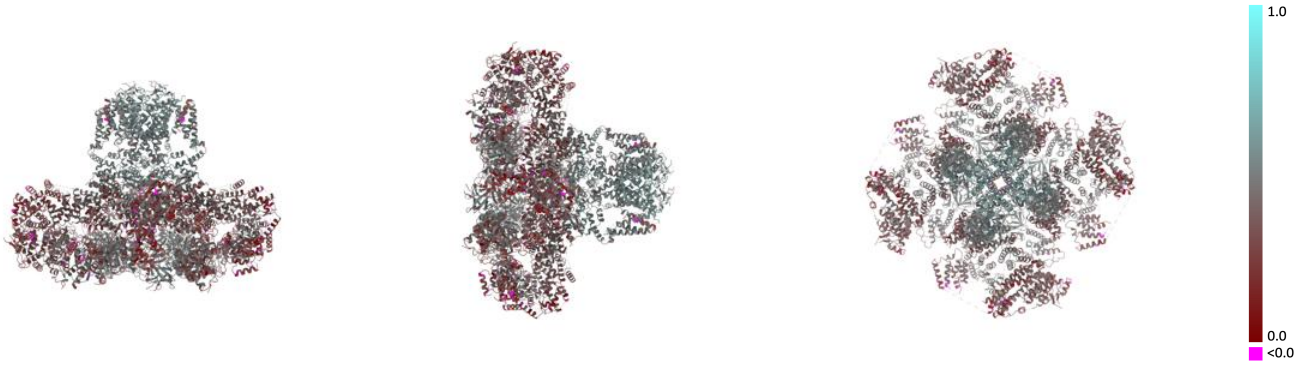
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

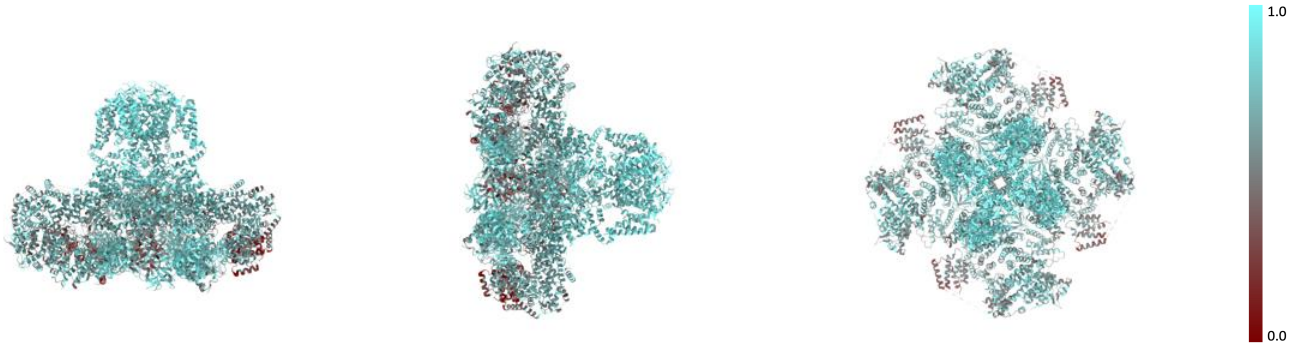
9.2 Q-score mapped to coordinate model (i)



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.

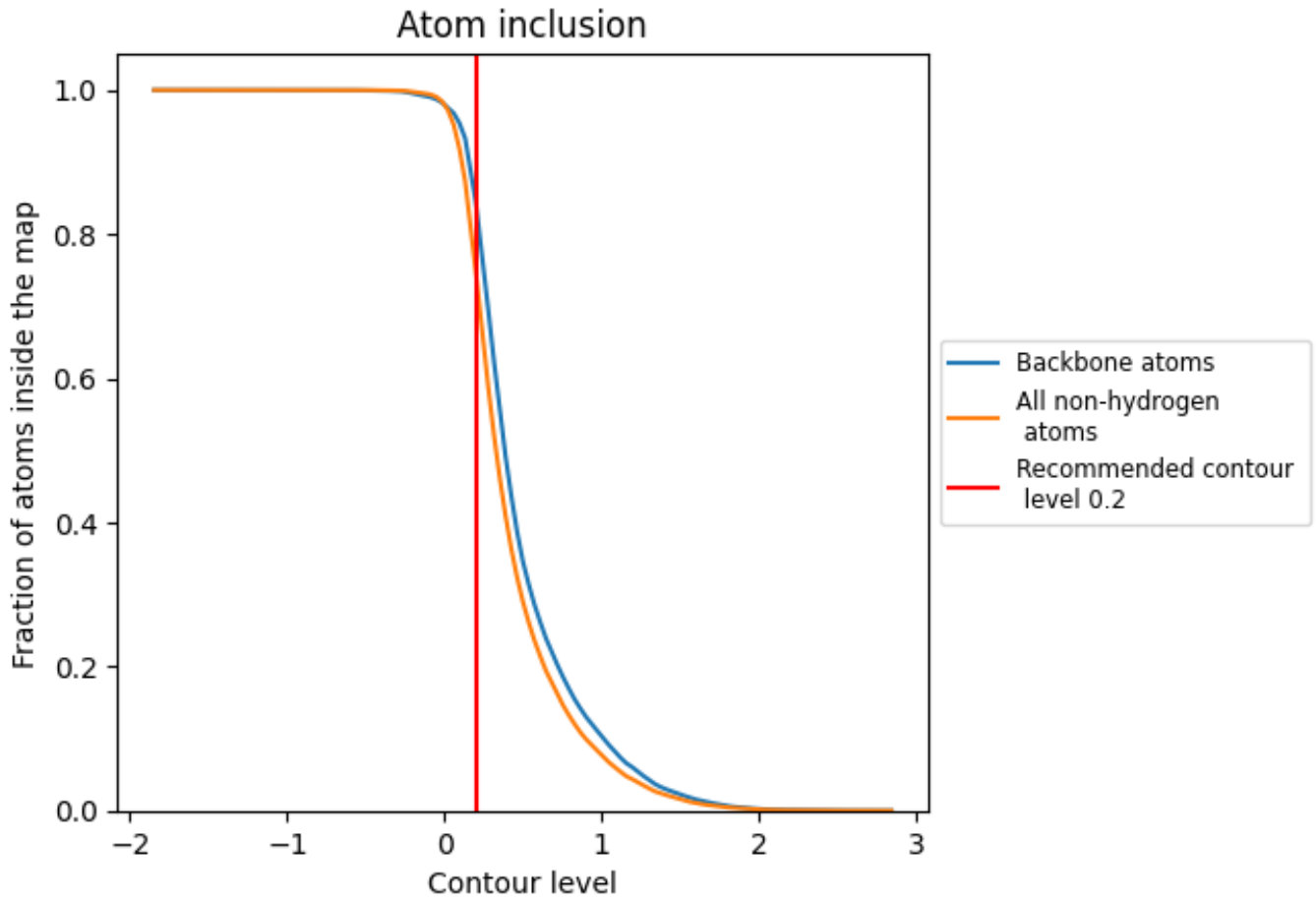
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 75% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7496	0.3990
A	0.7512	0.4020
B	0.7445	0.3910
C	0.7514	0.4020
D	0.7513	0.4020