



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:46 PM UTC

PDB ID : 7T3P / pdb_00007t3p
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

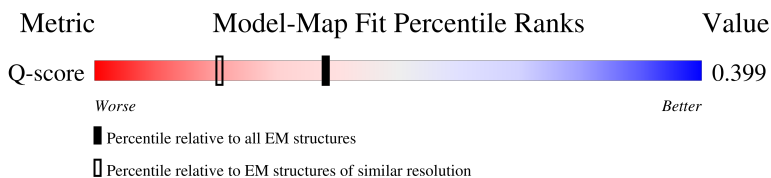
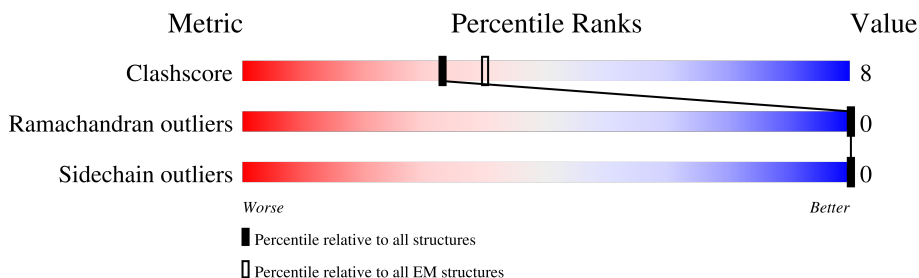
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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 $\leq 5\%$. 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% 15% 22%
1	B	2633	7% 63% 15% 22%
1	C	2633	6% 64% 15% 22%
1	D	2633	6% 63% 15% 22%

2 Entry composition

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.

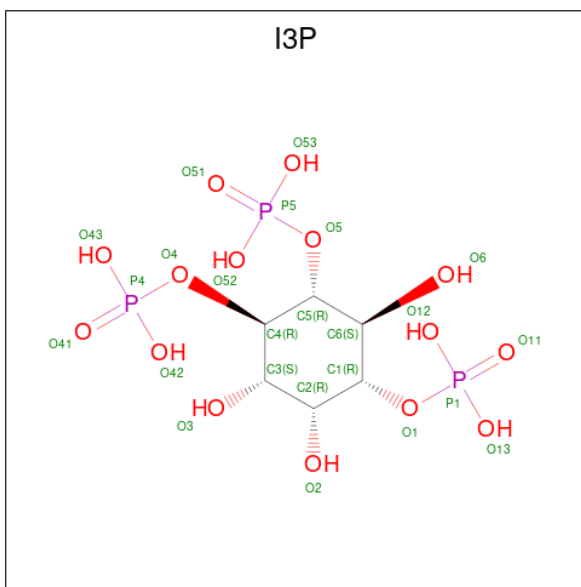
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

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 (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

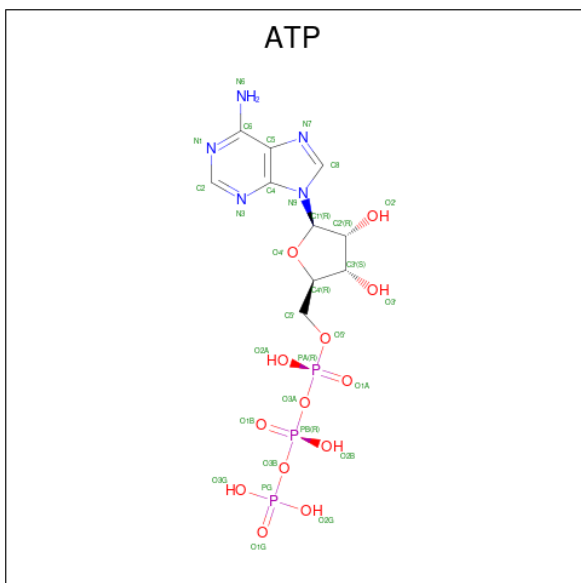
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: I3P) (formula: C₆H₁₅O₁₅P₃) (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 (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

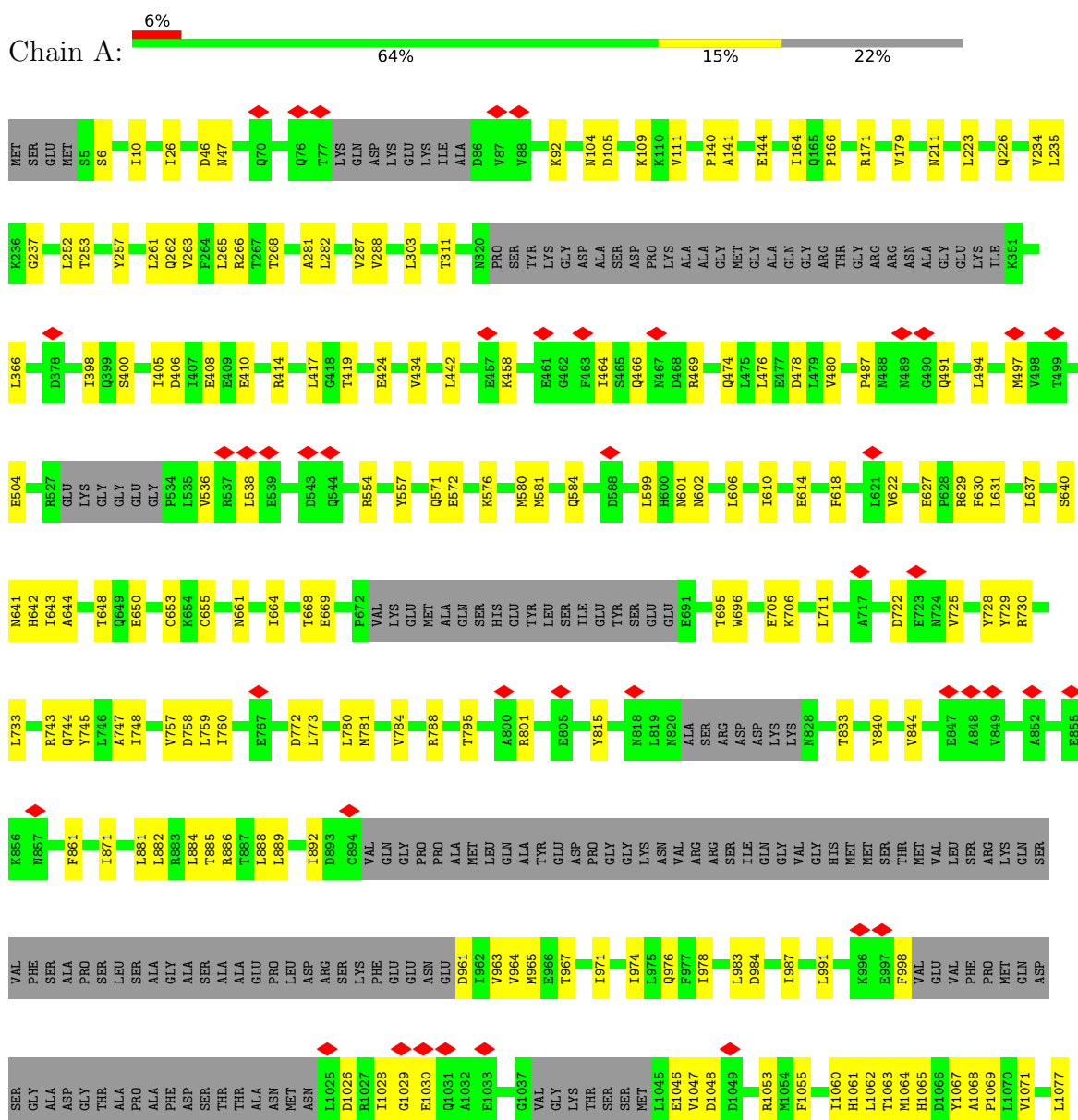


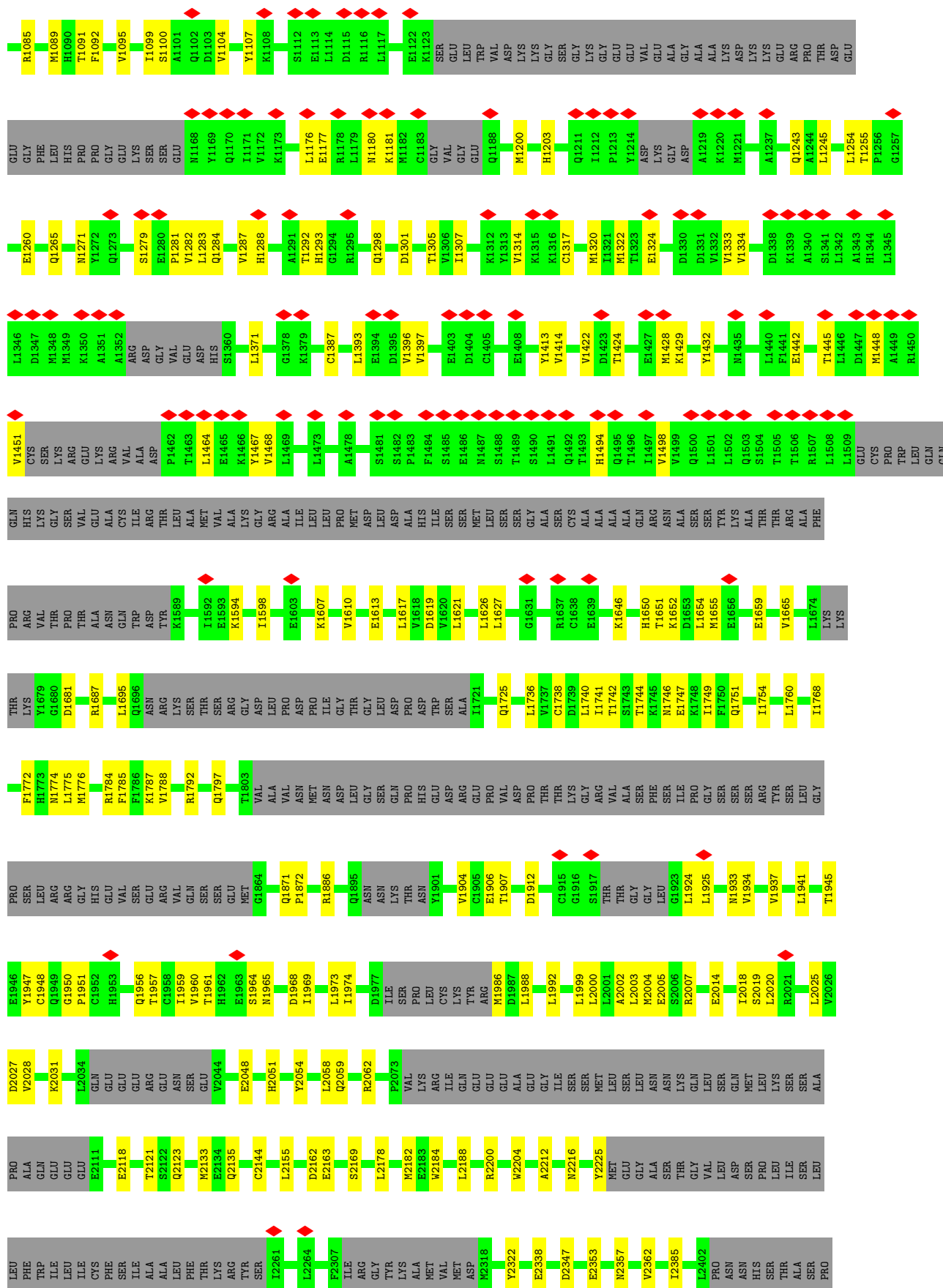
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0

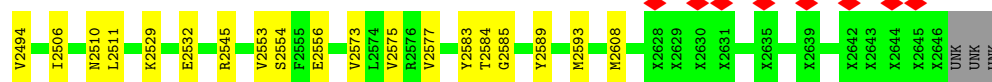
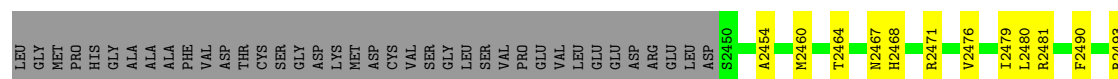
3 Residue-property plots

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.

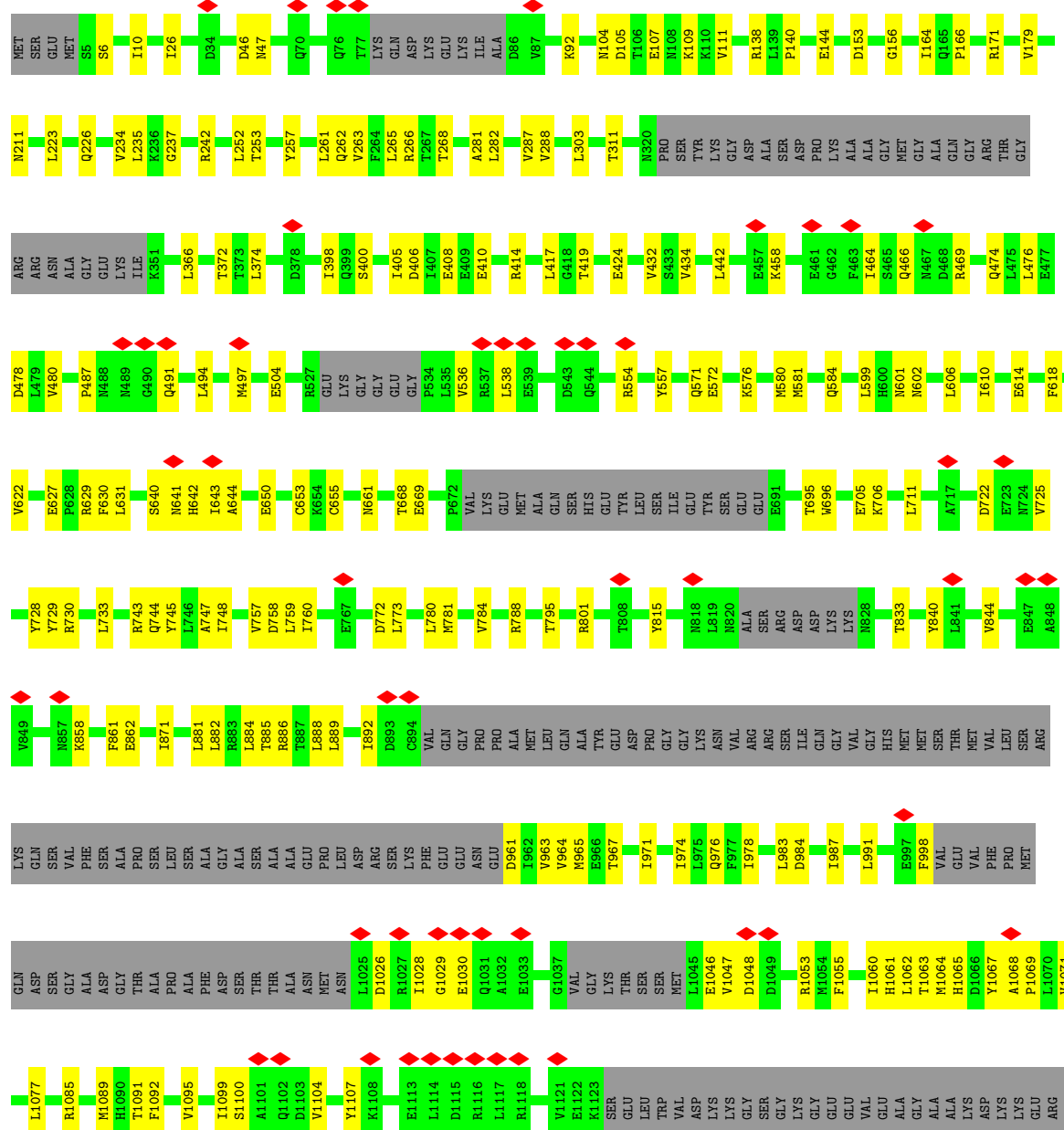
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3







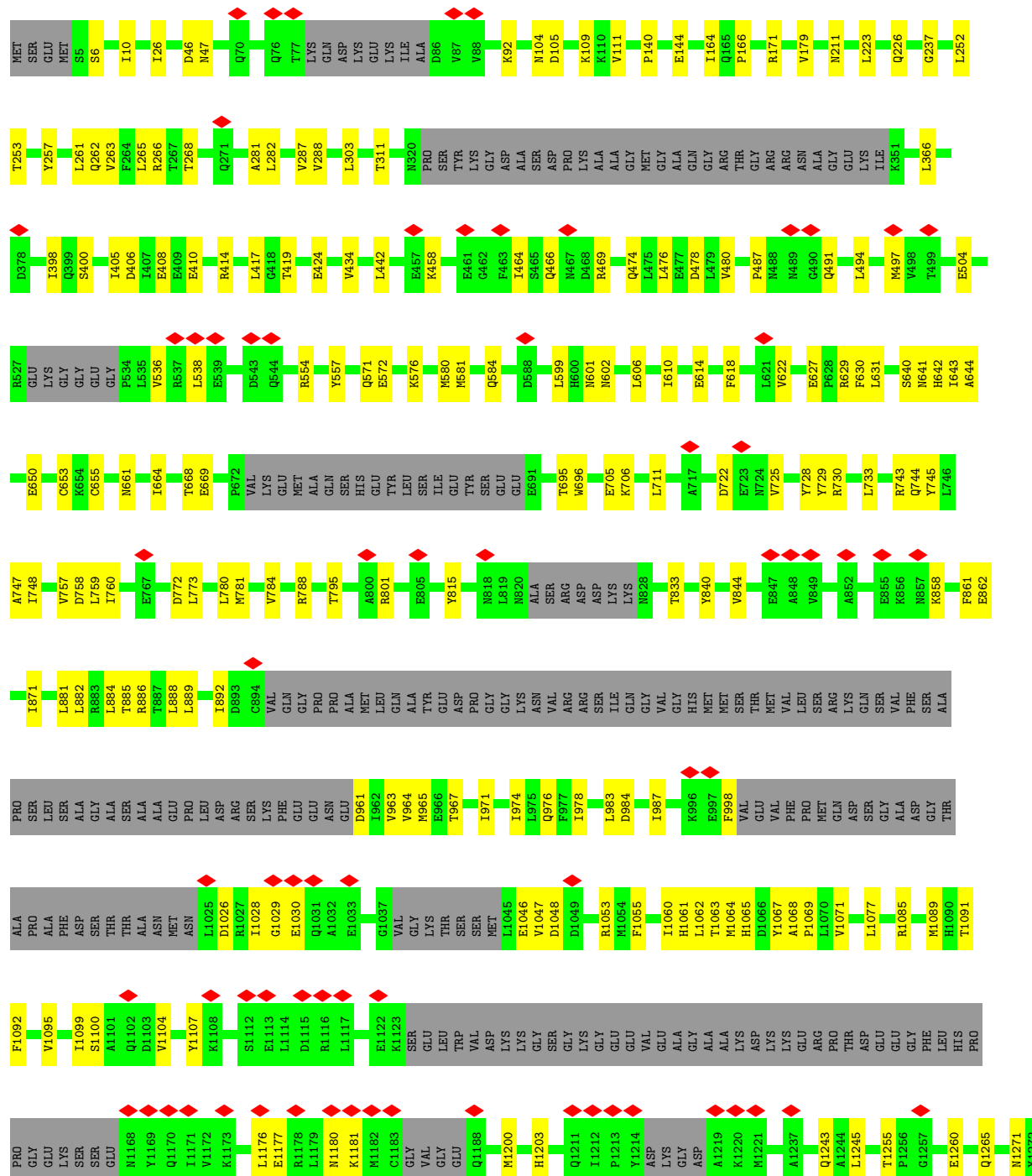
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3



THR	ASP	GLU	GLU	GLY	PHE	LEU	HIS	PRO	PRO	GLY	GLU	LYS	SER	SER	GLU	M168	Y169	Q1170	I1171	V1172	K1173	G1174	I1175	L1176	E1177	R1178	L1179	N1180	K1181	M1182	C1183	GLY	VAL	GLY	GLU	Q1188	M1200	H1203	Q1211	I1212	P1213	Y1214	ASP	LYS	GLY	ASP	A1219	K1220	M1221	M1222	E1223	R1226	A1237	
Q1243	A1244	L1245	T1255	E1260	Q1265	N1271	S1279	E1280	P1281	V1282	L1283	Q1284	V1287	H1288	T1292	H1293	G1294	R1295	Q1298	D1301	T1305	V1306	I1307	K1312	Y1313	V1314	K1315	K1316	C1317	Q1318	D1319	M1320	I1321	M1322	E1323	N1327	D1330	D1331	V1332	V1333	V1334	D1338	K1339	A1340										
S1341	L1342	A1343	L1346	D1347	K1350	A1351	A1352	ARG	ASP	GLY	VAL	GLU	ASP	HIS	S1360	M1363	L1371	K1379	M1380	C1387	L1393	E1394	D1395	V1396	V1397	E1403	D1404	C1405	E1408	Y1413	V1414	V1422	D1423	T1424	E1427	M1428	K1429	Y1432	M1435	L1440	M1443	D1447												
M1448	A1449	R1450	V1451	CYS	SER	LYS	VAL	ARG	ALA	LYS	ARG	VAL	P1462	T1463	L1464	E1465	K1466	Y1467	Y1468	L1469	S1470	L1473	A1478	S1481	S1482	S1485	E1486	N1487	S1488	T1489	S1490	L1491	Q1492	T1493	H1494	Q1495	T1496	I1497	V1498	V1499	Q1500	L1501	L1502	Q1503	T1504	T1505	T1506	R1507	L1508	L1509	GLU	CYS	PRO	TRP
LEU	GLN	GLN	HIS	LYS	GLY	SER	VAL	GLU	ALA	LYS	ILE	ARG	THR	ALA	ALA	LYS	GLY	ARG	ALA	ILE	LEU	LEU	PRO	MET	SER	SER	GLY	ALA	SER	CYS	ALA	ALA	ALA	GLN	ARG	ASN	ALA	SER	SER	TYR	LYS	THR	THR											
ARG	ALA	PHE	PRO	ARG	VAL	THR	PRO	ASN	GLN	TRP	ASP	K1589	I1592	E1593	K1594	I1598	K1607	V1610	E1613	L1617	V1618	D1619	V1620	L1621	L1626	L1627	E1633	R1637	C1638	E1639	K1646	H1650	T1651	K1652	D1653	L1654	M1655	E1656	S1657	E1658	E1659	V1665	L1674											
LYS	LYS	THR	LYS	Y1679	G1680	D1681	R1687	L1695	Q1696	ASN	ARG	LYS	THR	SER	ARG	GLY	LEU	PRO	ASP	ILE	THR	GLY	LEU	ASP	ALA	I1721	Q1725	L1736	V1737	C1738	L1740	I1741	T1742	S1743	T1744	K1745	N1746	E1747	K1748	F1750	Q1751	I1754	L1760											
I1768	F1772	H1773	N1774	L1775	M1776	K1781	R1784	F1785	F1786	K1787	V1788	R1792	T1803	VAL	ALA	VAL	ASN	MET	ASP	GLY	LEU	ASN	GLN	PRO	HIS	GLU	ASP	ARG	GLU	PRO	VAL	ASP	THR	THR	LYS	ARG	VAL	SER	PHE	SER	ILE	PRO	GLY	LEU										
LEU	GLY	PRO	SER	LEU	ARG	GLY	HIS	VAL	GLU	SER	GLU	VAL	G1864	Q1871	P1872	R1886	Q1895	ASN	ASN	LYS	THR	ASN	Y1901	T1907	D1912	C1915	G1916	S1917	THR	THR	GLY	GLY	LEU	G1923	L1924	L1925	N1933	V1934	V1937	L1941	T1945	E1946												
Y1947	C1948	Q1949	G1950	P1951	C1952	H1953	Q1956	I1959	V1960	T1961	S1964	N1965	D1968	I1969	L1973	I1974	D1977	ILE	SER	PRO	LEU	ARG	CYS	LYS	TYR	M1986	D1987	L1988	L1992	L1999	L2000	L2001	L2003	M2004	E2005	S2006	R2007	E2014	T2018	S2019	L2020	R2021	L2025	V2026	D2027	V2028								
K2031	L2034	GLN	GLU	GLU	GLU	ARG	Q1956	I1959	V1960	T1961	S1964	N1965	D1968	I1969	L1973	I1974	D1977	ILE	SER	PRO	LEU	ARG	CYS	LYS	TYR	M1986	D1987	L1988	L1992	L1999	L2000	L2001	L2003	M2004	E2005	S2006	R2007	E2014	T2018	S2019	L2020	R2021	L2025	V2026	D2027	V2028								
GLU	GLU	E2111	E2118	T2121	Q2123	E2133	E2134	Q2135	C2144	L2155	D2162	E2163	S2169	L2178	M2182	E2183	W2184	L2188	R2200	W2204	A2212	N2216	Y2225	GLU	GLY	ALA	SER	THR	GLY	VAL	LEU	ASP	SER	PRO	LEU	ILE	SER	LEU	LEU	PHE	TRP													
ILE	LEU	ILE	CYS	PHE	ILE	ALA	ALA	ALA	VAL	THR	LYS	ARG	TYR	SER	I2261	L2264	F2307	ILE	ARG	GLY	TYR	ALA	VAL	MET	M2318	L2321	Y2322	H2323	V2324	S2342	D2347	E2353	N2357	V2362	A2376	L2402	PRO	ASN	ASN	HIS	SER	THR	ALA	SER	PRO									
LEU	GLY	MET	PRO	HIS	GLY	ALA	ALA	VAL	THR	LYS	CYS	SER	GLY	ASP	MET	VAL	CYS	VAL	SER	GLY	LEU	SER	GLU	GLU	ASP	S2450	A2454	N2460	T2464	N2467	H2468	R2471	V2476	I2479	L2480	R2481	F2490	R2493																



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





Chain D: 6% 63% 15% 22%





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.18	0/16897	0.29	0/22813
1	B	0.18	0/16897	0.29	0/22813
1	C	0.18	0/16897	0.29	0/22813
1	D	0.18	0/16897	0.29	0/22813
All	All	0.18	0/67588	0.29	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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16692	0	16773	286	0
1	B	16692	0	16773	295	0
1	C	16692	0	16773	290	0
1	D	16692	0	16773	287	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	1124	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 1124 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:140:PRO:HD2	1:C:1428:MET:HE2	1.33	1.10
1:B:140:PRO:CD	1:C:1428:MET:HE2	1.87	1.03
1:A:1428:MET:HE2	1:D:140:PRO:HD2	1.45	0.99
1:C:140:PRO:HD2	1:D:1428:MET:HE2	1.46	0.97
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.09	0.86

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 ⓘ

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%)	1865 (100%)	0	100	100
1	B	1865/2329 (80%)	1865 (100%)	0	100	100
1	C	1865/2329 (80%)	1865 (100%)	0	100	100
1	D	1865/2329 (80%)	1865 (100%)	0	100	100
All	All	7460/9316 (80%)	7460 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1930	ASN
1	D	1773	HIS
1	C	744	GLN
1	D	1487	ASN
1	D	744	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	0
4	ATP	D	2703	-	32,33,33	0.35	0	48,52,52	0.69	1 (2%)
3	I3P	A	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	0
3	I3P	C	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	0
3	I3P	B	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	0
4	ATP	C	2703	-	32,33,33	0.35	0	48,52,52	0.69	1 (2%)
4	ATP	A	2703	-	32,33,33	0.35	0	48,52,52	0.69	1 (2%)
4	ATP	B	2703	-	32,33,33	0.35	0	48,52,52	0.69	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	-	-	3/15/39/39	0/1/1/1
4	ATP	D	2703	-	-	4/22/38/38	0/3/3/3
3	I3P	A	2702	-	-	3/15/39/39	0/1/1/1
3	I3P	C	2702	-	-	4/15/39/39	0/1/1/1
3	I3P	B	2702	-	-	3/15/39/39	0/1/1/1
4	ATP	C	2703	-	-	4/22/38/38	0/3/3/3
4	ATP	A	2703	-	-	4/22/38/38	0/3/3/3
4	ATP	B	2703	-	-	4/22/38/38	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	3.10	1.65	1.59
3	A	2702	I3P	P4-O4	3.07	1.64	1.59
3	C	2702	I3P	P4-O4	3.07	1.64	1.59
3	D	2702	I3P	P4-O4	3.07	1.64	1.59
3	A	2702	I3P	P5-O5	2.99	1.64	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2703	ATP	O3'-C3'-C2'	-2.03	105.32	111.82
4	D	2703	ATP	O3'-C3'-C2'	-2.03	105.32	111.82
4	A	2703	ATP	O3'-C3'-C2'	-2.02	105.33	111.82
4	B	2703	ATP	O3'-C3'-C2'	-2.02	105.33	111.82

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

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

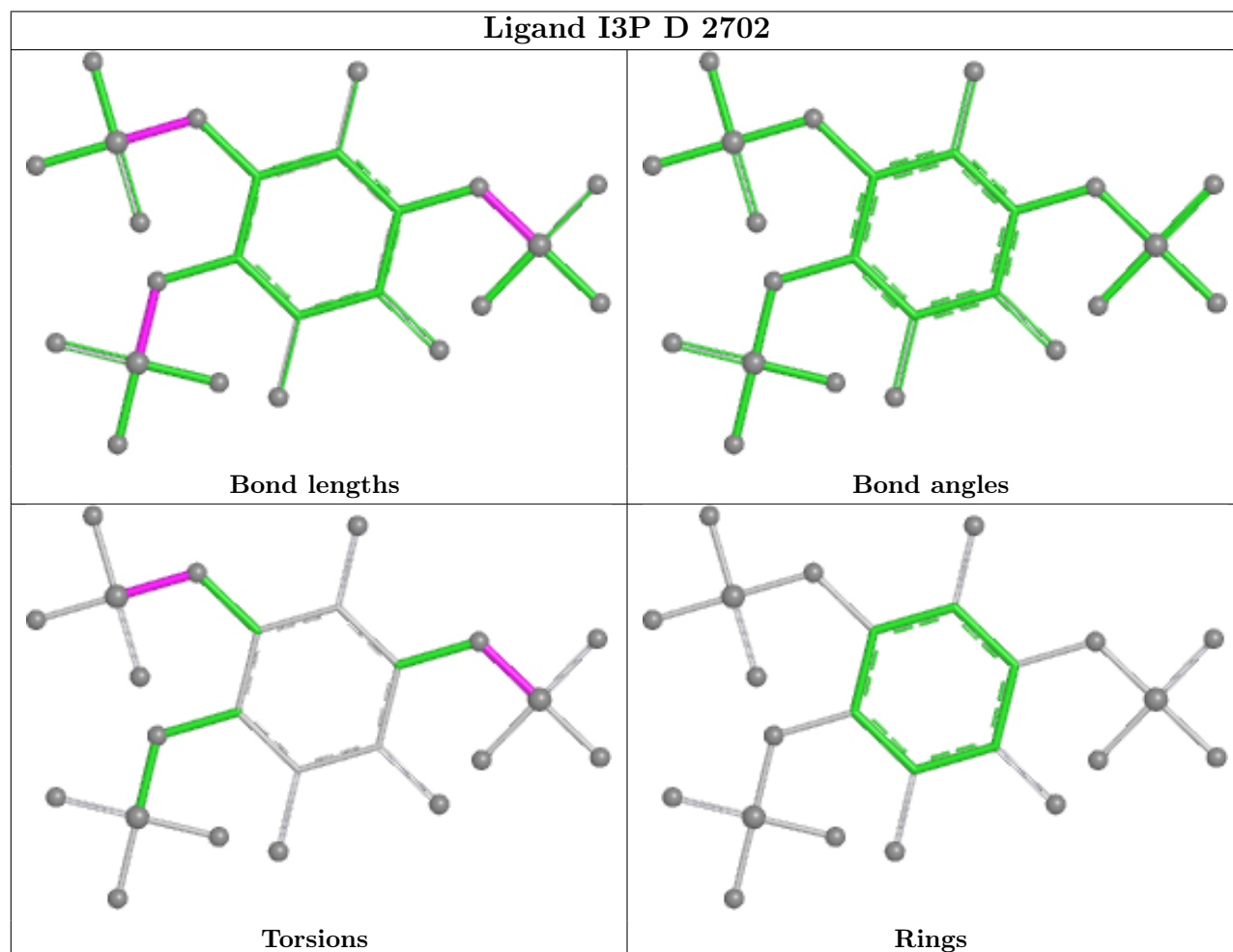
There are no ring outliers.

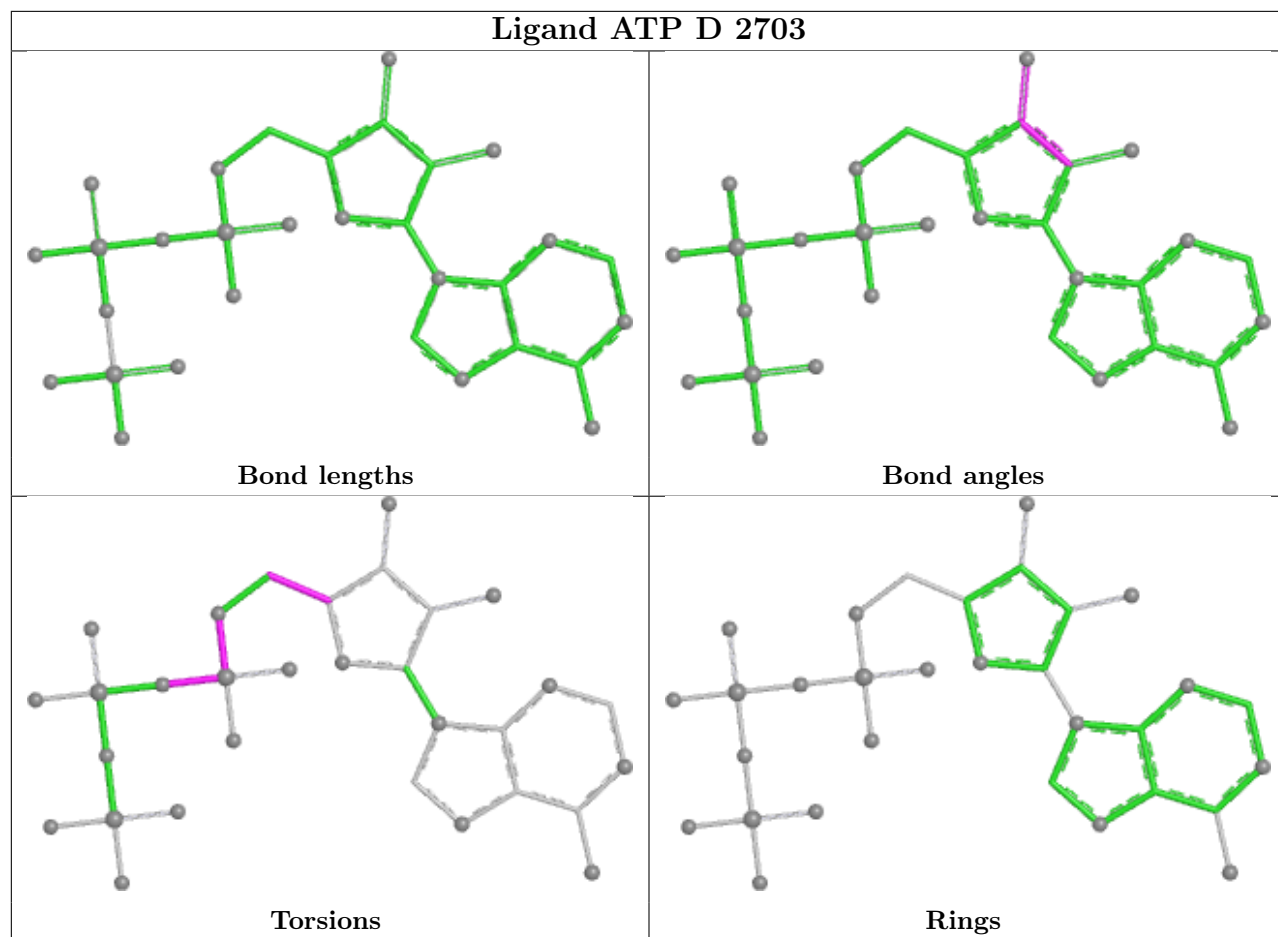
4 monomers are involved in 8 short contacts:

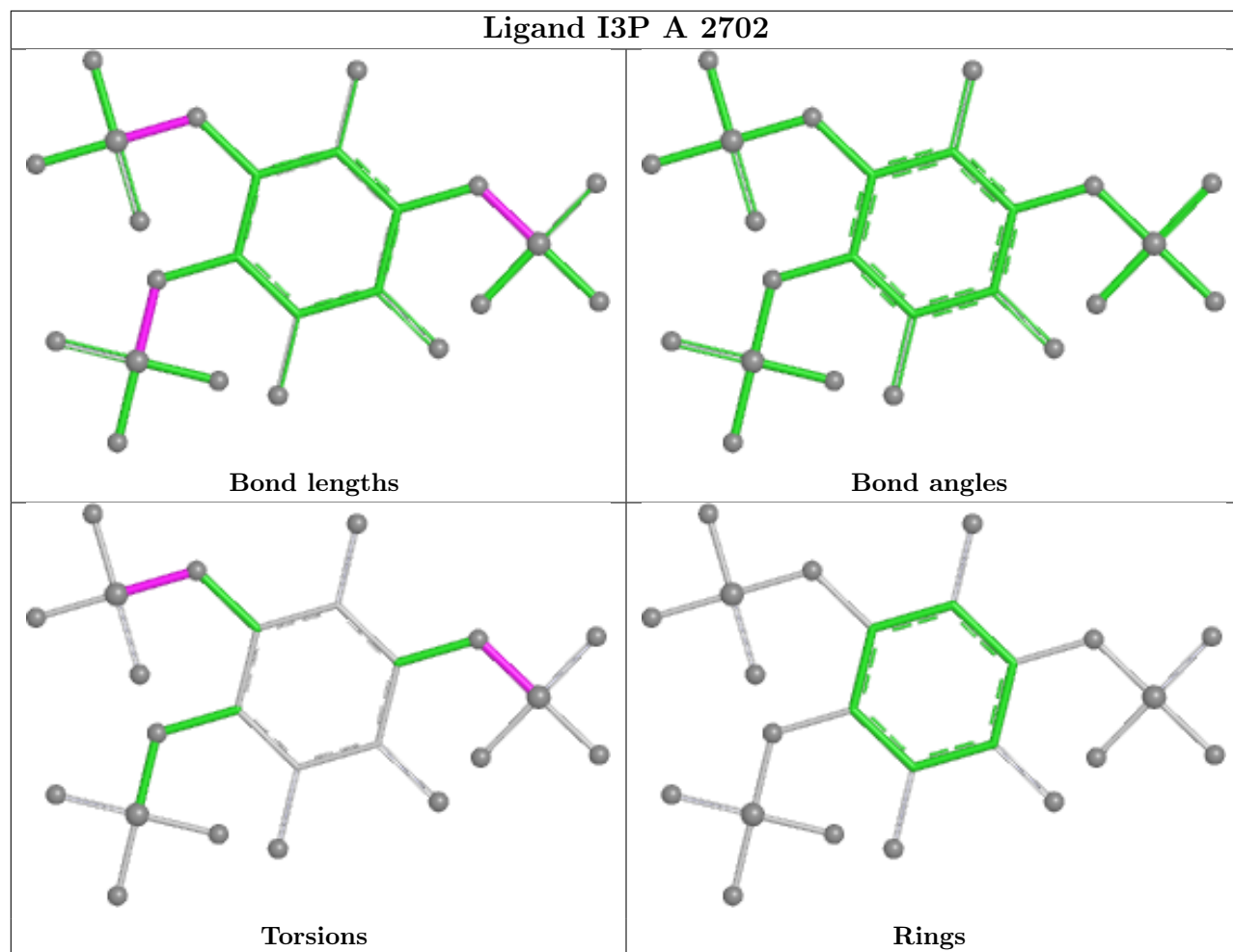
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2702	I3P	2	0
3	A	2702	I3P	2	0
3	C	2702	I3P	2	0
3	B	2702	I3P	2	0

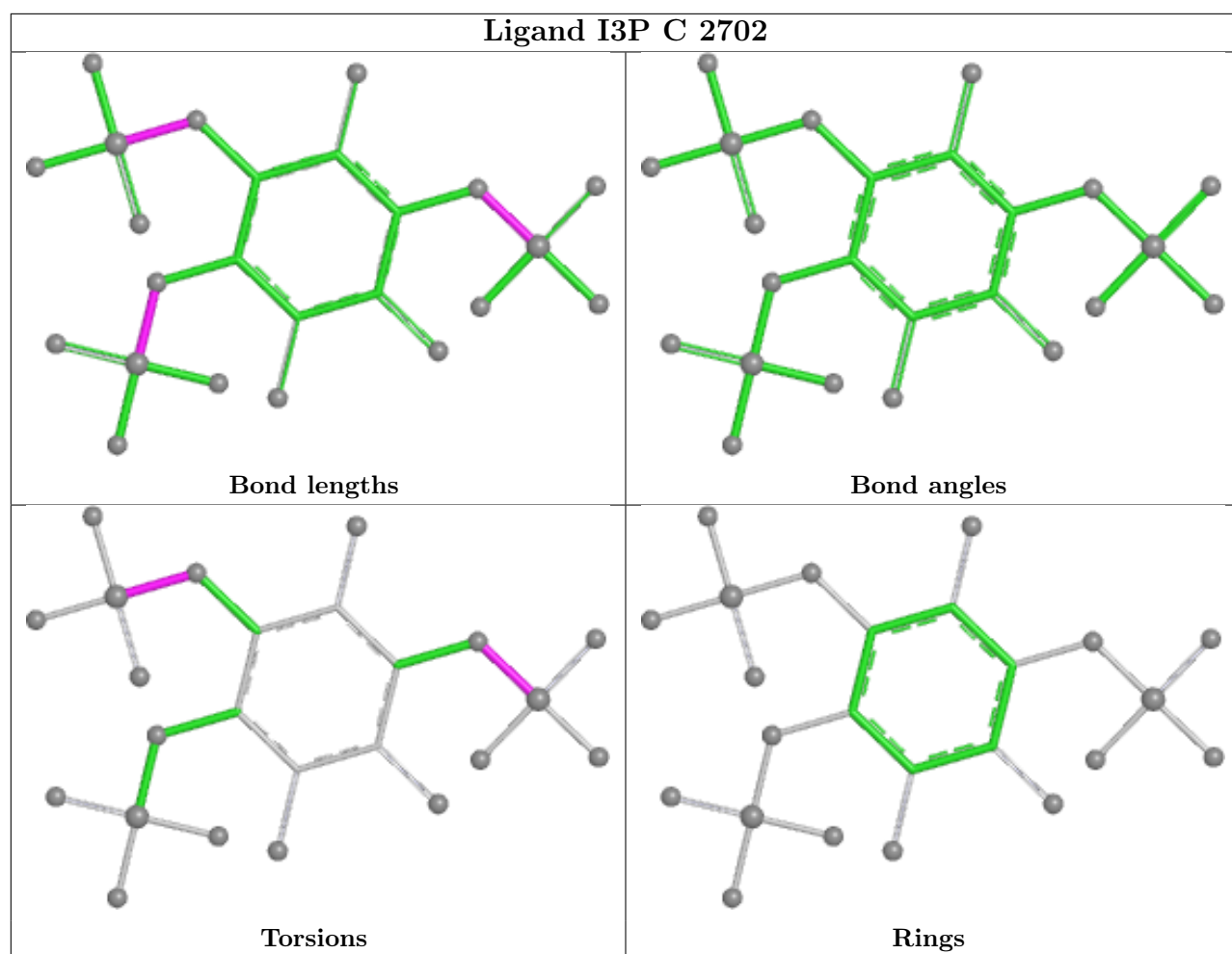
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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

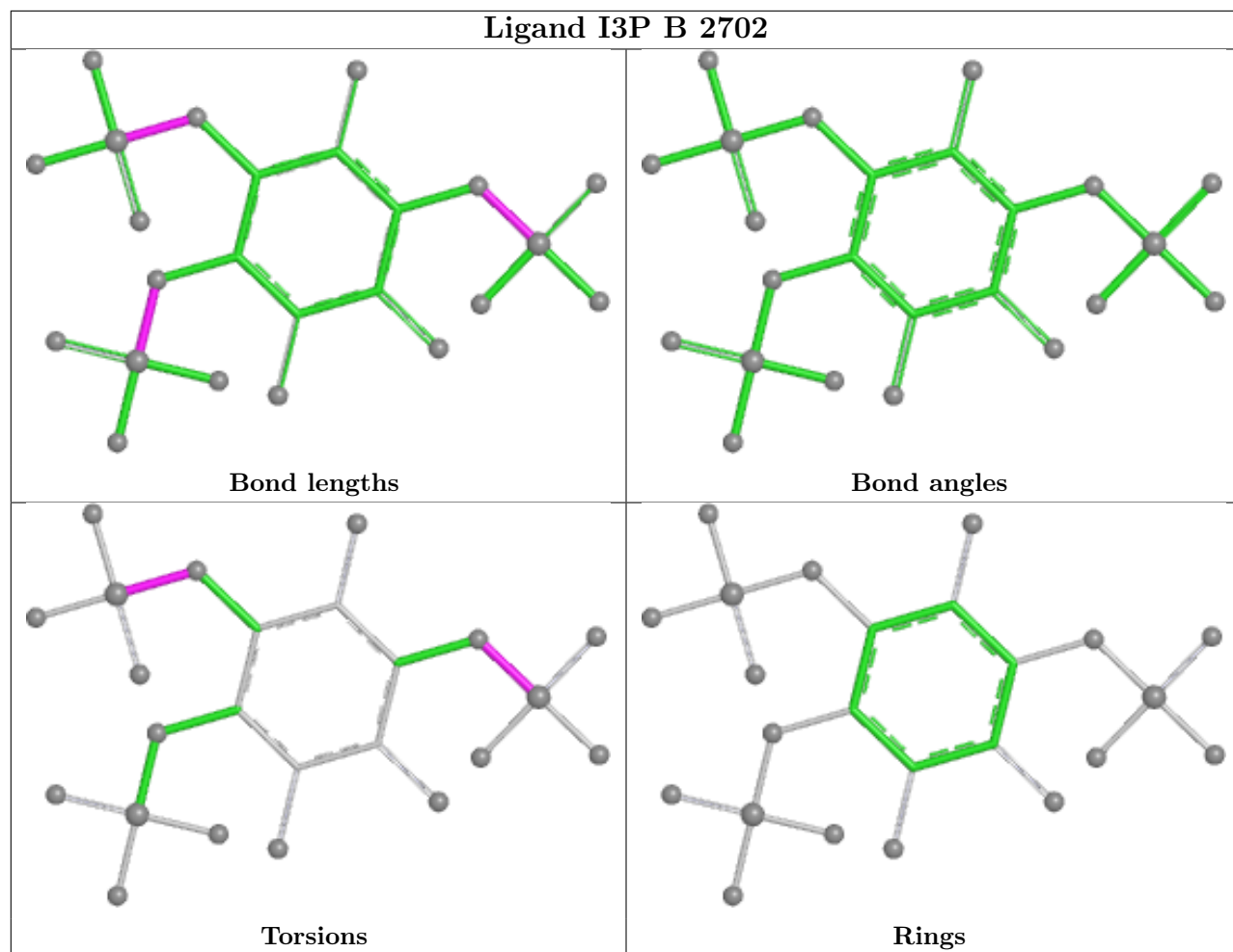
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

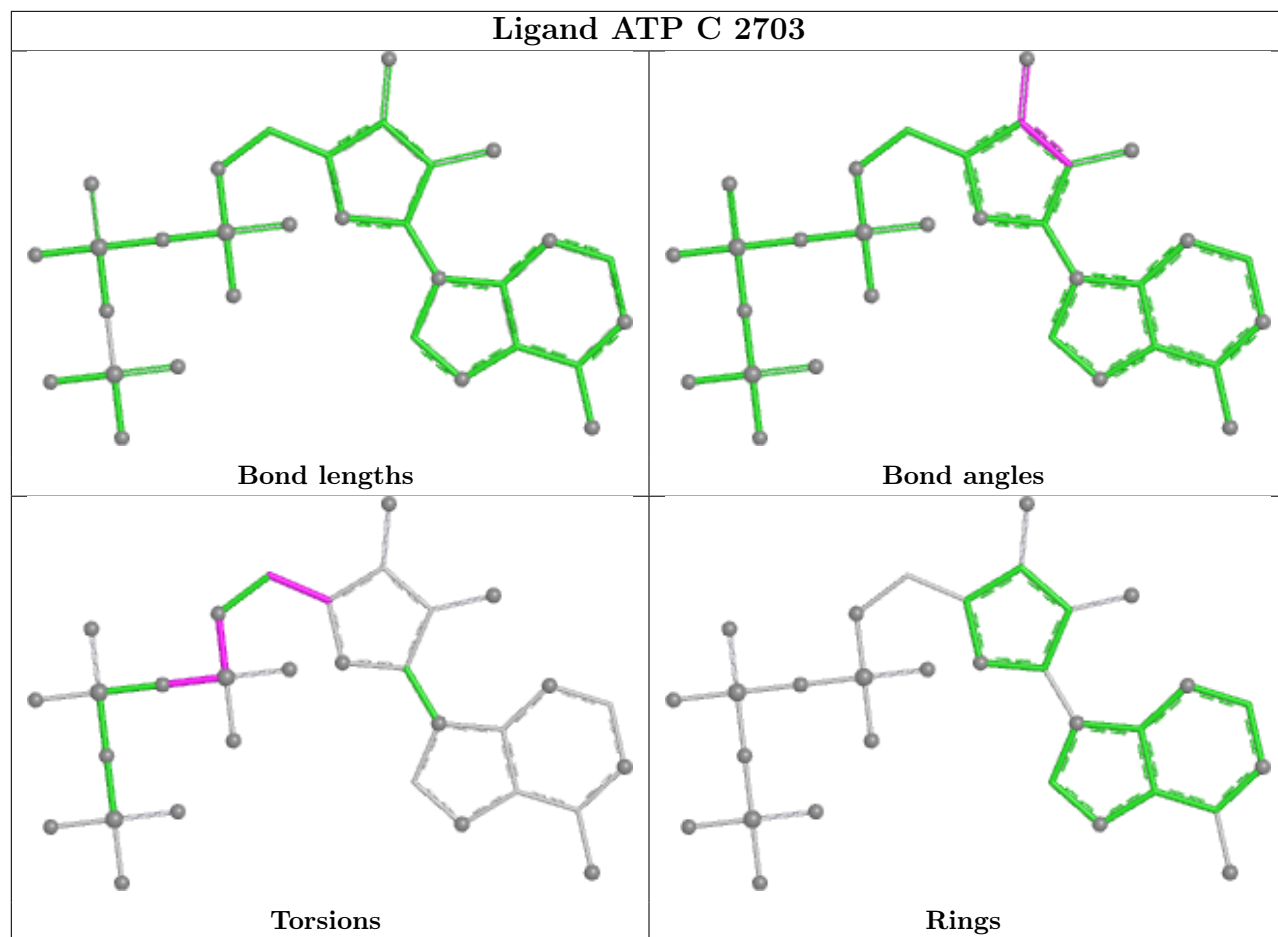


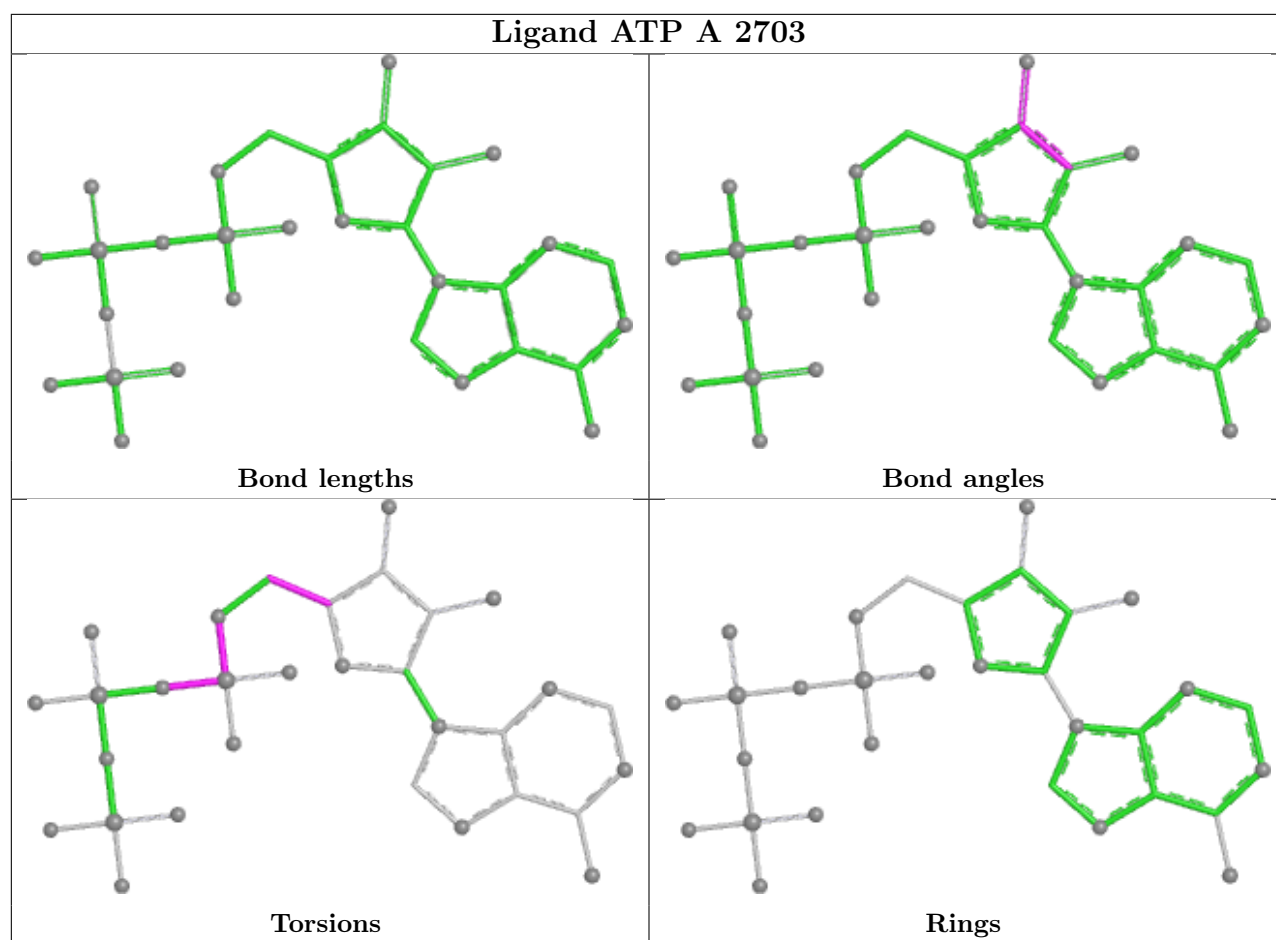


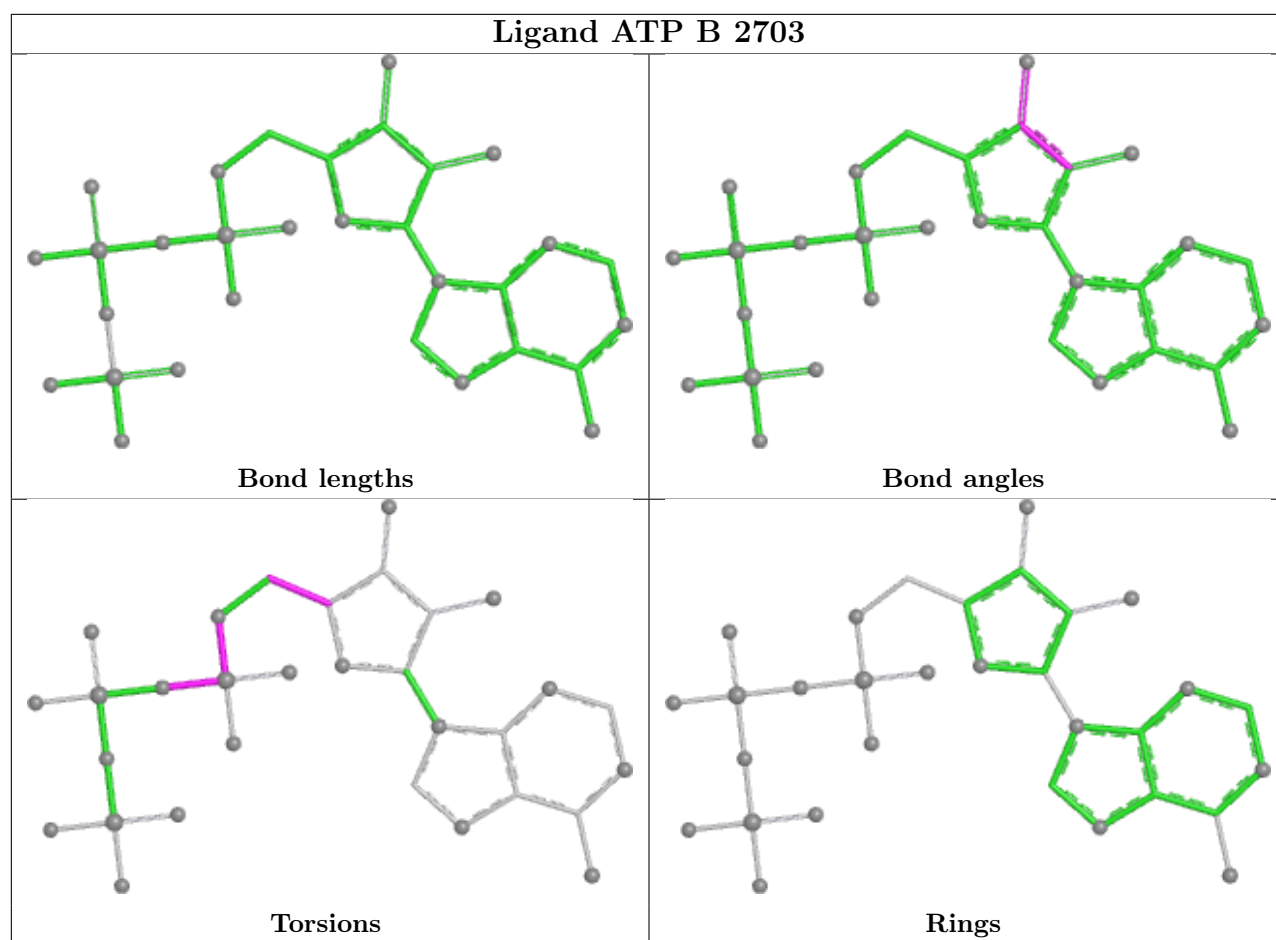












5.7 Other polymers [i](#)

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

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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

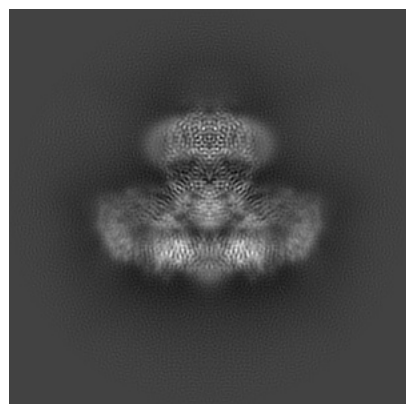
6 Map visualisation [i](#)

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.

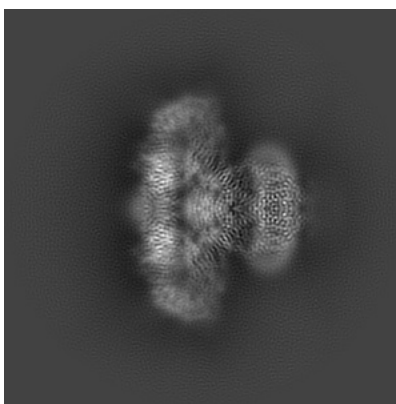
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

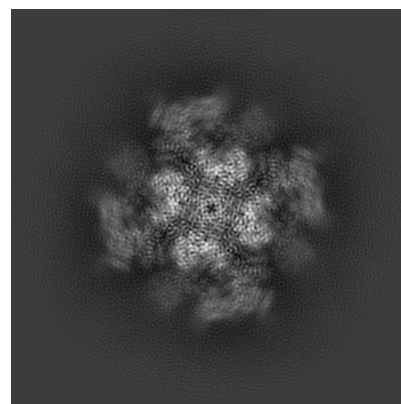
6.1.1 Primary map



X

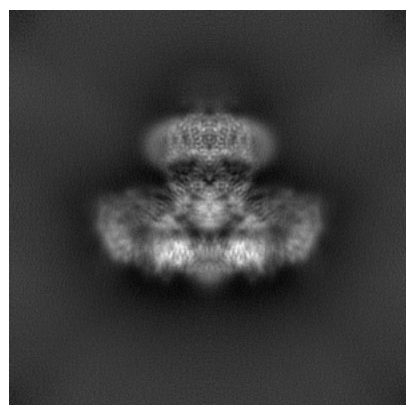


Y

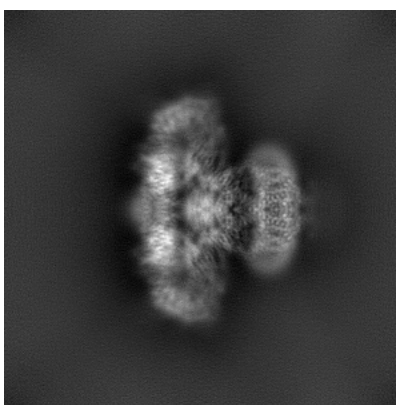


Z

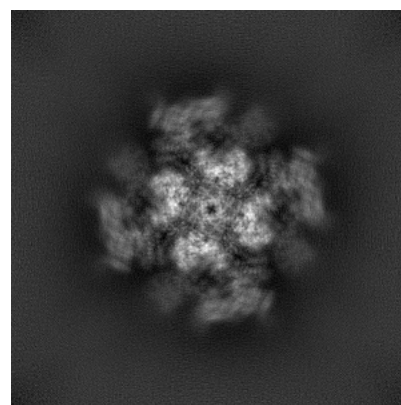
6.1.2 Raw map



X



Y

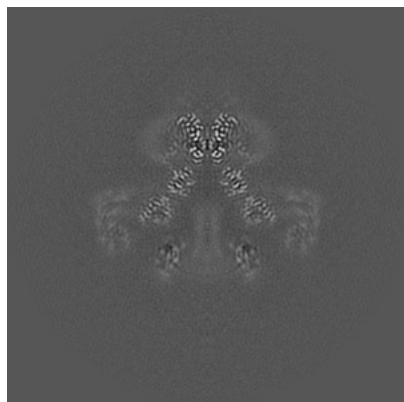


Z

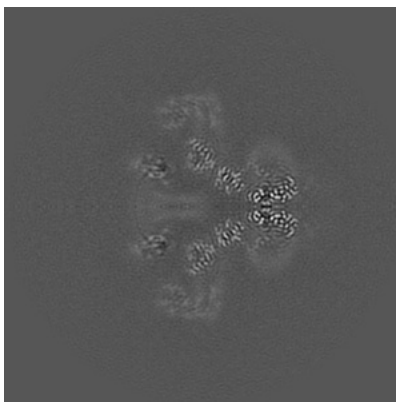
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

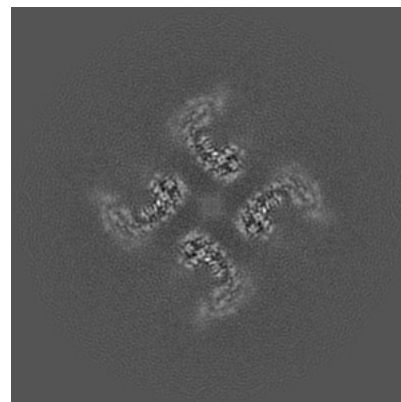
6.2.1 Primary map



X Index: 240

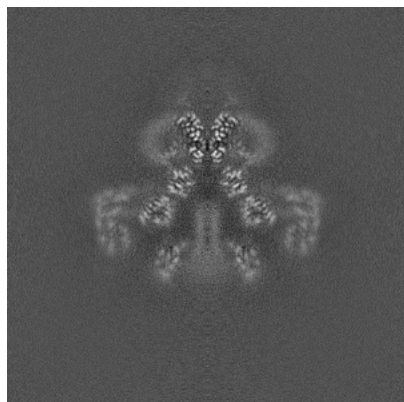


Y Index: 240

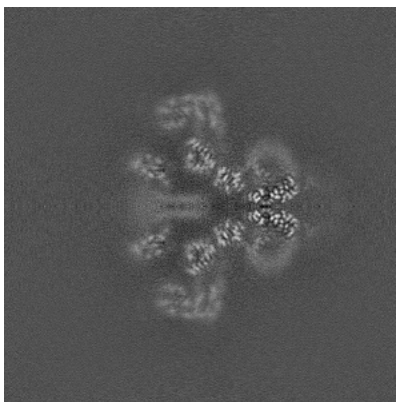


Z Index: 240

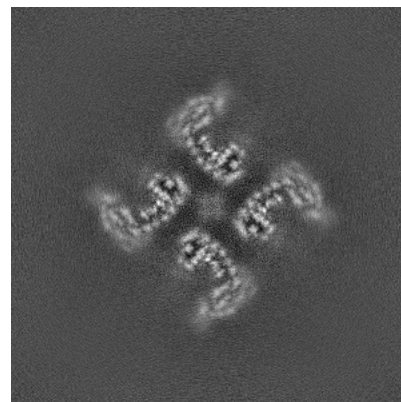
6.2.2 Raw map



X Index: 240



Y Index: 240

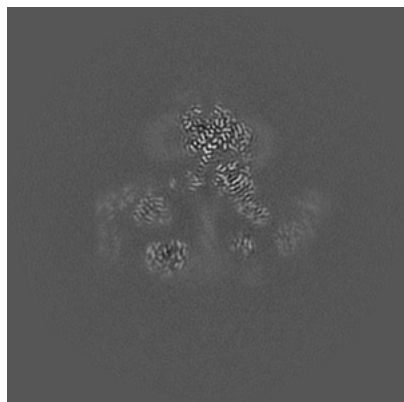


Z Index: 240

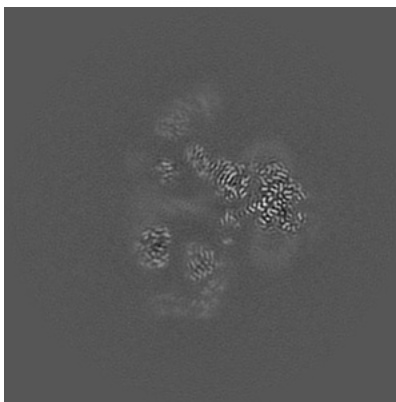
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

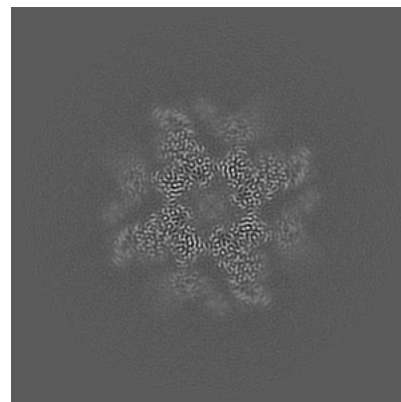
6.3.1 Primary map



X Index: 250

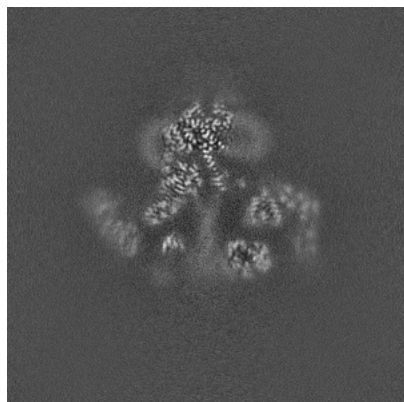


Y Index: 230

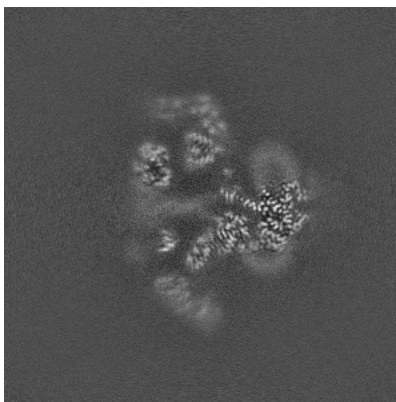


Z Index: 188

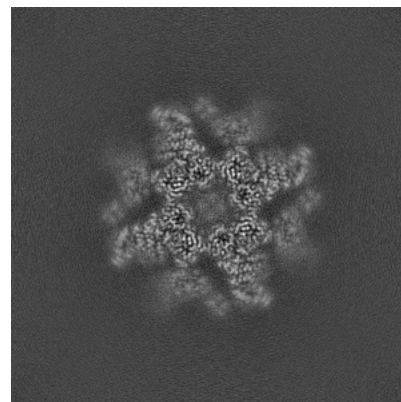
6.3.2 Raw map



X Index: 229



Y Index: 251

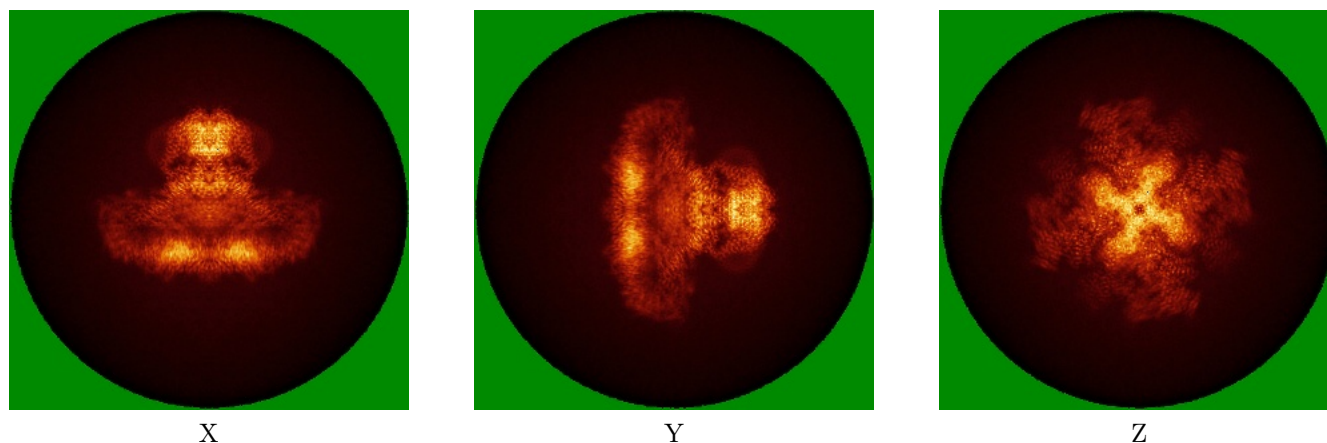


Z Index: 189

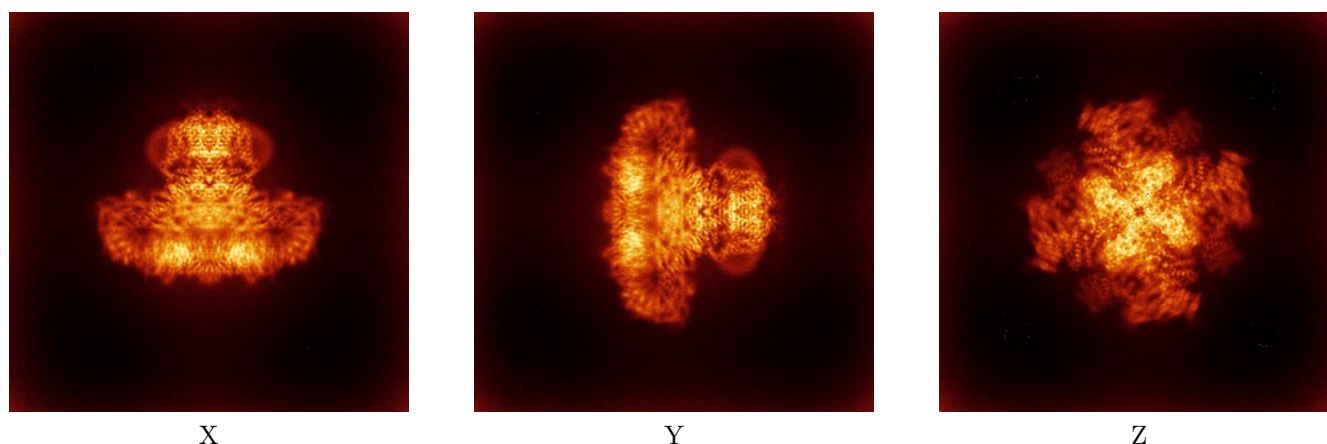
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

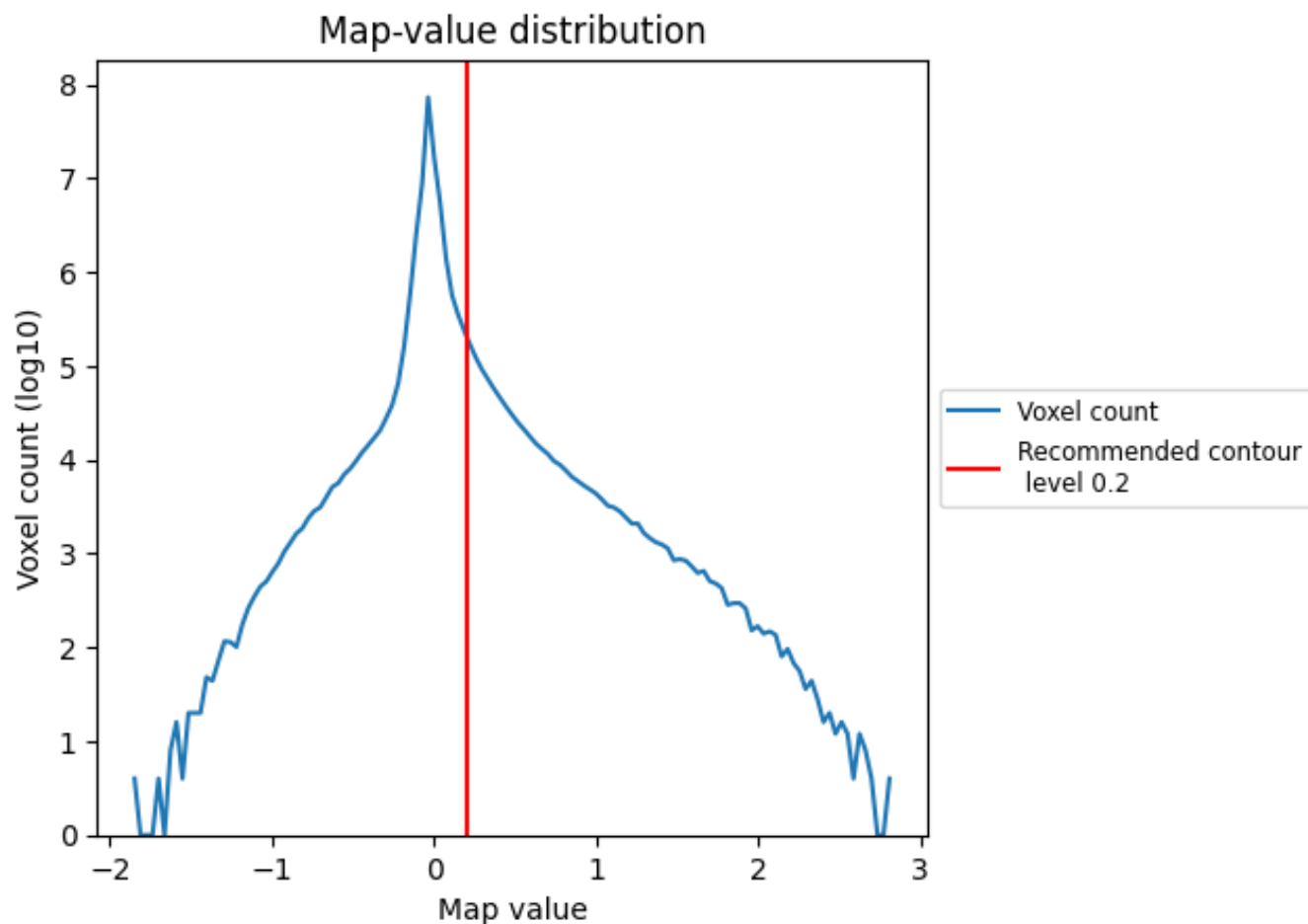
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

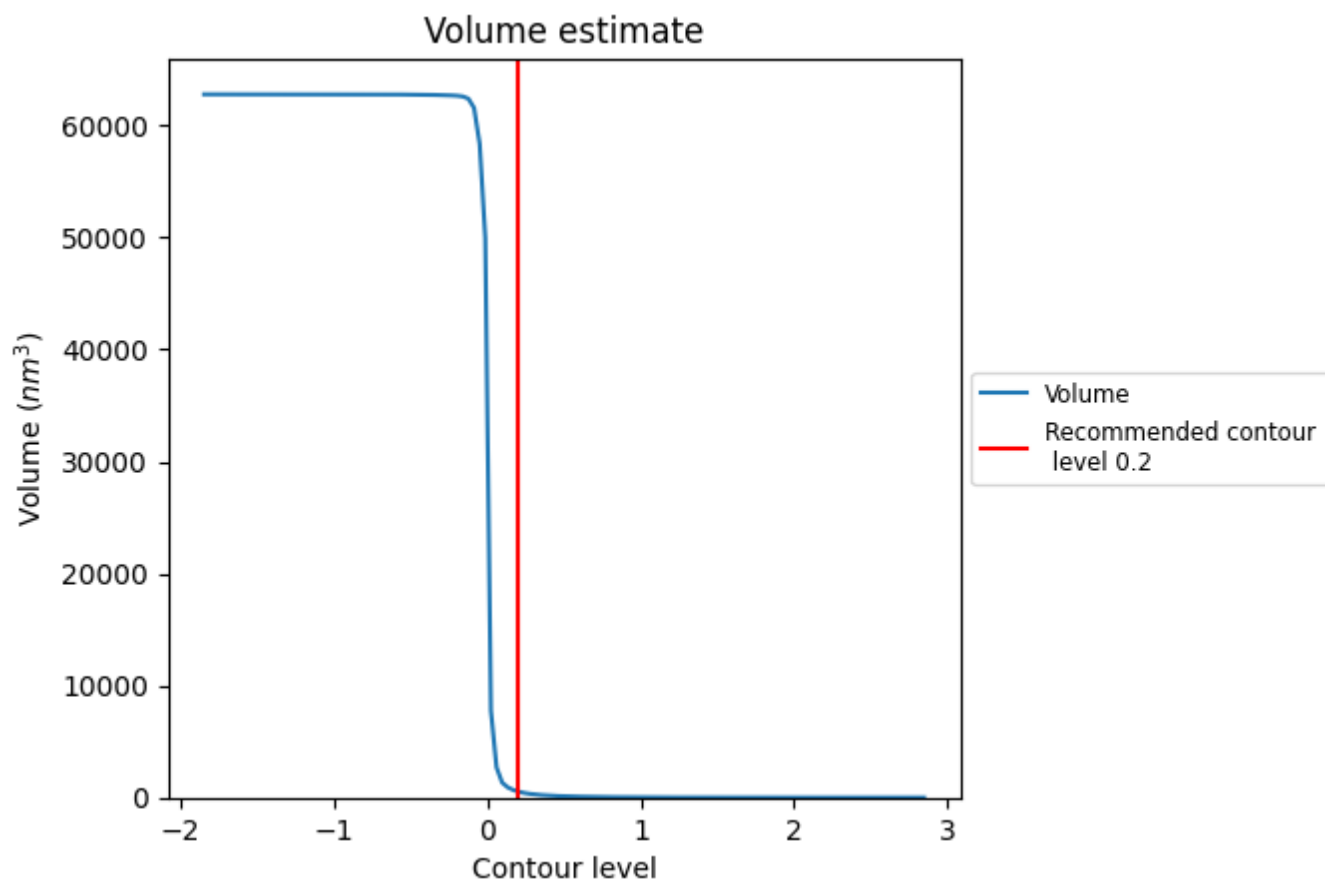
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

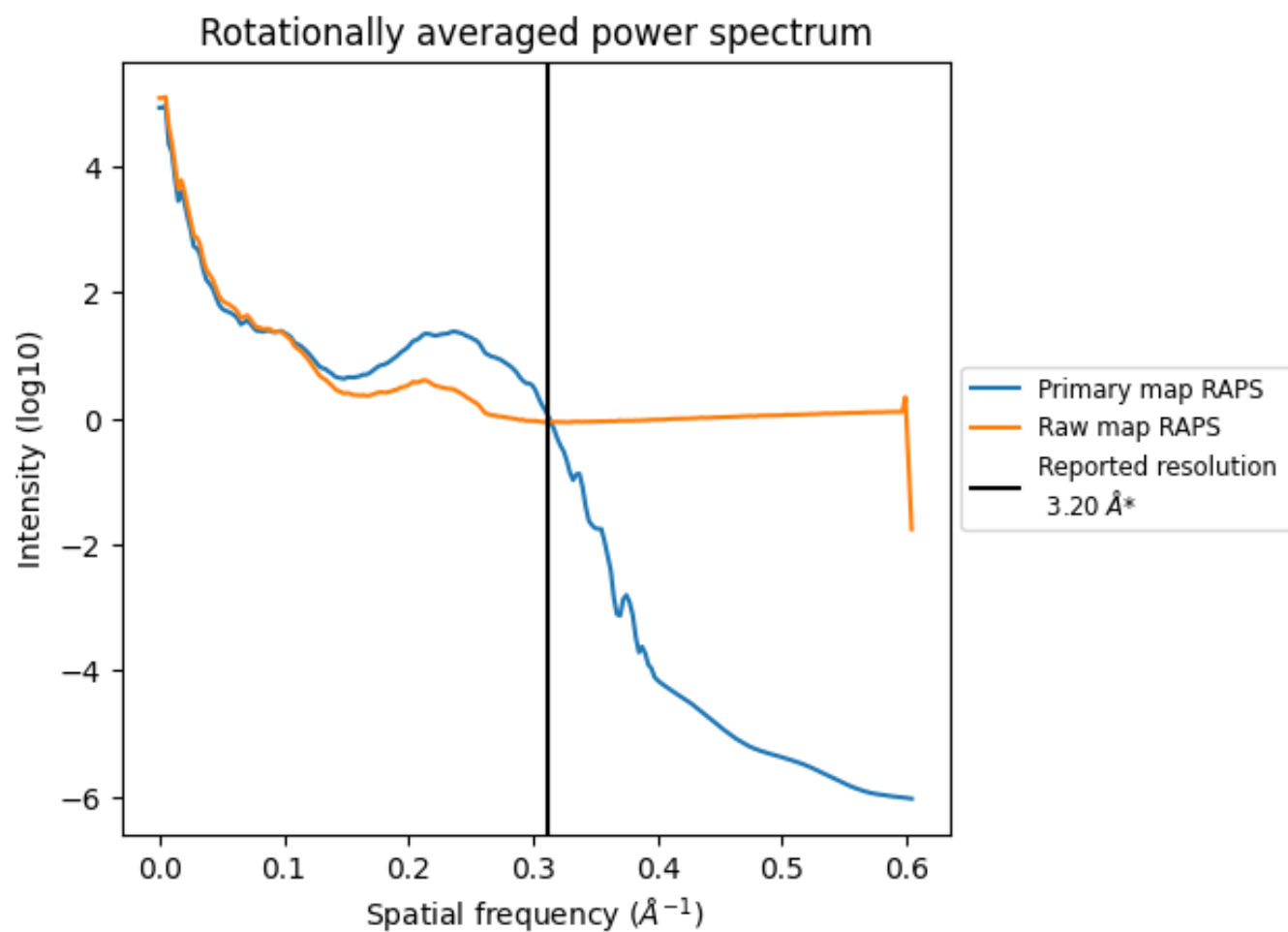
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 544 nm³; 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 ⓘ

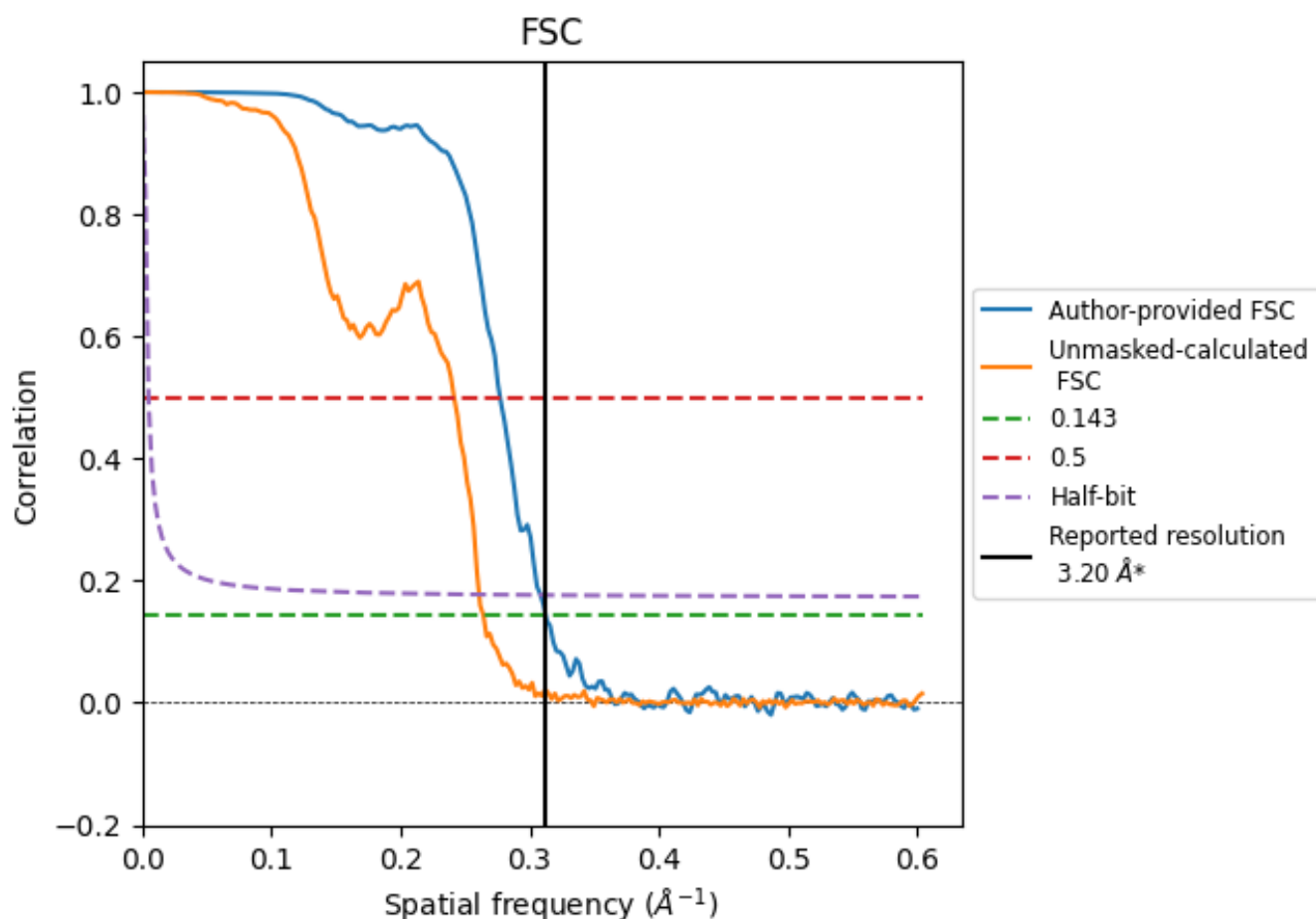


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

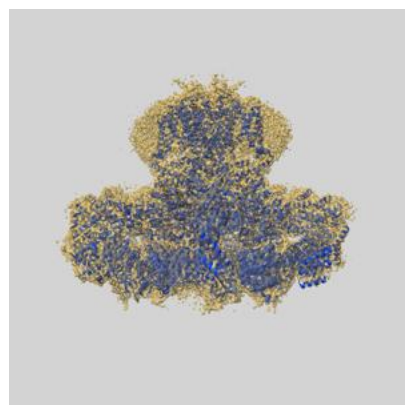
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.61	3.24
Unmasked-calculated*	3.79	4.14	3.83

*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 %

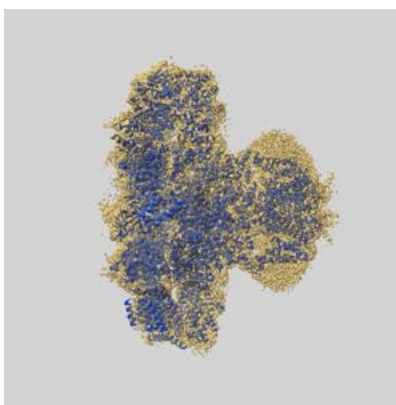
9 Map-model fit [i](#)

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](#).

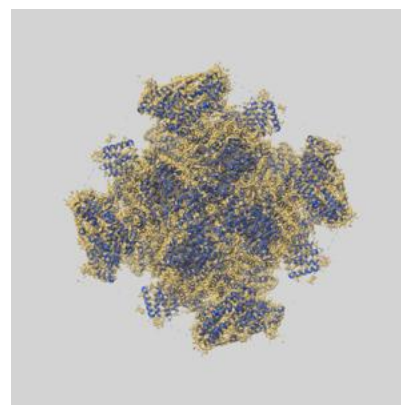
9.1 Map-model overlay [i](#)



X



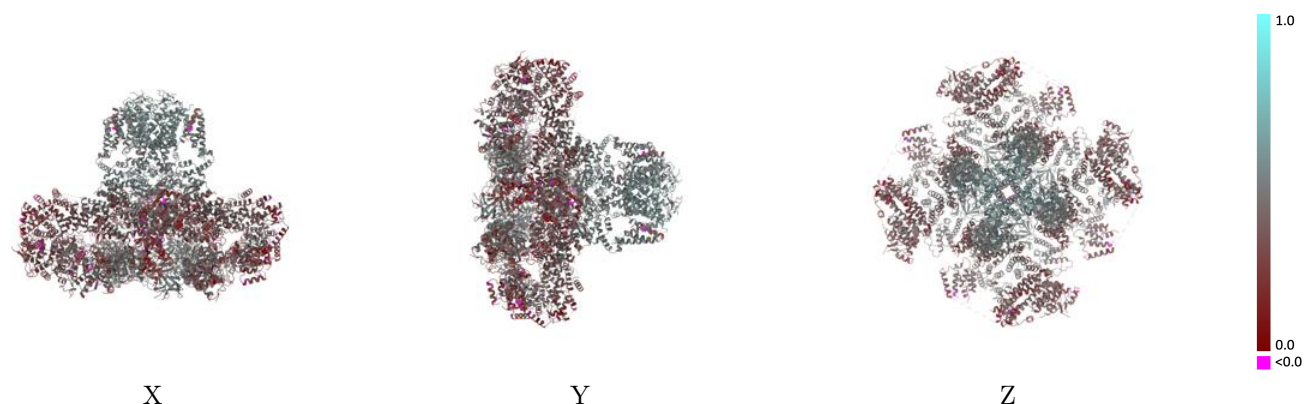
Y



Z

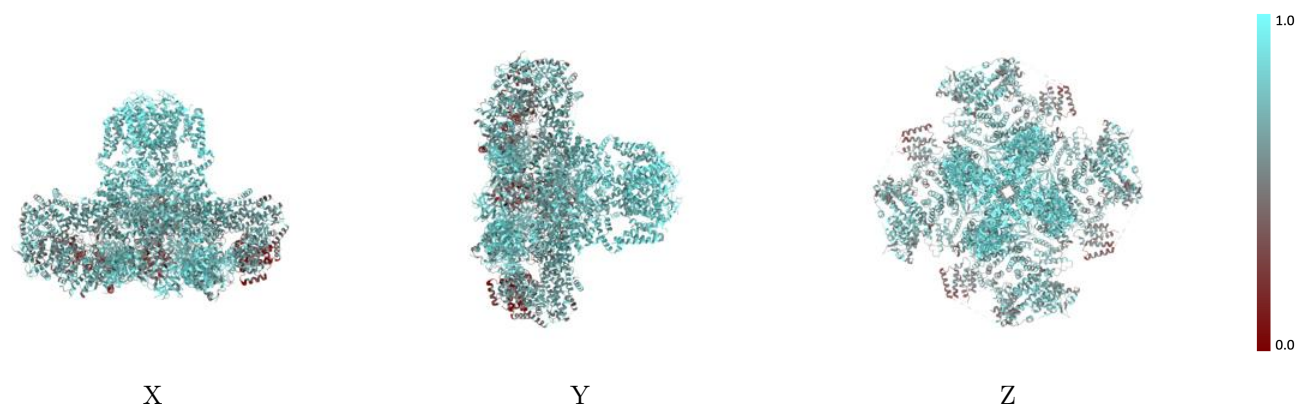
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



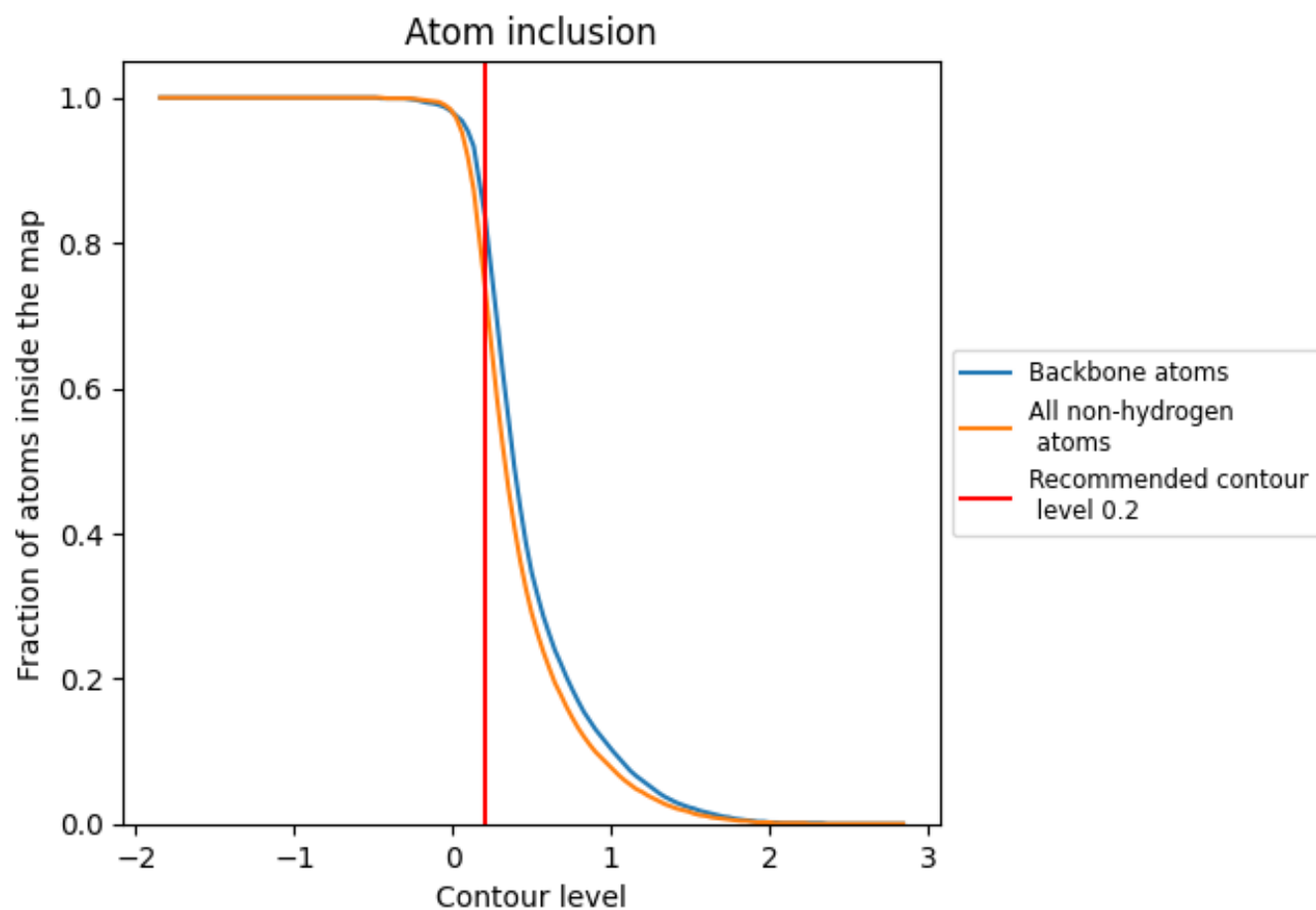
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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	0.7500	0.3990
A	0.7510	0.4020
B	0.7450	0.3910
C	0.7510	0.4020
D	0.7510	0.4020

