



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:19 PM UTC

PDB ID : 8TKI / pdb_00008tki
EMDB ID : EMD-41352
Title : Human Type 3 IP3 Receptor - Labile Resting State 2 (+IP3/ATP)
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.
Deposited on : 2023-07-25
Resolution : 3.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.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 EMDB 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

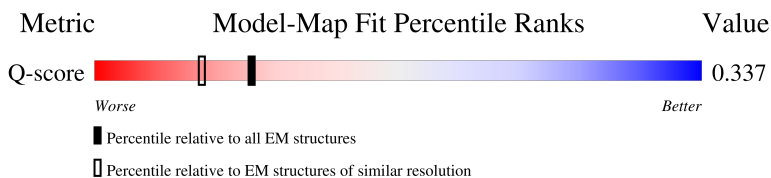
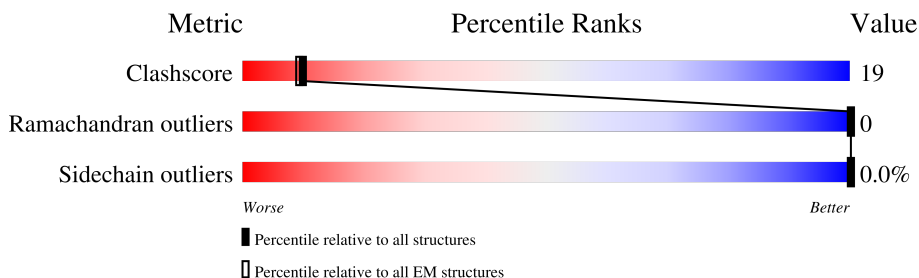
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	2671	 5% 71% 14% 10%
1	B	2671	 5% 61% 24% 10%
1	C	2671	 5% 64% 20% 11%
1	D	2671	 5% 61% 24% 10%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 145900 atoms, of which 72928 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

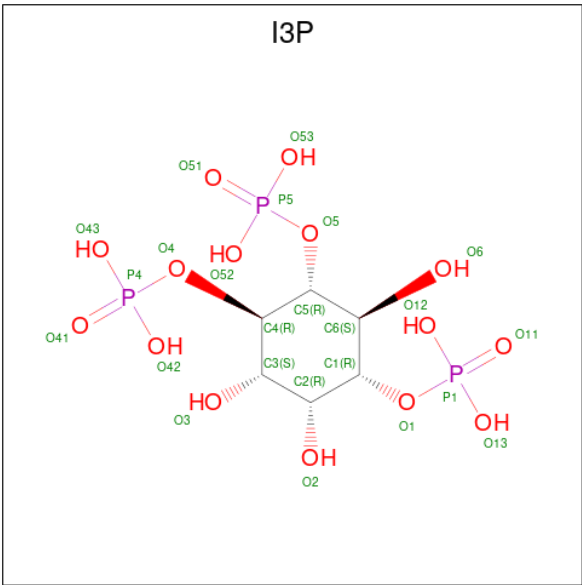
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

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

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

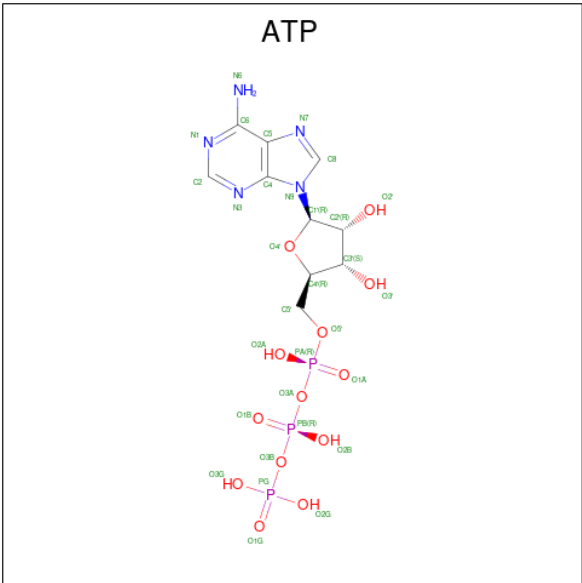
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

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



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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

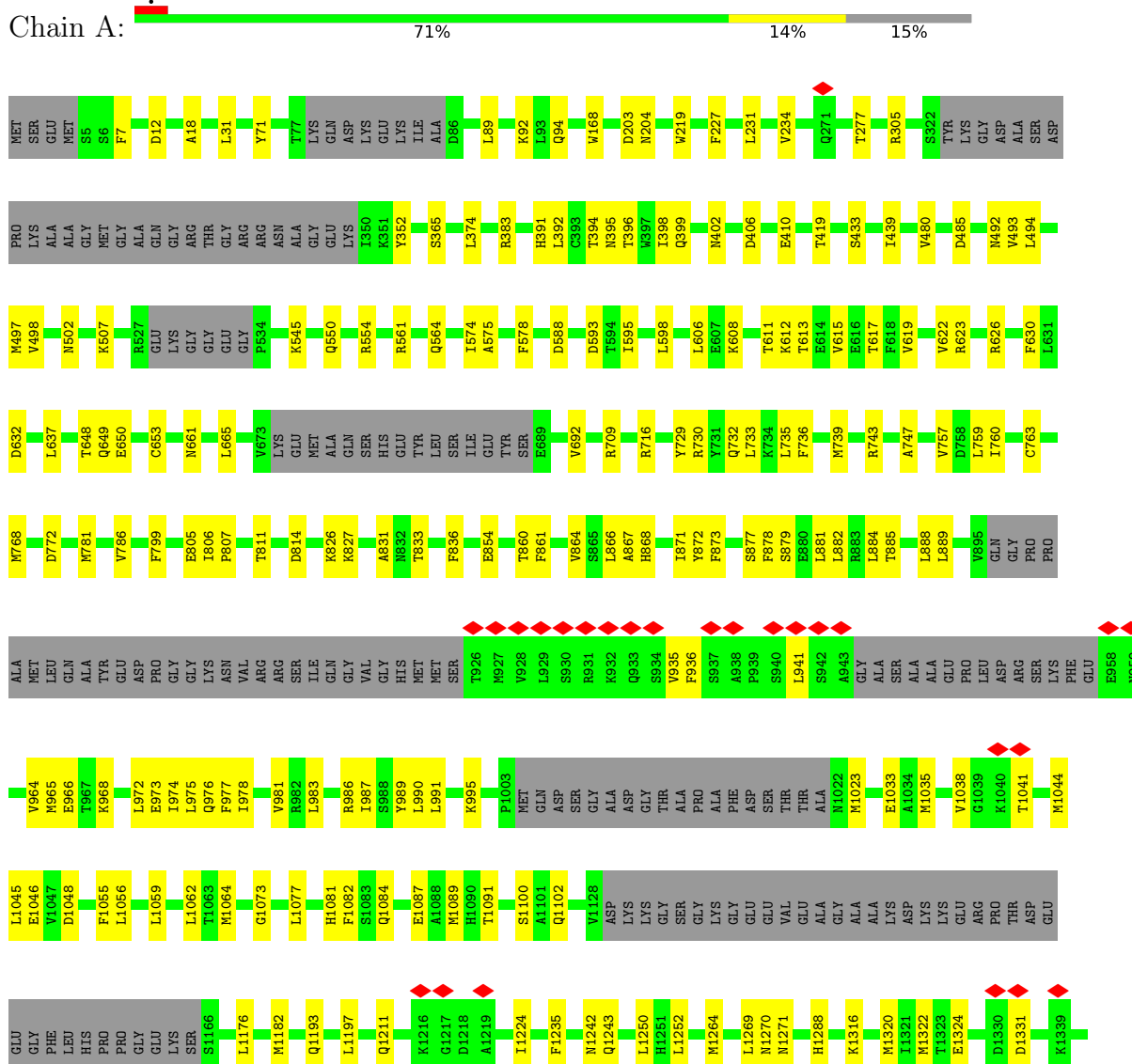


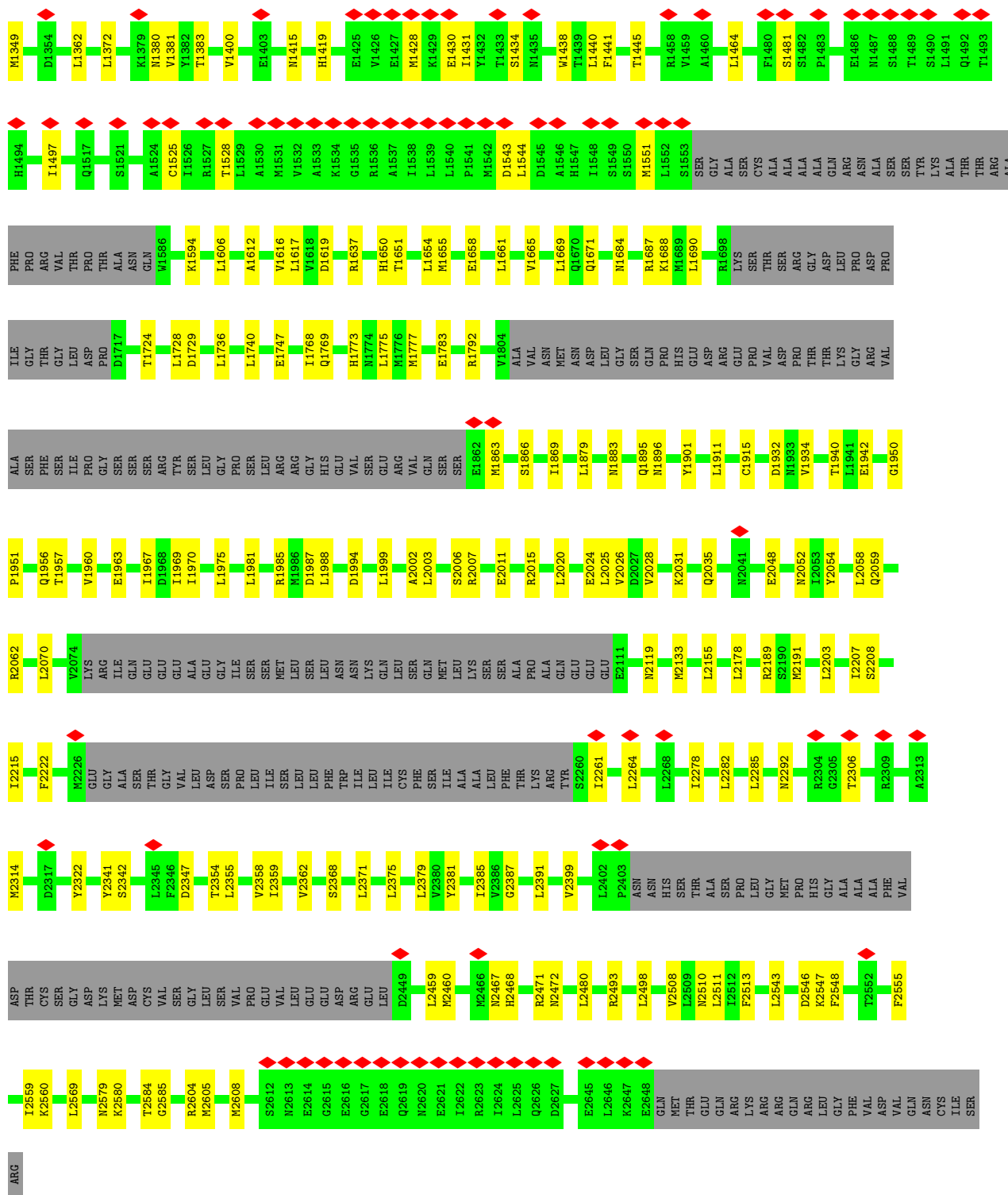
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

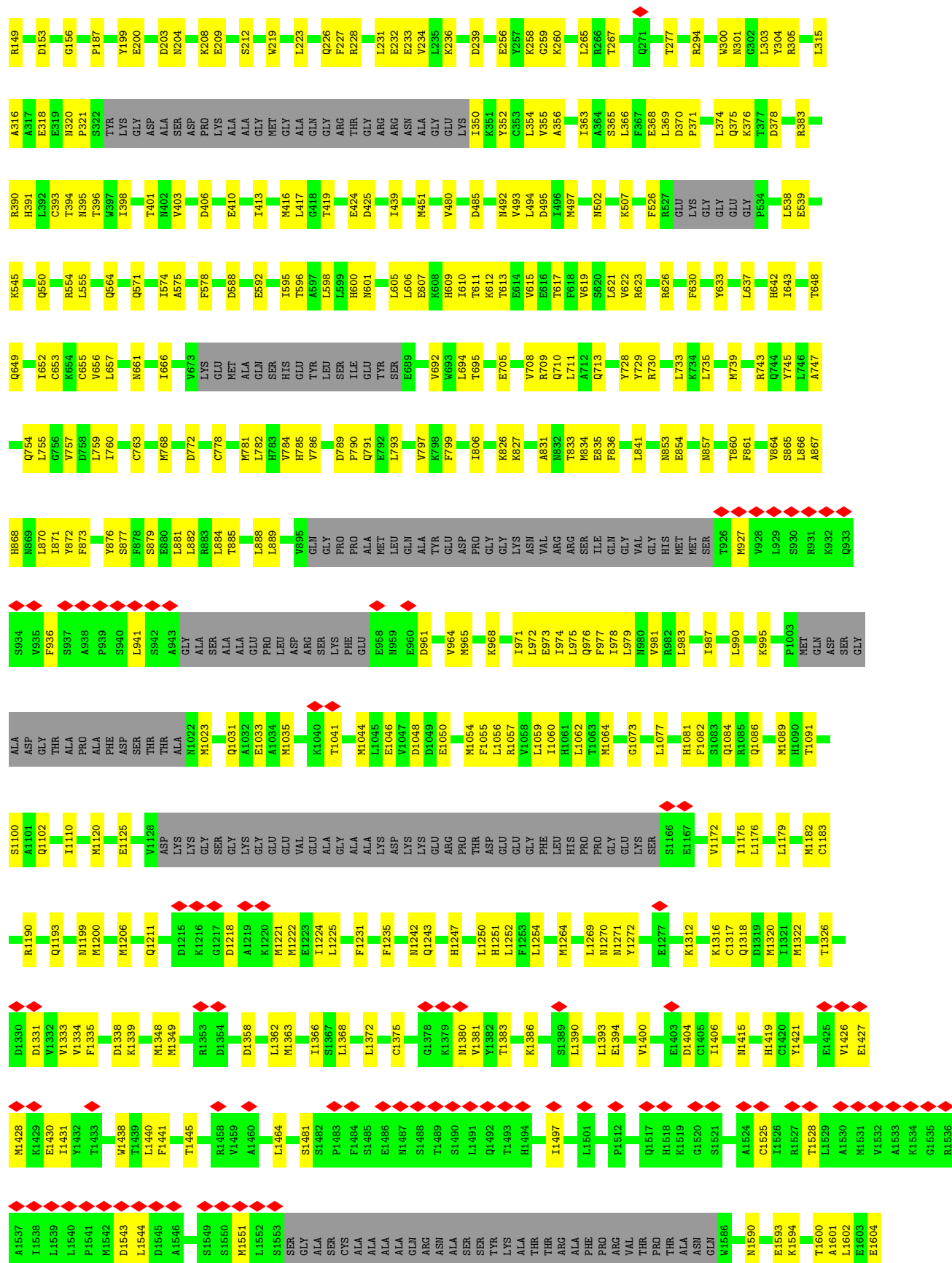
3 Residue-property plots

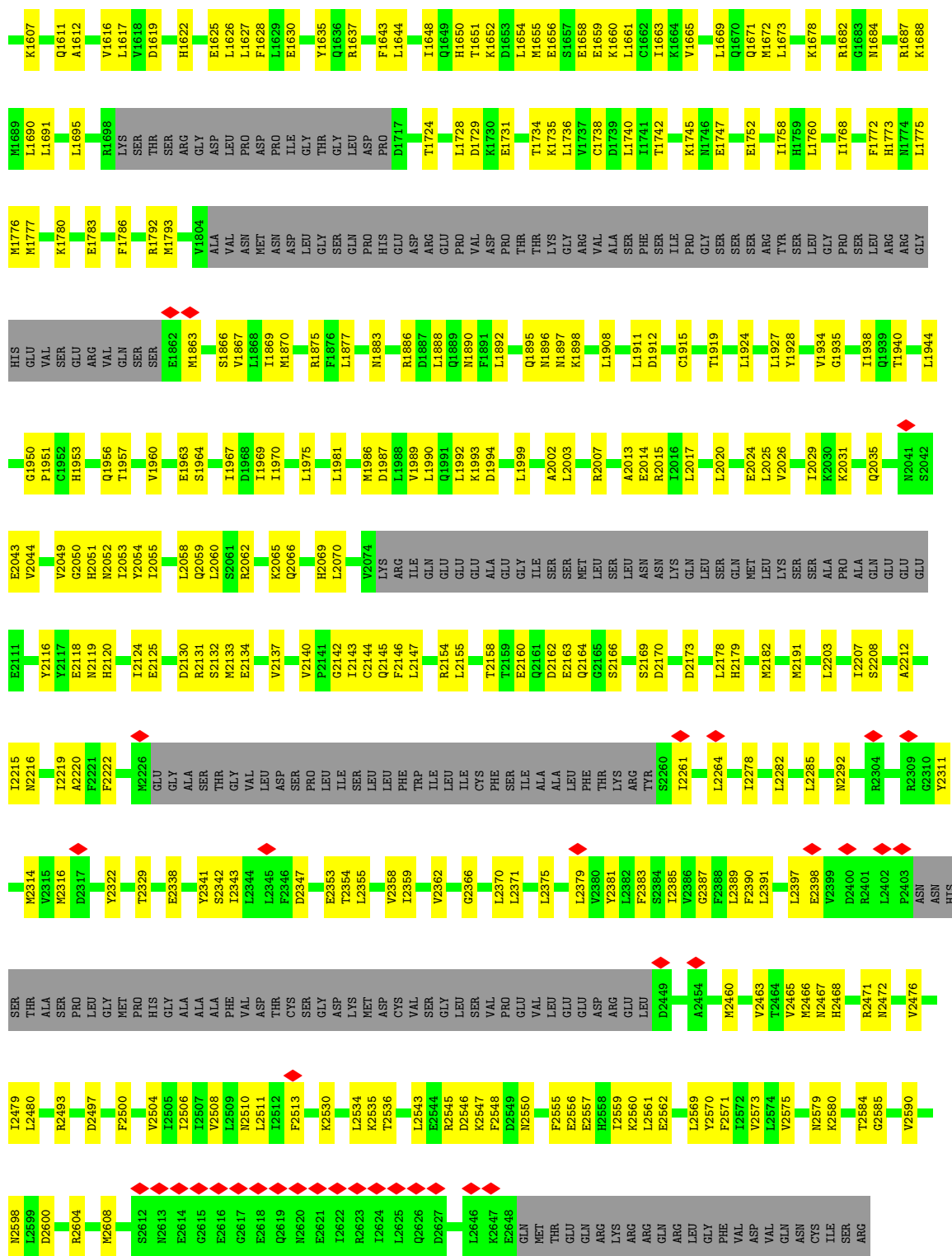
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

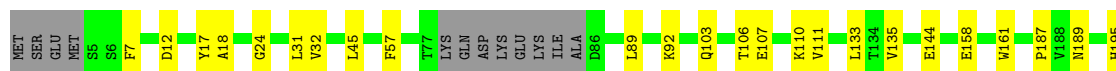




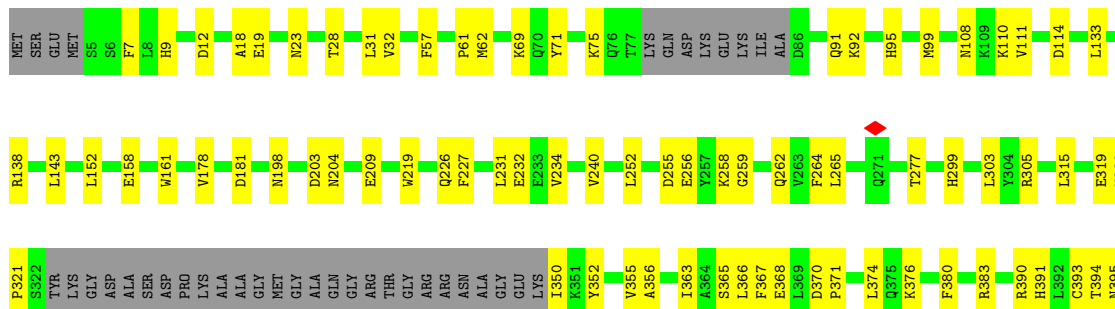
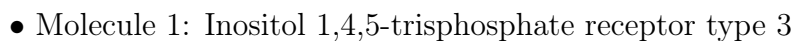




- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3







K1688	M1689	L1690	L1695	R1698	LYS	LYS	V1616	V1617	V1618	D1619	E1625	L1626	L1627	F1628	R1637	G1641	G1642	F1643	L1644	S1645	I1648	Q1649	H1650	T1651	K1652	D1653	L1654	M1655	S1656	S1657	E1658	L1661	C1662	K1664	V1665	R1666	R1667	T1668	F1669	Q1670	Q1671	S1672	M1673	L1674	L1675	K1678	Y1679	G1680	N1684	F1772	H1773	N1774			
A1533	K1534	G1535	R1536	A1537	I1538	L1539	L1540	P1541	M1542	D1543	L1544	D1545	A1546	H1547	I1548	S1549	S1550	M1551	L1552	S1553	SER	GLY	ALA	CYS	ALA	ALA	ALA	ALA	GLN	ASN	ALA	SER	SER	TYR	LYS	ALA	THR	THR	THR	ARG	ALA	PHE	PRO	ARG	VAL	THR	THR	THR	ALA	ASN	GLN	W1586	K1589	E1593	K1594
K1429	E1430	I1431	T1432	S1434	W1438	T1439	L1440	F1441	T1445	R1458	V1459	A1460	L1464	F1480	S1481	S1482	P1483	F1484	S1485	E1486	N1487	T1488	S1490	L1491	Q1492	T1493	H1494	I1497	L1501	E1510	C1511	P1512	Q1517	H1518	K1519	G1520	S1521	V1522	E1523	A1524	C1525	I1526	R1527	T1528	L1529	A1530	M1531	V1532							
D1301	K1316	C1317	Q1318	D1319	M1320	I1321	M1322	T1323	E1324	L1325	T1326	D1330	D1331	D1338	K1339	M1348	M1349	S1481	P1483	F1484	S1485	E1486	N1487	T1488	S1490	L1491	Q1492	T1493	H1494	I1497	L1501	E1510	C1511	P1512	Q1517	H1518	K1519	G1520	S1521	V1522	E1523	A1524	C1525	I1526	R1527	T1528	L1529	A1530	M1531	V1532					
L1175	L1176	L1179	M1182	E1187	Q1188	M1189	Q1193	L1197	M1206	Q1211	K1216	G1217	D1218	A1219	K1220	M1221	M1222	E1223	I1224	L1225	R1226	Q1230	F1231	L1232	F1235	N1239	M1242	Q1243	L1246	H1247	L1250	H1251	L1252	T1255	E1260	M1264	N1270	N1271	E1277																
H1090	T1091	F1092	K1093	Q1094	V1095	Q1096	S1100	A1101	Q1102	I1110	M1120	E1125	V1128	ASP	LYS	GLY	GLY	SER	GLY	LYS	GLY	GLU	VAL	GLY	ALA	GLY	ALA	LYS	ASP	LYS	LYS	GLY	ARG	PRO	THR	THR	ASP	GLU	GLU	GLY	PHE	LEU	HIS	PRO	PRO	GLY	GLY	LYS	S1166	E1167	V1172				
GLN	ASP	SER	GLY	ALA	ASP	GLY	THR	ALA	ALA	PRO	THR	THR	ALA	M1022	M1023	H1024	L1025	E1033	GLU	A1034	M1035	V1038	G1039	K1040	T1041	M1044	E1050	R1053	M1054	F1055	L1056	R1057	V1058	I1059	I1060	H1061	L1062	T1063	M1064	H1065	L1070	G1073	L1077	F1082	Q1086	M1089									
S930	R931	R932	Q933	S934	V935	F936	S937	A938	P939	S940	L941	S942	A943	GLY	ALA	SER	ALA	GLU	PRO	LEU	ASP	ARG	LYS	PHE	E958	N959	F960	D961	M965	K968	L971	L972	E973	L974	L975	Q976	F977	L978	V981	R982	L983	R986	S988	Y989	L990	K995	P1003	MET							
T860	V864	S865	L866	R867	H868	R869	L870	I871	Y872	F873	S877	F878	S879	E880	L881	L882	R883	L884	T885	L888	V895	GLN	GLY	PRO	PRO	ALA	MET	LEU	GLN	ALA	TYR	GLU	ASP	PRO	GLY	LYS	ASN	VAL	ARG	SER	ILE	GLN	GLY	VAL	GLY	HIS	MET	SER	T926	M927	V928	L929			
R743	Q744	Y745	L746	A747	Q754	L755	L756	D757	L758	L759	I760	F761	L762	C763	M764	A765	L766	L769	M781	L782	H783	V784	H785	V786	D789	P790	Q791	V797	K798	F799	I806	Y815	K826	K827	A831	N832	T833	F836	L841	E847	A848	Y853	E854	N857											
T648	Q649	I652	C653	V656	N661	L665	V673	LYS	GLU	MET	ALA	GLN	SER	HIS	GLU	TYR	LEU	SER	ILE	GLU	TYR	SER	E689	V692	V693	L694	T695	T611	K612	L494	D495	L496	M497	V498	N502	K507	F526	R527	GLY	LYS	GLY	GLY	F630	L631	D632	Y633	P534	R537	L538	E539	E540	L541			

L1775	L1776	M1777	E1783	F1786	H1790	D1791	R1792	V1804	ALA	VAL	ASN	MET	ASN	ASP	LEU	GLY	SER	GLN	PRO	HIS	GLU	ASP	ARG	GLU	PRO	THR	THR	LYS	GLY	ARG	VAL	ALA	SER	PHE	SER	ILE	PRO	GLY	SER	SER	ARG	TYR	SER	LEU	GLY	PRO	SER	LEU	ARG	ARG	GLY
HIS	GLU	VAL	SER	GLU	ARG	VAL	GLN	SER	E1862	M1863	S1866	V1867	L1868	I1869	R1875	F1876	L1877	C1881	E1882	N1883	H1884	N1885	R1886	D1887	L1888	Q1889	N1890	F1891	L1892	Q1895	N1896	Y1901	Q1909	D1912	I1913	M1914	C1915	T1919	L1924	L1927	Y1928	I1929	N1930	V1934	G1935	L1936	V1937				
I1938	Q1939	T1940	T1943	L1944	Y1947	C1948	Q1949	G1950	P1951	C1952	H1953	Q1956	T1957	V1960	E1963	G1966	I1967	D1968	I1969	I1970	L1973	I1974	L1975	I1978	S1979	P1980	L1981	C1982	K1983	M1986	D1987	L1988	V1989	L1990	Q1991	K1993	D1994	L1999	L2000	A2001	L2002	L2003	M2004	R2007	S2010						
E2014	R2015	L2020	E2024	L2025	V2026	D2027	I2029	K2030	K2031	Q2035	N2041	V2044	V2049	G2050	I2053	Y2054	I2058	Q2059	R2062	H2063	N2064	K2065	Q2066	H2069	L2070	L2071	V2074	LYS	ARG	ILE	GLN	GLU	GLU	ALA	GLY	ILE	SER	SER	MET	LEU	SER	LEU	ASN	ASN	LYS						
GLN	LEU	SER	MET	LYS	SER	SER	ALA	PRO	ALA	GLN	GLU	GLU	F2111	L2114	H2120	I2124	E2125	D2130	R2131	S2132	M2133	L2136	V2140	C2144	Q2145	F2146	L2147	R2154	L2155	T2158	T2159	E2160	Q2161	D2162	E2163	Q2164	Q2165	S2166	L2178	H2179	M2182	R2186	M2191								
P2192	L2193	I2194	L2203	L2207	S2208	V2213	F2214	I2215	N2216	I2217	I2218	I2219	A2220	F2221	F2222	M2226	GLU	GLY	SER	THR	GLY	VAL	LEU	ASP	SER	PRO	ILE	SER	LEU	PHE	TRP	ILE	LEU	CYS	PHE	ILE	ALA	LEU	THR	LYS	ARG	T2260	I2261	L2264	L2278						
L2282	L2285	N2292	R2304	R2309	K2312	A2313	M2314	V2315	M2316	D2317	M2318	F2319	F2320	Y2322	T2329	E2338	Y2341	S2342	L2343	L2344	L2345	F2346	D2347	L2348	I2349	Y2350	T2354	L2355	V2358	I2359	V2362	S2368	L2371	L2375	L2379	V2380	Y2381	L2382	F2383	S2384	I2385	V2386									
G2387	L2391	L2397	E2398	L2402	P2403	ASN	ASN	HIS	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	VAL	SER	PRO	GLU	VAL	GLU	GLU	ASP	ARG	GLU	LEU	D2449	A2454	M2460
H2468	R2471	N2472	G2477	D2478	I2479	L2480	S2484	E2493	D2497	F2500	V2508	L2509	N2510	L2511	I2512	F2513	E2531	L2534	K2535	L2543	D2546	K2547	F2548	D2549	N2550	K2551	F2555	E2556	L2559	E2562	L2569	Y2570	F2571	T2572	V2573	L2574	V2575	N2579	K2580	T2584	G2585										
N2596	R2604	M2605	L2610	V2611	S2612	N2613	E2614	G2615	E2616	G2617	E2618	Q2619	N2620	E2621	L2622	R2623	L2624	L2625	Q2626	D2627	K2628	L2629	F2648	GLN	MET	THR	GLU	GLN	ARG	LYS	ARG	ARG	GLN	ARG	LEU	GLY	PHE	VAL	ASP	VAL	GLN	ASN	CYS	ILE	SER	ARG					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155671	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.933	Depositor
Minimum map value	-0.374	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.826, 0.826, 0.826	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: ZN, 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	0.10	0/18521	0.25	0/25031
1	B	0.10	0/18521	0.25	0/25031
1	C	0.10	0/18521	0.25	0/25031
1	D	0.10	0/18521	0.25	0/25031
All	All	0.10	0/74084	0.25	0/100124

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	18187	18211	18206	383	0
1	B	18187	18211	18209	912	0
1	C	18187	18211	18208	782	0
1	D	18187	18211	18207	954	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	9	9	0	0
3	C	24	9	9	0	0
3	D	24	9	9	0	0
4	A	31	12	12	1	0
4	B	31	12	12	0	0
4	C	31	12	12	1	0
4	D	31	12	12	0	0
All	All	72972	72928	72914	2842	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 19.

The worst 5 of 2842 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2238/2671 (84%)	2202 (98%)	36 (2%)	0	100	100
1	B	2238/2671 (84%)	2202 (98%)	36 (2%)	0	100	100
1	C	2238/2671 (84%)	2203 (98%)	35 (2%)	0	100	100
1	D	2238/2671 (84%)	2203 (98%)	35 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8952/10684 (84%)	8810 (98%)	142 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2021/2385 (85%)	2020 (100%)	1 (0%)	100	100
1	B	2021/2385 (85%)	2021 (100%)	0	100	100
1	C	2021/2385 (85%)	2021 (100%)	0	100	100
1	D	2021/2385 (85%)	2019 (100%)	2 (0%)	88	87
All	All	8084/9540 (85%)	8081 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	ASN
1	D	641	ASN
1	D	1270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2066	GLN
1	D	1247	HIS
1	C	2592	GLN
1	D	359	HIS
1	D	1518	HIS

5.3.3 RNA ⓘ

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 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	A	3003	-	32,33,33	0.26	0	48,52,52	0.67	0
4	ATP	D	3003	-	32,33,33	0.26	0	48,52,52	0.67	0
4	ATP	C	3003	-	32,33,33	0.26	0	48,52,52	0.67	0
3	I3P	A	3002	-	24,24,24	2.17	3 (12%)	39,39,39	0.86	0
3	I3P	C	3002	-	24,24,24	2.17	3 (12%)	39,39,39	0.86	0
4	ATP	B	3003	-	32,33,33	0.26	0	48,52,52	0.67	0
3	I3P	D	3002	-	24,24,24	2.17	3 (12%)	39,39,39	0.87	0
3	I3P	B	3002	-	24,24,24	2.18	3 (12%)	39,39,39	0.86	0

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	A	3003	-	-	10/22/38/38	0/3/3/3
4	ATP	D	3003	-	-	10/22/38/38	0/3/3/3
4	ATP	C	3003	-	-	10/22/38/38	0/3/3/3
3	I3P	A	3002	-	-	0/15/39/39	0/1/1/1
3	I3P	C	3002	-	-	0/15/39/39	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	3003	-	-	10/22/38/38	0/3/3/3
3	I3P	D	3002	-	-	0/15/39/39	0/1/1/1
3	I3P	B	3002	-	-	0/15/39/39	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3002	I3P	P4-O4	6.07	1.70	1.59
3	A	3002	I3P	P4-O4	6.04	1.70	1.59
3	C	3002	I3P	P4-O4	6.02	1.70	1.59
3	D	3002	I3P	P4-O4	6.01	1.70	1.59
3	B	3002	I3P	P5-O5	5.89	1.69	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3003	ATP	PB-O3B-PG-O3G
4	A	3003	ATP	C5'-O5'-PA-O2A
4	A	3003	ATP	C5'-O5'-PA-O3A
4	B	3003	ATP	PB-O3B-PG-O3G
4	B	3003	ATP	C5'-O5'-PA-O2A

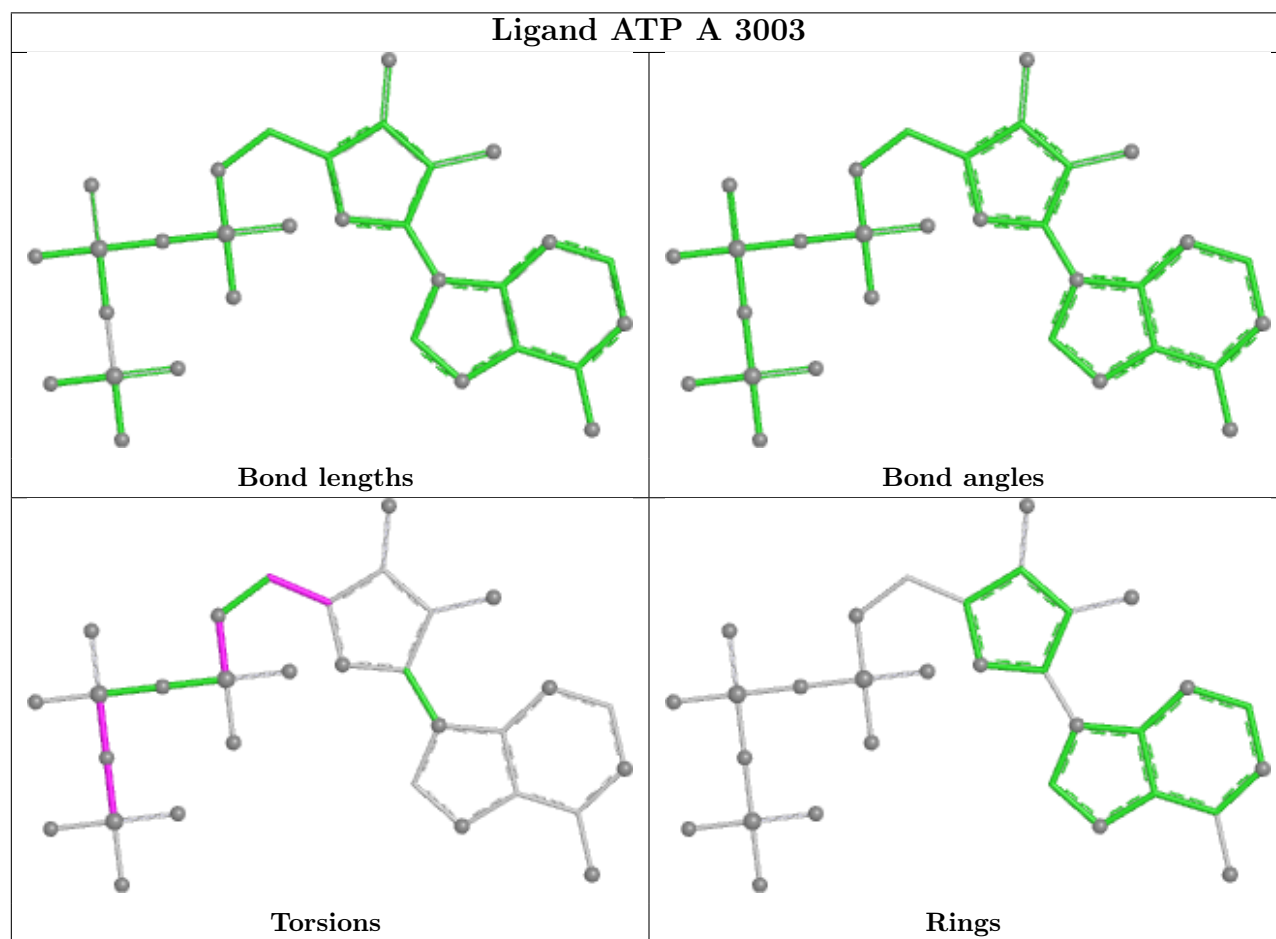
There are no ring outliers.

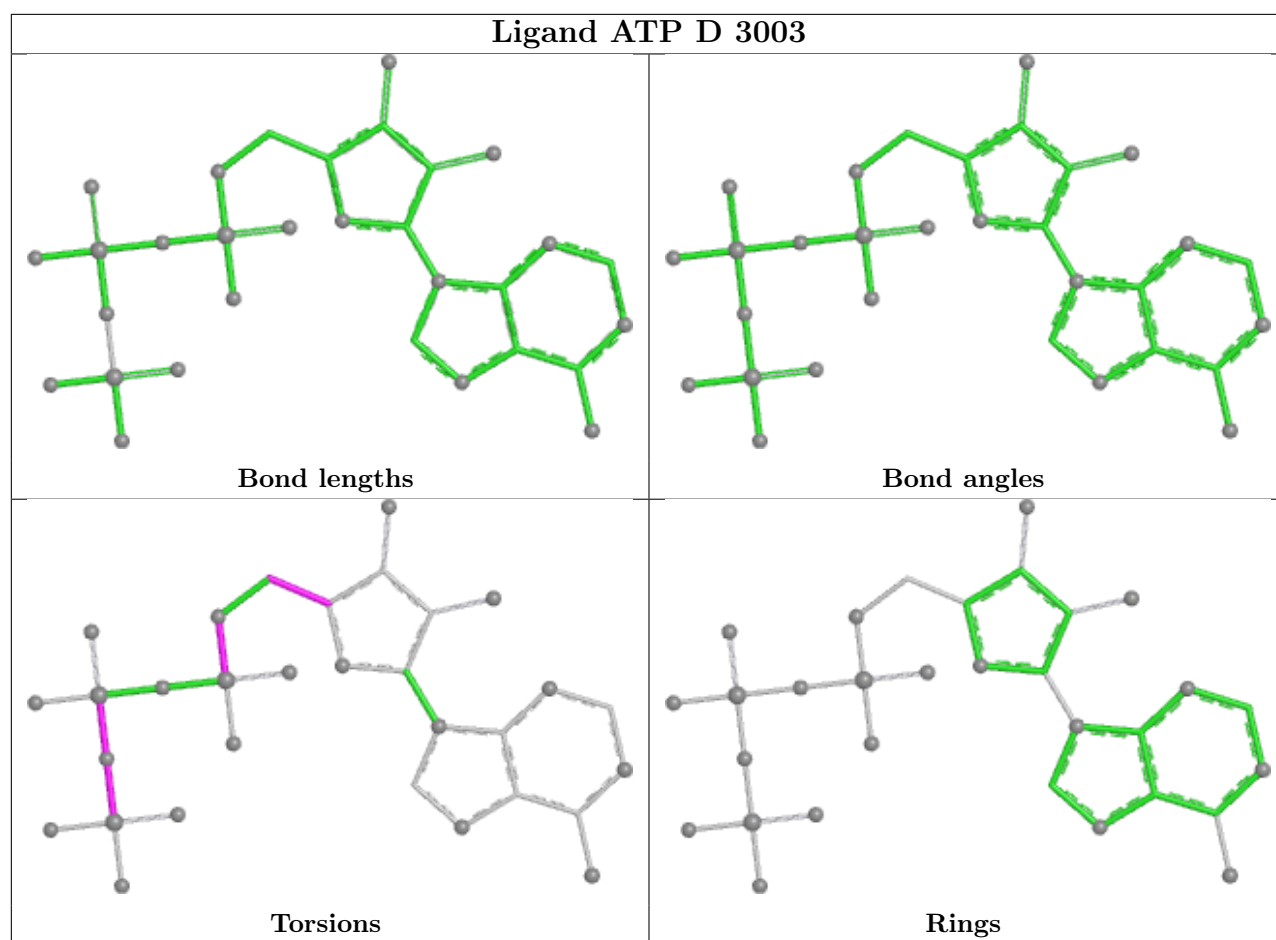
2 monomers are involved in 2 short contacts:

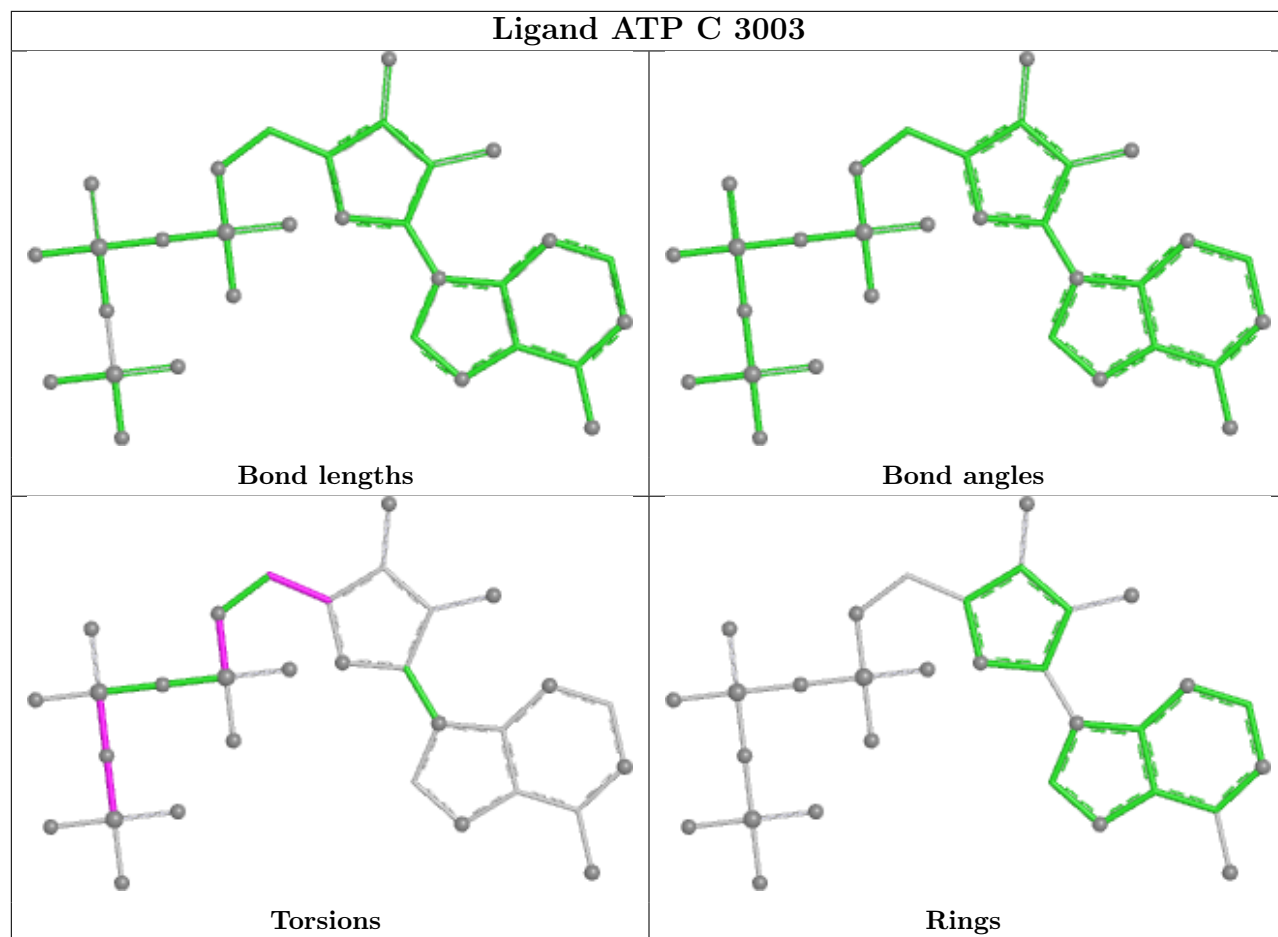
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3003	ATP	1	0
4	C	3003	ATP	1	0

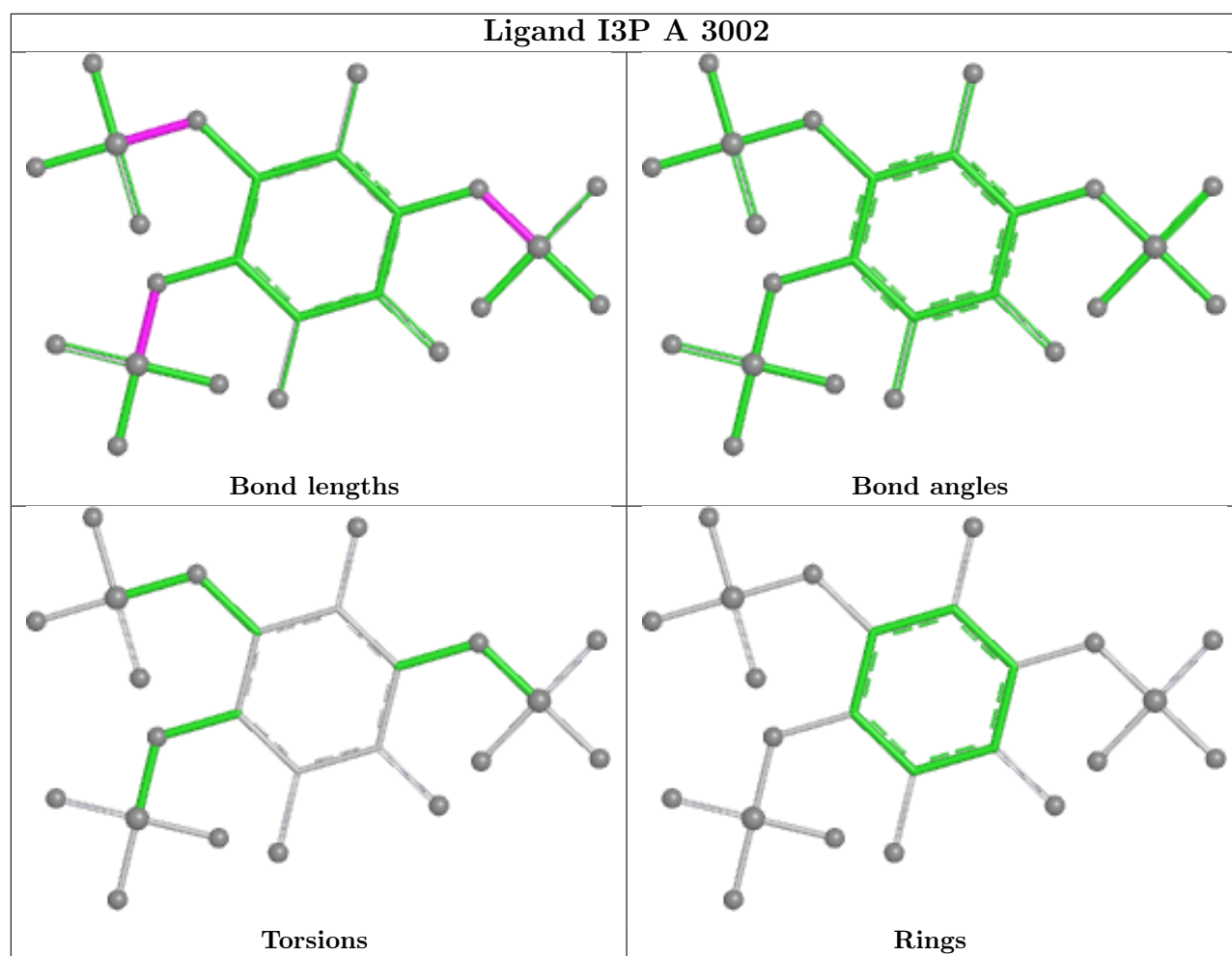
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

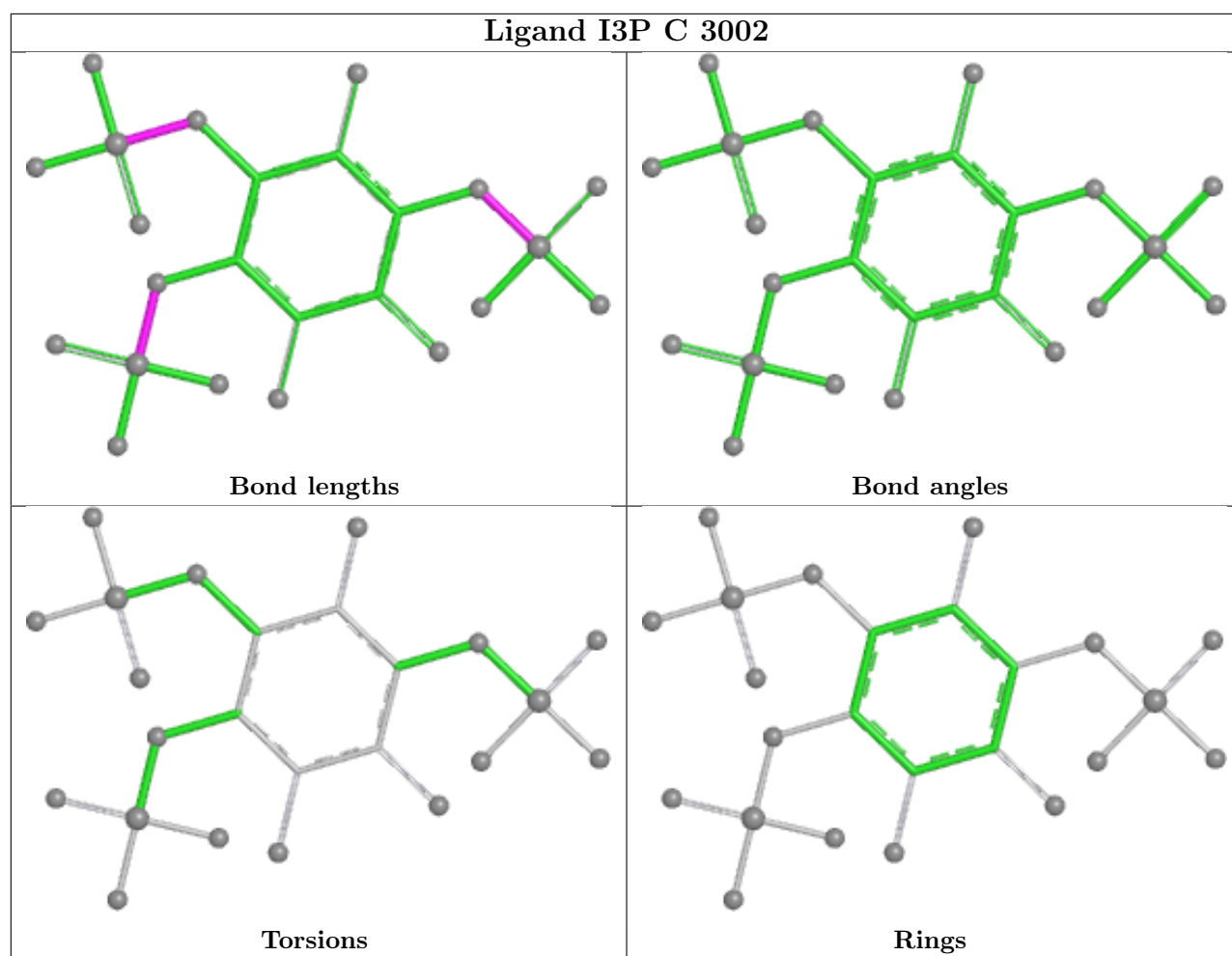
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

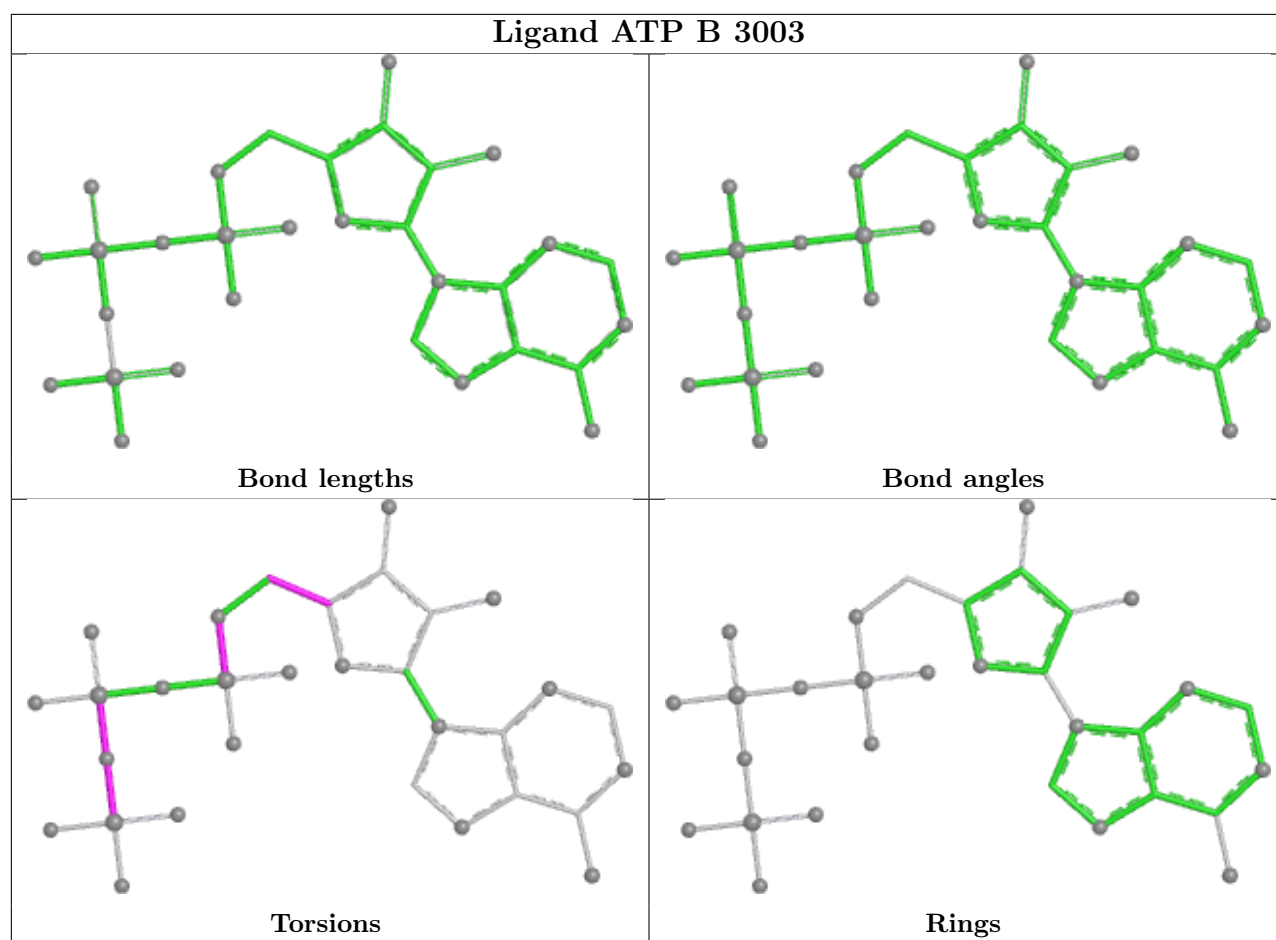


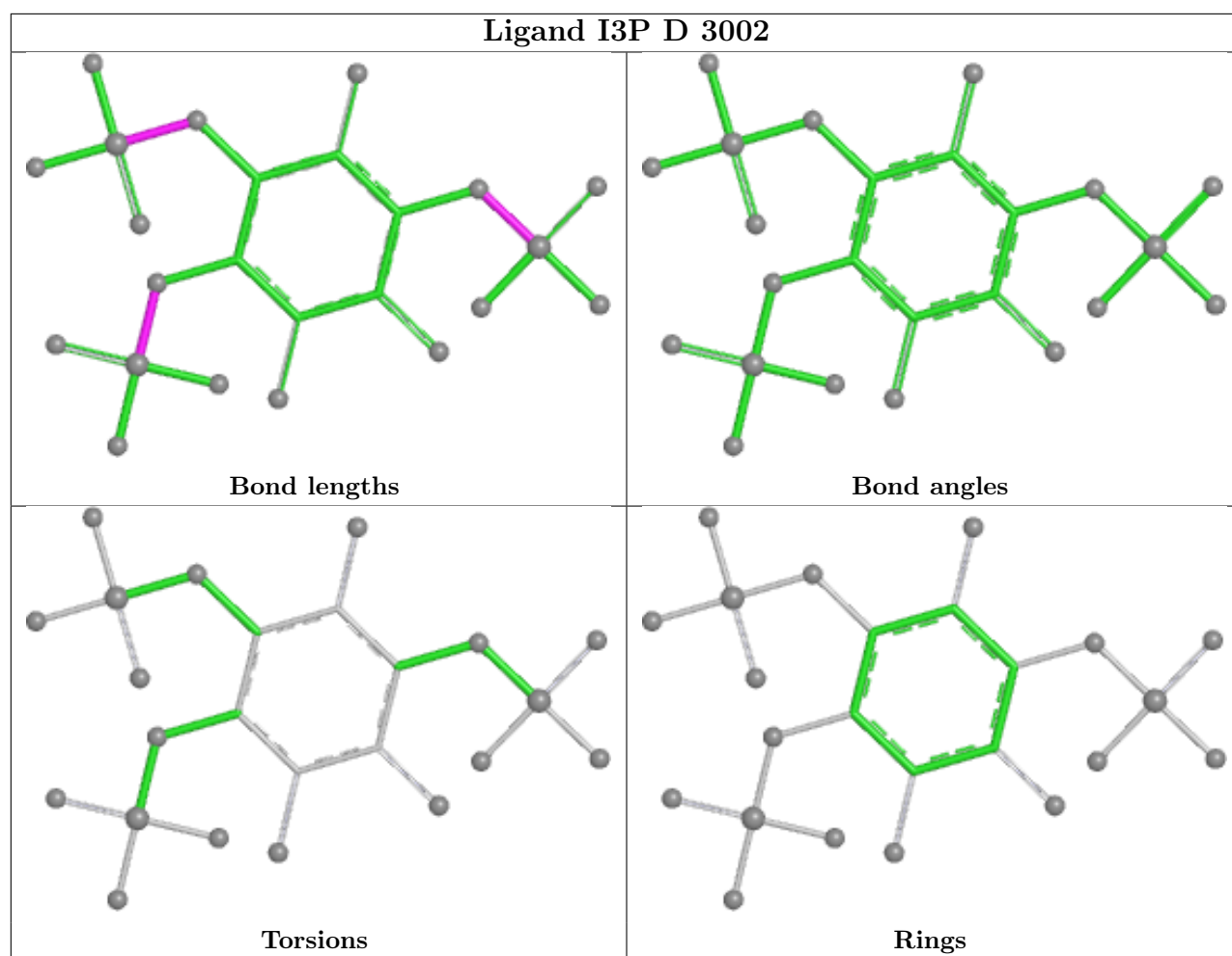


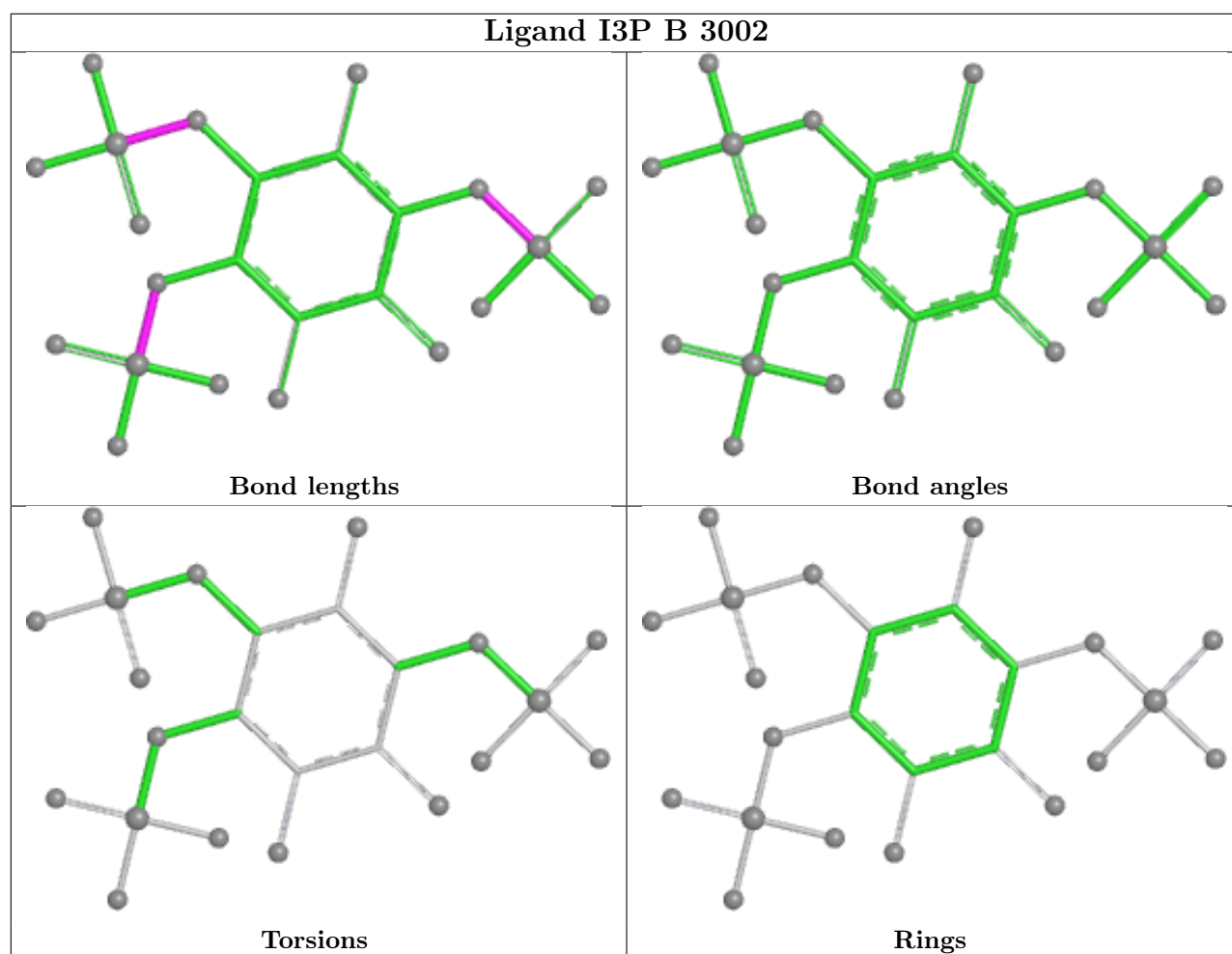












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

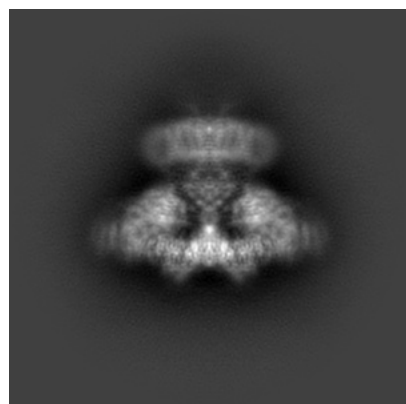
6 Map visualisation [i](#)

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

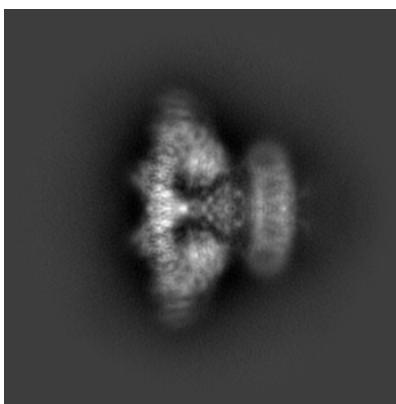
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

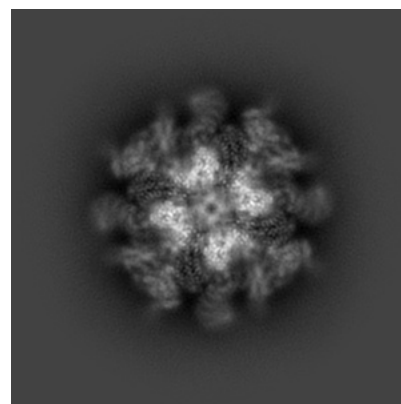
6.1.1 Primary map



X

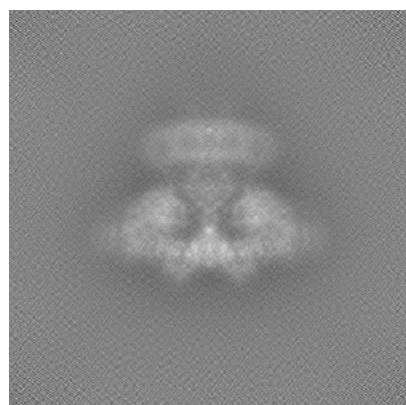


Y

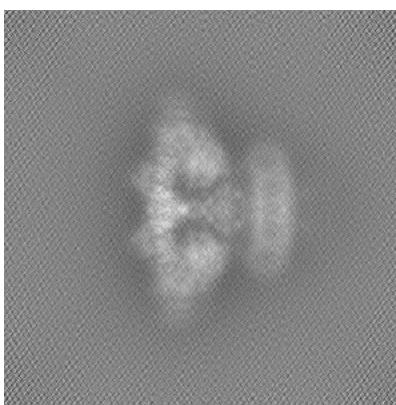


Z

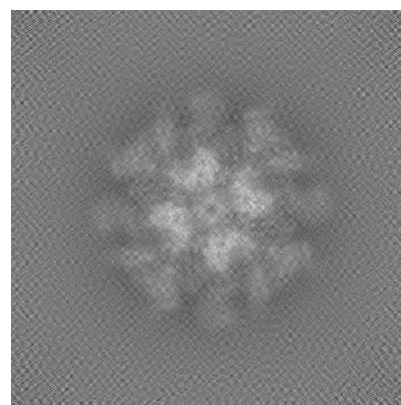
6.1.2 Raw map



X



Y

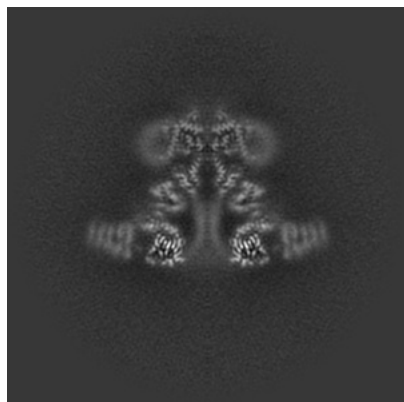


Z

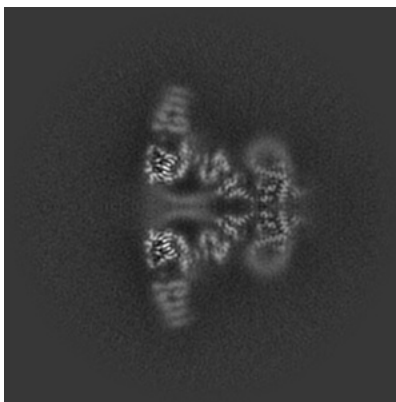
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

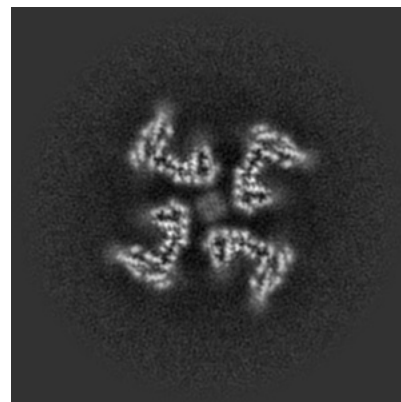
6.2.1 Primary map



X Index: 256

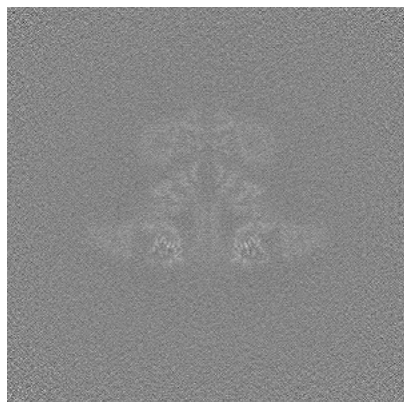


Y Index: 256

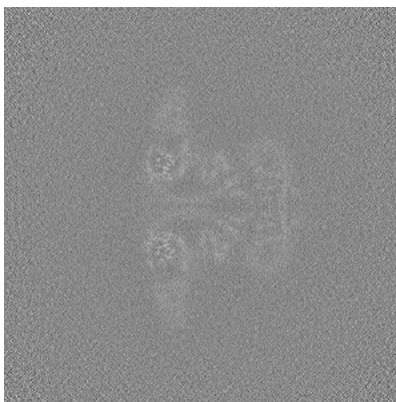


Z Index: 256

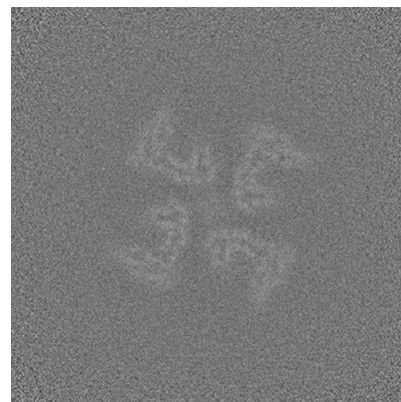
6.2.2 Raw map



X Index: 256



Y Index: 256

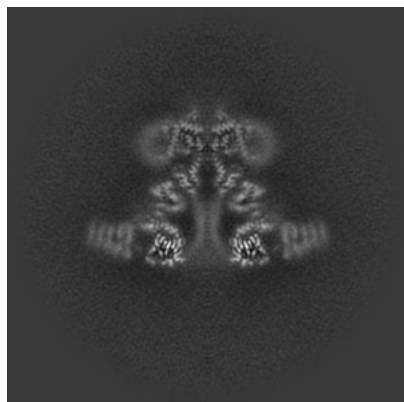


Z Index: 256

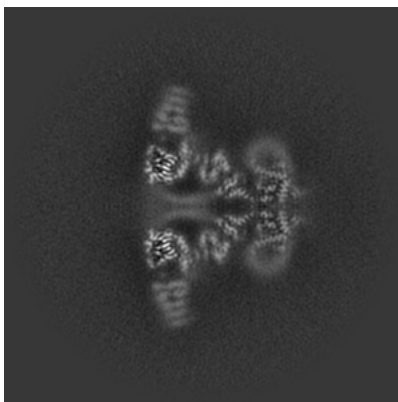
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

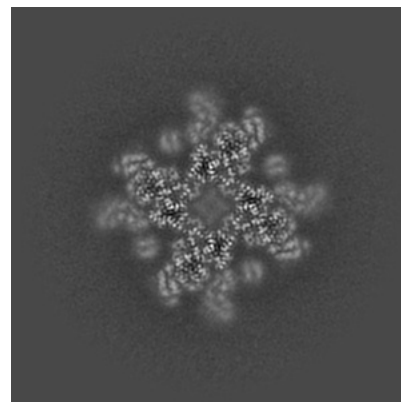
6.3.1 Primary map



X Index: 256

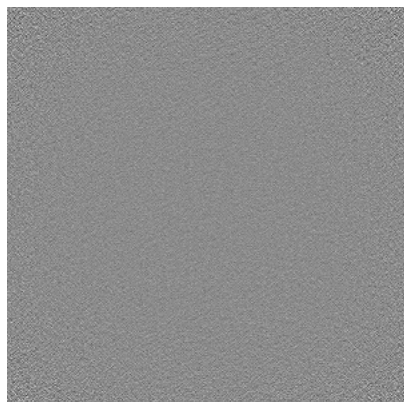


Y Index: 256

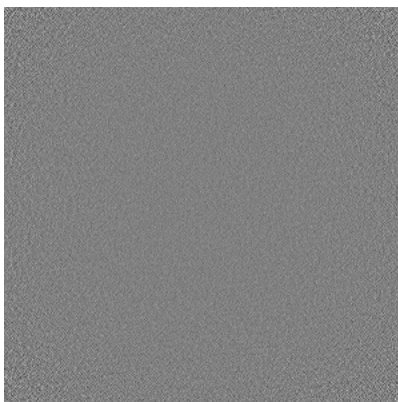


Z Index: 205

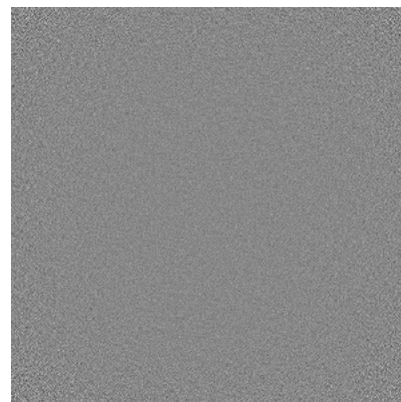
6.3.2 Raw map



X Index: 0



Y Index: 0

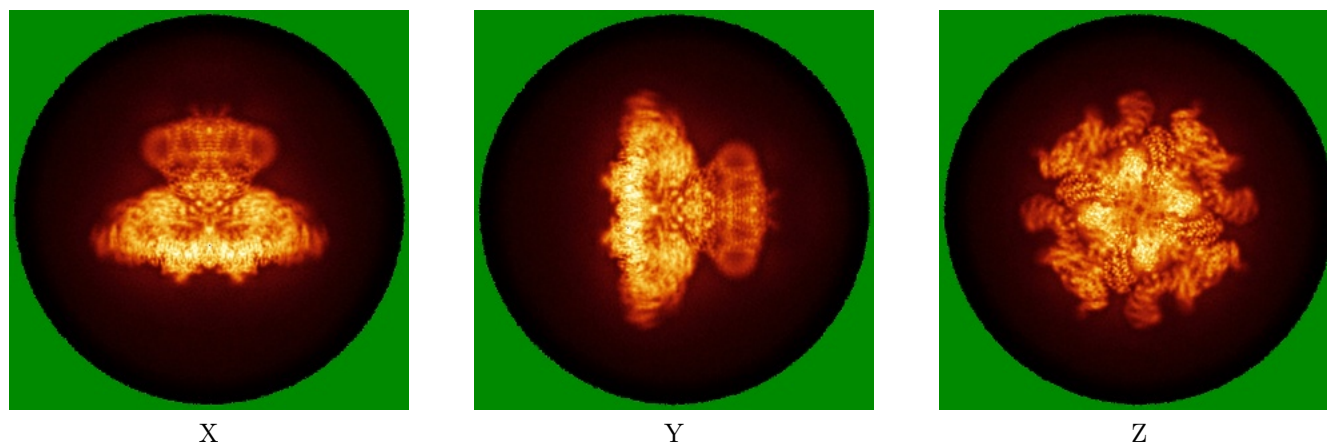


Z Index: 0

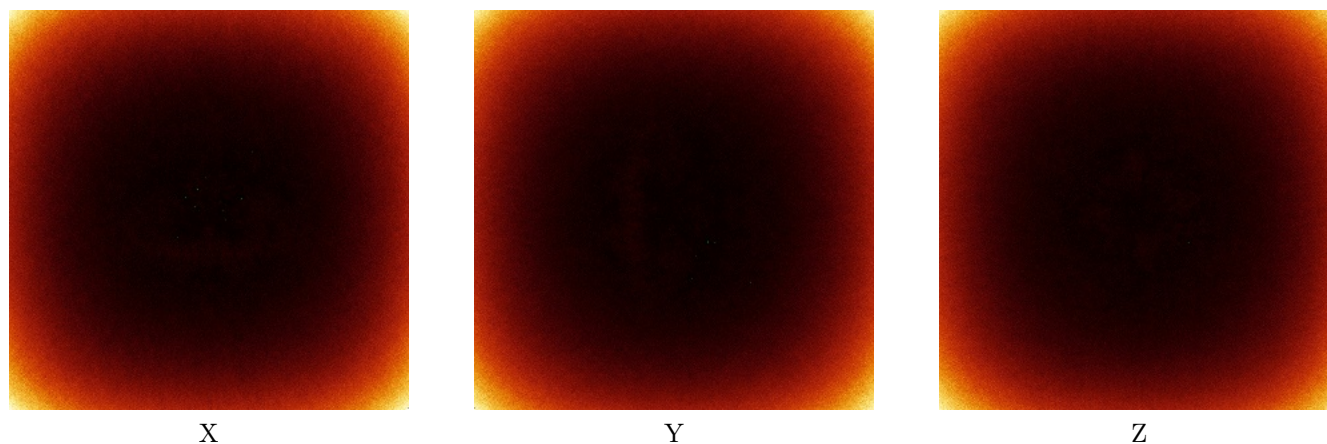
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



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.

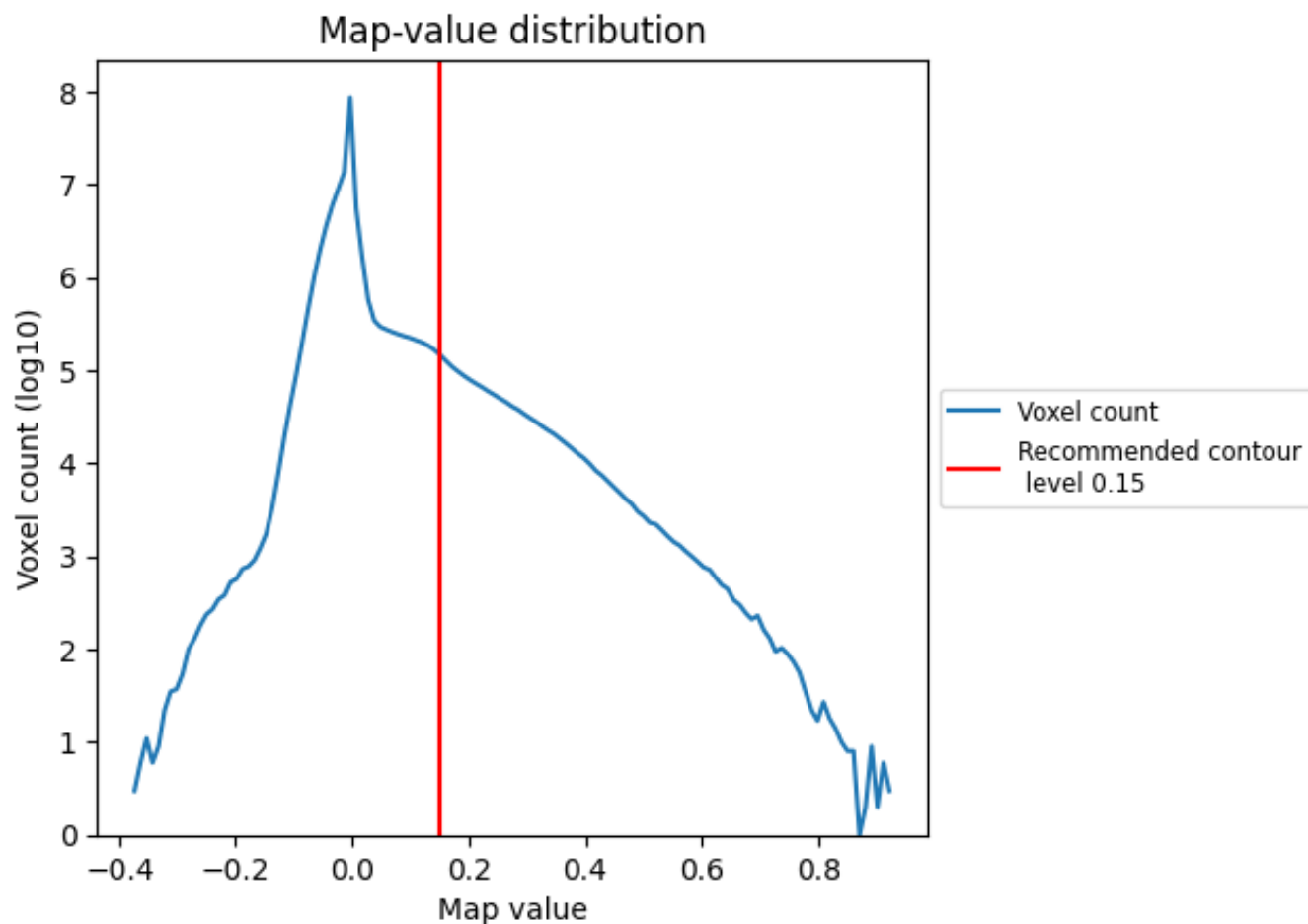
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

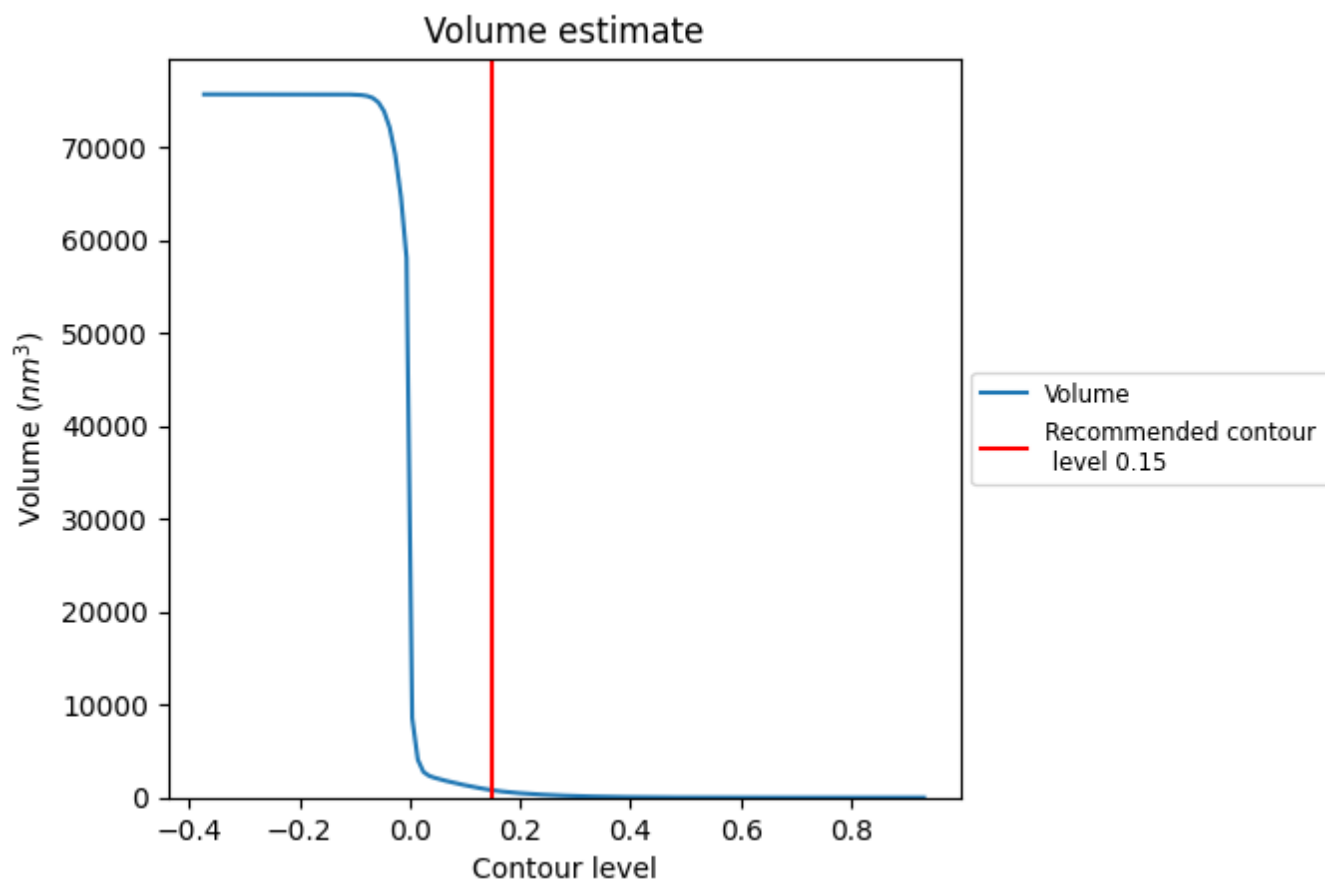
This section contains the results of statistical analysis of the map.

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.

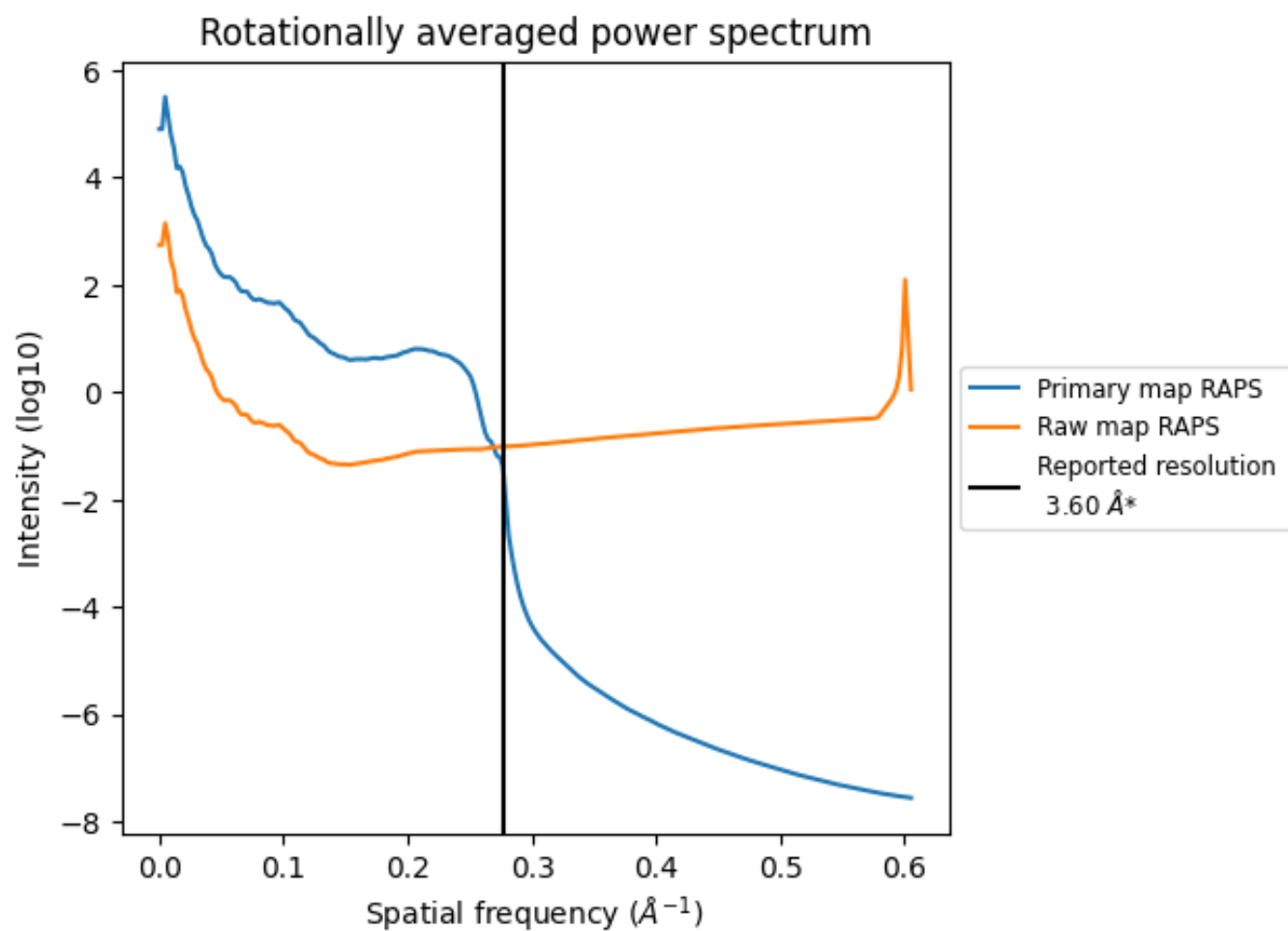
7.2 Volume estimate [i](#)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

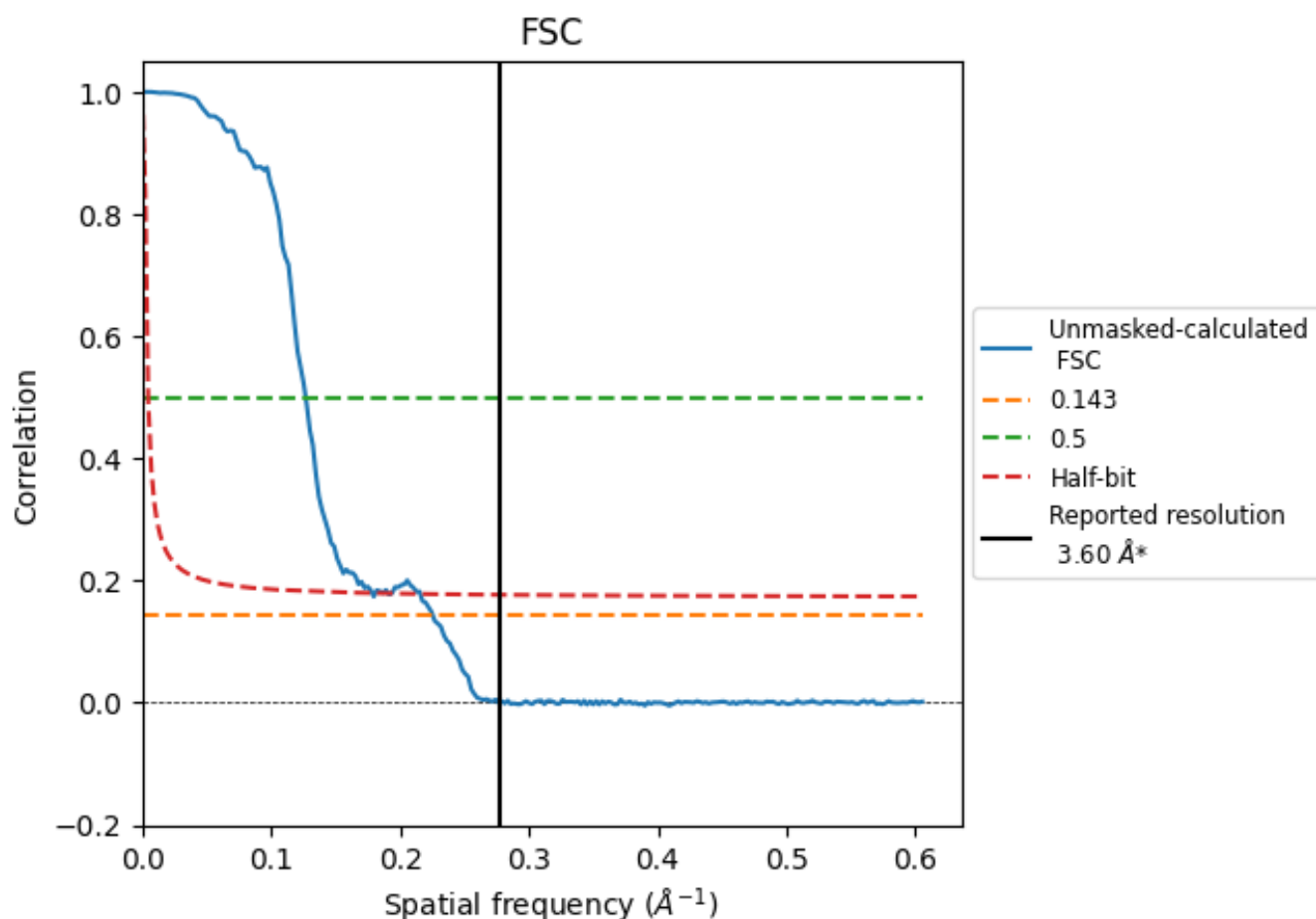


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

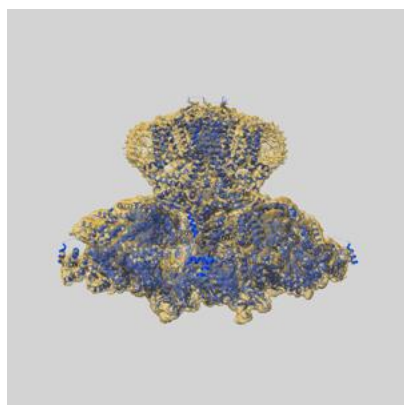
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.43	7.89	5.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.43 differs from the reported value 3.6 by more than 10 %

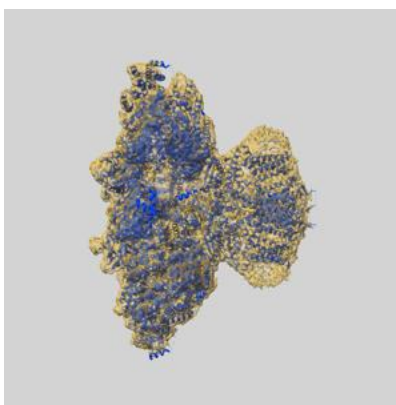
9 Map-model fit [i](#)

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

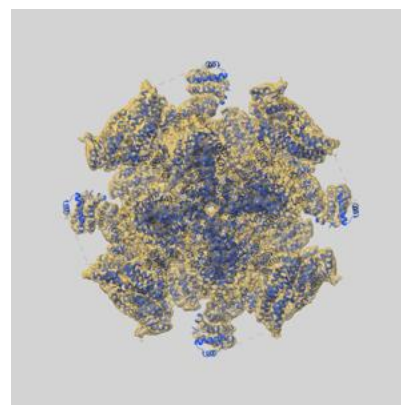
9.1 Map-model overlay [i](#)



X



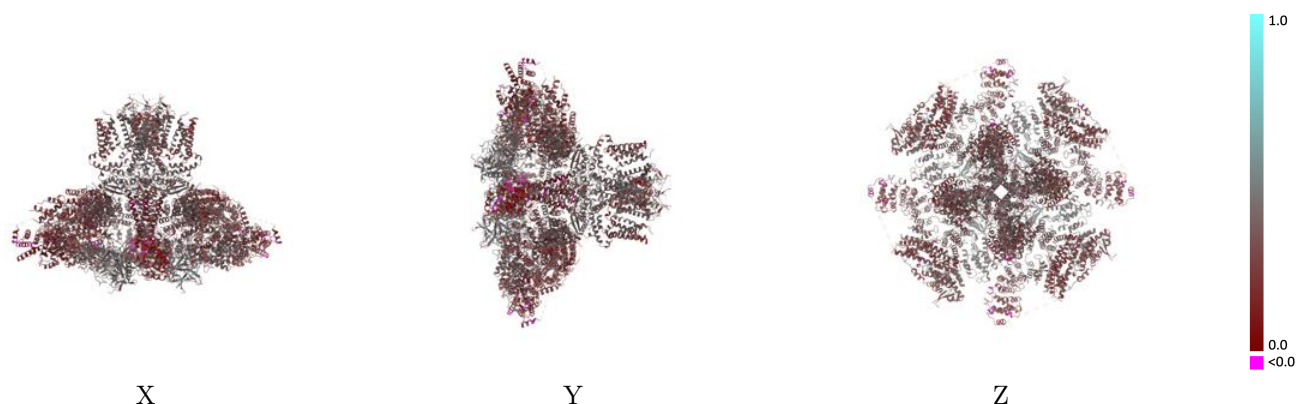
Y



Z

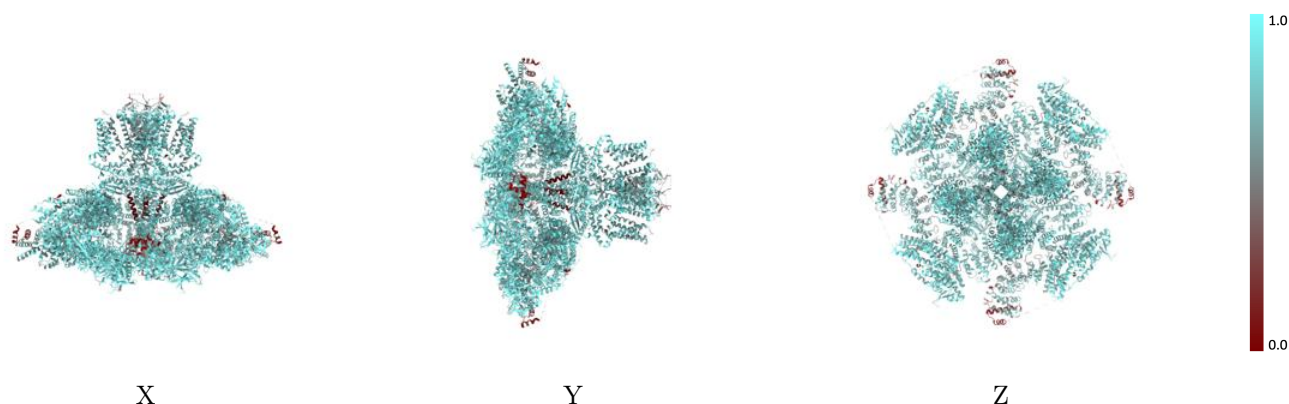
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



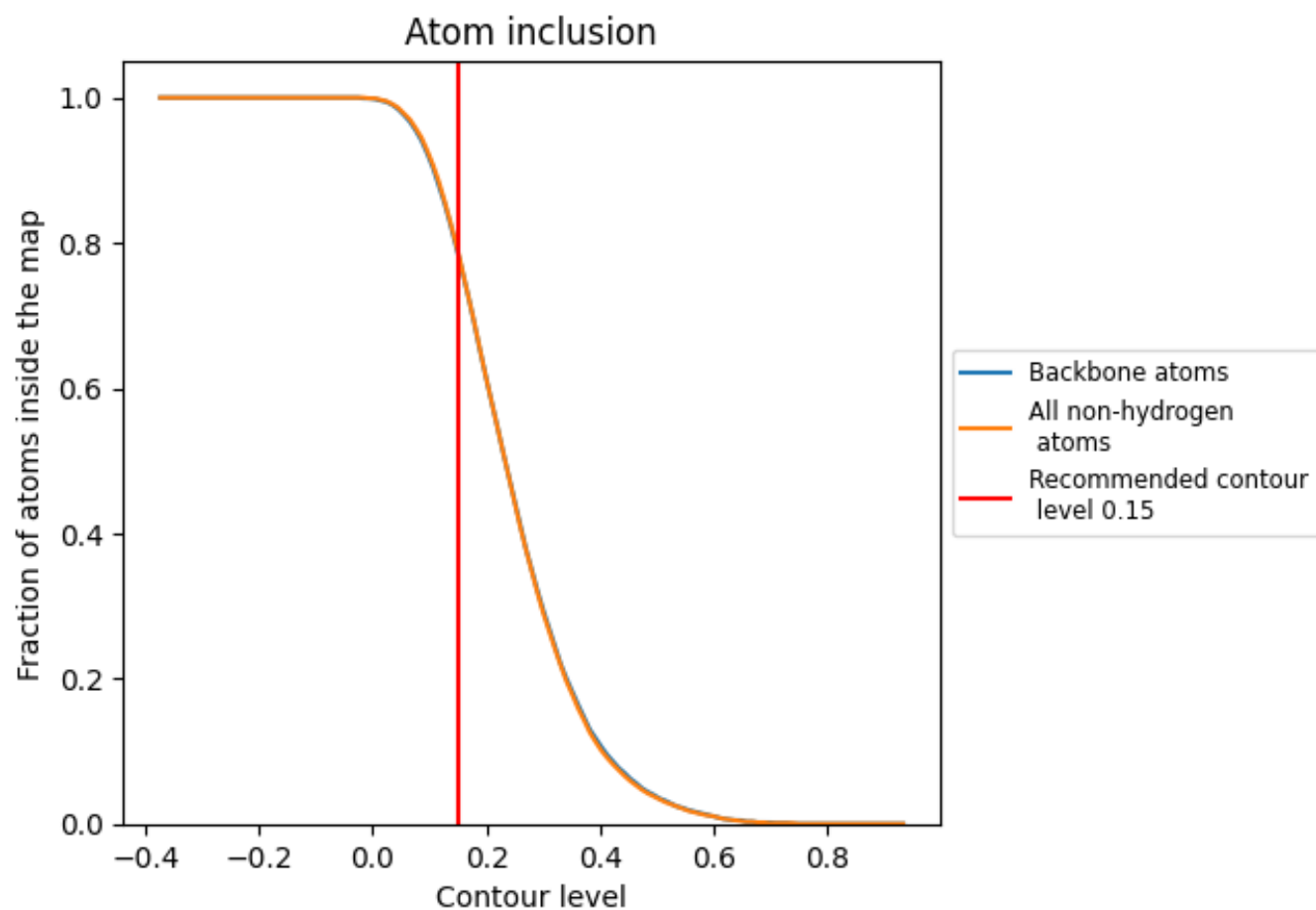
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

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

