



# wwPDB EM Validation Summary Report ⓘ

Oct 30, 2023 – 04:13 PM EDT

PDB ID : 8TL9  
EMDB ID : EMD-41365  
Title : Human Type 3 IP3 Receptor - Resting State (+IP3/ATP)  
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.  
Deposited on : 2023-07-26  
Resolution : 3.30 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

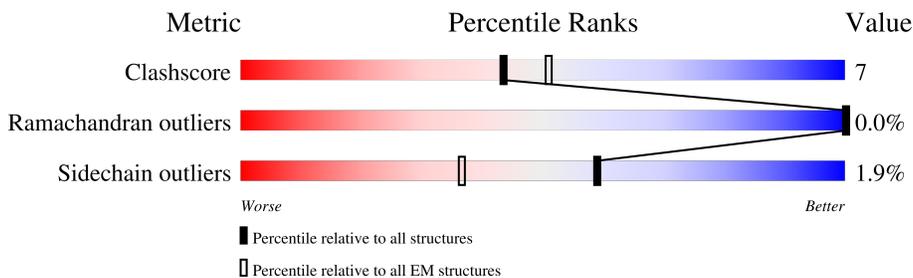
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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  $\geq 3$ , 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	
1	B	2671	
1	C	2671	
1	D	2671	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 130518 atoms, of which 65442 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.

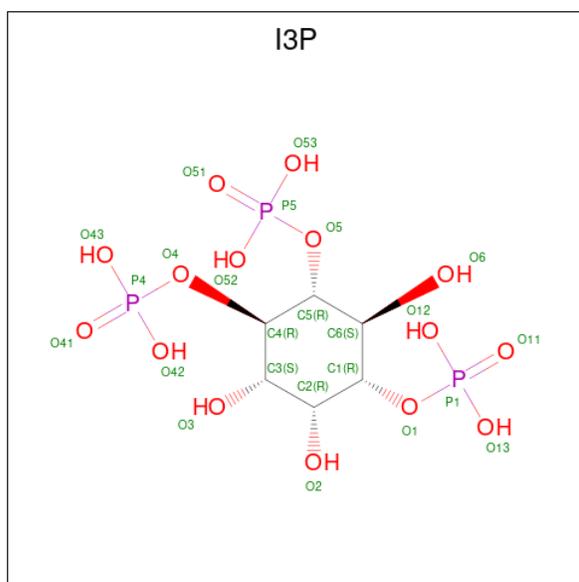
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1989	32350	10293	16244	2749	2960	104	0	0
1	B	1987	32312	10283	16225	2743	2957	104	0	0
1	C	2005	32587	10375	16353	2768	2987	104	0	0
1	D	2034	32957	10480	16536	2807	3029	105	0	0

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

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

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



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).







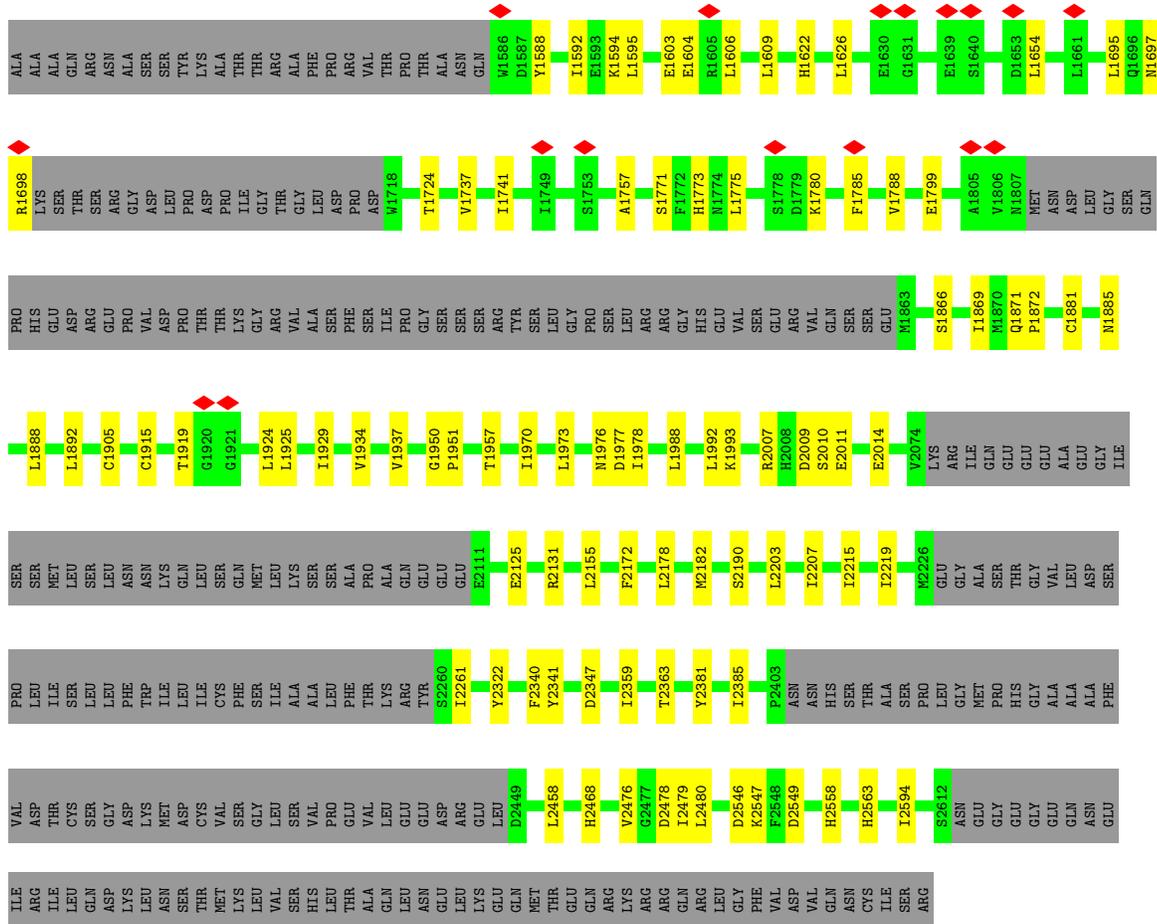




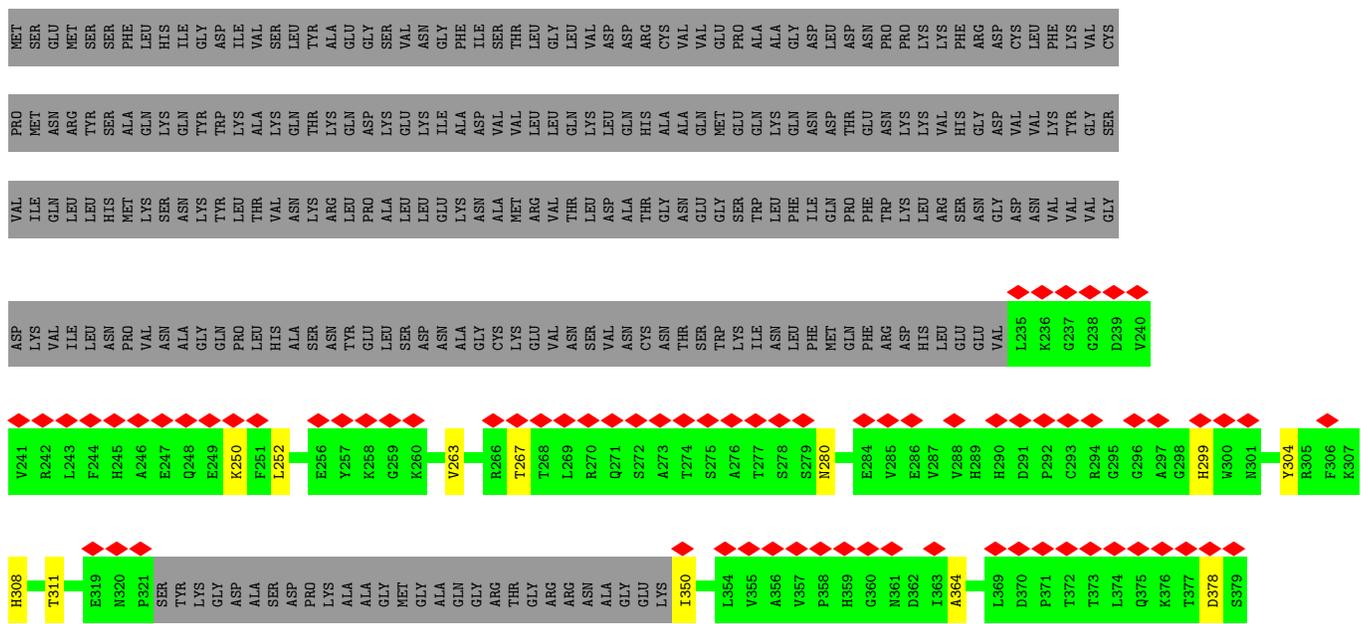
Q1031	A1032	E1033	M1034	H1035	F1036	G1037	VAL	GLY	LYS	THR	SER	S1043	M1044	L1045	E1046	V1047	D1048	D1049	E1050	M1054	R1057	L1062	T1063	M1064	H1065	D1066	Y1067	A1068	F1069	L1070	Y1071	S1072	L1075	Q1076	F1079	F1082	Q1086	E1087	A1088	M1089	H1090	H1091	F1092	K1093	Q1094	V1095	Q1096	L1097	M1101	Q1102											
E1105	K1108	Q1170	I1171	I1110	K1111	L1114	D1115	R1116	L1117	R1118	M1119	M1120	K1123	S1124	E1125	Y1126	L1126	W1127	V1128	D1129	LYS	GLY	GLY	GLY	GLY	GLY	GLU	VAL	GLU	ALA	GLY	ALA	ALA	ALA	ASP	L1207	LYS	LYS	GLU	ARG	PRU	THR	ASP	GLU	GLU	GLY	PHE	LEU	HIS	PRO	PRO	GLY	LYS	SER	S1166	E1167					
M1168	Y1169	Q1170	I1171	I1110	K1111	L1114	D1115	R1116	L1117	R1118	M1119	M1120	K1123	S1124	E1125	Y1126	L1126	W1127	V1128	D1129	LYS	GLY	GLY	GLY	GLY	GLU	VAL	GLU	ALA	GLY	ALA	ALA	ASP	L1207	LYS	LYS	GLU	ARG	PRU	THR	ASP	GLU	GLU	GLY	PHE	LEU	HIS	PRO	PRO	GLY	LYS	SER	S1166	E1167							
M1168	Y1169	Q1170	I1171	I1110	K1111	L1114	D1115	R1116	L1117	R1118	M1119	M1120	K1123	S1124	E1125	Y1126	L1126	W1127	V1128	D1129	LYS	GLY	GLY	GLY	GLY	GLU	VAL	GLU	ALA	GLY	ALA	ALA	ASP	L1207	LYS	LYS	GLU	ARG	PRU	THR	ASP	GLU	GLU	GLY	PHE	LEU	HIS	PRO	PRO	GLY	LYS	SER	S1166	E1167							
F1231	L1232	Q1233	F1234	R1235	C1236	A1237	G1238	M1239	F1240	G1241	M1242	Q1243	A1244	L1245	L1246	H1247	K1248	H1249	L1250	H1251	L1252	F1253	L1254	T1255	P1256	G1257	L1258	L1259	E1260	A1261	E1262	K1263	T1264	M1265	Q1266	H1266	I1267	F1268	L1269	M1270	Q1271	M1271	Y1272	Q1273	L1274	C1275	S1276	E1277	I1278	K1279	S1280	P1281	V1282	L1283	Q1284	H1285	F1286	V1287	H1288	L1289	L1290
A1291	T1292	H1293	G1294	R1295	H1296	V1297	Q1298	Y1299	L1300	D1301	F1302	L1303	H1304	T1305	V1306	L1307	K1308	A1309	E1310	G1311	K1312	Y1313	V1314	K1315	K1316	C1317	Q1318	D1319	M1320	I1321	M1322	T1323	L1324	L1325	T1326	M1327	A1328	G1329	D1330	V1331	V1332	V1333	V1334	F1335	Y1336	L1337	D1338	K1339	A1340	S1341	L1342	A1343	H1344	L1345	L1346	D1347	M1348	K1349	K1350		
A1351	A1352	R1353	D1354	G1355	V1356	E1357	D1358	H1359	S1360	P1361	L1362	M1363	H1364	H1365	I1366	S1367	L1368	V1369	D1370	L1371	L1372	A1373	A1374	E1377	G1378	K1379	M1380	V1381	Y1382	L1383	E1384	I1385	K1386	C1387	L1388	S1389	A1390	L1391	P1392	L1393	E1394	D1395	V1396	V1397	S1398	A1399	V1400	T1401	H1402	E1403	D1404	C1405	V1406	T1407	E1408	V1409	M1410	M1411			
A1412	Y1413	F1416	V1417	M1418	H1419	C1420	Y1421	Y1422	D1423	T1424	E1425	Y1426	E1427	M1428	K1429	E1430	I1431	Y1432	T1433	S1434	N1435	H1436	I1437	M1438	T1439	L1440	F1441	E1442	M1443	F1444	T1445	L1446	D1447	M1448	A1449	R1450	V1451	C1452	S1453	K1454	R1455	E1456	K1457	R1458	V1459	H1518	K1519	G1520	S1521	V1522	E1523	A1524	C1525	I1526	R1527	T1528	L1529	A1530	M1531	V1532	
L1473	D1474	T1475	T1476	M1477	A1478	F1479	F1480	S1481	S1482	P1483	F1484	S1485	E1486	M1487	S1488	T1489	S1490	L1491	Q1492	T1493	H1494	Q1495	T1496	I1497	V1498	V1499	Q1500	L1501	L1502	Q1503	S1504	S1505	T1506	R1507	L1508	L1509	E1510	C1511	P1512	M1513	L1514	Q1515	Q1516	Q1517	H1518	K1519	G1520	S1521	V1522	E1523	A1524	C1525	I1526	R1527	T1528	L1529	A1530	M1531	V1532		
A1533	K1534	G1535	R1536	A1537	L1538	L1539	L1540	P1541	M1542	D1543	L1544	D1545	E1546	H1547	I1548	S1549	M1551	L1552	S1553	S1554	G1555	A1556	S1557	CYS	ALA	ALA	ALA	ALA	GLN	ARG	ASN	ALA	SER	SER	TYR	LYS	ALA	THR	THR	ARG	ALA	PHE	PRO	VAL	VAL	THR	PRO	THR	ALA	ASN	GLN	V1556	D1557	Y1558	K1559	M1590	I1591	I1592			
E1593	K1594	L1595	Q1596	D1597	I1598	I1599	T1600	A1601	L1602	E1603	E1604	R1605	L1606	K1607	L1621	H1622	E1630	G1631	S1632	R1637	C1638	E1639	S1640	F1643	L1647	Q1648	H1650	T1651	K1652	D1653	L1654	M1655	E1656	S1657	E1658	E1659	K1660	L1661	V1665	M1672	L1673	L1674	K1675	K1676	T1677	K1678	Y1679	G1680	D1681	R1682											
Q1696	ASN	ARG	LYS	THR	SER	ARG	GLY	ASP	LEU	PRO	ALA	ASP	PRO	ILE	GLY	THR	GLY	LEU	ASP	PRO	ASP	ASP	W1718	L1728	D1729	K1730	E1731	D1739	L1740	I1741	T1742	S1743	I1744	K1745	I1749	S1771	F1785	E1799	V1804	A1805	V1806	N1807	MET	ASN	ASP	LEU	GLY	SER	GLN	PRO	HIS	GLU	ASP								
ARG	GLU	PRO	VAL	ASP	THR	THR	LYS	GLY	ARG	VAL	ALA	SER	PHE	SER	ILE	PRO	GLY	LEU	ASP	SER	SER	ARG	TYR	SER	LEU	GLY	HIS	GLU	VAL	SER	GLN	VAL	GLU	ARG	ARG	GLU	ARG	M1863	S1866	L1869	M1870	Q1871	L1877	C1894	Q1895	M1896	N1897	P2021	K1898	T1899											
M1900	Y1901	M1902	C1905	M1914	C1915	T1919	G1920	G1921	L1922	G1923	L1924	V1934	Y1947	C1948	G1949	G1950	P1951	I1959	V1960	T1961	H1962	E1963	I1969	L1973	I1974	L1975	M1976	D1977	S1978	L1981	C1982	L1988	L2003	B2009	S2010	E2011	N2012	A2013	E2014	S2019	L2020	R2021	P2022	L2025																	







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





P2022	V2026	E2048	K2065	V2074	LYS	ARG	ILE	GLN	GLU	GLU	GLU	ALA	THR	GLY	GLY	VAL	LEU	ILE	SER	ASP	SER	MET	LEU	SER	LEU	ASN	LYS	GLN	LEU	SER	GLN	GLN	E2111	I2143	L2155	T2159	D2162	E2163	Q2164	K2167	F2172																					
S2175	L2178	M2182	R2199	A2220	M2226	GLY	ALA	SER	THR	GLY	VAL	LEU	ASP	SER	PRO	LEU	ILE	SER	ASP	SER	PRO	LEU	ILE	SER	SER	LEU	LEU	ASN	PHE	TRP	TRP	ILE	LEU	ILE	LEU	ILE	CYS	PHE	LEU	SER	LYS	ILE	ALA	ALA	PRO	ALA	ALA	THR	THR	LYS	ARG	TYR	S2260	I2261	L2290	I2294	V2295	F2296	V2297	V2298	R2309	V2331
R2367	S2368	I2369	L2389	F2403	ASN	ASN	HIS	SER	THR	ALA	SER	PRO	LEU	GLY	MET	PRO	HIS	GLY	ALA	ALA	ALA	PHE	VAL	ASP	THR	THR	CYS	SER	GLY	ASP	LYS	MET	ASP	VAL	SER	GLY	VAL	SER	GLY	VAL	SER	PRO	VAL	VAL	LEU	LEU	GLU	GLU	GLU	ASP	ARG	GLU	LEU	D2449	M2460	C2461	H2468	V2476				
I2479	P2491	V2495	I2512	E2531	L2543	D2549	N2550	V2553	H2558	E2562	H2563	R2576	I2594	L2610	V2611	S2612	ASN	GLU	GLY	GLY	GLY	GLY	GLN	ASN	GLU	ILE	ILE	ILE	LEU	GLN	ASP	LYS	ASN	SER	THR	MET	LYS	LEU	VAL	SER	HIS	LEU	THR	ALA	GLN																	
LEU	ASN	GLU	LEU	LYS	GLN	MET	THR	GLU	GLN	ARG	LYS	ARG	ARG	ARG	GLN	ARG	LEU	GLY	PHE	VAL	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	88082	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	0.869	Depositor
Minimum map value	-0.421	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/16403	0.47	0/22156
1	B	0.25	0/16384	0.46	0/22131
1	C	0.25	0/16535	0.46	0/22337
1	D	0.25	0/16726	0.46	0/22603
All	All	0.25	0/66048	0.46	0/89227

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	16106	16244	16243	255	0
1	B	16087	16225	16224	248	0
1	C	16234	16353	16362	210	0
1	D	16421	16536	16535	203	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	1	0
3	C	24	9	9	0	0
3	D	24	9	9	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	12	12	0	0
5	B	31	12	12	0	0
5	C	31	12	12	0	0
5	D	31	12	12	0	0
All	All	65076	65442	65448	911	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 7.

The worst 5 of 911 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:1962:HIS:HD1	1:A:1964:SER:HG	0.98	0.96
1:B:1799:GLU:OE1	1:B:1866:SER:OG	1.91	0.89
1:C:354:LEU:HD12	1:C:417:LEU:HD12	1.55	0.87
1:D:1510:GLU:OE2	1:D:1547:HIS:NE2	2.08	0.84
1:A:1262:GLU:O	1:A:1266:HIS:ND1	2.11	0.83

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	1961/2671 (73%)	1930 (98%)	30 (2%)	1 (0%)	51 81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1959/2671 (73%)	1937 (99%)	22 (1%)	0	100	100
1	C	1979/2671 (74%)	1948 (98%)	31 (2%)	0	100	100
1	D	2010/2671 (75%)	1975 (98%)	35 (2%)	0	100	100
All	All	7909/10684 (74%)	7790 (98%)	118 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1697	ASN

### 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	1807/2385 (76%)	1760 (97%)	47 (3%)	46	71
1	B	1805/2385 (76%)	1758 (97%)	47 (3%)	46	71
1	C	1821/2385 (76%)	1803 (99%)	18 (1%)	76	86
1	D	1838/2385 (77%)	1811 (98%)	27 (2%)	65	81
All	All	7271/9540 (76%)	7132 (98%)	139 (2%)	59	77

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	778	CYS
1	D	1043	SER
1	D	1894	CYS
1	B	444	PHE
1	B	251	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2292	ASN
1	C	1622	HIS
1	D	1622	HIS
1	C	1065	HIS
1	C	2598	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ATP	D	3004	-	26,33,33	0.60	0	31,52,52	1.06	2 (6%)
3	I3P	C	3002	-	24,24,24	2.08	3 (12%)	36,39,39	0.85	0
3	I3P	A	3002	-	24,24,24	2.08	3 (12%)	36,39,39	0.84	0
3	I3P	B	3002	-	24,24,24	2.08	3 (12%)	36,39,39	0.91	0
5	ATP	B	3004	-	26,33,33	0.60	0	31,52,52	1.08	3 (9%)
3	I3P	D	3002	-	24,24,24	2.08	3 (12%)	36,39,39	0.84	0
5	ATP	A	3004	-	26,33,33	0.60	0	31,52,52	1.08	3 (9%)
5	ATP	C	3004	-	26,33,33	0.60	0	31,52,52	1.07	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	D	3004	-	-	2/18/38/38	0/3/3/3
3	I3P	C	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	A	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	B	3002	-	-	2/15/39/39	0/1/1/1
5	ATP	B	3004	-	-	4/18/38/38	0/3/3/3
3	I3P	D	3002	-	-	2/15/39/39	0/1/1/1
5	ATP	A	3004	-	-	5/18/38/38	0/3/3/3
5	ATP	C	3004	-	-	2/18/38/38	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	A	3002	I3P	P4-O4	5.74	1.70	1.59
3	B	3002	I3P	P4-O4	5.74	1.70	1.59
3	C	3002	I3P	P4-O4	5.74	1.70	1.59
3	D	3002	I3P	P4-O4	5.73	1.70	1.59
3	C	3002	I3P	P5-O5	5.64	1.70	1.59

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3004	ATP	C5'-C6'-N6	2.31	123.86	120.35
5	B	3004	ATP	C5'-C6'-N6	2.31	123.86	120.35
5	C	3004	ATP	C5'-C6'-N6	2.30	123.85	120.35
5	D	3004	ATP	C5'-C6'-N6	2.30	123.85	120.35
5	B	3004	ATP	O4'-C1'-C2'	-2.17	103.75	106.93

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

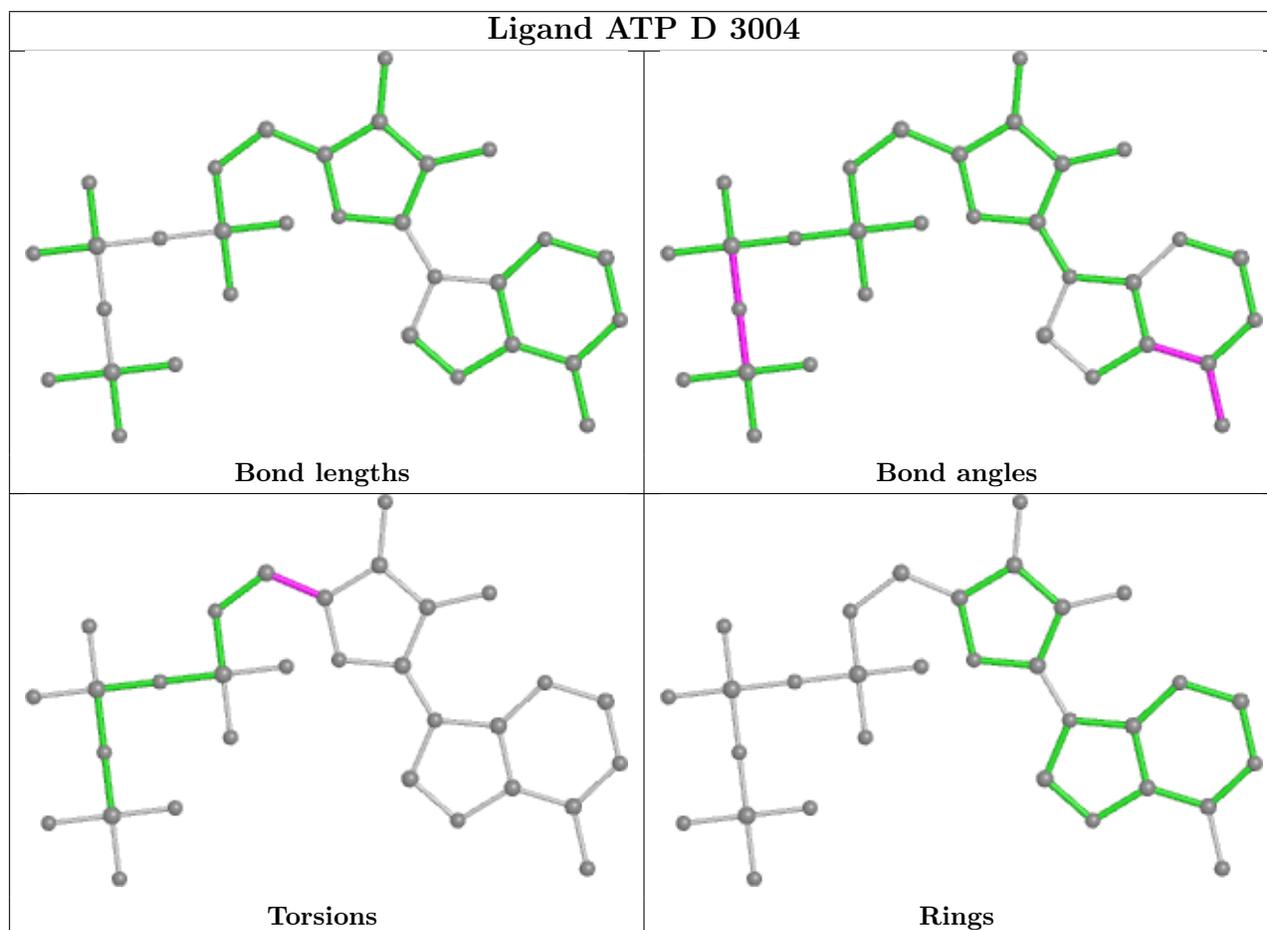
Mol	Chain	Res	Type	Atoms
5	A	3004	ATP	C5'-O5'-PA-O2A
5	A	3004	ATP	C3'-C4'-C5'-O5'
5	A	3004	ATP	O4'-C4'-C5'-O5'
5	D	3004	ATP	O4'-C4'-C5'-O5'
5	D	3004	ATP	C3'-C4'-C5'-O5'

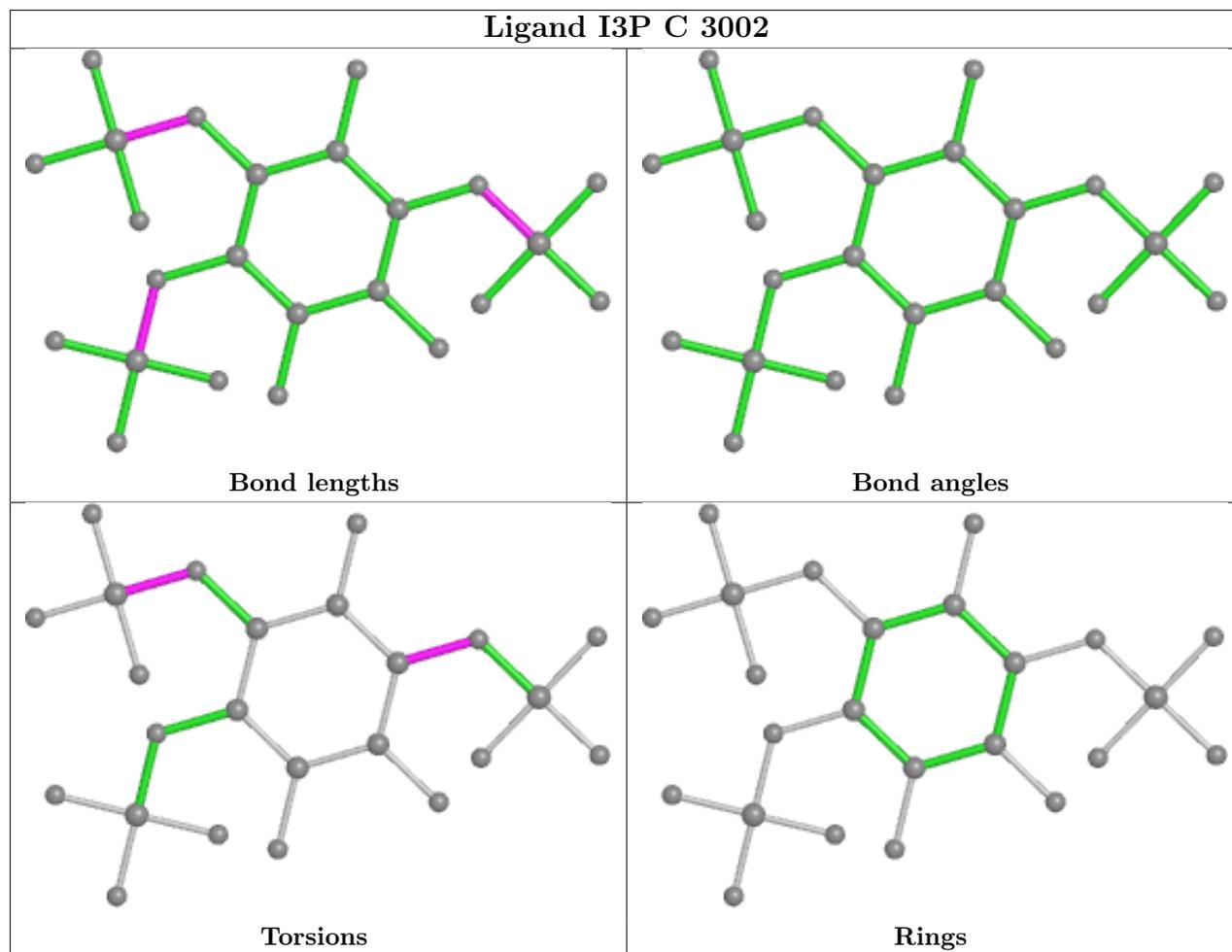
There are no ring outliers.

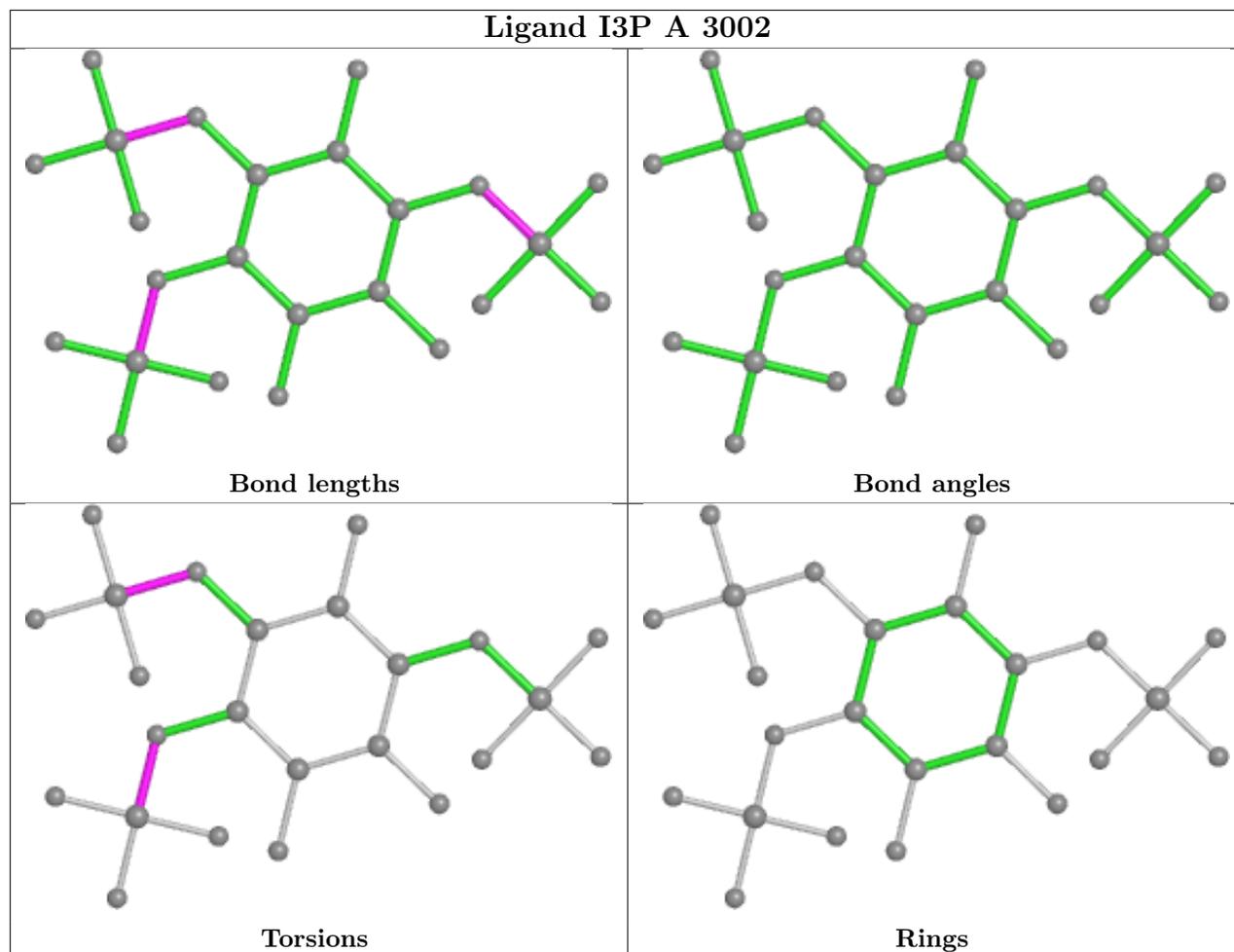
1 monomer is involved in 1 short contact:

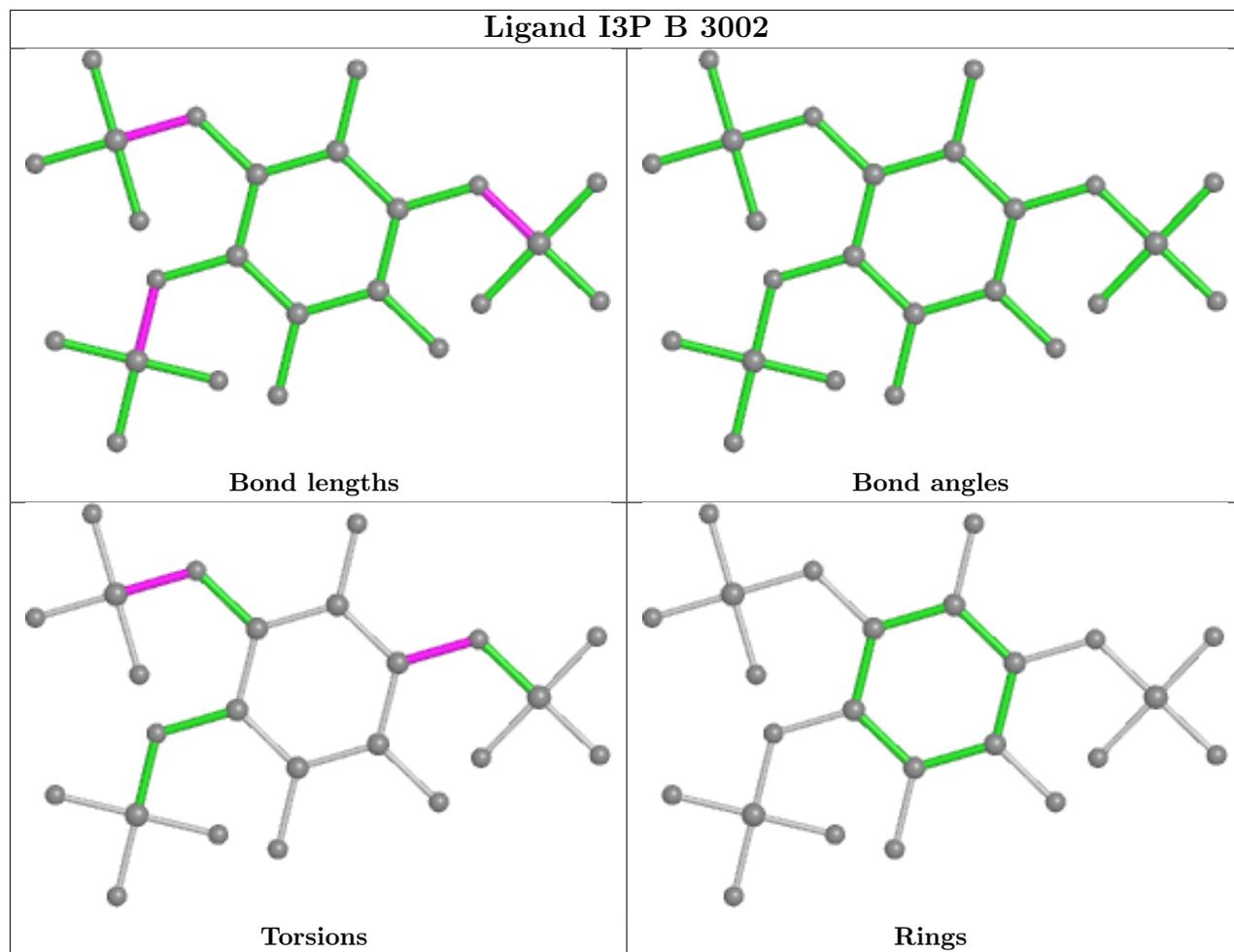
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3002	I3P	1	0

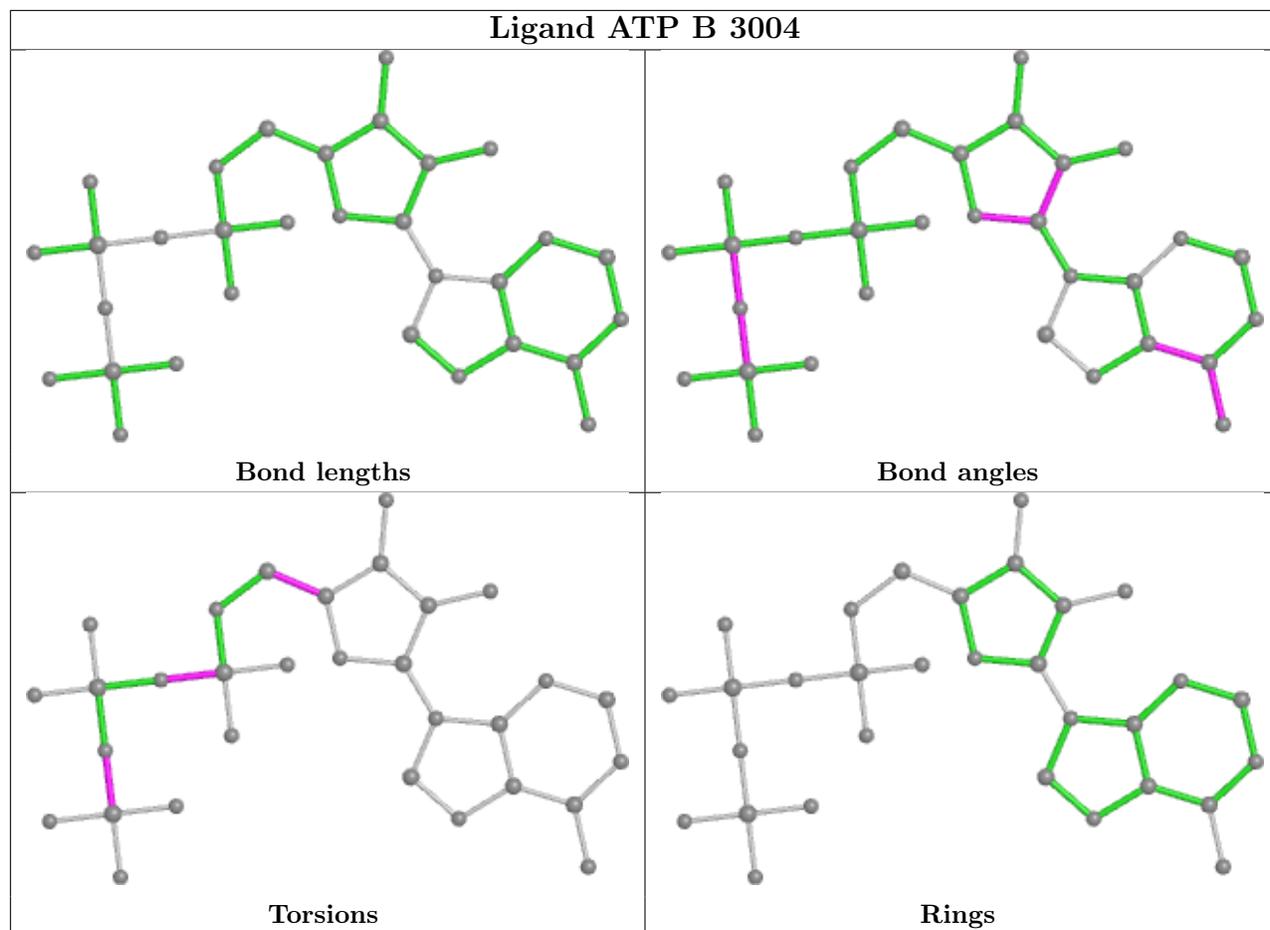
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

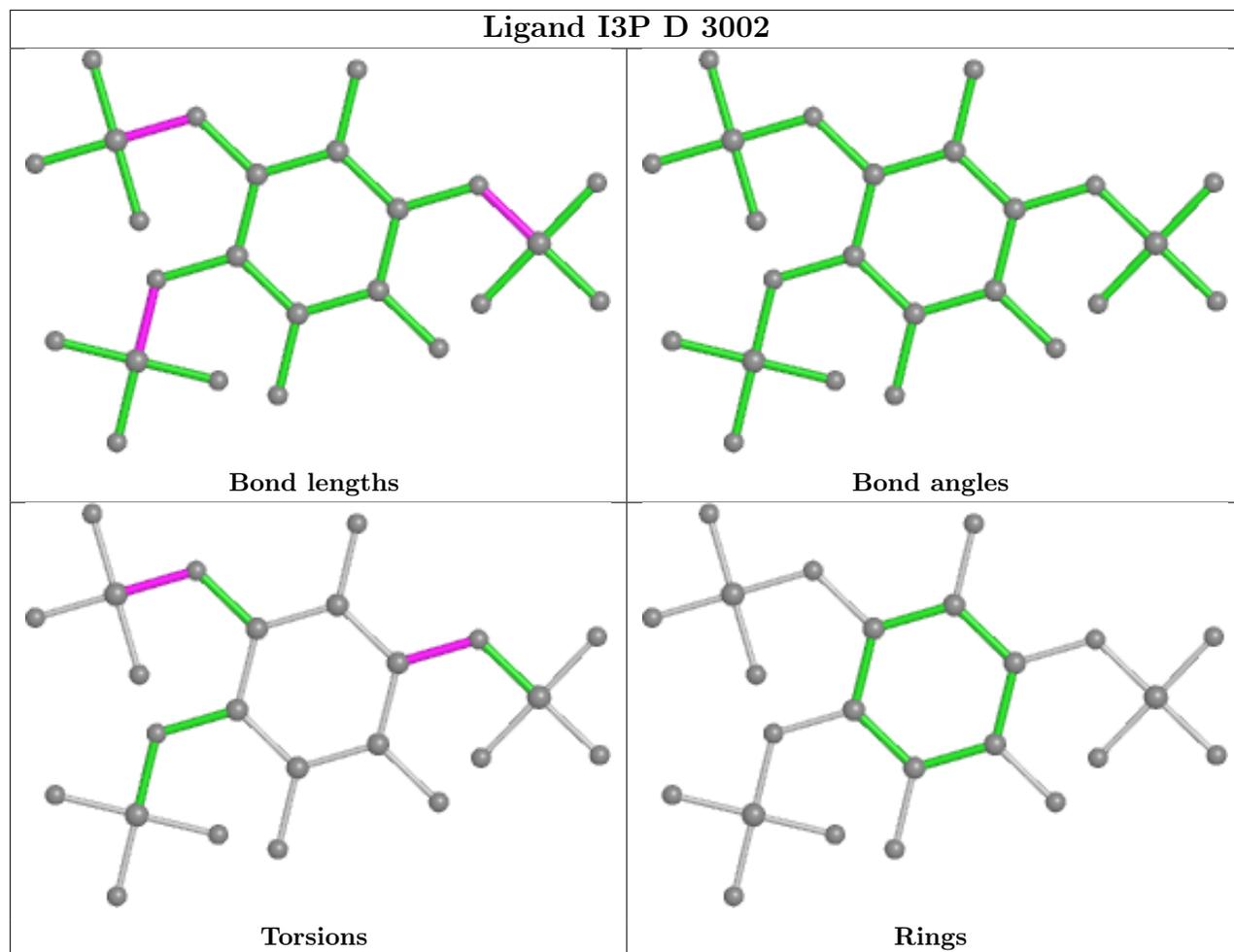


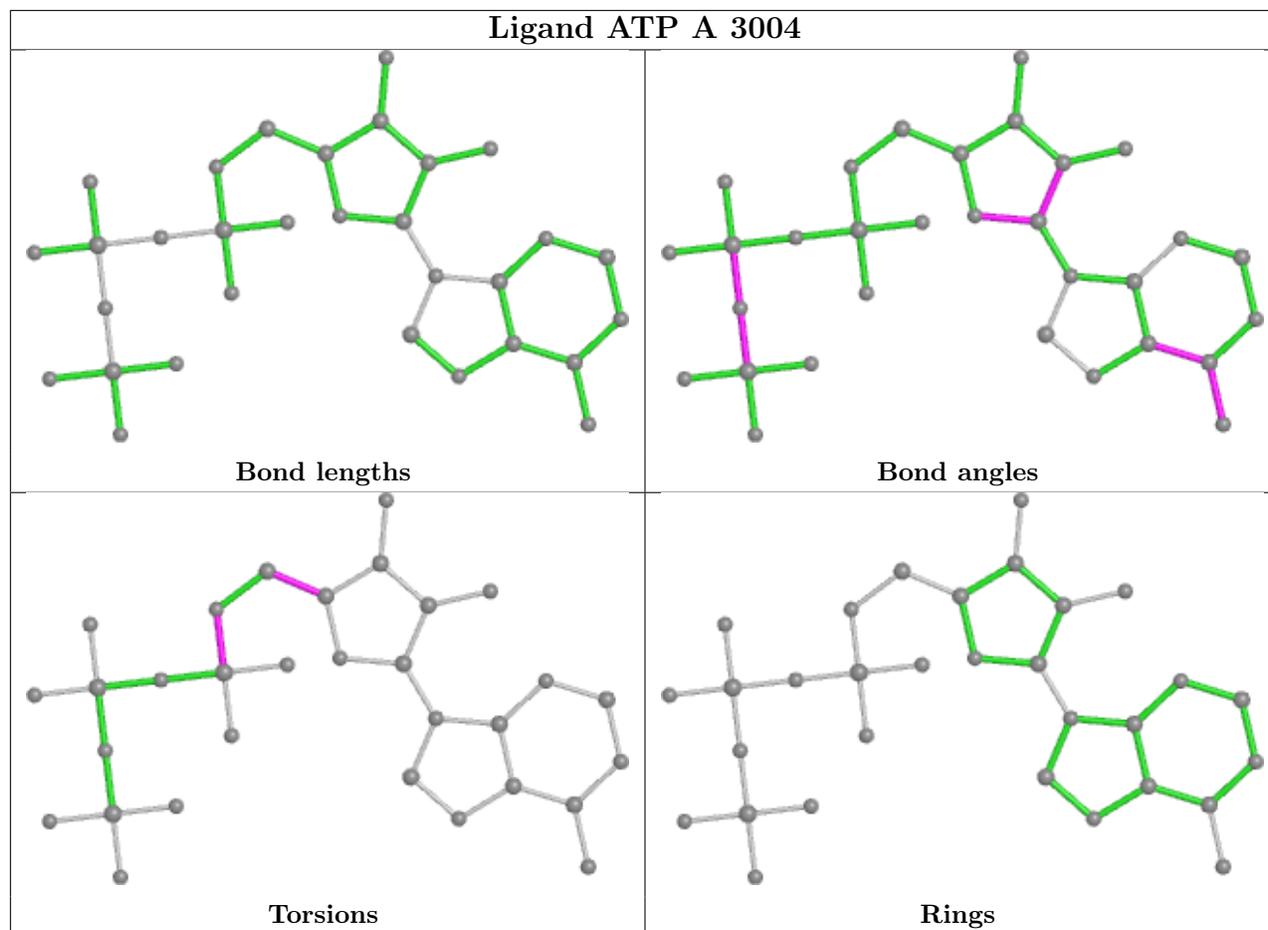


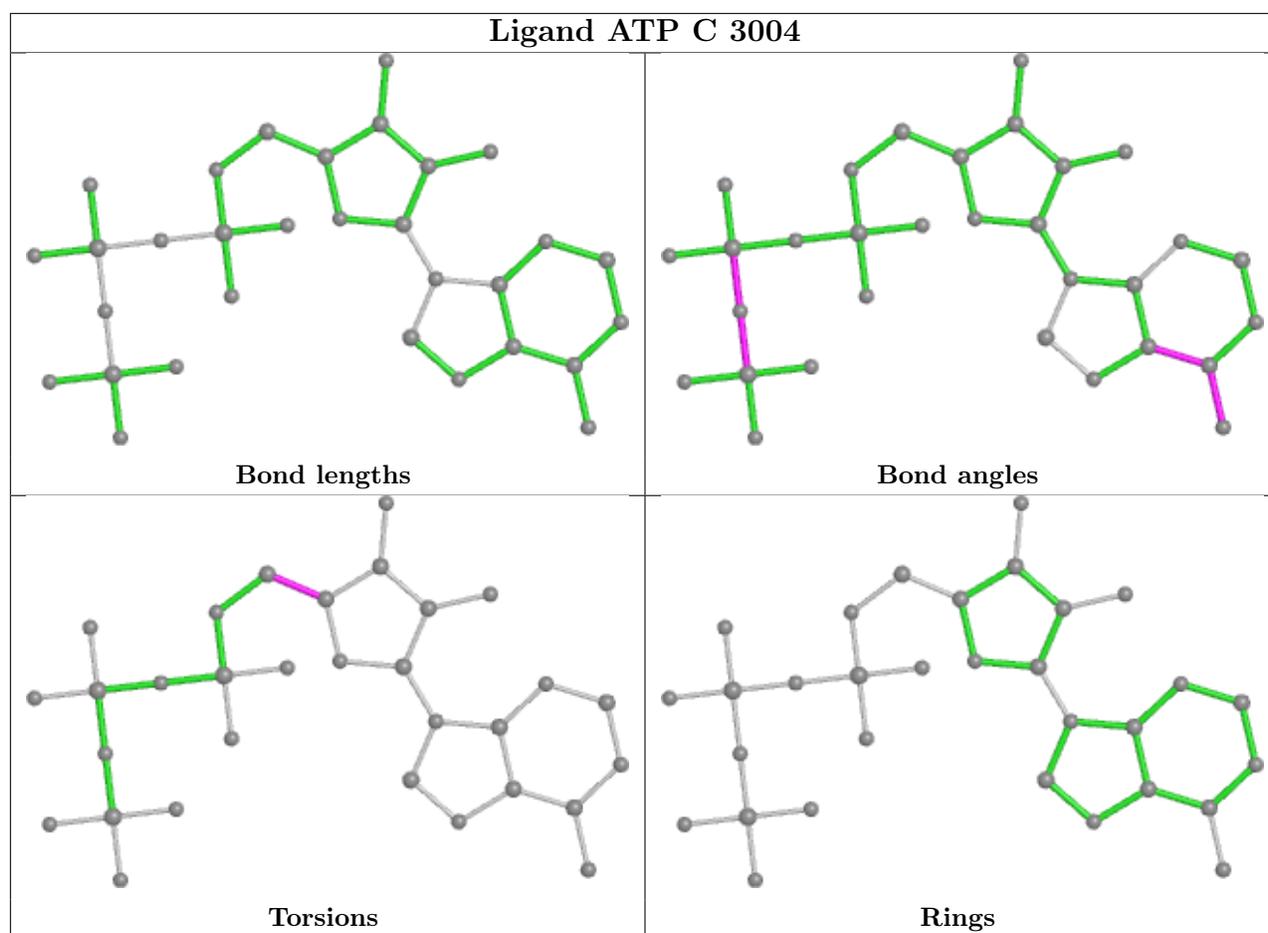












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

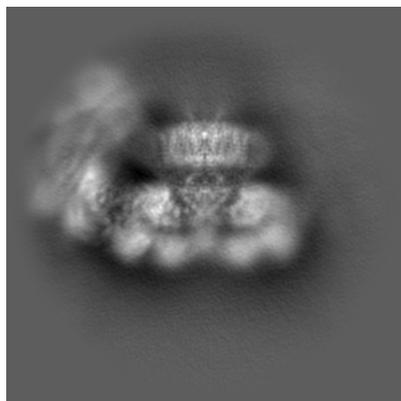
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41365. These allow visual inspection of the internal detail of the map and identification of artifacts.

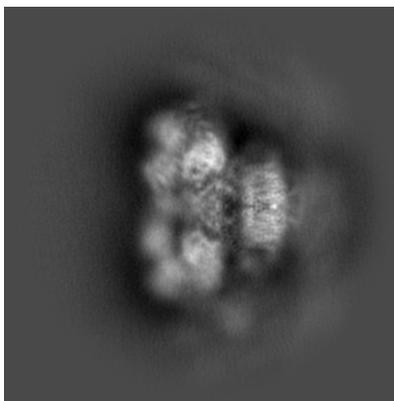
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

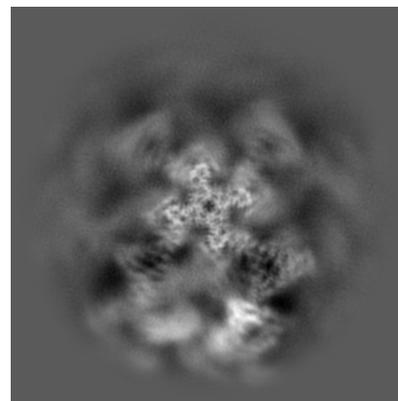
#### 6.1.1 Primary map



X

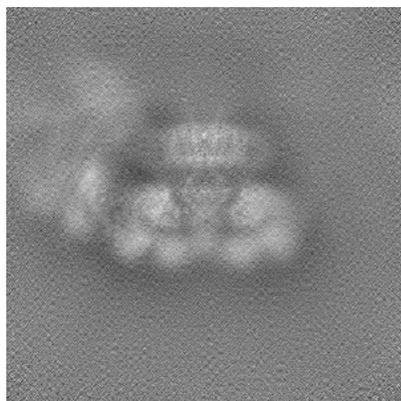


Y

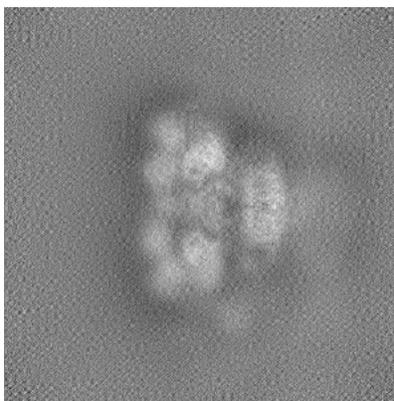


Z

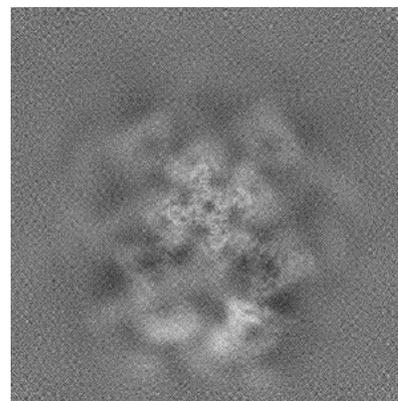
#### 6.1.2 Raw map



X



Y

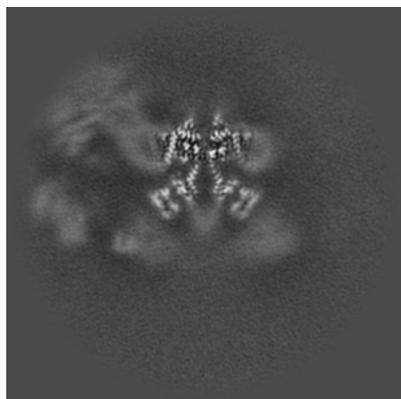


Z

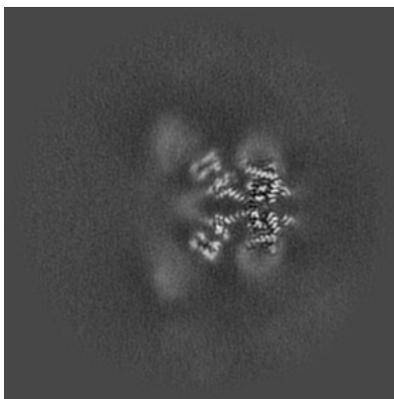
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

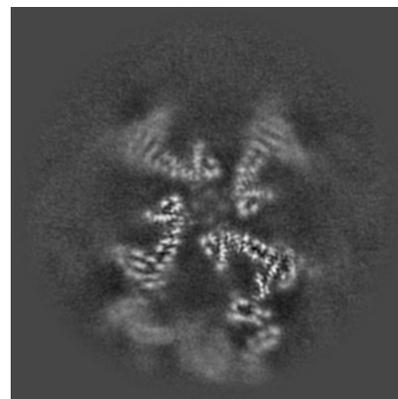
### 6.2.1 Primary map



X Index: 256

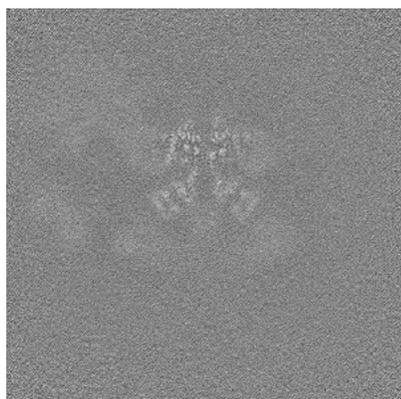


Y Index: 256



Z Index: 256

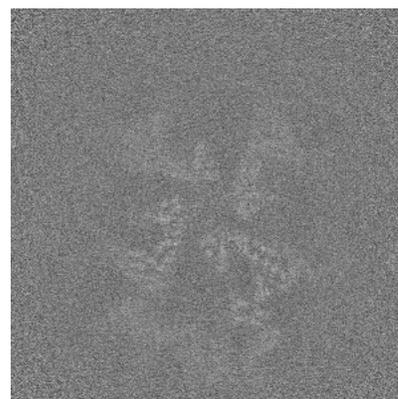
### 6.2.2 Raw map



X Index: 256



Y Index: 256

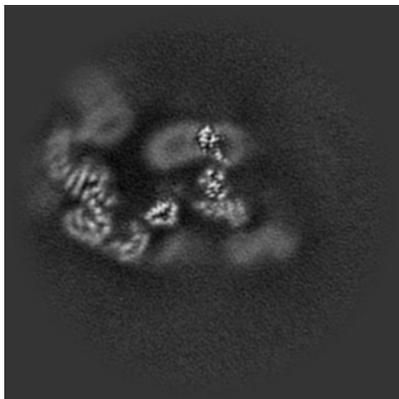


Z Index: 256

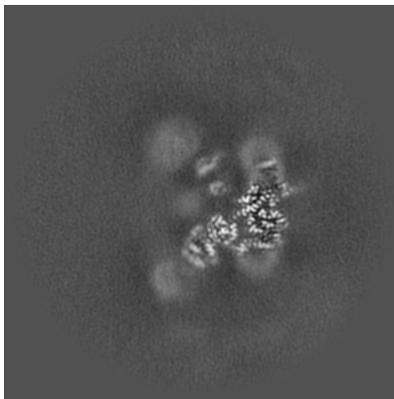
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

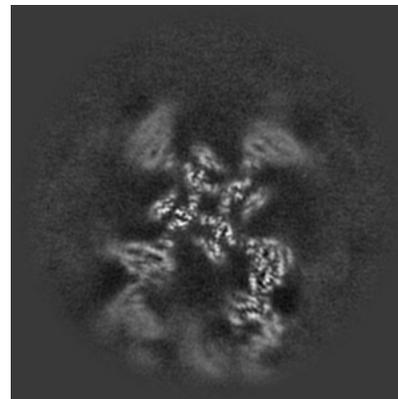
### 6.3.1 Primary map



X Index: 293

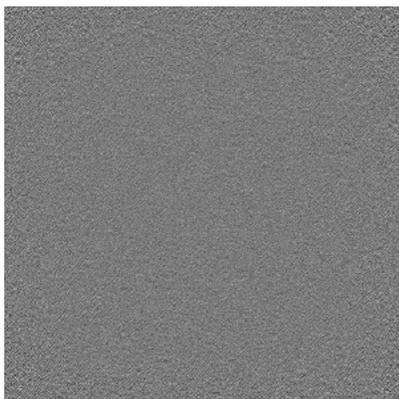


Y Index: 247

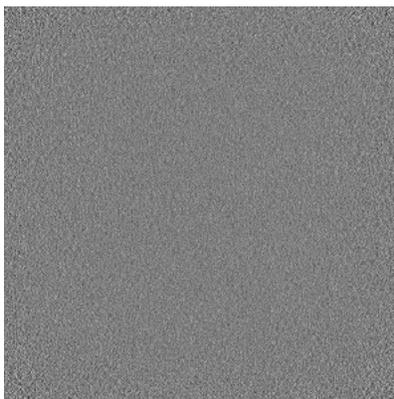


Z Index: 266

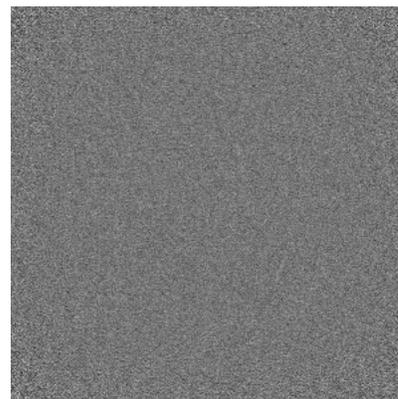
### 6.3.2 Raw map



X Index: 0



Y Index: 0

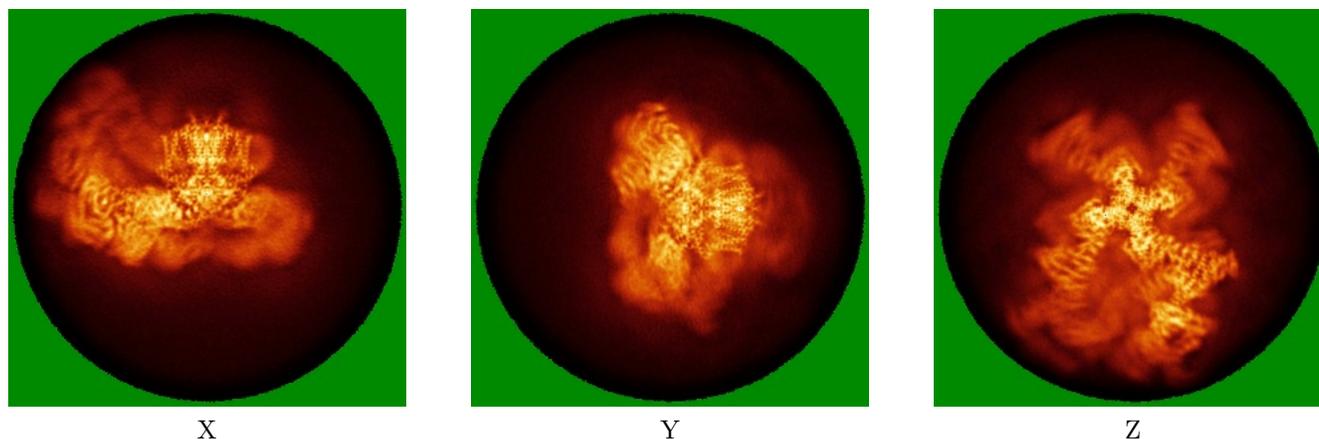


Z Index: 0

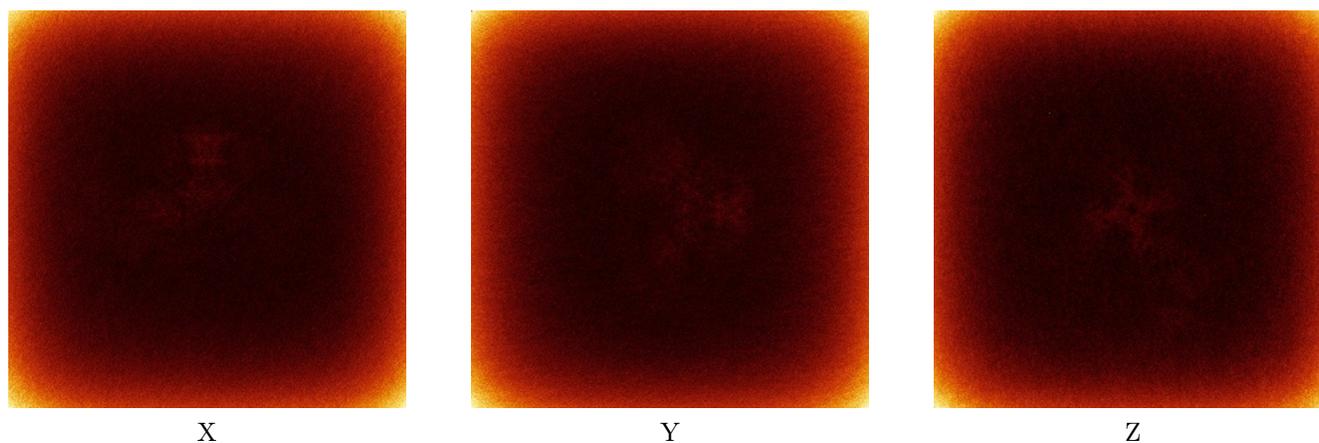
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



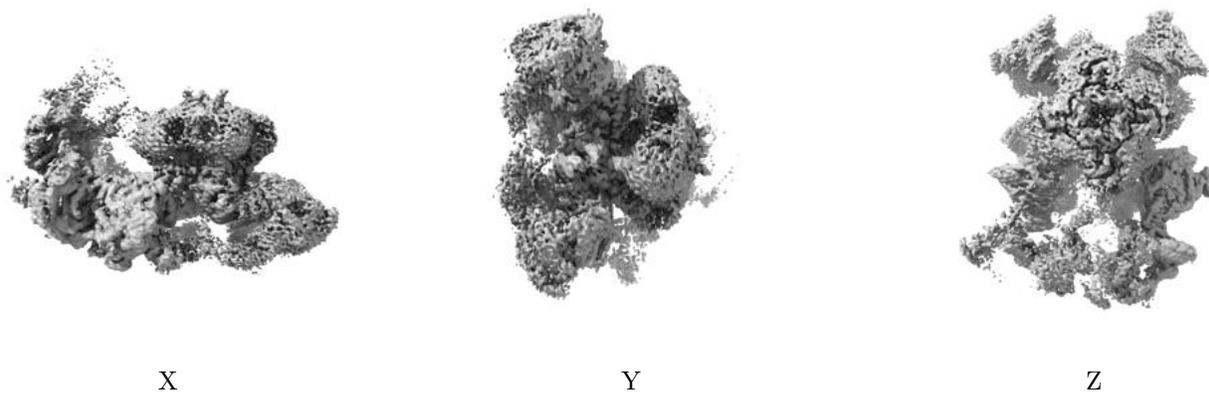
### 6.4.2 Raw map



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.

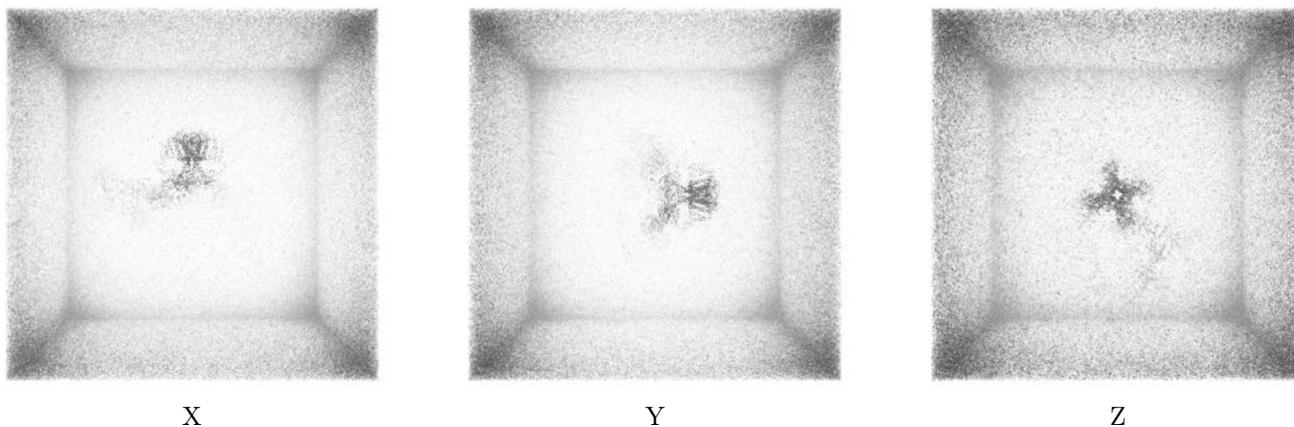
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

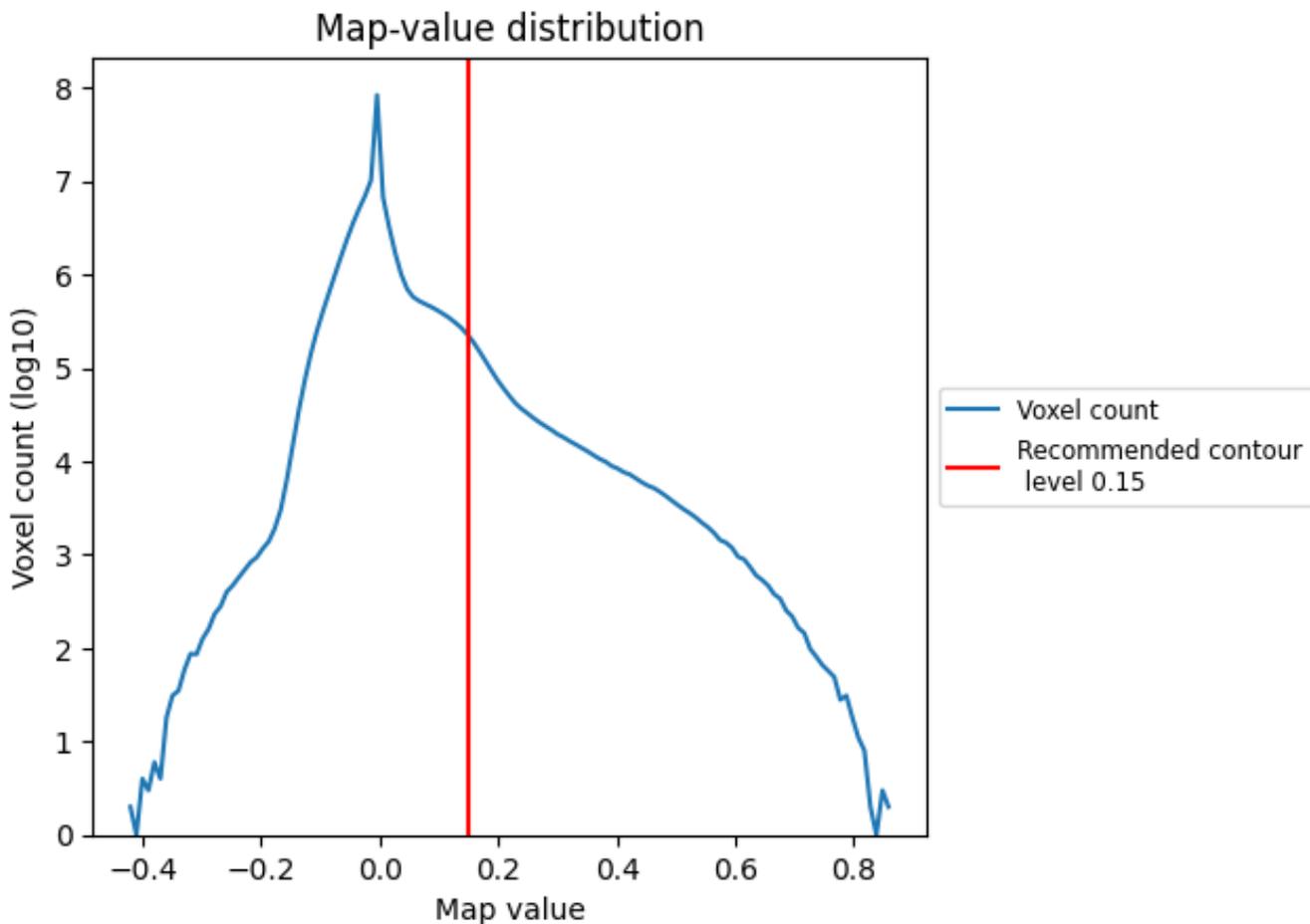
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

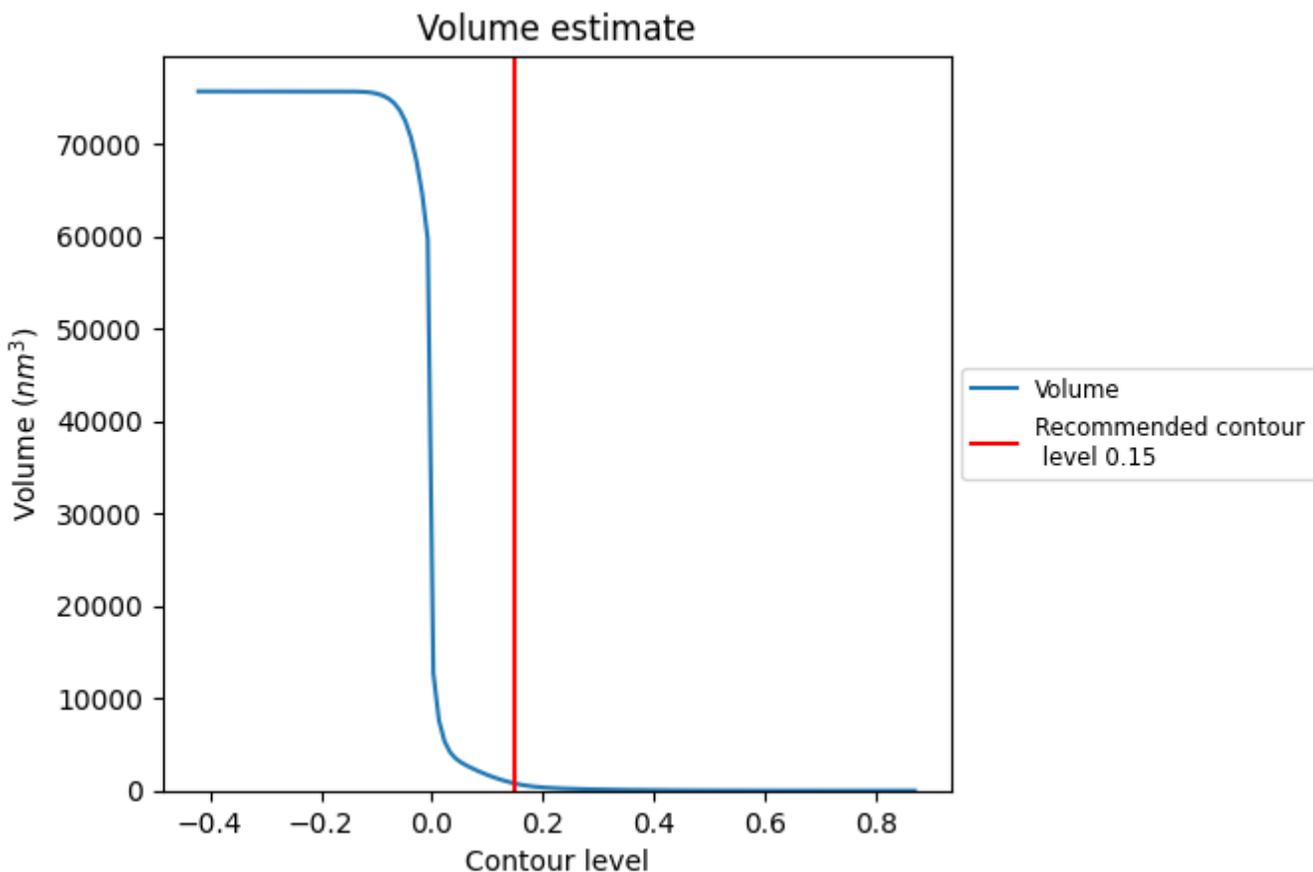
This section contains the results of statistical analysis of the map.

### 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.

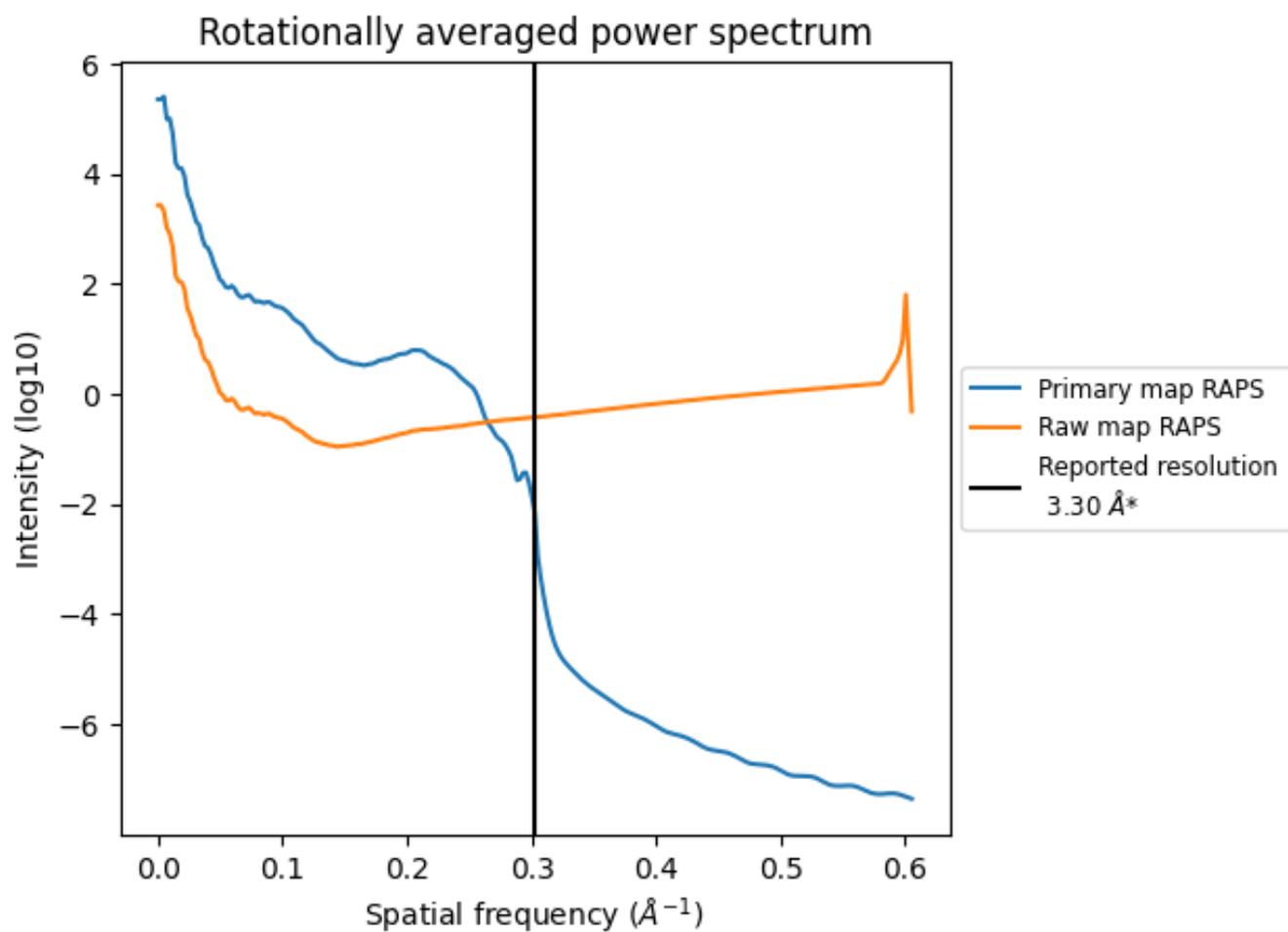
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 764  $\text{nm}^3$ ; this corresponds to an approximate mass of 690 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](#)

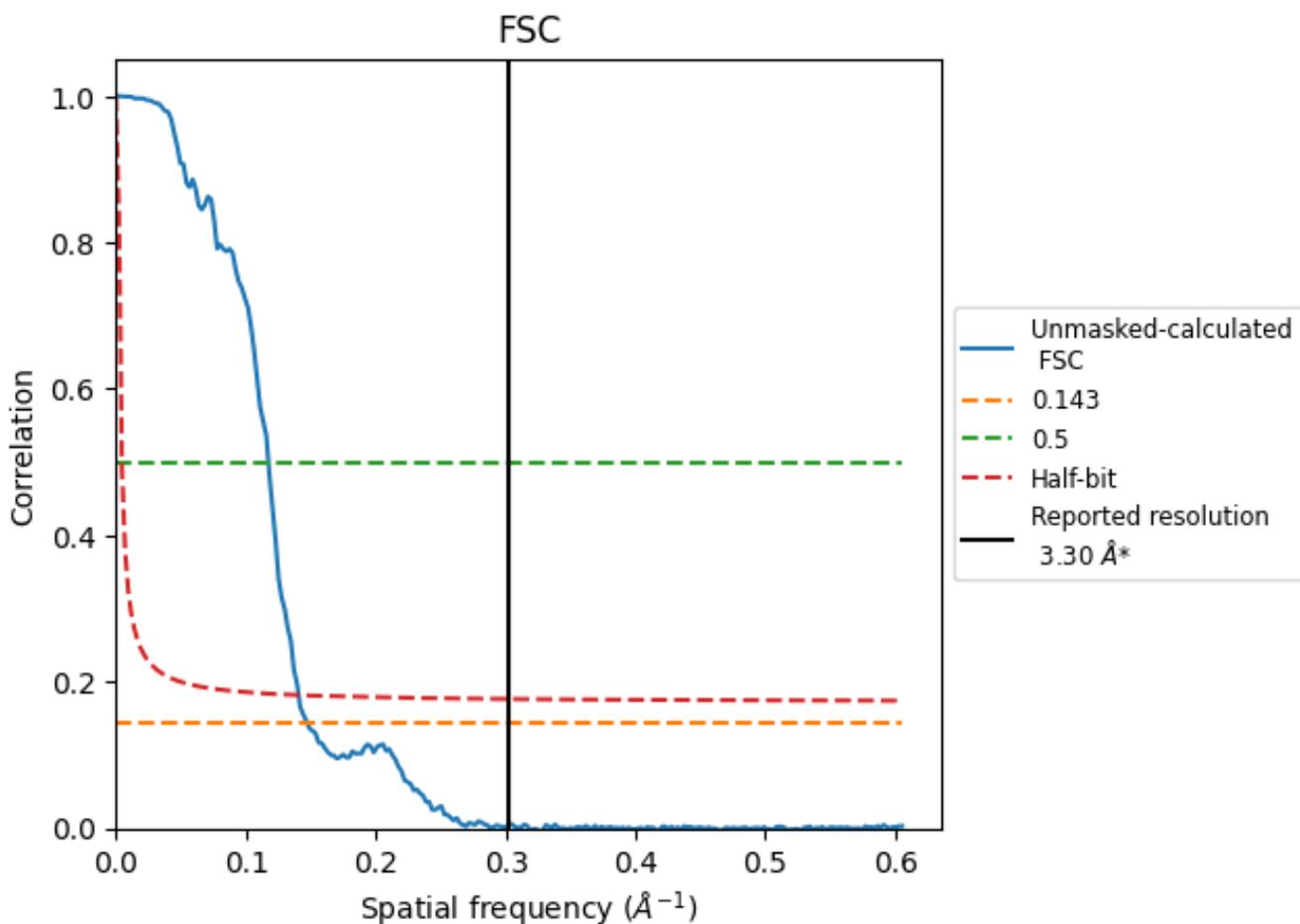


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

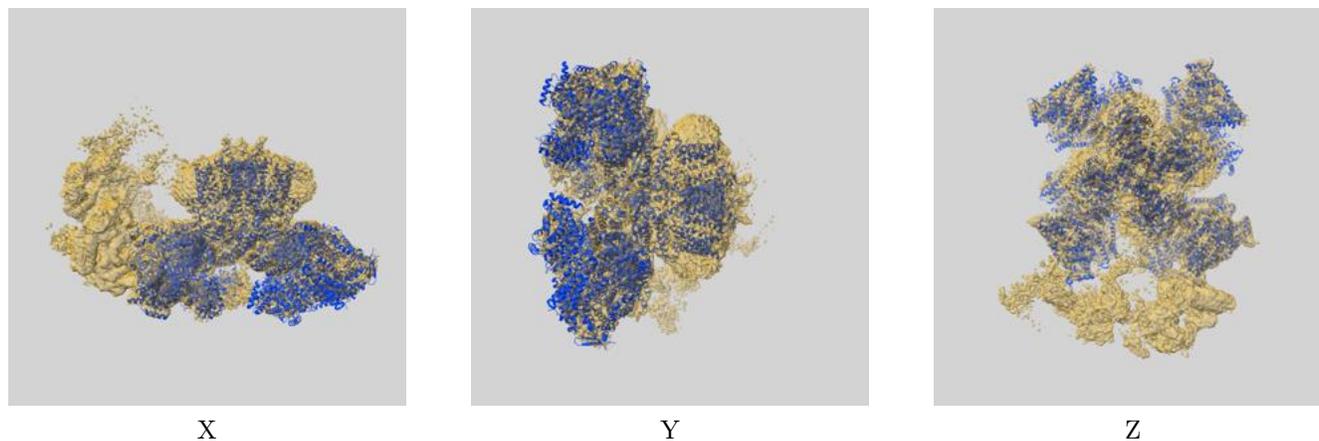
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.78	8.52	7.11

\*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 6.78 differs from the reported value 3.3 by more than 10 %

## 9 Map-model fit [i](#)

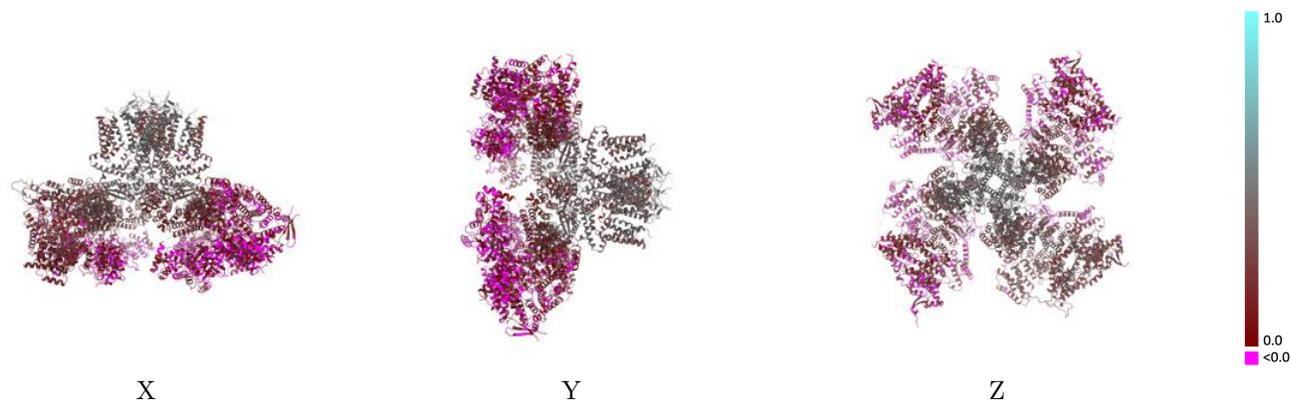
This section contains information regarding the fit between EMDB map EMD-41365 and PDB model 8TL9. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



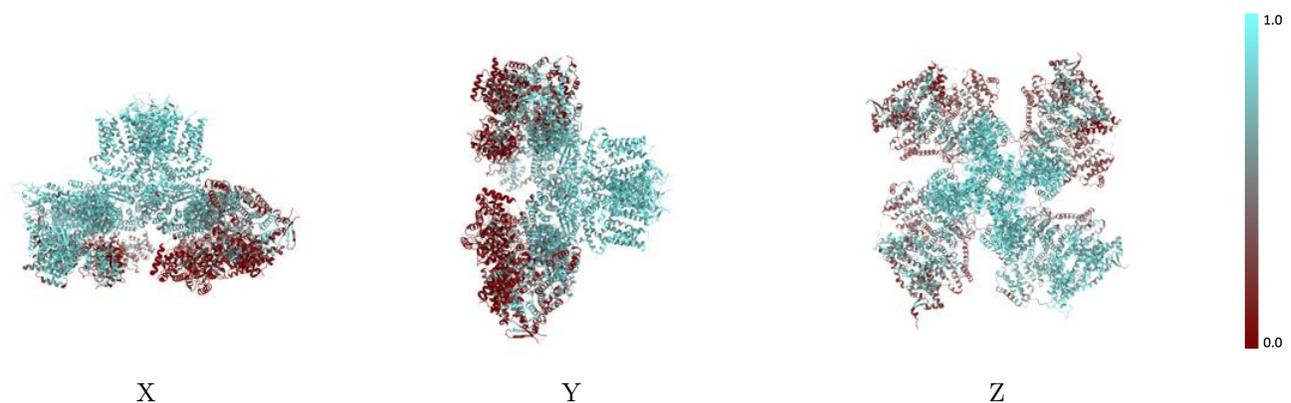
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



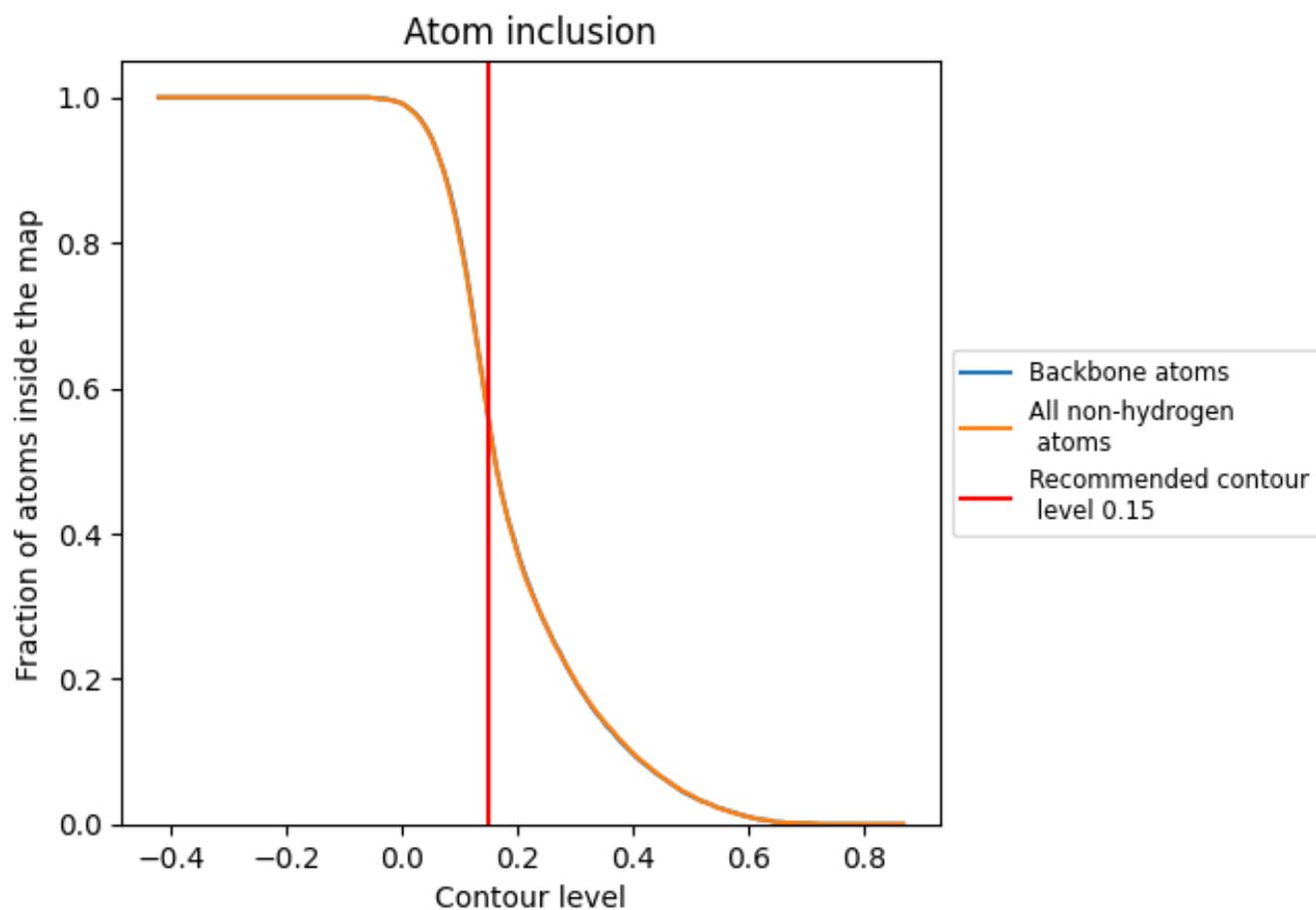
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 56% of all backbone atoms, 56% 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	 0.5580	 0.1960
A	 0.4890	 0.1590
B	 0.4520	 0.1630
C	 0.5790	 0.1900
D	 0.7300	 0.2700

