



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 01:52 AM UTC

PDB ID : 7T3R / pdb_00007t3r
EMDB ID : EMD-25669
Title : IP3 and ATP bound type 3 IP3 receptor in the pre-active C state
Authors : Schmitz, E.A.; Takahashi, H.; Karakas, E.
Deposited on : 2021-12-08
Resolution : 3.40 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 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

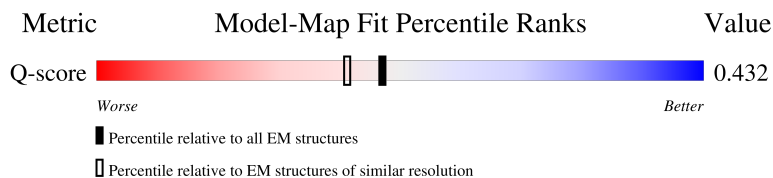
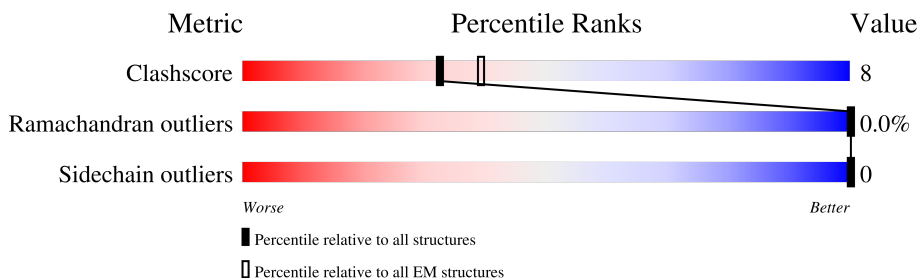
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	
1	B	2633	
1	C	2633	
1	D	2633	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 68780 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.

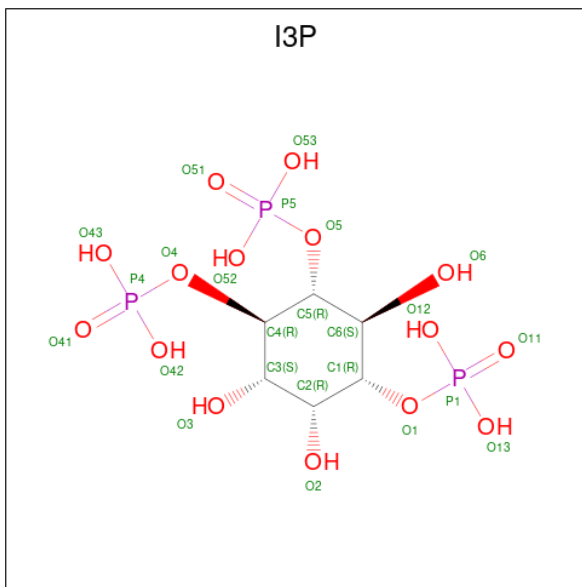
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2130	Total	C	N	O	S	0	0
			17139	10950	2934	3151	104		
1	B	2130	Total	C	N	O	S	0	0
			17139	10950	2934	3151	104		
1	C	2130	Total	C	N	O	S	0	0
			17139	10950	2934	3151	104		
1	D	2130	Total	C	N	O	S	0	0
			17139	10950	2934	3151	104		

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

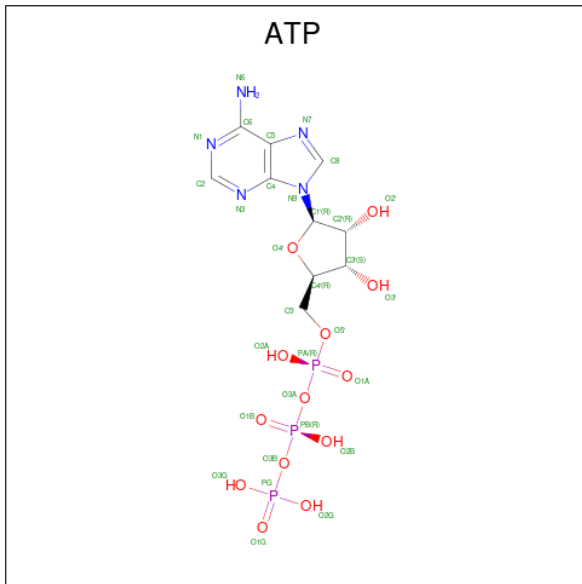
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: I3P) (formula: C₆H₁₅O₁₅P₃).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 24	C 6	O 15	P 3	0
3	B	1	Total 24	C 6	O 15	P 3	0
3	C	1	Total 24	C 6	O 15	P 3	0
3	D	1	Total 24	C 6	O 15	P 3	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).

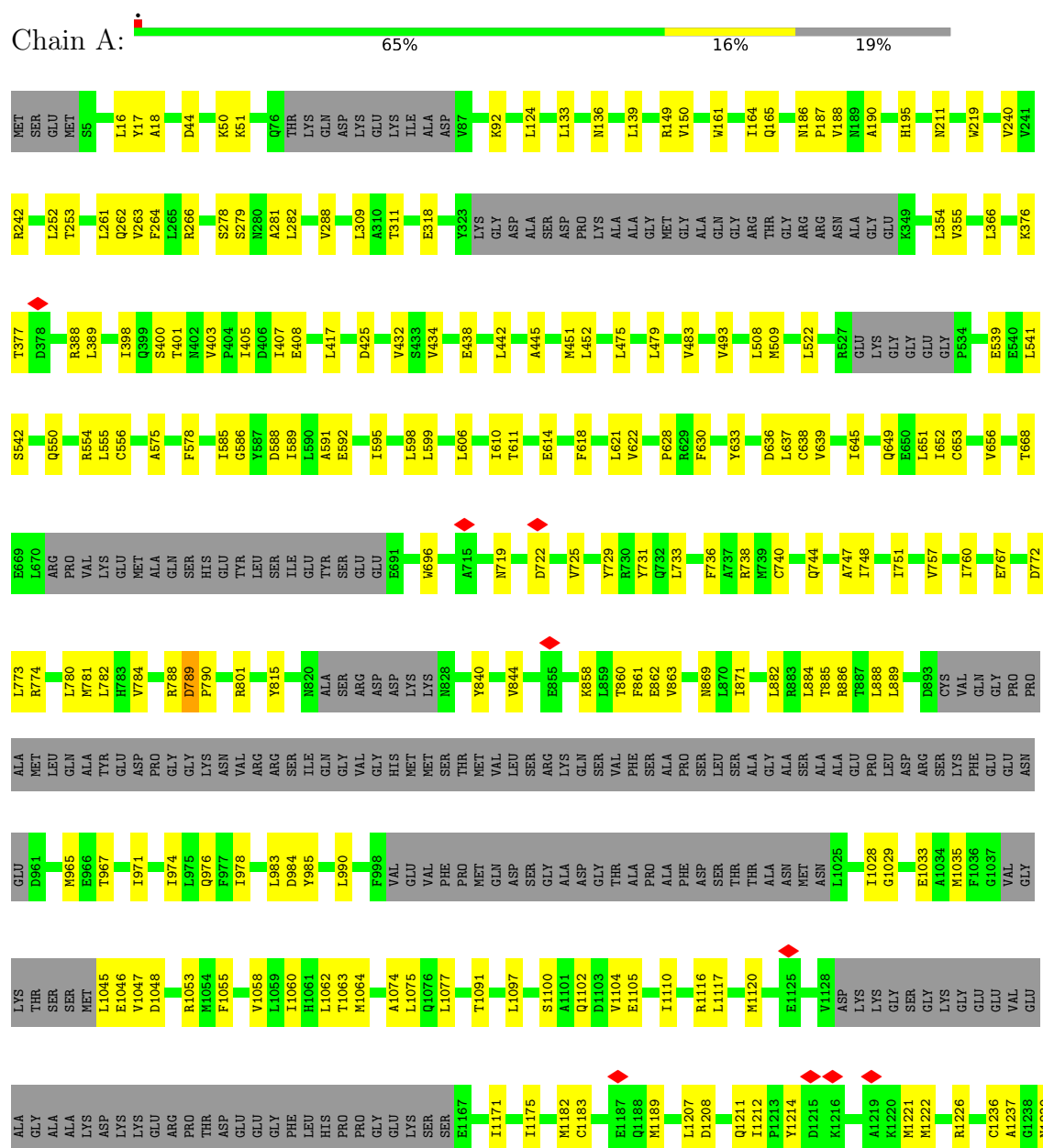


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0

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.

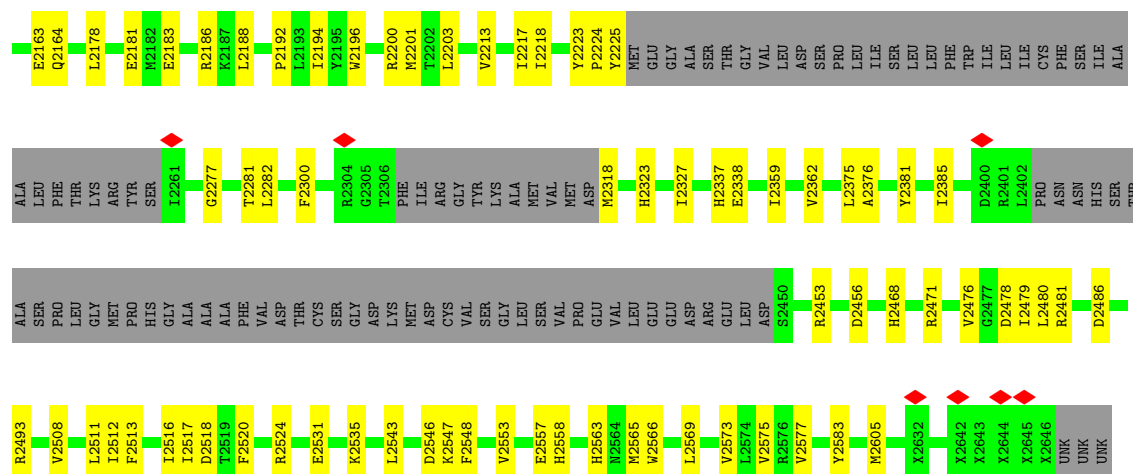
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





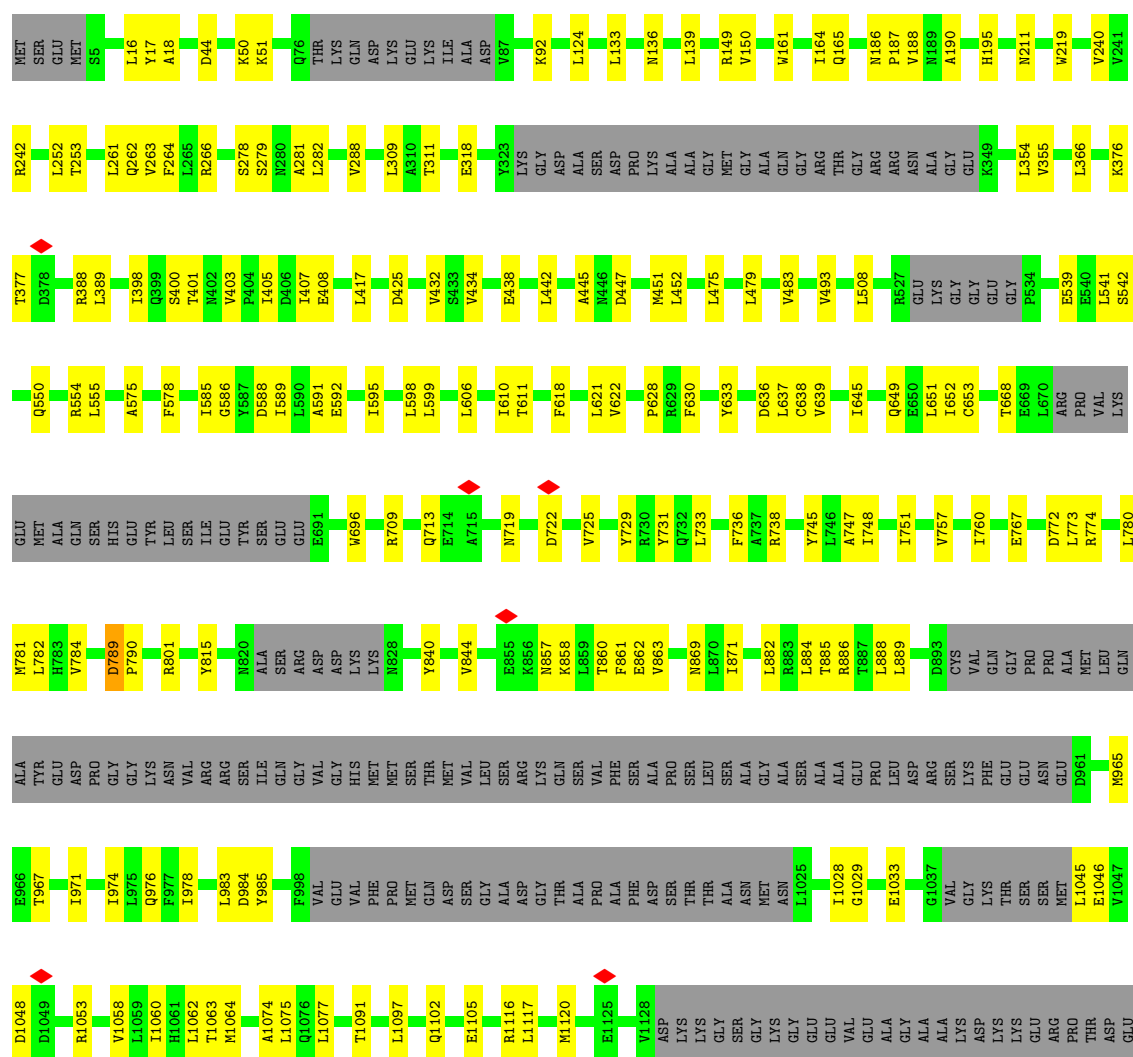
W1586	L1595	Q1596	D1597	I1598	I1599	T1600	A1601	L1602	R1605	L1606	K1607	P1608	V1610	Q1611	A1612	E1613	L1614	S1615	D1619	W1623	L1626	F1643	L1644	T1651	M1655	E1656	V1665	R1682	R1687	K1688	Q1692	N1693	Y1694	N1697	ARG	LYS	SER	THR	ALA	ALA	ALA	GLN	ASN	ASN	SER	THR	TYR	LYS	ALA	ALA	THR	THR	ARG	ALA	PHE	PRO	CYS	PRO	ARG	VAL	THR	PRO	ASP	LEU	THR	ALA	ASN	GLN
G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	LEU	LEU	LEU	PRO	PRO	MET	ASP	LEU	ASP	ALA	HIS	ILE	SER	SER	GLY	SER	ALA	SER	CYS	ALA	ALA	ALA	GLN	ASN	ASN	SER	GLN	T1493	H1494	Q1495	L1501	L1508	LEU	GLU	CYS	PRO	ARG	VAL	THR	PRO	ASP	LEU	THR	ALA	ASN	GLN													
E1408	V1409	Y1421	T1424	E1425	V1426	E1427	M1428	K1429	E1442	T1445	L1446	D1447	R1450	V1451	CYS	SER	LYS	ARG	GLU	LYS	ARG	VAL	ALA	ASP	P1462	L1469	E1486	N1487	S1488	T1489	SER	LEU	GLN	T1493	H1494	Q1495	L1501	L1508	LEU	GLU	CYS	PRO	ARG	VAL	THR	PRO	ASP	LEU	THR	ALA	ASN	GLN																
L1259	E1260	T1263	M1264	Q1265	Y1272	E1280	P1281	V1282	L1283	Q1298	D1301	T1305	V1306	T1307	K1308	A1309	C1317	T1321	D1330	V1334	K1339	L1342	L1346	M1349	K1350	A1351	A1352	D1358	H1359	M1363	T1366	K1379	N1380	L1391	E1394	E1403	E1405	L1219	K1220	M1221	G1236	A1237	G1238	M1239	L1246	H1251	F1253	L1254	T1255	L1258																		
LYS	LYS	ARG	PRO	THR	ASP	GLU	GLY	PHE	HIS	PRO	PRO	GLY	GLU	LYS	SER	SER	Q1170	I1175	E1187	L1196	M1200	L1207	D1208	Q1211	I1212	P1213	Y1214	D1215	K1216	A1219	M1221	G1236	A1237	G1238	M1239	L1246	H1251	F1253	L1254	T1255	L1258																											
SER	MET	L1045	E1046	V1047	D1048	D1049	R1053	M1054	F1055	L1056	R1057	V1058	L1059	I1060	H1061	L1062	T1063	M1064	L1070	A1074	L1075	Q1076	L1077	T1091	L1097	Q1102	E1105	R1116	L1117	E1125	V1128	ASP	LYS	LYS	GLY	SER	GLY	GLY	GLY	GLU	VAL	VAL	GLU	ALA	ALA	LYS	LYS	ASP																				
TYR	GLU	ASP	PRO	GLY	GLY	LYS	ASN	VAL	ARG	ARG	SER	ILE	GLN	GLY	VAL	HIS	GLY	MET	MET	SER	THR	MET	VAL	LEU	SER	ARG	GLN	LYS	N869	L870	I871	L882	R883	L884	T885	R886	T887	L888	L889	D893	CYS	VAL	GLN	GLY	PRO	GLU	ASN	PRO	ALA	MET	LEU	GLN	ALA															
E669	L670	ARG	VAL	LYS	GLU	MET	ALA	GLN	SER	SER	HIS	GLU	TYR	SER	SER	E691	W696	K706	S707	V708	R709	Q710	L711	A715	N719	D722	V725	Y729	R730	Y731	Q732	L733	F736	A737	R738	A747	I748	I751	V757	D758	L759	I760																										
S542	Q550	R554	L555	Y567	R568	K569	N570	A575	F578	G586	Y587	D588	I589	L590	E592	I595	L598	L599	L606	I610	T611	E614	F618	L621	V622	P628	R629	F630	Y633	L637	C638	V639	I645	Q649	E650	L651	I652	O653	T668																													
K376	T377	D378	R388	L389	T398	Q399	S400	T401	N402	V403	P404	Y405	D406	I407	E408	L417	D425	V432	S433	V434	E438	I439	L442	A445	L452	R470	L479	V483	V493	L508	M509	R527	GLU	LYS	GLY	GLY	GLU	GLY	P534	E539	E540	L541																										
V240	V241	R242	L252	T253	L261	Q262	V263	F264	L265	R266	S278	S279	N280	A281	L282	V288	L309	A310	T311	E318	Y323	GLY	ASP	ALA	SER	ASP	PRO	LYS	ALA	ALA	GLY	MET	GLY	ALA	GLN	GLY	ARG	THR	GLY	ARG	ASN	ALA	GLY	GLU	K349	L354	V355	L366																				
MET	SER	GLU	MET	S5	L16	Y17	A18	D44	K50	K51	Q76	THR	LYS	GLN	ASP	LYS	GLU	LYS	ILE	ALA	ASP	V87	K92	L124	L133	N136	L139	R149	V150	W161	T164	Q165	N186	P187	V188	W189	A190	G191	Q192	H195	N211	W219																										





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

Chain D: 66% 15% 19%



E2567	E2568	M2565	M2566	L2569	V2573	L2574	R2575	R2576	V2577	Y2583	Y2589	M2593	M2605	X2630	X2631	X2632	X2633	X2634	X2642	X2643	X2644	X2645	X2646	UNK	UNK	UNK		
SER	GLY	SER	VAL	PRO	GLU	VAL	ASP	ARG	GLU	ASP	S2450	R2453	D2456	H2468	R2471	V2476	G2477	D2478	L2479	L2480	R2481	R2482	R2493	N2510	L2511	L2512	F2513	
TYR	LYS	ALA	MET	VAL	MET	ASP	M2318	H2323	I2327	H2337	E2338	I2359	V2362	L2375	Y2381	I2385	D2400	R2401	L2402	PRO	ASN	ASN	HIS	THR	ALA	SER	PRO	GLY
W2196	R2200	M2201	T2202	L2203	Y2223	P2224	Y2225	MET	GLU	GLY	ALA	GLU	GLY	THR	VAL	LEU	ASP	SER	PRO	LEU	ILE	SER	LEU	ALA	ALA	ALA	ALA	GLY
C1948	Q1949	G1950	P1951	I1959	H1962	E1963	S1964	I1967	T1971	I1974	L1975	N1976	D1977	I1978	S1979	P1980	L1988	L1989	M2004	E2011	E2014	S2019	L2020	L2025	V2028	Y2033	L2034	
PRO	SER	LEU	ARG	GLY	HIS	GLU	VAL	GLU	VAL	GLN	SER	SER	GLU	M1863	S1866	R1886	M1890	R1893	C1894	Q1895	M1896	N1897	M1900	T1907	L1911	M1914	C1915	
N1746	I1749	A1757	L1764	S1765	N1774	L1775	S1778	F1785	V1788	A1796	T1803	VAL	ALA	VAL	ASN	MET	ASN	ASP	GLY	SER	GLN	PRO	HIS	SER	THR	LYS	ASP	ALA
ILE	LEU	PRO	MET	ASP	LEU	ASP	ALA	ILE	SER	SER	ILE	SER	SER	GLY	ALA	ALA	ALA	ALA	GLN	ARG	ASN	ALA	SER	TYR	LYS	ASP	ALA	THR
V1610	Q1611	A1612	E1613	L1614	S1615	D1619	L1626	F1643	L1644	M1655	E1656	R1682	R1687	K1688	Q1692	N1693	Y1694	L1695	Q1696	M1697	ARG	LYS	SER	THR	LYS	ASP	ALA	THR
GLU	GLY	PHE	LEU	HIS	PRO	PRO	GLY	LYS	SER	LYS	SER	E1167	I1171	I1175	E1187	L1196	M1200	L1207	D1208	Q1211	I1212	P1213	Y1214	D1215	K1216	G1217	D1218	
Y1272	Q1273	L1274	E1280	P1281	Q1298	F1301	F1302	T1305	V1306	K1308	A1309	I1321	D1330	K1339	L1342	K1350	A1351	A1352	D1358	H1359	M1363	Y1364	H1365	I1366	S1367	L1368	C1379	N1380
E1442	T1445	L1446	D1447	R1450	V1451	CYS	SER	LYS	ARG	GLU	LYS	VAL	ALA	ASP	P1462	L1469	E1486	N1487	S1488	T1489	SER	LEU	GLN	T1493	H1494	Q1495	L1501	L1508
Y1421	T1424	E1425	V1426	E1427	M1428	R1535	R1536	K1429	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
E1403	E1408	V1409	Y1421	T1424	E1425	V1426	E1427	M1428	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A1601	L1602	R1605	L1596	Q1596
F1253	L1254	T1255	L1258	L1259	E1260	T1263	M1264	Q1265	G1520	S1521	V1522	E1523	R1527	V1532	G1535	R1536	ALA	ILE	L1585	Q1596	D1597	I1598	I1599	A16				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	75994	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	2.476	Depositor
Minimum map value	-1.428	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.18	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	0.17	0/17356	0.29	0/23440
1	B	0.18	0/17356	0.30	0/23440
1	C	0.17	0/17356	0.30	0/23440
1	D	0.17	0/17356	0.29	0/23440
All	All	0.17	0/69424	0.29	0/93760

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	17139	0	17153	305	0
1	B	17139	0	17153	305	0
1	C	17139	0	17153	299	0
1	D	17139	0	17153	282	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	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	9	2	0
3	C	24	0	9	1	0
3	D	24	0	9	1	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	1	0
4	D	31	0	12	0	0
All	All	68780	0	68696	1162	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 1162 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:1214:TYR:CG	1:A:1221:MET:HE1	2.08	0.89
1:D:1214:TYR:CG	1:D:1221:MET:HE1	2.09	0.88
1:A:2213:VAL:O	1:A:2217:ILE:HD12	1.78	0.83
1:B:2213:VAL:O	1:B:2217:ILE:HD12	1.79	0.83
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.14	0.81

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	2069/2633 (79%)	1975 (96%)	93 (4%)	1 (0%)	100	100
1	B	2069/2633 (79%)	1968 (95%)	100 (5%)	1 (0%)	100	100
1	C	2069/2633 (79%)	1970 (95%)	98 (5%)	1 (0%)	100	100
1	D	2069/2633 (79%)	1974 (95%)	94 (4%)	1 (0%)	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8276/10532 (79%)	7887 (95%)	385 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	789	ASP
1	B	789	ASP
1	C	789	ASP
1	D	789	ASP

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	1903/2329 (82%)	1903 (100%)	0	100	100
1	B	1903/2329 (82%)	1903 (100%)	0	100	100
1	C	1903/2329 (82%)	1903 (100%)	0	100	100
1	D	1903/2329 (82%)	1903 (100%)	0	100	100
All	All	7612/9316 (82%)	7612 (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 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1596	GLN
1	D	2164	GLN
1	C	136	ASN
1	D	2023	GLN
1	D	980	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	I3P	A	2702	-	24,24,24	1.29	3 (12%)	39,39,39	0.78	1 (2%)
3	I3P	B	2702	-	24,24,24	1.29	3 (12%)	39,39,39	0.77	1 (2%)
4	ATP	C	2703	-	32,33,33	0.29	0	48,52,52	0.68	0
4	ATP	D	2703	-	32,33,33	0.29	0	48,52,52	0.68	0
3	I3P	D	2702	-	24,24,24	1.29	3 (12%)	39,39,39	0.77	1 (2%)
3	I3P	C	2702	-	24,24,24	1.29	3 (12%)	39,39,39	0.77	1 (2%)
4	ATP	A	2703	-	32,33,33	0.29	0	48,52,52	0.68	0
4	ATP	B	2703	-	32,33,33	0.29	0	48,52,52	0.68	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
3	I3P	A	2702	-	-	1/15/39/39	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	I3P	B	2702	-	-	1/15/39/39	0/1/1/1
4	ATP	C	2703	-	-	4/22/38/38	0/3/3/3
4	ATP	D	2703	-	-	4/22/38/38	0/3/3/3
3	I3P	D	2702	-	-	2/15/39/39	0/1/1/1
3	I3P	C	2702	-	-	3/15/39/39	0/1/1/1
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	D	2702	I3P	P1-O1	3.15	1.65	1.59
3	B	2702	I3P	P4-O4	3.12	1.65	1.59
3	A	2702	I3P	P4-O4	3.12	1.65	1.59
3	A	2702	I3P	P1-O1	3.10	1.65	1.59
3	D	2702	I3P	P4-O4	3.10	1.65	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2702	I3P	P1-O1-C1	-2.30	117.30	123.43
3	C	2702	I3P	P1-O1-C1	-2.29	117.31	123.43
3	A	2702	I3P	P1-O1-C1	-2.28	117.35	123.43
3	D	2702	I3P	P1-O1-C1	-2.26	117.41	123.43

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 6 short contacts:

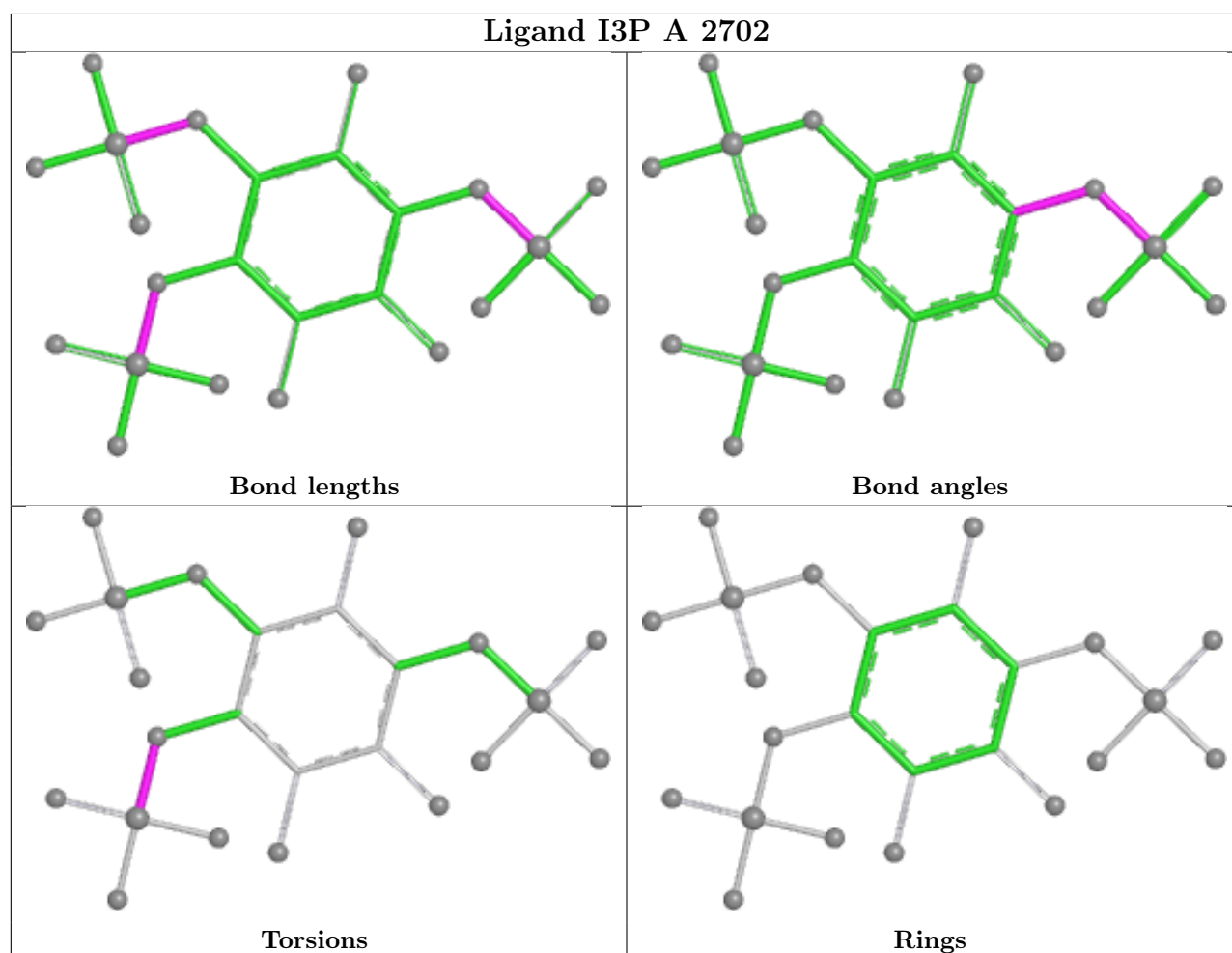
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2702	I3P	1	0

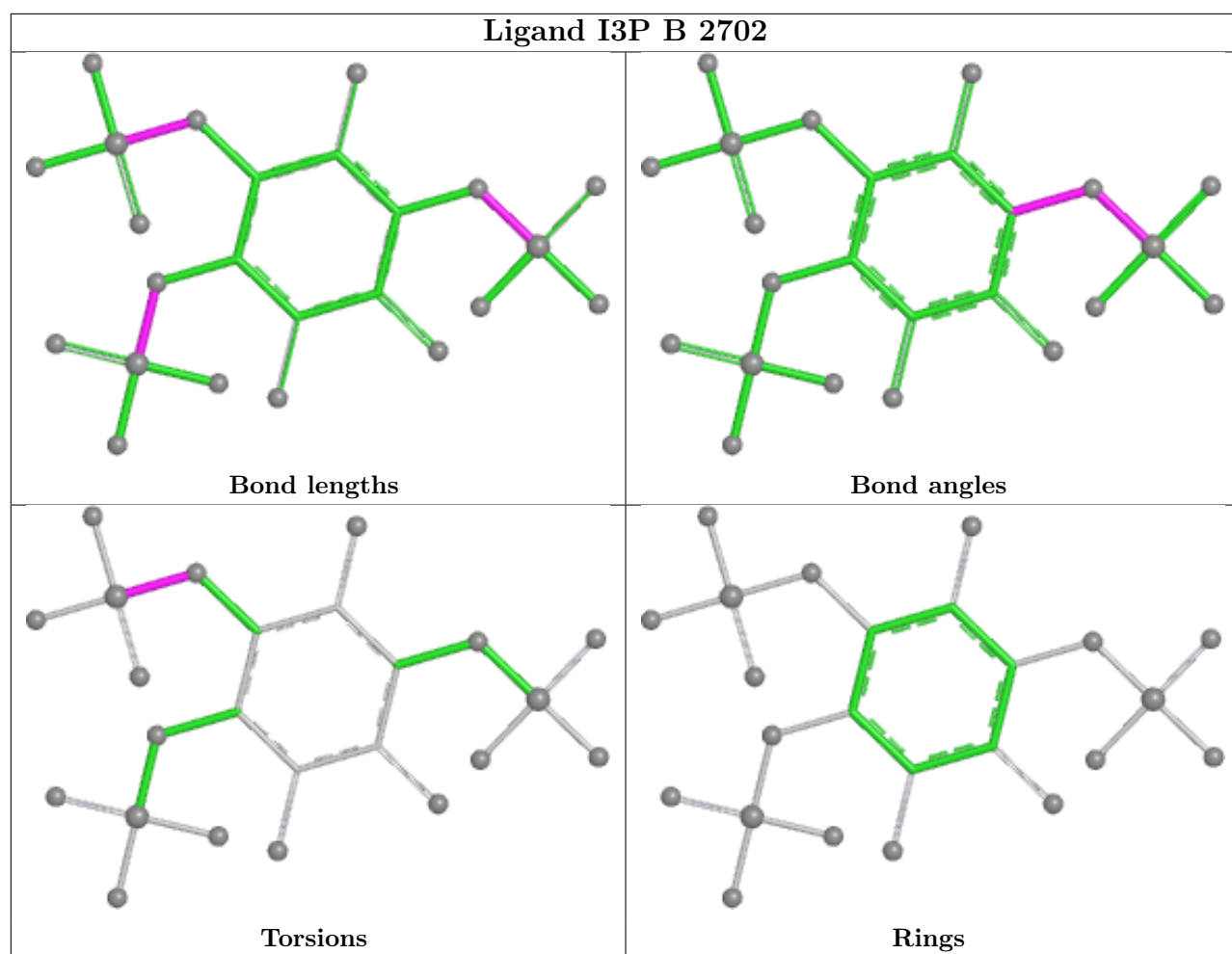
Continued on next page...

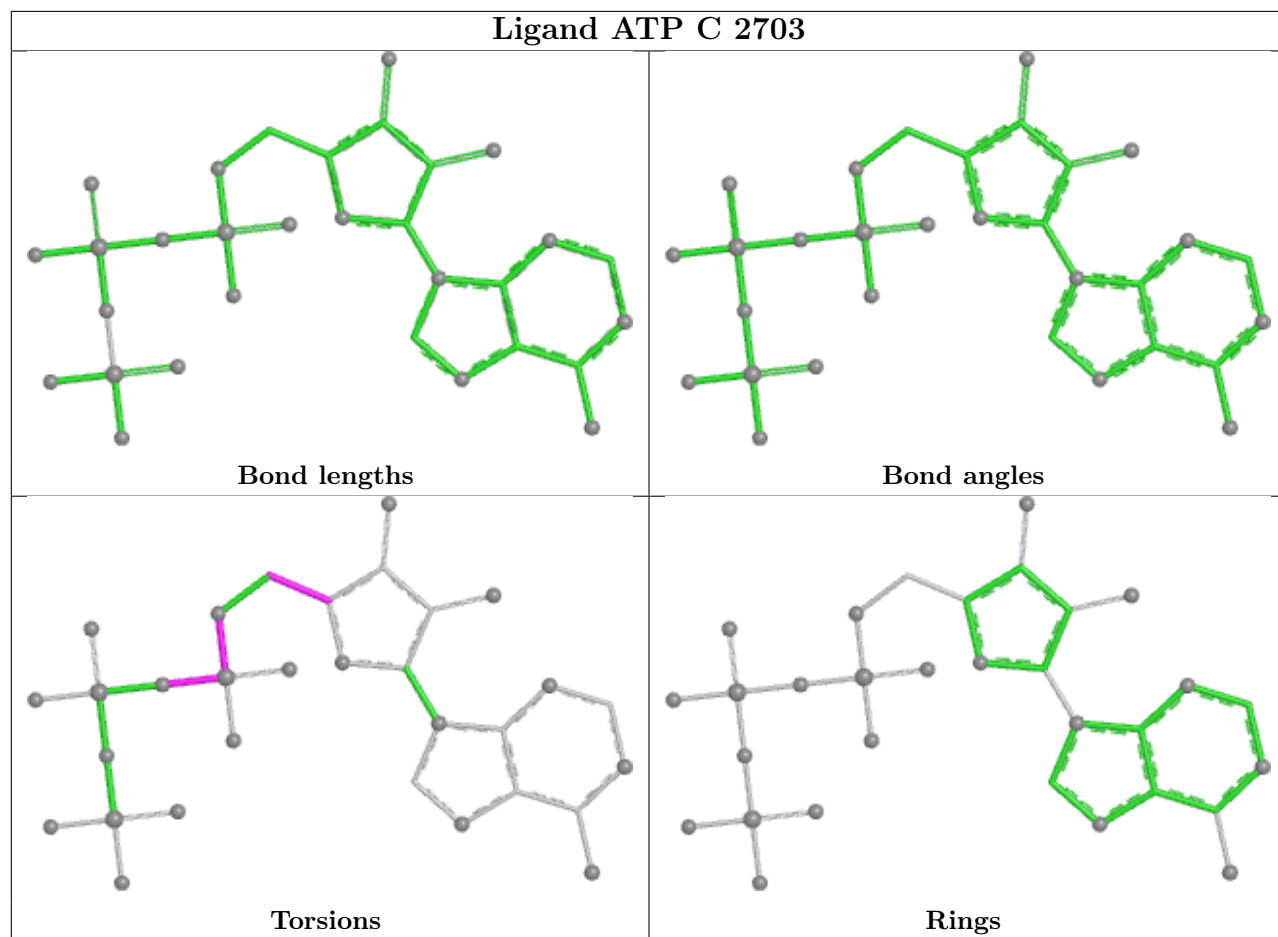
Continued from previous page...

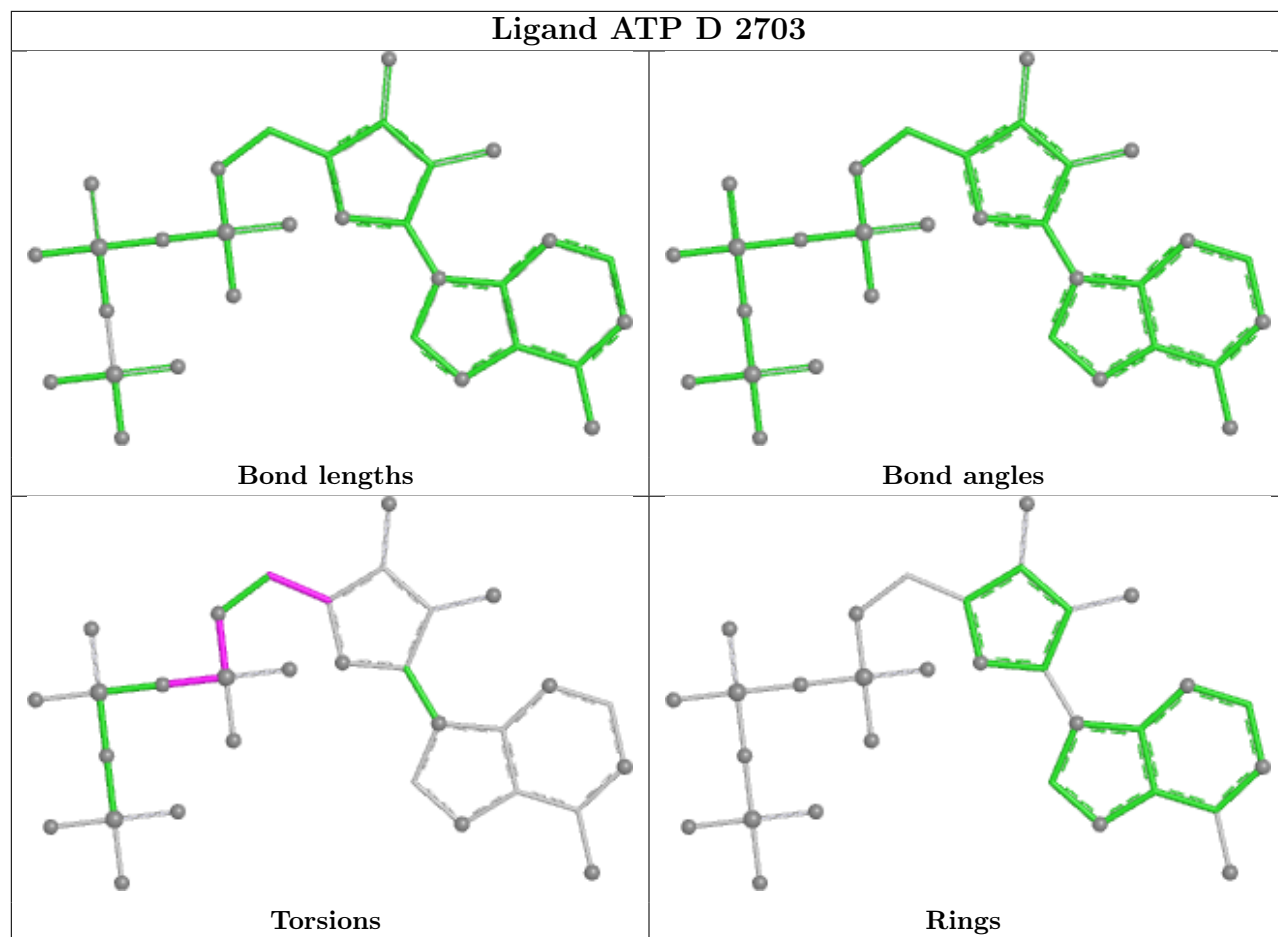
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2702	I3P	2	0
4	C	2703	ATP	1	0
3	D	2702	I3P	1	0
3	C	2702	I3P	1	0

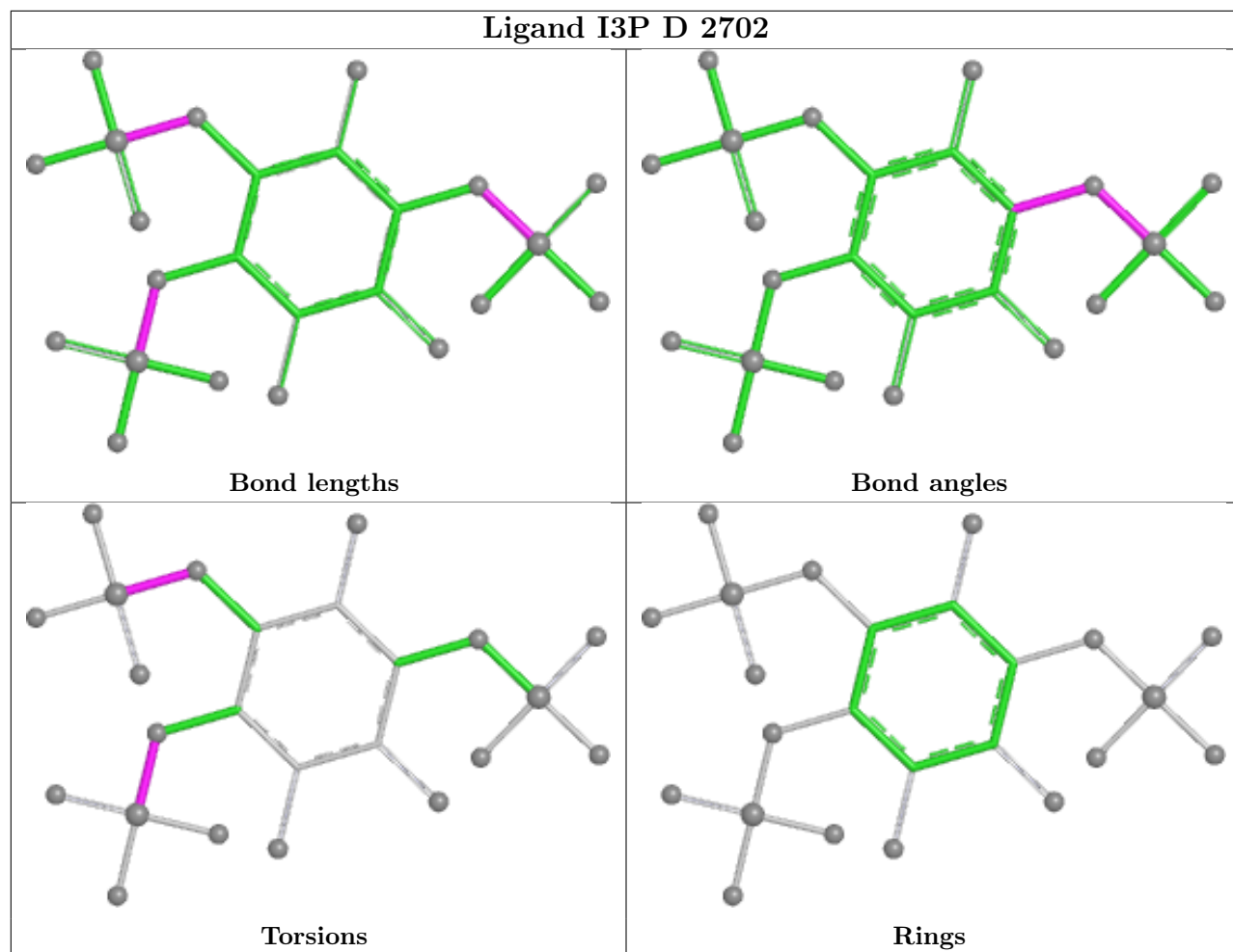
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

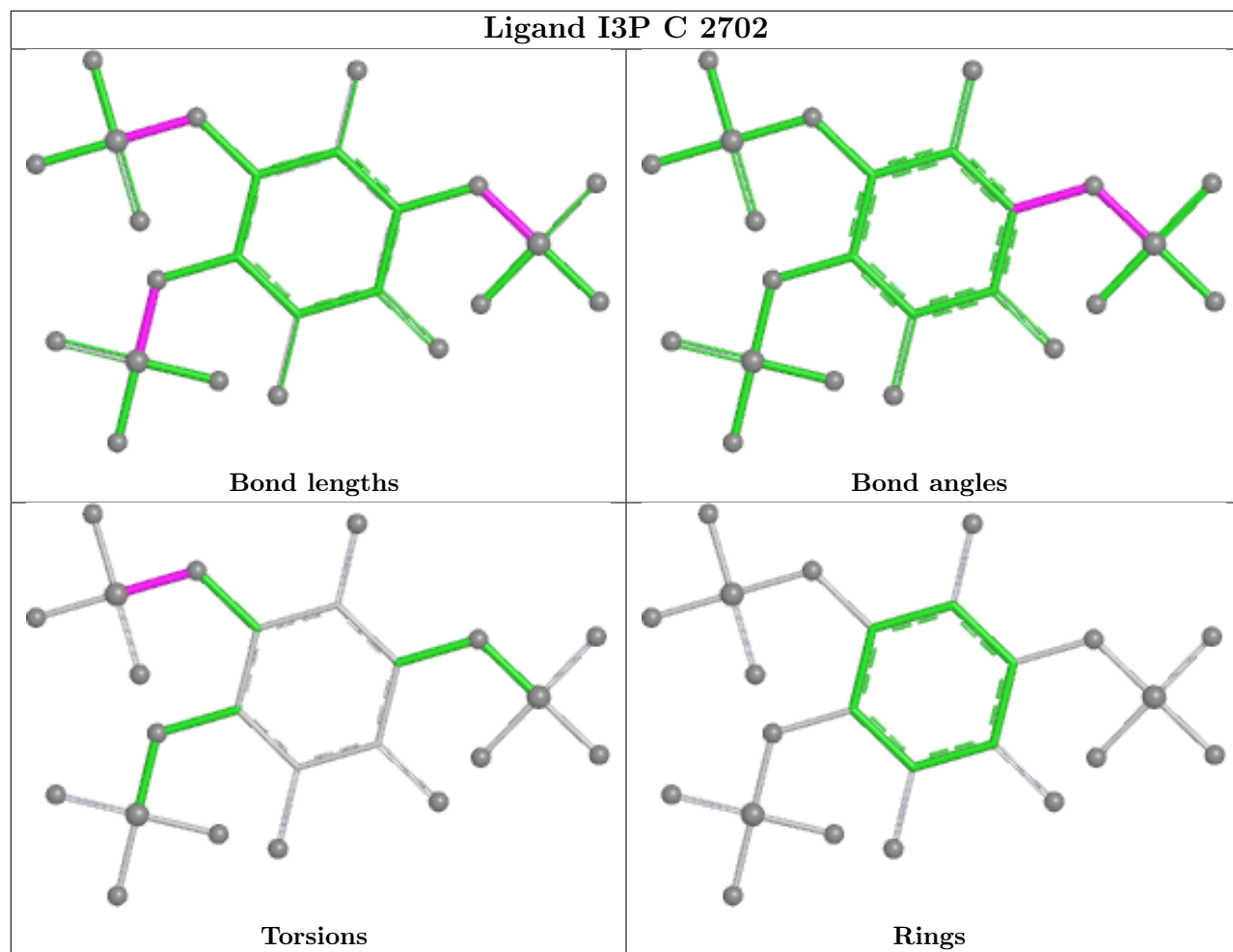


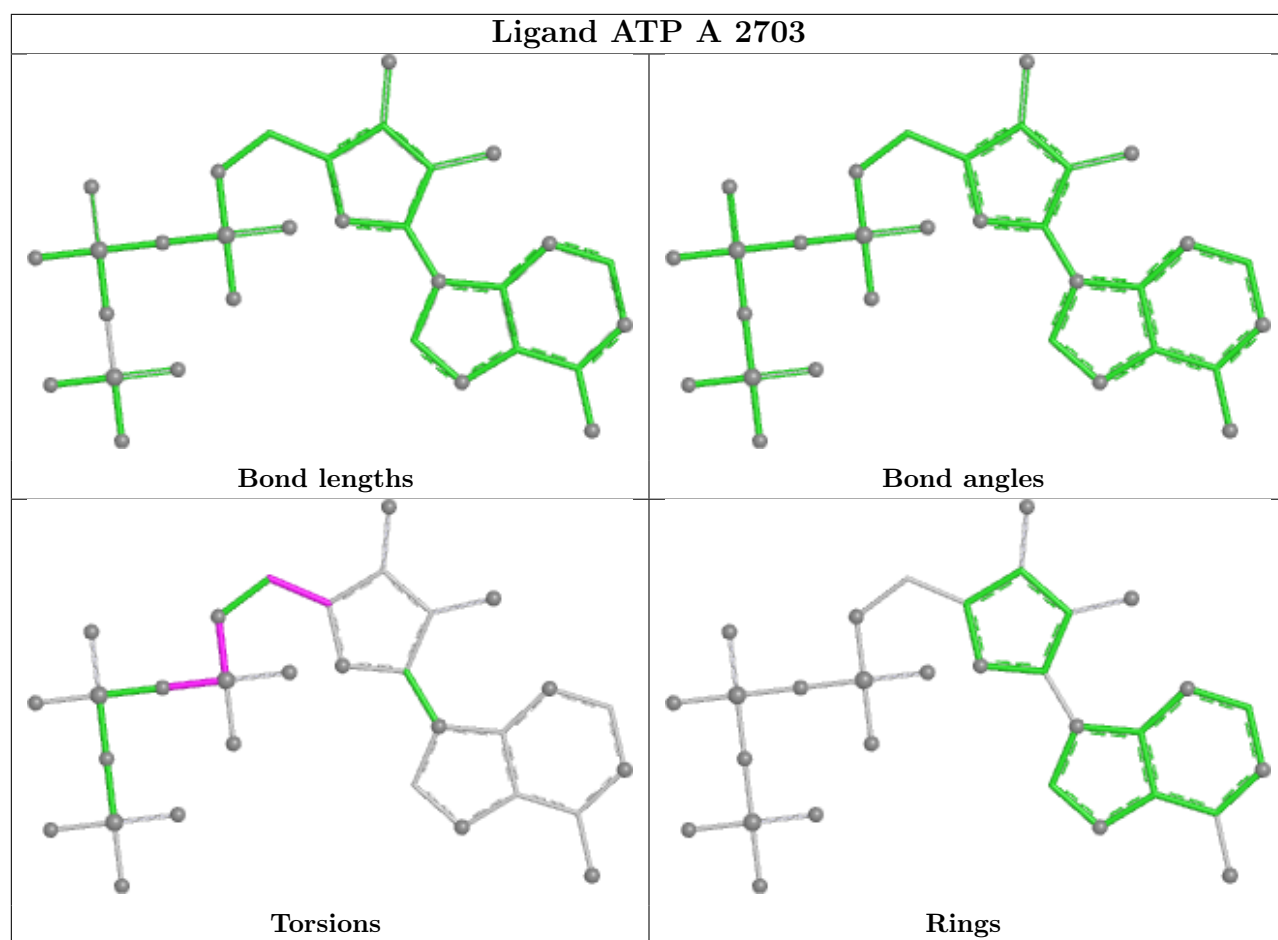


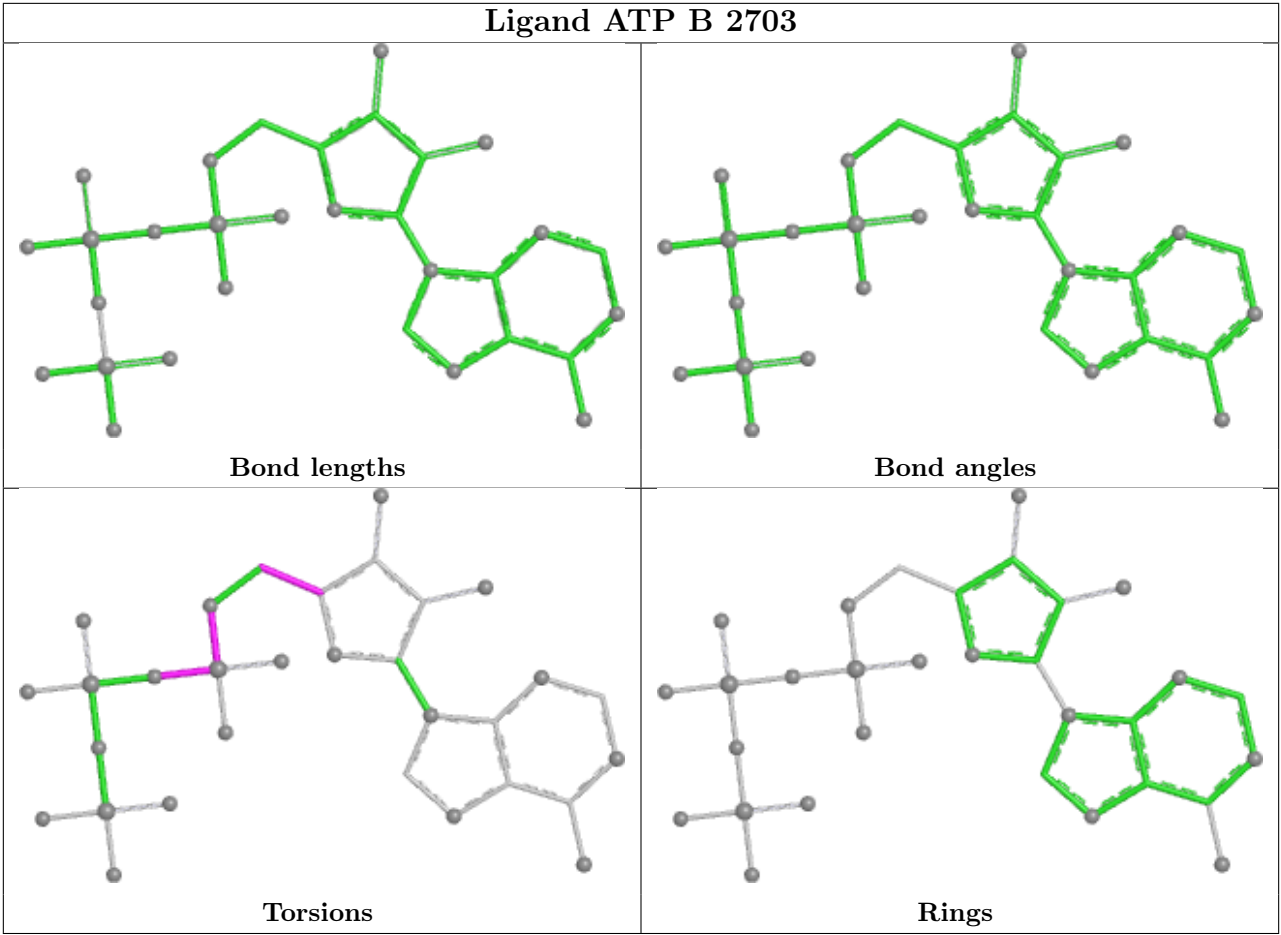












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	D	1
1	C	1
1	B	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	27.59
1	D	2611:VAL	C	2628:UNK	N	27.58

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2611:VAL	C	2628:UNK	N	27.54
1	B	2611:VAL	C	2628:UNK	N	27.53

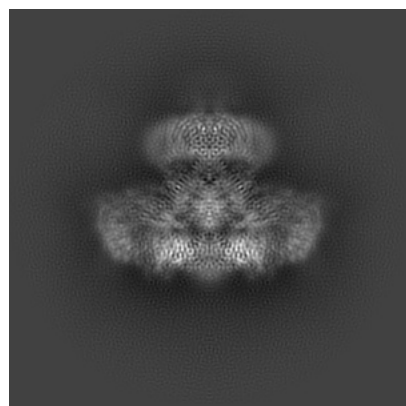
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25669. These allow visual inspection of the internal detail of the map and identification of artifacts.

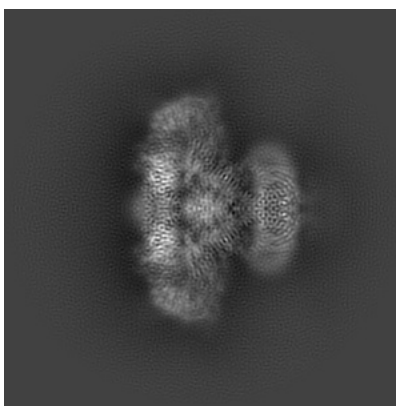
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

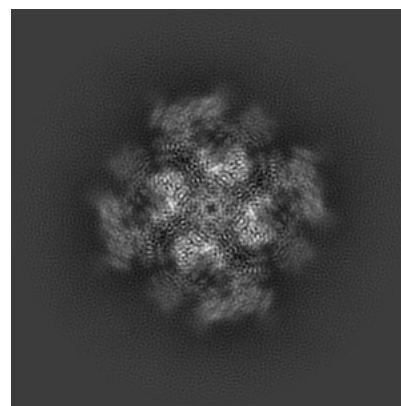
6.1.1 Primary map



X

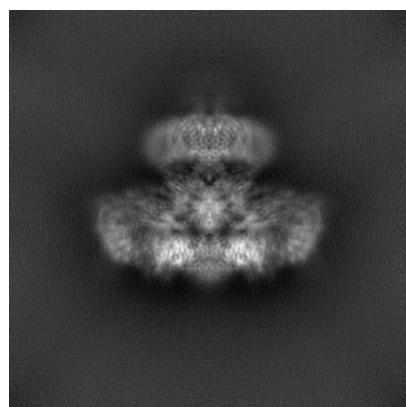


Y

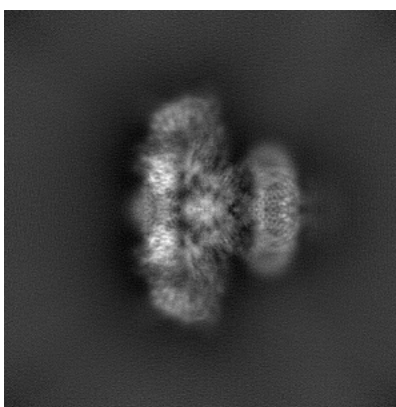


Z

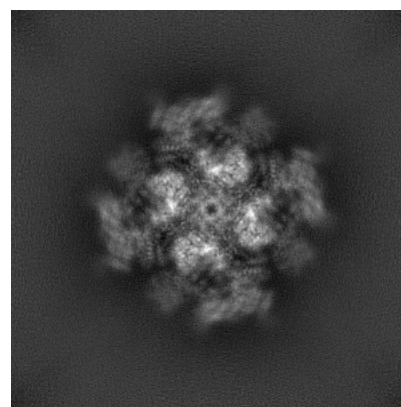
6.1.2 Raw map



X



Y

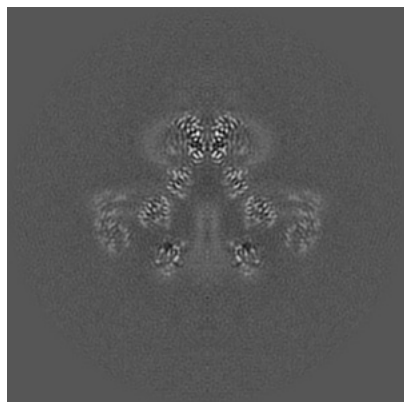


Z

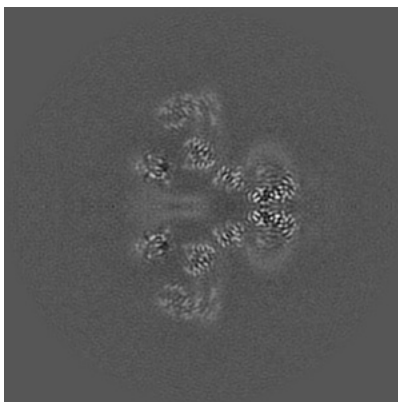
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

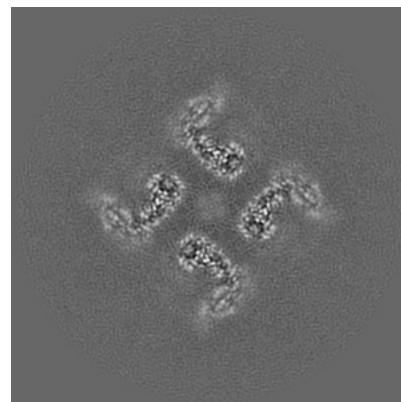
6.2.1 Primary map



X Index: 240

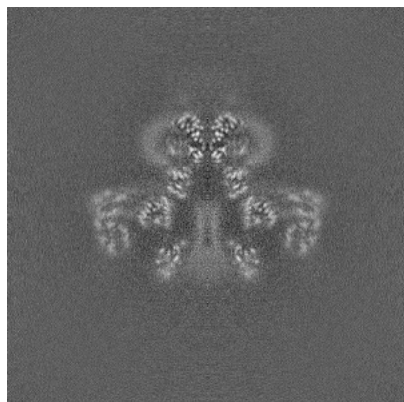


Y Index: 240

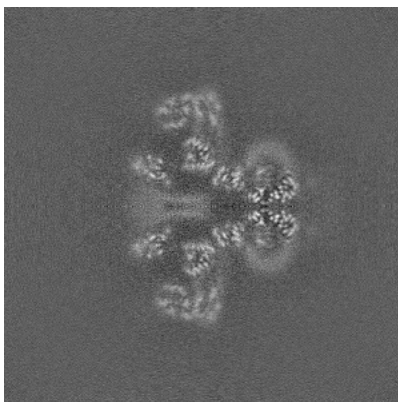


Z Index: 240

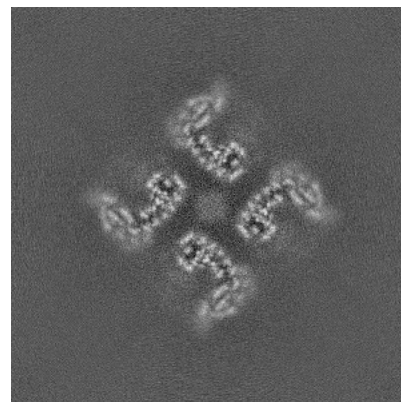
6.2.2 Raw map



X Index: 240



Y Index: 240

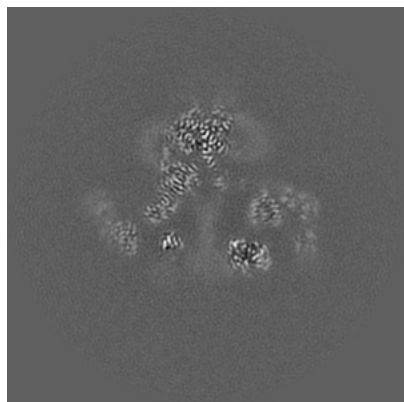


Z Index: 240

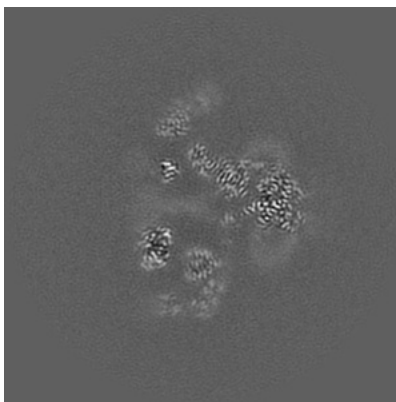
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

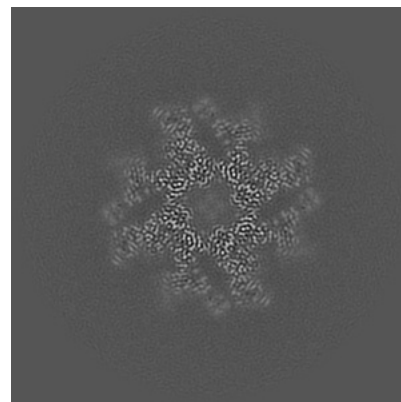
6.3.1 Primary map



X Index: 229

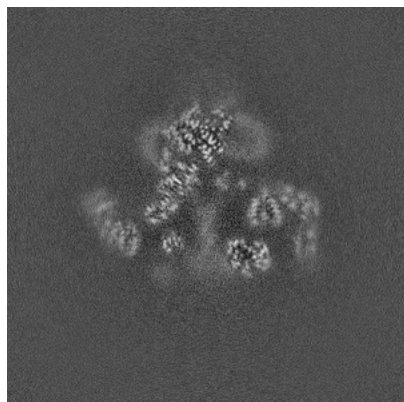


Y Index: 229

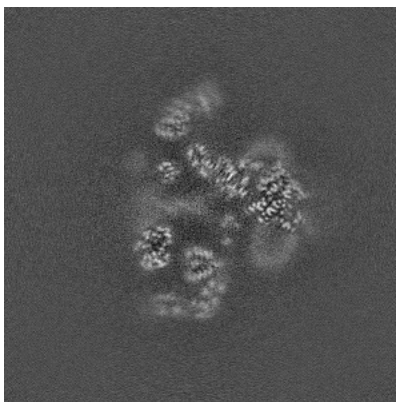


Z Index: 191

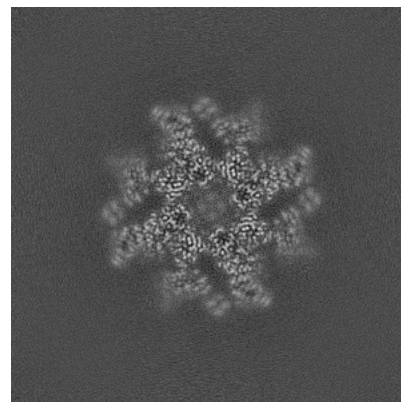
6.3.2 Raw map



X Index: 230



Y Index: 230

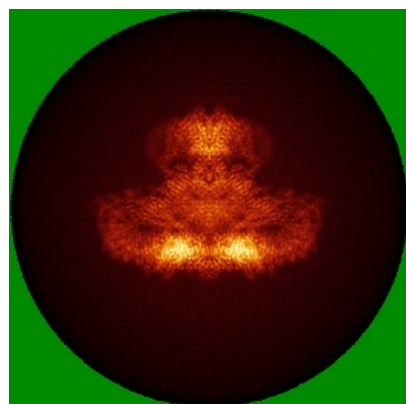


Z Index: 190

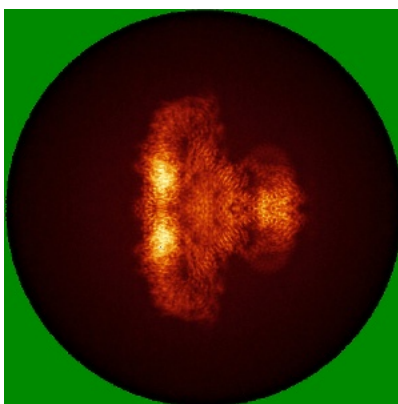
The images above show the largest variance slices of the map in three orthogonal directions.

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

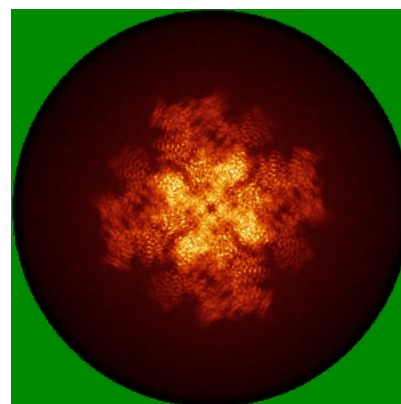
6.4.1 Primary map



X

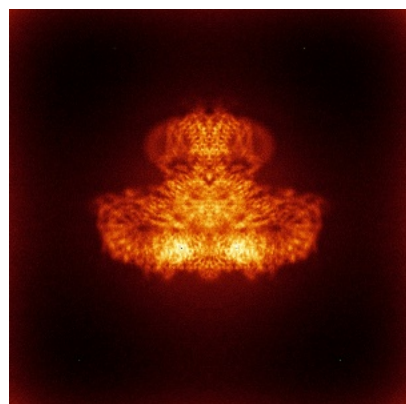


Y

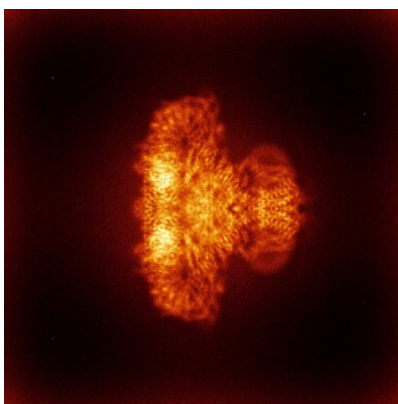


Z

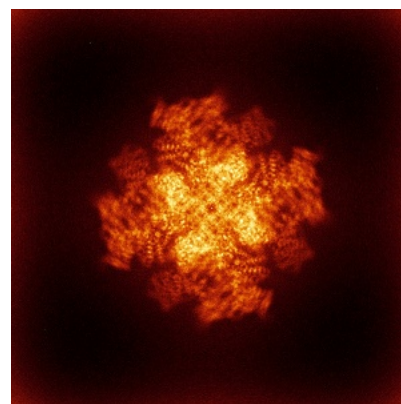
6.4.2 Raw map



X



Y

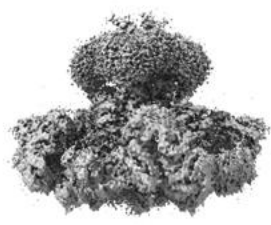


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

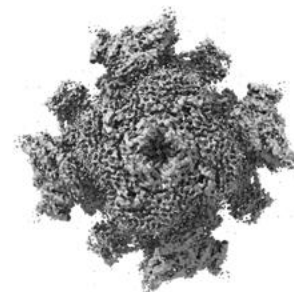
6.5.1 Primary map



X



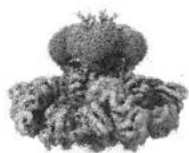
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

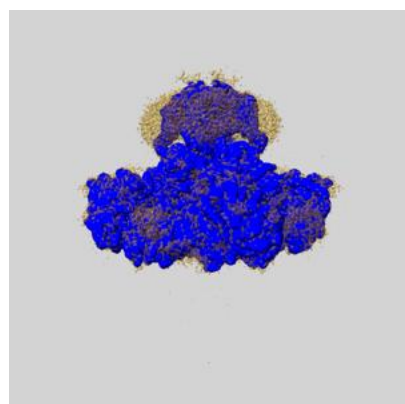
6.6 Mask visualisation [i](#)

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

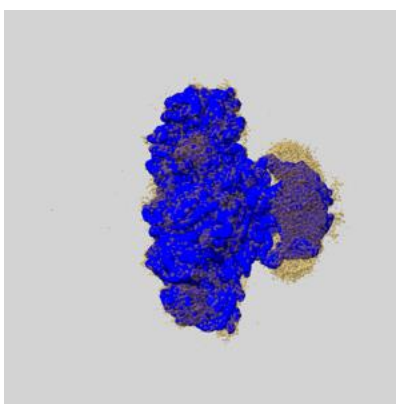
A mask typically either:

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

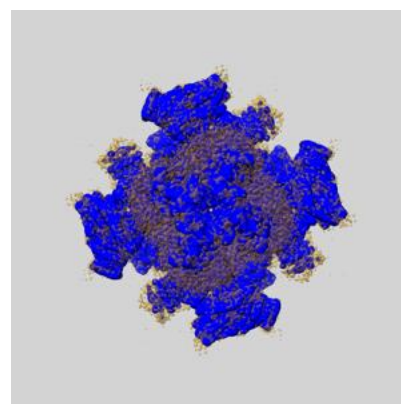
6.6.1 emd_25669_msk_1.map [i](#)



X



Y

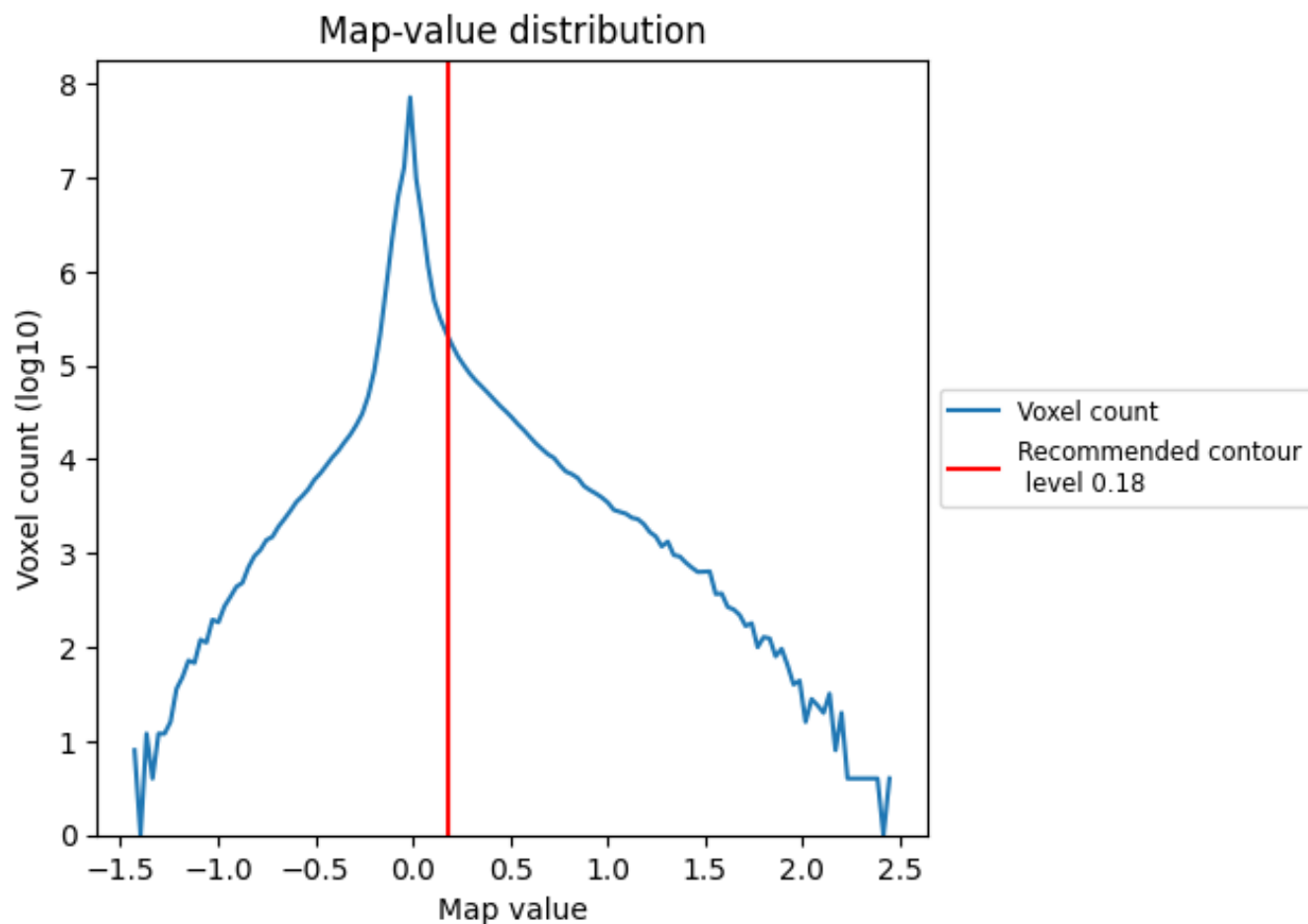


Z

7 Map analysis [i](#)

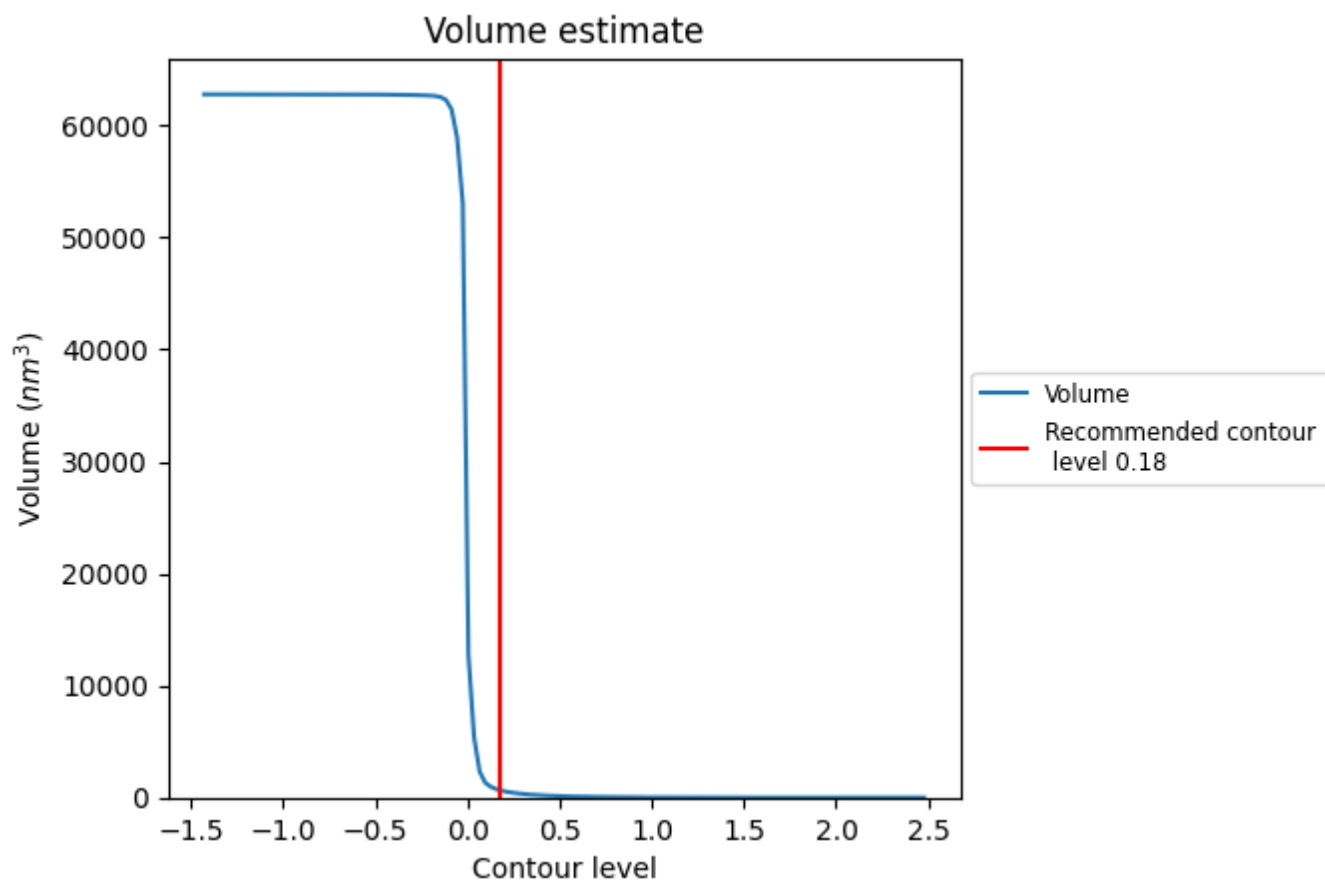
This section contains the results of statistical analysis of the map.

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.

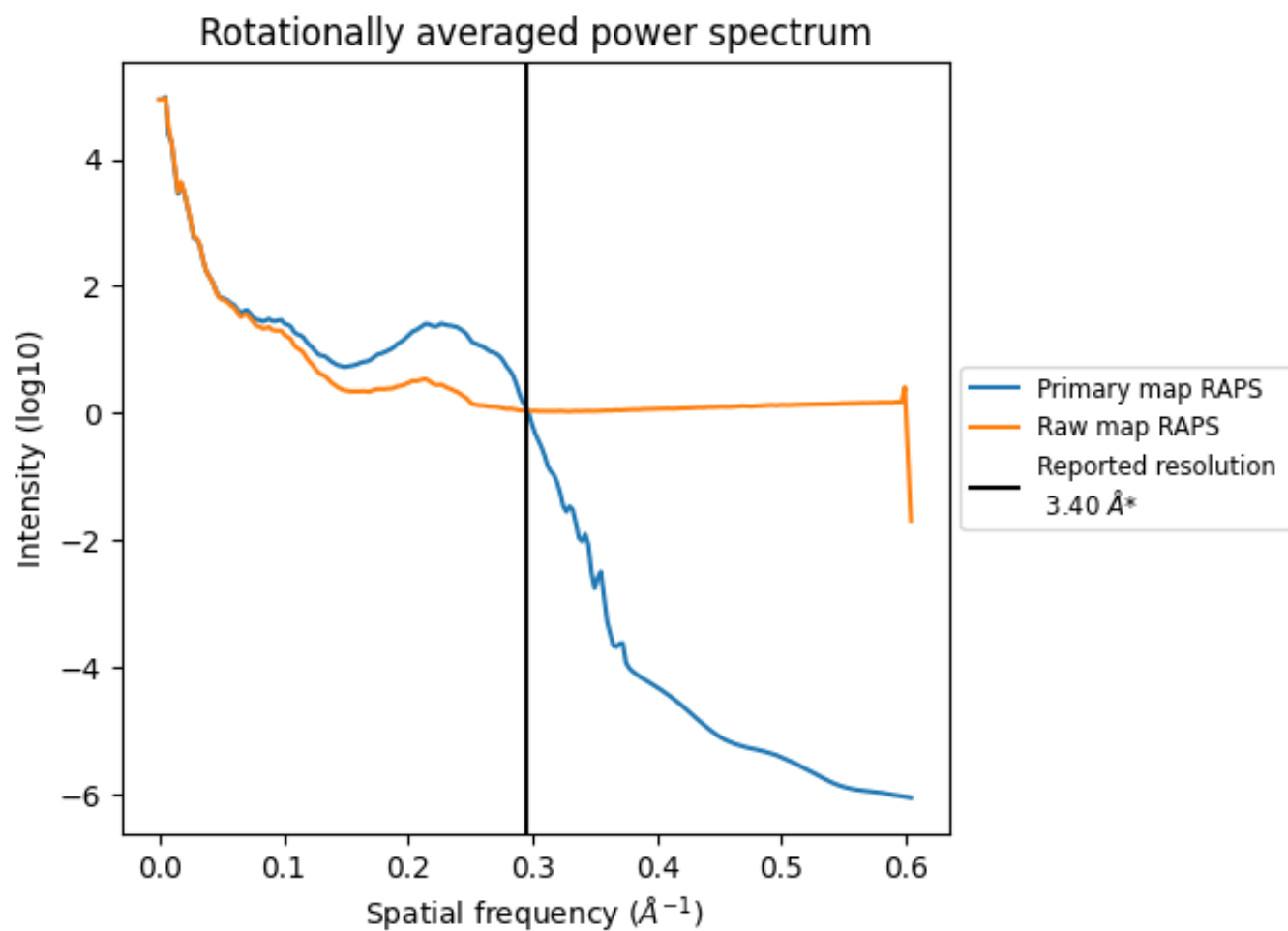
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 645 nm³; this corresponds to an approximate mass of 583 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 ⓘ

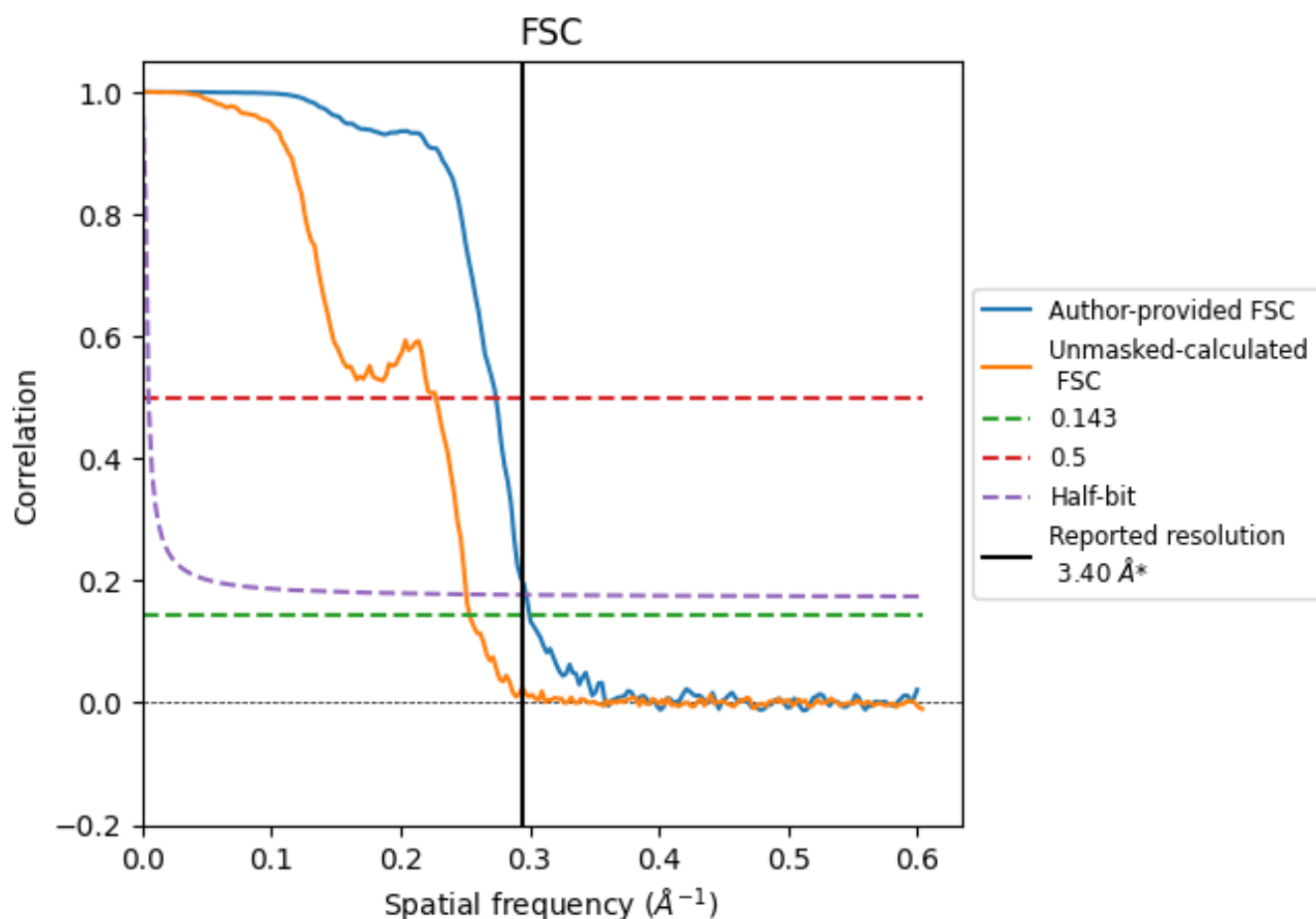


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

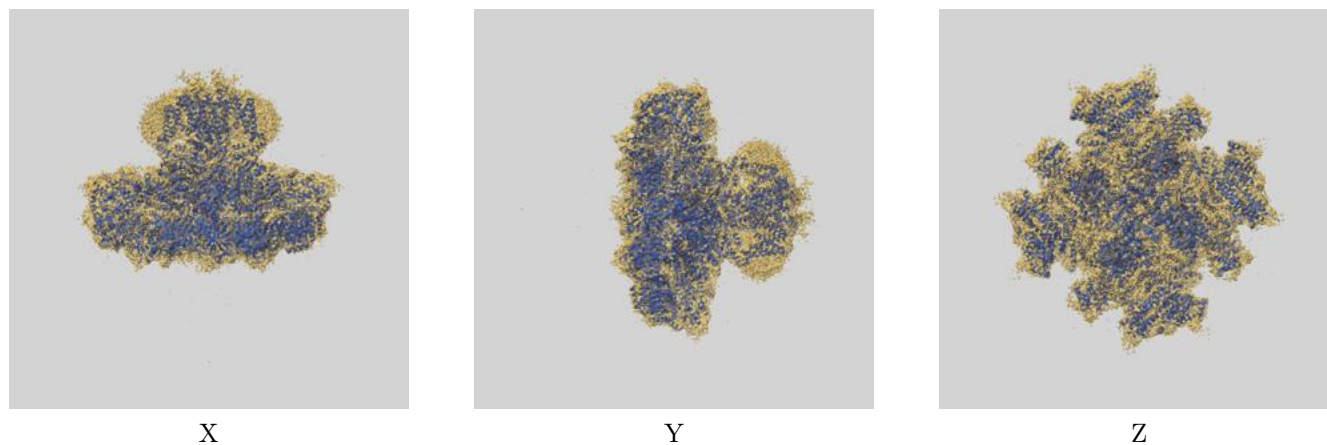
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.33	3.65	3.36
Unmasked-calculated*	3.94	4.40	3.99

*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 3.94 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

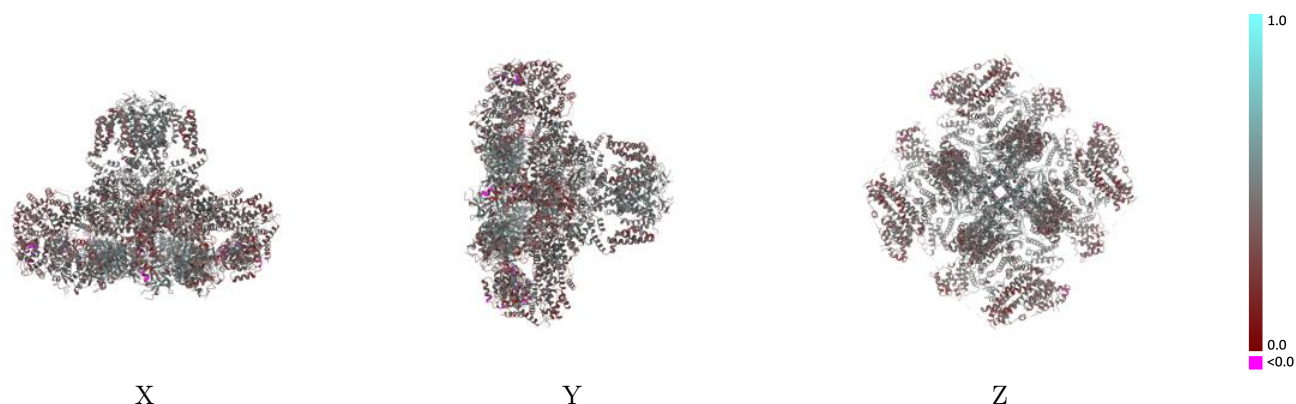
This section contains information regarding the fit between EMDB map EMD-25669 and PDB model 7T3R. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



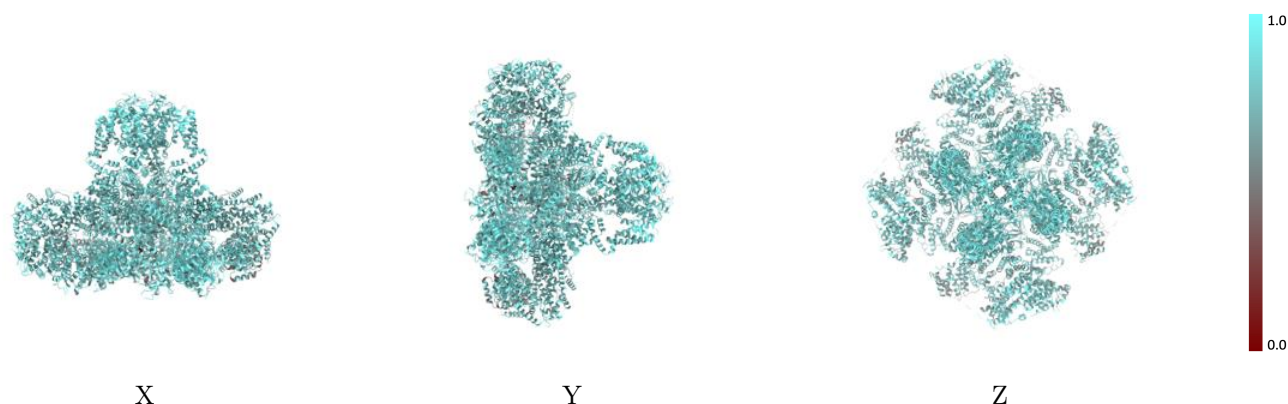
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



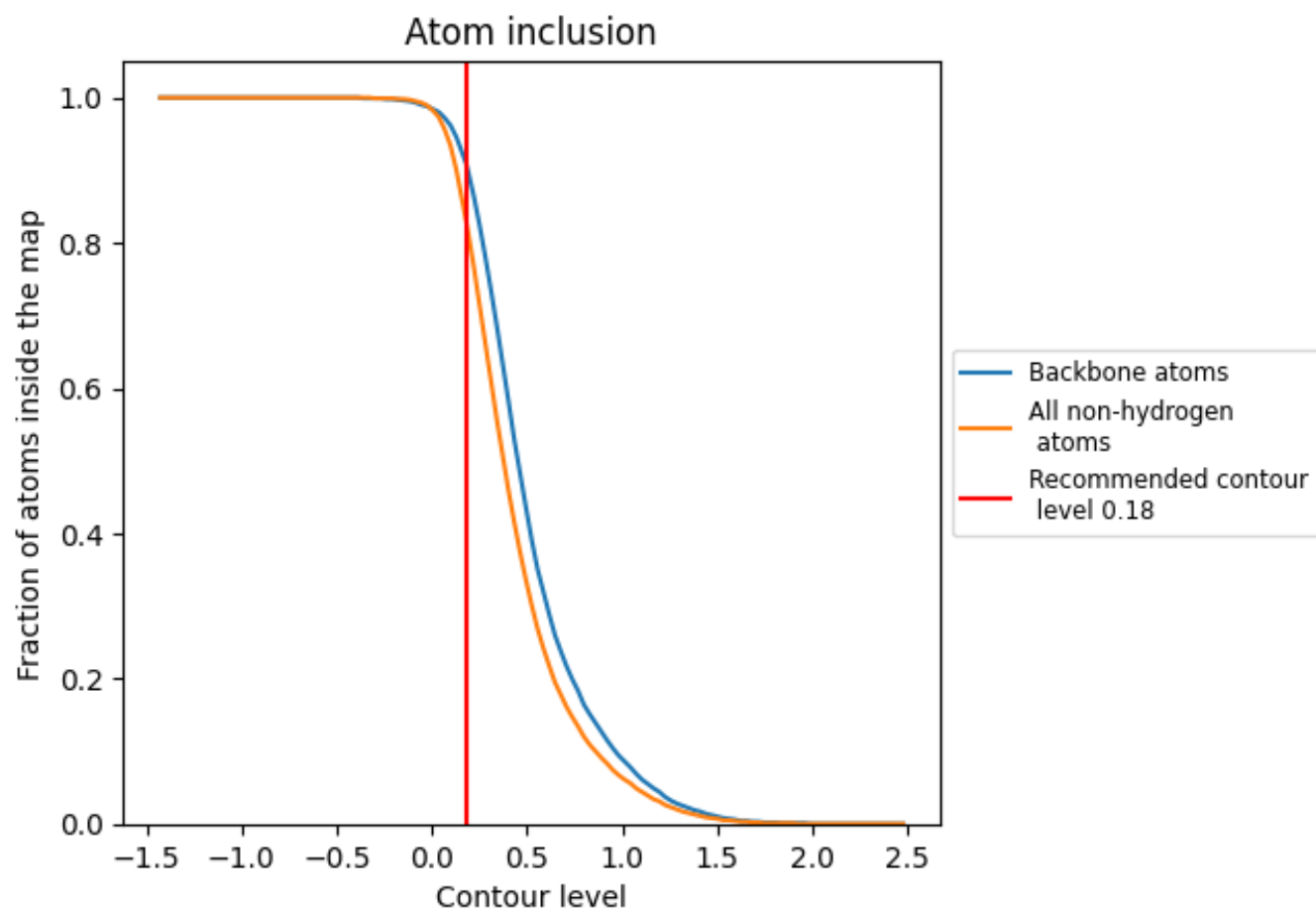
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 83% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.4320
A	0.8300	0.4320
B	0.8300	0.4320
C	0.8300	0.4310
D	0.8300	0.4320

