



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 12:12 AM UTC

PDB ID : 9CTL / pdb_00009ctl
EMDB ID : EMD-45910
Title : Full length EcPKS2 - malonylCoA inhibited dataset
Authors : Schubert, H.L.; Hill, C.P.
Deposited on : 2024-07-25
Resolution : 3.15 Å (reported)
Based on initial model : .

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:

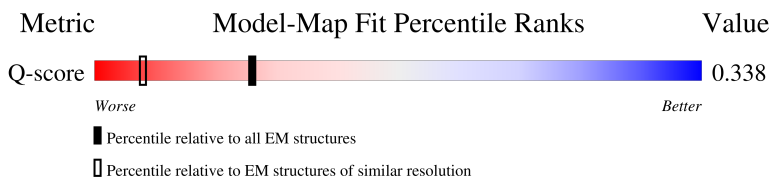
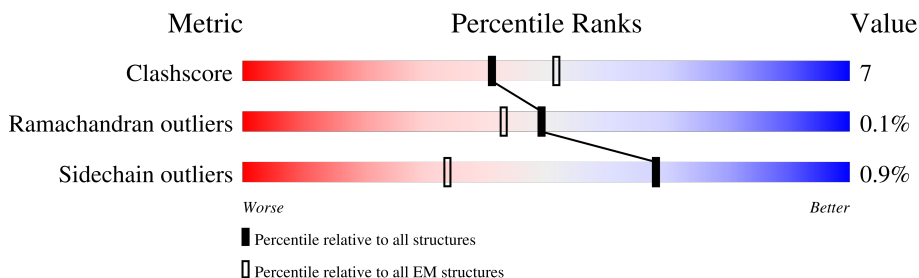
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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	14486 (2.65 - 3.65)

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	2287	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">14%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">83%</div> <div style="text-align: center;">15%</div> <div style="text-align: center;">•</div> </div>
1	B	2287	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">19%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">82%</div> <div style="text-align: center;">15%</div> <div style="text-align: center;">•</div> </div>

2 Entry composition [i](#)

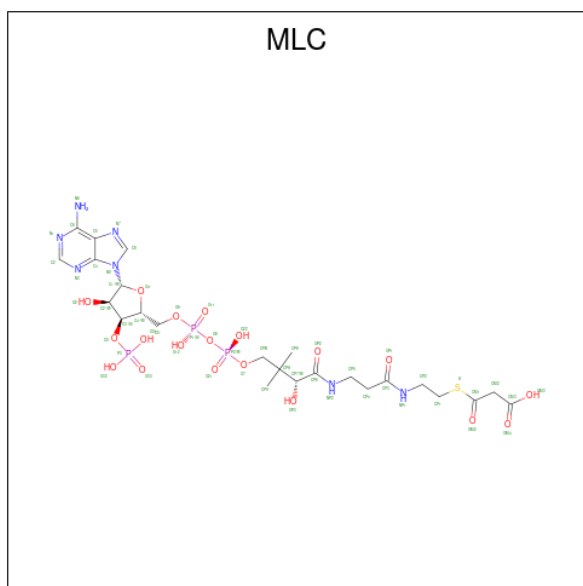
There are 3 unique types of molecules in this entry. The entry contains 69882 atoms, of which 34789 are hydrogens and 0 are deuteriums.

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 Polyketide synthase 2.

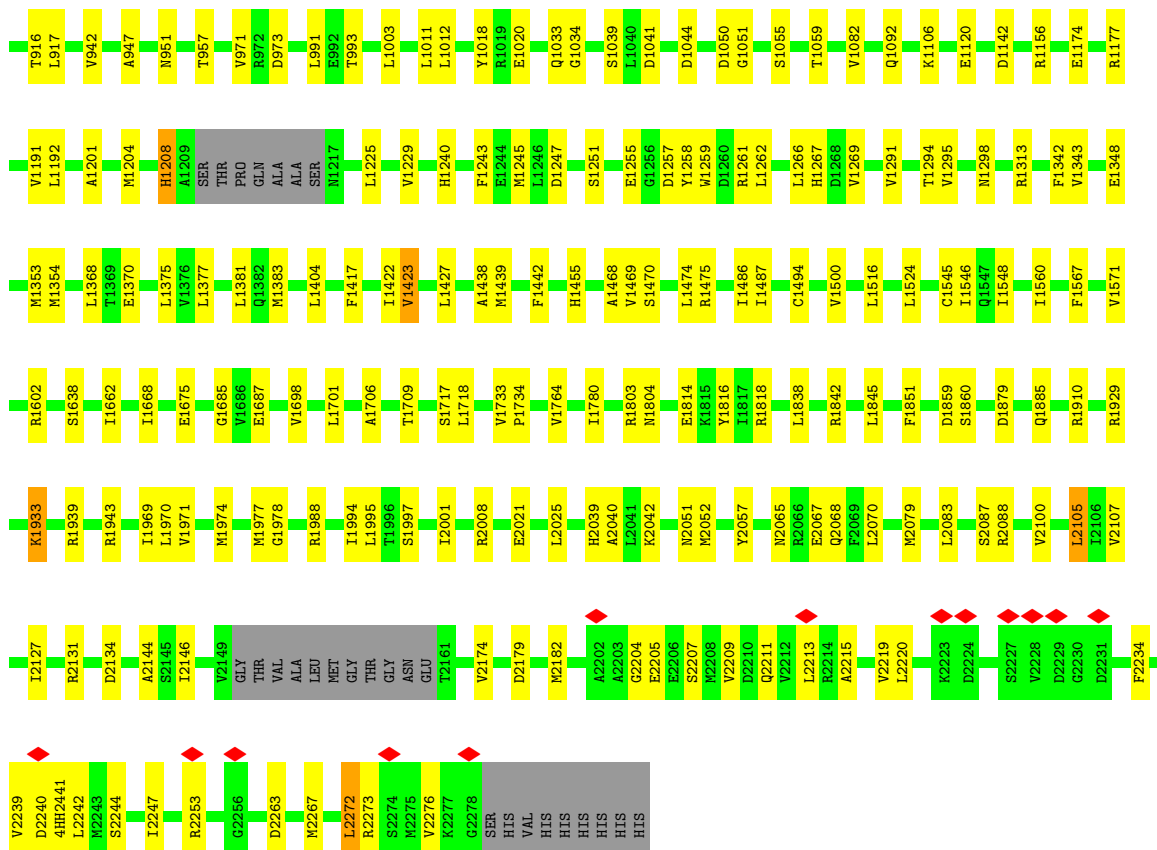
Mol	Chain	Residues	Atoms							AltConf	Trace
			Total	C	H	N	O	P	S		
1	A	2240	Total	C	H	N	O	P	S	3	0
			34802	11075	17346	2969	3301	1	110		
1	B	2236	Total	C	H	N	O	P	S	3	0
			34760	11062	17327	2965	3295	1	110		

- Molecule 2 is MALONYL-COENZYME A (CCD ID: MLC) (formula: $C_{24}H_{38}N_7O_{19}P_3S$) (labeled as "Ligand of Interest" by depositor).

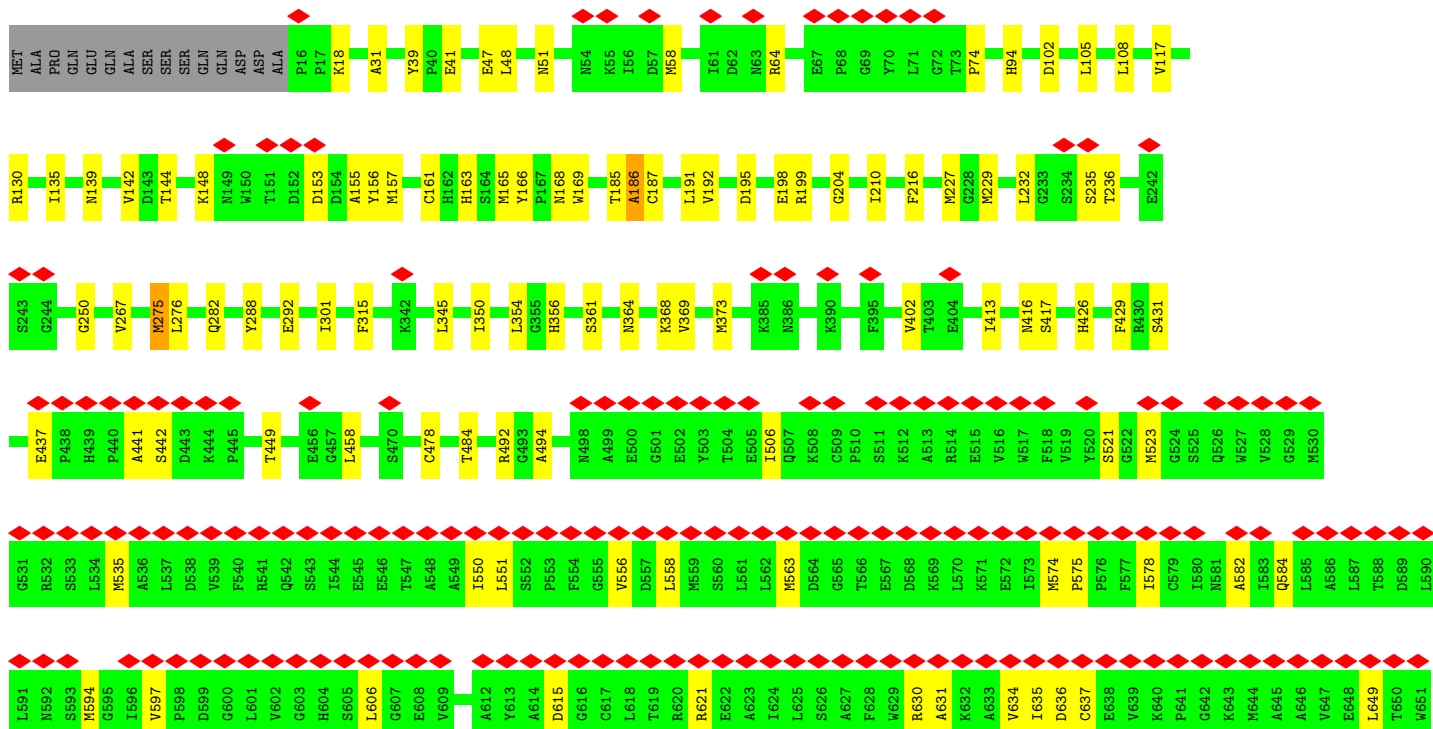
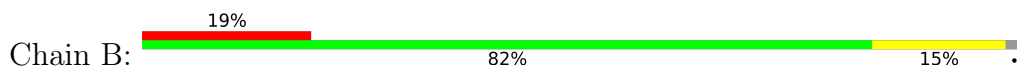


Mol	Chain	Residues	Atoms							AltConf
			Total	C	H	N	O	P	S	
2	A	1	Total	C	H	N	O	P	S	0
			87	24	33	7	19	3	1	
2	B	1	Total	C	H	N	O	P	S	0
			87	24	33	7	19	3	1	

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



● Molecule 1: Polyketide synthase 2



G2238	V2239	D2240	4HHZ241	L2242	M2243	S2244	V2245	E2246	I2247	K2248	Q2249	A2250	L2251	E2252	R2253	D2254	A2255	G2256	L2257	V2258	I2259	S2260	T2261	K2262	D2263	T2264	Q2265	L2266	M2267	F2268	N2270	T2271	L2272	R2273	S2274	M2275	V2276	K2277	G2278	SER	HIS	VAL	HIS	HIS	HIS	HIS	HIS	HIS											
E652	E653	A654	K655	R656	L657	C658	P659	P660	G661	V662	V663	A664	C666	H667	N668	S669	Q670	D671	S672	V673	T674	I675	S676	G677	G678	A679	Q680	E681	M682	T683	K684	F685	M686	A687	E688	L689	S690	A691	G692	V694	T695	V696	K697	E698	V699	N700	S701	N702	N703	I704	S705	Y706	H707	S708	F710	M711			
T712	E713	P714	A715	A716	Y717	L718	K719	K720	G721	L722	E723	K724	E725	I726	V727	P728	K729	P730	R731	S732	K733	K734	W735	I736	S737	T738	S739	I740	P741	E742	E743	R744	W745	G746	N747	P748	E749	A750	Q751	T752	A753	D754	A755	S756	Y757	Q758	A759	N760	N761	L762	L763	S764	S765	V766	L767	F768	Y769	E770	G771
L772	Q773	K774	I775	P776	S777	N778	A779	I780	A781	I782	E783	I784	A787	G788	L789	L790	Q791	S792	S793	I794	K795	K796	S797	L798	G799	Q800	D801	C802	T803	I804	V805	W806	A806	L807	Q808	K809	R810	K811	S812	P813	N814	N815	L816	E817	V818	F819	F820	S821	A822	L823	H829	G830	V831	P832	M833	N834	L838		
Y839	P840	A841	W842	Q843	L853	W857	A779	S864	A865	K866	P870	E873	E876	E877	GLY	GLY	SER	SER	SER	S883	D888	E889	D894	L901	M909	T916	L917	T957	V971	R972	D973	E987	R989	R810	K811	S812	P813	N814	L1012	Y1018	H1019	E1020	Q1033	G1034															
D1044	D1050	G1051	S1055	T1059	V1082	Q1092	K1106	W1107	D1108	Q1112	E1120	D1136	E1174	F1175	S1176	V1191	L1192	P1193	N1194	H1208	A1209	SER	THR	GLN	ALA	ALA	SER	N1217	L1225	V1229	H1240	F1243	E1244	M1245	E1265	G1266	I1267	Y1268	W1269																				
D1360	R1261	L1263	M1264	K1265	L1266	H1267	V1269	D1275	L1282	V1291	T1294	V1295	M1298	M1304	E1308	Q1334	Y1335	T1337	V1343	M1353	M1354	L1368	T1369	E1370	L1375	V1376	L1377	L1381	V1385	L1404	L1413	I1419	M1424	I1422	V1423	L1427	G1428																						
D1436	R1437	A1438	M1439	F1442	Y1443	A1468	V1469	S1470	M1471	R1475	I1486	I1487	C1494	V1500	Q1501	L1516	L1524	L1531	V1535	C1545	I1548	K1559	I1560	F1567	V1571	R1572	K1573	D1585	R1602	S1638	E1647	N1657	L1668	R1659	I1662	I1668																							
E1675	G1685	V1686	E1687	S1693	V1698	L1701	A1706	T1709	S1717	L1718	V1733	P1734	A1760	S1763	V1764	I1780	R1803	M1804	E1814	K1815	Y1816	I1817	R1818	L1838	R1842	R1843	L1844	L1845	F1851	D1859	S1860	D1879	Q1885	R1910	M1915	K1933																							
R1939	F1954	I1969	L1970	V1971	M1977	G1978	R1988	L1994	L1995	S1997	R2008	E2021	V2022	L2023	V2027	M2028	T2029	H2039	K2042	F2050	M2051	M2052	F2061	L2070	S2075	M2079	T2080	L2083	S2087	R2088	V2100	M2101	V2107	T2127	R2131	D2134																							
I2146	V2149	THR	VAL	ALA	LEU	MET	THR	GLY	ASN	T2161	V2174	D2179	M2182	V2201	ALA	ALA	GLY	GLU	E2206	S2207	M2208	V2209	D2210	Q2211	L2213	R2214	A2215	V2216	G2217	K2218	V2219	L2220	G2221	I2222	K2223	D2224	V2225	S2226	S2227	V2228	D2229	G2230	K2232	E2233	F2234	I2235	D2236	M2237											
G2238	V2239	D2240	4HHZ241	L2242	M2243	S2244	V2245	E2246	I2247	K2248	Q2249	A2250	L2251	E2252	R2253	D2254	A2255	G2256	L2257	V2258	I2259	S2260	T2261	K2262	D2263	T2264	Q2265	L2266	M2267	F2268	N2270	T2271	L2272	R2273	S2274	M2275	V2276	K2277	G2278	SER	HIS	VAL	HIS	HIS	HIS	HIS	HIS												

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	258974	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.794	Depositor
Minimum map value	-0.282	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.105	Depositor
Map size (\AA)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	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: 4HH, MLC, NAP

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	0.11	0/17814	0.26	1/24118 (0.0%)
1	B	0.11	0/17790	0.26	0/24084
All	All	0.11	0/35604	0.26	1/48202 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1423	VAL	N-CA-C	-5.05	108.37	113.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2253	ARG	Sidechain

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	17456	17346	17347	240	0
1	B	17433	17327	17327	247	0
2	A	54	33	33	2	0
2	B	54	33	33	4	0
3	A	48	25	25	1	0
3	B	48	25	25	3	0
All	All	35093	34789	34790	480	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 480 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:125:SER:OG	1:A:126:MET:SD	2.27	0.92
1:A:993:THR:OG1	1:A:1120:GLU:OE2	1.90	0.88
1:A:130:ARG:NH2	1:A:204:GLY:O	2.16	0.79
1:A:772:LEU:HD21	1:A:794:ILE:HD13	1.64	0.79
1:B:198:GLU:OE1	1:B:199:ARG:NH2	2.17	0.77

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	2234/2287 (98%)	2169 (97%)	64 (3%)	1 (0%)	100	100
1	B	2228/2287 (97%)	2159 (97%)	67 (3%)	2 (0%)	48	76
All	All	4462/4574 (98%)	4328 (97%)	131 (3%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	ALA
1	A	1468	ALA
1	B	1468	ALA

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	1895/1929 (98%)	1879 (99%)	16 (1%)	73	78
1	B	1894/1929 (98%)	1875 (99%)	19 (1%)	68	76
All	All	3789/3858 (98%)	3754 (99%)	35 (1%)	68	77

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1996	THR
1	B	2029	THR
1	B	2248	LYS
1	A	1994	ILE
1	A	1933	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1194	ASN
1	B	1767	GLN
1	B	2249	GLN
1	B	1877	GLN
1	A	1799	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	4HH	B	2241	1	22,26,27	0.45	0	27,35,37	0.60	0
1	4HH	A	2441	1	22,26,27	0.45	0	27,35,37	0.51	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
1	4HH	B	2241	1	-	15/33/35/37	-
1	4HH	A	2441	1	-	7/33/35/37	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2441	4HH	N-CA-CB-OG
1	A	2441	4HH	NN-CL3-CM-OM
1	A	2441	4HH	CJ-O3P-P-O2P
1	A	2441	4HH	CT-CS-NR-CQ
1	B	2241	4HH	C-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	2241	4HH	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2441	4HH	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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
2	MLC	A	3001	-	53,56,56	3.20	21 (39%)	77,83,83	1.90	15 (19%)
3	NAP	A	5001	-	50,52,52	1.69	4 (8%)	71,80,80	1.04	5 (7%)
2	MLC	B	3001	-	53,56,56	3.20	21 (39%)	77,83,83	1.95	19 (24%)
3	NAP	B	5001	-	50,52,52	1.69	4 (8%)	71,80,80	1.02	5 (7%)

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
2	MLC	A	3001	-	-	27/54/71/71	0/3/3/3
3	NAP	A	5001	-	-	8/35/67/67	0/5/5/5
2	MLC	B	3001	-	-	27/54/71/71	0/3/3/3
3	NAP	B	5001	-	-	8/35/67/67	0/5/5/5

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	MLC	C2'-C3'	-9.11	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3001	MLC	C2'-C3'	-9.05	1.33	1.53
3	A	5001	NAP	P2B-O2B	8.26	1.74	1.59
3	B	5001	NAP	P2B-O2B	8.26	1.74	1.59
2	B	3001	MLC	P2-O6	8.07	1.68	1.59

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3001	MLC	N6-C6-N1	-6.16	104.65	118.38
2	A	3001	MLC	N6-C6-N1	-6.11	104.76	118.38
2	B	3001	MLC	N1-C2-N3	-5.28	120.58	128.58
2	A	3001	MLC	N1-C2-N3	-5.21	120.70	128.58
2	B	3001	MLC	C5-C4-N3	-4.96	119.89	126.72

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	MLC	C4'-C5'-O5'-P1
2	A	3001	MLC	C5'-O5'-P1-O12
2	A	3001	MLC	C5'-O5'-P1-O6
2	A	3001	MLC	CPB-O7-P2-O22
2	A	3001	MLC	CP7-CPA-CPB-O7

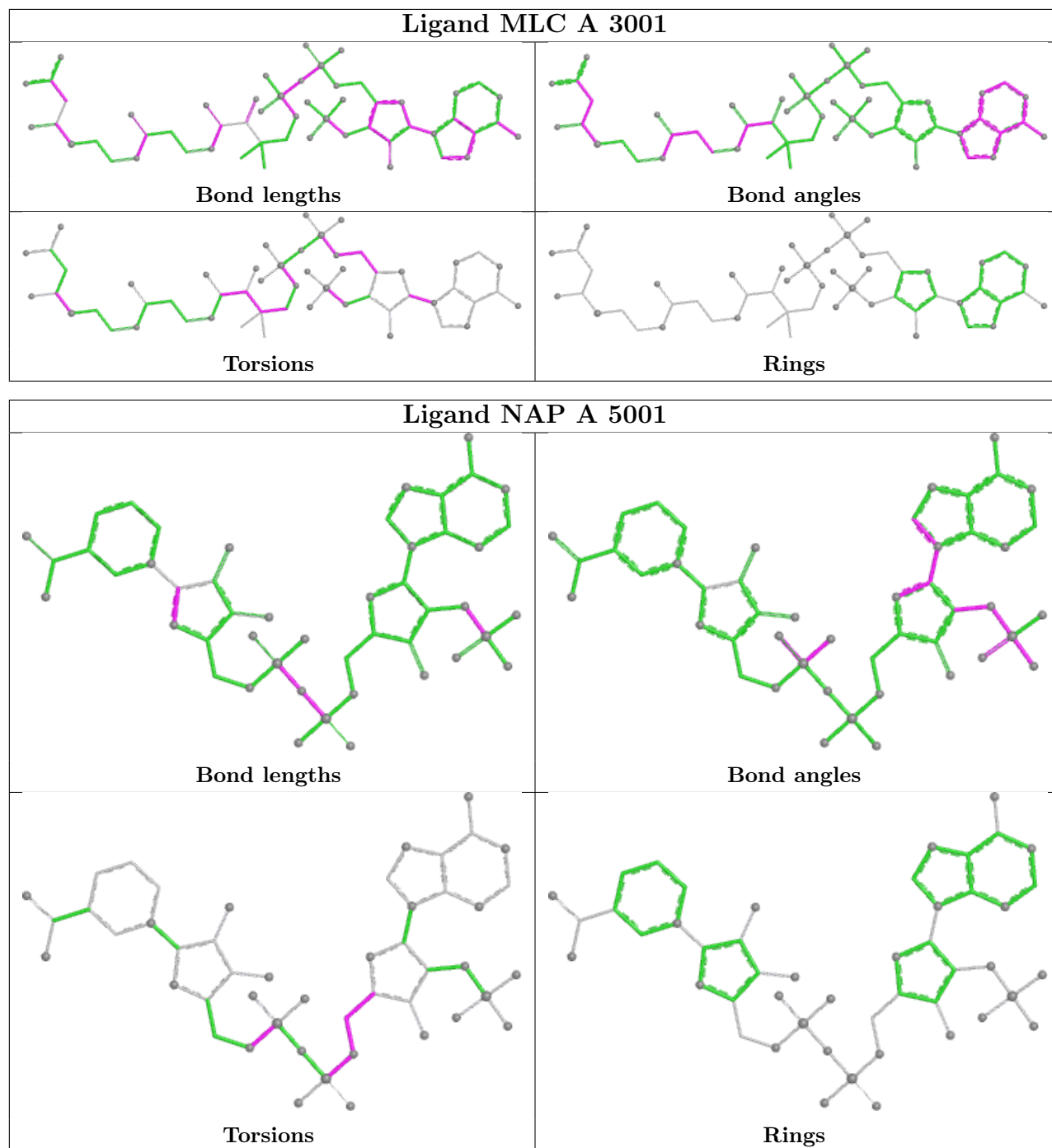
There are no ring outliers.

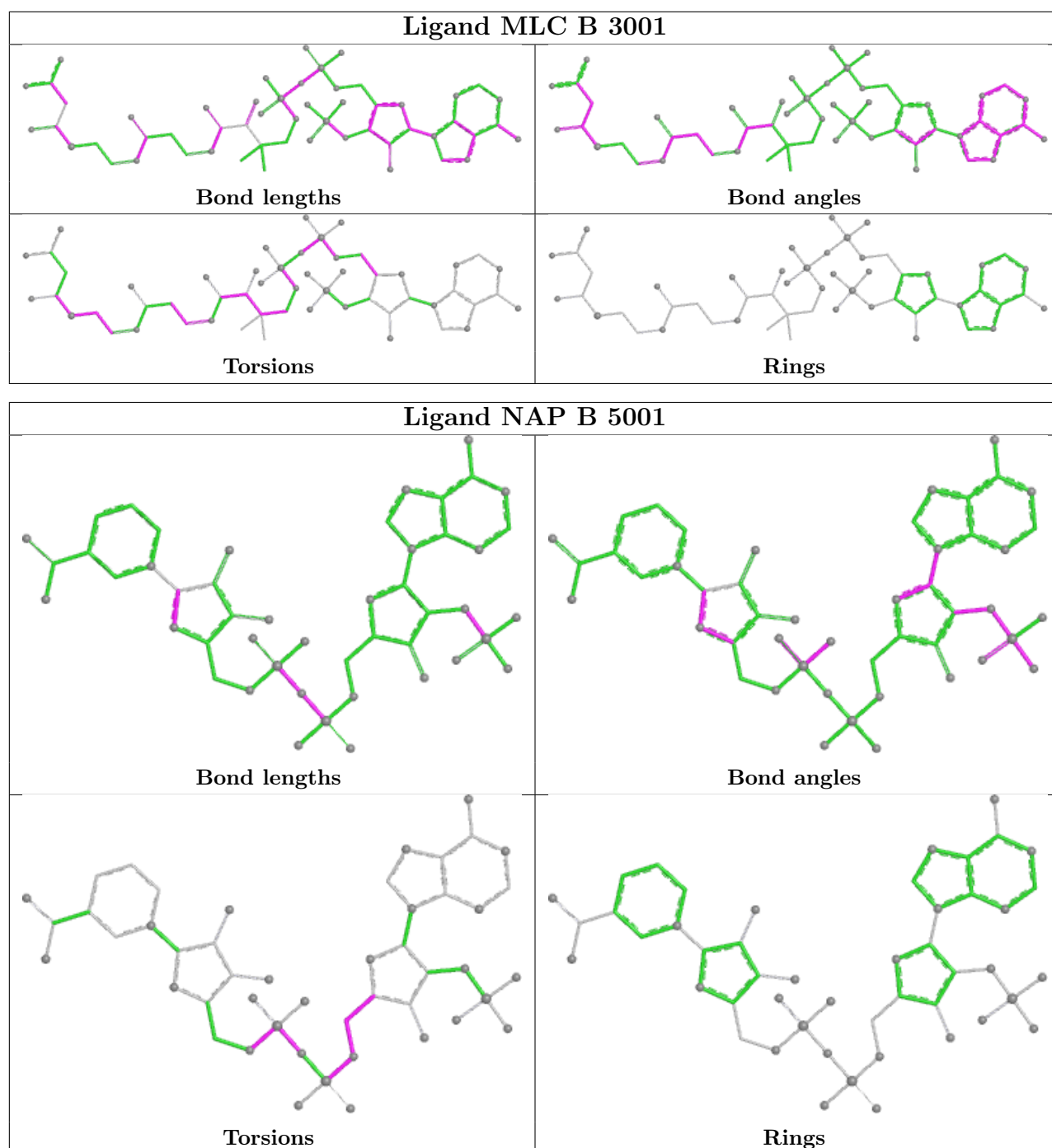
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	MLC	2	0
3	A	5001	NAP	1	0
2	B	3001	MLC	4	0
3	B	5001	NAP	3	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.

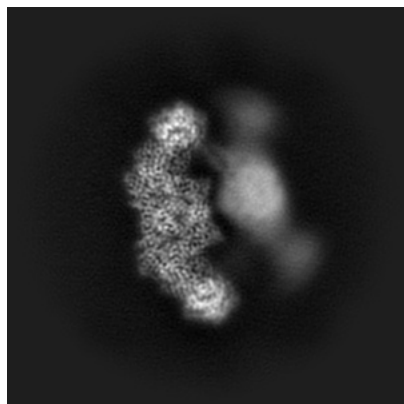
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45910. These allow visual inspection of the internal detail of the map and identification of artifacts.

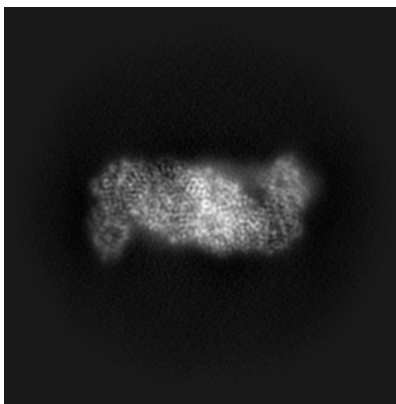
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

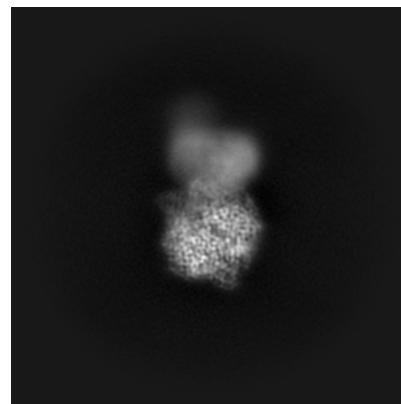
6.1.1 Primary map



X

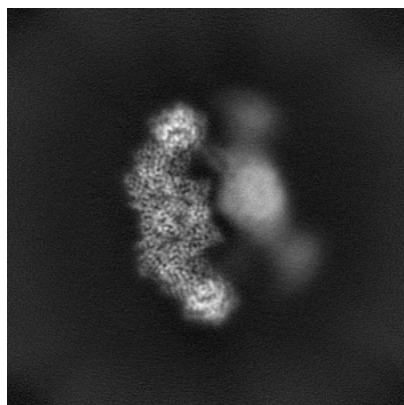


Y

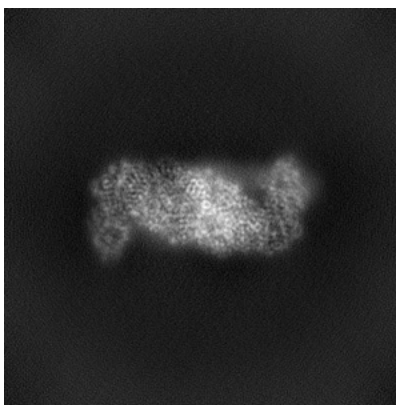


Z

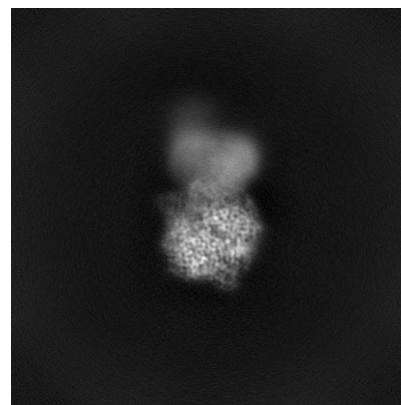
6.1.2 Raw map



X



Y

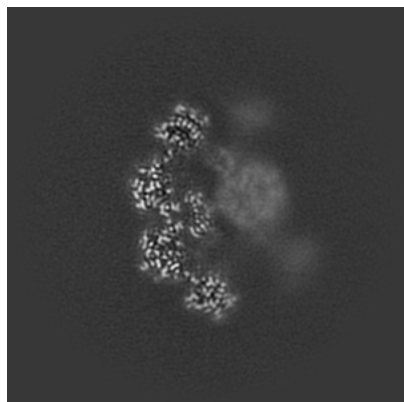


Z

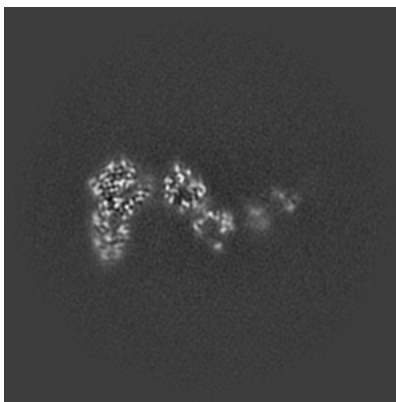
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

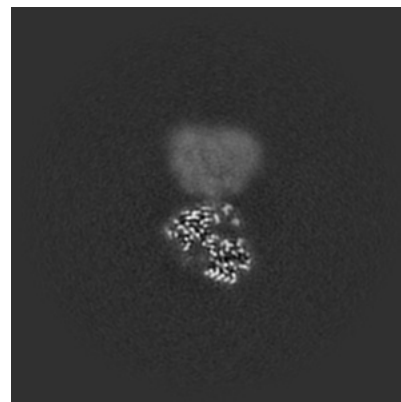
6.2.1 Primary map



X Index: 160

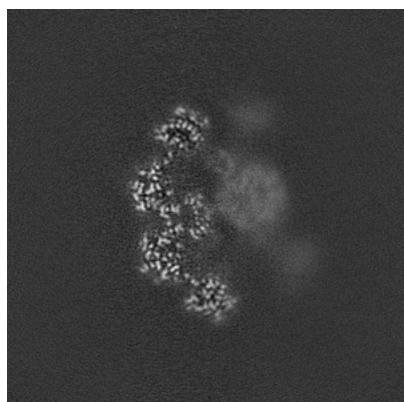


Y Index: 160

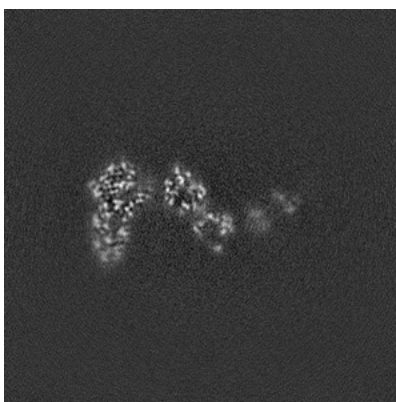


Z Index: 160

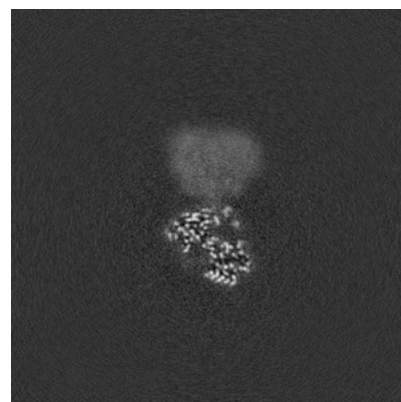
6.2.2 Raw map



X Index: 160



Y Index: 160

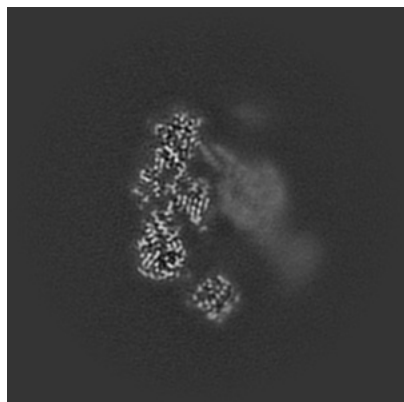


Z Index: 160

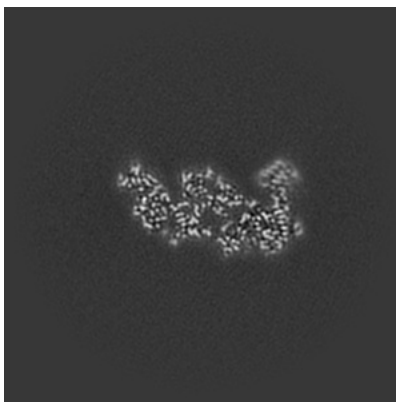
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

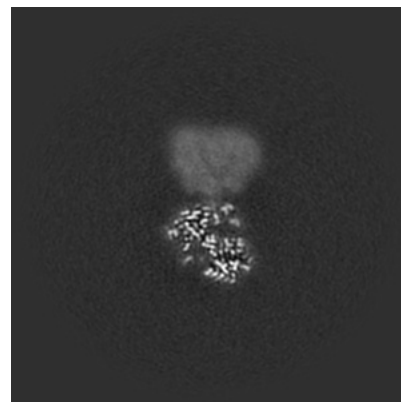
6.3.1 Primary map



X Index: 154

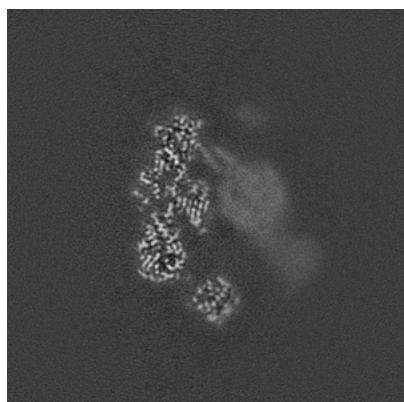


Y Index: 127

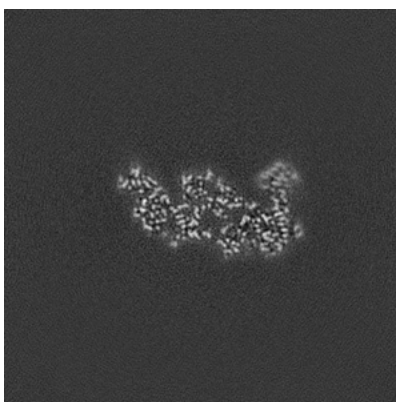


Z Index: 159

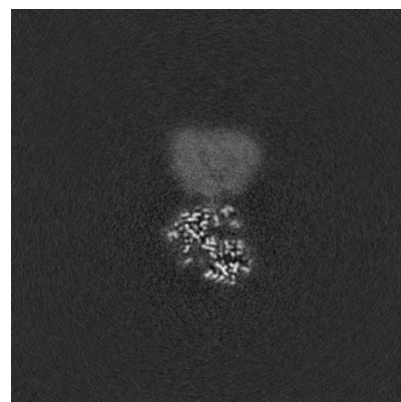
6.3.2 Raw map



X Index: 154



Y Index: 127

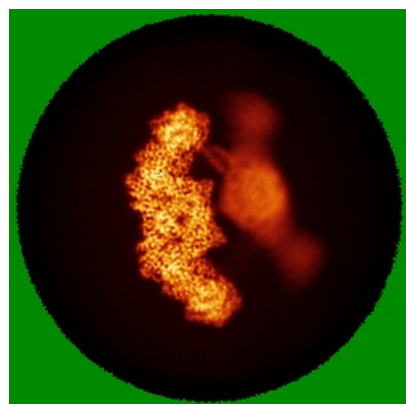


Z Index: 159

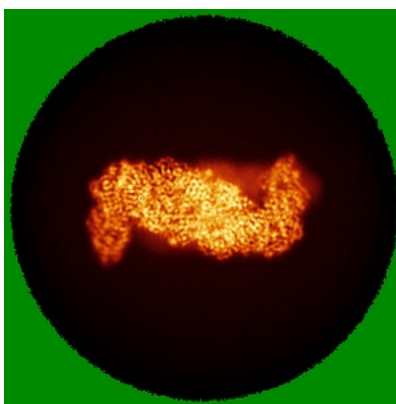
The images above show the largest variance slices of the map in three orthogonal directions.

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

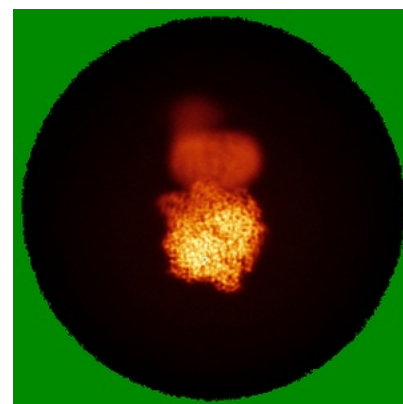
6.4.1 Primary map



X

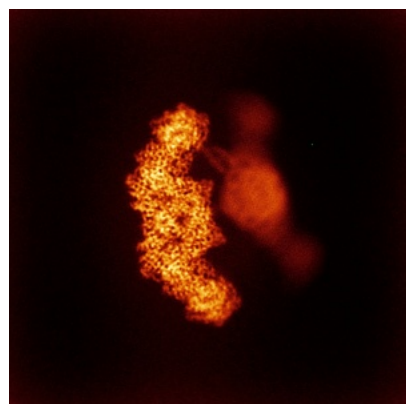


Y

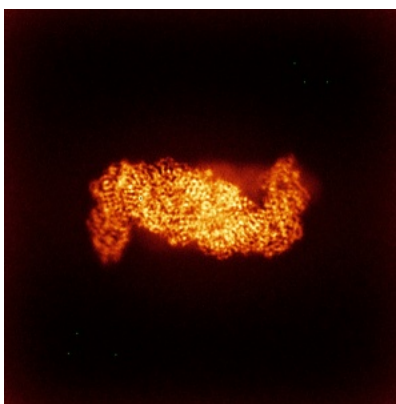


Z

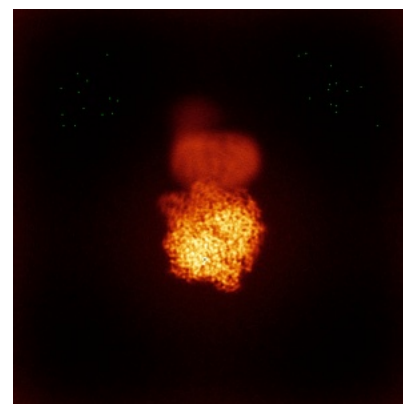
6.4.2 Raw map



X



Y

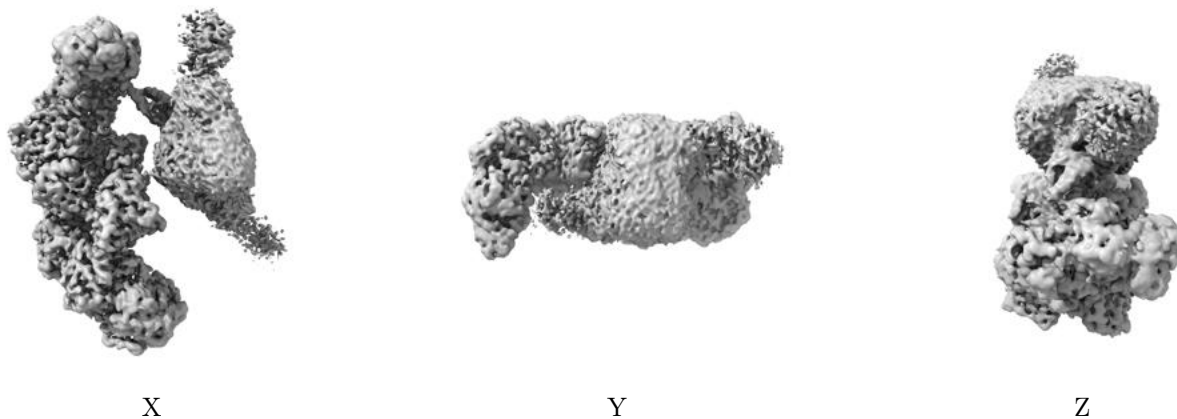


Z

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.

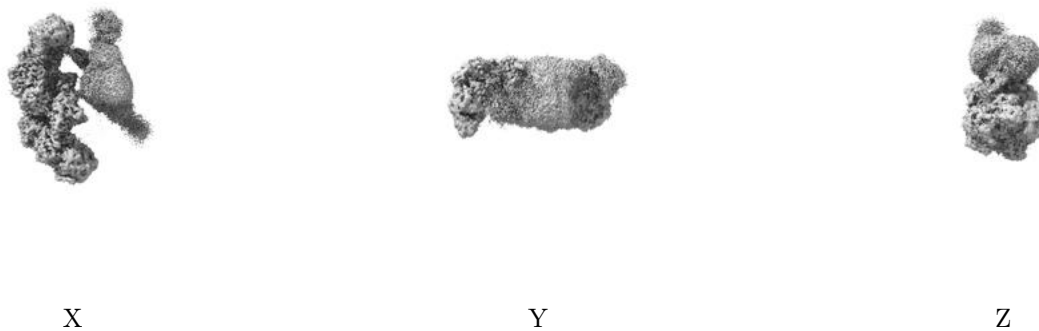
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.105. 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.

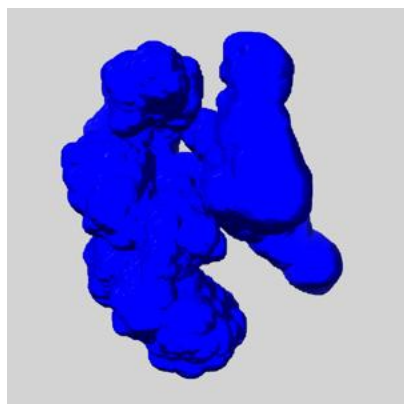
6.6 Mask visualisation [i](#)

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

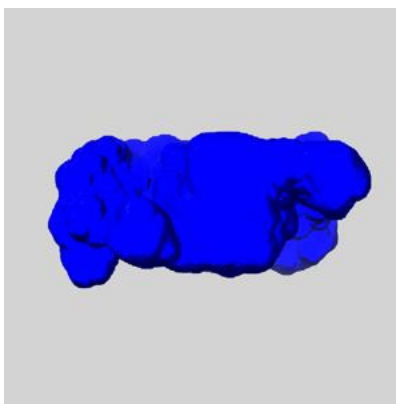
A mask typically either:

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

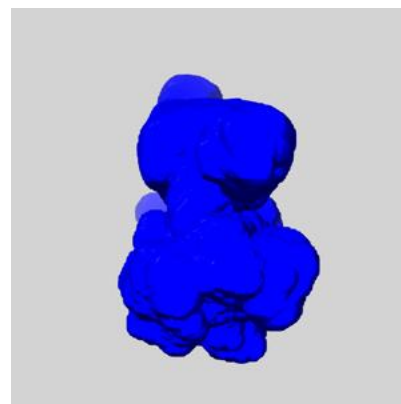
6.6.1 emd_45910_msk_1.map [i](#)



X



Y

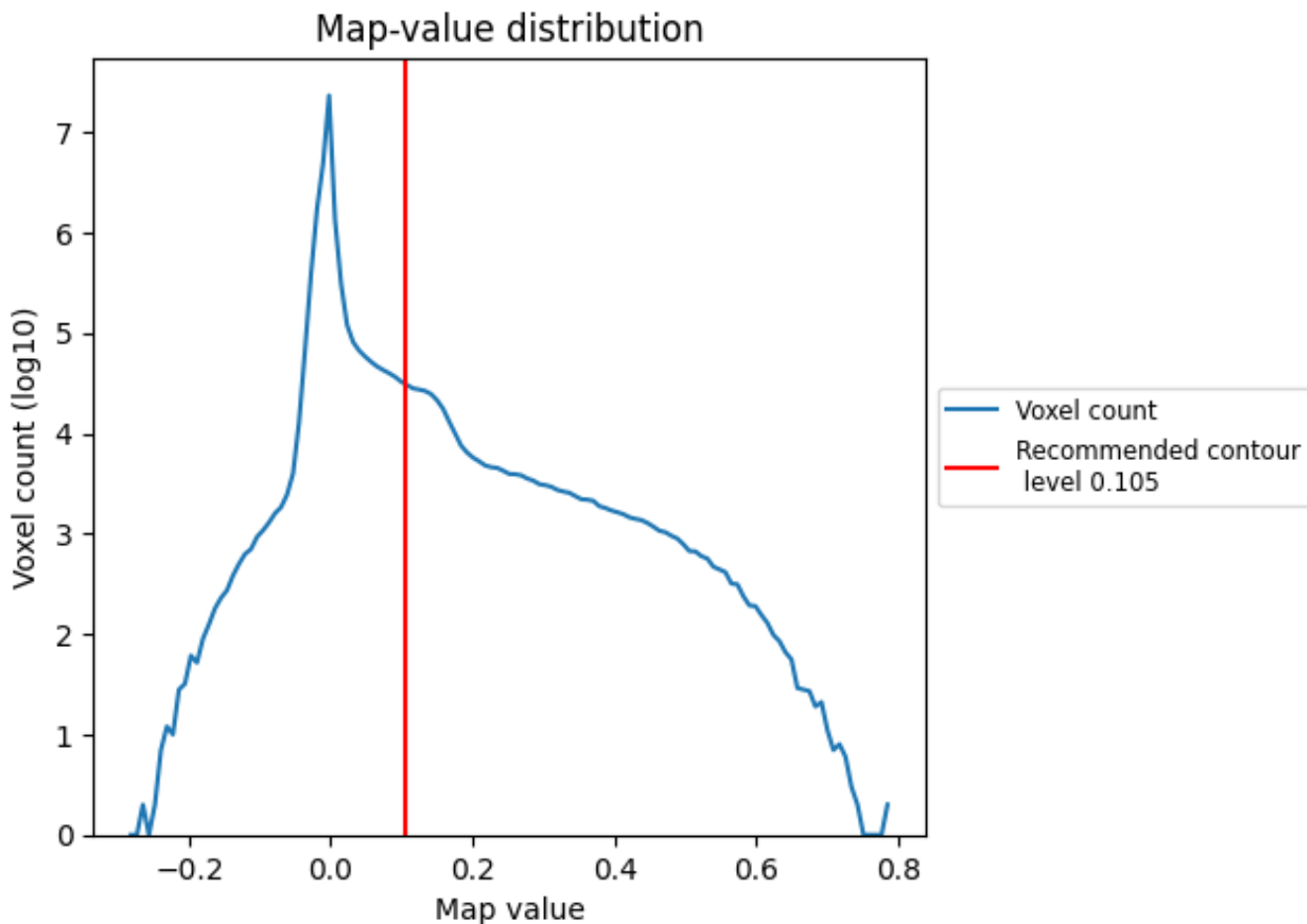


Z

7 Map analysis [i](#)

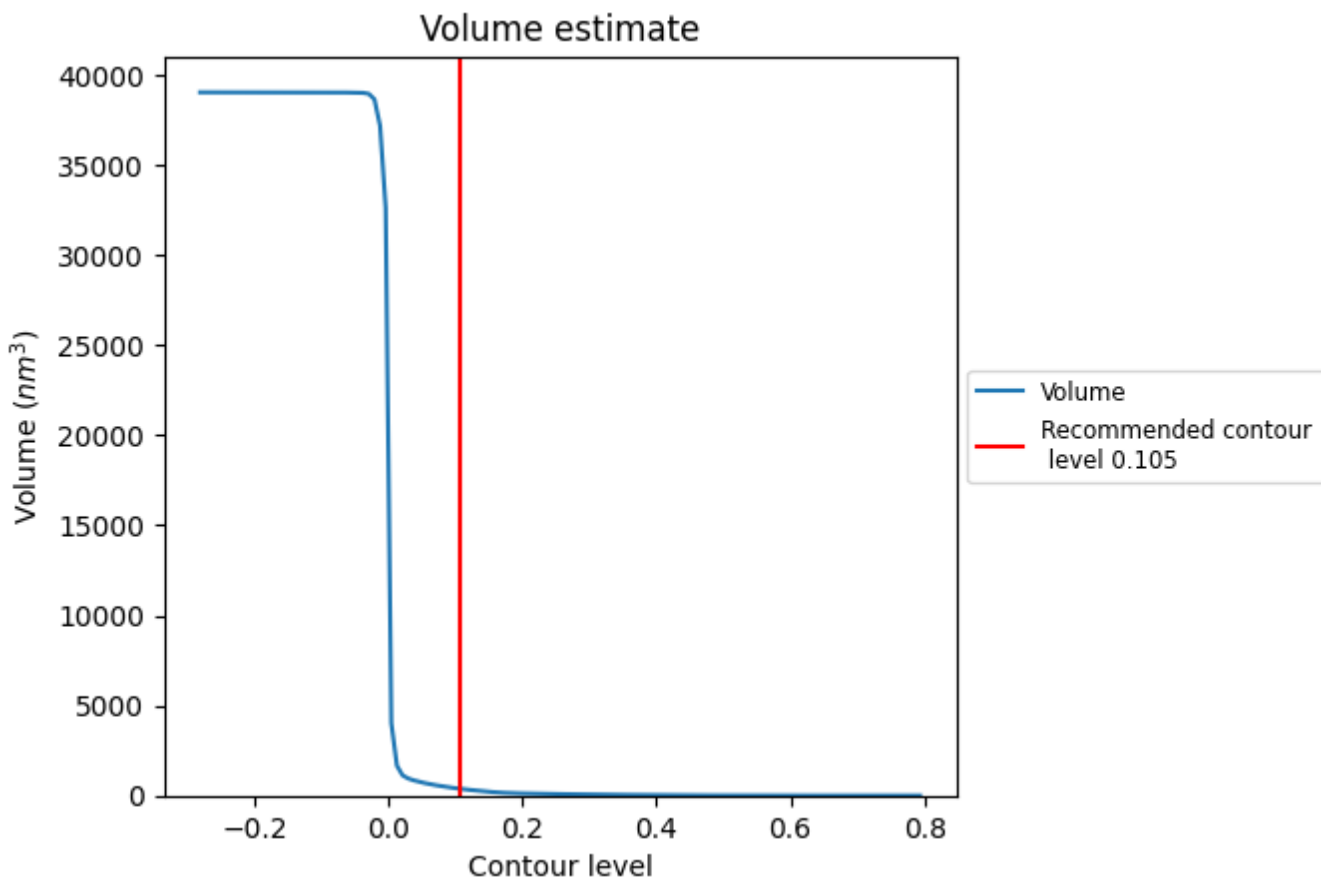
This section contains the results of statistical analysis of the map.

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.

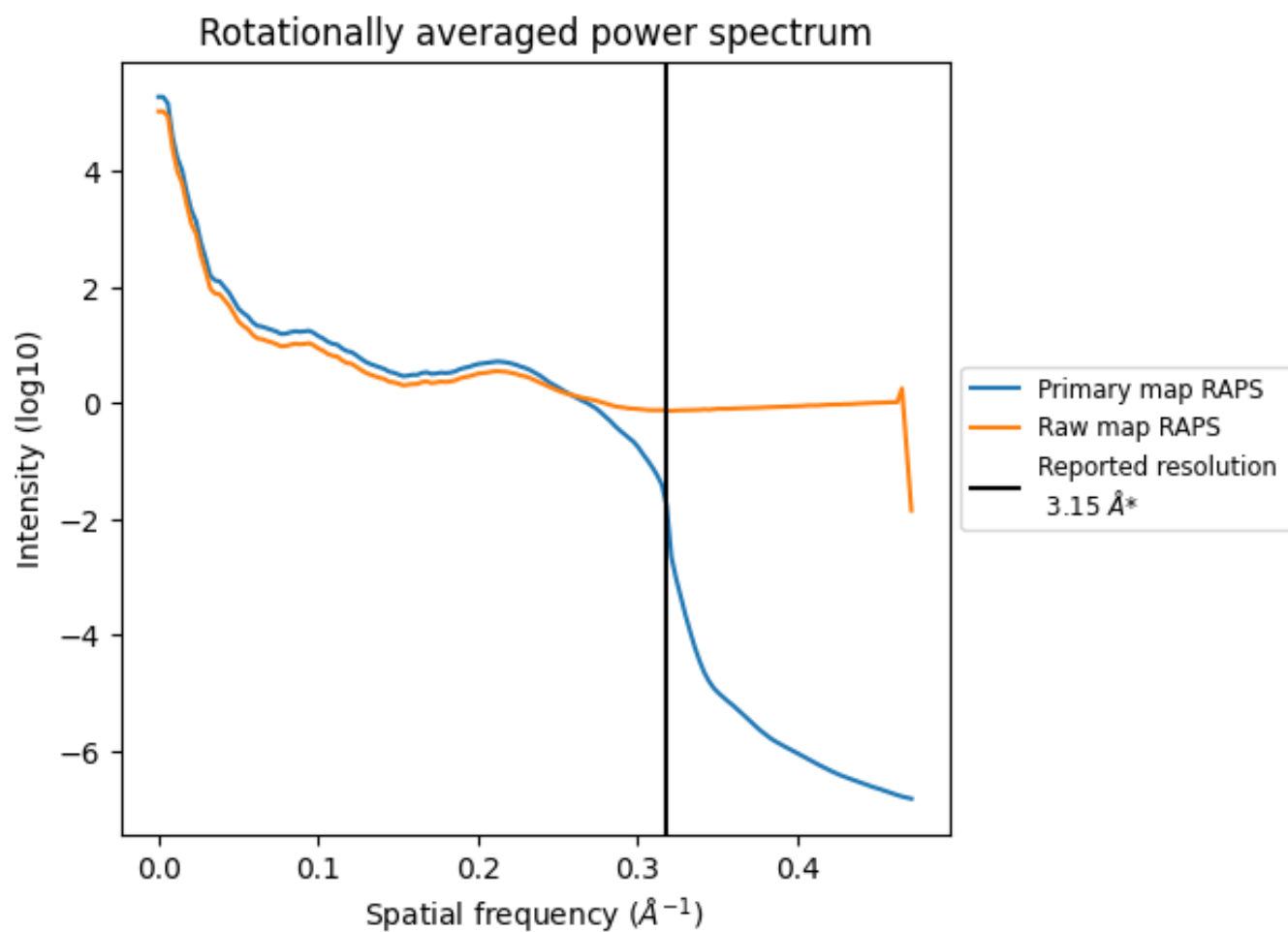
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 383 nm³; this corresponds to an approximate mass of 346 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

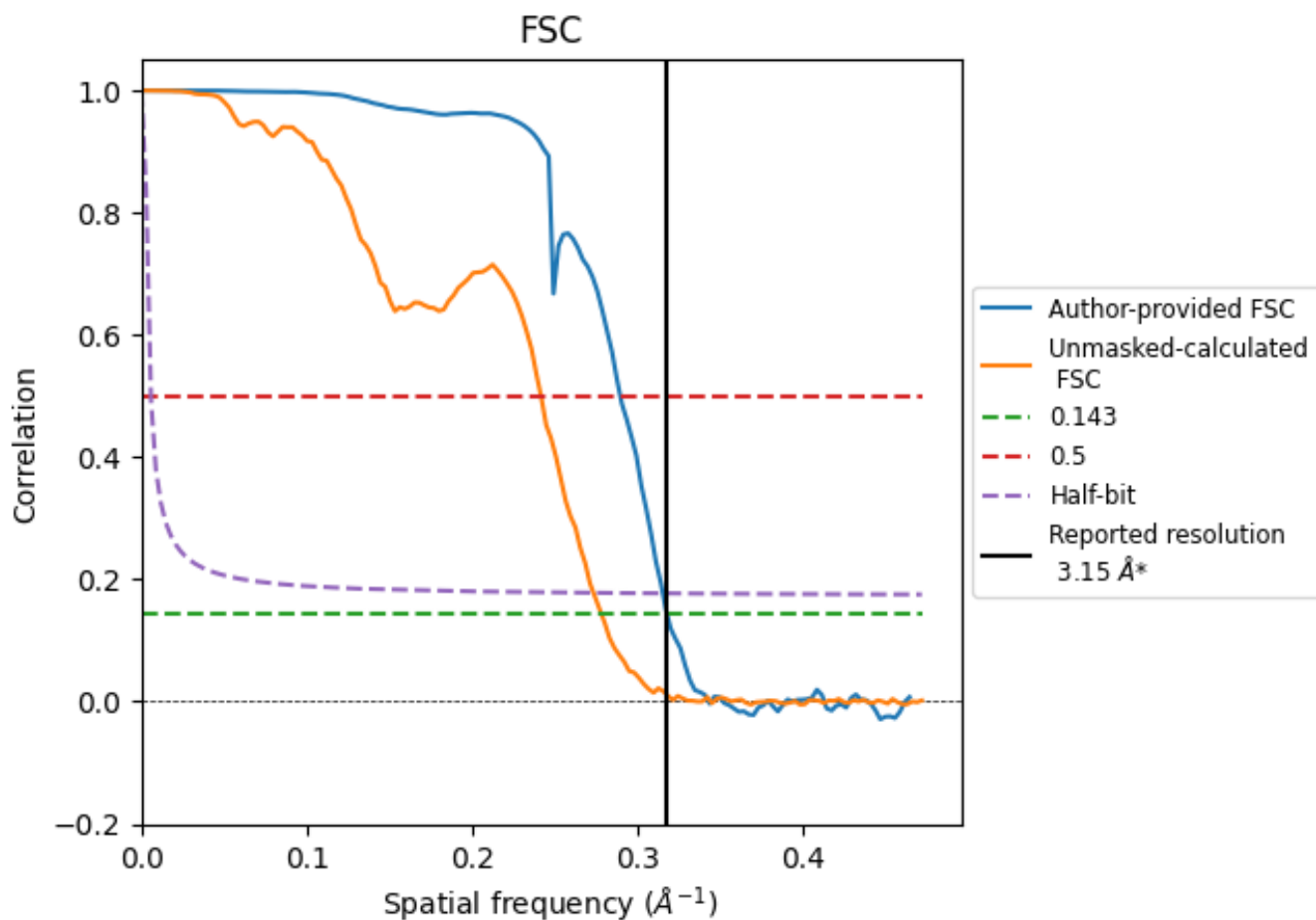


*Reported resolution corresponds to spatial frequency of 0.317 \AA^{-1}

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 0.317 Å⁻¹

8.2 Resolution estimates [i](#)

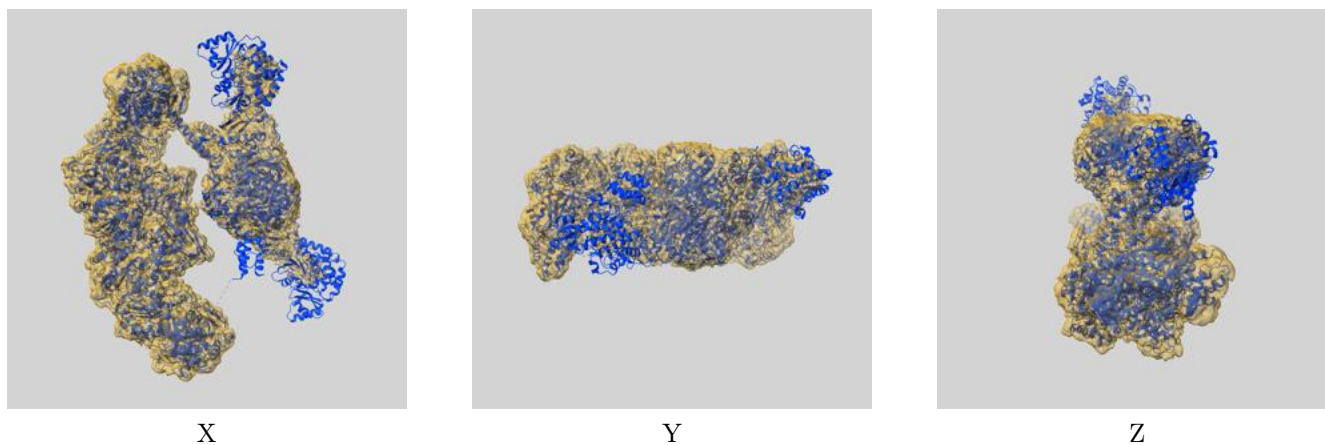
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.15	3.45	3.17
Unmasked-calculated*	3.60	4.14	3.66

*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 3.60 differs from the reported value 3.15 by more than 10 %

9 Map-model fit [i](#)

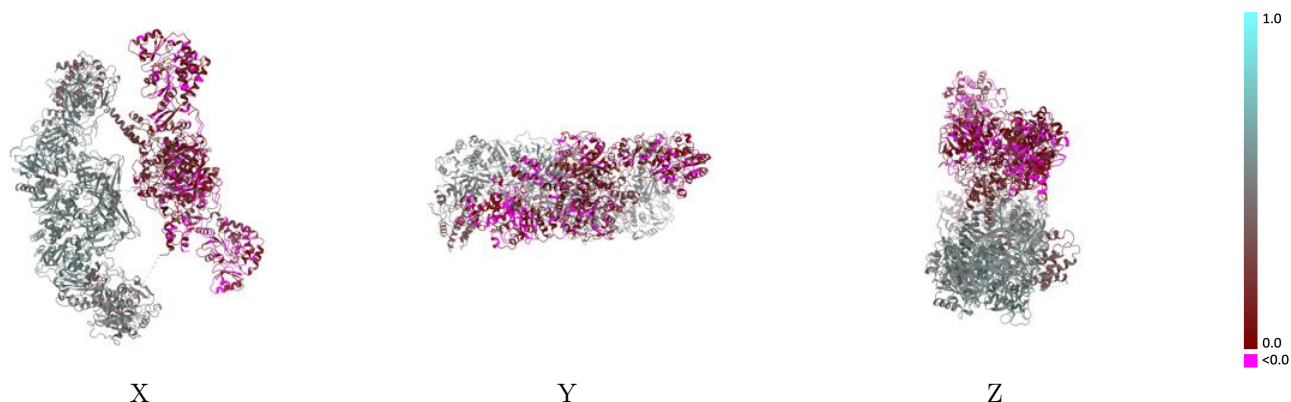
This section contains information regarding the fit between EMDB map EMD-45910 and PDB model 9CTL. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



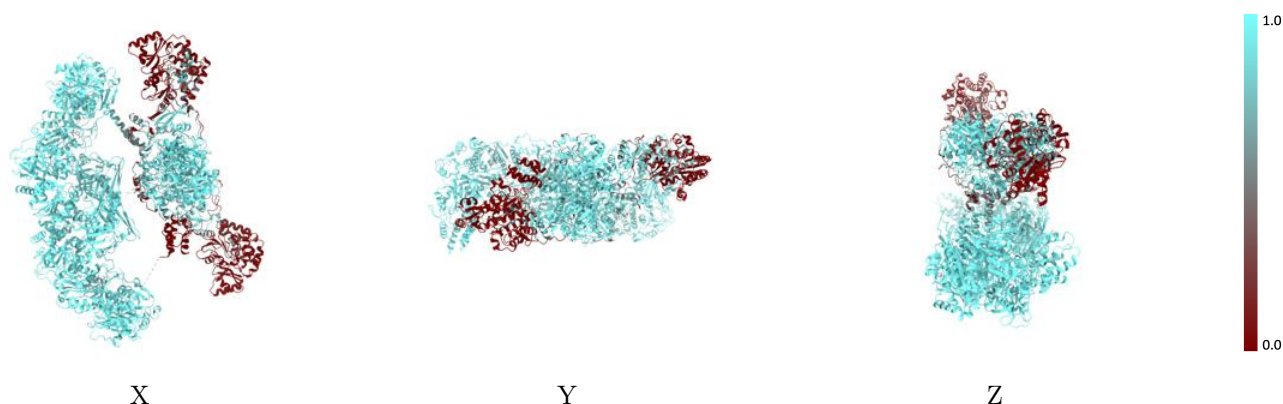
The images above show the 3D surface view of the map at the recommended contour level 0.105 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



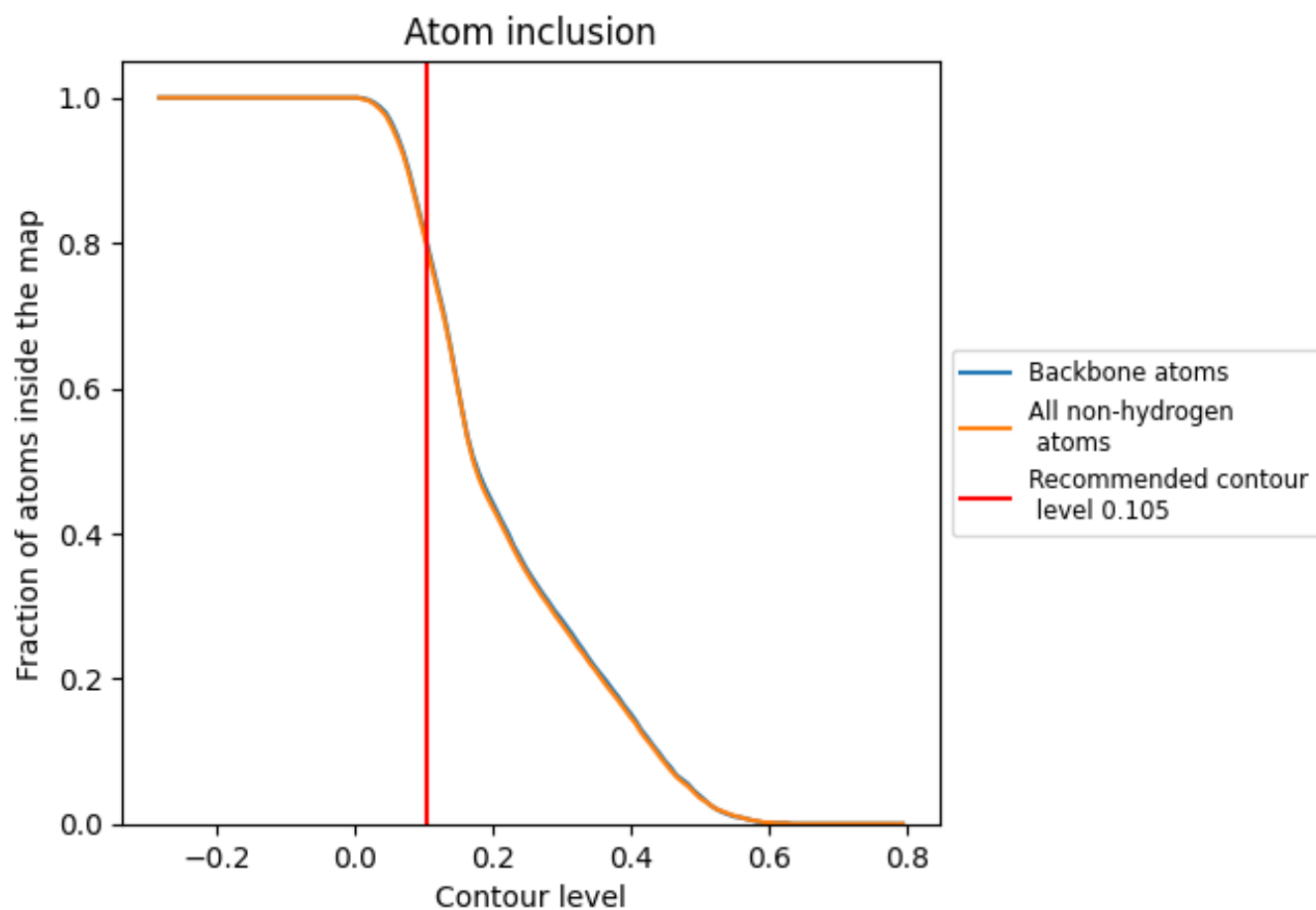
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.105).


9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.105) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7940	 0.3380
A	 0.8130	 0.3480
B	 0.7760	 0.3270

