



wwPDB EM Validation Summary Report ⓘ

Aug 19, 2026 – 04:31 pm BST

PDB ID : 9TU9 / pdb_00009tu9
EMDB ID : EMD-56253
Title : CryoEM structure of DruE:ATPgammaS:DNA from Druantia type III - dimer 2
Authors : Grass, L.M.; Himpich, S.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on : 2026-01-08
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

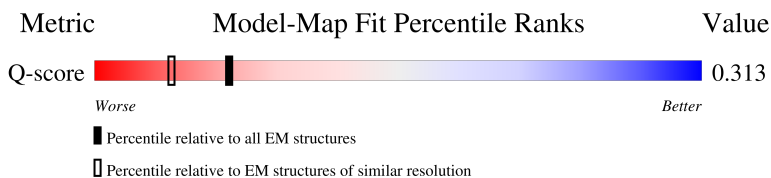
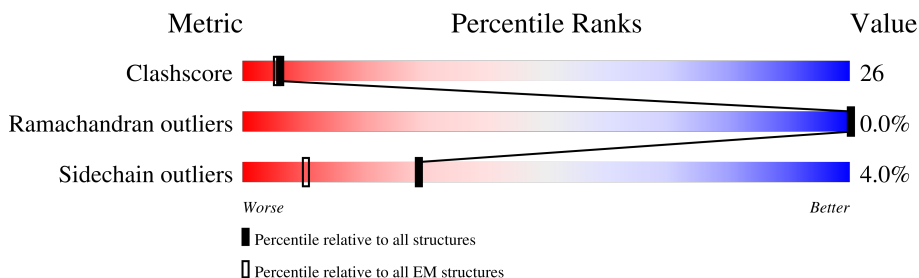
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

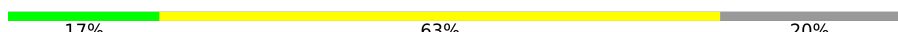
The reported resolution of this entry is 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Y	2108	
1	y	2108	
2	G	30	
3	I	30	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33663 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 DEAD/DEAH box helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	2075	Total	C	N	O	S	0	0
			16471	10380	2939	3080	72		
1	y	2050	Total	C	N	O	S	0	0
			16275	10265	2912	3026	72		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
Y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
Y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
Y	0	PHE	-	expression tag	UNP A0A4P8BDA5
y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
y	0	PHE	-	expression tag	UNP A0A4P8BDA5

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*AP*CP*CP*GP*TP*CP*GP*GP*AP*AP*GP*AP*GP*AP*CP*TP*AP*TP*CP*GP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	24	Total	C	N	O	P	0	0
			497	235	98	140	24		

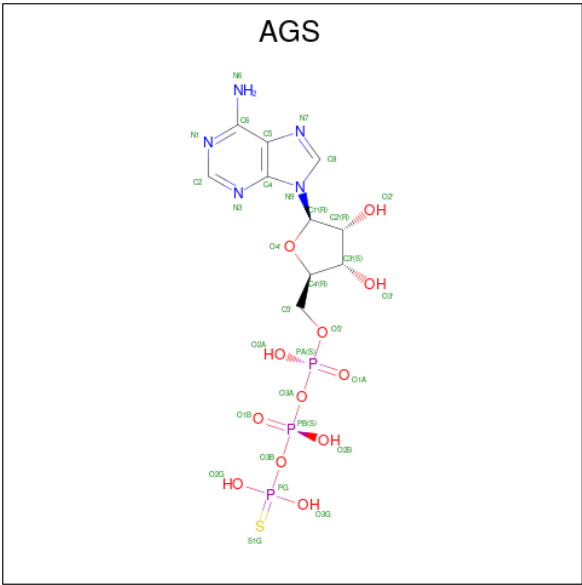
- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*TP*CP*GP*AP*TP*AP*GP*TP*CP*TP*CP*TP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	17	Total	C	N	O	P	0	0
			348	166	62	103	17		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	Y	5	Total	Zn	0
			5	5	
4	y	5	Total	Zn	0
			5	5	

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

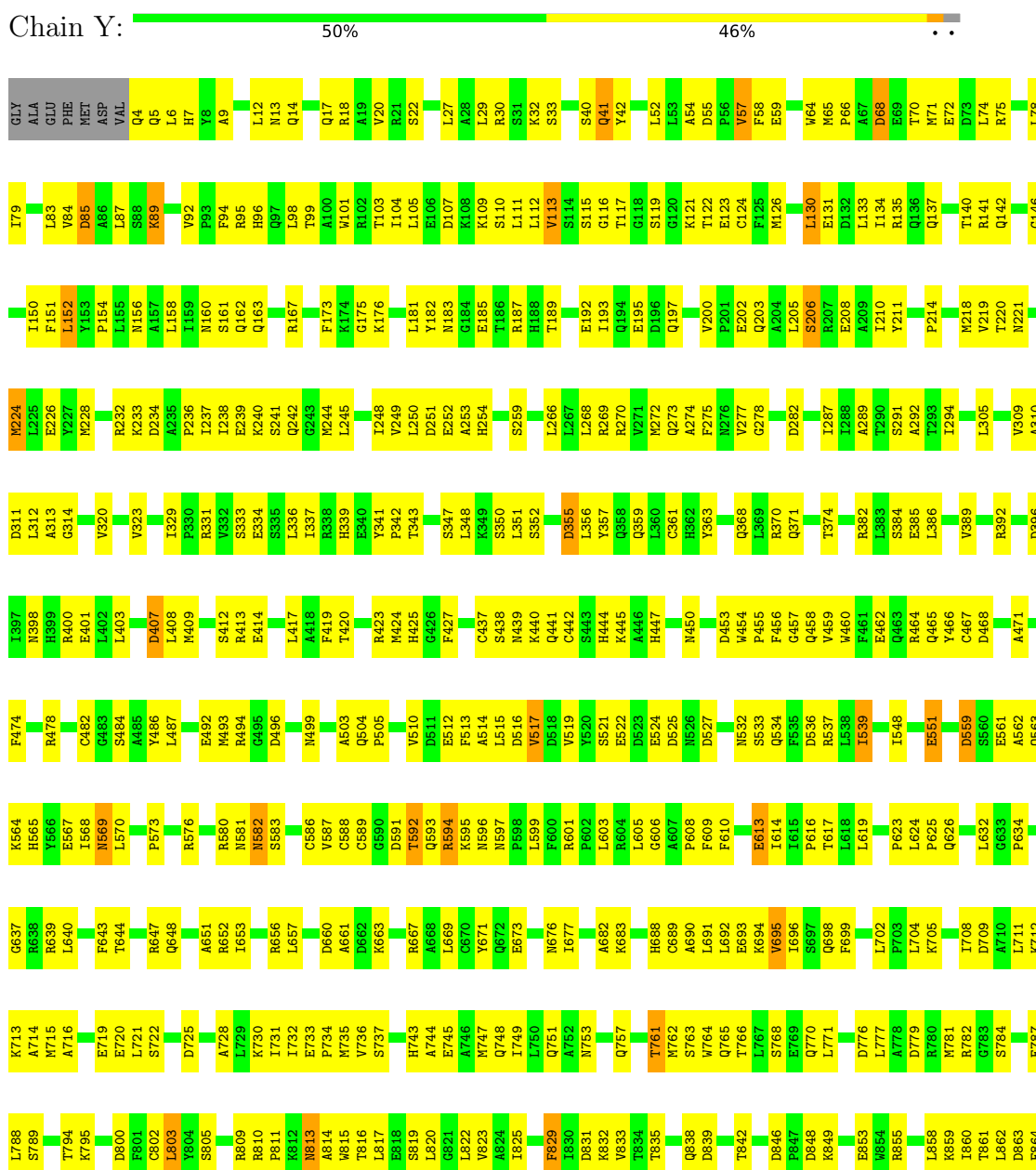


Mol	Chain	Residues	Atoms						AltConf
5	Y	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	y	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

3 Residue-property plots

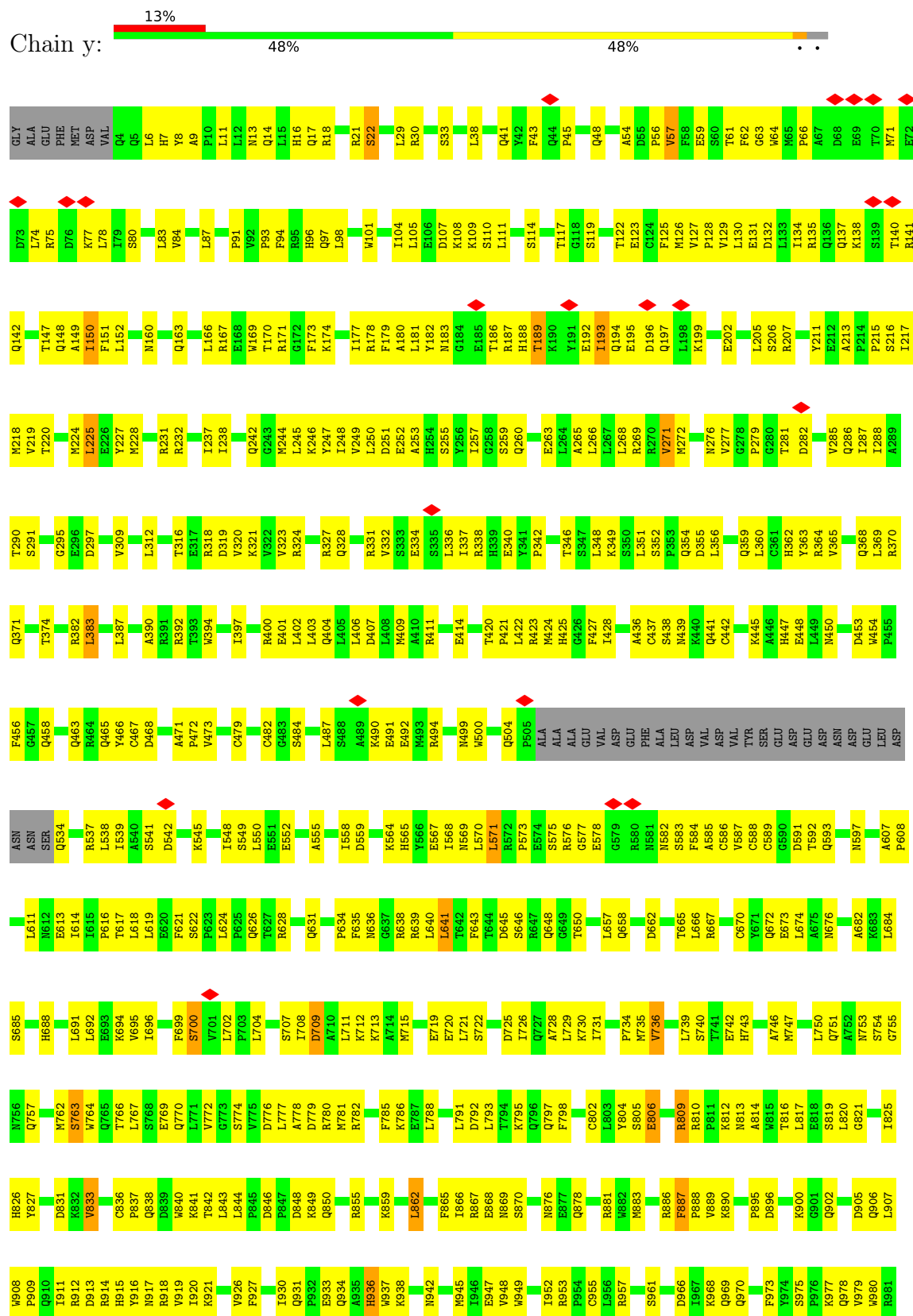
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

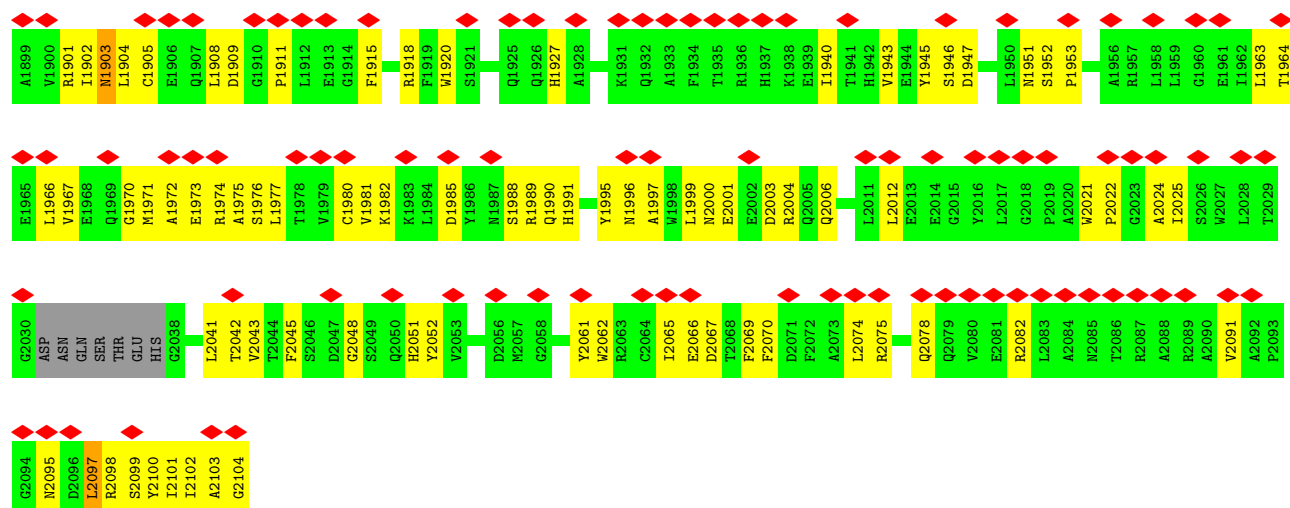




• Molecule 1: DEAD/DEAH box helicase

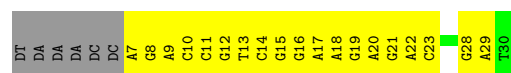


Q1827	S1757	F1672	I1602	T1541	A1468	M1400	Y1336	S1272	A1204	M1119	W1056	C982
L1828	L1758	C1681	R1603	P1542	S1473	L1401	L1337	Q1273	T1205	N1120	S1057	P983
N1829	V1759	M1543	D1604	E1543	S1473	G1402	T1338	L1274	K1206	N1121		
R1834	A1761	S1682	E1605	N1544	M1474	K1403	A1339	A1275	L1207	V1122		
W1835	G1762	D1682	A1607	L1545	P1475	V1404	D1340	I1276	P1207	P1123	S1060	R986
	P1763	K1682	R1608	K1546	P1475	L1405	E1343	L1277	S1208	P1124	D1061	R987
Q1838	Q1764	F1686	R1609	N1547	Q1476	L1406	E1341	L1278	G1209	A1125	E1062	A988
V1839	E1765	C1687	S1610	P1548	Q1477	A1406	L1342	E1279	K1210	P1126	L1063	L989
T1840	E1766	H1688	R1611	P1479	P1479	S1407	E1343	M1280			K1066	Y991
R1841	W1767	H1689	A1612	R1550	W1480	G1408	K1344	L1129	A1127	L1130	W1069	T992
E1842	P1767	C1690	V1613	E1551	L1481	Q1409	R1346	I1281	A1133			Y996
	Q1771	G1693	L1615	E1552	D1482	E1410	E1346	E1282				Y999
Q1844	W1772	L1692	L1615	E1553	P1483	E1410	A1347	A1283				L1000
S1845	P1773	S1693	R1616	T1553	R1484	L1411	A1347	L1284				P1001
	L1774	Y1694	E1617	H1554	Y1485	S1412	I1348	L1284				G1002
W1848	F1775		K1622	Y1555	Y1485	G1413	K1349	A1286				S1003
	Q1776	Q1697	L1556	L1557	Y1487	D1414	A1350	A1286				E1004
D1851	E1777	H1698	L1557	R1558	P1488	H1415	T1351	D1287				K1004
D1852	L1778	Y1699	I1625	G1559	S1489	I1416	ALA	E1287				E1005
T1855	L1779	V1700	E1629	G1560	S1489	I1417	ASP	A1290				K1006
	Q1780	R1702	L1630	S1561	V1493	P1418	PRO	W1291				T1006
P1858	F1781	L1703	G1631	S1561	W1419	W1419	ASN	E1292				A1007
G1859	S1783	D1704	V1632	D1497	F1420	F1420	GLU	E1292				P1008
	S1784	R1705	T1633	M1562	W1421	H1422	GLY	P1294				
E1860		H1706	T1634	R1564	L1500		GLY	T1294				
	V1768	H1707	R1638	Q1565	G1501	G1427	GLU	P1295				
G1863	E1769	D1639	D1639	S1567	R1502	A1428	SER	A1296				L1013
Q1864	L1790	I1641	I1641	N1568	E1510	G1429	PHE	A1296				L1014
	L1791	L1711	N1640	K1569	E1510	A1430	ARG	A1299				E1015
S1868	V1792	L1717	G1642	S1567	S1506	T1431	ARG	A1299				M1016
P1869	A1793		Y1643	C1571	F1512	T1433	ILE	A1299				P1017
V1870		L1722	T1644	H1572	H1512	T1433	GLU	A1299				F1086
	L1796	Y1726	G1645	H1572	H1512	T1433	GLU	A1299				E1087
L1872	A1797		Y1646	G1573	H1513	V1437	K1368	A1299				L1018
	N1798		S1647	H1574	E1516	E1438	R1372	A1299				L1019
G1875	L1799	F1729	S1647	H1574	E1516	E1438	R1372	A1299				L1019
	T1800	G1730	I1648	V1575	G1517	C1439	D1373	A1299				P1020
		D1731	F1649	H1576	G1517	S1440	L1374	A1299				F1091
Q1876	G1732	G1730	F1649	K1577	E1518	H1441	P1376	A1299				R1022
L1879	S1803	S1733	D1652	D1578	F1519	H1441	T1375	A1299				H1023
H1880	Q1804	R1734	L1579	W1580	G1520	A1444	T1376	A1299				W1024
F1881	Q1806	V1735	L1581	L1581	G1521	D1445	A1377	A1299				R1025
S1882	L1807	E1736	A1655	G1582	Y1523	Q1447	A1377	A1299				
G1883	S1808	T1737	A1655	Y1583	A1524	Q1448	A1377	A1299				
	A1809	N1738	A1658	S1584	T1525	L1449	A1377	A1299				
Q1884	L1810	P1739	G1859	S1585	G1526	D1450	A1377	A1299				
L1886		L1740	Y1660	R1586	L1527	Q1447	A1377	A1299				
S1887	P1814	L1742	A1661	T1587	S1528	K1451	A1377	A1299				
	R1817	A1745	Q1663	R1588	G1529	V1454	A1377	A1299				
E1889	V1820		L1664	M1589	G1530	Y1454	A1377	A1299				
D1890	L1821		I1665	V1590	R1531		A1377	A1299				
L1891	S1822		W1668	E1591	A1532		A1377	A1299				
L1892	T1823		A1669	Q1593	Q1535		A1377	A1299				
P1893	A1824		L1594	L1594	T1536		A1377	A1299				
A1894	T1825		D1670	N1595	Q1537		A1377	A1299				
	A1826		V1671	D1596	P1538		A1377	A1299				
L1895				D1597	Q1539		A1377	A1299				
P1896				N1598	R1540		A1377	A1299				
T1897				G1599			A1377	A1299				
G1898							A1377	A1299				



- Molecule 2: DNA (5'-D(P*AP*GP*AP*CP*CP*GP*TP*CP*GP*GP*AP*AP*GP*AP*GP*A P*CP*TP*AP*TP*CP*GP*AP*T)-3')

Chain G: 17% 63% 20%



- Molecule 3: DNA (5'-D(P*AP*TP*CP*GP*AP*TP*AP*GP*TP*CP*TP*CP*TP*AP*GP*G P*C)-3')

Chain I: 13% 43% 43%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27507	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.374	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1093334, 1.1093334, 1.1093334	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, AGS

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	Y	0.33	0/16840	0.42	0/22830
1	y	0.17	0/16641	0.35	0/22555
2	G	0.29	0/559	0.45	0/861
3	I	0.25	0/389	0.41	0/598
All	All	0.26	0/34429	0.39	0/46844

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	Y	16471	0	16231	822	0
1	y	16275	0	16083	867	0
2	G	497	0	269	39	0
3	I	348	0	193	23	0
4	Y	5	0	0	0	0
4	y	5	0	0	0	0
5	Y	31	0	12	6	0
5	y	31	0	12	3	0
All	All	33663	0	32800	1721	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 26.

The worst 5 of 1721 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:Y:1529:CYS:SG	1:Y:1554:HIS:CD2	2.49	1.05
1:y:1622:LYS:HZ3	1:y:1671:VAL:HA	1.29	0.96
2:G:21:DG:N2	3:I:10:DC:O2	2.00	0.92
1:Y:65:MET:HE3	1:Y:66:PRO:HD2	1.51	0.92
2:G:21:DG:N1	3:I:10:DC:N3	2.19	0.90

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	Y	2069/2108 (98%)	1919 (93%)	149 (7%)	1 (0%)	100	100
1	y	2042/2108 (97%)	1934 (95%)	108 (5%)	0	100	100
All	All	4111/4216 (98%)	3853 (94%)	257 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	1208	SER

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	Y	1768/1795 (98%)	1683 (95%)	85 (5%)	23	50
1	y	1746/1795 (97%)	1691 (97%)	55 (3%)	34	58
All	All	3514/3590 (98%)	3374 (96%)	140 (4%)	29	54

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	y	1169	THR
1	y	1251	THR
1	y	1574	HIS
1	Y	1201	VAL
1	Y	1153	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	y	1083	GLN
1	y	1688	HIS
1	y	1128	ASN
1	y	1576	HIS
1	y	1805	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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	AGS	Y	2206	-	29,33,33	0.46	0	39,52,52	0.75	1 (2%)
5	AGS	y	2206	-	29,33,33	0.47	1 (3%)	39,52,52	0.75	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AGS	Y	2206	-	-	6/21/38/38	0/3/3/3
5	AGS	y	2206	-	-	7/21/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	y	2206	AGS	PG-S1G	2.09	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	2206	AGS	PA-O3A-PB	-3.90	119.45	132.83
5	y	2206	AGS	PA-O3A-PB	-3.76	119.93	132.83

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

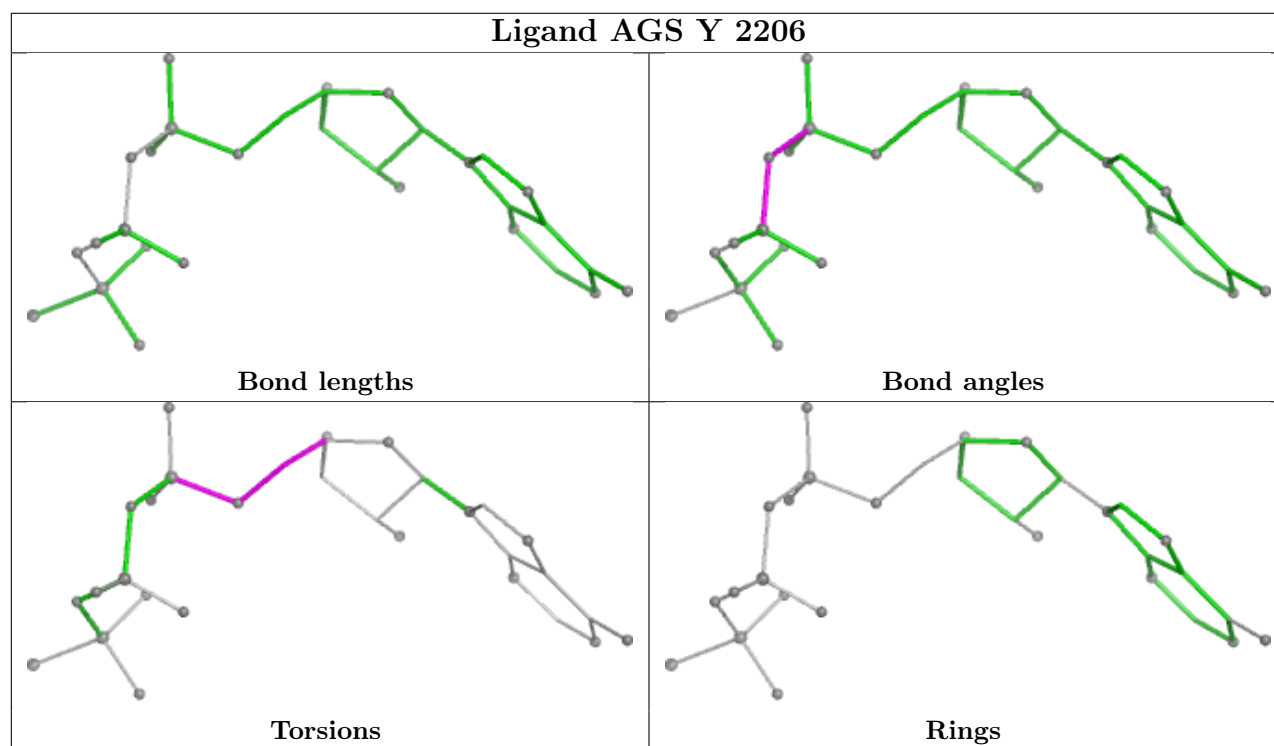
Mol	Chain	Res	Type	Atoms
5	Y	2206	AGS	C5'-O5'-PA-O2A
5	y	2206	AGS	PB-O3B-PG-O2G
5	y	2206	AGS	PB-O3B-PG-O3G
5	Y	2206	AGS	O4'-C4'-C5'-O5'
5	y	2206	AGS	O4'-C4'-C5'-O5'

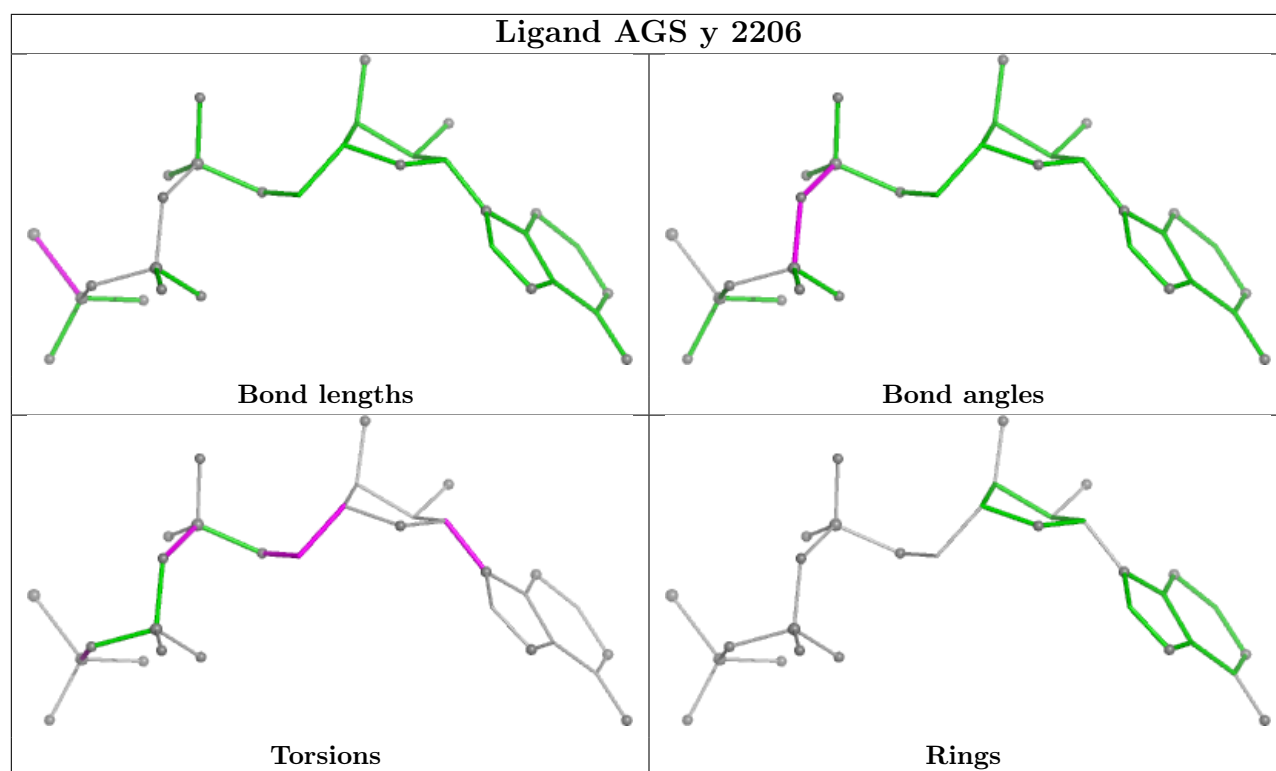
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	2206	AGS	6	0
5	y	2206	AGS	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.

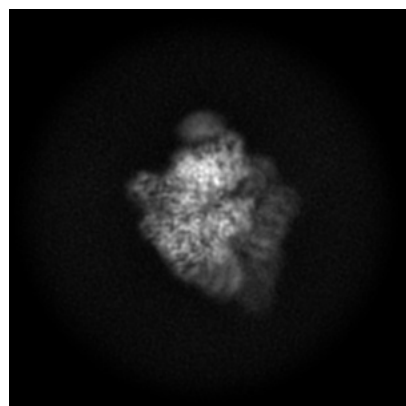
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56253. These allow visual inspection of the internal detail of the map and identification of artifacts.

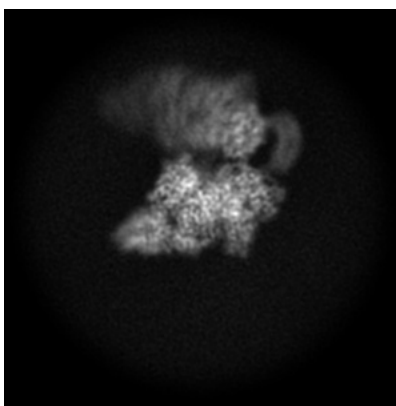
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

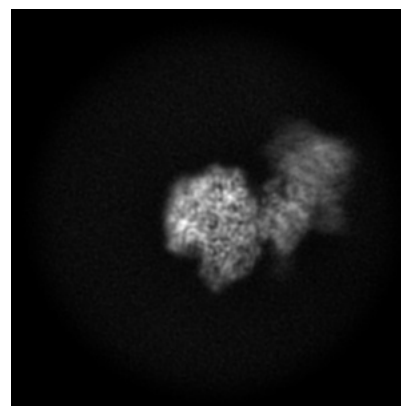
6.1.1 Primary map



X

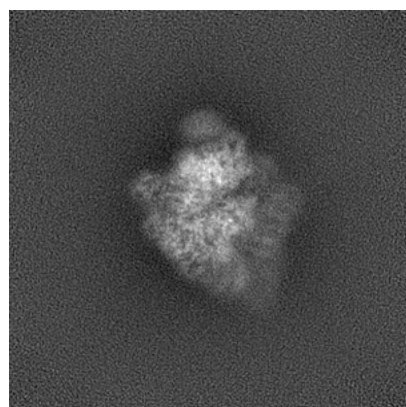


Y

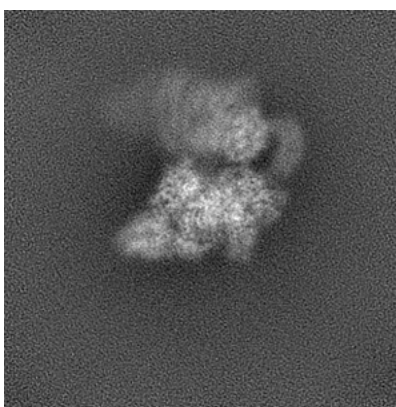


Z

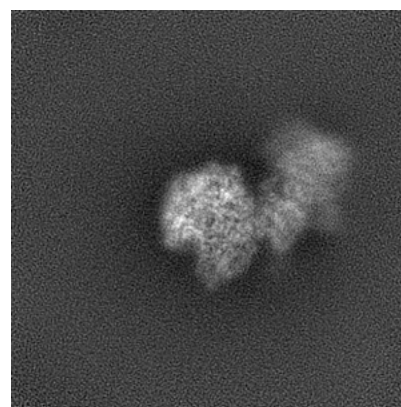
6.1.2 Raw map



X



Y

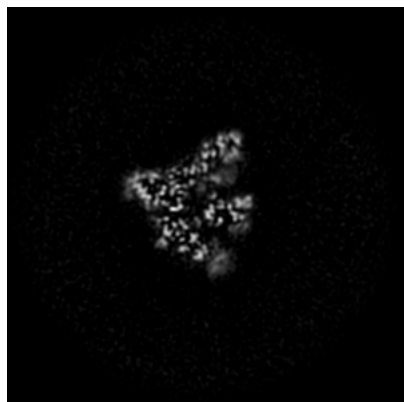


Z

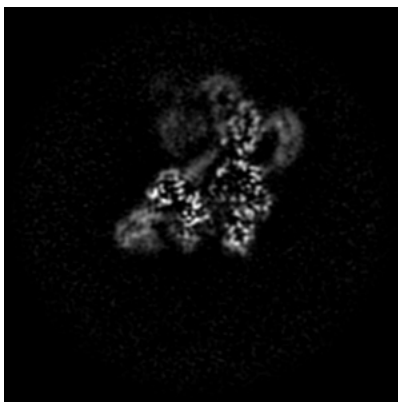
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

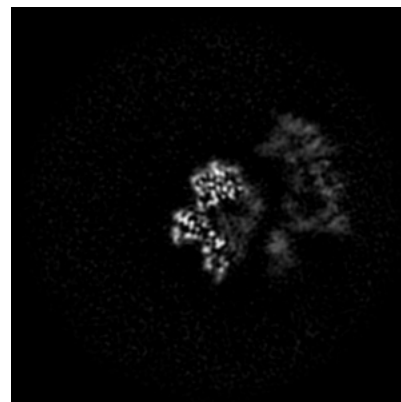
6.2.1 Primary map



X Index: 144

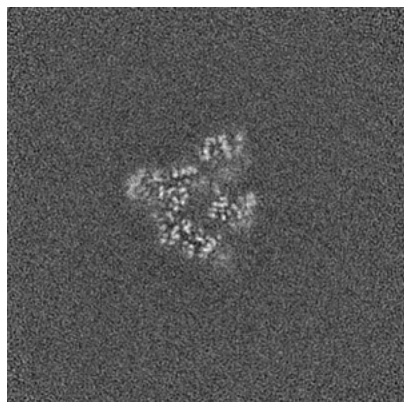


Y Index: 144

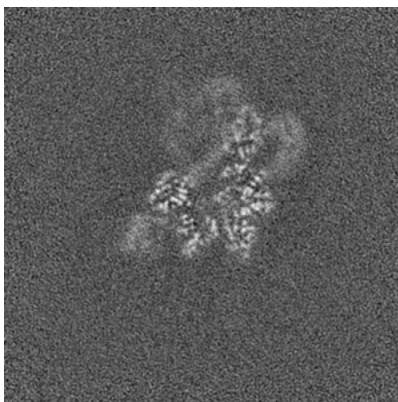


Z Index: 144

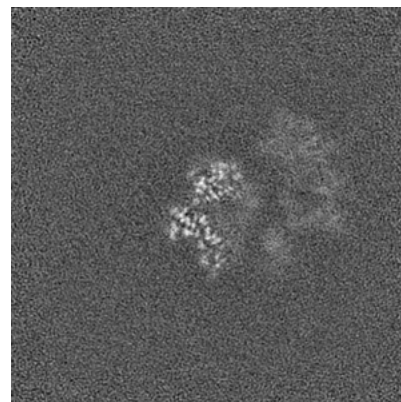
6.2.2 Raw map



X Index: 144



Y Index: 144

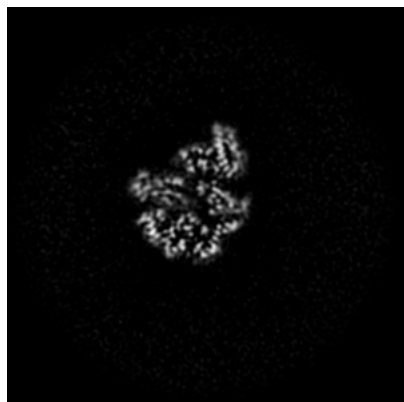


Z Index: 144

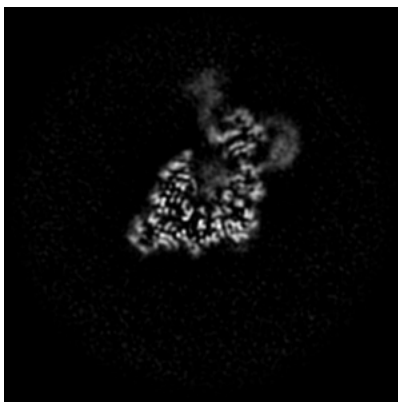
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

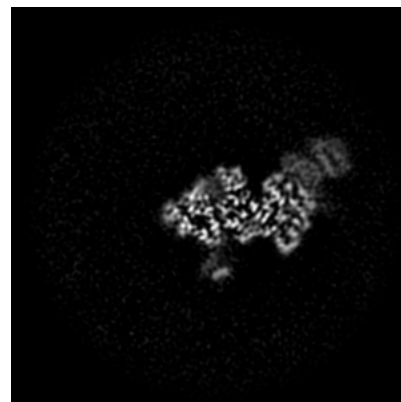
6.3.1 Primary map



X Index: 157

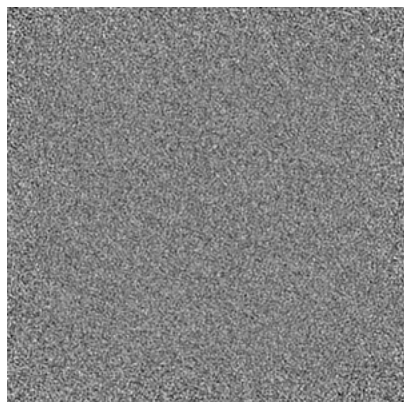


Y Index: 129

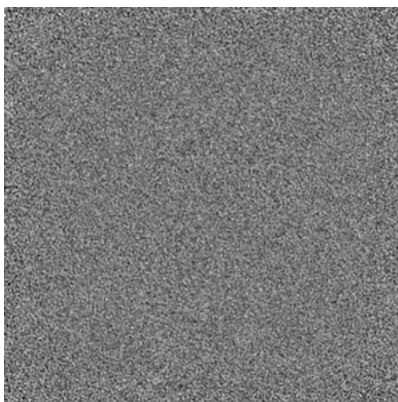


Z Index: 170

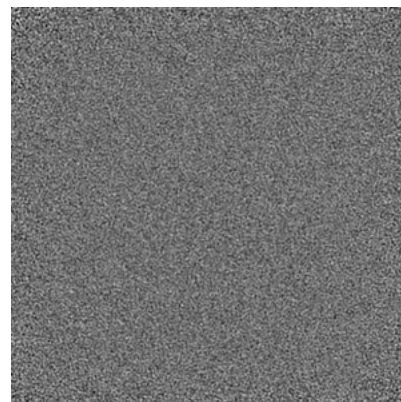
6.3.2 Raw map



X Index: 0



Y Index: 0

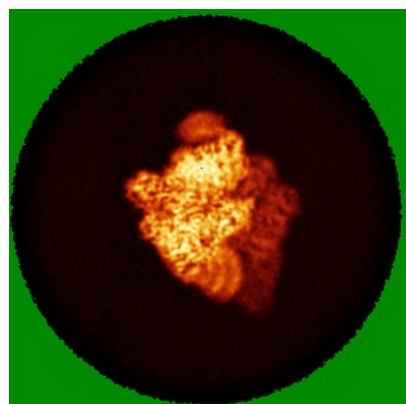


Z Index: 0

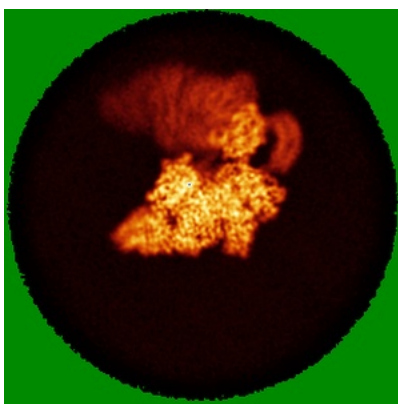
The images above show the largest variance slices of the map in three orthogonal directions.

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

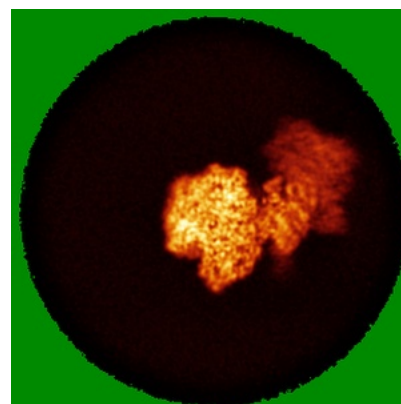
6.4.1 Primary map



X

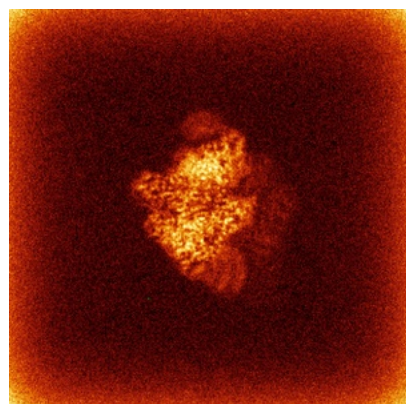


Y

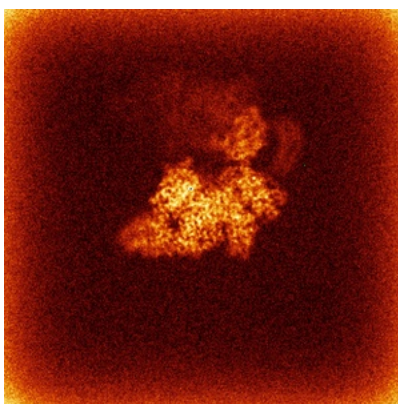


Z

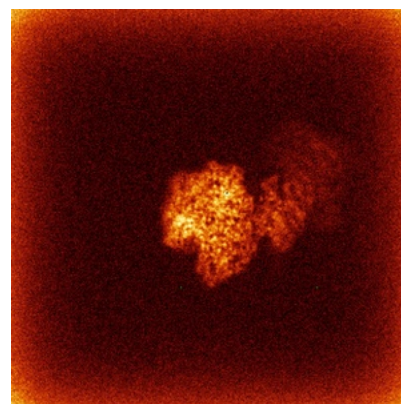
6.4.2 Raw map



X



Y

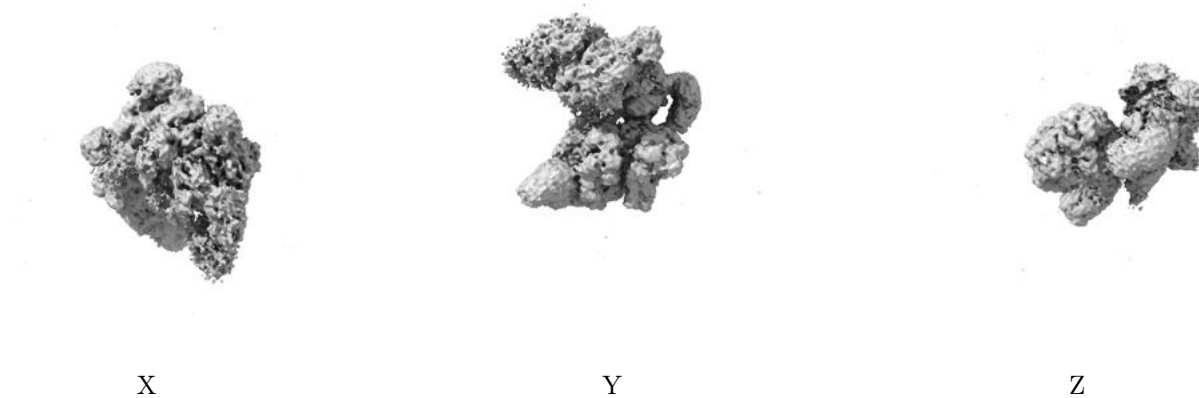


Z

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.

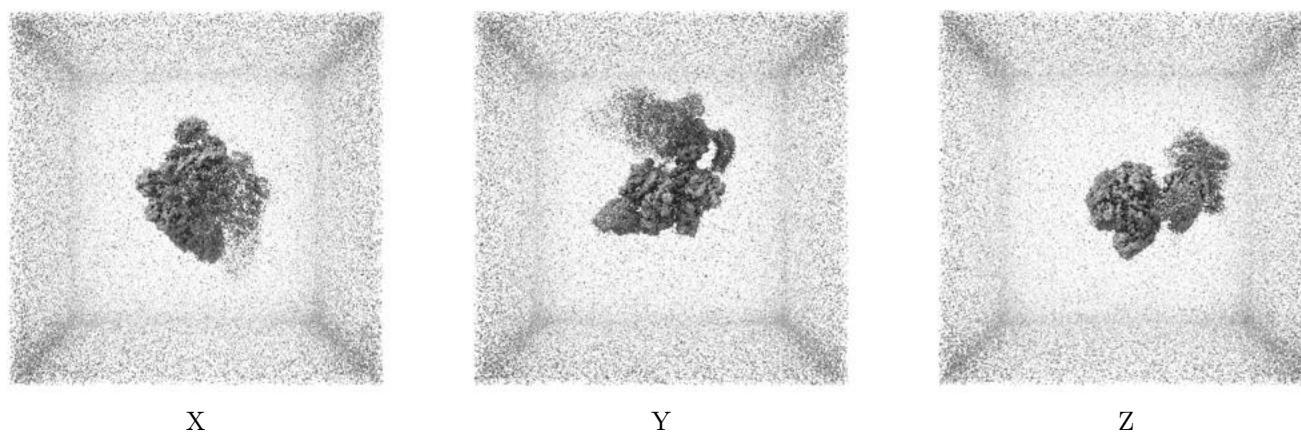
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

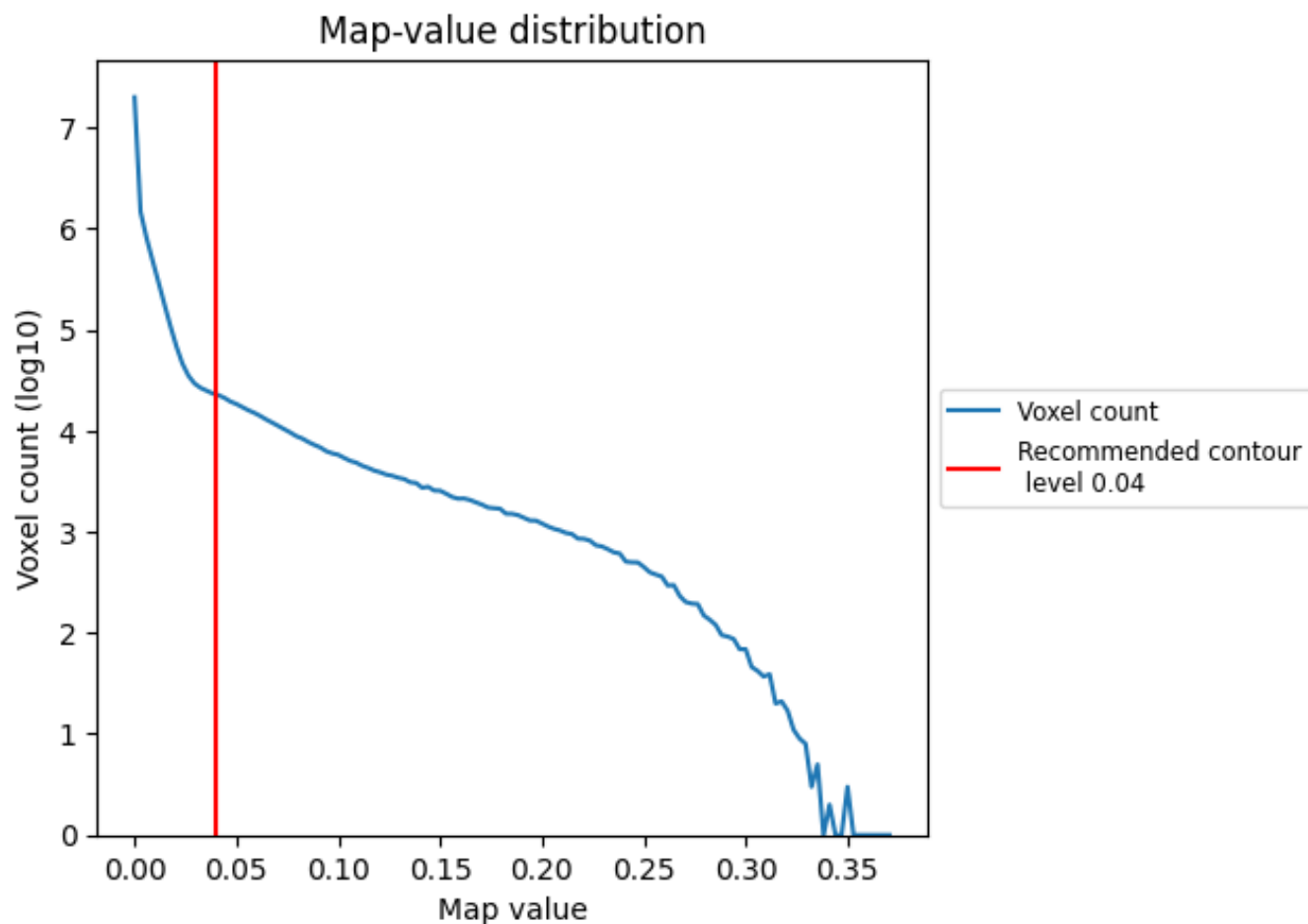
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

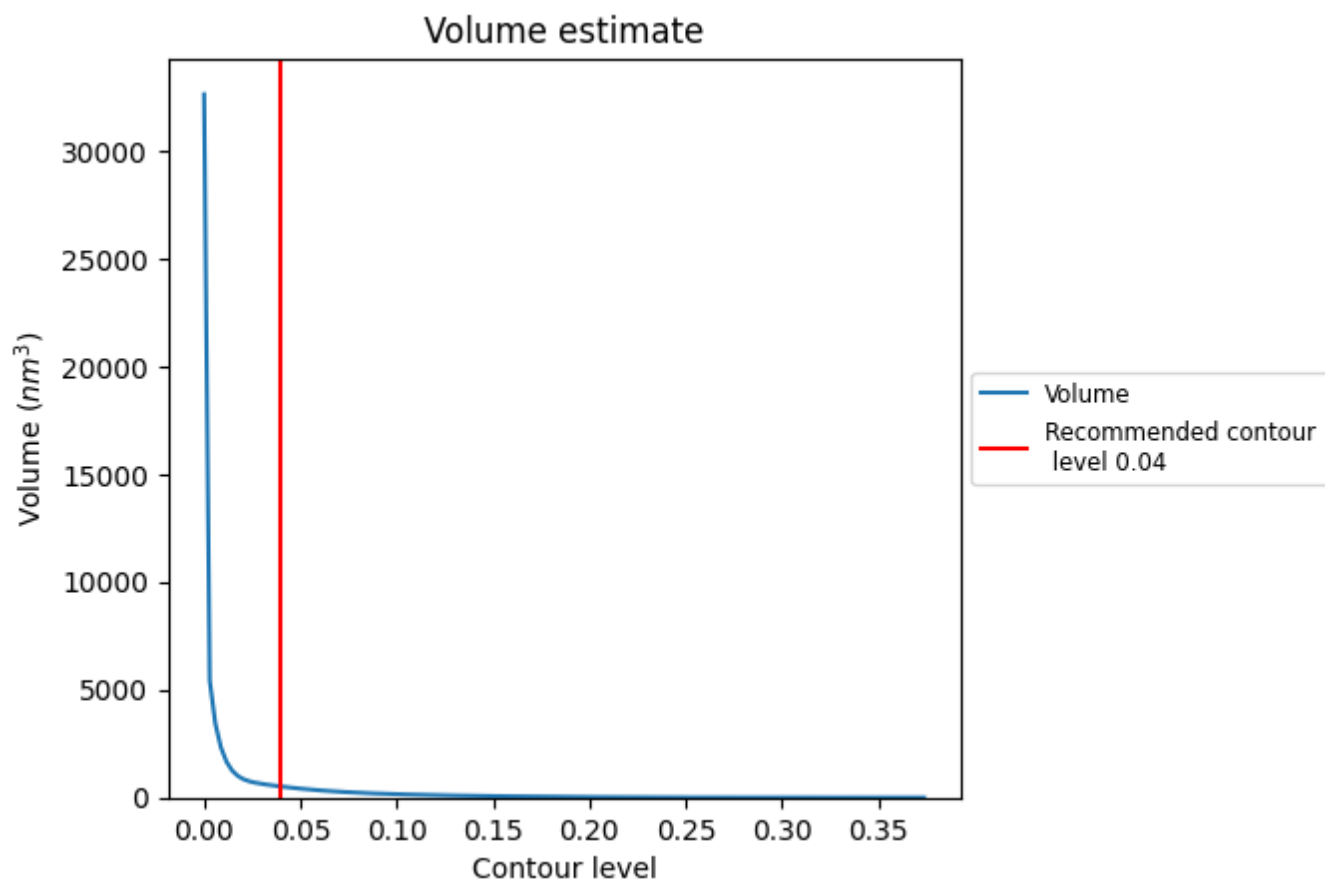
This section contains the results of statistical analysis of the map.

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.

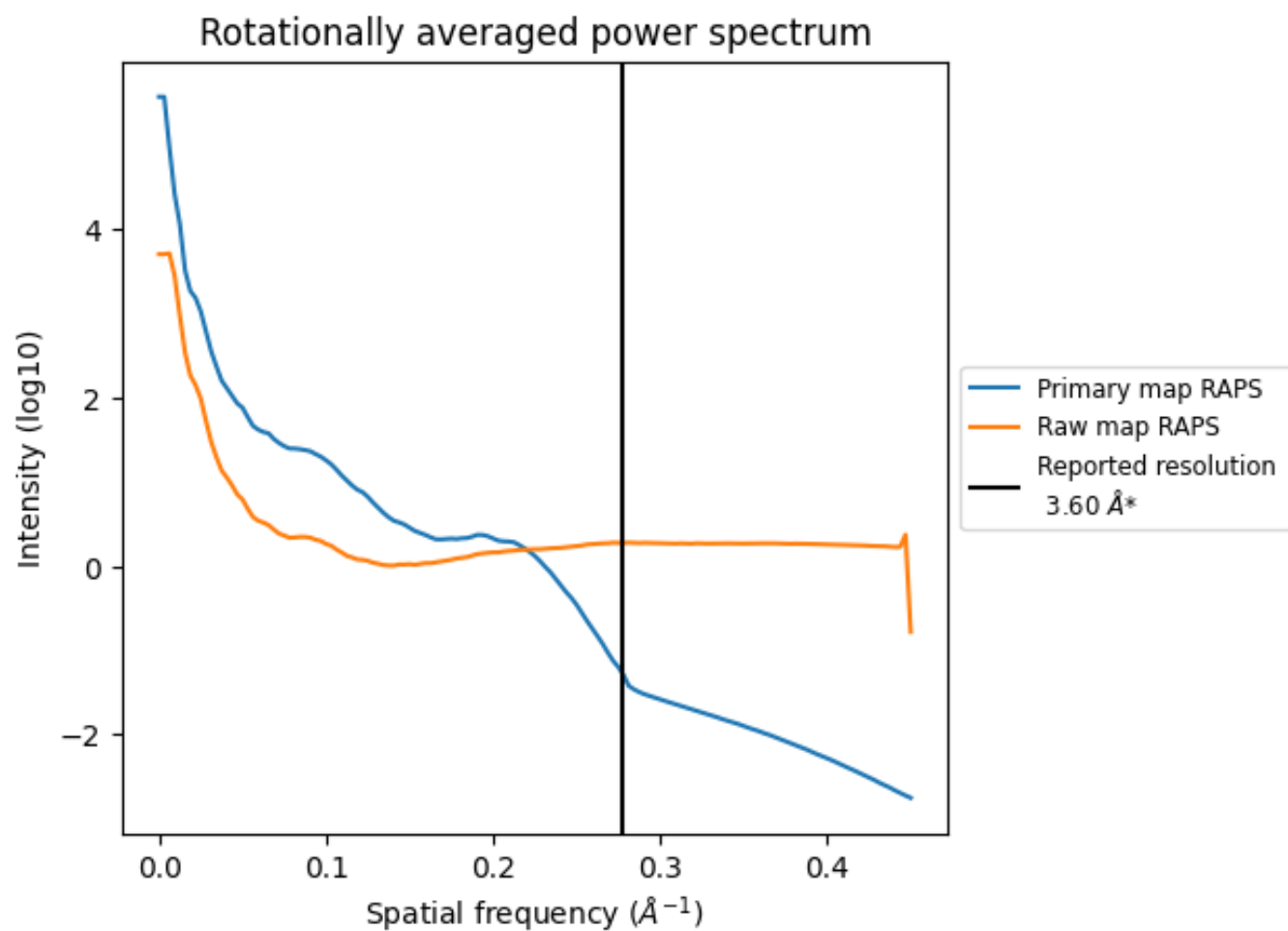
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 512 nm³; this corresponds to an approximate mass of 463 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

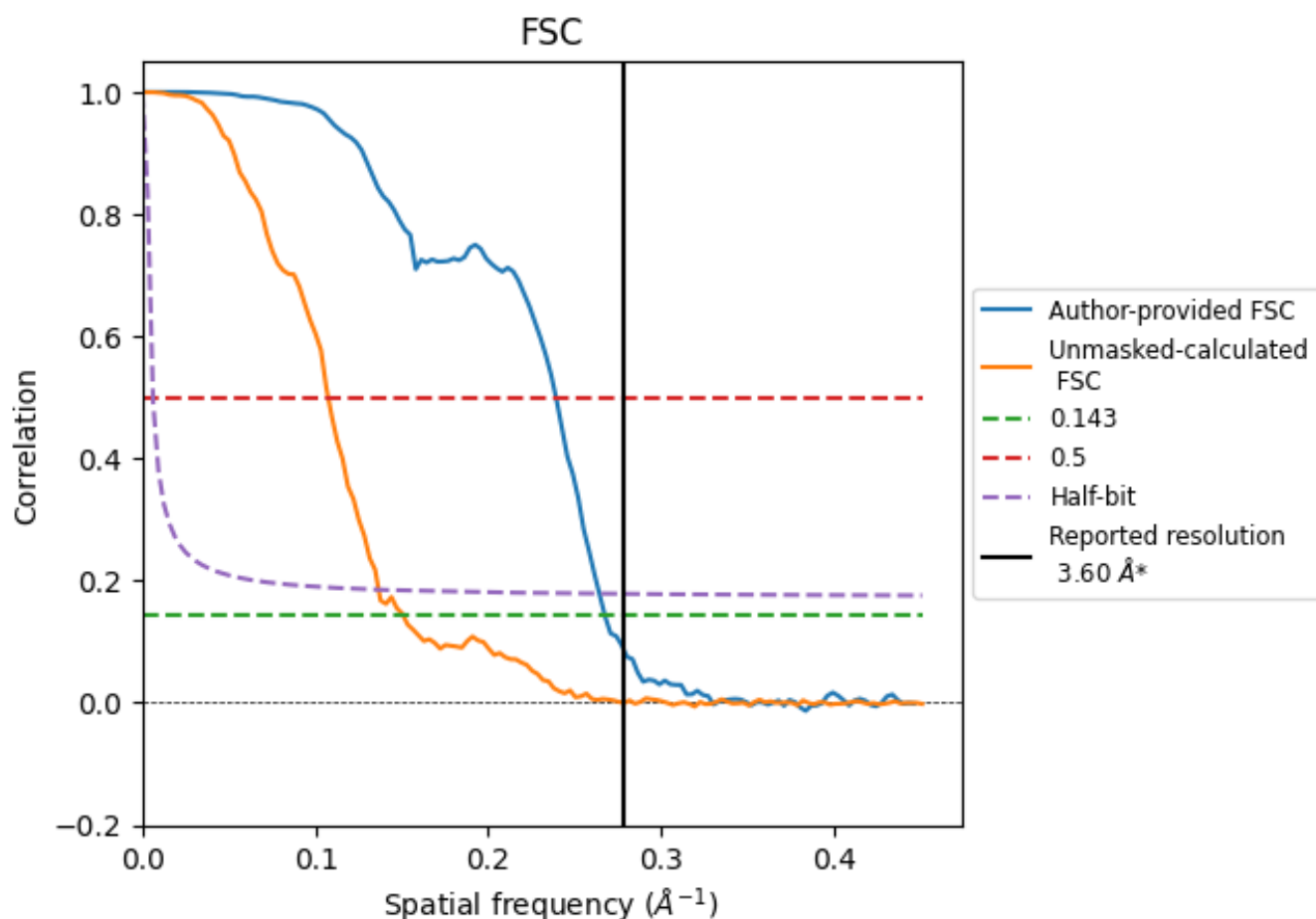


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

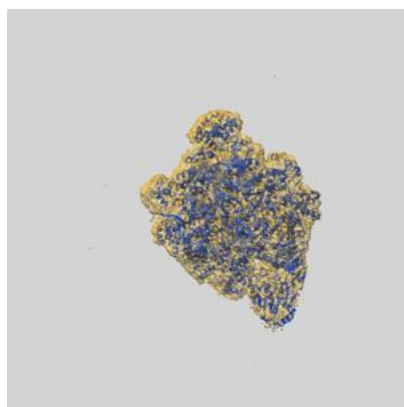
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.74	4.18	3.79
Unmasked-calculated*	6.63	9.31	7.32

*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 6.63 differs from the reported value 3.6 by more than 10 %

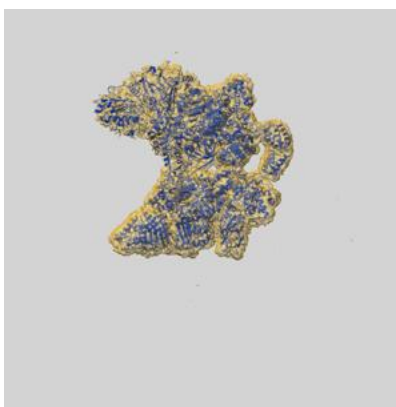
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56253 and PDB model 9TU9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

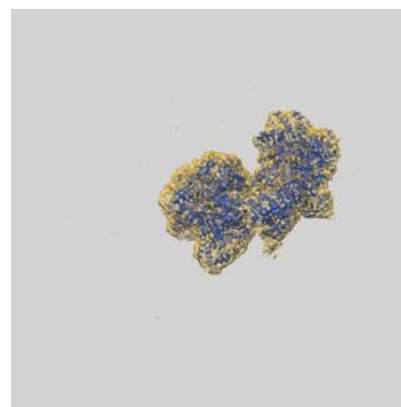
9.1 Map-model overlay [i](#)



X



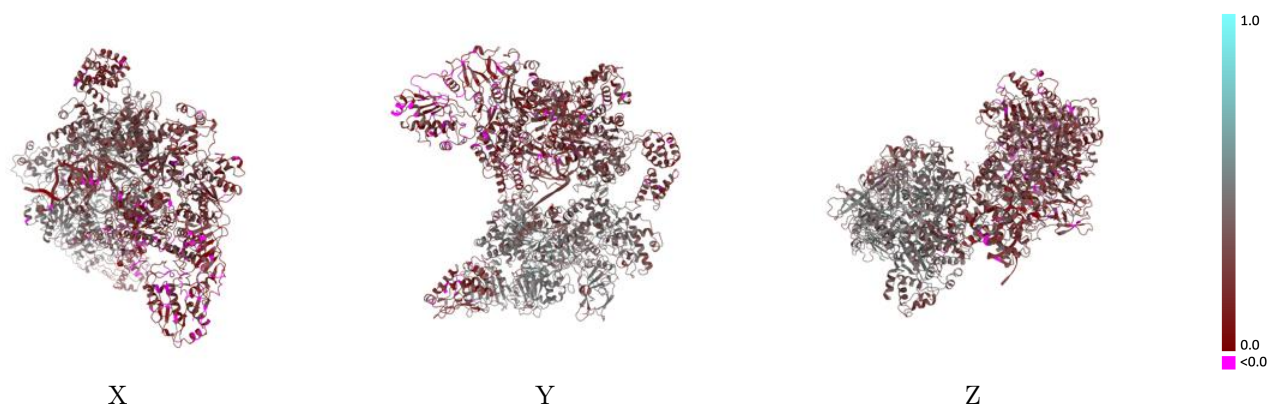
Y



Z

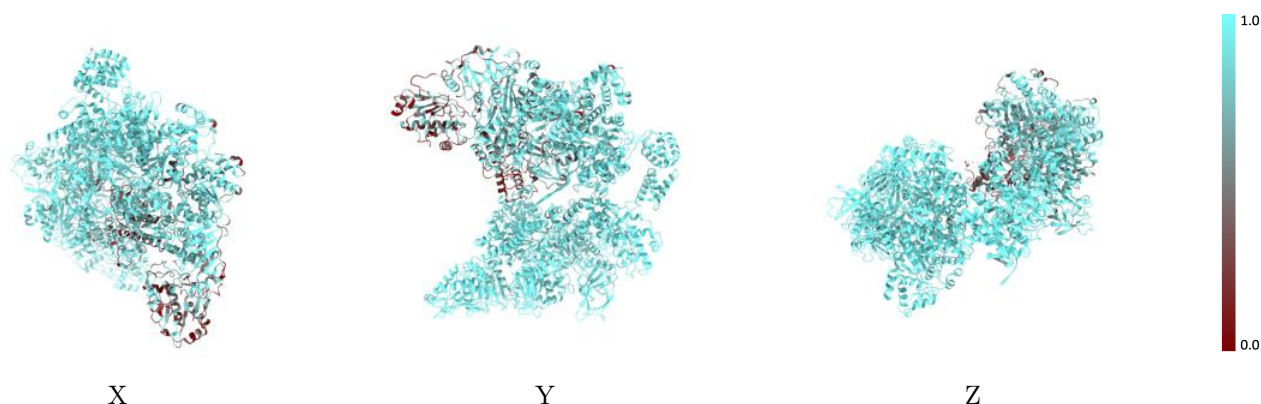
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



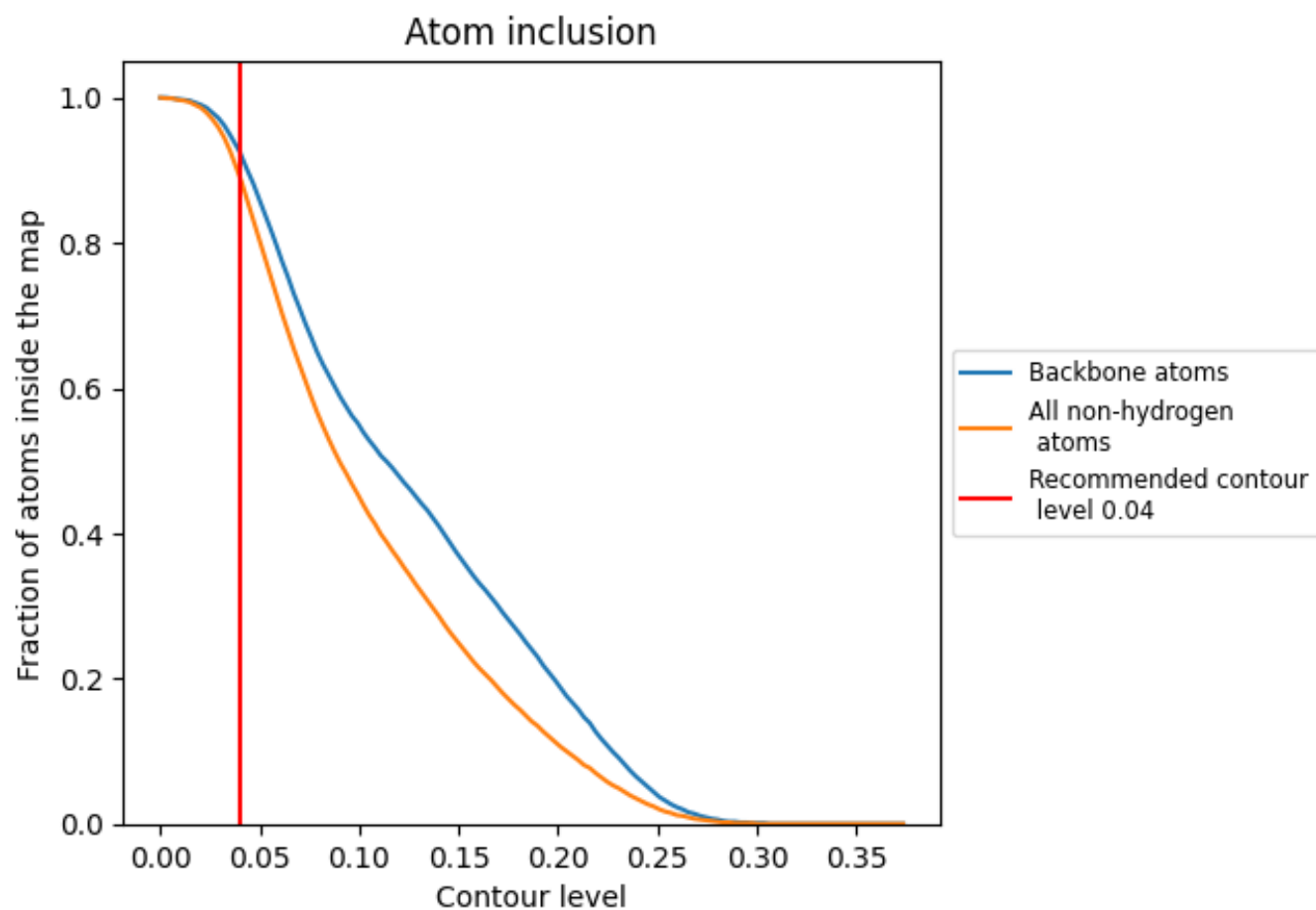
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.3130
G	0.9380	0.2590
I	0.9400	0.2340
Y	0.9890	0.3870
y	0.7890	0.2420

