



wwPDB EM Validation Summary Report ⓘ

Aug 28, 2025 – 03:15 PM EDT

PDB ID : 9CI3 / pdb_00009ci3
EMDB ID : EMD-45609
Title : Structure of the LRRK2/14-3-3 complex
Authors : Martinez Fiesco, J.A.; Zhang, P.
Deposited on : 2024-07-02
Resolution : 3.96 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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

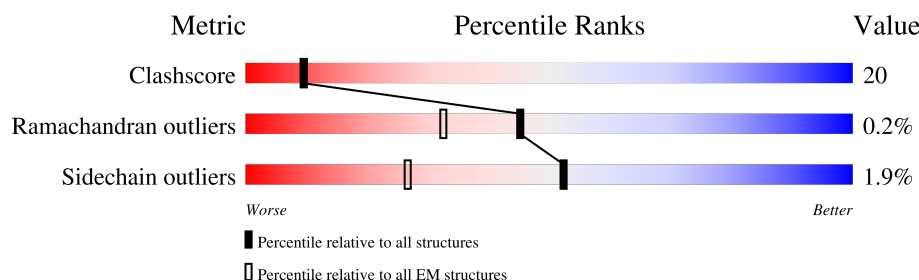
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.96 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	265	<div> <div>43%</div> <div>55%</div> <div>35%</div> <div>9%</div> </div>
1	C	265	<div> <div>32%</div> <div>54%</div> <div>34%</div> <div>11%</div> </div>
2	A	2562	<div> <div>28%</div> <div>36%</div> <div>23%</div> <div>41%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15926 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 14-3-3 protein gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	237	Total	C	N	O	S	0	0
			1909	1190	325	384	10		
1	B	240	Total	C	N	O	S	0	0
			1935	1204	330	391	10		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	initiating methionine	UNP P61981
C	-16	GLY	-	expression tag	UNP P61981
C	-15	SER	-	expression tag	UNP P61981
C	-14	HIS	-	expression tag	UNP P61981
C	-13	HIS	-	expression tag	UNP P61981
C	-12	HIS	-	expression tag	UNP P61981
C	-11	HIS	-	expression tag	UNP P61981
C	-10	HIS	-	expression tag	UNP P61981
C	-9	HIS	-	expression tag	UNP P61981
C	-8	SER	-	expression tag	UNP P61981
C	-7	GLY	-	expression tag	UNP P61981
C	-6	GLU	-	expression tag	UNP P61981
C	-5	ASN	-	expression tag	UNP P61981
C	-4	LEU	-	expression tag	UNP P61981
C	-3	TYR	-	expression tag	UNP P61981
C	-2	PHE	-	expression tag	UNP P61981
C	-1	GLN	-	expression tag	UNP P61981
C	0	GLY	-	expression tag	UNP P61981
B	-17	MET	-	initiating methionine	UNP P61981
B	-16	GLY	-	expression tag	UNP P61981
B	-15	SER	-	expression tag	UNP P61981
B	-14	HIS	-	expression tag	UNP P61981
B	-13	HIS	-	expression tag	UNP P61981
B	-12	HIS	-	expression tag	UNP P61981
B	-11	HIS	-	expression tag	UNP P61981
B	-10	HIS	-	expression tag	UNP P61981

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP P61981
B	-8	SER	-	expression tag	UNP P61981
B	-7	GLY	-	expression tag	UNP P61981
B	-6	GLU	-	expression tag	UNP P61981
B	-5	ASN	-	expression tag	UNP P61981
B	-4	LEU	-	expression tag	UNP P61981
B	-3	TYR	-	expression tag	UNP P61981
B	-2	PHE	-	expression tag	UNP P61981
B	-1	GLN	-	expression tag	UNP P61981
B	0	GLY	-	expression tag	UNP P61981

- Molecule 2 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	1521	Total	C	N	O	P	S	0	0
			12054	7711	2074	2197	2	70		

There are 36 discrepancies between the modelled and reference sequences:

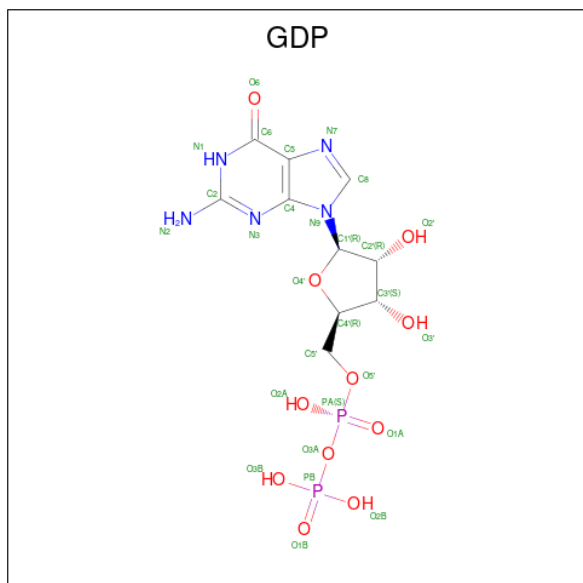
Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP Q5S007
A	-33	GLY	-	expression tag	UNP Q5S007
A	-32	SER	-	expression tag	UNP Q5S007
A	-31	ASP	-	expression tag	UNP Q5S007
A	-30	TYR	-	expression tag	UNP Q5S007
A	-29	LYS	-	expression tag	UNP Q5S007
A	-28	ASP	-	expression tag	UNP Q5S007
A	-27	HIS	-	expression tag	UNP Q5S007
A	-26	ASP	-	expression tag	UNP Q5S007
A	-25	GLY	-	expression tag	UNP Q5S007
A	-24	ASP	-	expression tag	UNP Q5S007
A	-23	TYR	-	expression tag	UNP Q5S007
A	-22	LYS	-	expression tag	UNP Q5S007
A	-21	ASP	-	expression tag	UNP Q5S007
A	-20	HIS	-	expression tag	UNP Q5S007
A	-19	ASP	-	expression tag	UNP Q5S007
A	-18	ILE	-	expression tag	UNP Q5S007
A	-17	ASP	-	expression tag	UNP Q5S007
A	-16	TYR	-	expression tag	UNP Q5S007
A	-15	LYS	-	expression tag	UNP Q5S007
A	-14	ASP	-	expression tag	UNP Q5S007
A	-13	ASP	-	expression tag	UNP Q5S007

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ASP	-	expression tag	UNP Q5S007
A	-11	ASP	-	expression tag	UNP Q5S007
A	-10	LYS	-	expression tag	UNP Q5S007
A	-9	LEU	-	expression tag	UNP Q5S007
A	-8	GLY	-	expression tag	UNP Q5S007
A	-7	LEU	-	expression tag	UNP Q5S007
A	-6	GLU	-	expression tag	UNP Q5S007
A	-5	VAL	-	expression tag	UNP Q5S007
A	-4	LEU	-	expression tag	UNP Q5S007
A	-3	PHE	-	expression tag	UNP Q5S007
A	-2	GLN	-	expression tag	UNP Q5S007
A	-1	GLY	-	expression tag	UNP Q5S007
A	0	PRO	-	expression tag	UNP Q5S007
A	50	HIS	ARG	variant	UNP Q5S007

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			28	10	5	11	2	

T1912	D1844	L1749	D1675	I1606	S1536	GLN	W1376	F1308	L1243	M1183	N1117	F1050
S1913	H1676	V1750	H1676	M1607	E1537	ARG	P1377	K1309	W1244	K1184	K1118	P1051
L1914	R1677	A1608	R1677	A1608	R1538	K1463	I1378	H1310	S1245	F1185	I1119	S1052
R1915	P1846	H1768	I1680	L1611	K1539	K1468	R1381	I1311	R1246	S1186	G1121	Y1053
L1916	R1847	L1763	E1681	V1615	I1543	L1474	D1382	G1312	K1249	I1188	I1122	L1055
R1917	P1846	K1764	P1683	E1616	F1544	N1475	K1383	K1314	L1250	P1189	C1123	L1056
R1918	R1847	V1767	P1683	G1617	F1545	K1476	R1384	K1316	H1251	M1057		M1056
Q1919	P1851	V1767	H1684	E1618	I1548	R1477	K1385	K1317	L1252	A1190		S1058
E1920	Q1854	R1771	C1685	C1618	D1549	P1480	D1387	D1316	L1257	I1192		C1059
L1921	D1858	K1772	E1686	P1619	R1550	L1481	L1388	I1319	K1258	L1193		C1059
V1922	D1858	K1772	M1687	K1620	K1551	I1482	V1389	I1320	E1259	N1194		I1060
V1923	A1862	I1775	S1688	H1621	R1552	Y1485	V1392	F1321	I1260	L1195		A1061
L1924	D1863	I1776	S1688	P1622	Q1555	V1488	F1395	L1322		P1196		N1062
G1925	P1865	L1777	E1688	K1623	L1556	N1488	F1395	Q1323	E1263	H1197		S1066
L1926	P1865	L1777	E1688	L1556	V1557	M1489	F1401	Q1324	I1264	L1198		R1067
L1927	R1866	V1780	P1695	V1557	R1558	N1490	Y1402	R1325	G1265	R1199		N1068
H1928	I1868	V1781	I1625	R1558	E1559	T1491	S1403	L1326	C1266	S1200		G1071
H1929	I1868	I1784	I1625	E1559	E1492	E1492	T1404	K1327	L1267	M1203		P1072
P1930	M1869	W1791	E1632	E1559	E1493	E1493	H1405	K1328	E1288	D1202		S1073
S1931	M1869		K1633	Q1561	L1497	L1497	H1407	A1329	N1269	M1203		V1074
L1932	L1870		F1634	L1562	A1498	A1498	F1408	V1330	L1270	S1204		V1075
I1933	D1873		L1635	Q1563	L1564	L1564	M1409	G1424	T1271	N1206		L1076
S1934	E1874		L1636	L1564	D1565	K1499	Y1415	N1333	S1272	D1207		D1077
L1935	L1875		S1637	L1564	E1566	L1500	Y1416	K1334	L1273	L1208		P1078
G1939	E1876		LVS	LVS	E1567	R1501	L1416	M1335	L1274	Q1209		T1079
I1940	F1877		ARG	ARG	N1567	K1502	A1417	K1336	V1275	Y1210		V1080
R1941	E1878		LVS	LVS	E1568	T1503	V1418	L1337	S1276	L1211		K1081
P1942	Q1879		PHE	PHE	L1569	I1504		M1338	L1277	P1212		C1082
R1943	A1880		LVS	LVS	H1574	N1506	Q1425	I1339	L1279	G1213		P1083
M1944	P1881		N1644	N1644	F1575	E1507		G1340	E1281	P1214		T1084
L1945	E1882		M1645	M1645	L1576	S1508		V1341	L1281	A1215		L1085
V1946	F1883		S1647	S1647		L1509		G1342	R1282	H1216		K1086
M1947	Y1718		Q1648	Q1648	S1579	K1512	D1429	G1346	R1282	W1217		Q1087
E1948	Y1814		Y1649	Y1649	V1581	I1513	A1430	L1351	S1283	K1218		F1088
A1950	S1815		GLY	GLY	L1582		K1432	Q1352	F1284	S1219		S1091
L1955	D1818		ARG	ARG	L1583	Q1516	P1433	Q1353	P1285	K1218		Y1092
D1956	G1819		K1651	K1651	H1584	L1517	W1434	L1354	M1286	M1221		M1093
R1957	E1820		L1652	L1652	F1585	V1518	F1436	M1355	E1287	L1222		Q1094
L1958	E1821		L1653	L1653	Q1586	G1520	I1437	K1356	M1288	R1223		L1095
L1959	E1822		E1654	E1654	D1587	Q1521	I1438	T1357	G1289	E1224		S1096
Q1960	L1826		K1655	K1655	P1588	L1522	K1439	K1358	L1291	L1225		F1097
Q1961	L1827		F1656	F1656	A1589	D1525	S1444	K1359	Q1290	L1226		S1096
D1962	D1828		Q1657	Q1657	I1523	C1526	I1448	S1360	S1292	F1227		E1100
K1963	L1829		I1658	I1658	P1524	G1526	L1449	D1361	K1228	H1229		N1101
A1964	L1830		A1659	A1659	Q1591	C1526	L1449	L1362	M1168	W1230		L1102
S1965	M1831		LEU	LEU	L1592	Y1527	L1454	G1363	P1169	Q1231		T1103
S1965	G1736		ILE	ILE	S1593	V1528	D1455	L1364	F1170	L1232		L1104
L1966	Q1736		GLY	GLY	D1594	V1529	V1456	Q1231	L1171	S1233		V1105
T1967	I1738		GLU	GLU	L1595	L1530	V1456	Q1365	P1172	I1234		V1106
R1968	Y1739		TVA	TVA	Y1596	I1533	S1457	V1369	P1173	L1235		E1107
E1902	W1742		LEU	LEU	F1597	I1534	ASP	G1370	S1174	D1236		K1108
V1905			L1668	L1668	V1598	L1535	GLU	I1371	M1175	L1237		L1109
K1906			V1669	V1669	E1599		LYS	D1372	M1176	D1237		E1110
I1907								K1373	L1177	E1239		L1114
A1975								K1374	L1178	K1240		E1115
L1976								D1375	L1179	A1241		G1116
H1977									S1181	Y1242		

L2493	T2494	V2495	W2496	D2497	L2498	N2499	L2500	P2501	H2502	E2503	V2504	Q2505	N2506	L2507	E2508	K2509	H2510	L2511	E2512	V2513	R2514	K2515	E2516	L2517	A2518	E2519	K2520	M2521	R2522	R2523	T2524	S2525	V2526	E2527																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	2.360	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.122	Depositor
Map size (Å)	325.62, 325.62, 325.62	wwPDB
Map dimensions	402, 402, 402	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, GDP

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	B	0.17	0/1963	0.46	0/2648
1	C	0.17	0/1937	0.43	0/2613
2	A	0.19	0/12271	0.46	6/16603 (0.0%)
All	All	0.18	0/16171	0.46	6/21864 (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
2	A	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	938	PRO	CA-N-CD	-9.96	98.06	112.00
2	A	938	PRO	CB-CA-C	7.04	123.18	111.56
2	A	938	PRO	N-CA-CB	-6.67	96.25	103.25
2	A	2142	ARG	N-CA-C	6.30	116.77	107.88
2	A	2500	LEU	N-CA-C	5.83	122.68	109.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2142	ARG	Sidechain

5.2 Too-close contacts

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	B	1935	0	1898	84	0
1	C	1909	0	1878	82	0
2	A	12054	0	12234	475	0
3	A	28	0	12	0	0
All	All	15926	0	16022	626	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 20.

The worst 5 of 626 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)
2:A:1240:LYS:HD2	2:A:1243:LEU:HD22	1.54	0.90
1:C:225:LEU:O	1:C:229:ASN:ND2	2.08	0.87
2:A:1437:ASN:HD21	2:A:1702:MET:HE3	1.37	0.86
1:C:57:ARG:NH2	2:A:935:SEP:O2P	2.11	0.84
2:A:2456:ARG:NH1	2:A:2475:TYR:OH	2.11	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	B	238/265 (90%)	236 (99%)	2 (1%)	0	100	100
1	C	235/265 (89%)	231 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	1499/2562 (58%)	1356 (90%)	140 (9%)	3 (0%)	44	76
All	All	1972/3092 (64%)	1823 (92%)	146 (7%)	3 (0%)	45	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	938	PRO
2	A	940	PHE
2	A	1713	LEU

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	B	211/231 (91%)	209 (99%)	2 (1%)	75	83
1	C	208/231 (90%)	203 (98%)	5 (2%)	44	62
2	A	1346/2310 (58%)	1320 (98%)	26 (2%)	52	69
All	All	1765/2772 (64%)	1732 (98%)	33 (2%)	52	69

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2397	MET
2	A	2436	LEU
2	A	2500	LEU
2	A	1192	ILE
2	A	1175	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	1854	GLN
2	A	2420	GLN

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Mol	Chain	Res	Type
2	A	2506	ASN
2	A	1986	HIS
2	A	1068	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
2	SEP	A	910	2	8,9,10	1.60	1 (12%)	7,12,14	1.30	1 (14%)
2	SEP	A	935	2	8,9,10	1.57	1 (12%)	7,12,14	1.52	1 (14%)

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	SEP	A	910	2	-	1/6/8/10	-
2	SEP	A	935	2	-	5/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	935	SEP	P-O1P	3.47	1.61	1.50
2	A	910	SEP	P-O1P	3.47	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	935	SEP	OG-CB-CA	3.57	111.62	108.14
2	A	910	SEP	OG-CB-CA	2.88	110.94	108.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	935	SEP	N-CA-CB-OG
2	A	935	SEP	C-CA-CB-OG
2	A	935	SEP	CB-OG-P-O1P
2	A	935	SEP	CB-OG-P-O2P
2	A	935	SEP	CB-OG-P-O3P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	910	SEP	3	0
2	A	935	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	GDP	A	2601	-	25,30,30	0.95	1 (4%)	30,47,47	1.13	3 (10%)

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	GDP	A	2601	-	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	GDP	C6-N1	-2.20	1.34	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	GDP	C8-N7-C5	2.96	107.58	102.55
3	A	2601	GDP	O4'-C1'-N9	2.34	111.84	108.75
3	A	2601	GDP	C5-C6-N1	2.08	118.03	114.07

There are no chirality outliers.

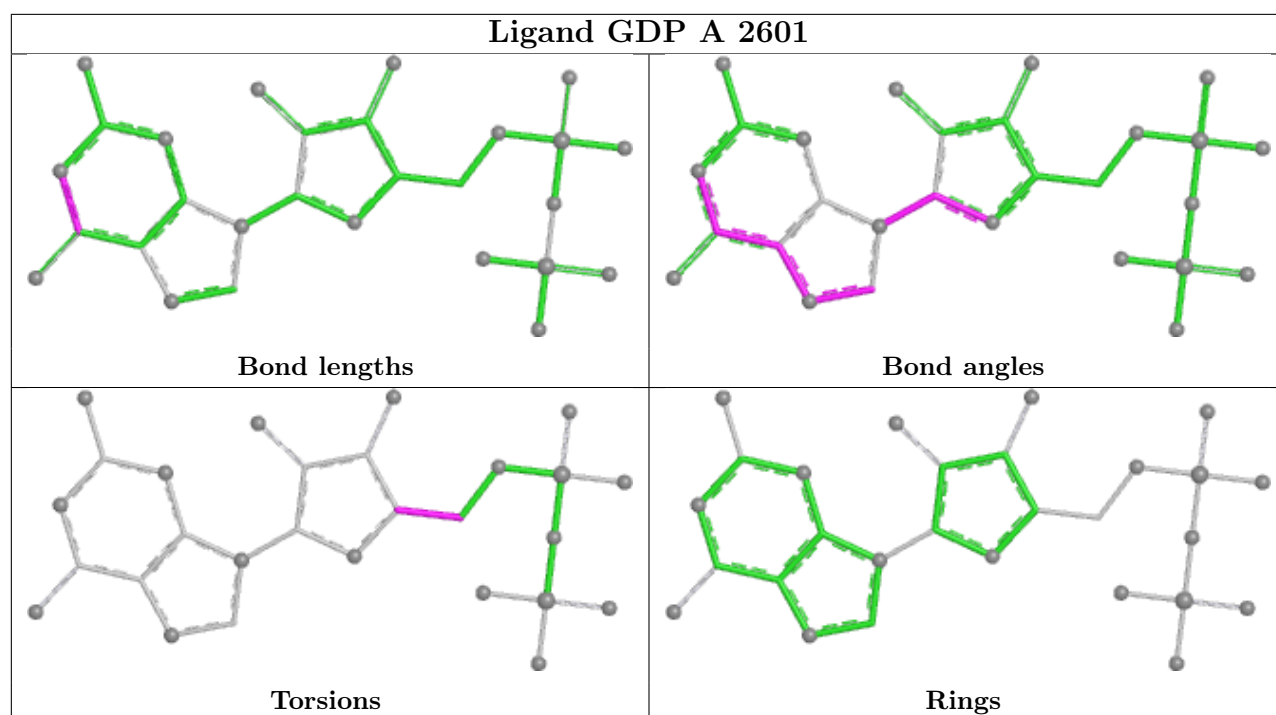
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2601	GDP	O4'-C4'-C5'-O5'
3	A	2601	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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.

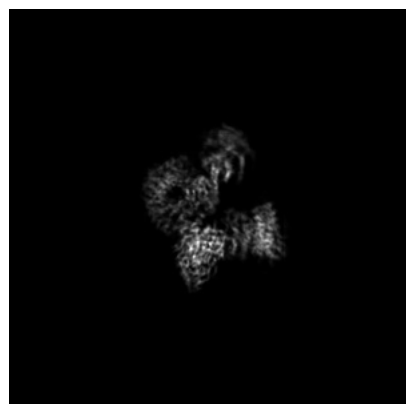
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45609. These allow visual inspection of the internal detail of the map and identification of artifacts.

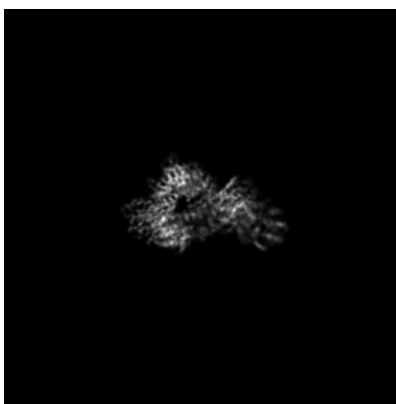
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

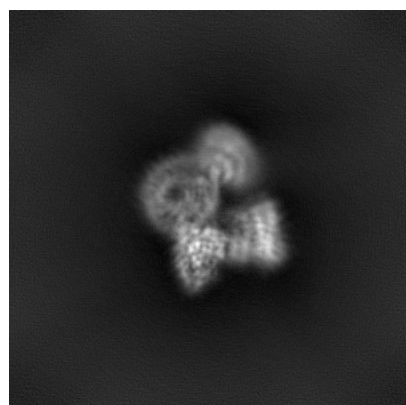


Y

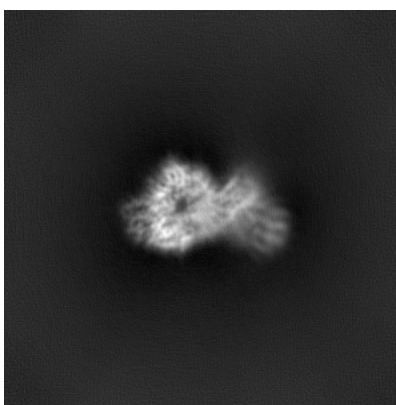


Z

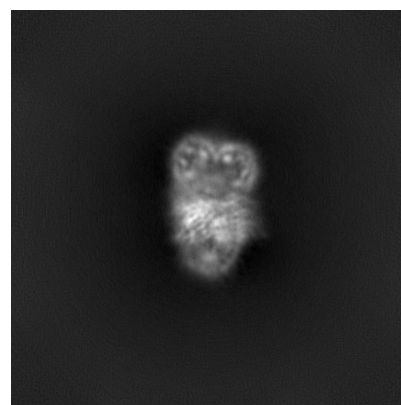
6.1.2 Raw map



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: 201

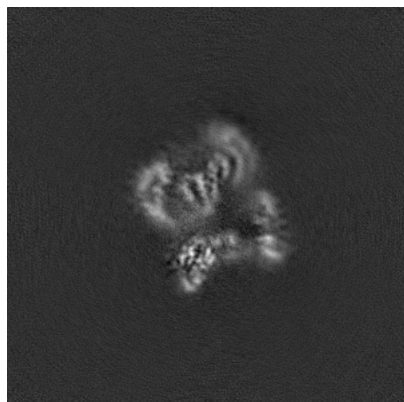


Y Index: 201

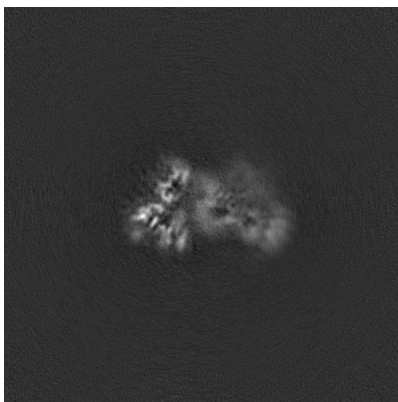


Z Index: 201

6.2.2 Raw map



X Index: 201



Y Index: 201



Z Index: 201

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: 193

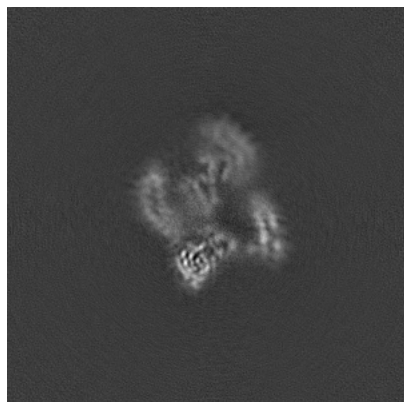


Y Index: 189

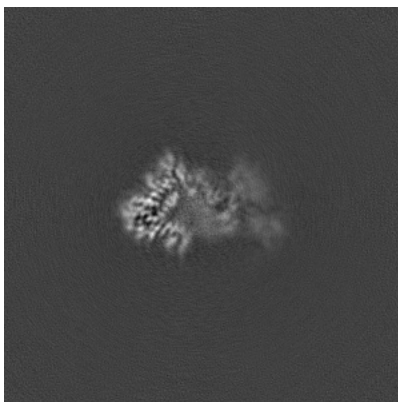


Z Index: 167

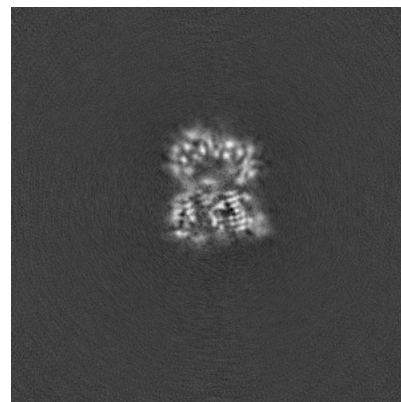
6.3.2 Raw map



X Index: 193



Y Index: 189

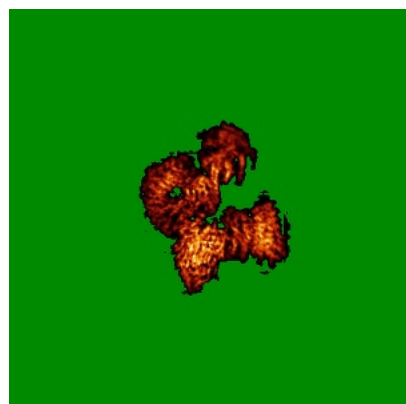


Z Index: 166

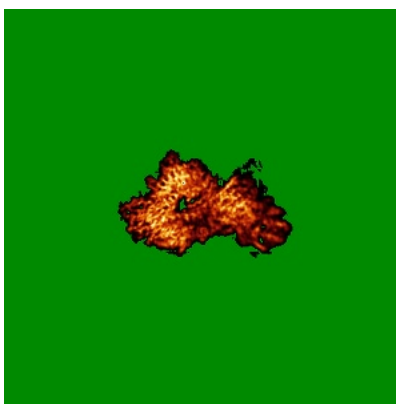
The images above show the largest variance slices of the map in three orthogonal directions.

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

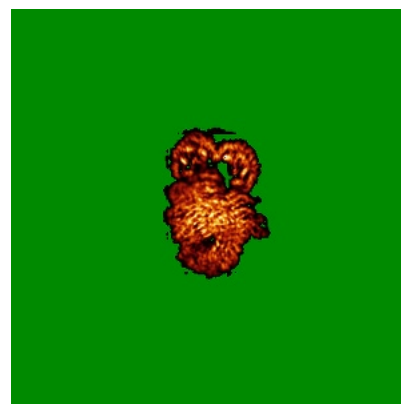
6.4.1 Primary map



X

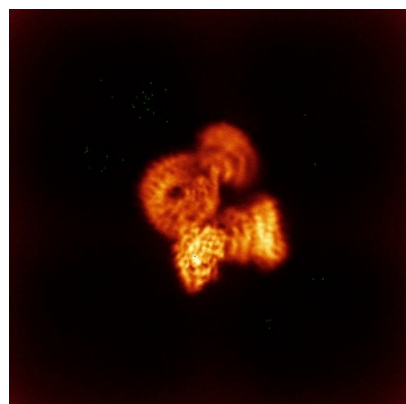


Y

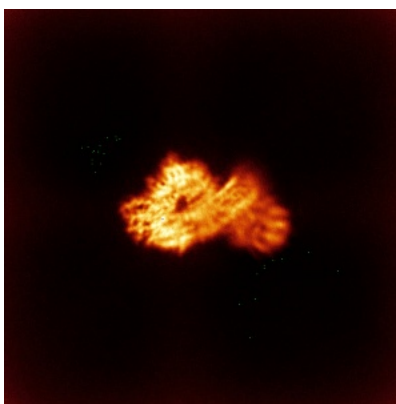


Z

6.4.2 Raw map



X



Y

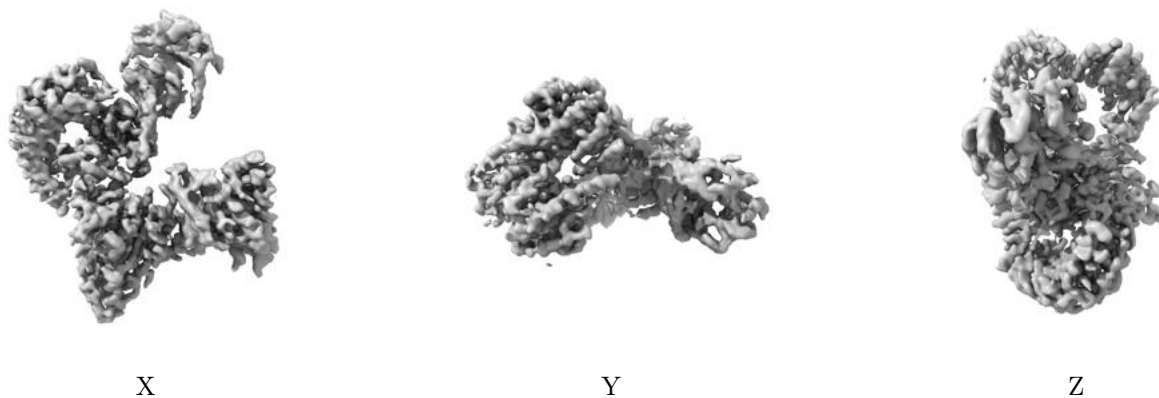


Z

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.

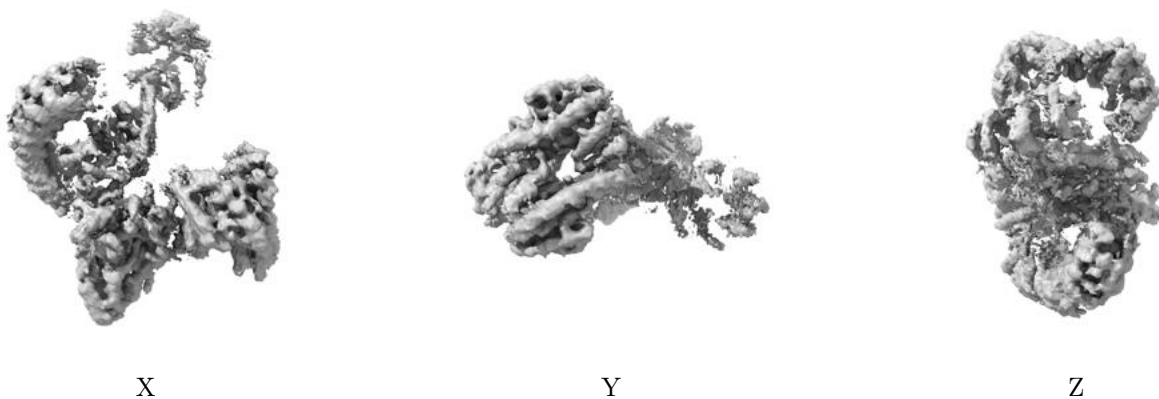
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.122. 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.

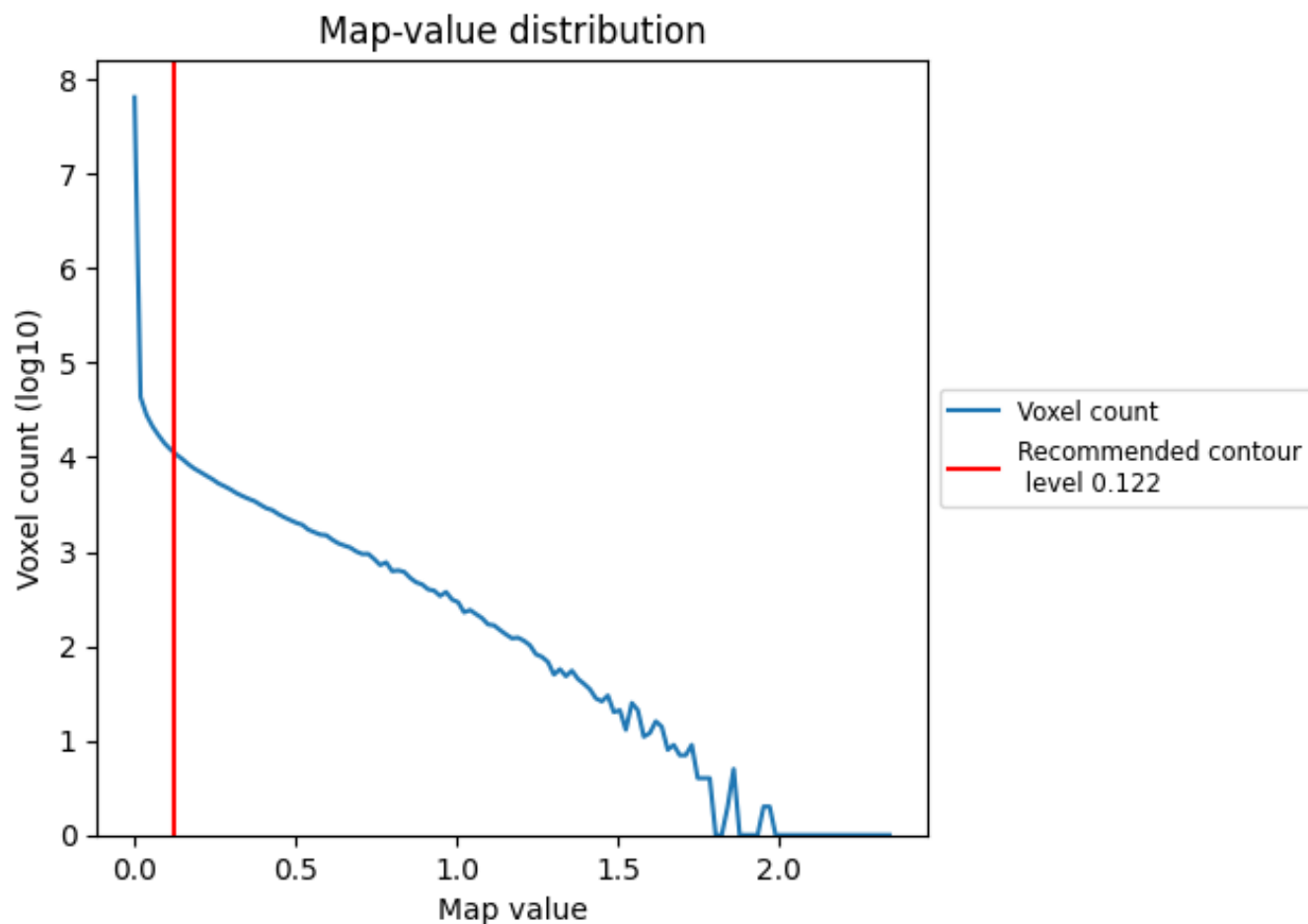
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

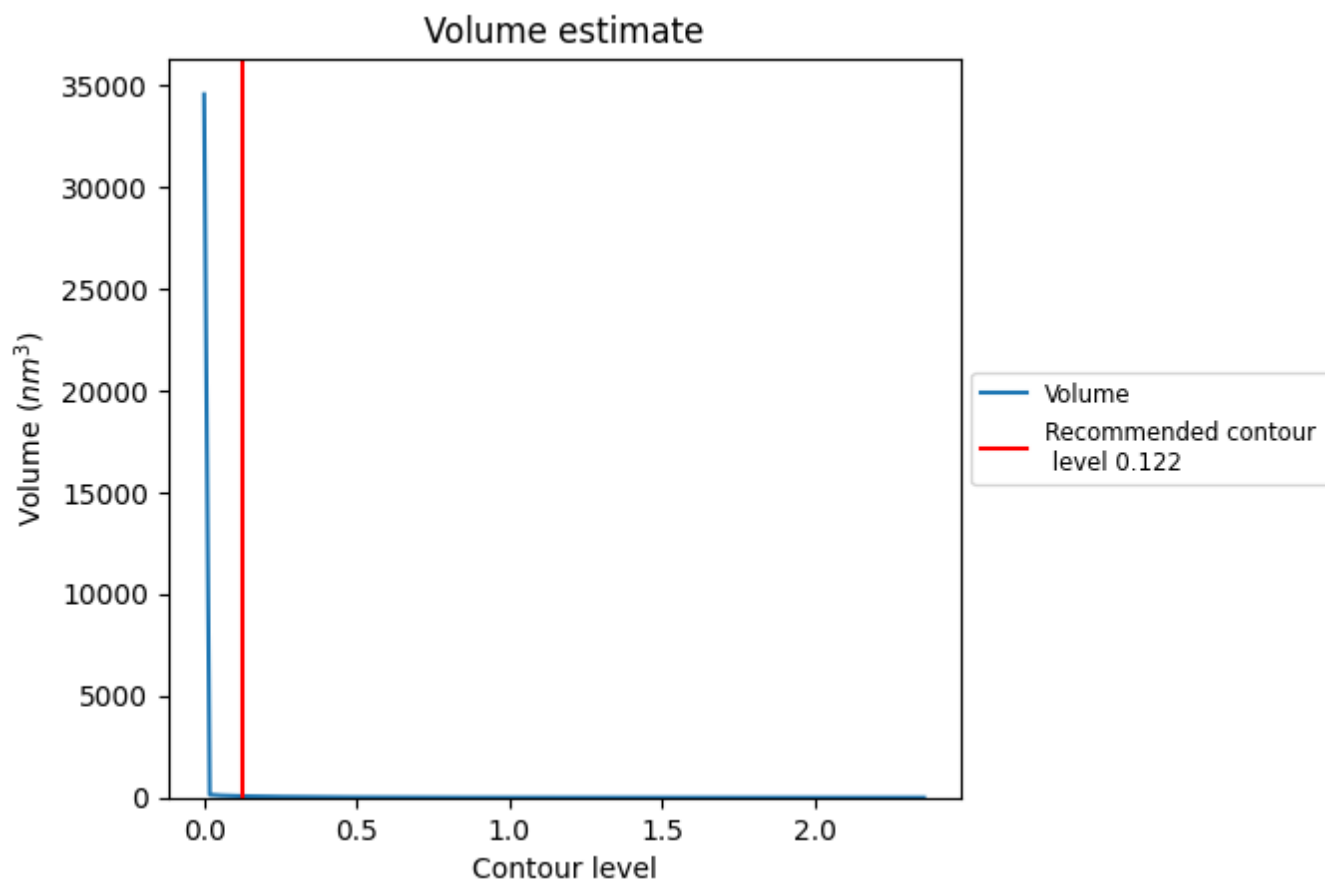
This section contains the results of statistical analysis of the map.

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.

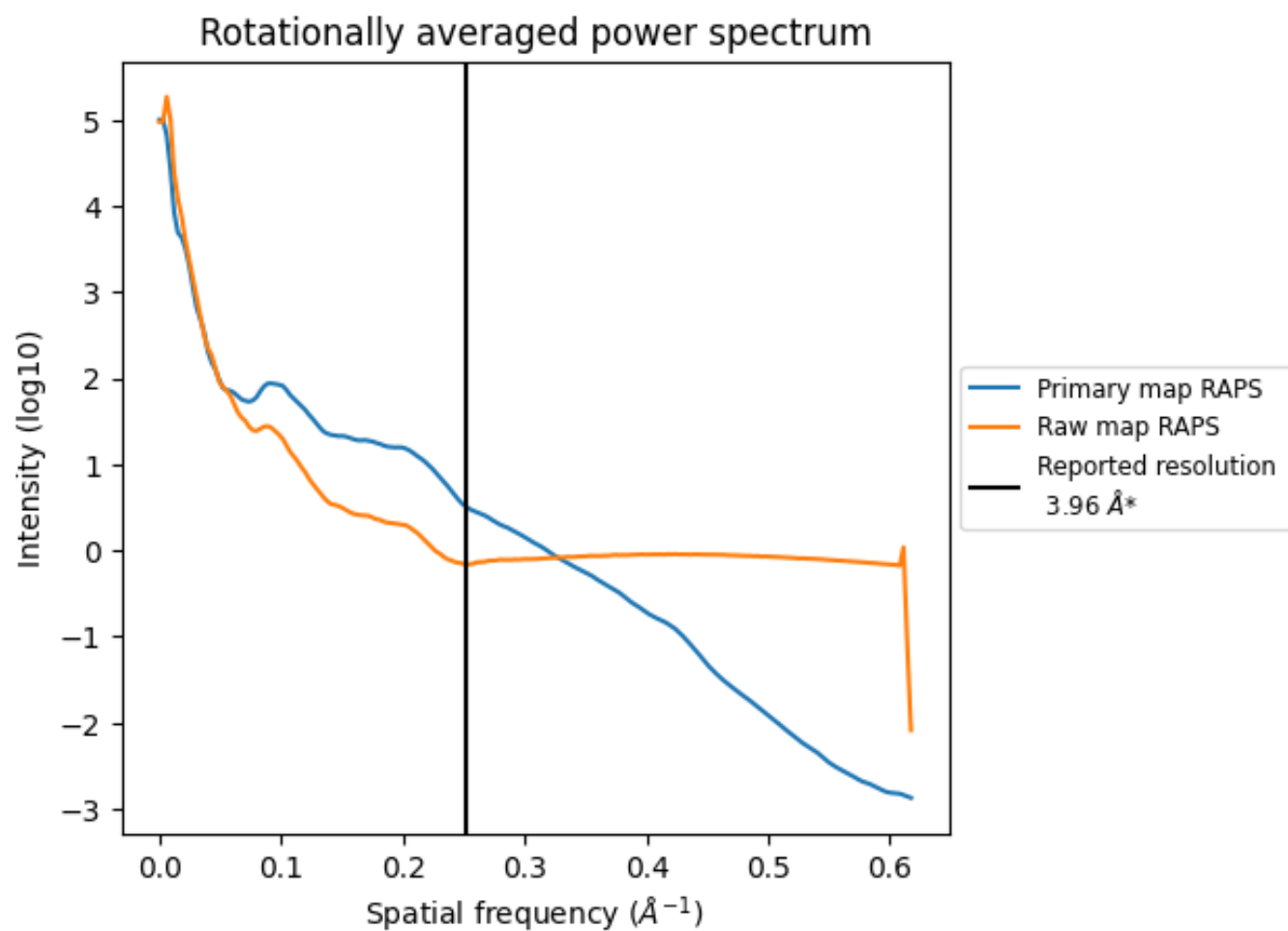
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm³; this corresponds to an approximate mass of 64 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 ⓘ

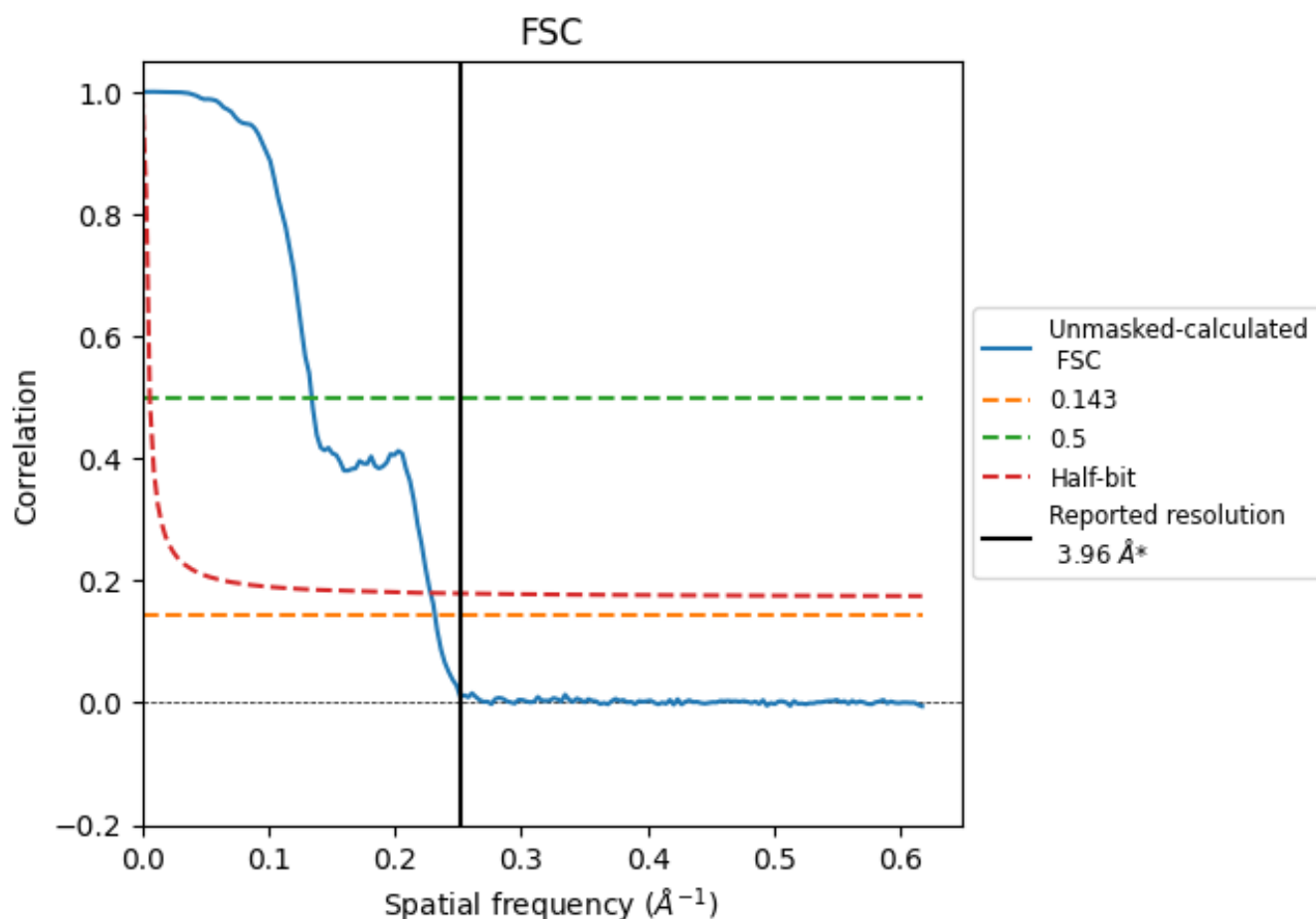


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

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 0.253 Å⁻¹

8.2 Resolution estimates [i](#)

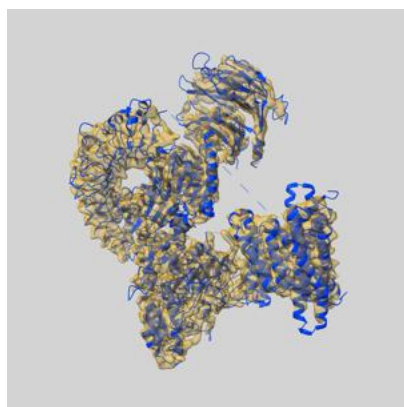
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.32	7.45	4.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

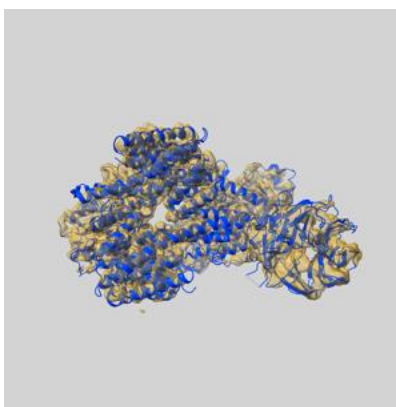
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45609 and PDB model 9CI3. Per-residue inclusion information can be found in section 3 on page 6.

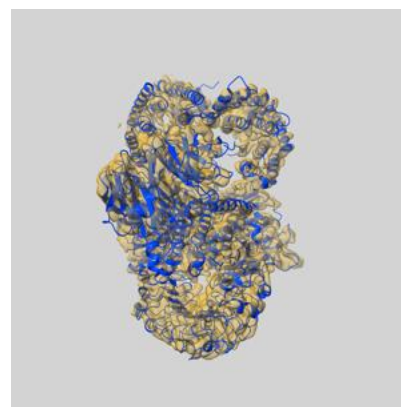
9.1 Map-model overlay [i](#)



X



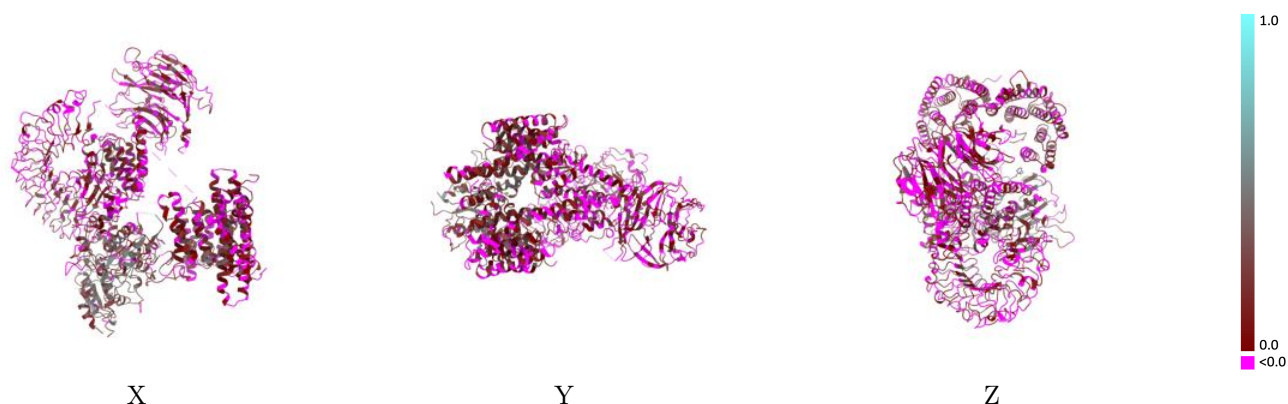
Y



Z

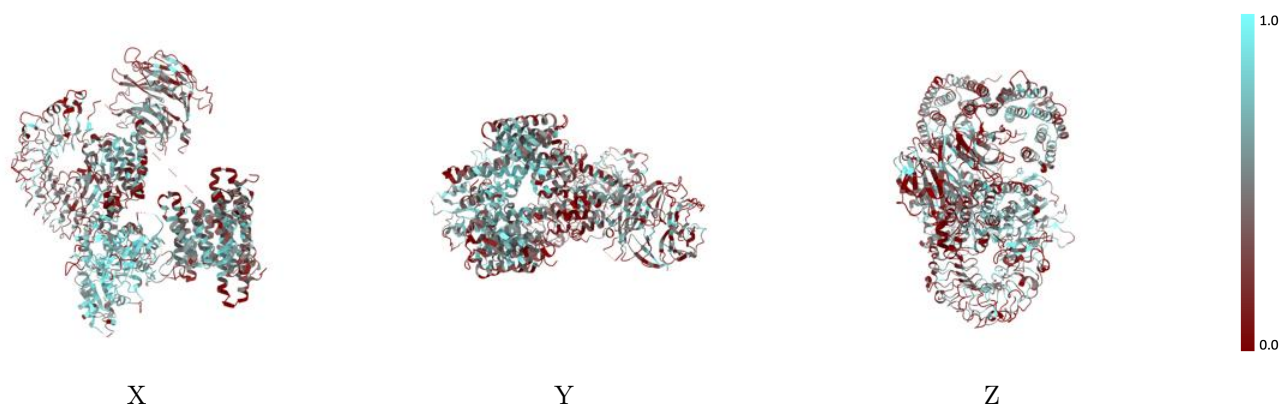
The images above show the 3D surface view of the map at the recommended contour level 0.122 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



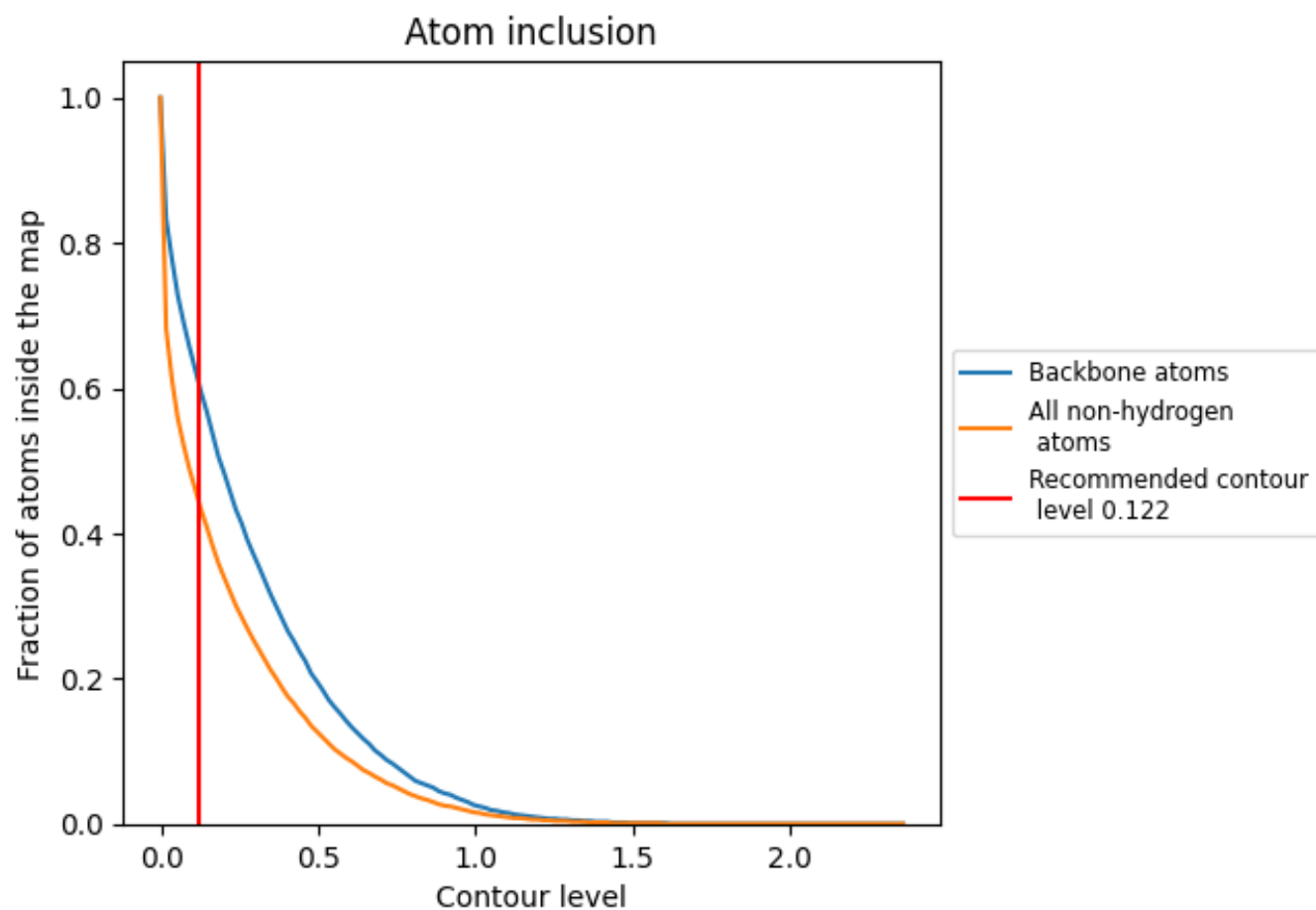
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.122).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 44% 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 (0.122) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4410	<div></div> 0.1120
A	<div></div> 0.4380	<div></div> 0.1170
B	<div></div> 0.3980	<div></div> 0.0800
C	<div></div> 0.5030	<div></div> 0.1170

