



wwPDB EM Validation Summary Report ⓘ

Oct 16, 2025 – 01:50 pm BST

PDB ID : 9SZR / pdb_00009szr
EMDB ID : EMD-55382
Title : shutdown state non-muscle myosin 2A heads region
Authors : Peckham, M.; Carrington, G.
Deposited on : 2025-10-15
Resolution : 6.30 Å(reported)

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

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

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:

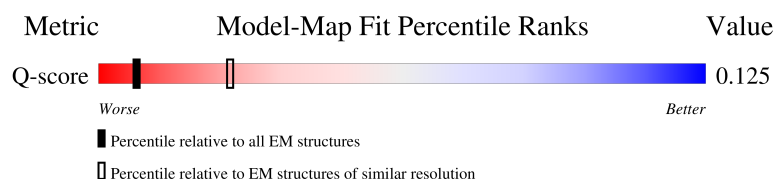
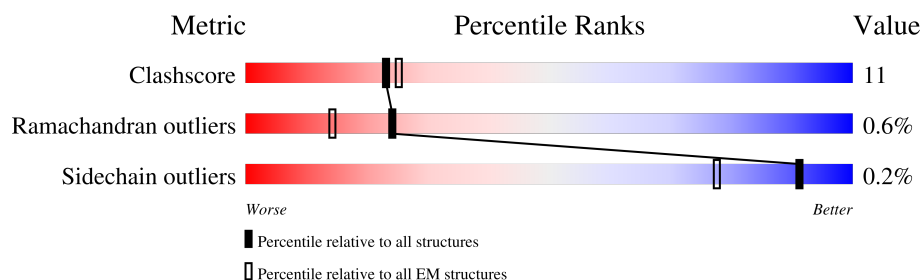
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up 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) : 2.46

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 6.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	550 (5.80 - 6.80)

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	1960	
1	B	1960	
2	C	151	
2	D	151	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	172	<div><div></div><div>79%</div><div>9% • 12%</div></div>
3	F	172	<div><div></div><div>78%</div><div>13% 8%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36487 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 Isoform 1 of Myosin-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1947	Total	C	N	O	S	0	0
			15790	9772	2822	3125	71		
1	B	1945	Total	C	N	O	S	0	0
			15770	9761	2816	3122	71		

- Molecule 2 is a protein called Isoform 1 of Myosin light polypeptide 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	150	Total	C	N	O	S	0	0
			1174	729	195	238	12		
2	D	150	Total	C	N	O	S	0	0
			1175	729	195	239	12		

- Molecule 3 is a protein called Myosin regulatory light polypeptide 9.

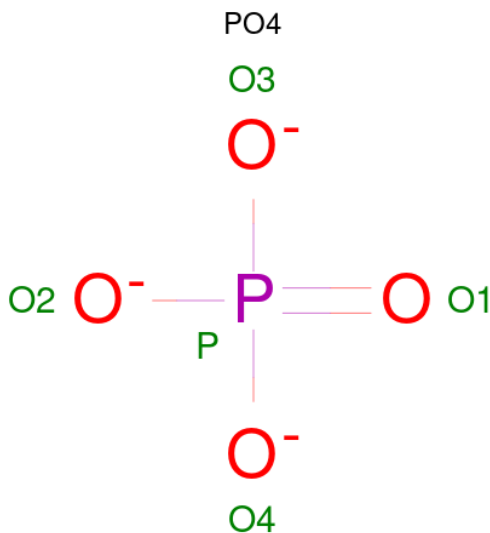
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	152	Total	C	N	O	S	0	0
			1229	771	200	249	9		
3	F	158	Total	C	N	O	S	0	0
			1281	803	212	257	9		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	O	P	0
			5	4	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	O	P	0
			5	4	1	

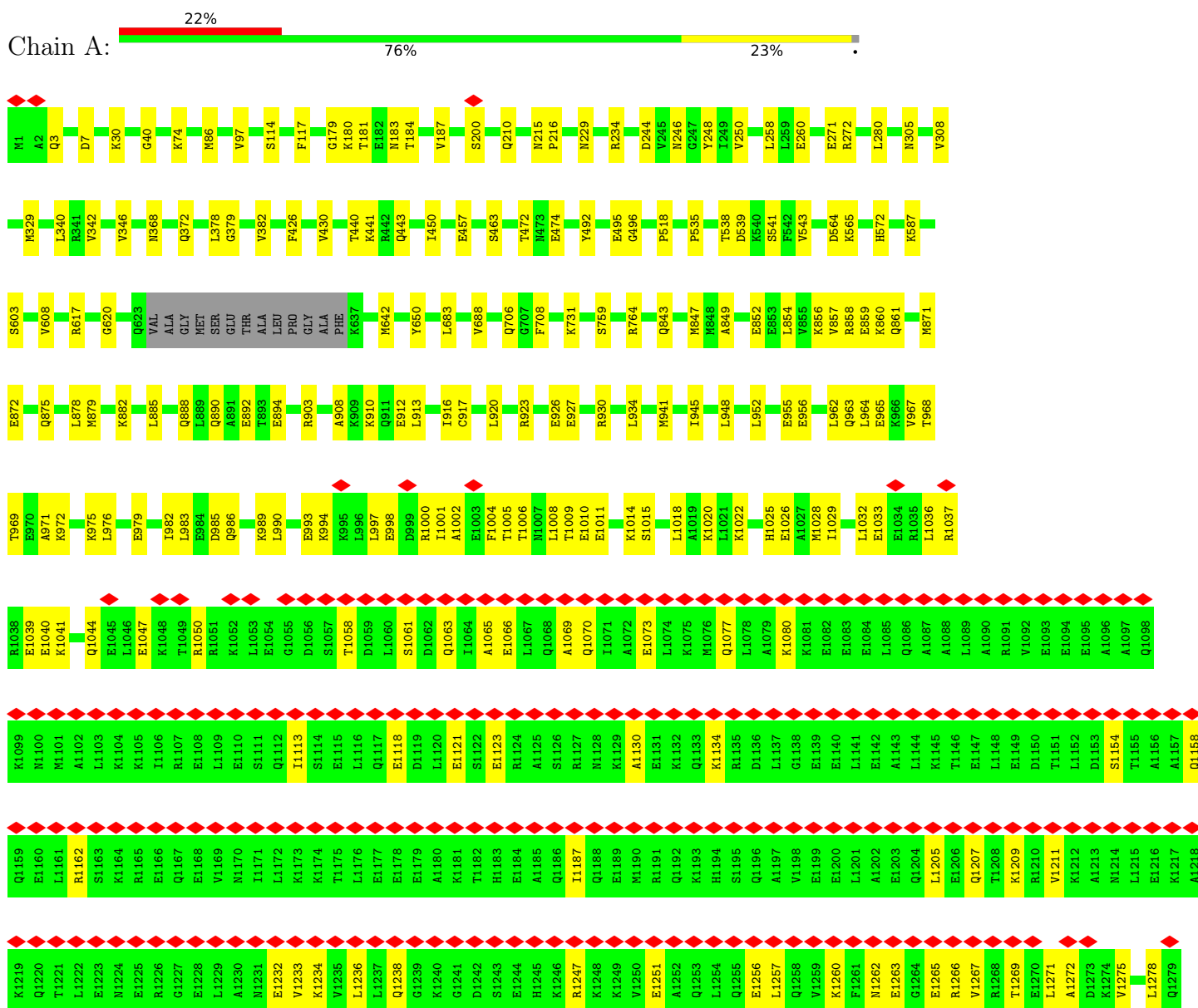
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

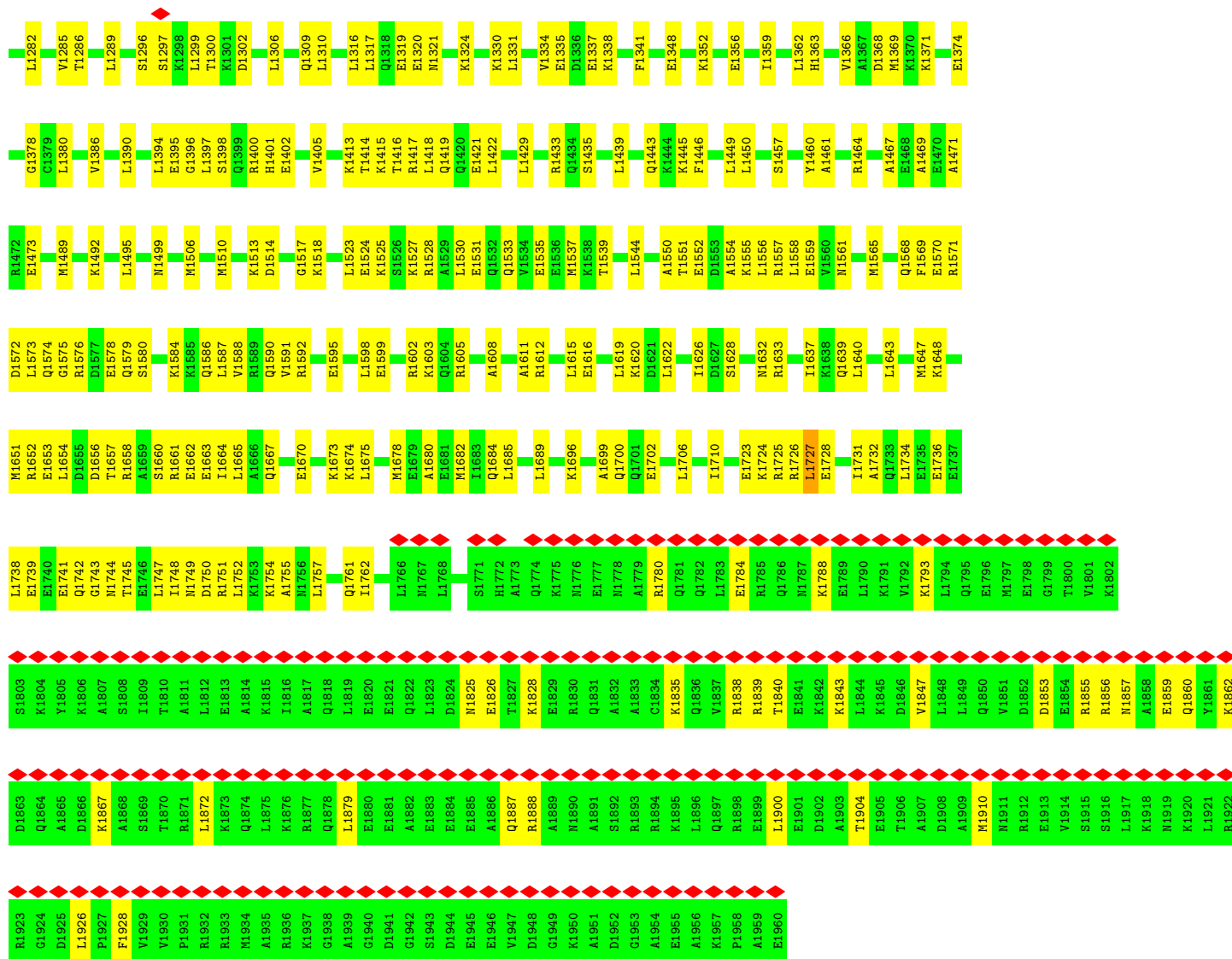
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	
6	E	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	

3 Residue-property plots

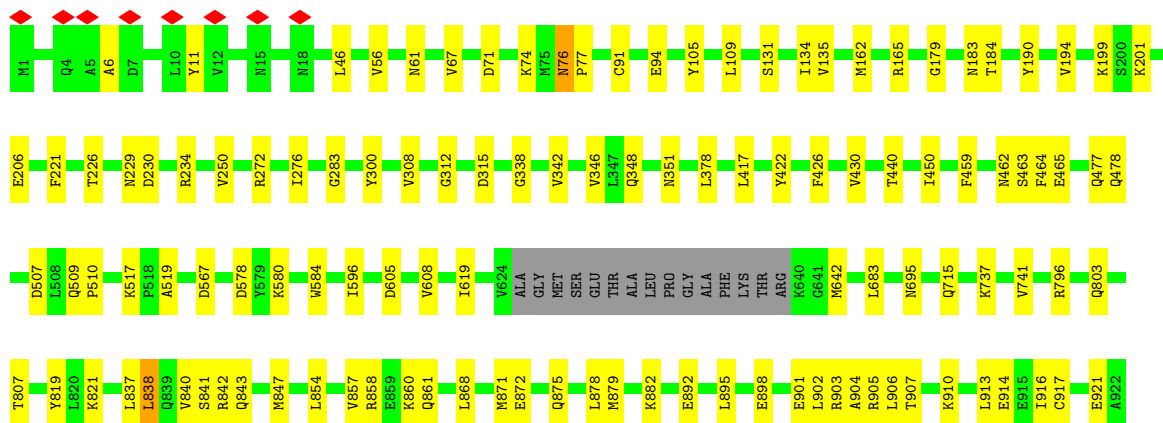
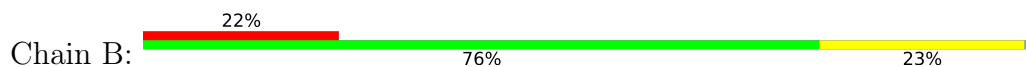
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Isoform 1 of Myosin-9

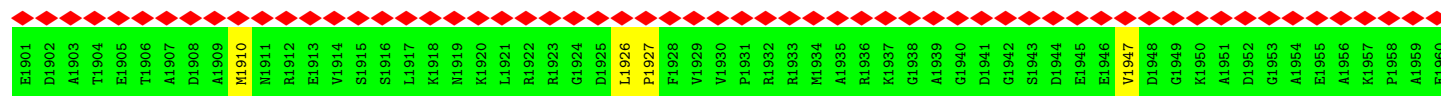




● Molecule 1: Isoform 1 of Myosin-9



E1841	Q1761	E1702	L1622	E1545	D1428	V1334	K1260	E1200	E1140	K1080	E1012	R923
K1842	Q1762	R1703	H1625	L1548	L1429	Q1344	F1261	L1201	L1141	K1081	E1013	E926
K1843	L1763	L1706	I1626	T1551	Q1432	Q1434	N1262	A1202	E1142	E1082	K1014	E927
L1844	E1764	E1709	D1627	T1555	Q1434	E1348	G1264	F1203	A1143	E1083	K1016	E928
K1846	R1765	L1710	S1628	K1555	S1435	E1349	E1265	Q1204	L1144	E1084	S1017	Q932
V1847	Q1766	A1711	N1632	L1556	L1439	E1350	R1266	E1206	K1145	L1018	L1018	H933
L1848	R1767	M1712	R1633	L1558	K1442	K1352	V1267	Q1207	T1146	L1085	A1019	H934
L1849	E1768	S1713	Q1637	E1559	K1442	H1353	R1268	T1208	E1147	Q1086	K1020	L934
K1850	K1769	G1715	T1638	V1560	A1451	K1354	E1270	K1209	L1148	A1087	L1021	Q935
V1851	L1790	K1716	Q1639	M1561	A1451	L1355	E1271	M1210	E1149	L1088	K1022	A936
D1852	V1792	E1723	L1640	L1562	T1455	I1359	L1271	V1211	D1150	L1089	M1023	E937
D1853	K1724	K1724	R1641	Q1563	I1456	I1362	A1272	V1092	T1151	R1091	K1024	K938
L1854	L1727	L1727	K1642	M1565	S1457	H1363	D1273	E1093	L1152	L1092	H1025	K939
R1855	L1730	R1730	Q1644	Q1568	A1458	K1366	K1274	E1094	S1154	E1094	L1032	Q946
R1856	I1731	I1731	Q1647	F1569	K1459	V1366	V1275	E1095	T1155	E1095	L1036	E947
E1857	E1734	E1734	E1653	R1571	Y1460	M1369	T1276	A1096	A1156	A1096	R1035	E949
E1858	L1734	L1734	E1653	D1572	R1464	L1278	K1277	E1097	A1157	A1097	L1036	E950
E1859	L1738	L1738	T1657	L1573	A1471	L1380	Q1279	Q1098	Q1158	Q1098	R1037	Q951
Y1861	E1741	R1658	R1658	R1576	R1472	E1384	V1280	K1219	Q1159	K1099	E1038	E955
D1863	Q1742	A1659	S1660	E1581	T1476	V1385	E1281	E1160	Q1159	M1100	E1039	E956
K1864	G1743	R1661	R1661	E1582	T1476	V1386	N1284	T1221	L1161	M1101	R1043	R959
A1865	E1746	E1662	E1662	K1583	L1495	R1387	M1285	L1222	R1162	A1102	Q1044	Q960
D1866	L1747	K1664	L1665	K1584	E1496	K1388	T1286	E1223	S1163	L1103	E1045	K961
K1867	I1748	L1665	L1665	K1585	L1509	L1390	G1287	M1224	K1164	K1104	L1046	L962
S1868	K1752	K1669	K1669	Q1586	L1509	Q1391	L1288	E1225	R1165	K1105	E1047	Q963
S1869	L1753	E1670	E1670	L1587	S1512	K1392	L1289	A1226	E1166	I1106	L1063	E970
T1870	K1753	R1589	R1589	K1590	D1514	D1394	K1298	G1227	Q1167	R1107	E1054	L973
R1871	M1756	E1672	E1672	V1591	D1515	L1396	K1298	E1228	Q1168	E1108	G1065	Q880
L1872	L1757	K1673	K1673	E1592	S1519	L1397	S1297	L1229	V1169	L1109	D1066	K989
K1873	Q1758	L1675	L1675	M1594	L1523	R1400	T1300	A1230	N1170	E1110	D1059	E993
K1874	L1759	K1676	K1676	E1595	E1524	E1403	K1301	E1232	I1171	S1111	L1060	K994
L1875	D1760	M1682	M1682	A1596	K1525	K1404	D1302	V1233	K1173	T1113	L1060	K995
K1876	Q1761	I1683	I1683	E1597	S1526	Y1408	F1303	K1234	K1174	S1114	S1061	L996
R1877	M1762	Q1686	Q1686	L1598	K1527	A1305	S1304	V1235	T1175	E1115	D1062	E998
K1878	M1763	E1687	E1687	D1600	R1528	L1411	L1306	L1236	L1176	Q1117	Q1063	L999
L1879	L1766	E1688	E1688	E1601	A1529	E1412	L1306	L1237	E1177	Q1117	I1064	D999
E1880	M1767	L1689	L1689	Q1604	L1530	K1413	Q1309	Q1238	E1178	E1118	A1065	R1000
E1881	L1768	A1690	A1690	R1605	Q1533	T1414	L1310	G1239	E1179	D1119	E1066	I1001
E1882	E1769	A1691	A1691	K1415	E1536	K1415	Q1311	K1240	A1180	L1120	A1002	A1002
L1883	R1770	A1692	A1692	T1416	M1537	R1416	D1312	G1241	A1181	E1121	Q1067	E1003
E1883	R1771	A1695	A1695	R1418	K1538	R1417	T1313	G1242	T1182	S1122	L1068	F1004
L1884	H1772	L1615	L1615	L1418	T1539	L1418	Q1314	D1242	H1183	E1123	A1069	T1005
E1885	A1773	Q1698	Q1698	E1421	Q1540	E1421	E1315	S1243	H1184	R1124	Q1070	L1006
E1886	D1618	Q1700	Q1700	L1425	E1542	L1425	L1316	E1244	A1185	A1125	I1071	N1007
Q1887	L1619	Q1701	Q1701	E1542	E1542	E1542	E1319	H1245	Q1186	A1072	L1008	L1008
R1888	M1776	E1777	E1777	E1542	E1542	E1542	N1321	K1246	Q1186	S1126	E1073	E1011
A1889	A1779	M1778	M1778	E1542	E1542	E1542	R1322	R1247	I1187	R1127	L1074	L1074
N1890	K1828	E1829	E1829	E1542	E1542	E1542	Q1330	K1248	Q1188	M1128	K1075	K1075
A1891	E1829	E1829	E1829	E1542	E1542	E1542	L1331	K1249	E1189	K1129	M1076	M1076
S1892	Q1831	E1832	E1832	E1542	E1542	E1542	E1330	V1250	M1190	A1130	Q1077	Q1077
R1893	E1833	E1833	E1833	E1542	E1542	E1542	E1331	E1251	R1191	E1131	L1078	L1078
R1894	A1833	E1833	E1833	E1542	E1542	E1542	L1331	A1252	Q1192	K1132	A1079	A1079
K1895	C1834	E1834	E1834	E1542	E1542	E1542	E1331	Q1253	K1193	Q1133	E1073	E1073
L1896	K1835	E1835	E1835	E1542	E1542	E1542	E1331	L1254	H1194	K1134	L1074	L1074
Q1897	Q1836	E1836	E1836	E1542	E1542	E1542	E1331	Q1255	S1195	R1135	K1075	K1075
R1898	V1837	E1837	E1837	E1542	E1542	E1542	E1331	E1256	Q1196	L1136	M1076	M1076
E1899	R1838	E1838	E1838	E1542	E1542	E1542	E1331	L1257	A1197	L1137	Q1077	Q1077
L1900	R1839	E1839	E1839	E1542	E1542	E1542	E1331	Q1258	V1198	G1138	L1078	L1078
	T1840	E1840	E1840	E1542	E1542	E1542	E1331	V1259	E1199	E1139	A1079	A1079



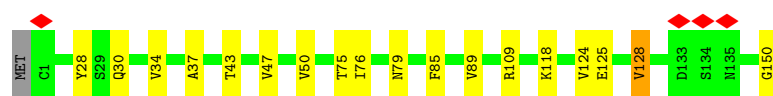
- Molecule 2: Isoform 1 of Myosin light polypeptide 6

Chain C: 87% 12% ..



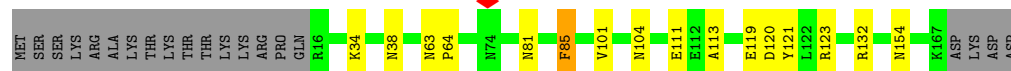
- Molecule 2: Isoform 1 of Myosin light polypeptide 6

Chain D: 87% 11% ..



- Molecule 3: Myosin regulatory light polypeptide 9

Chain E: 79% 9% 12%



- Molecule 3: Myosin regulatory light polypeptide 9

Chain F: 78% 13% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15167	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 ($e^-/\text{\AA}^2$)	36.94	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.051	Depositor
Minimum map value	-0.432	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	839.68, 839.68, 839.68	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	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: PO4, MG, ADP

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	0.06	0/15951	0.14	0/21339
1	B	0.06	0/15930	0.14	0/21311
2	C	0.09	0/1189	0.19	0/1594
2	D	0.10	0/1190	0.21	0/1594
3	E	0.07	0/1252	0.18	0/1685
3	F	0.07	0/1305	0.18	0/1755
All	All	0.06	0/36817	0.15	0/49278

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15790	0	15952	532	0
1	B	15770	0	15927	539	0
2	C	1174	0	1138	11	0
2	D	1175	0	1138	10	0
3	E	1229	0	1154	13	0
3	F	1281	0	1215	12	0
4	A	27	0	12	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	12	1	0
5	A	5	0	0	1	0
5	B	5	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	36487	0	36548	794	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 11.

The worst 5 of 794 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:1570:GLU:HA	1:A:1574:GLN:HB2	1.44	0.96
1:A:971:ALA:HB2	1:B:1687:GLU:HG3	1.49	0.94
1:A:1595:GLU:HG2	1:B:1594:MET:HG3	1.53	0.90
1:A:847:MET:HE1	1:B:843:GLN:HB3	1.52	0.90
1:A:1317:LEU:HD13	1:B:1316:LEU:HD23	1.52	0.89

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	1943/1960 (99%)	1865 (96%)	69 (4%)	9 (0%)	25 64
1	B	1939/1960 (99%)	1850 (95%)	81 (4%)	8 (0%)	30 68
2	C	148/151 (98%)	134 (90%)	11 (7%)	3 (2%)	6 31
2	D	148/151 (98%)	134 (90%)	12 (8%)	2 (1%)	9 40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	150/172 (87%)	130 (87%)	19 (13%)	1 (1%)	19	57
3	F	156/172 (91%)	133 (85%)	18 (12%)	5 (3%)	3	21
All	All	4484/4566 (98%)	4246 (95%)	210 (5%)	28 (1%)	24	60

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	276	ILE
2	C	20	ARG
1	B	838	LEU
3	E	154	ASN
3	F	16	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1708/1716 (100%)	1707 (100%)	1 (0%)	92	95
1	B	1706/1716 (99%)	1702 (100%)	4 (0%)	92	94
2	C	129/130 (99%)	127 (98%)	2 (2%)	58	73
2	D	129/130 (99%)	129 (100%)	0	100	100
3	E	132/151 (87%)	131 (99%)	1 (1%)	79	85
3	F	138/151 (91%)	138 (100%)	0	100	100
All	All	3942/3994 (99%)	3934 (100%)	8 (0%)	91	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	85	PHE
2	C	70	LEU
1	B	683	LEU
1	B	619	ILE
2	C	13	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1311	GLN
1	B	1686	GLN
1	B	1353	HIS
1	B	1501	GLN
1	B	1758	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](#)

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
4	ADP	B	2001	-	24,29,29	0.96	1 (4%)	29,45,45	1.53	5 (17%)
5	PO4	A	2002	6	4,4,4	1.52	1 (25%)	6,6,6	0.45	0
5	PO4	B	2002	6	4,4,4	1.50	1 (25%)	6,6,6	0.46	0
4	ADP	A	2001	6	24,29,29	0.96	1 (4%)	29,45,45	1.52	4 (13%)

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
4	ADP	B	2001	-	-	2/12/32/32	0/3/3/3
4	ADP	A	2001	6	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2002	PO4	P-O1	2.61	1.57	1.50
5	B	2002	PO4	P-O1	2.59	1.56	1.50
4	B	2001	ADP	C5-C4	2.41	1.47	1.40
4	A	2001	ADP	C5-C4	2.40	1.47	1.40

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	ADP	PA-O3A-PB	-3.76	119.91	132.83
4	A	2001	ADP	PA-O3A-PB	-3.69	120.15	132.83
4	B	2001	ADP	N3-C2-N1	-3.66	122.96	128.68
4	A	2001	ADP	N3-C2-N1	-3.65	122.97	128.68
4	B	2001	ADP	C3'-C2'-C1'	3.30	105.95	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

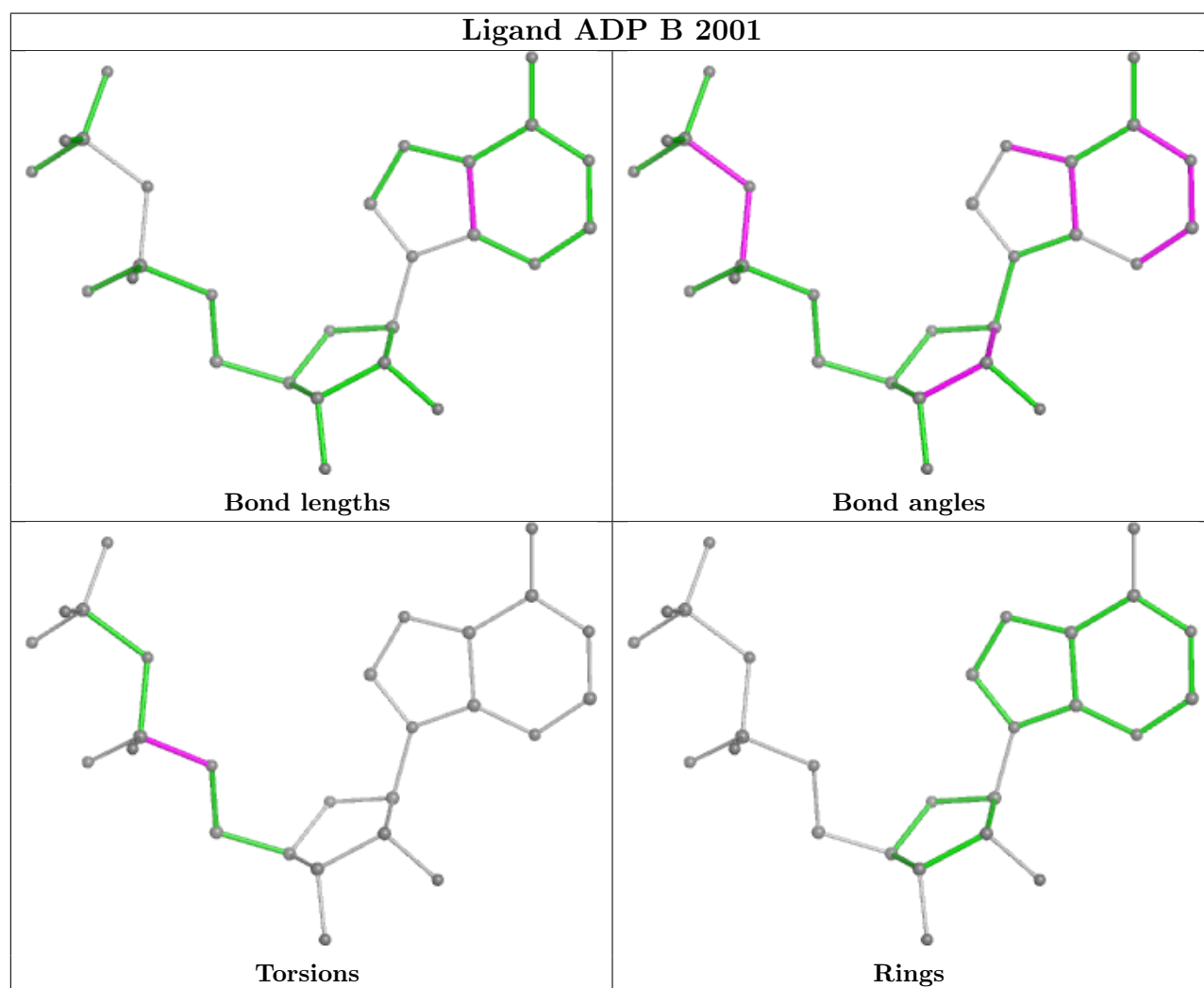
Mol	Chain	Res	Type	Atoms
4	A	2001	ADP	C5'-O5'-PA-O1A
4	A	2001	ADP	C5'-O5'-PA-O3A
4	B	2001	ADP	C5'-O5'-PA-O3A
4	B	2001	ADP	C5'-O5'-PA-O1A

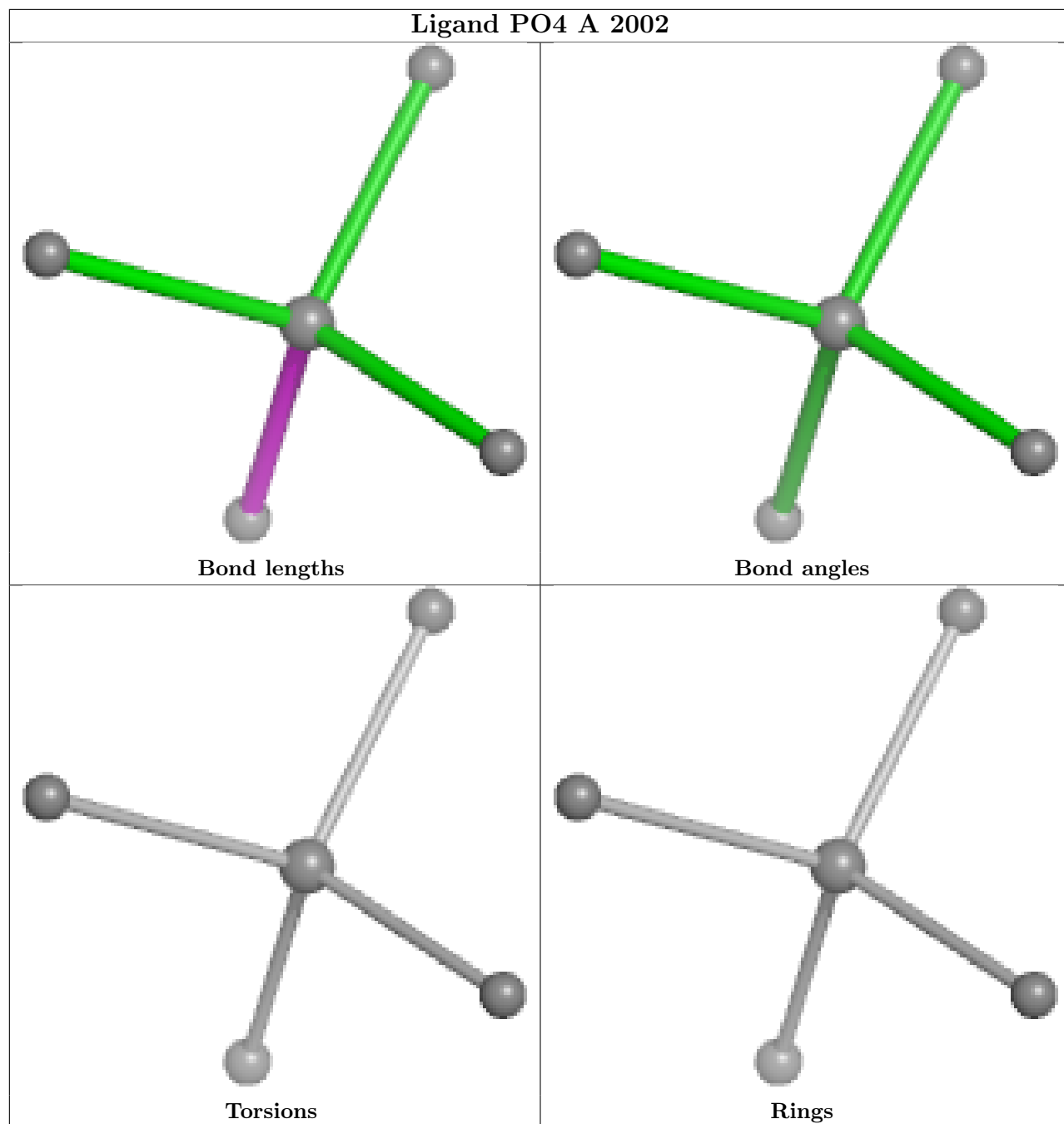
There are no ring outliers.

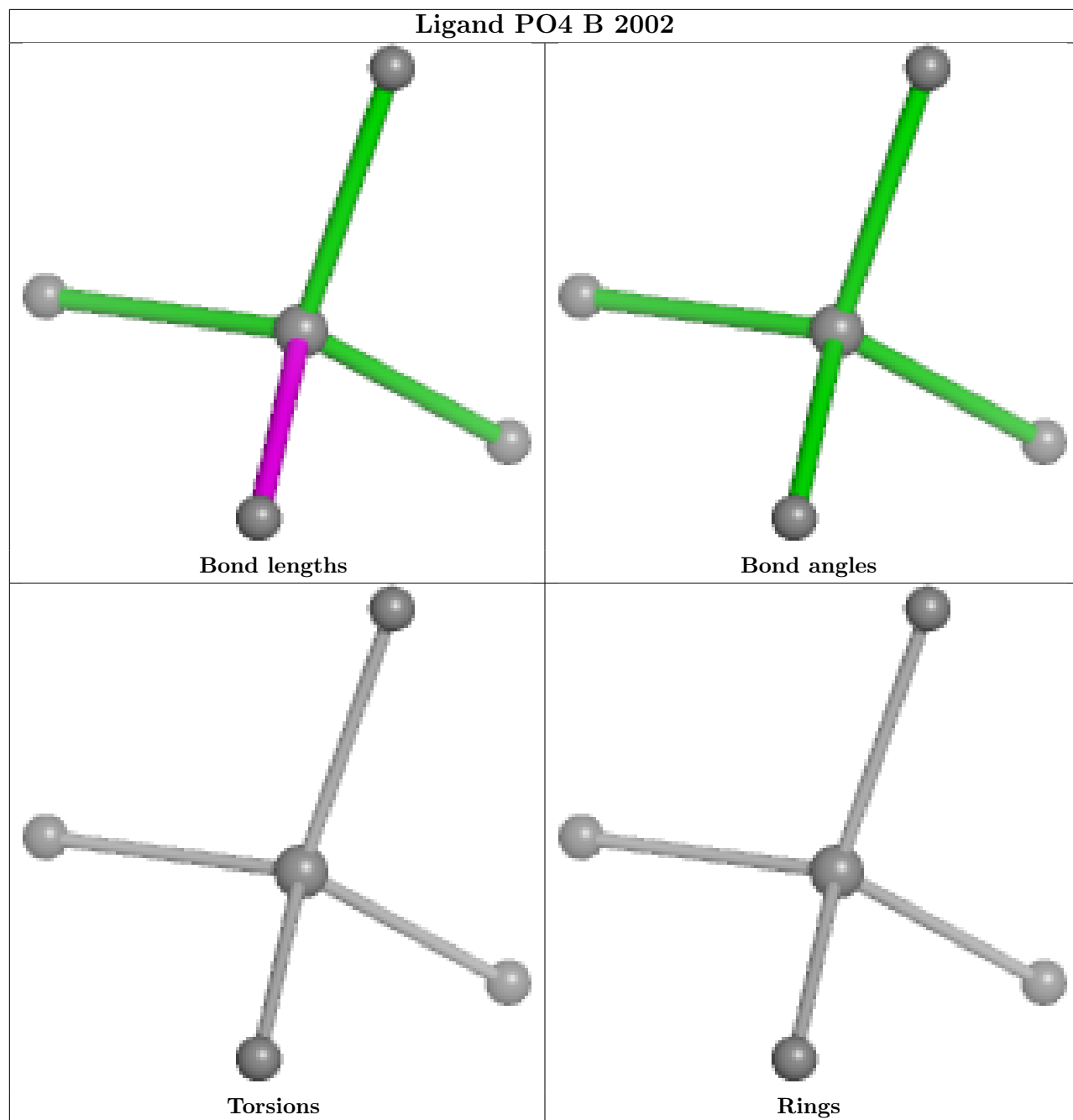
4 monomers are involved in 6 short contacts:

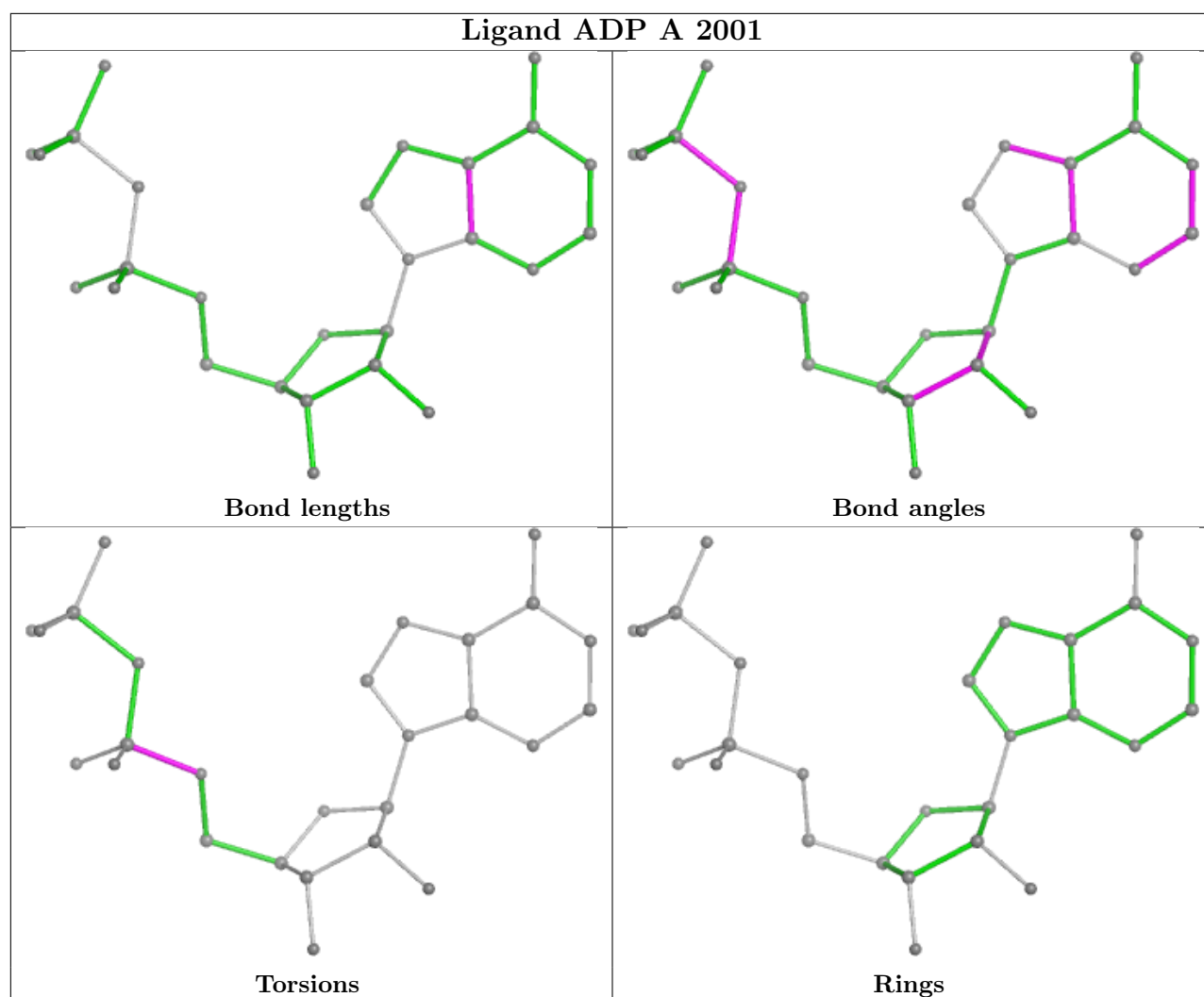
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2001	ADP	1	0
5	A	2002	PO4	1	0
5	B	2002	PO4	1	0
4	A	2001	ADP	3	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1830:ARG	C	1831:GLN	N	3.54

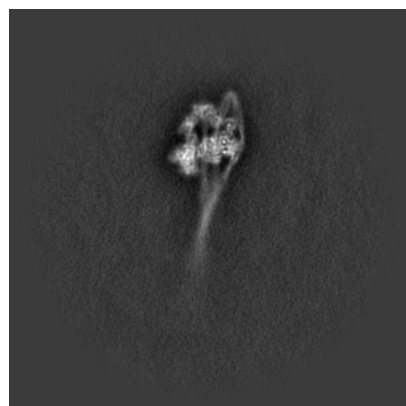
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55382. These allow visual inspection of the internal detail of the map and identification of artifacts.

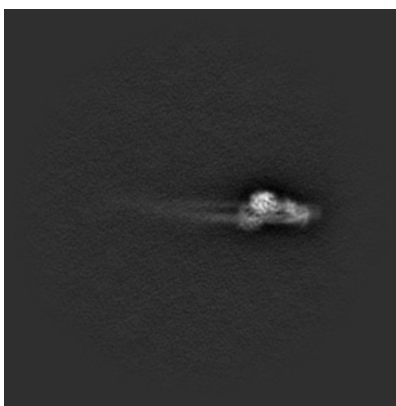
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

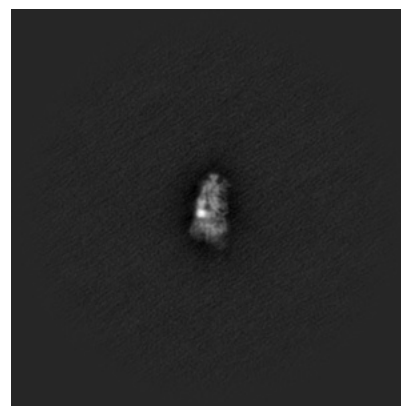
6.1.1 Primary map



X

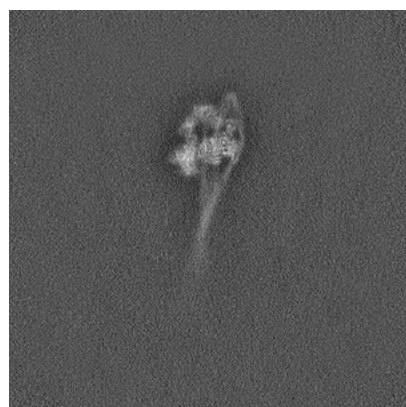


Y

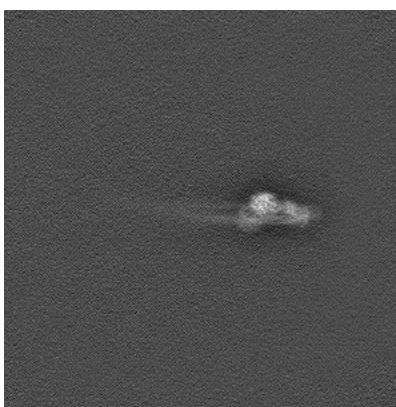


Z

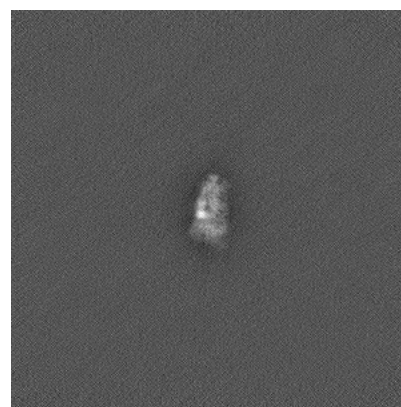
6.1.2 Raw map



X



Y

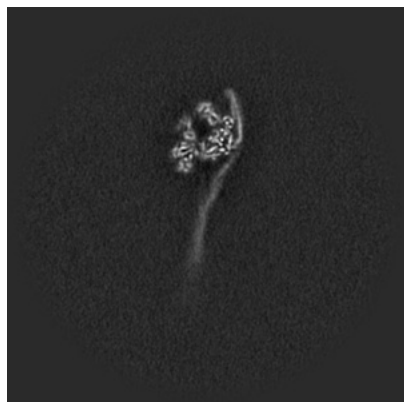


Z

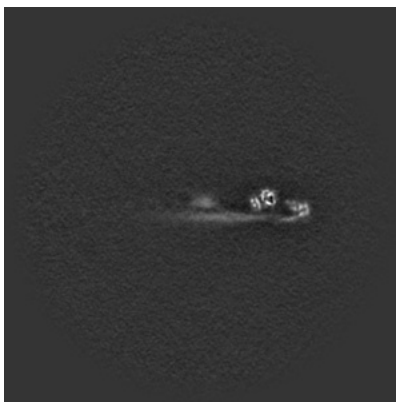
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

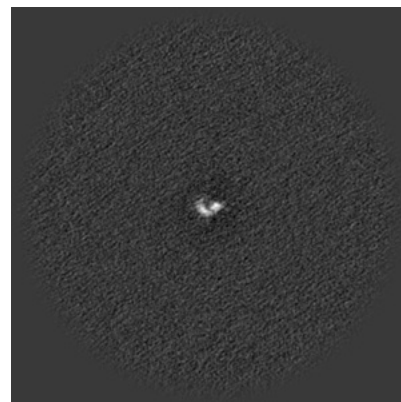
6.2.1 Primary map



X Index: 256



Y Index: 256

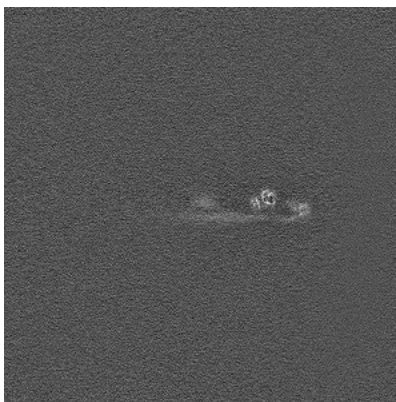


Z Index: 256

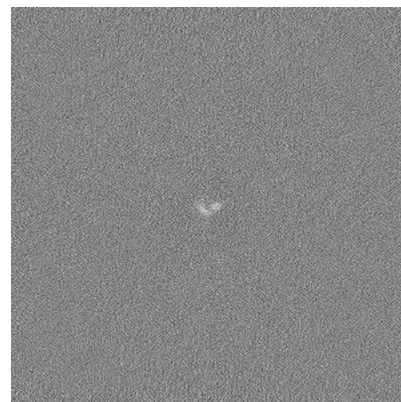
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

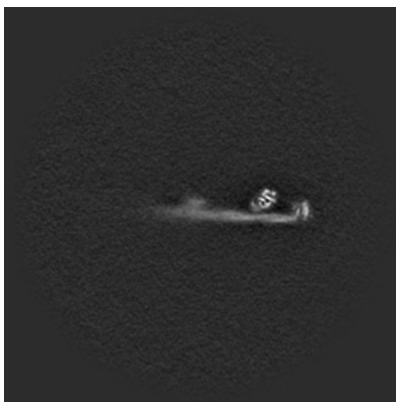
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

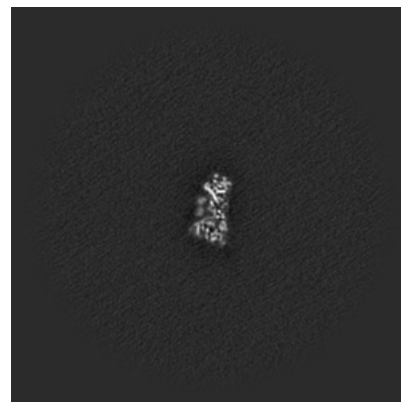
6.3.1 Primary map



X Index: 260

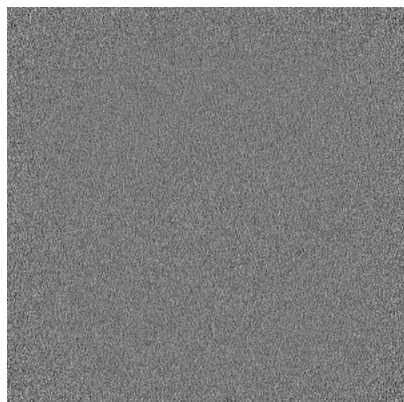


Y Index: 251

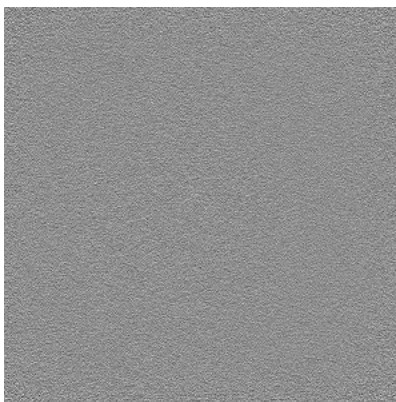


Z Index: 328

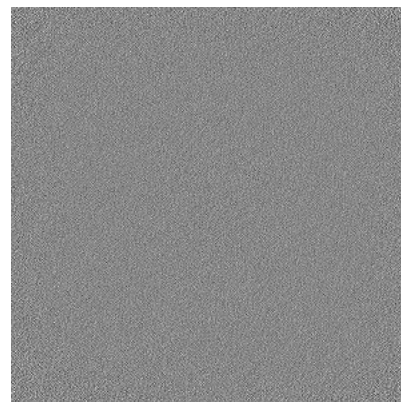
6.3.2 Raw map



X Index: 0



Y Index: 0

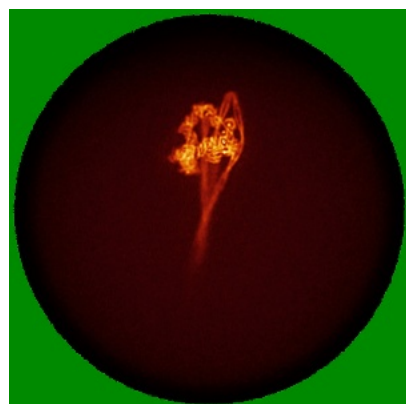


Z Index: 511

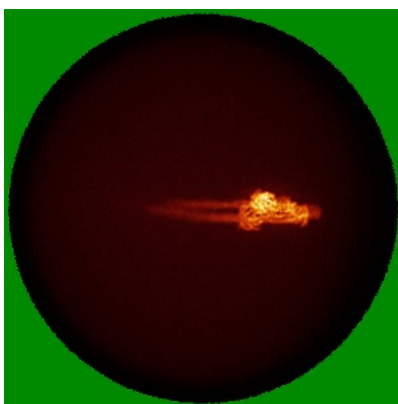
The images above show the largest variance slices of the map in three orthogonal directions.

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

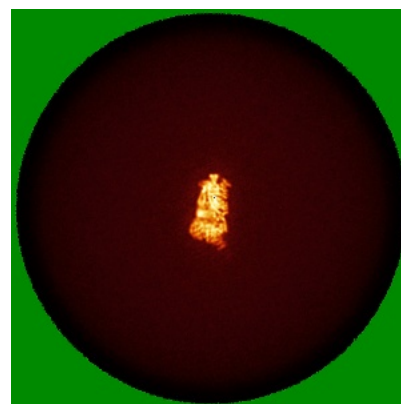
6.4.1 Primary map



X

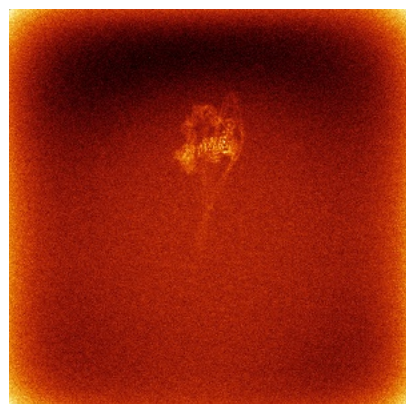


Y

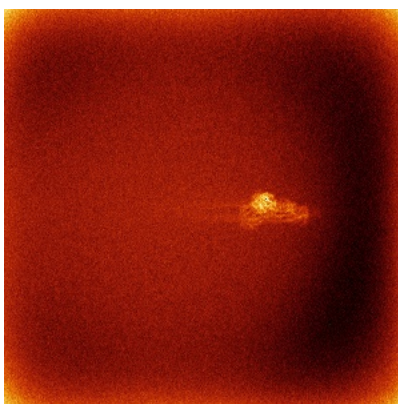


Z

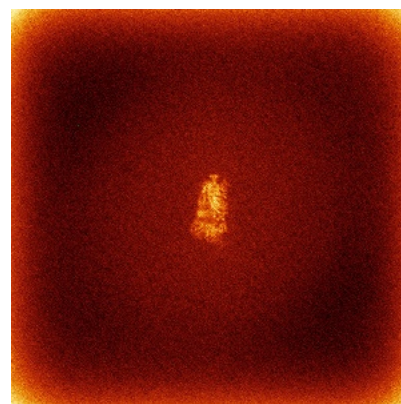
6.4.2 Raw map



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.

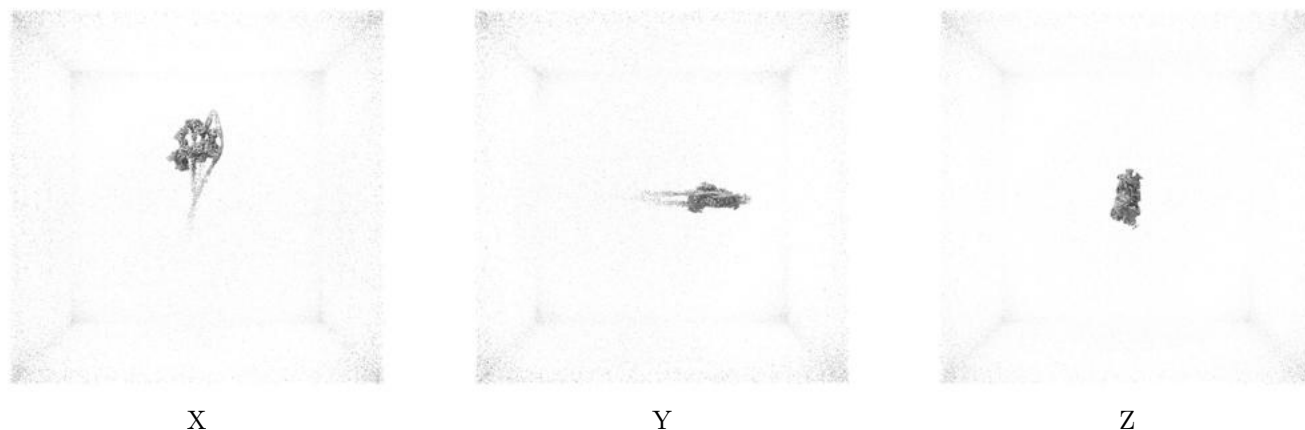
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

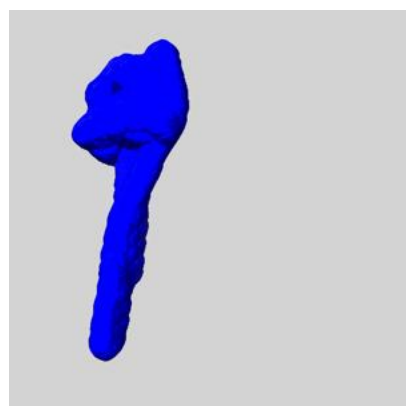
6.6 Mask visualisation [i](#)

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

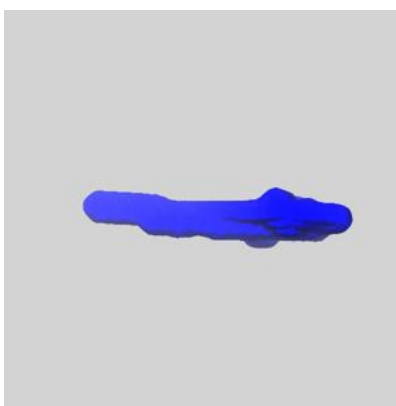
A mask typically either:

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

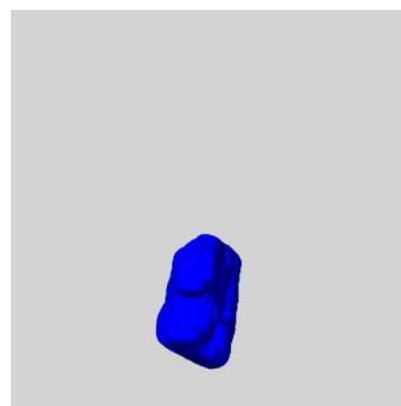
6.6.1 emd_55382_msk_1.map [i](#)



X



Y

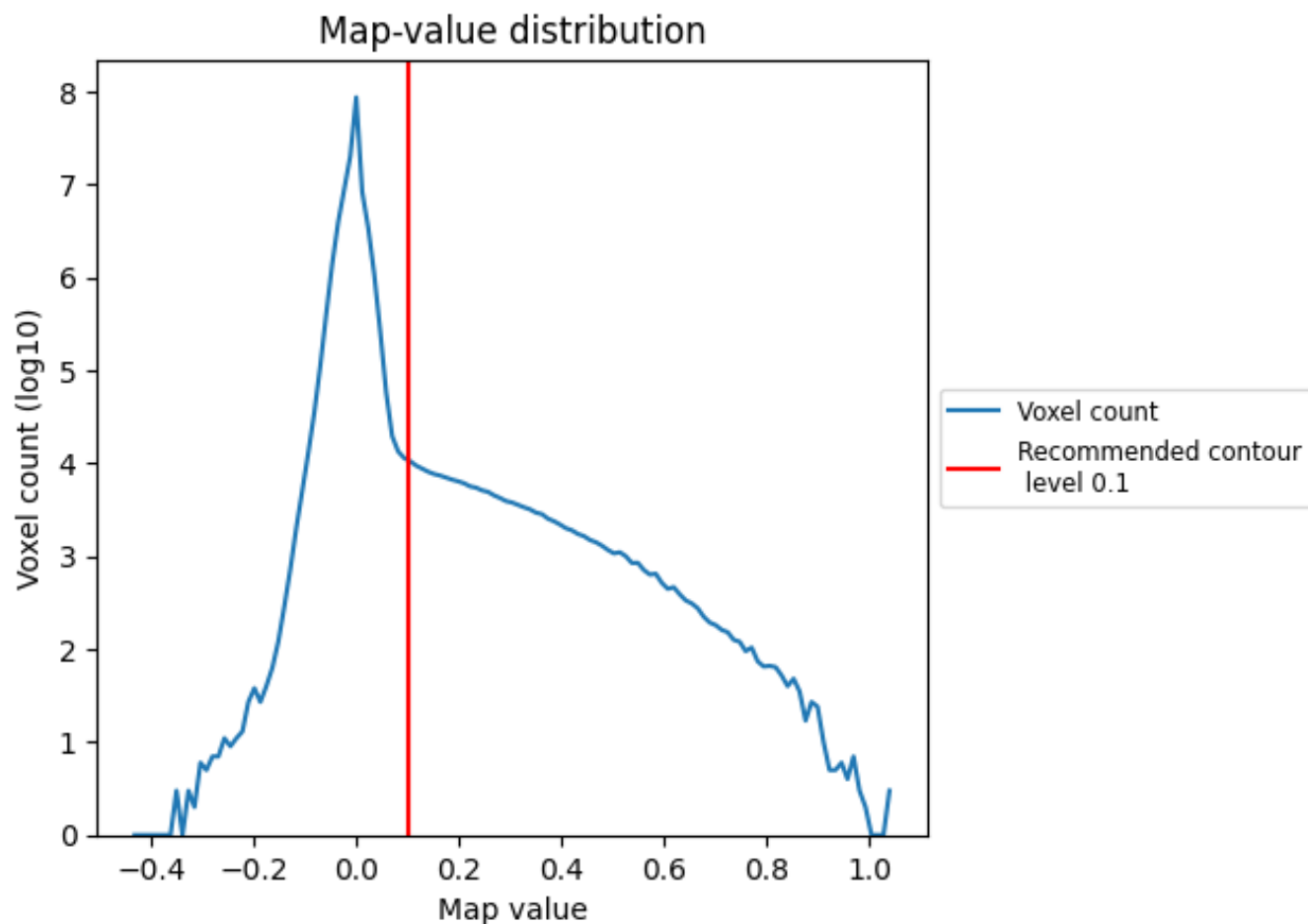


Z

7 Map analysis [i](#)

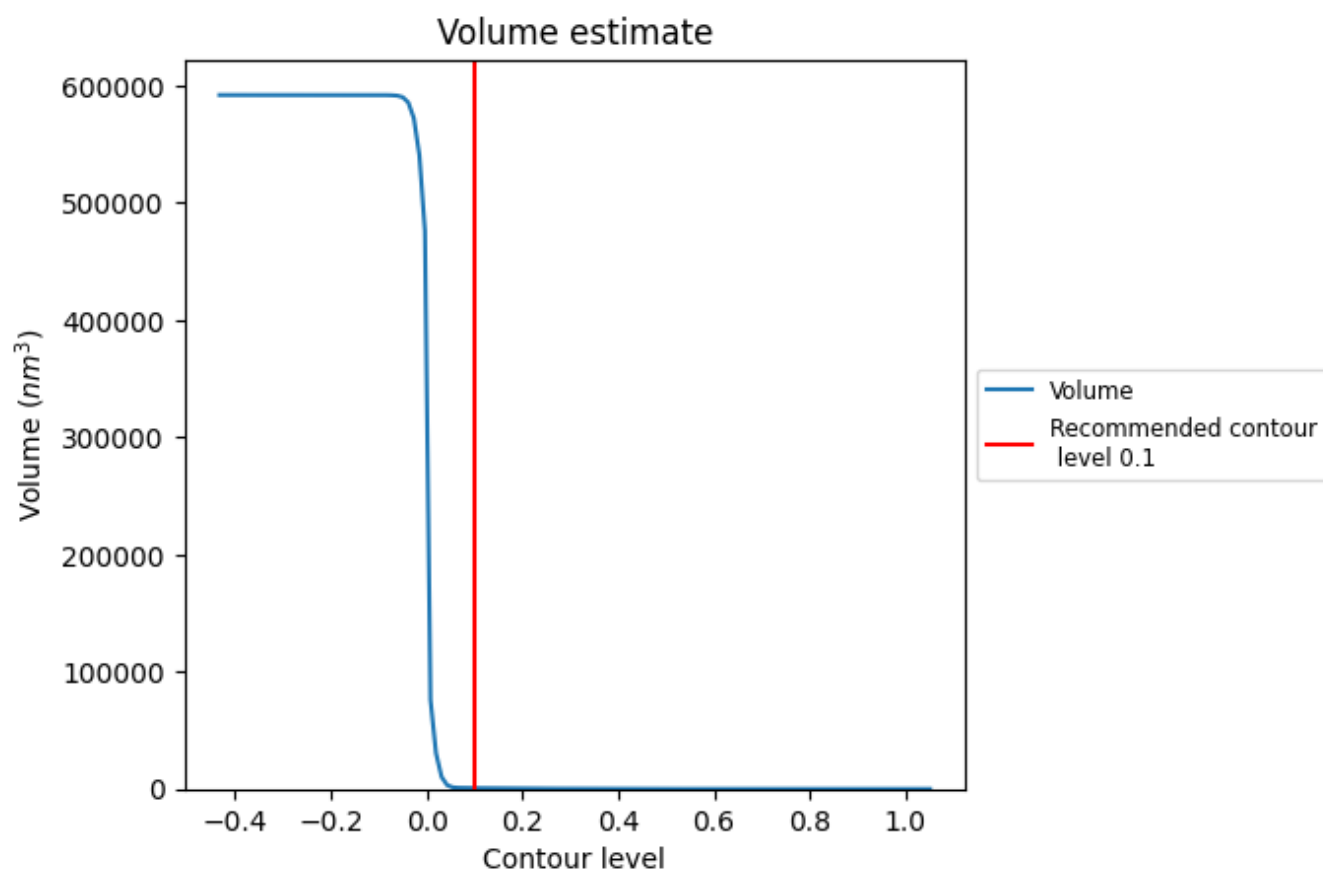
This section contains the results of statistical analysis of the map.

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.

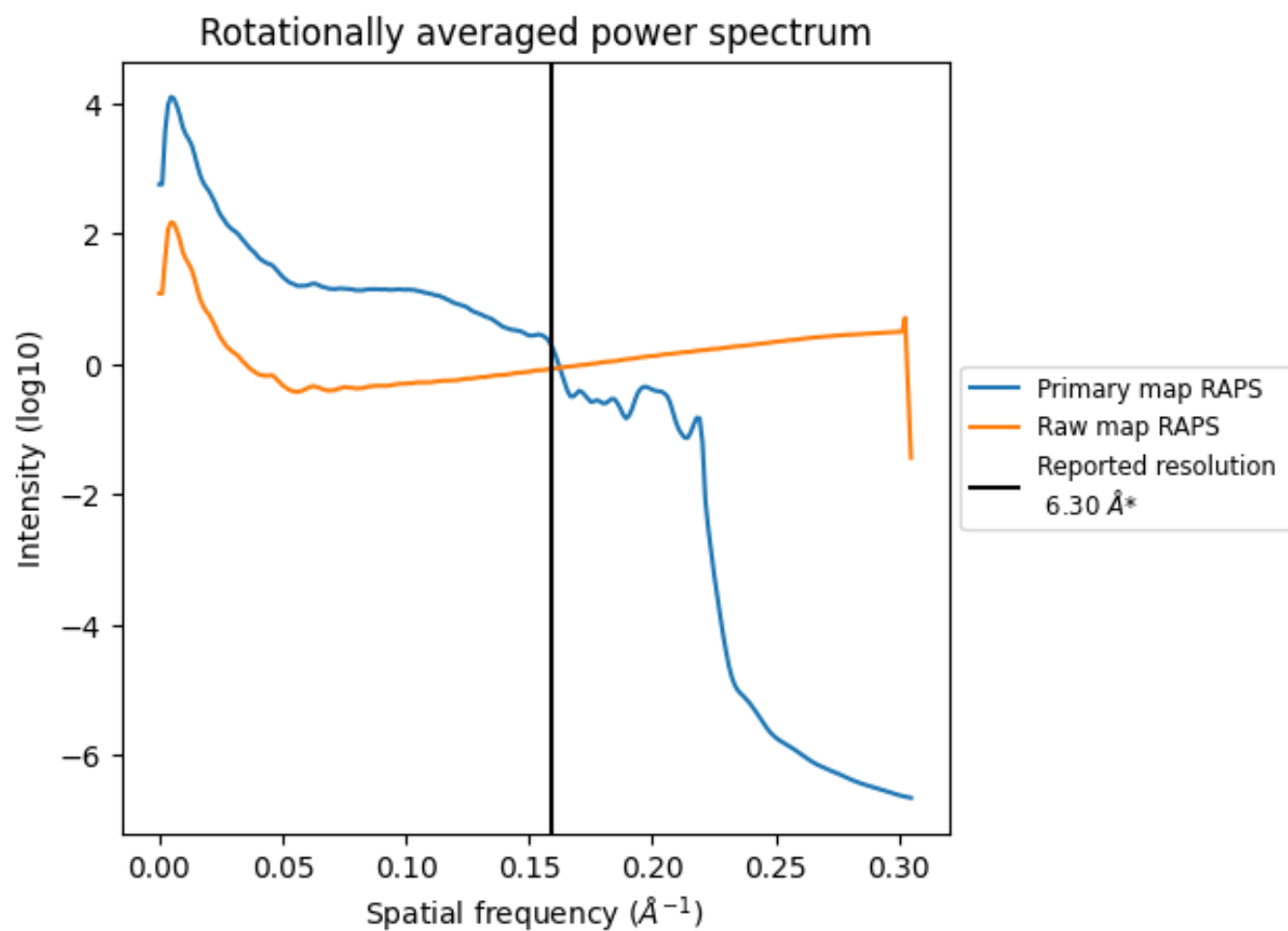
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 737 nm^3 ; this corresponds to an approximate mass of 666 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 ⓘ

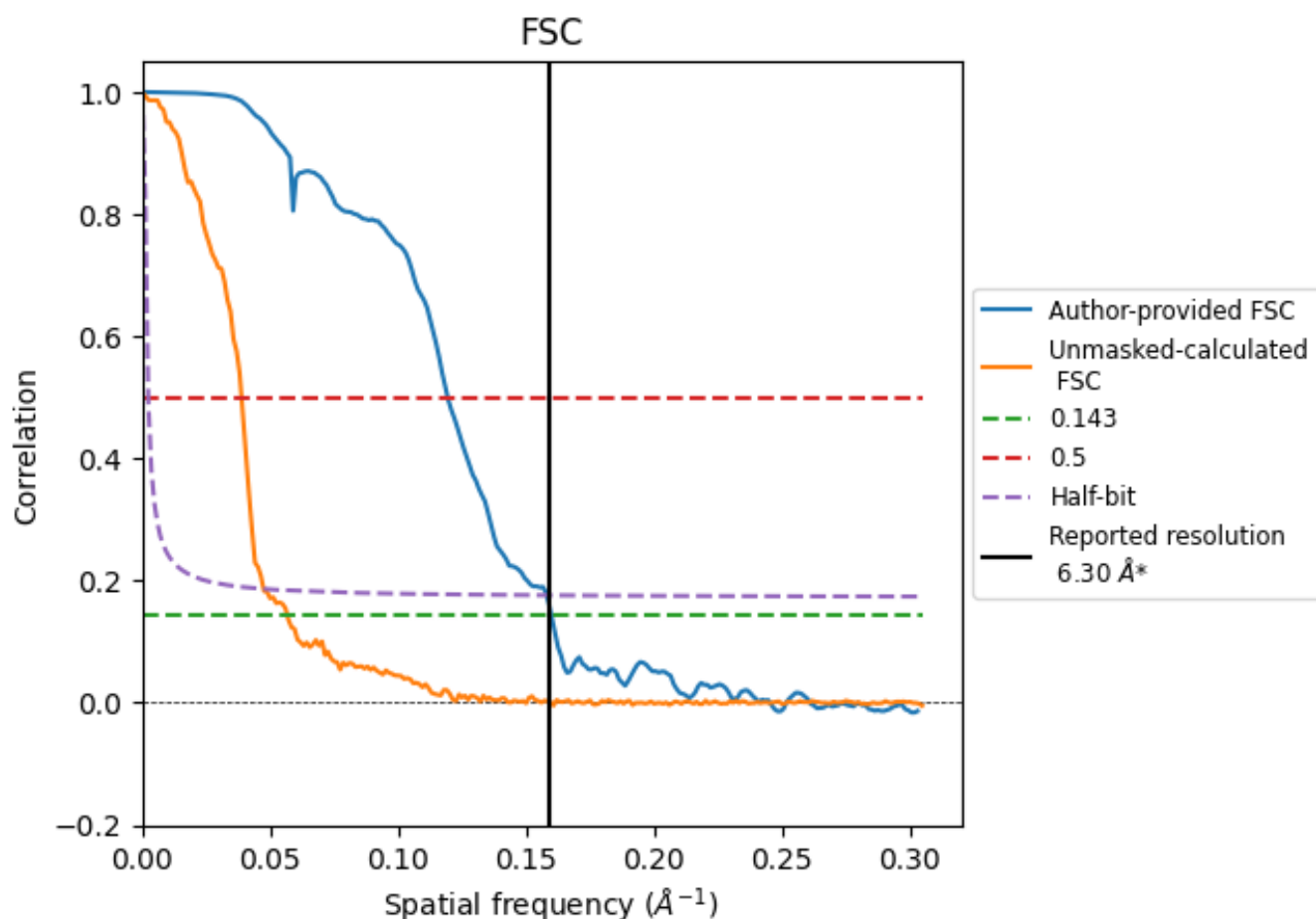


*Reported resolution corresponds to spatial frequency of 0.159 Å⁻¹

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 0.159 \AA^{-1}

8.2 Resolution estimates [i](#)

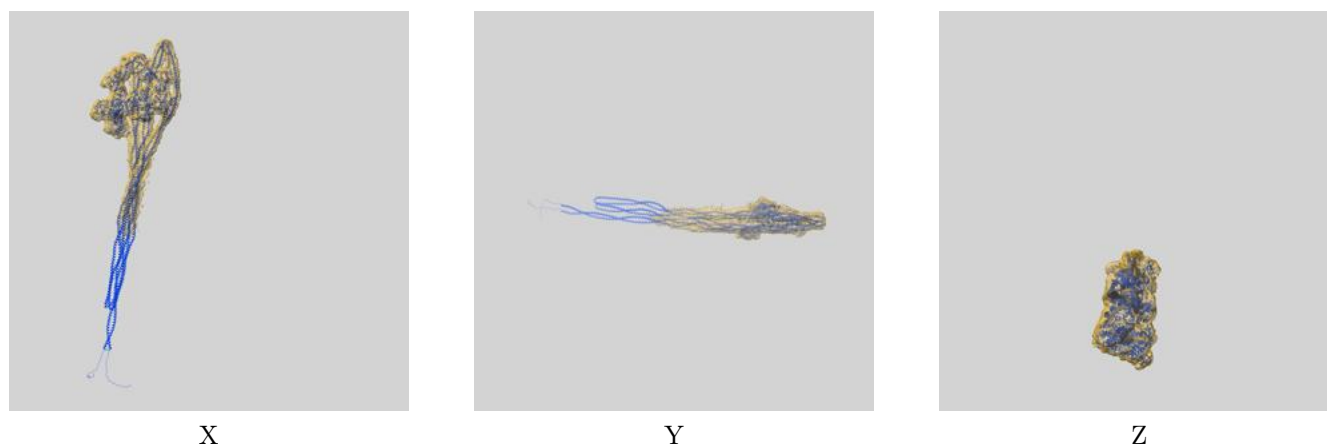
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.25	8.38	6.33
Unmasked-calculated*	17.64	25.77	21.05

*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 17.64 differs from the reported value 6.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55382 and PDB model 9SZR. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



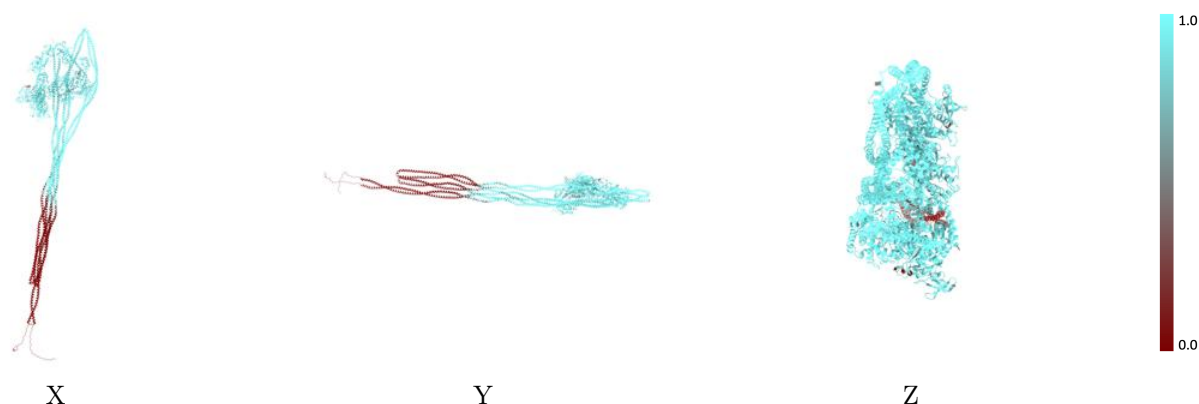
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



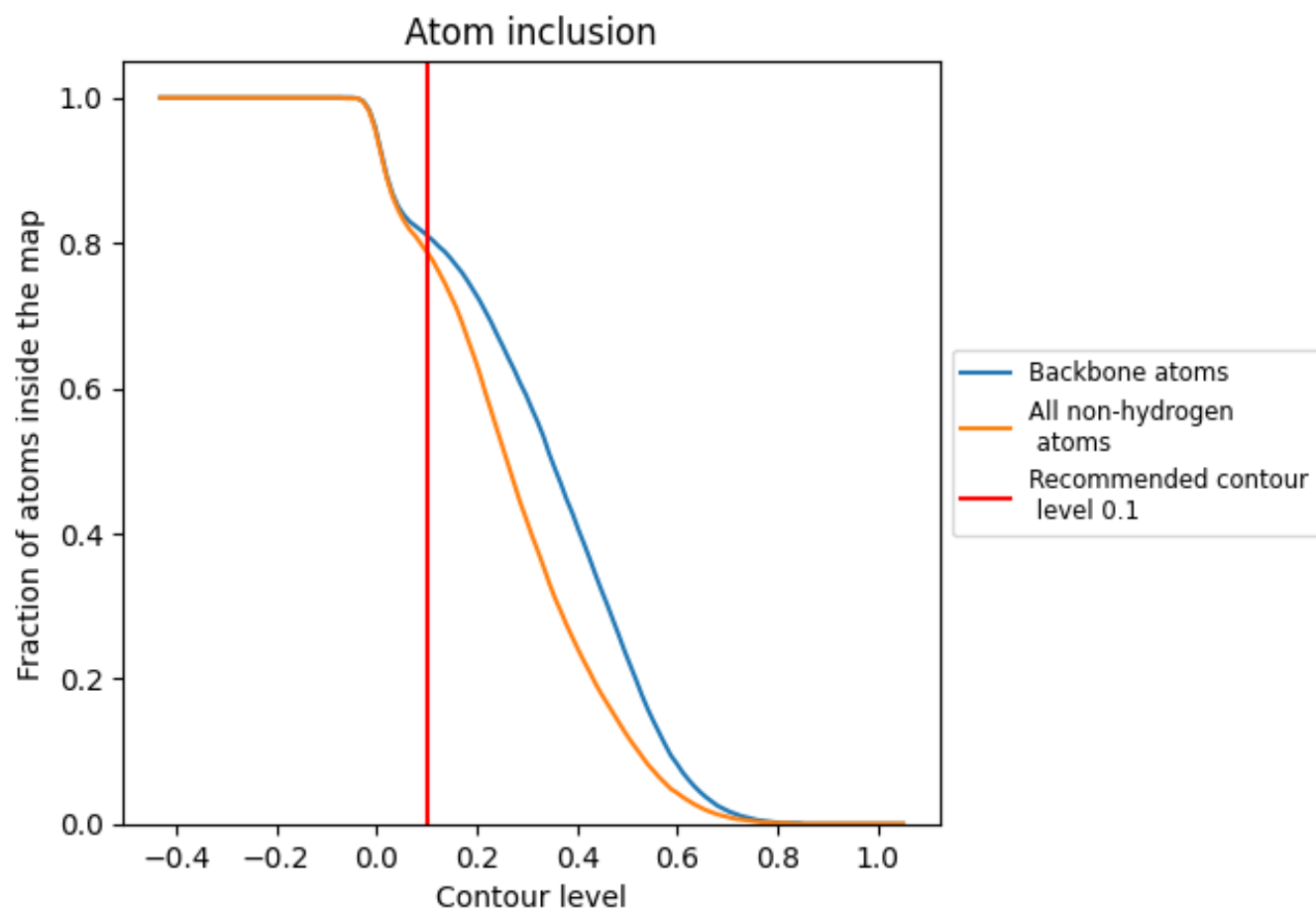
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7870	<div></div> 0.1250
A	<div></div> 0.7570	<div></div> 0.1240
B	<div></div> 0.7610	<div></div> 0.1180
C	<div></div> 0.9710	<div></div> 0.1800
D	<div></div> 0.9530	<div></div> 0.1540
E	<div></div> 0.9720	<div></div> 0.1440
F	<div></div> 0.9890	<div></div> 0.1340

1.0

0.0

<0.0