



## wwPDB EM Validation Summary Report ⓘ

Jun 29, 2024 – 09:01 am BST

PDB ID : 8QOZ  
EMDB ID : EMD-18542  
Title : Cryo-EM Structure of Pre-B+5'ss+ATPgammaS Complex (core part)  
Authors : Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.  
Deposited on : 2023-09-29  
Resolution : 3.10 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](mailto: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>.

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

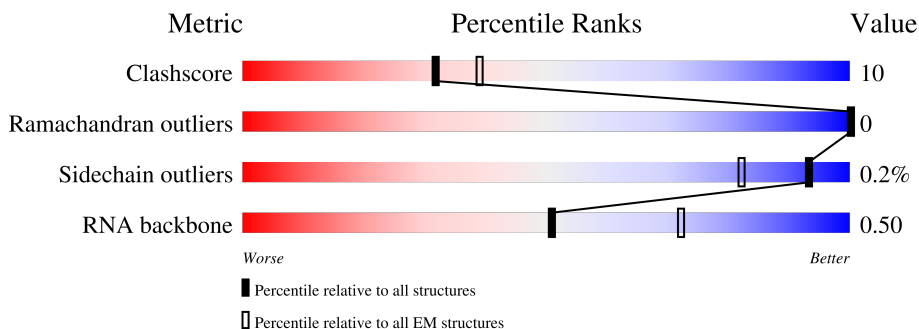
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	160	11% 86%
2	G	820	12% 85%
3	J	683	9% 88%
4	L	499	60% 16% 25%
5	F	522	7% 88%
6	N	941	5% 37% 11% 51%
7	A	2335	62% 22% 15%

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Mol	Chain	Length	Quality of chain
8	U	565	
9	S	800	
10	C	972	
11	M	128	
12	D	142	
13	5	117	
14	z	11	
15	7	793	
16	4	144	
17	6	106	

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 44360 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 U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	22	158	97	28	32	1	0	0

- Molecule 2 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	122	1077	673	205	197	2	0	0

- Molecule 3 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	84	679	419	138	119	3	0	0

- Molecule 4 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	376	2886	1796	526	552	12	0	0

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	61	488	297	97	93	1	0	0

- Molecule 6 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	457	3502	2191	655	644	12	0	0

- Molecule 7 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A	1977	16419	10577	2865	2907	70	0	0

- Molecule 8 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	U	456	3749	2427	635	673	14	0	0

- Molecule 9 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	S	148	1164	724	216	222	2	0	0

- Molecule 10 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	836	6592	4211	1110	1238	33	0	0

- Molecule 11 is a protein called NHP2-like protein 1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	124	962	608	171	178	5	0	0

- Molecule 12 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	141	1170	751	194	215	10	0	0

- Molecule 13 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	5	79	1660	744	275	562	79	0	0

- Molecule 14 is a RNA chain called 5'ss RNA oligo.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	z	11	239	107	46	75	11	0	0

- Molecule 15 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	7	107	846	522	152	169	3	0	0

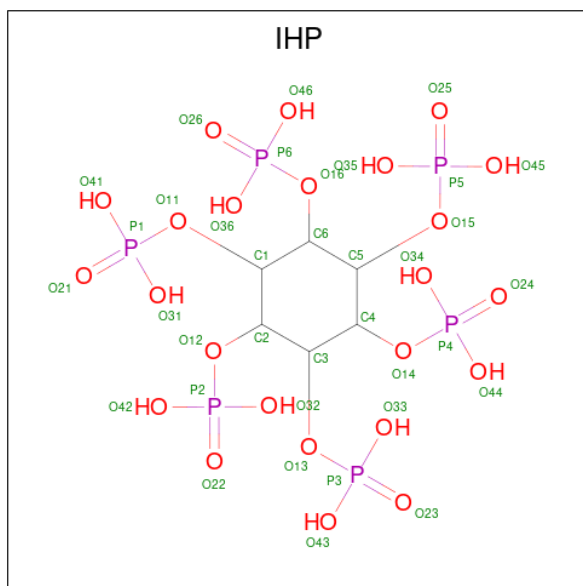
- Molecule 16 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	4	80	1699	760	297	562	80	0	0

- Molecule 17 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	6	48	1034	462	196	328	48	0	0

- Molecule 18 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ) (labeled as "Ligand of Interest" by depositor).

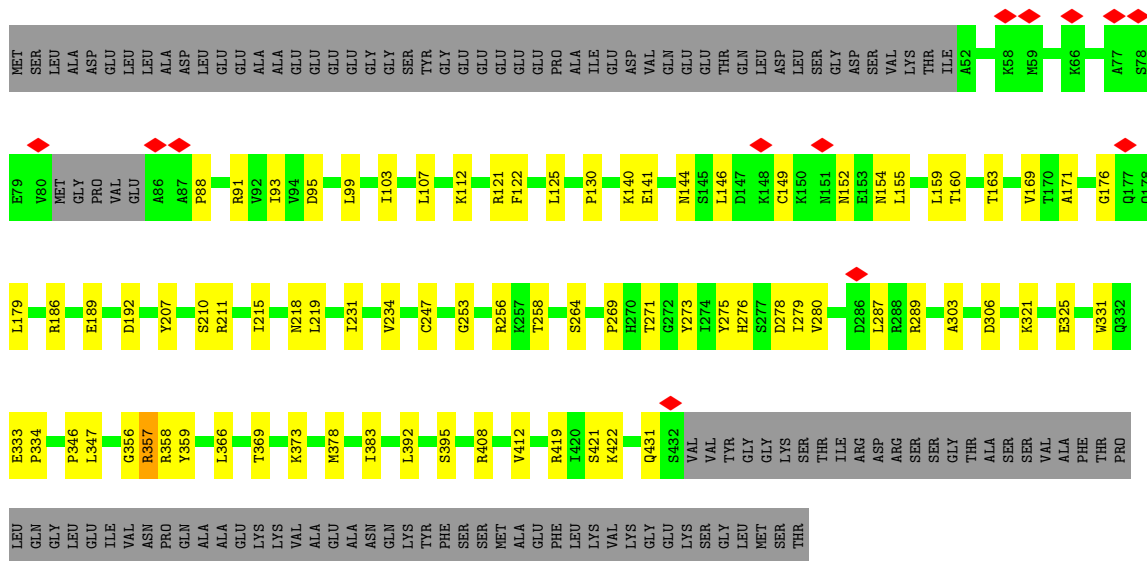


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	A	1	36	6	24	6	0

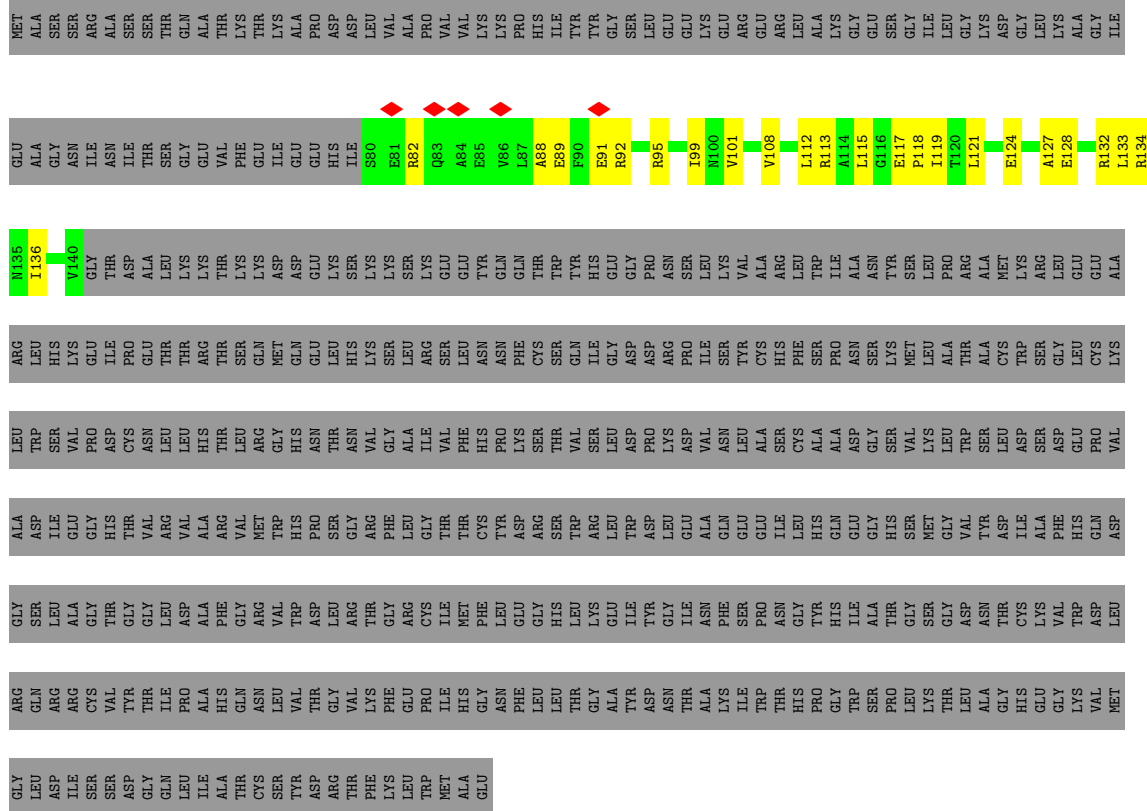




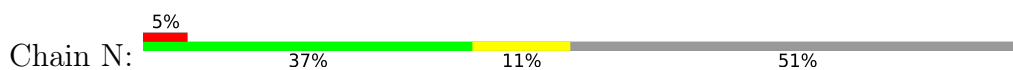


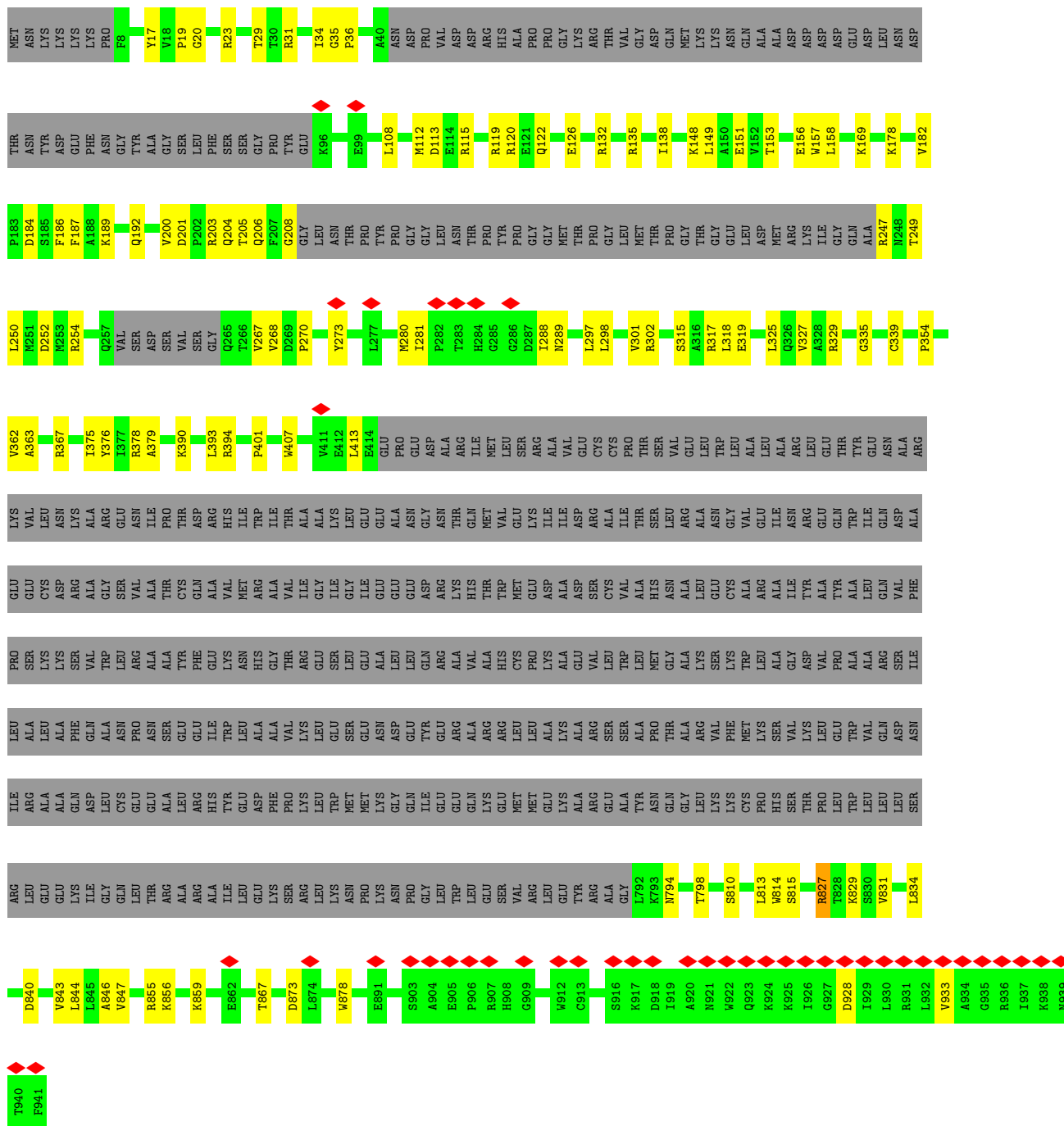


• Molecule 5: U4/U6 small nuclear ribonucleoprotein Prp4

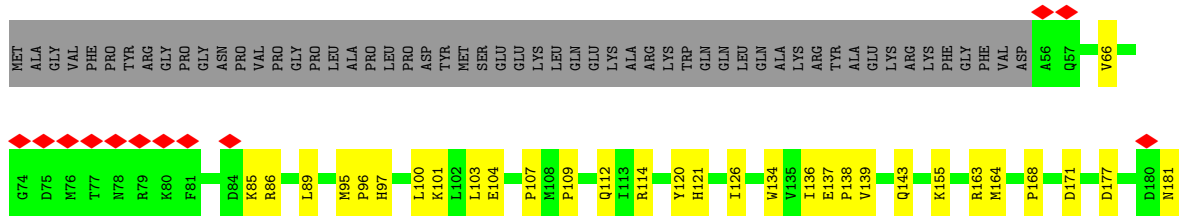


• Molecule 6: Pre-mRNA-processing factor 6

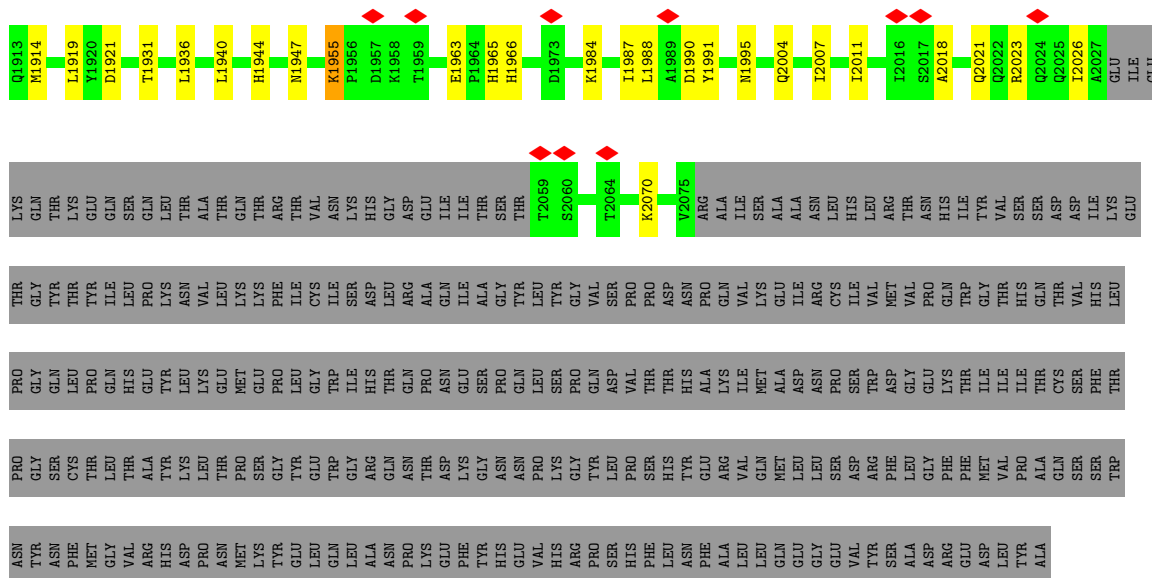




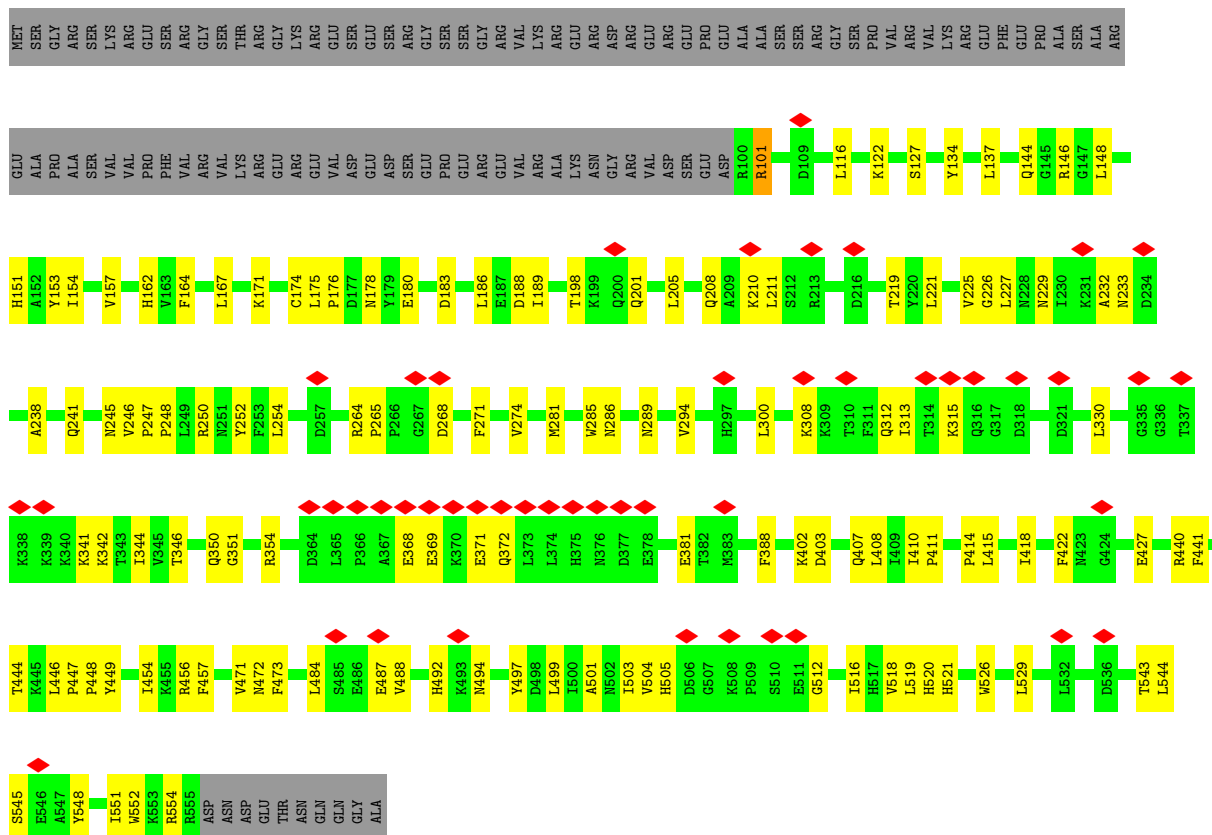
• Molecule 7: Pre-mRNA-processing factor 8



P1812	L1817	F1818	L1819	L1820	L1821	L1822	Q1830	L1831	L1832	L1833	G1834	Q1835	L1836	W1839	K1840	T1841	E1844	V1845	A1846	L1848	I1849	R1850	K1859	Q1860	I1861	M1868	L1872	E1873	L1876	F1879	R1878	V1878	V1877	K1792	F1793	F1794	E1795	G1796	L1798	P1802	I1803	N1804	G1805	A1806	L1807	F1808	I1809	P1812
D1706	M1710	M1717	P1720	A1729	M1737	L1740	E1757	P1758	T1759	Y1762	L1763	L1771	Q1775	I1776	W1777	F1779	V1780	D1781	D1782	V1785	Y1786	R1787	V1788	K1792	F1793	F1794	E1795	G1796	L1798	P1802	I1803	N1804	G1805	A1806	L1807	F1808	I1809	P1812	D1904	P1912								
Q1589	E1600	L1601	L1604	E1605	L1606	E1607	L1608	K1618	S1619	Y1620	K1621	M1622	M1623	S1624	S1625	I1629	L1630	L1631	F1632	A1633	S1634	W1637	M1638	V1639	S1640	R1641	P1642	M1652	D1653	K1659	Y1660	V1661	I1662	D1663	I1664	R1667	Y1671	D1672	S1673	I1676	Y1679	K1683	D1686	Y1687	D1690	N1691		
Y1494	F1495	W1498	L1501	F1502	W1503	E1504	A1506	S1507	E1510	M1513	K1514	W1515	K1516	Q1522	L1536	W1537	W1538	S1539	P1540	T1541	R1544	Y1548	L1555	G1559	I1560	S1572	L1573	I1574	Q1575	L1576	F1577	R1578	Q1582	Q1583	L1589	M1591	D1592	L1593	C1594	Q1595	V1596	F1597	D1598					
G1363	L1364	I1365	Y1369	I1372	W1375	E1376	S1377	E1378	F1379	I1380	S1381	D1382	V1385	W1386	L1403	D1410	S1411	W1412	R1414	G1415	I1416	P1417	I1418	I1419	M1420	T1421	Q1424	D1433	R1437	V1438	R1439	T1440	D1441	Q1444	P1452	H1460	W1465	L1478	L1485	F1490	T1493							
M1249	T1265	R1275	E1276	V1279	N1280	L1281	Q1282	Q1283	L1284	L1285	L1288	V1289	K1290	C1291	K1294	M1307	P1308	S1309	R1310	F1311	P1312	P1313	V1314	V1315	T1318	E1321	G1324	M1330	V1333	L1334	I1335	S1338	W1342	D1347	F1353	R1354	M1357	S1358	H1359	E1361	D1362							
R1136	D1137	R1141	M1143	D1146	V1147	L1148	L1149	A1152	V1153	F1154	W1155	R1160	F1174	V1175	S1176	V1177	D1181	N1182	L1186	R1195	I1196	L1197	P1198	T1202	S1203	Y1204	E1205	F1207	T1208	H1209	W1214	N1215	L1216	E1219	R1224	T1225	A1226	Q1227	C1228	R1231	M1237	V1244						
I1005	M1009	M1022	N1023	H1024	G1033	Y1043	L1046	D1049	V1052	R1057	E1060	G1063	P1064	M1067	L1072	I1085	R1086	L1087	F1088	C1089	R1090	V1091	I1092	H1096	I1097	F1098	F1099	R1107	D1108	L1109	N1110	Q1111	R1112	E1116	D1119	M1124	C1133											
Q860	R861	I867	L878	I881	K882	Q888	R889	F898	M899	D900	L901	Y902	S903	H904	L905	Y909	P913	L914	E915	K916	I917	T918	D923	E929	R933	W939	P942	P947	L950	I959	N960	N961	V965	N974	V975	M976	M984	I988	L999									
L731	P732	I735	M738	I739	Y742	W750	I761	R762	T766	V767	D768	K769	N775	L776	G777	R778	L779	T780	R781	L784	K785	Q788	E789	Y810	R820	I825	P828	Y832	D835	T836	I840	K847	Y850	K853	R855	Q858	S859											
P625	W630	A631	A632	G633	W634	F639	M641	R642	G643	I644	T645	E649	L652	L655	L656	G662	HIS	SER	GLY	VAL	ALA	LYS	THR	VAL	THR	LYS	Q675	R676	V677	E678	S679	H680	F681	D682	L683	E684	V689	M696	K606	D607	L608	K609	H610	T618	G622	K623	S624	W720
L487	D488	W489	V490	E491	L494	Q495	L507	R510	L516	D519	Y520	V521	F522	N523	K536	C547	E549	V550	L551	R552	E585	T554	V562	Q563	Y564	T418	R419	L422	D423	I424	P425	L428	V443	K449	K465	D467	K468	R470	F476	Q483	S484	T485	K486					
I182	V185	L188	L189	A190	I191	V203	F207	P212	R227	T247	D251	L257	T265	L269	R284	D285	I286	N287	L288	Q289	D290	E291	D292	V293	I299	I302	P307	Y312	K313	I314	A315	Y318	N321	V327	P335	M336	V337	V338										
D344	L347	P348	D353	P354	L355	I356	N357	R362	H363	S364	V365	K366	L371	P372	D373	D374	D375	L380	P381	V384	E385	L388	G416	R417	T418	R419	L422	D423	I424	P425	L428	V443	K449	K465	D467	K468	R470	F476	Q483	S484	T485	K486						

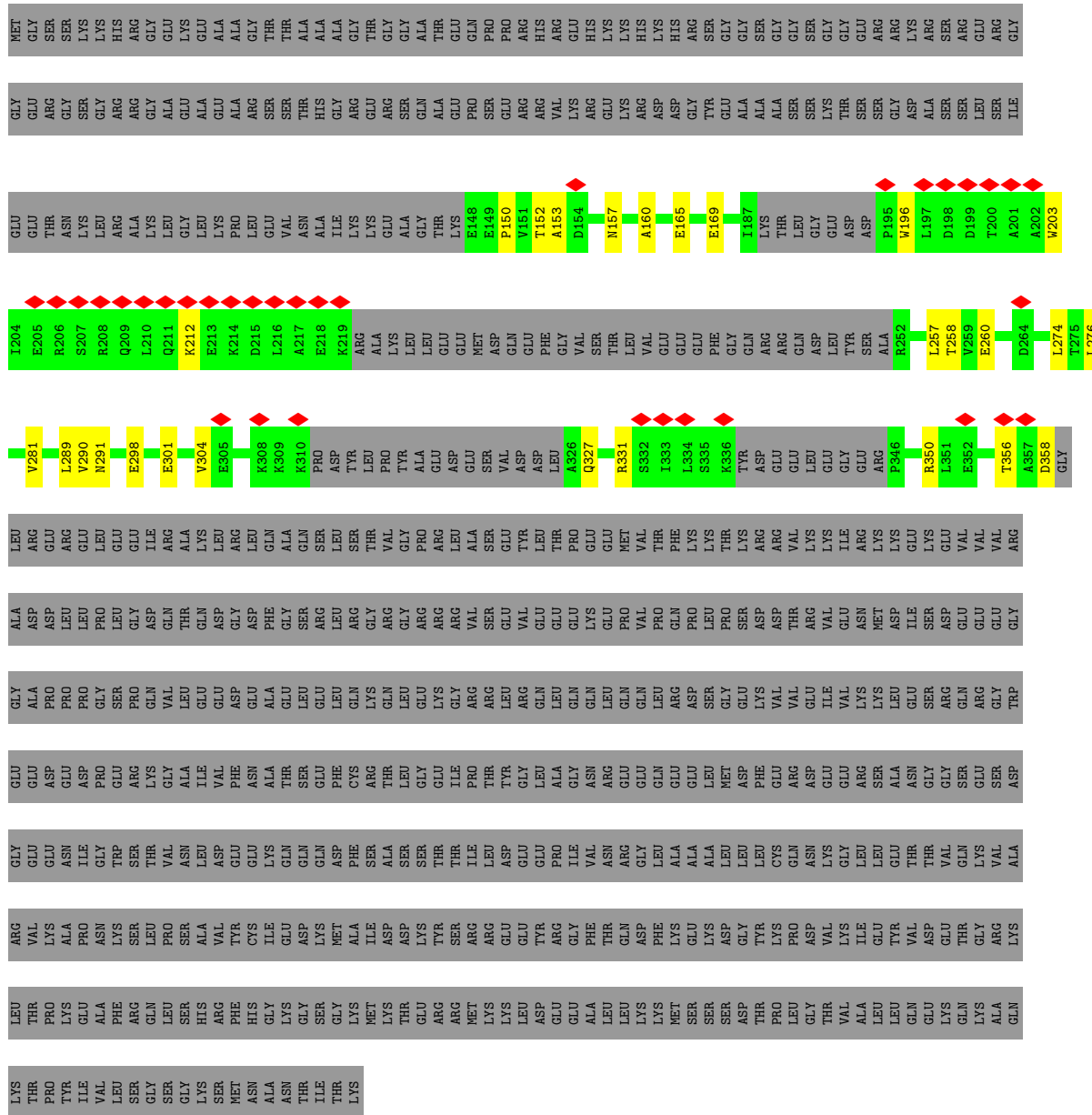


• Molecule 8: Ubiquitin carboxyl-terminal hydrolase 39

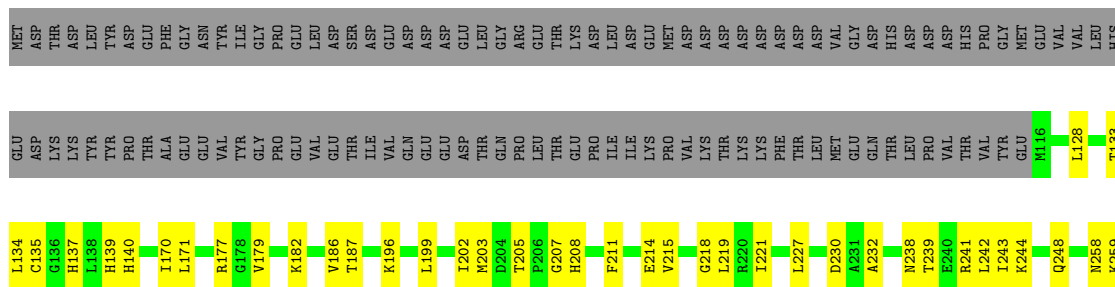


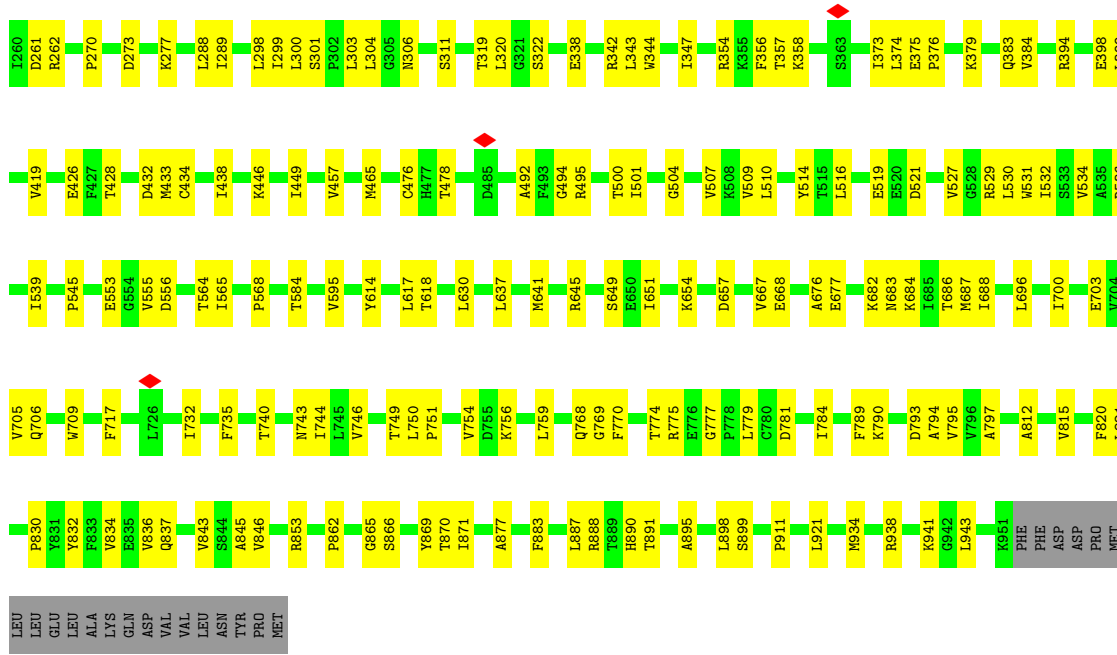
• Molecule 9: U4/U6.U5 tri-snRNP-associated protein 1



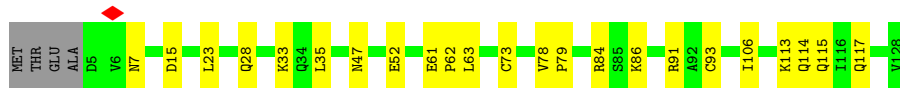
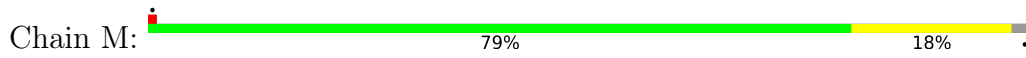


- Molecule 10: 116 kDa U5 small nuclear ribonucleoprotein component

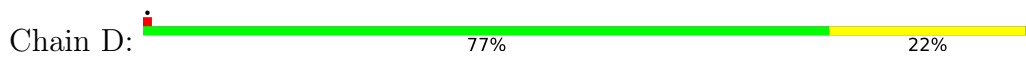




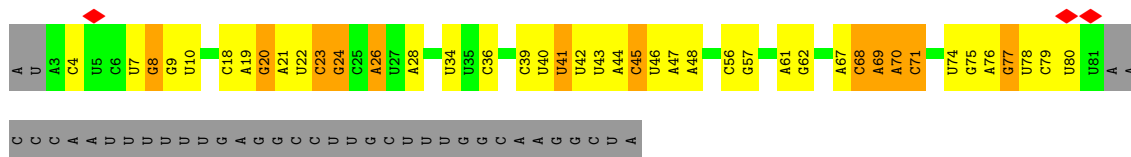
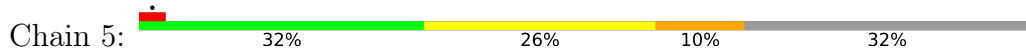
- Molecule 11: NHP2-like protein 1, N-terminally processed



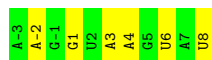
- Molecule 12: Thioredoxin-like protein 4A



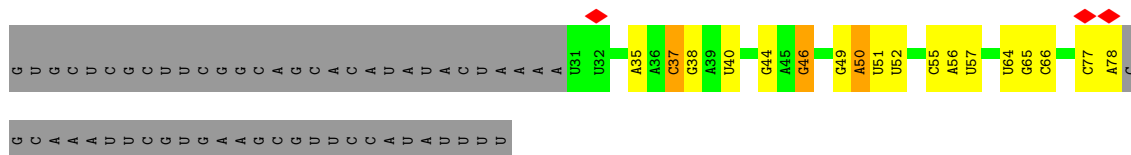
- Molecule 13: U5 snRNA



- Molecule 14: 5'ss RNA oligo









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	411185	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.224	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	556.8, 556.8, 556.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	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: IHP

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	0.24	0/158	0.57	0/209
2	G	0.23	0/1096	0.49	0/1455
3	J	0.25	0/686	0.54	0/914
4	L	0.25	0/2924	0.48	0/3938
5	F	0.24	0/491	0.58	0/657
6	N	0.24	0/3565	0.49	0/4818
7	A	0.25	0/16866	0.48	0/22880
8	U	0.24	0/3845	0.46	0/5208
9	S	0.23	0/1172	0.48	0/1567
10	C	0.25	0/6739	0.47	0/9151
11	M	0.24	0/974	0.47	0/1316
12	D	0.26	0/1199	0.45	0/1620
13	5	0.21	0/1850	0.75	0/2875
14	z	0.23	0/268	0.68	0/416
15	7	0.23	0/858	0.49	0/1152
16	4	0.19	0/1898	0.68	0/2954
17	6	0.20	0/1159	0.73	0/1806
All	All	0.24	0/45748	0.52	0/62936

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	B	158	0	166	8	0
2	G	1077	0	1066	21	0
3	J	679	0	728	20	0
4	L	2886	0	2885	61	0
5	F	488	0	499	16	0
6	N	3502	0	3379	84	0
7	A	16419	0	16348	377	0
8	U	3749	0	3769	81	0
9	S	1164	0	1173	21	0
10	C	6592	0	6615	140	0
11	M	962	0	1012	17	0
12	D	1170	0	1141	23	0
13	5	1660	0	842	24	0
14	z	239	0	119	0	0
15	7	846	0	837	19	0
16	4	1699	0	858	15	0
17	6	1034	0	521	11	0
18	A	36	0	6	2	0
All	All	44360	0	41964	808	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 10.

The worst 5 of 808 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)
7:A:1809:ILE:HB	7:A:1818:PHE:HB2	1.60	0.83
7:A:781:ARG:HA	7:A:1022:MET:HE1	1.60	0.83
2:G:253:ARG:HH12	7:A:313:LYS:HZ3	1.29	0.80
7:A:1775:GLN:HB2	7:A:1859:LYS:HE3	1.66	0.76
10:C:846:VAL:HG22	10:C:887:LEU:HD11	1.68	0.76

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	B	20/160 (12%)	19 (95%)	1 (5%)	0	100	100
2	G	118/820 (14%)	116 (98%)	2 (2%)	0	100	100
3	J	82/683 (12%)	82 (100%)	0	0	100	100
4	L	372/499 (74%)	362 (97%)	10 (3%)	0	100	100
5	F	59/522 (11%)	59 (100%)	0	0	100	100
6	N	447/941 (48%)	441 (99%)	6 (1%)	0	100	100
7	A	1971/2335 (84%)	1883 (96%)	88 (4%)	0	100	100
8	U	454/565 (80%)	437 (96%)	17 (4%)	0	100	100
9	S	138/800 (17%)	135 (98%)	3 (2%)	0	100	100
10	C	834/972 (86%)	818 (98%)	16 (2%)	0	100	100
11	M	122/128 (95%)	119 (98%)	3 (2%)	0	100	100
12	D	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
15	7	103/793 (13%)	101 (98%)	2 (2%)	0	100	100
All	All	4859/9360 (52%)	4708 (97%)	151 (3%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	B	17/140 (12%)	17 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	113/721 (16%)	113 (100%)	0	100	100
3	J	72/599 (12%)	71 (99%)	1 (1%)	67	86
4	L	303/424 (72%)	302 (100%)	1 (0%)	92	96
5	F	52/442 (12%)	52 (100%)	0	100	100
6	N	341/792 (43%)	339 (99%)	2 (1%)	86	94
7	A	1788/2108 (85%)	1784 (100%)	4 (0%)	93	97
8	U	418/511 (82%)	417 (100%)	1 (0%)	93	97
9	S	120/681 (18%)	119 (99%)	1 (1%)	81	92
10	C	738/866 (85%)	738 (100%)	0	100	100
11	M	108/111 (97%)	108 (100%)	0	100	100
12	D	129/130 (99%)	129 (100%)	0	100	100
15	7	91/709 (13%)	91 (100%)	0	100	100
All	All	4290/8234 (52%)	4280 (100%)	10 (0%)	93	97

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	1965	HIS
8	U	101	ARG
9	S	212	LYS
6	N	827	ARG
7	A	362	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
7	A	1752	GLN
8	U	275	GLN
7	A	775	ASN
7	A	1246	GLN
7	A	1522	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	5	78/117 (66%)	26 (33%)	3 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	z	10/11 (90%)	6 (60%)	0
16	4	79/144 (54%)	23 (29%)	0
17	6	47/106 (44%)	8 (17%)	2 (4%)
All	All	214/378 (56%)	63 (29%)	5 (2%)

5 of 63 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	5	8	G
13	5	9	G
13	5	10	U
13	5	20	G
13	5	21	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	5	70	A
13	5	77	G
13	5	78	U
17	6	51	U
17	6	77	C

## 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 monosaccharides 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	$\# Z  > 2$
18	IHP	A	2401	-	36,36,36	0.97	1 (2%)	54,60,60	1.35	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	IHP	A	2401	-	-	6/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	2401	IHP	P2-O12	2.26	1.63	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	2401	IHP	C5-C6-C1	4.11	119.41	110.41
18	A	2401	IHP	C6-C1-C2	3.89	118.93	110.41
18	A	2401	IHP	C6-C5-C4	3.31	117.66	110.41
18	A	2401	IHP	C4-C3-C2	2.26	115.35	110.41

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

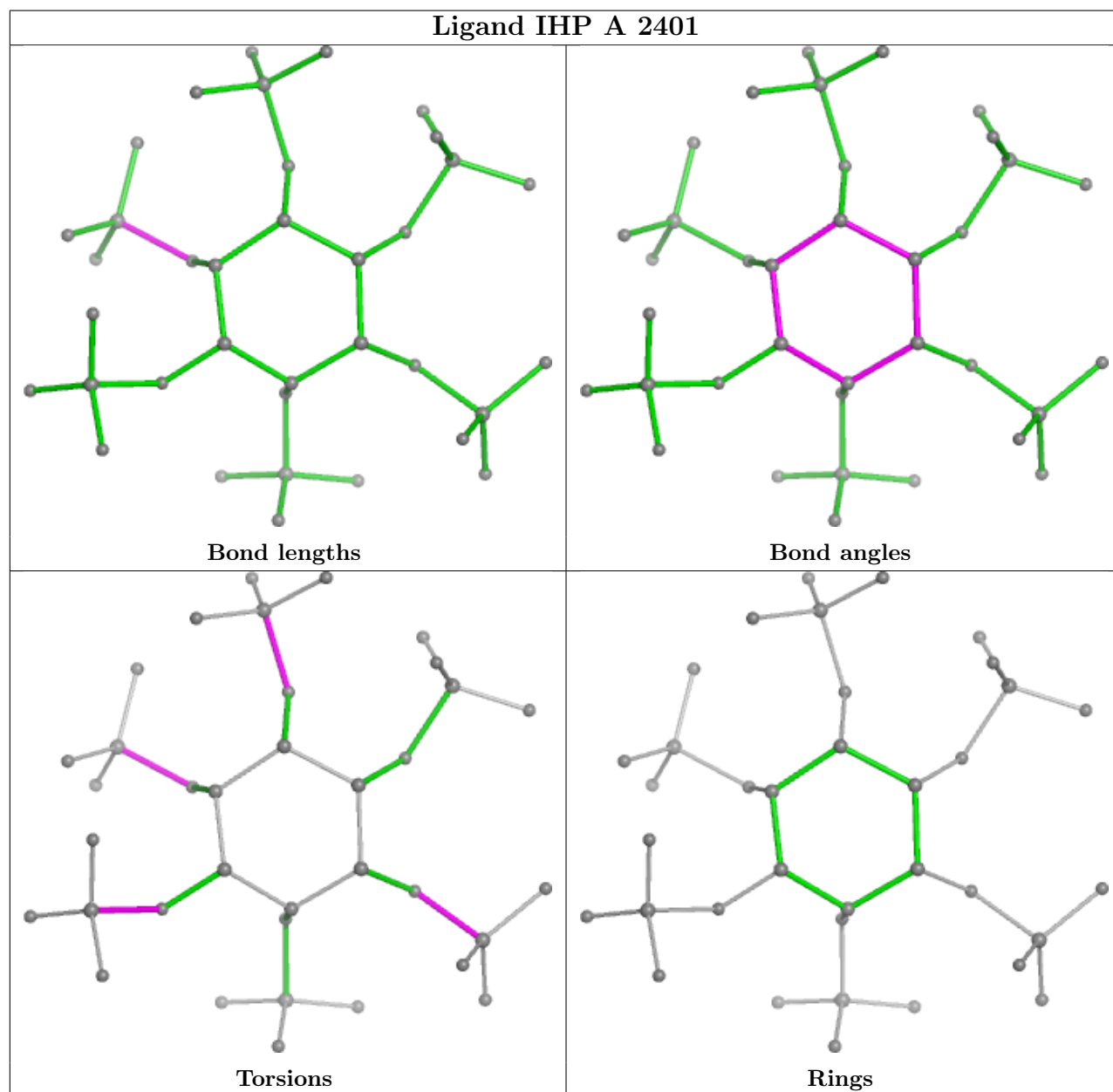
Mol	Chain	Res	Type	Atoms
18	A	2401	IHP	C1-O11-P1-O31
18	A	2401	IHP	C1-O11-P1-O21
18	A	2401	IHP	C5-O15-P5-O25
18	A	2401	IHP	C2-O12-P2-O32
18	A	2401	IHP	C3-O13-P3-O33

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	2401	IHP	2	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.

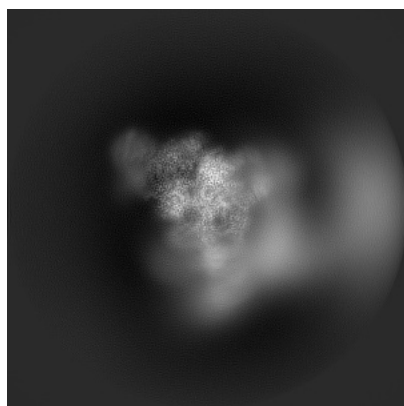
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18542. These allow visual inspection of the internal detail of the map and identification of artifacts.

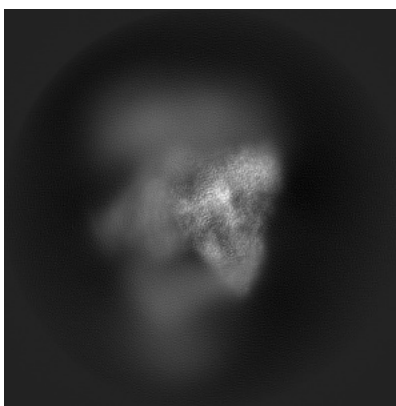
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

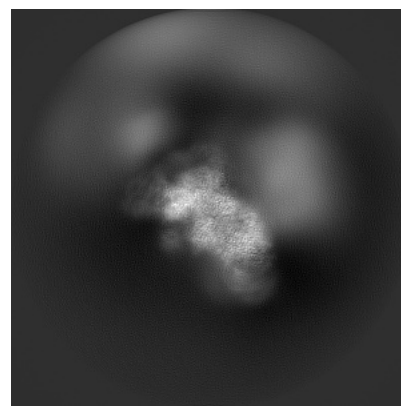
#### 6.1.1 Primary map



X

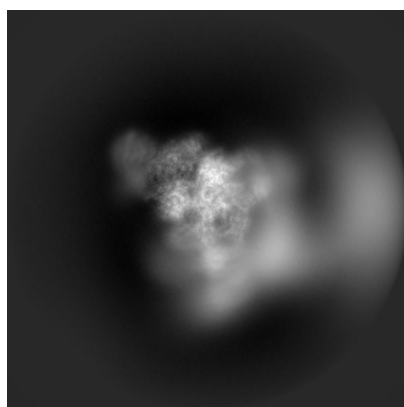


Y

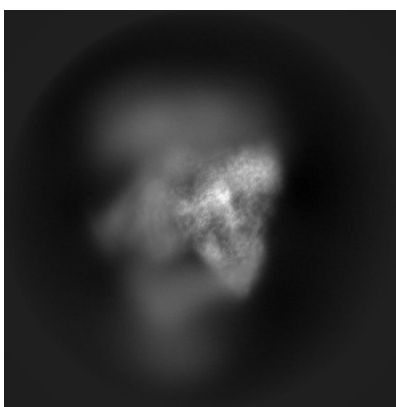


Z

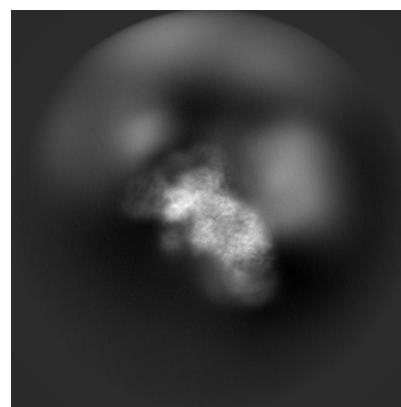
#### 6.1.2 Raw map



X



Y

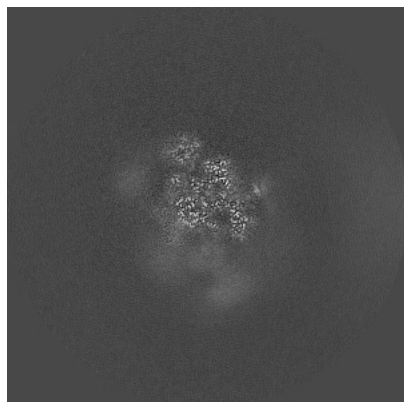


Z

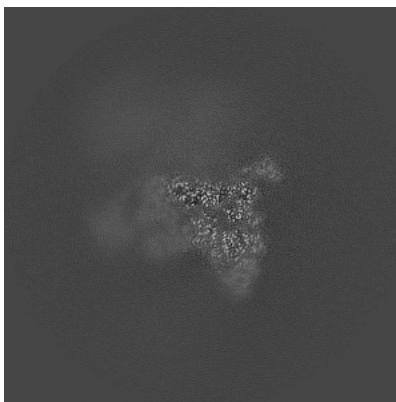
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

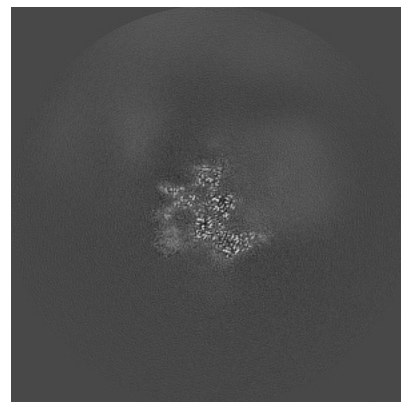
### 6.2.1 Primary map



X Index: 240

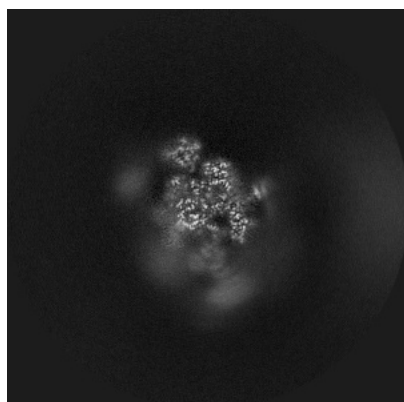


Y Index: 240

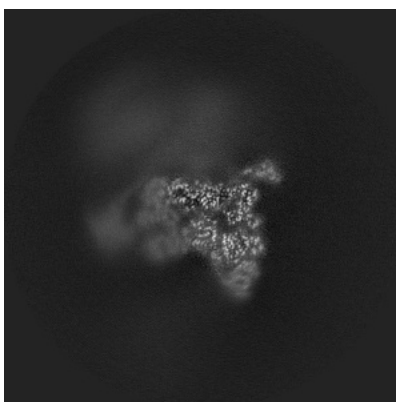


Z Index: 240

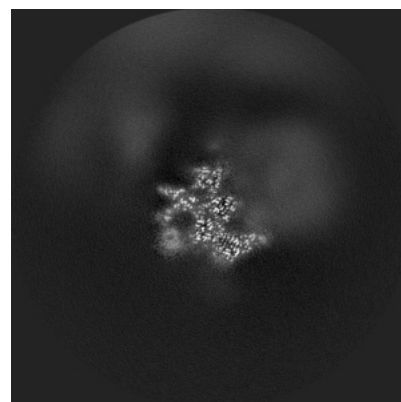
### 6.2.2 Raw map



X Index: 240



Y Index: 240

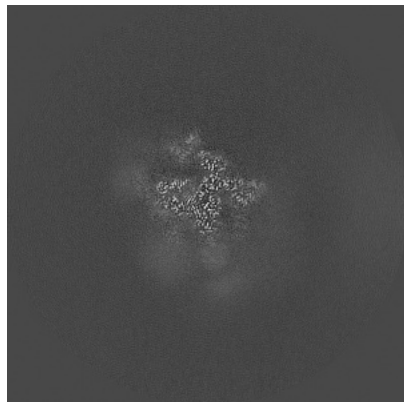


Z Index: 240

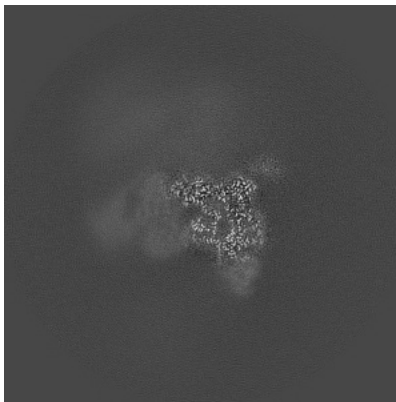
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

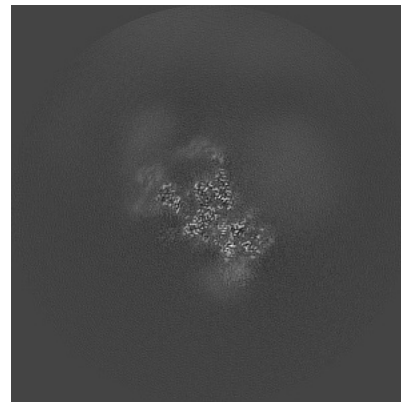
### 6.3.1 Primary map



X Index: 252

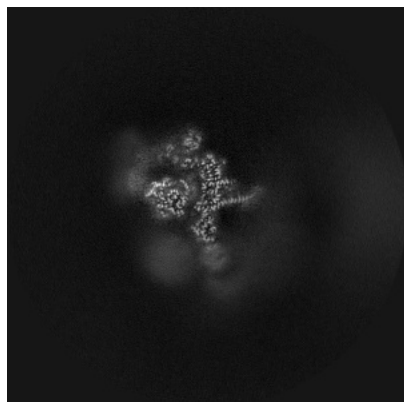


Y Index: 245

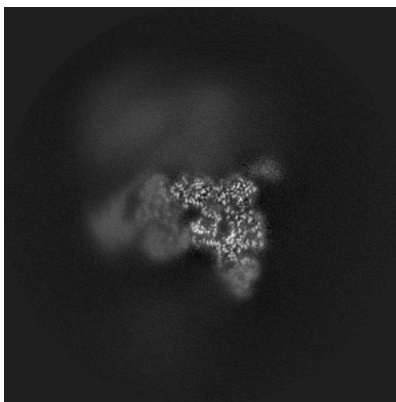


Z Index: 267

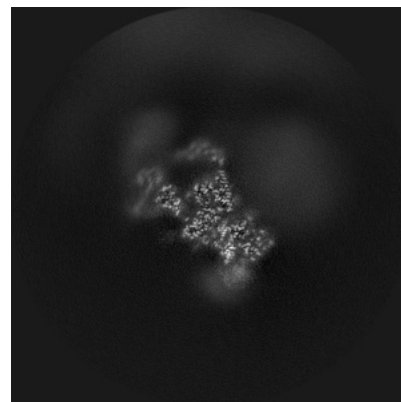
### 6.3.2 Raw map



X Index: 260



Y Index: 245

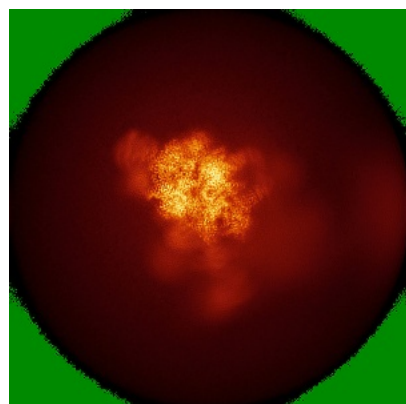


Z Index: 267

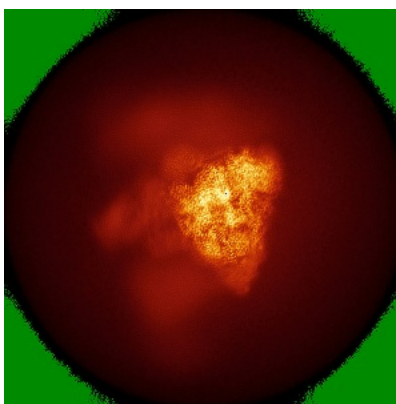
The images above show the largest variance slices of the map in three orthogonal directions.

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

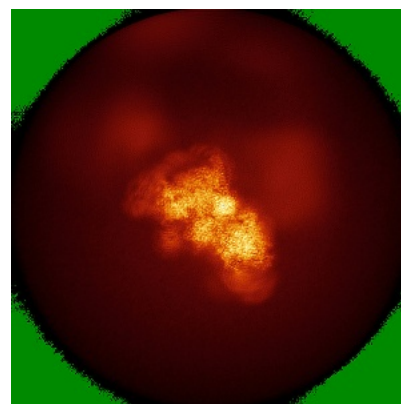
### 6.4.1 Primary map



X

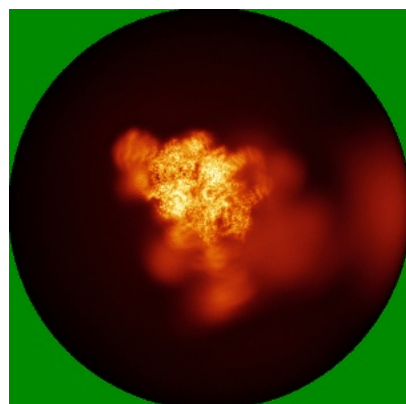


Y

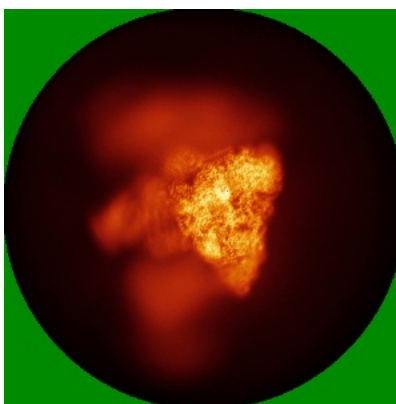


Z

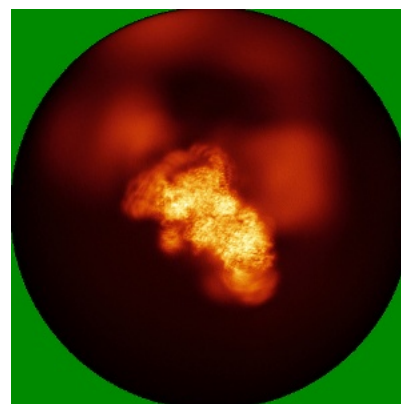
### 6.4.2 Raw map



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 0.032. 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.

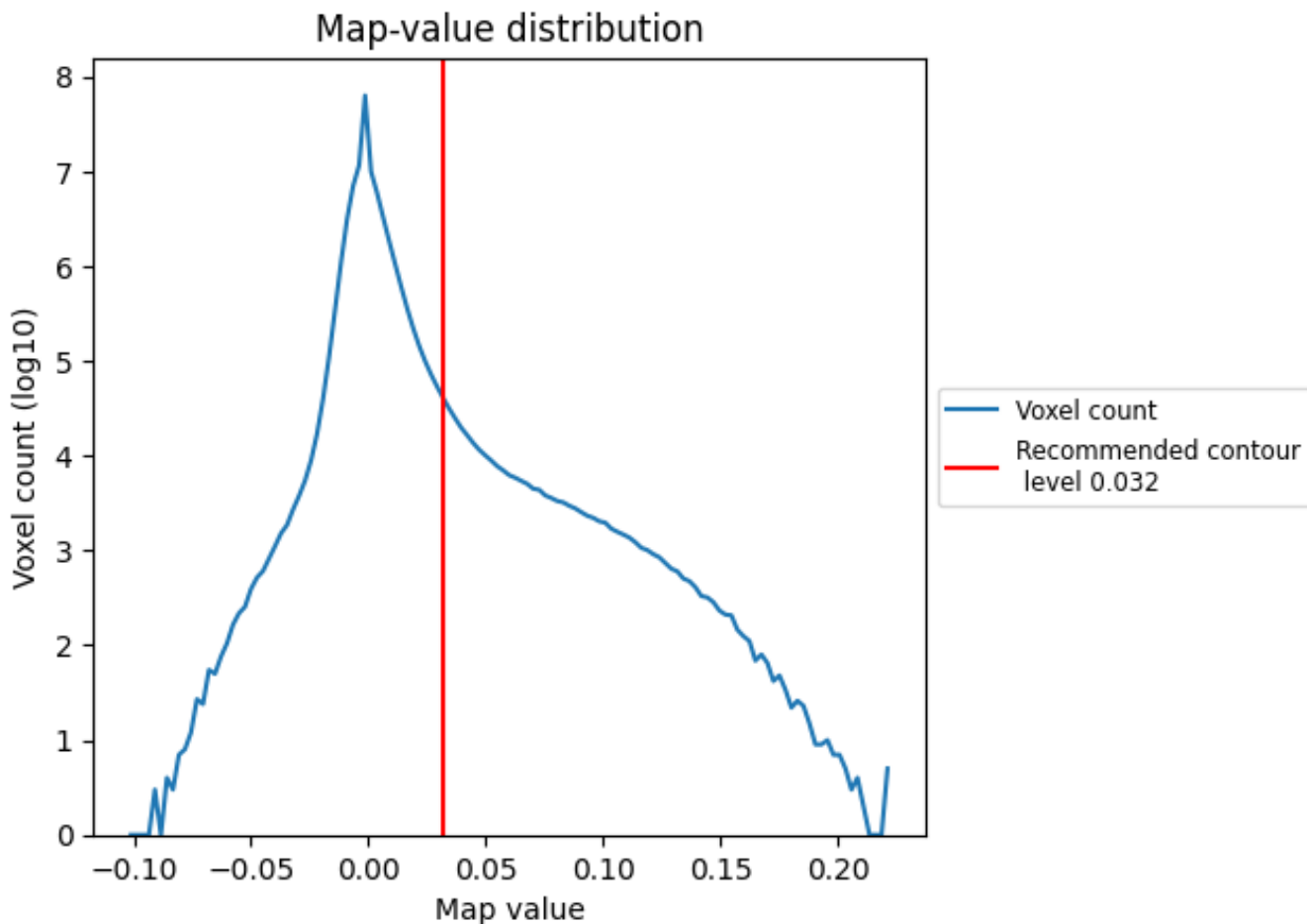
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

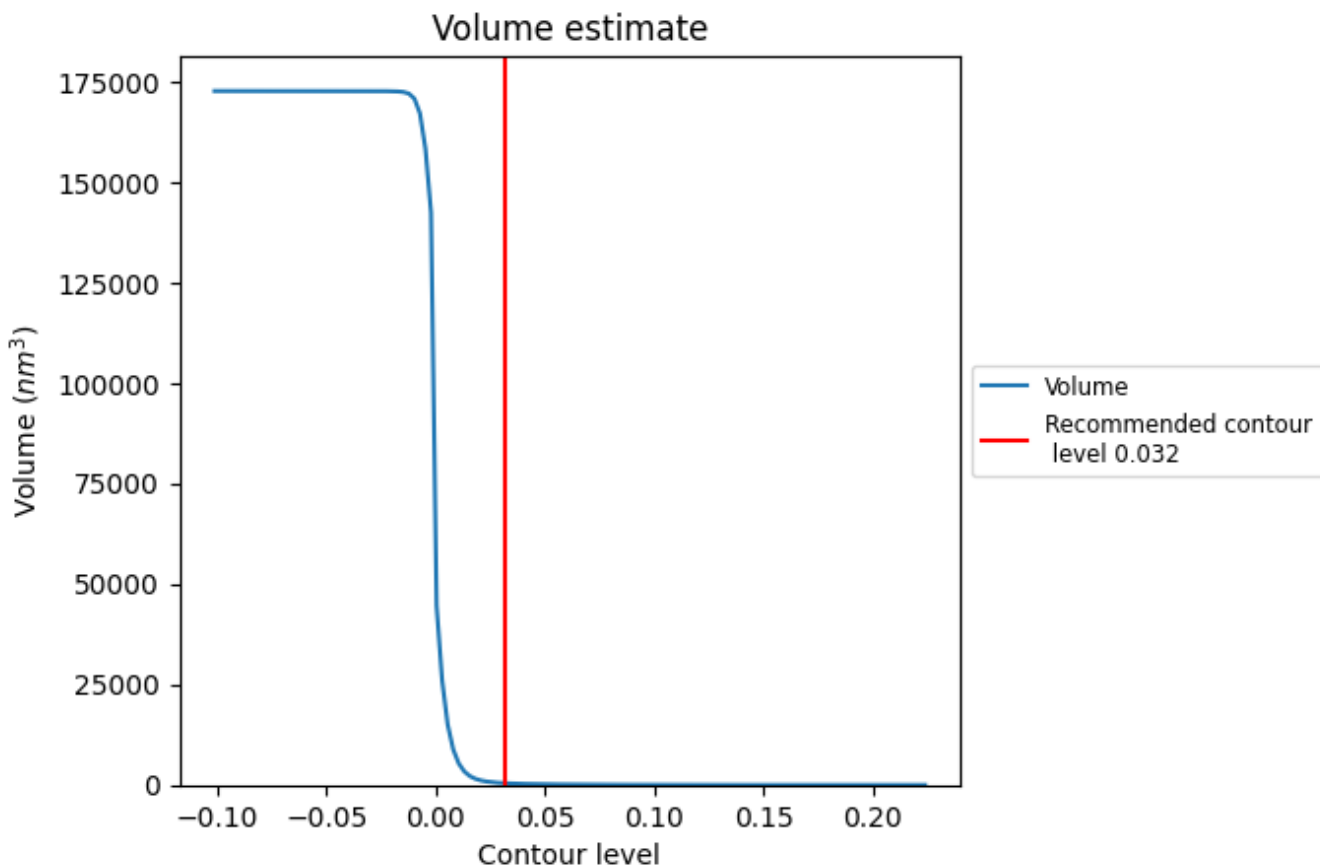
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

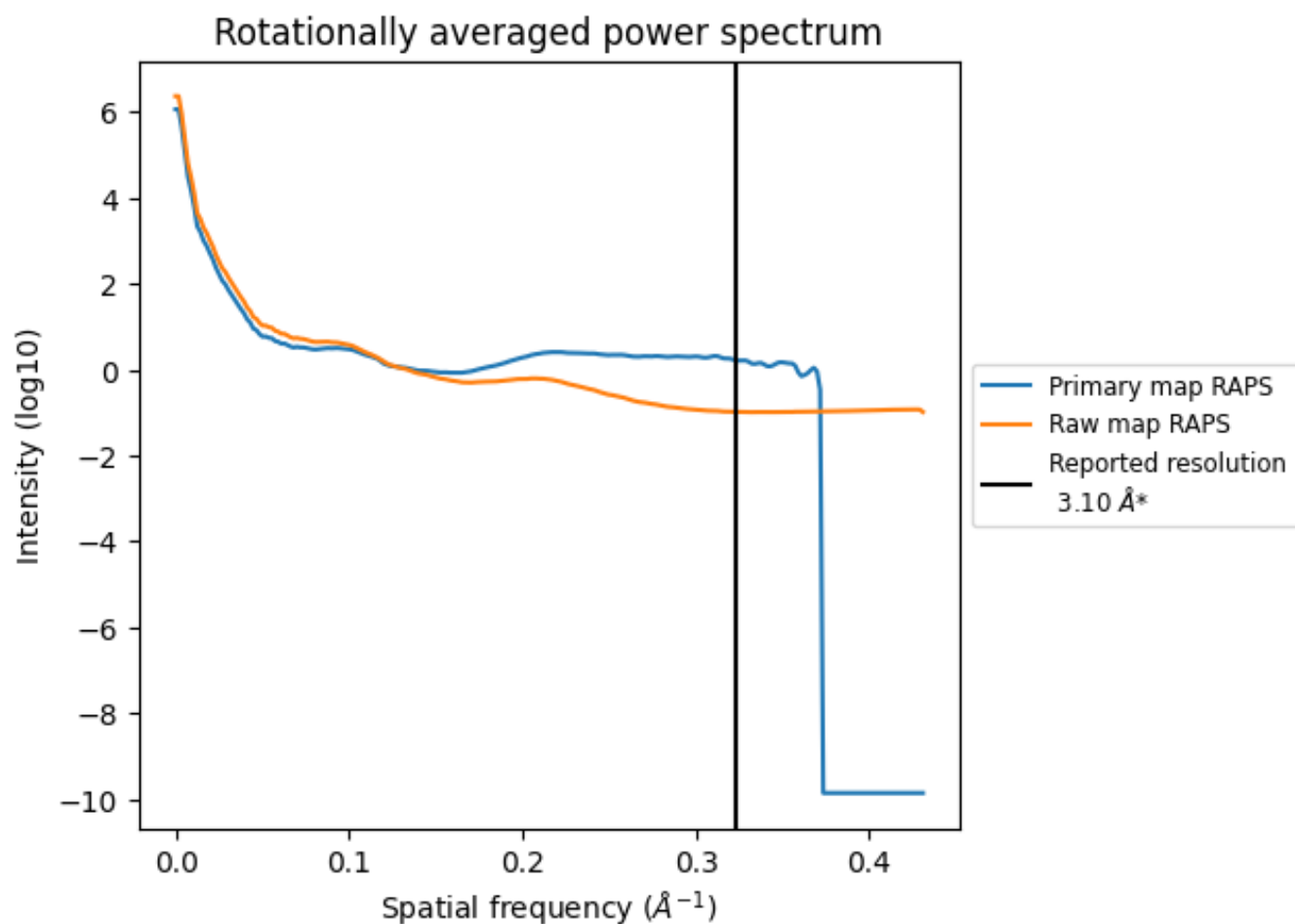


The volume at the recommended contour level is 424  $\text{nm}^3$ ; this corresponds to an approximate mass of 383 kDa.

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



### 7.3 Rotationally averaged power spectrum [i](#)

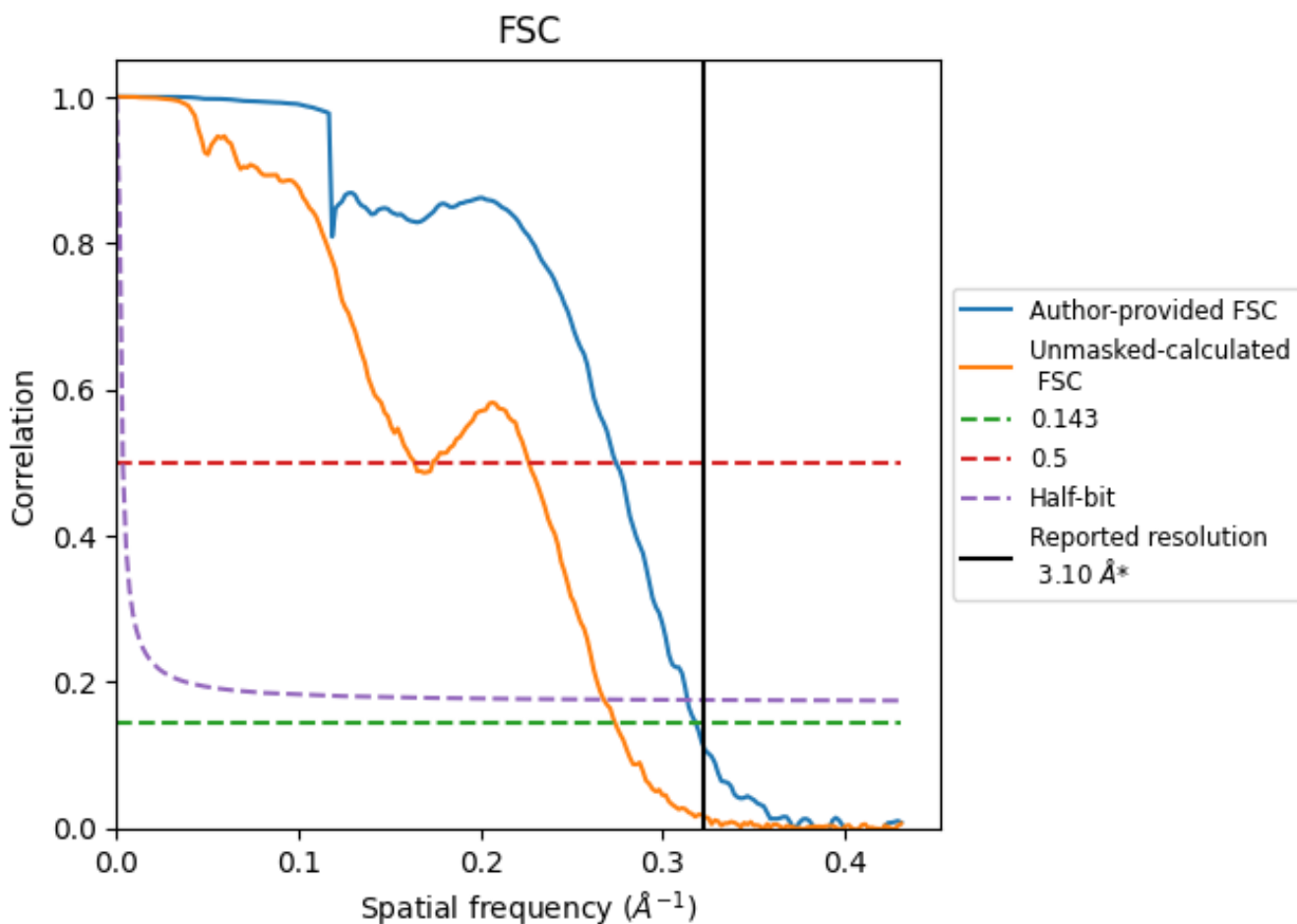


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

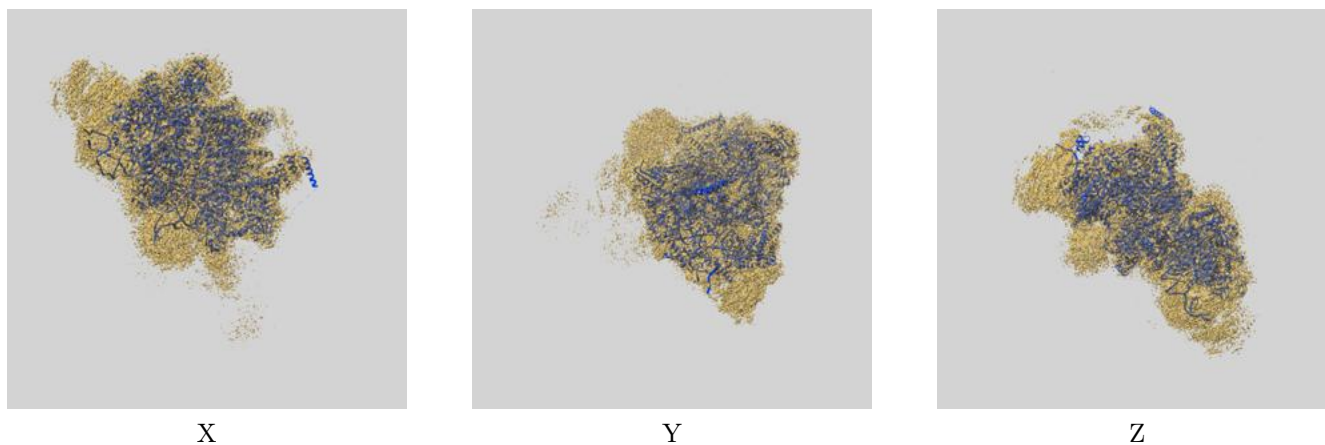
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.14	3.65	3.19
Unmasked-calculated*	3.65	6.11	3.74

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.65 differs from the reported value 3.1 by more than 10 %

## 9 Map-model fit [i](#)

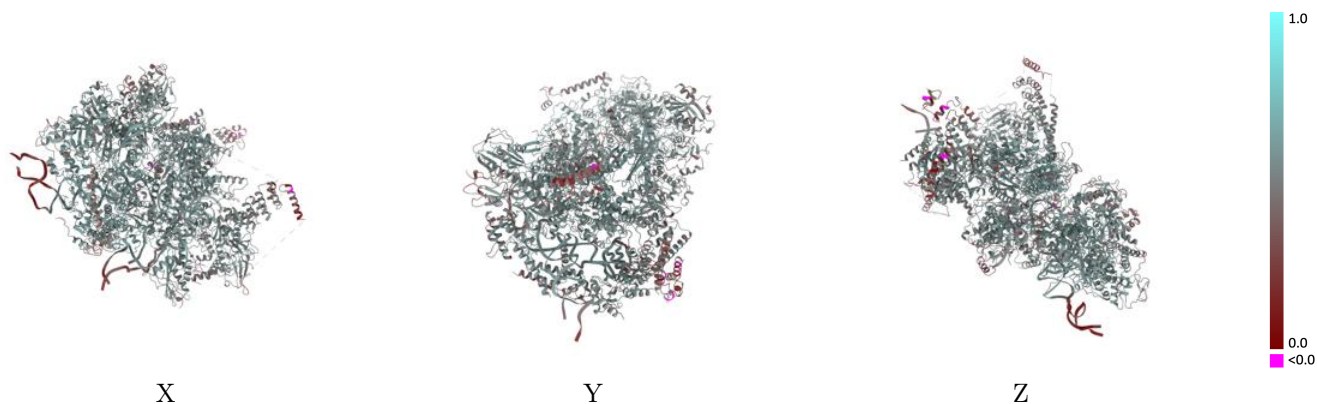
This section contains information regarding the fit between EMDB map EMD-18542 and PDB model 8QOZ. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



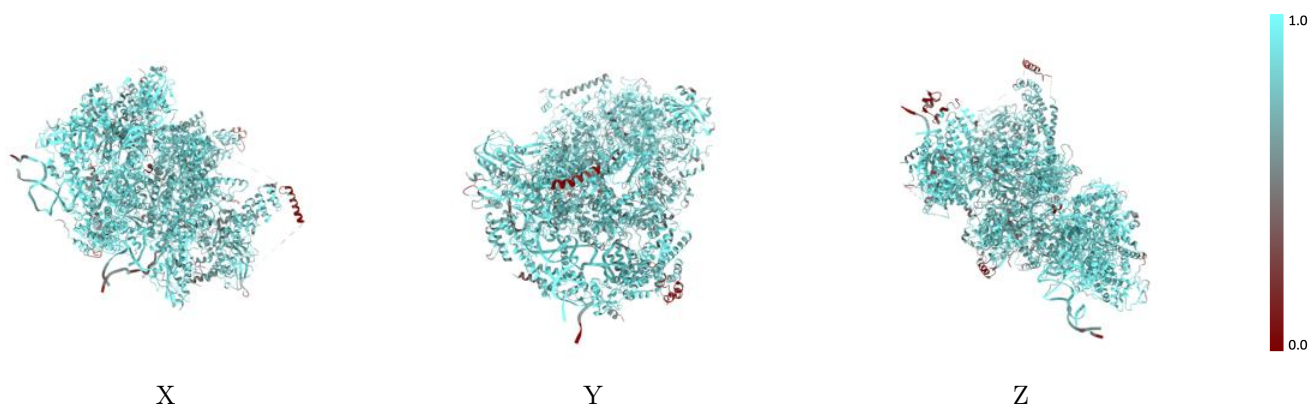
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



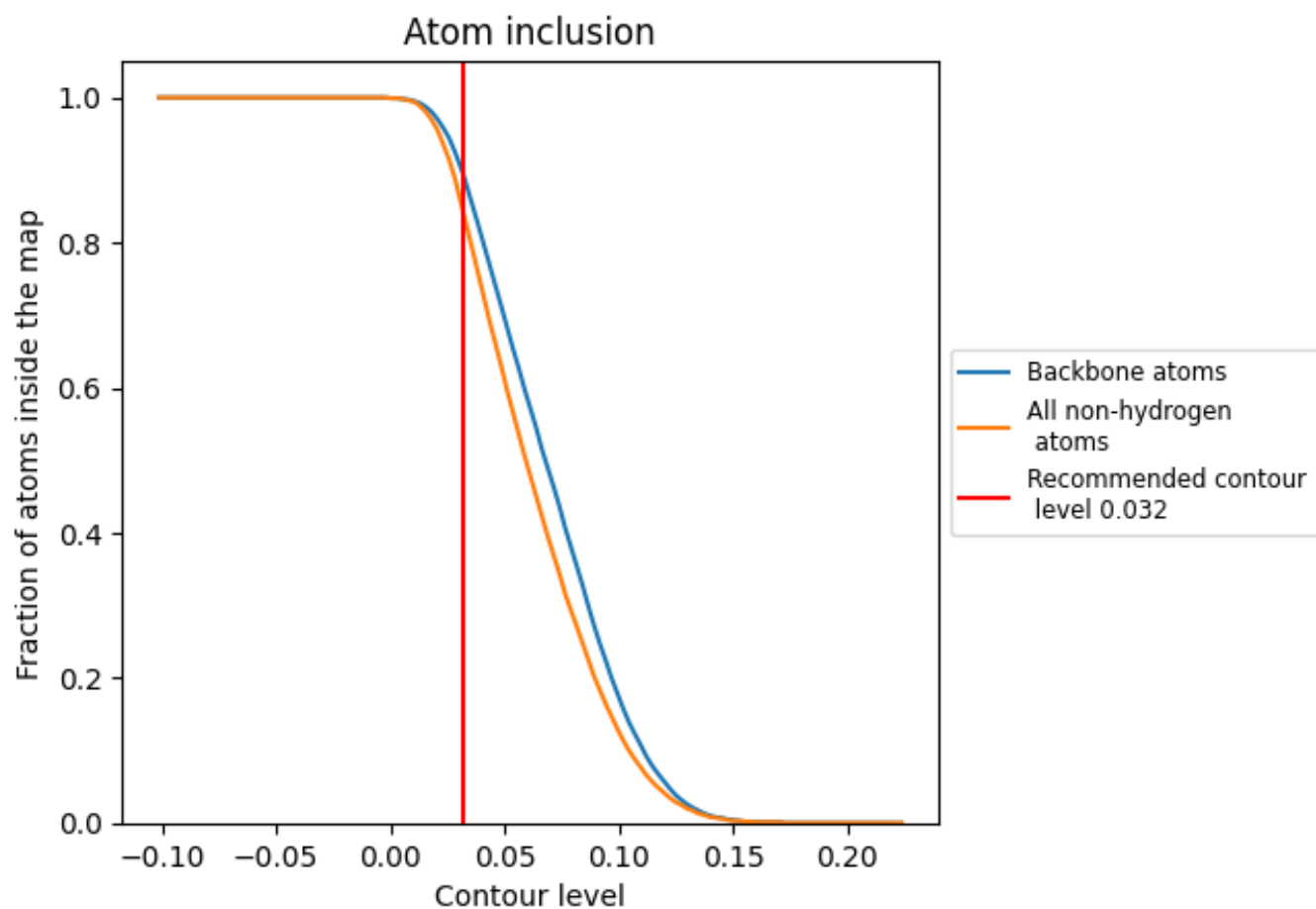
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).





































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.5190
4	 0.8380	 0.4980
5	 0.8820	 0.4560
6	 0.8650	 0.5070
7	 0.7720	 0.4840
A	 0.8740	 0.5460
B	 0.7950	 0.4910
C	 0.8970	 0.5390
D	 0.9250	 0.5880
F	 0.7390	 0.4420
G	 0.7680	 0.4890
J	 0.8840	 0.5320
L	 0.8480	 0.5050
M	 0.8720	 0.5180
N	 0.7870	 0.4830
S	 0.5910	 0.4350
U	 0.7170	 0.4800
z	 0.9460	 0.5540

