



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 08:12 AM UTC

PDB ID : 6ZXF / pdb_00006zxf
EMDB ID : EMD-11519
Title : Cryo-EM structure of a late human pre-40S ribosomal subunit - State G
Authors : Ameismeier, M.; Zemp, I.; van den Heuvel, J.; Thoms, M.; Berninghausen, O.;
Kutay, U.; Beckmann, R.
Deposited on : 2020-07-29
Resolution : 3.70 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

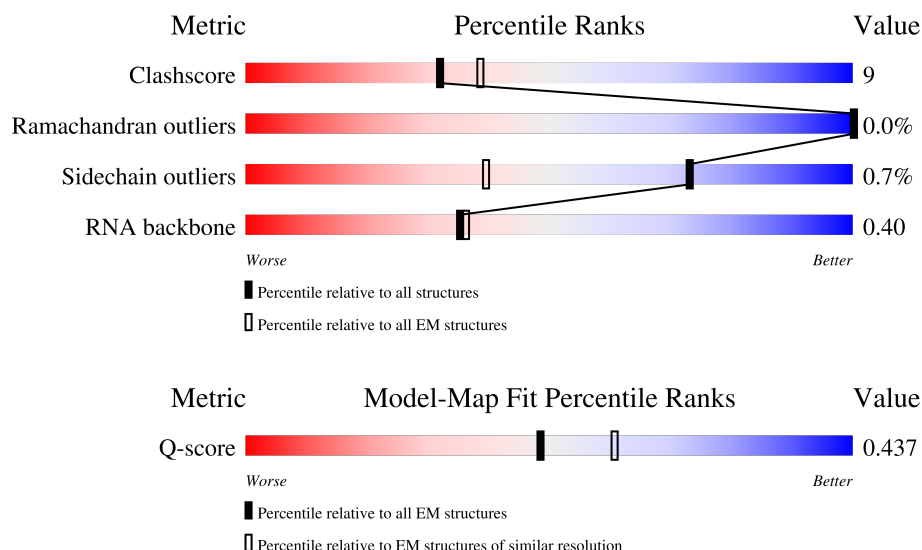
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

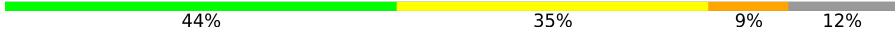
The reported resolution of this entry is 3.70 Å.

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



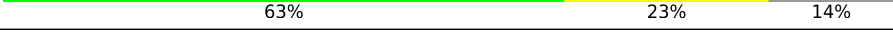
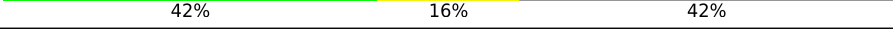
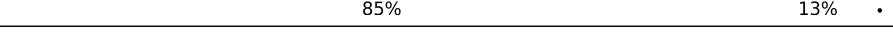
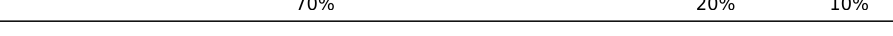
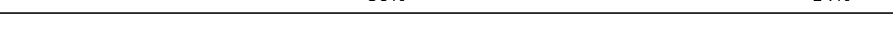
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	2	1874	
2	A	295	
3	B	264	

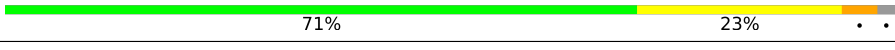
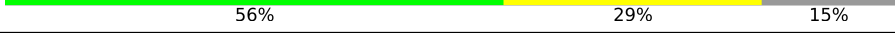
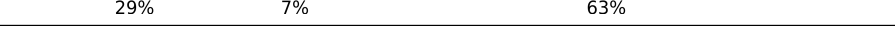
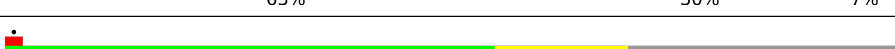
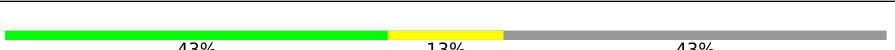
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Mol	Chain	Length	Quality of chain
4	C	293	
5	E	263	
6	D	243	
7	G	249	
8	H	194	
9	I	208	
10	J	194	
11	F	204	
12	L	158	
13	K	165	
14	N	151	
15	O	151	
16	M	132	
17	P	145	
18	R	135	
19	Q	146	
20	S	152	
21	T	145	
22	V	83	
23	W	130	
24	X	143	
25	Y	133	
26	U	119	
27	Z	125	
28	b	84	

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Mol	Chain	Length	Quality of chain
29	c	69	
30	d	56	
31	e	59	
32	f	156	
33	g	317	
34	j	165	
35	z	568	
36	y	412	
37	k	583	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 80133 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 RNA chain called pre-18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1656	Total	C	N	O	P	0	0
			35367	15787	6366	11558	1656		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	216	Total	C	N	O	S	0	0
			1674	1085	287	292	10		

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	255	Total	C	N	O	S	0	0
			2031	1299	377	347	8		

- Molecule 6 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	223	Total	C	N	O	S	0	0
			1802	1128	358	309	7		

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	179	Total	C	N	O	S	0	0
			1446	927	264	254	1		

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	199	Total	C	N	O	S	0	0
			1638	1027	322	284	5		

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	176	Total	C	N	O	S	0	0
			1465	934	295	234	2		

- Molecule 11 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 12 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	136	Total	C	N	O	S	0	0
			1127	719	212	190	6		

- Molecule 13 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 14 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	126	Total	C	N	O	S	0	0
			947	580	188	173	6		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	108	Total	C	N	O	S	0	0
			837	530	147	153	7		

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	131	Total	C	N	O	S	0	0
			1072	682	201	182	7		

- Molecule 18 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	121	Total	C	N	O	S	0	0
			983	617	183	180	3		

- Molecule 19 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	140	Total	C	N	O	S	0	0
			1116	710	211	192	3		

- Molecule 20 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	141	Total	C	N	O	S	0	0
			1162	731	232	198	1		

- Molecule 21 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	141	Total	C	N	O	S	0	0
			1094	685	210	196	3		

- Molecule 22 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 23 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 24 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 25 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	122	Total	C	N	O	S	0	0
			987	624	193	165	5		

- Molecule 26 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	98	Total	C	N	O	S	0	0
			774	486	145	139	4		

- Molecule 27 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	70	Total	C	N	O	S	0	0
			557	358	101	97	1		

- Molecule 28 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	77	Total	C	N	O	S	0	0
			611	386	113	107	5		

- Molecule 29 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 30 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 31 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	50	Total	C	N	O	S	0	0
			398	244	90	63	1		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	57	Total	C	N	O	S	0	0
			465	295	89	74	7		

- Molecule 33 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	295	Total	C	N	O	S	0	0
			2306	1460	403	431	12		

- Molecule 34 is a protein called Probable RNA-binding protein EIF1AD.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	115	Total	C	N	O	S	0	0
			928	590	166	170	2		

- Molecule 35 is a protein called Serine/threonine-protein kinase RIO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	373	Total	C	N	O	S	0	0
			3041	1911	553	555	22		

- Molecule 36 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	y	233	Total	C	N	O	S	0	0
			1838	1167	335	327	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	10	ASN	ASP	conflict	UNP Q9ULX3

- Molecule 37 is a protein called Leucine-rich repeat-containing protein 47.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	430	Total	C	N	O	0	0
			2117	1257	430	430		

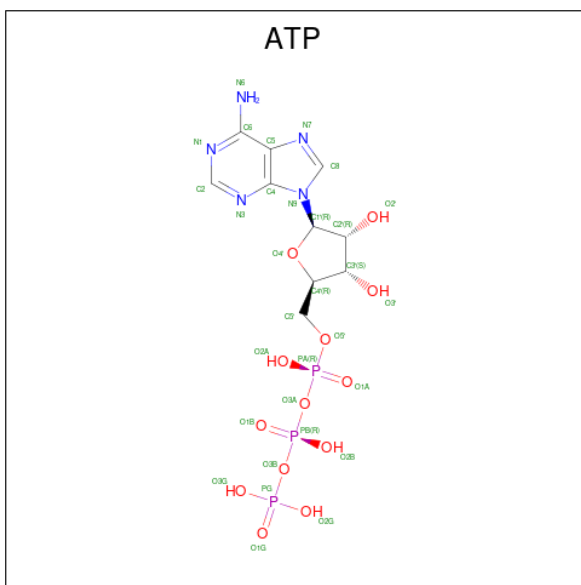
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	d	1	Total	Zn	0
			1	1	
38	f	1	Total	Zn	0
			1	1	
38	y	1	Total	Zn	0
			1	1	

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	z	2	Total	Mg	0
			2	2	

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
40	z	1	Total	C	N	O	P	0
			31	10	5	13	3	

G1857	G1780	C1701	U1622	G1550	C1453	A1379	G1298	U1202	A1084	A1001	G928	U866
G1861	A1781	G1702	A1623	U1551	A1454	A1382	A1299	G1203	C1085	A1002	G929	G967
G1862	G1782	G1706	C1628	C1553	A1455		A1299	A1204	G1086	U1002	G930	G968
G1784	C1783	U1707	C1629	C1554	G1461	G1387	G1301	C1213	A1087		G931	A869
C1785	U1708	C1708	A1630	U1555	U1462	A1388	C1303	A1214	G1096	A1009	G932	A870
U1786	C1709	G1709		A1556	U1463		U1304	C1215	G1096	G1010	G933	
			A1633	U1557	C1464	C1391	C1305	A1216		G1011		G873
		U1711	A1634	C1558	U1465		A1217	C1216	G1099	A1012	G936	
				C1559	G1466	C1395	U1307	C1218	A1100	U1013	G937	G874
		U1714	G1639	U1560	C1467	C1396	U1308		U1101	A1013	A938	A875
		A1715	A1640	A1561		U1397	C1309	G1221	G1102	G1014	U939	C876
		C1716	A1641	C1562	C1470	G1398	U1310	G1222		U1015		C877
				G1563	C1471				G1108	U1016	G942	G878
		C1717	C1646	C1564		A1401	A1313	G1226	C1109	U1017	G943	C879
		G1718	U1647	C1565	U1477	A1402	U1314		G1110	U1018	G981	G880
		U1720	G1648			C1403	A1228	A1227		C1019	U946	U882
		U1721	U1649	C1568	A1487	U1404	C1316	A1228	A1113		U947	U883
		G1722		U1569	C1488	A1405	C1317	G1229	U1114	A1023	C948	C884
		G1723	G1652	G1570	C1489	A1406	G1318		U	A1024	G949	U885
		A1724	U1653	C1570	U1490	U1407	U1319	C1233	C	U1025	C950	A
		U1725	G1654	G1576	G1491		G1320	G1233	C	A1027	G951	U
		G1726		U1577	U1492	C1410	G1321	G1236	A1119	A1028	C953	U
			U1659	U1578	C1493	G1411	G1322		U1120		U954	G
	A1735	G1736	C1660	A1579	U1494	G1412	U1323	U1242	G1121	G1033		U
	G1737		A1661	A1580	G1495	A1413	U1329	U1243	A1122	A1036	U960	U
	C1738			G1584	U1496	G1414	A1332	C1247	C1123	G1037	A962	U
			A1664	U1585	G1497	C1415			C1124	U1038	A963	G
	U1741		G1665	U1586	U1498	C1416			G1129		A964	U
	C1742		C1666	U1587	C1566	C1417			G1041		U965	U
	G1743		U1667	A1588	G1500	C1418	C1337	A1251	A1133		U966	U
	G1744		G1669	A1589	A1506	C	G1338	A1252		U1045		C900
	A1745		C1670	C1590	G1507	G	U1339	A1253	C1138	G1048	U969	G901
	U1746		G1671	C1593	A1508	G	U1340		C1139	A1049	G970	G902
	C1747		U1672	A1594			C1341	A1258	A1143		G971	A903
	G1748			U1595	U1511	G1423		A1259		A1052	G972	A904
			G1674	U1596	C1512		G1349		A1149	C1053	C974	C905
		C1753	A1675	C1597	C1513	G1428	U1350	U1263	A1150	G1054	G975	U906
	G1754	G1754	C1675	G1598	G1514	G1429	G1351	C1264	G1151	A1055	G976	G907
	C1755		U1676	U1599		C1430			U1152	U1056	C977	A908
	G1756		U1677	U1599	C1518	G1431	G1354	C1271	U1152	U1056		
	C1756		A1678	U1602	U1519	U1432	C1355		C1153	C1057	G909	
	U1838		A1679	G1603	G1520	C	G1356	G1274	U1154	A1058	A980	G910
	U1839		G1680	C1604	C1521	C	A1357	G1275	U1155	G1059	A981	C911
	A1840		G1759	G1605	A1522	C	U1358	A1276	U1156	A1060	G982	C912
	C1841			G1606	C1683	C	U1359		G1157	U1061	A983	A913
						C	C	G1280	A1062	A1062	C984	U914
	U1844		G1866	C1609	G1526	A1438	U1360	G1281	A1170	C1063	G985	G915
	A1845		C1687	C1609		A1439	G1361	A1282	G1171	C1064	G985	A916
	G1846		C1688	G1610	C1532	A1439	U1362	C1283	G1182	G1085	A987	U917
	C1746		C1689	G1611	C1533	U1441	C1363	A1284	A1182	U1066	C988	U918
	U1848		U1690	G1612	C1534			G1285			A919	A919
	G1849		C1691	G1613	U1535		U1367			U1069	A990	A920
	A1850		U1692	A1614	G1536	A1446	U1368	G1286	G1187	A1070	G991	A921
	C1851		C1693	U1615	A1537	G1447	U1371		A1188	G1071	A992	G922
	C1852		U1694	U1616		G1449	U1372	A1291	A1190	A1070	A992	G923
	C1853		A1695	G1617	C1544	G1450	C1373	A1295	A1195	A1090	A996	G924
	U1854			C1618	G1548	G1451	A1378			A1090	A997	G925
	G1855		C1699	U1621	U1549	G1452				A1093	A998	
	C1856		C1700									

• Molecule 2: 40S ribosomal protein SA

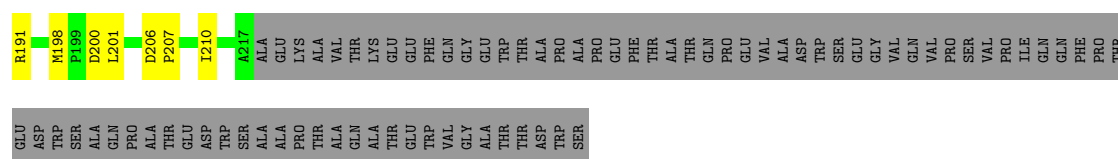
Chain A:

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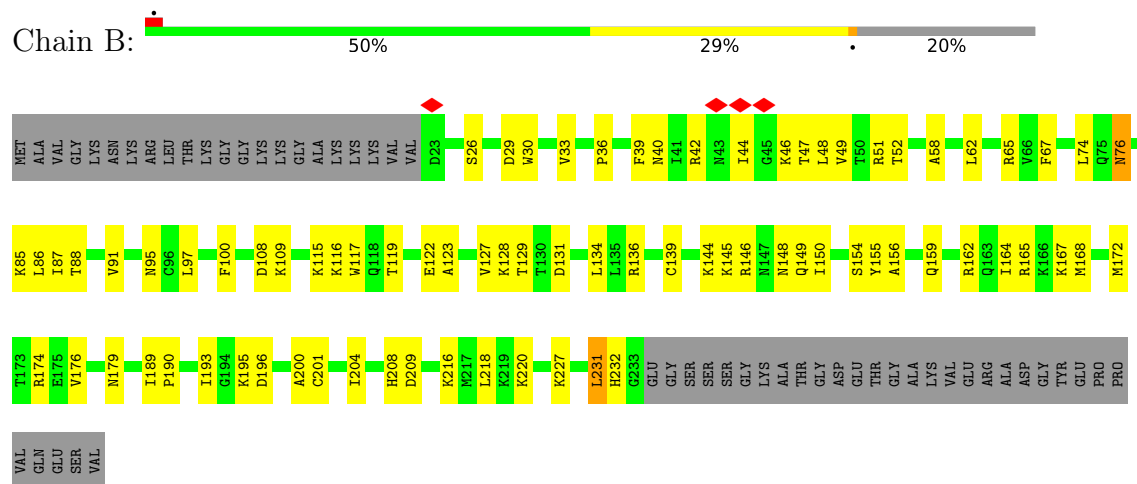
14%

27%

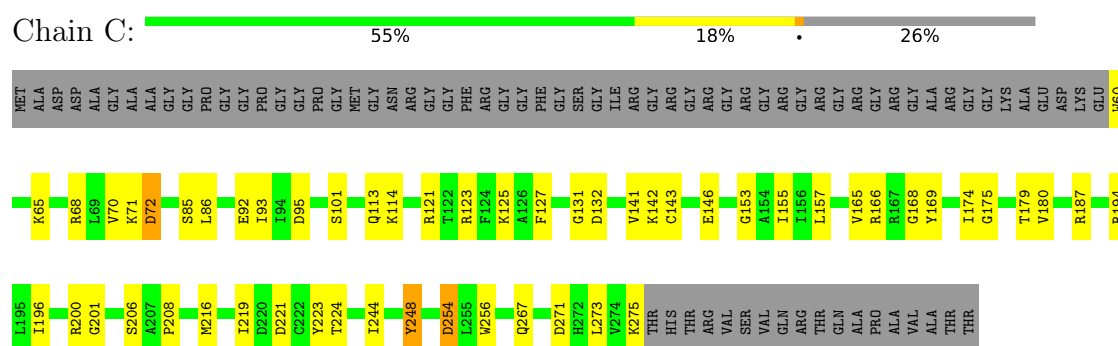
MET	S2	E12	N29	L30	Q33	N34	K40	R41	K42	K52	E56	K57	L58	N81	Q84	R85	K89	A100	T104	P105	R120	Q132	T135	E136	A137	S138	N141	L142	L147	D151	V157	P162	N165	M177	R184	S190
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



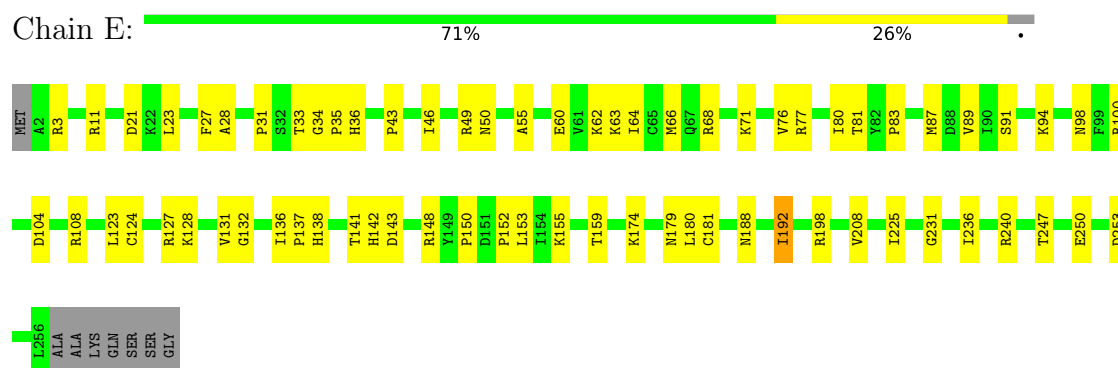
• Molecule 3: 40S ribosomal protein S3a



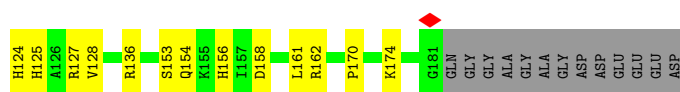
• Molecule 4: 40S ribosomal protein S2



• Molecule 5: 40S ribosomal protein S4, X isoform

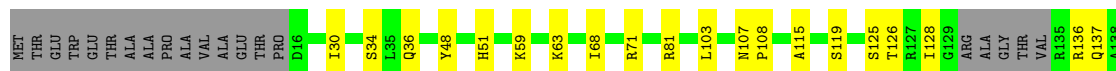


• Molecule 6: 40S ribosomal protein S3



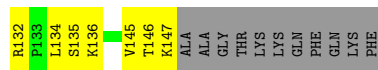
- Molecule 11: 40S ribosomal protein S5

Chain F: 77% 13% 10%



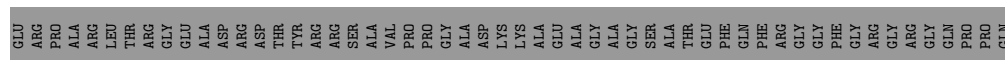
- Molecule 12: 40S ribosomal protein S11

Chain L: 63% 23% 14%



- Molecule 13: 40S ribosomal protein S10

Chain K: 42% 16% 42%



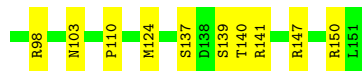
- Molecule 14: 40S ribosomal protein S13

Chain N: 85% 13%



- Molecule 15: 40S ribosomal protein S14

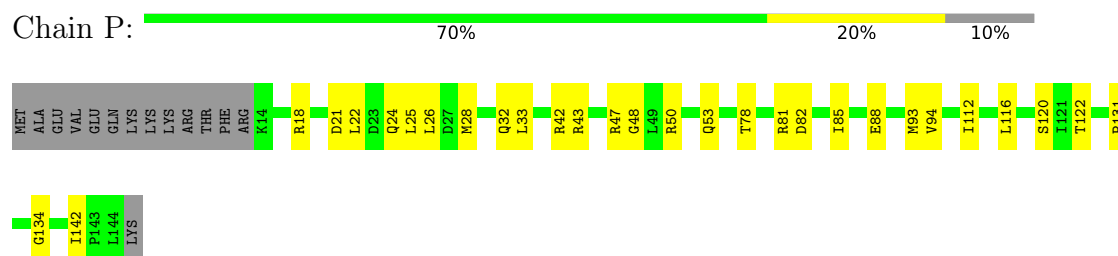
Chain O: 62% 22% 17%



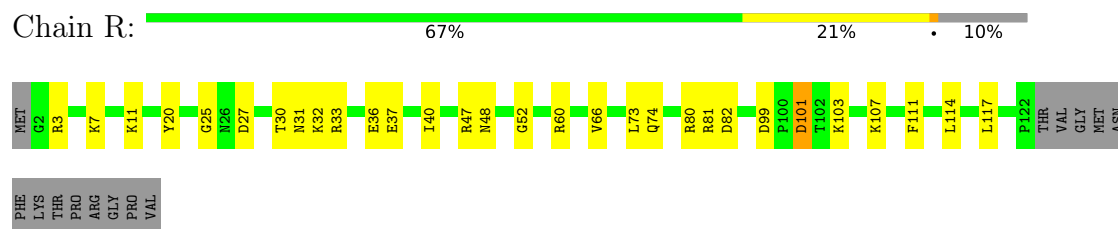
- Molecule 16: 40S ribosomal protein S12



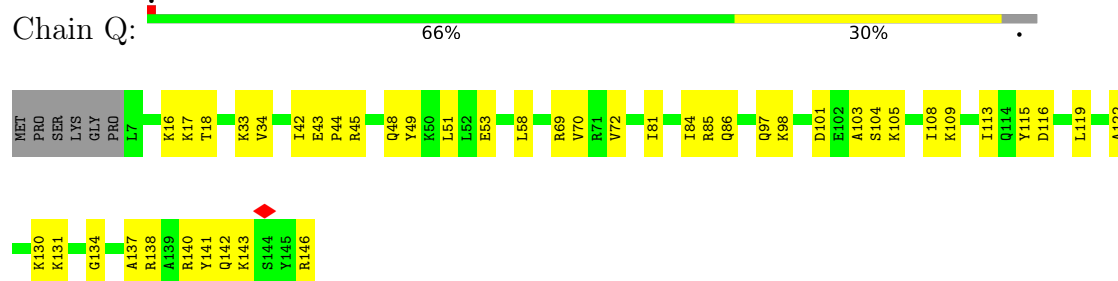
- Molecule 17: 40S ribosomal protein S15



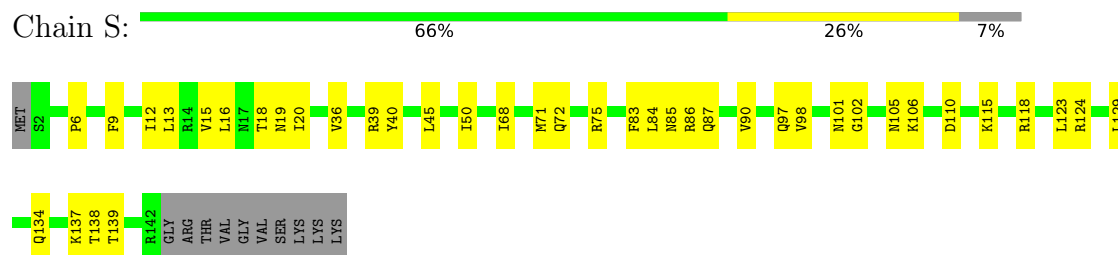
- Molecule 18: 40S ribosomal protein S17



- Molecule 19: 40S ribosomal protein S16

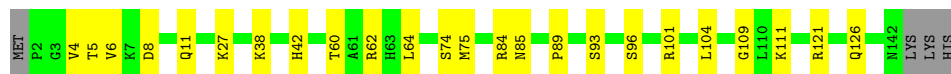


- Molecule 20: 40S ribosomal protein S18



- Molecule 21: 40S ribosomal protein S19

Chain T:  81% 17%



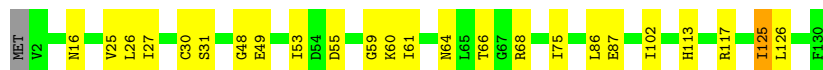
- Molecule 22: 40S ribosomal protein S21

Chain V:  86% 14%



- Molecule 23: 40S ribosomal protein S15a

Chain W:  81% 18%



- Molecule 24: 40S ribosomal protein S23

Chain X:  78% 20%



- Molecule 25: 40S ribosomal protein S24

Chain Y:  72% 20% 8%



PRO
LYS
GLU

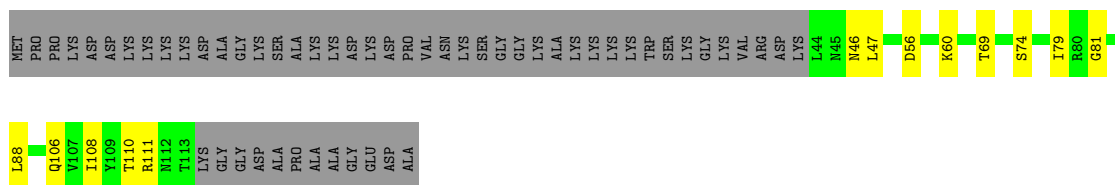
- Molecule 26: 40S ribosomal protein S20

Chain U:  63% 19% 18%



ASP
ALA

- Molecule 27: 40S ribosomal protein S25



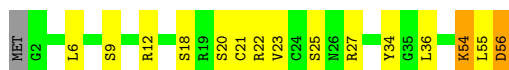
- Molecule 28: 40S ribosomal protein S27



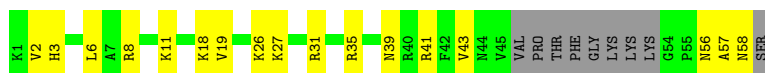
- Molecule 29: 40S ribosomal protein S28



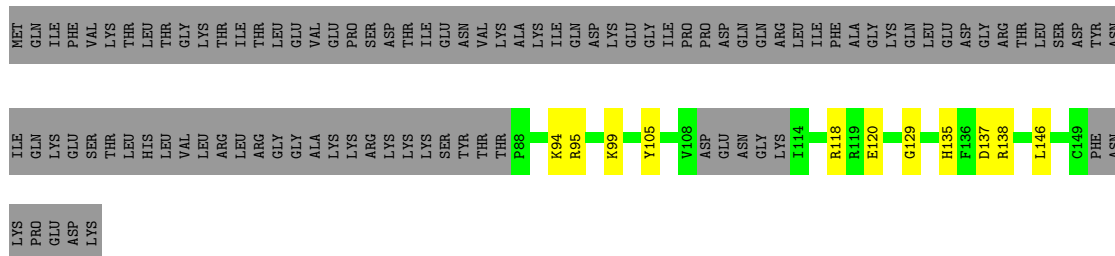
- Molecule 30: 40S ribosomal protein S29



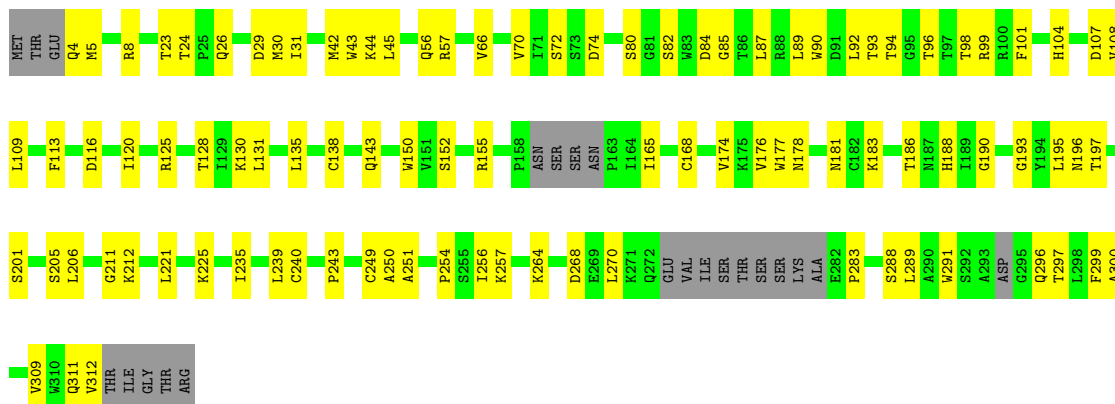
- Molecule 31: 40S ribosomal protein S30



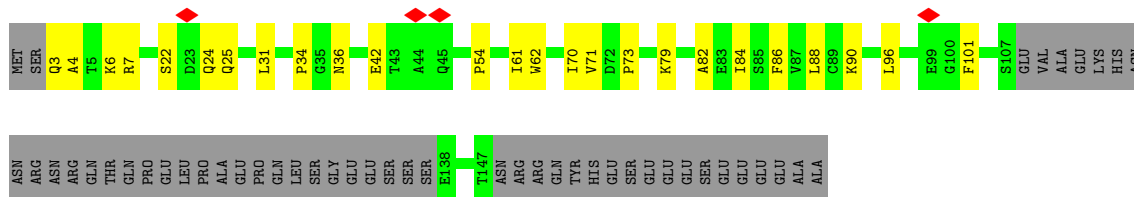
- Molecule 32: Ubiquitin-40S ribosomal protein S27a



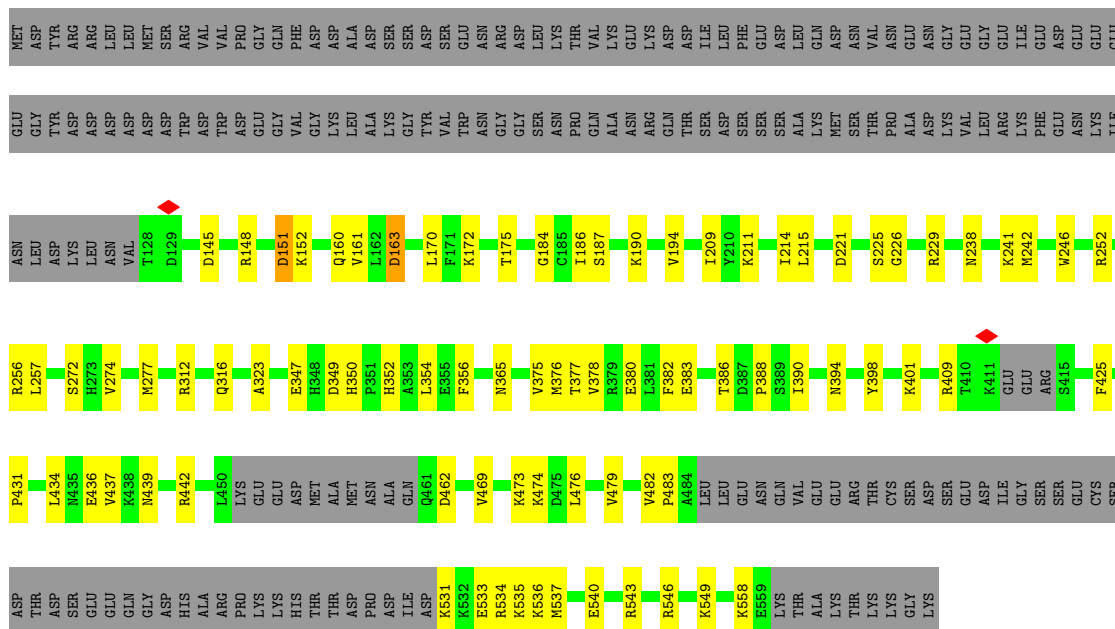
- Molecule 33: Receptor of activated protein C kinase 1



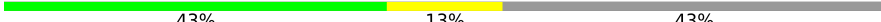
- Molecule 34: Probable RNA-binding protein EIF1AD

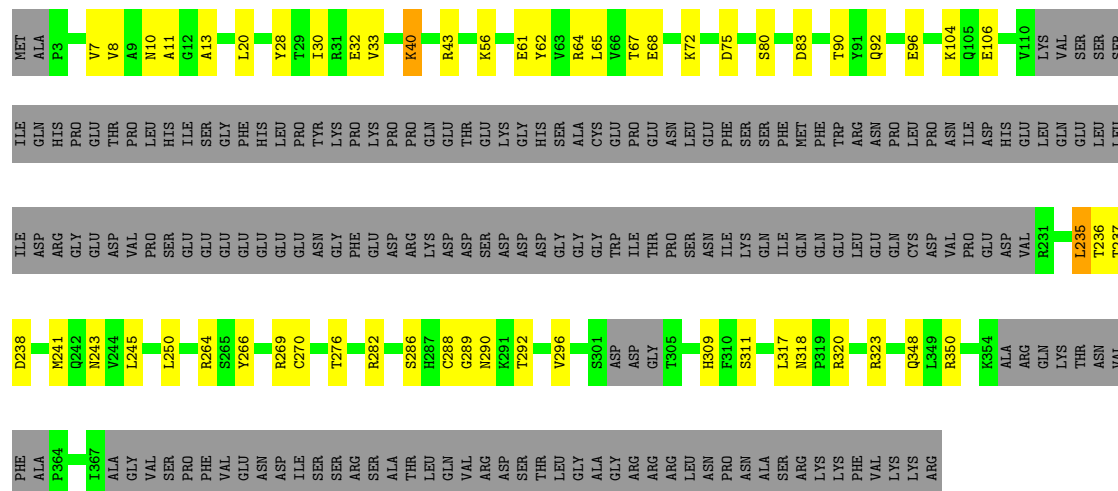


- Molecule 35: Serine/threonine-protein kinase RIO1



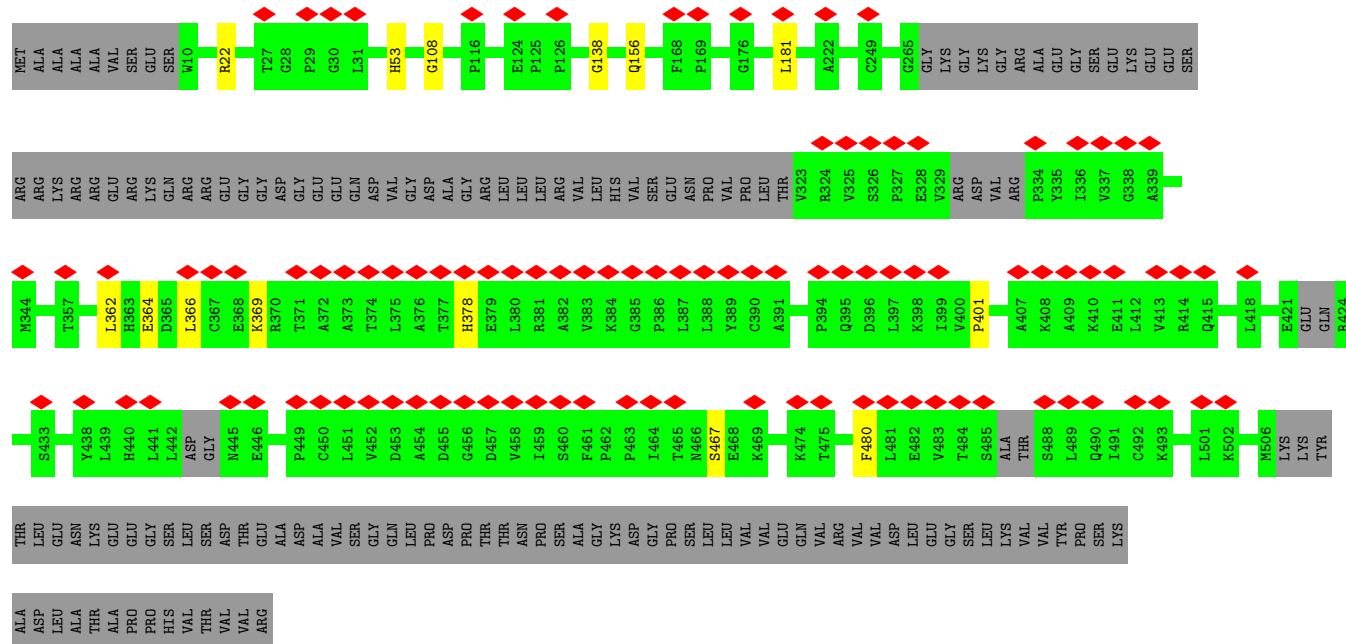
- Molecule 36: RNA-binding protein NOB1

Chain y:  43% 13% 43%



• Molecule 37: Leucine-rich repeat-containing protein 47

Chain k:  18% 71% 26%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140612	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.340	Depositor
Minimum map value	-0.135	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ZN

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	2	0.53	0/39549	0.49	1/61629 (0.0%)
2	A	0.51	0/1742	0.52	0/2367
3	B	0.44	0/1742	0.60	0/2330
4	C	0.55	0/1710	0.58	0/2310
5	E	0.43	0/2073	0.51	0/2791
6	D	0.41	0/1773	0.53	0/2387
7	G	0.33	0/1825	0.52	0/2431
8	H	0.35	0/1466	0.51	0/1959
9	I	0.43	0/1666	0.55	0/2223
10	J	0.41	0/1489	0.55	0/1987
11	F	0.43	0/1481	0.54	0/1988
12	L	0.53	0/1147	0.51	0/1535
13	K	0.40	0/823	0.51	0/1111
14	N	0.43	0/1226	0.48	0/1649
15	O	0.42	0/959	0.58	0/1286
16	M	0.26	0/845	0.49	0/1134
17	P	0.38	0/1094	0.55	0/1464
18	R	0.41	0/995	0.53	0/1335
19	Q	0.46	0/1133	0.58	0/1517
20	S	0.38	0/1180	0.53	0/1582
21	T	0.41	0/1113	0.49	0/1493
22	V	0.46	0/643	0.52	0/860
23	W	0.54	0/1051	0.59	0/1406
24	X	0.48	0/1097	0.54	0/1464
25	Y	0.35	0/1004	0.50	0/1337
26	U	0.44	0/783	0.54	0/1052
27	Z	0.30	0/563	0.53	0/758
28	b	0.43	0/623	0.51	0/834
29	c	0.41	0/481	0.62	0/643
30	d	0.56	0/469	0.76	0/623
31	e	0.36	0/401	0.51	0/526
32	f	0.30	0/474	0.54	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.37	0/2360	0.55	0/3207
34	j	0.31	0/946	0.54	0/1274
35	z	0.44	0/3088	0.58	0/4134
36	y	0.42	0/1874	0.57	0/2531
37	k	0.21	0/2111	0.51	0/2926
All	All	0.47	0/84999	0.52	1/122709 (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
19	Q	0	1
35	z	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1060	A	P-O3'-C3'	5.28	128.12	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	Q	103	ALA	Peptide
35	z	272	SER	Peptide

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	2	35367	0	17861	469	0
2	A	1705	0	1706	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1715	0	1785	60	0
4	C	1674	0	1764	42	0
5	E	2031	0	2133	47	0
6	D	1745	0	1839	36	0
7	G	1802	0	1954	58	0
8	H	1446	0	1540	27	0
9	I	1638	0	1710	45	0
10	J	1465	0	1583	41	0
11	F	1461	0	1511	22	0
12	L	1127	0	1190	24	0
13	K	799	0	823	19	0
14	N	1202	0	1289	18	0
15	O	947	0	976	25	0
16	M	837	0	870	21	0
17	P	1072	0	1121	23	0
18	R	983	0	1030	24	0
19	Q	1116	0	1185	29	0
20	S	1162	0	1215	30	0
21	T	1094	0	1120	19	0
22	V	636	0	637	10	0
23	W	1034	0	1080	17	0
24	X	1080	0	1147	20	0
25	Y	987	0	1038	18	0
26	U	774	0	839	14	0
27	Z	557	0	610	11	0
28	b	611	0	637	8	0
29	c	479	0	507	10	0
30	d	458	0	448	13	0
31	e	398	0	439	14	0
32	f	465	0	483	10	0
33	g	2306	0	2266	59	0
34	j	928	0	923	20	0
35	z	3041	0	3106	55	0
36	y	1838	0	1860	40	0
37	k	2117	0	957	7	0
38	d	1	0	0	0	0
38	f	1	0	0	0	0
38	y	1	0	0	0	0
39	z	2	0	0	0	0
40	z	31	0	12	3	0
All	All	80133	0	63194	1200	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 9.

The worst 5 of 1200 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)
1:2:878:G:H1	1:2:908:A:N6	1.63	0.95
1:2:878:G:H1	1:2:908:A:H61	0.97	0.94
1:2:880:G:H1	1:2:906:U:H3	1.12	0.93
9:I:31:ARG:HH11	9:I:31:ARG:HG3	1.33	0.92
1:2:1748:G:H1	1:2:1786:U:H3	0.93	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	
2	A	214/295 (72%)	199 (93%)	15 (7%)	0	100	100
3	B	209/264 (79%)	194 (93%)	15 (7%)	0	100	100
4	C	214/293 (73%)	198 (92%)	16 (8%)	0	100	100
5	E	253/263 (96%)	232 (92%)	21 (8%)	0	100	100
6	D	222/243 (91%)	211 (95%)	11 (5%)	0	100	100
7	G	221/249 (89%)	203 (92%)	18 (8%)	0	100	100
8	H	171/194 (88%)	165 (96%)	6 (4%)	0	100	100
9	I	195/208 (94%)	181 (93%)	14 (7%)	0	100	100
10	J	172/194 (89%)	159 (92%)	13 (8%)	0	100	100
11	F	180/204 (88%)	170 (94%)	10 (6%)	0	100	100
12	L	132/158 (84%)	128 (97%)	4 (3%)	0	100	100
13	K	93/165 (56%)	92 (99%)	1 (1%)	0	100	100
14	N	147/151 (97%)	140 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	124/151 (82%)	113 (91%)	11 (9%)	0	100	100
16	M	102/132 (77%)	97 (95%)	5 (5%)	0	100	100
17	P	129/145 (89%)	117 (91%)	12 (9%)	0	100	100
18	R	119/135 (88%)	110 (92%)	9 (8%)	0	100	100
19	Q	138/146 (94%)	124 (90%)	14 (10%)	0	100	100
20	S	139/152 (91%)	128 (92%)	11 (8%)	0	100	100
21	T	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
22	V	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
23	W	127/130 (98%)	114 (90%)	13 (10%)	0	100	100
24	X	137/143 (96%)	128 (93%)	8 (6%)	1 (1%)	18	50
25	Y	120/133 (90%)	113 (94%)	7 (6%)	0	100	100
26	U	96/119 (81%)	90 (94%)	6 (6%)	0	100	100
27	Z	68/125 (54%)	63 (93%)	5 (7%)	0	100	100
28	b	73/84 (87%)	67 (92%)	6 (8%)	0	100	100
29	c	59/69 (86%)	53 (90%)	6 (10%)	0	100	100
30	d	53/56 (95%)	44 (83%)	9 (17%)	0	100	100
31	e	46/59 (78%)	43 (94%)	3 (6%)	0	100	100
32	f	53/156 (34%)	46 (87%)	7 (13%)	0	100	100
33	g	287/317 (90%)	256 (89%)	31 (11%)	0	100	100
34	j	111/165 (67%)	98 (88%)	13 (12%)	0	100	100
35	z	365/568 (64%)	318 (87%)	47 (13%)	0	100	100
36	y	225/412 (55%)	187 (83%)	37 (16%)	1 (0%)	30	60
37	k	418/583 (72%)	359 (86%)	59 (14%)	0	100	100
All	All	5632/7089 (79%)	5152 (92%)	478 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	y	40	LYS
24	X	86	PRO

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	
2	A	180/243 (74%)	180 (100%)	0	100	100
3	B	192/231 (83%)	190 (99%)	2 (1%)	68	74
4	C	182/225 (81%)	178 (98%)	4 (2%)	45	63
5	E	220/225 (98%)	217 (99%)	3 (1%)	59	70
6	D	188/202 (93%)	187 (100%)	1 (0%)	81	80
7	G	194/218 (89%)	194 (100%)	0	100	100
8	H	160/174 (92%)	159 (99%)	1 (1%)	78	79
9	I	174/180 (97%)	171 (98%)	3 (2%)	53	67
10	J	156/168 (93%)	156 (100%)	0	100	100
11	F	156/170 (92%)	156 (100%)	0	100	100
12	L	126/142 (89%)	126 (100%)	0	100	100
13	K	86/136 (63%)	86 (100%)	0	100	100
14	N	130/131 (99%)	130 (100%)	0	100	100
15	O	99/119 (83%)	99 (100%)	0	100	100
16	M	91/108 (84%)	91 (100%)	0	100	100
17	P	117/130 (90%)	117 (100%)	0	100	100
18	R	109/122 (89%)	107 (98%)	2 (2%)	51	67
19	Q	116/121 (96%)	115 (99%)	1 (1%)	70	75
20	S	122/132 (92%)	122 (100%)	0	100	100
21	T	111/115 (96%)	111 (100%)	0	100	100
22	V	67/67 (100%)	67 (100%)	0	100	100
23	W	112/113 (99%)	110 (98%)	2 (2%)	51	67
24	X	111/115 (96%)	111 (100%)	0	100	100
25	Y	103/115 (90%)	103 (100%)	0	100	100
26	U	90/107 (84%)	89 (99%)	1 (1%)	65	73
27	Z	62/103 (60%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	b	70/76 (92%)	70 (100%)	0	100	100
29	c	54/62 (87%)	53 (98%)	1 (2%)	50	65
30	d	48/49 (98%)	45 (94%)	3 (6%)	16	43
31	e	40/48 (83%)	40 (100%)	0	100	100
32	f	51/140 (36%)	51 (100%)	0	100	100
33	g	255/275 (93%)	254 (100%)	1 (0%)	84	81
34	j	102/150 (68%)	102 (100%)	0	100	100
35	z	336/512 (66%)	332 (99%)	4 (1%)	63	72
36	y	201/367 (55%)	200 (100%)	1 (0%)	81	80
All	All	4611/5591 (82%)	4581 (99%)	30 (1%)	73	77

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	R	40	ILE
35	z	221	ASP
23	W	25	VAL
36	y	235	LEU
33	g	104	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
24	X	92	ASN
33	g	285	GLN
27	Z	89	GLN
33	g	14	HIS
35	z	309	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1645/1874 (87%)	428 (26%)	19 (1%)

5 of 428 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	11	A
1	2	14	C
1	2	17	C
1	2	25	A

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1679	A
1	2	1850	A
1	2	1872	G
1	2	1814	G
1	2	1060	A

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 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\# Z > 2$
40	ATP	z	603	39	32,33,33	1.32	5 (15%)	48,52,52	1.66	8 (16%)

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
40	ATP	z	603	39	-	1/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	z	603	ATP	C5-C4	4.14	1.46	1.39
40	z	603	ATP	C5-N7	-2.81	1.33	1.39
40	z	603	ATP	C4-N9	-2.52	1.32	1.37
40	z	603	ATP	C5-C6	2.16	1.47	1.41
40	z	603	ATP	C8-N7	2.10	1.35	1.31

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	z	603	ATP	C5-C4-N3	-5.55	119.08	126.72
40	z	603	ATP	N3-C4-N9	4.34	134.54	127.17
40	z	603	ATP	C2-N3-C4	3.36	120.03	111.83
40	z	603	ATP	C4-C5-N7	-3.10	107.04	110.58
40	z	603	ATP	N3-C2-N1	-2.78	124.38	128.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	z	603	ATP	C5'-O5'-PA-O3A

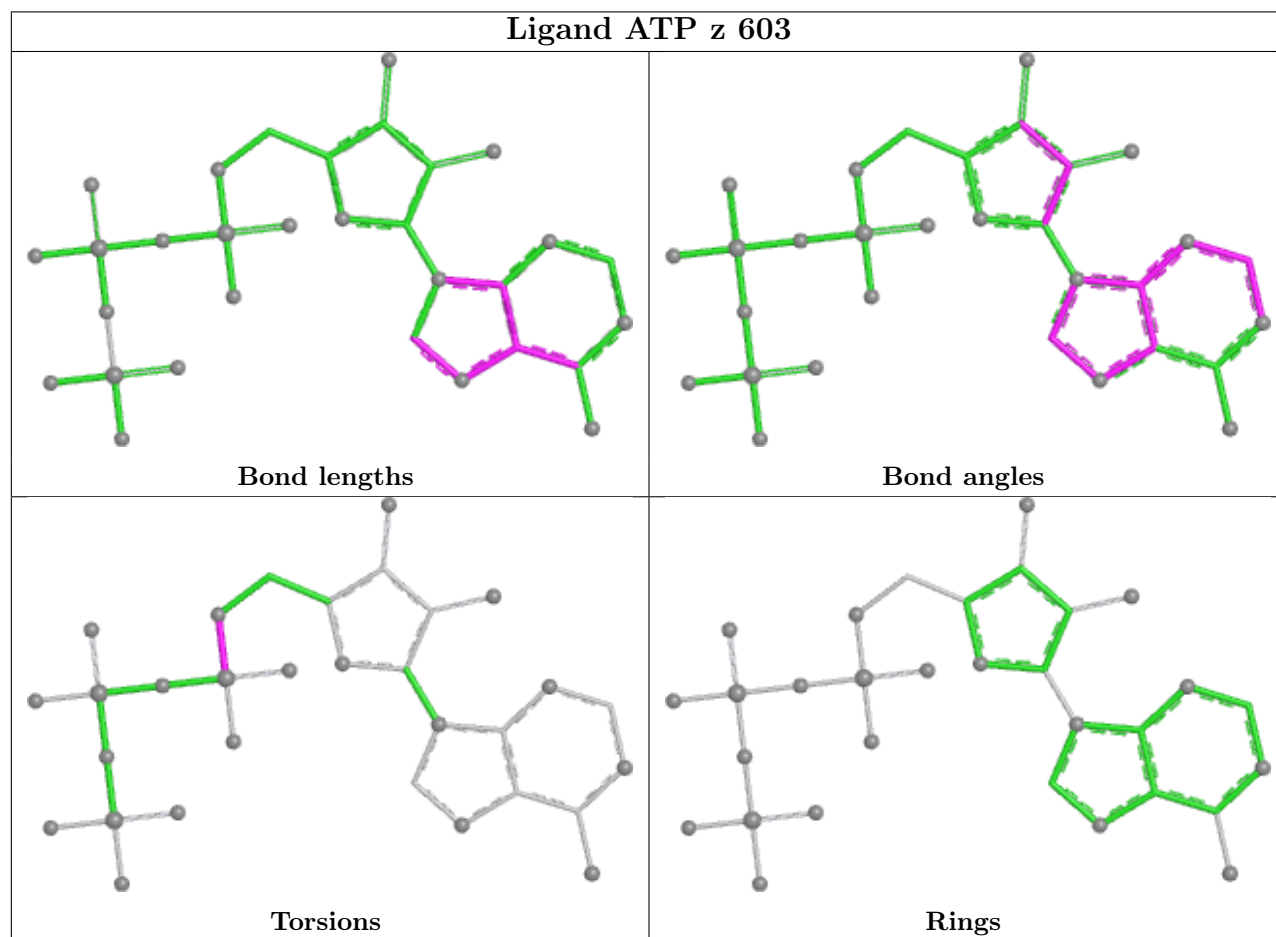
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	z	603	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

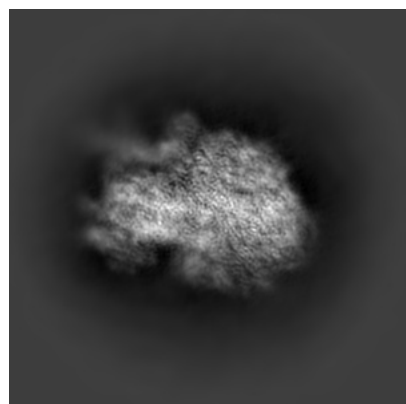
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11519. These allow visual inspection of the internal detail of the map and identification of artifacts.

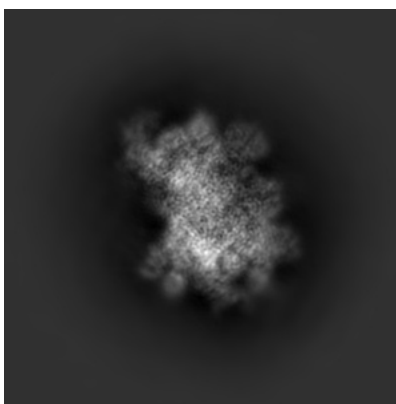
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

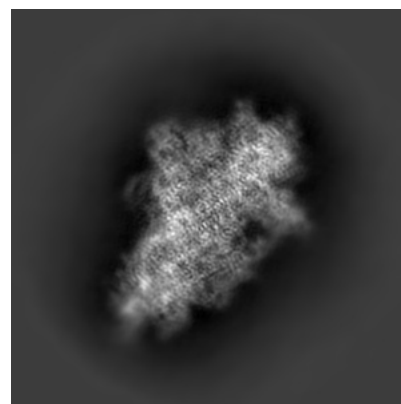
6.1.1 Primary map



X

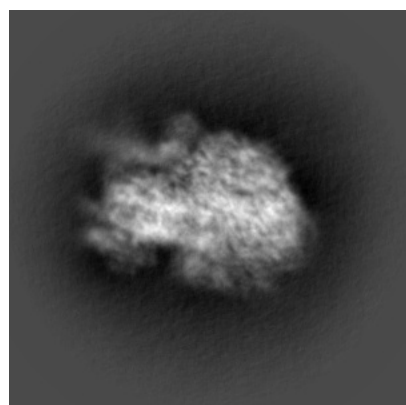


Y

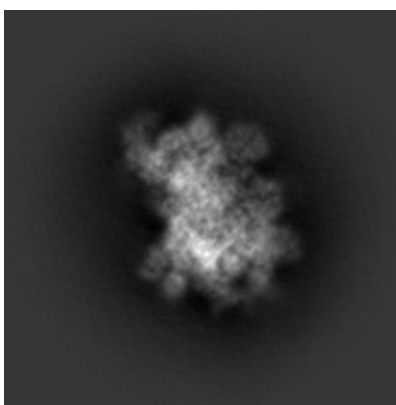


Z

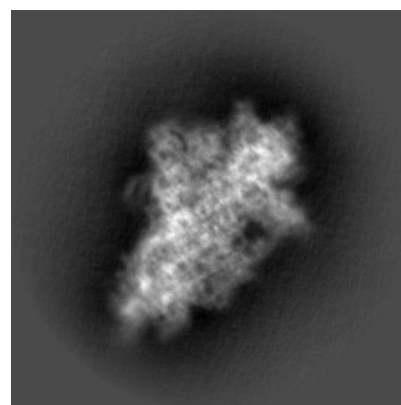
6.1.2 Raw map



X



Y

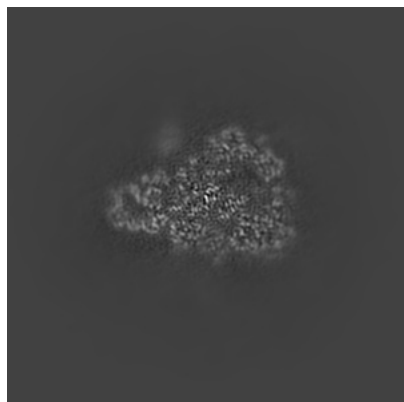


Z

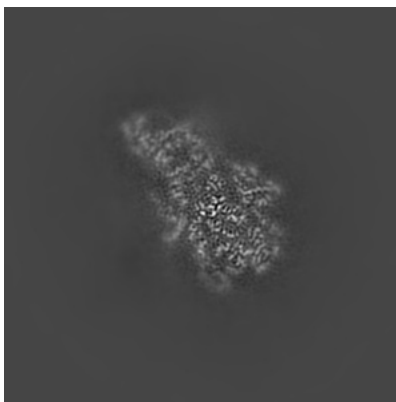
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

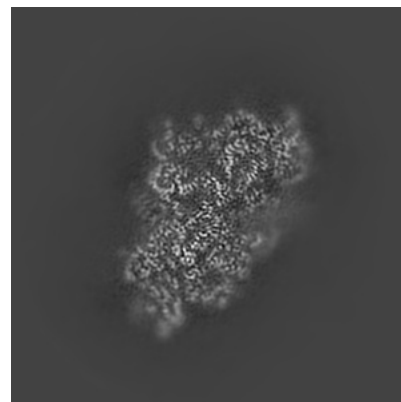
6.2.1 Primary map



X Index: 180

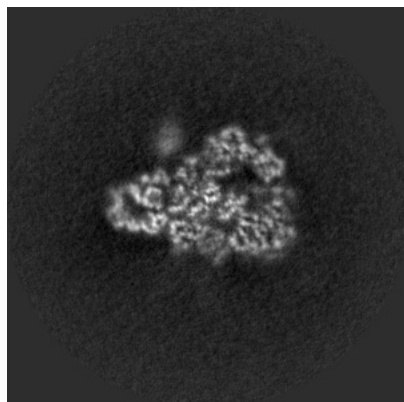


Y Index: 180

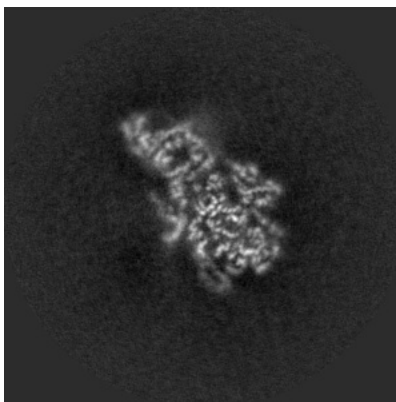


Z Index: 180

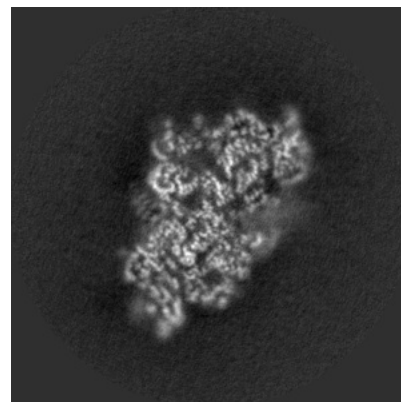
6.2.2 Raw map



X Index: 180



Y Index: 180

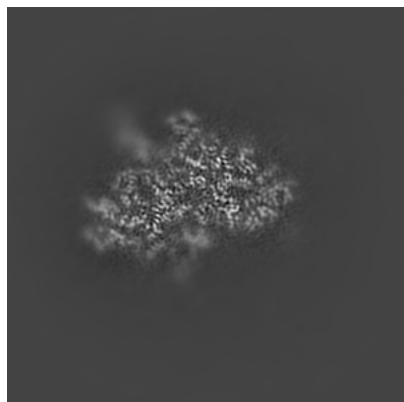


Z Index: 180

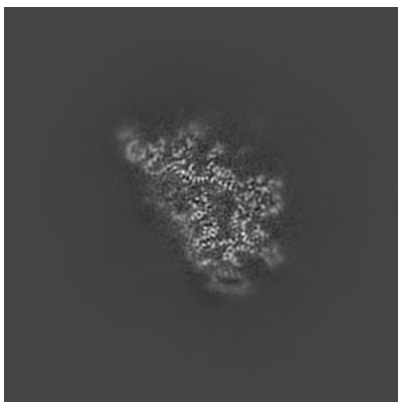
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

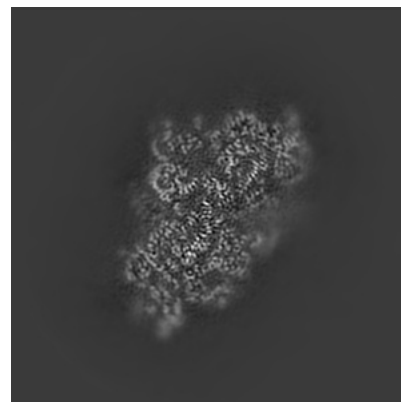
6.3.1 Primary map



X Index: 150

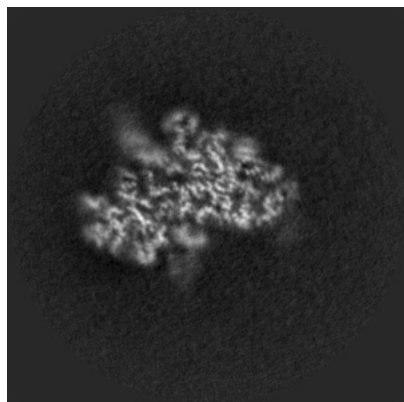


Y Index: 198

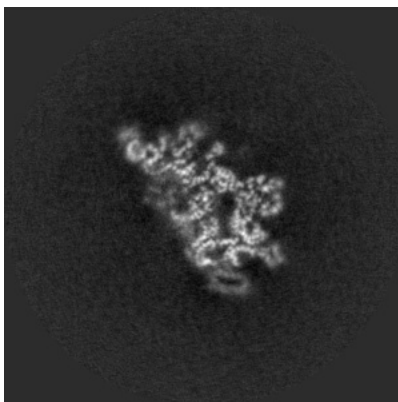


Z Index: 181

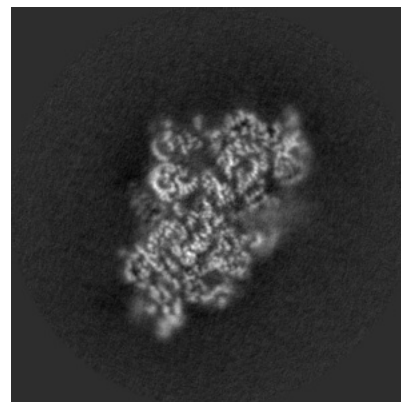
6.3.2 Raw map



X Index: 145



Y Index: 197

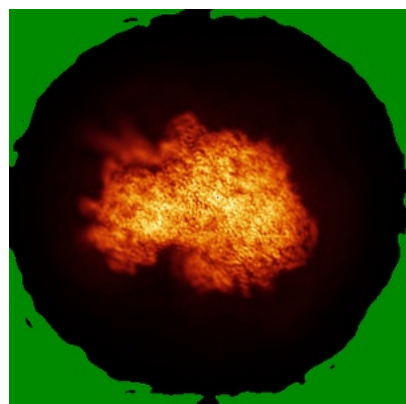


Z Index: 181

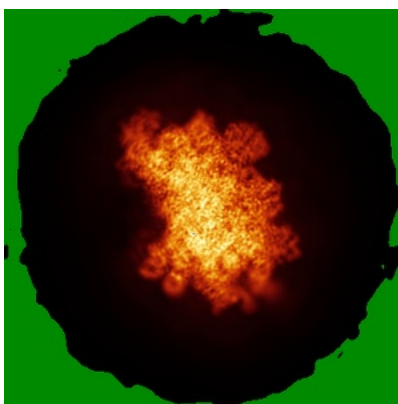
The images above show the largest variance slices of the map in three orthogonal directions.

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

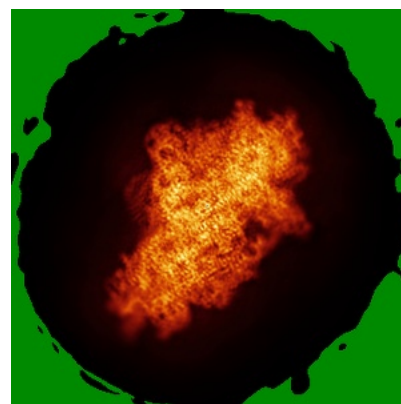
6.4.1 Primary map



X

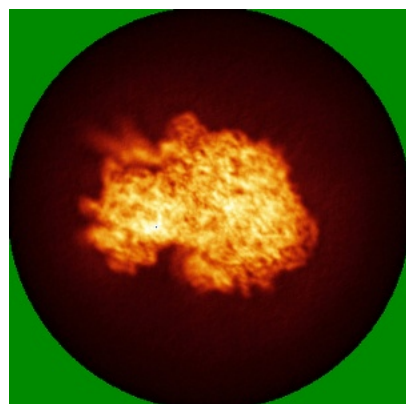


Y

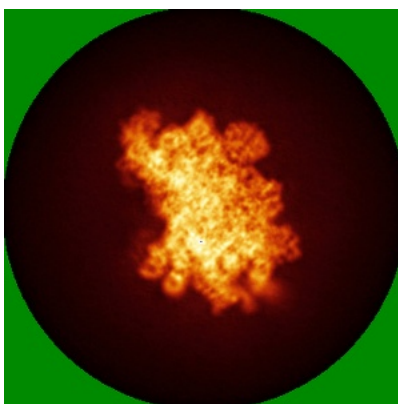


Z

6.4.2 Raw map



X



Y

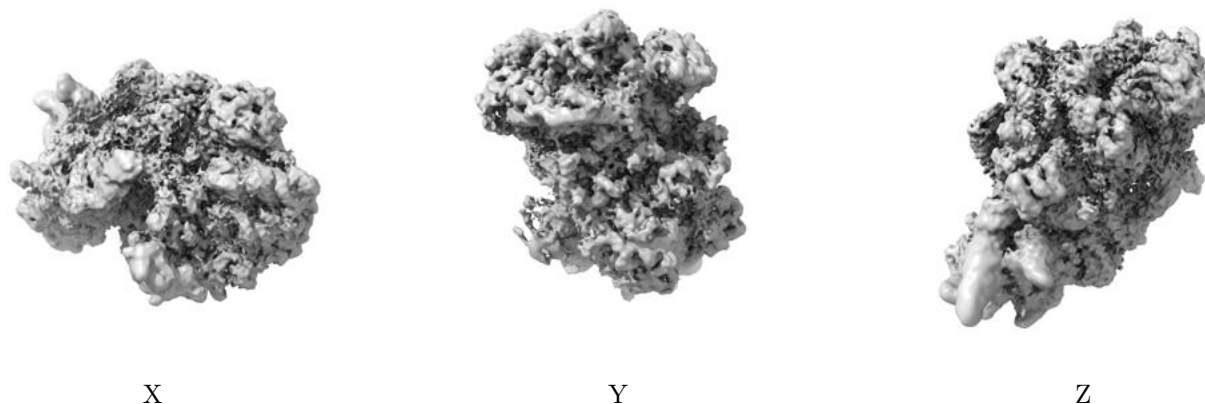


Z

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.

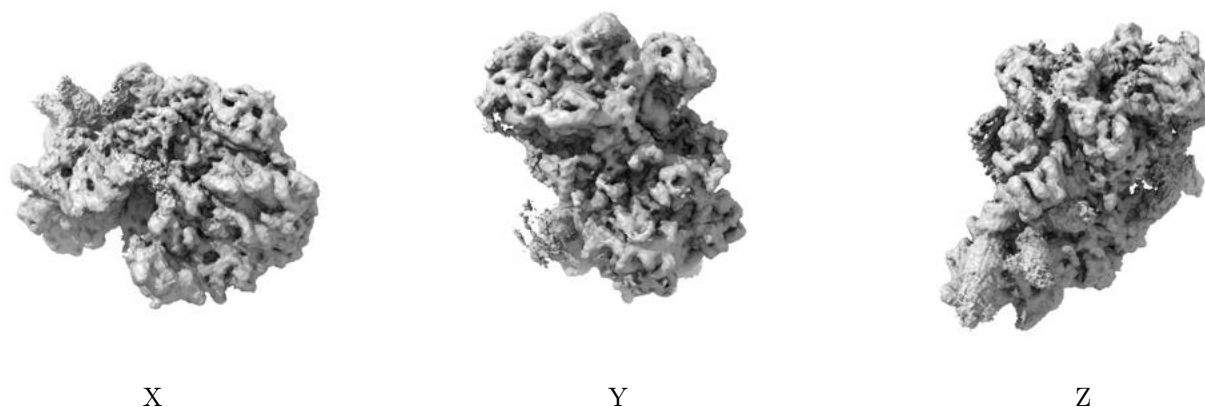
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

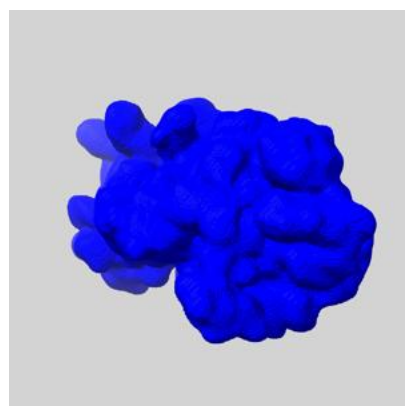
6.6 Mask visualisation [i](#)

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

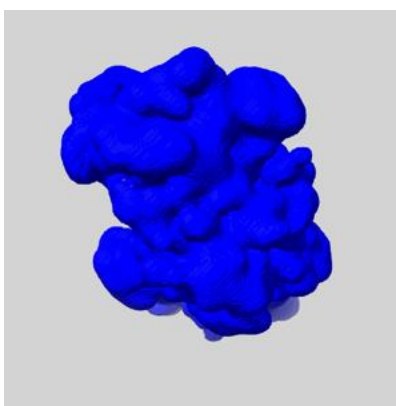
A mask typically either:

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

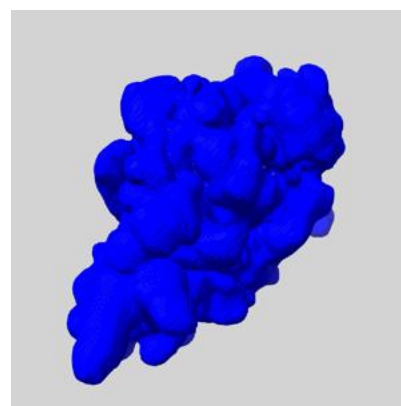
6.6.1 emd_11519_msk_1.map [i](#)



X



Y

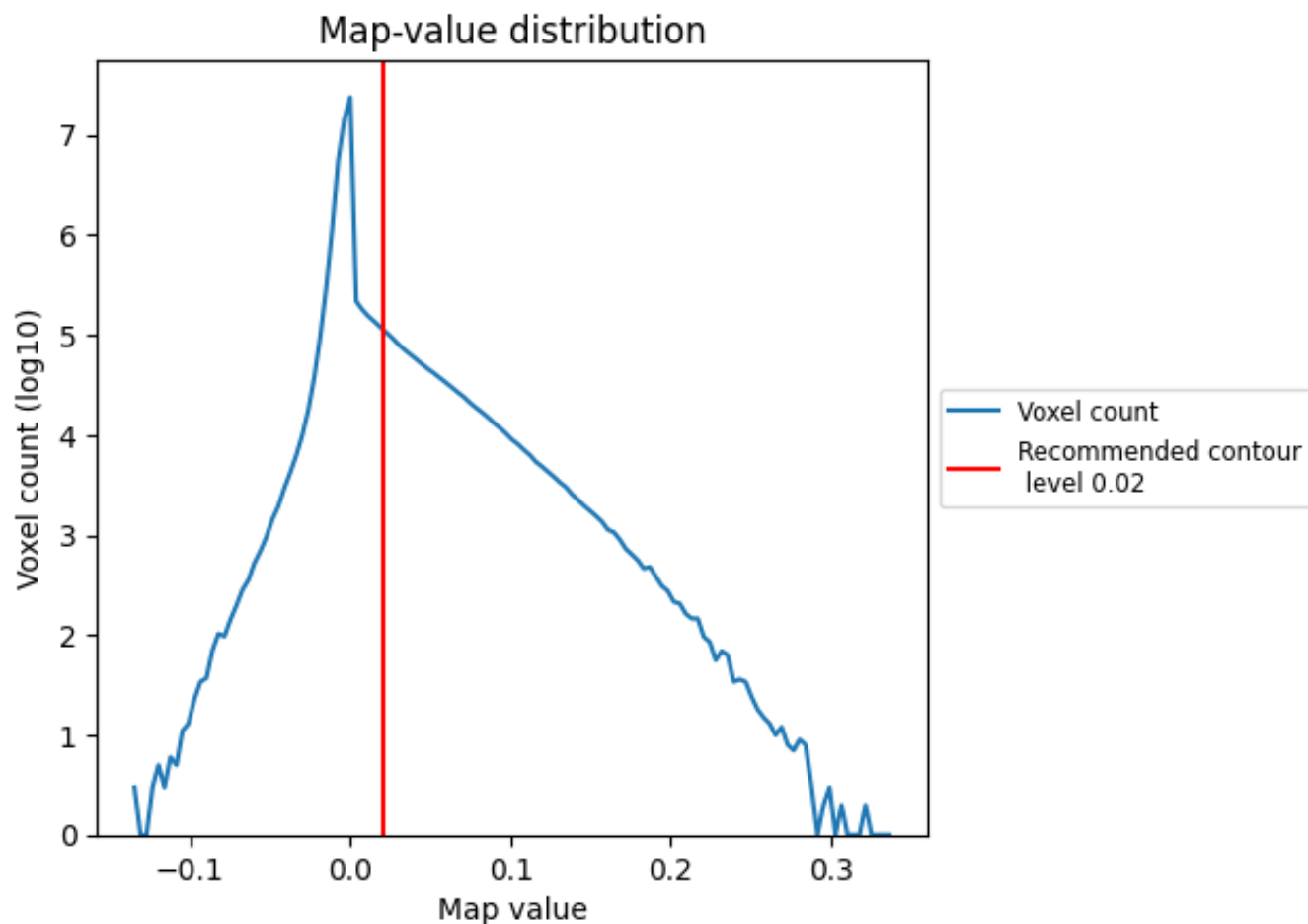


Z

7 Map analysis [i](#)

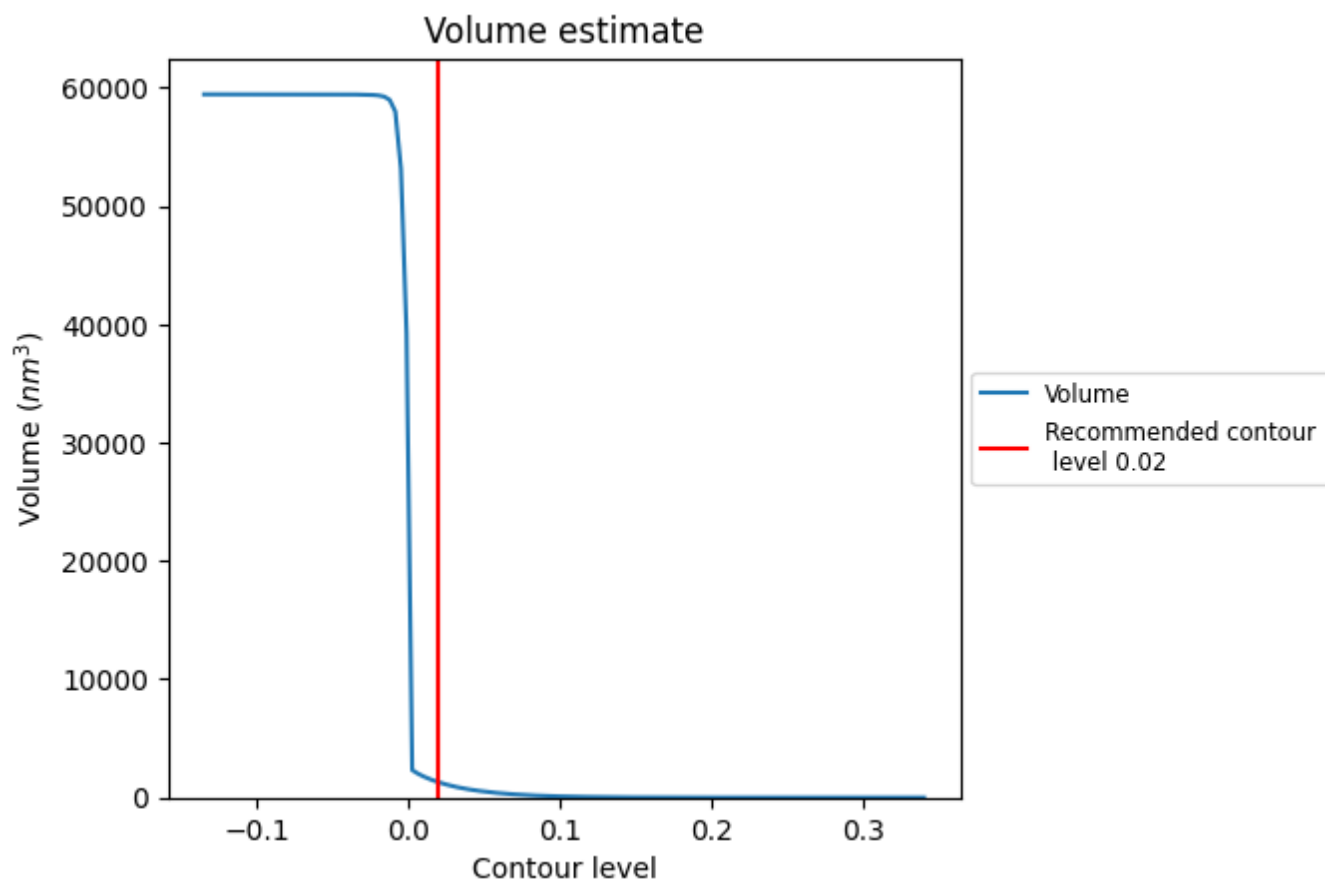
This section contains the results of statistical analysis of the map.

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.

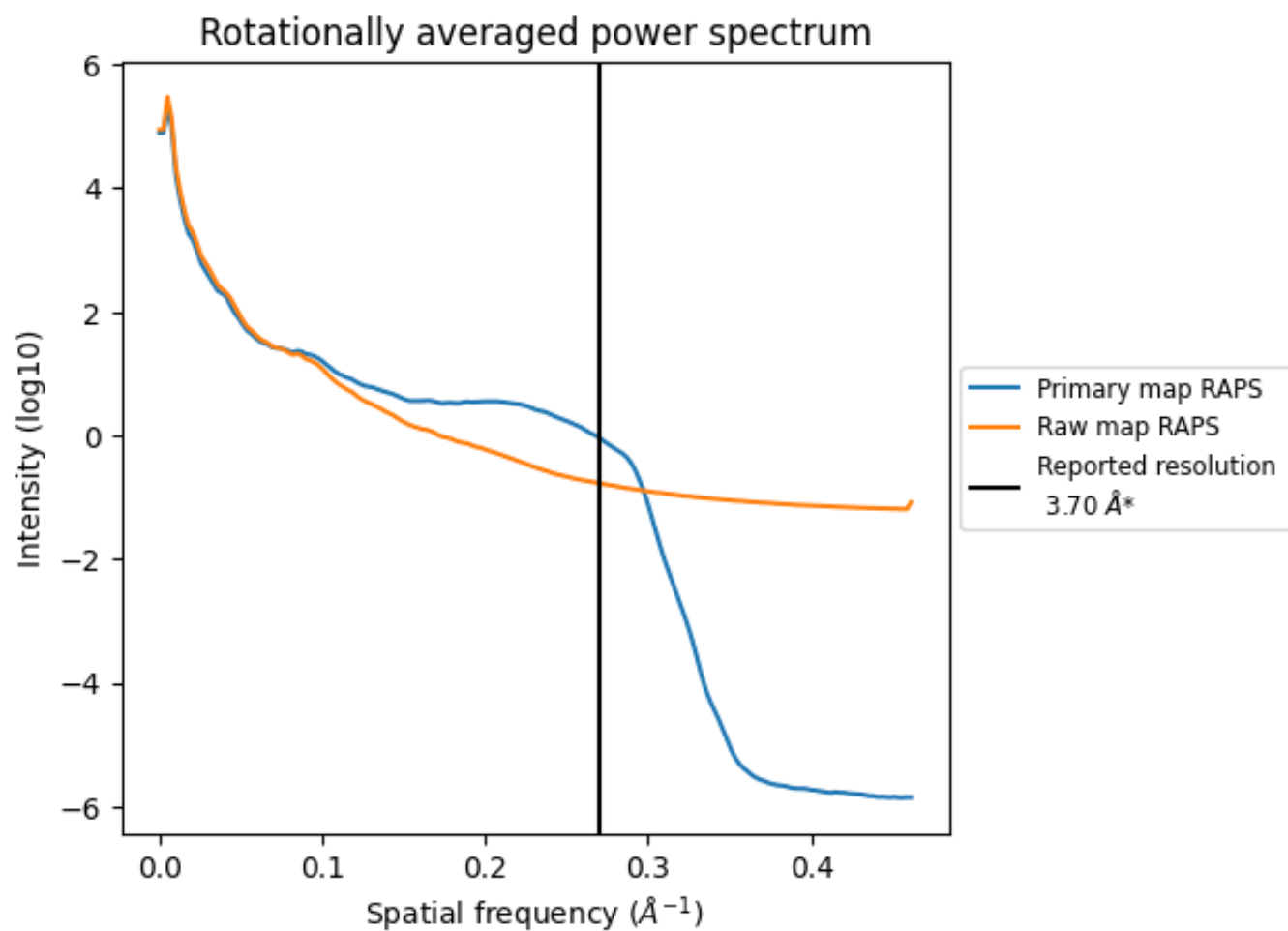
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1298 nm³; this corresponds to an approximate mass of 1173 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 ⓘ

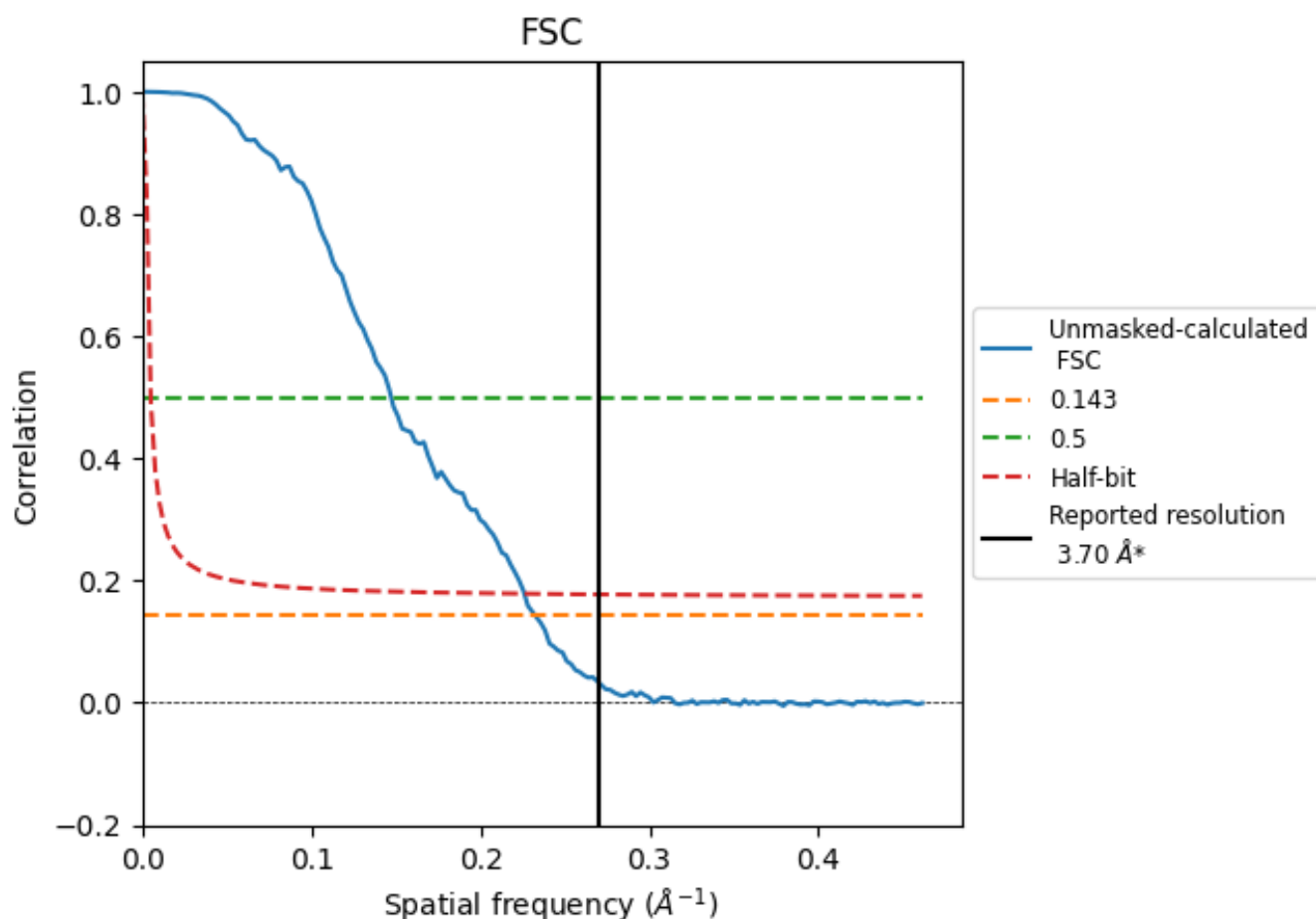


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

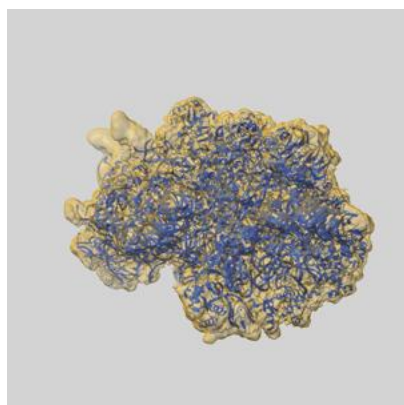
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.30	6.79	4.42

*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 4.30 differs from the reported value 3.7 by more than 10 %

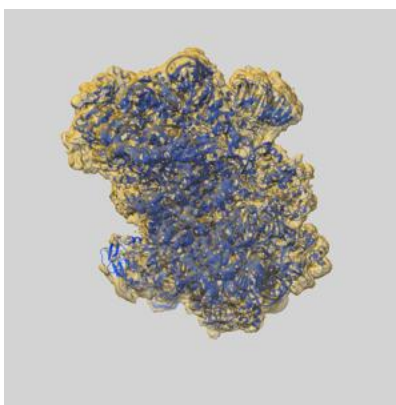
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11519 and PDB model 6ZXF. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

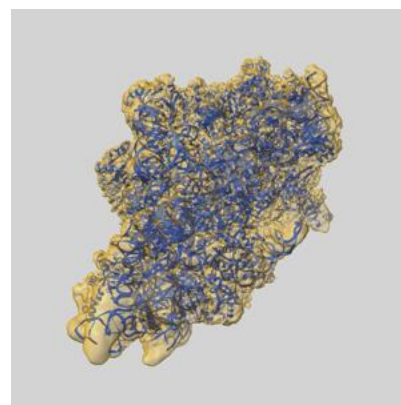
9.1 Map-model overlay [i](#)



X



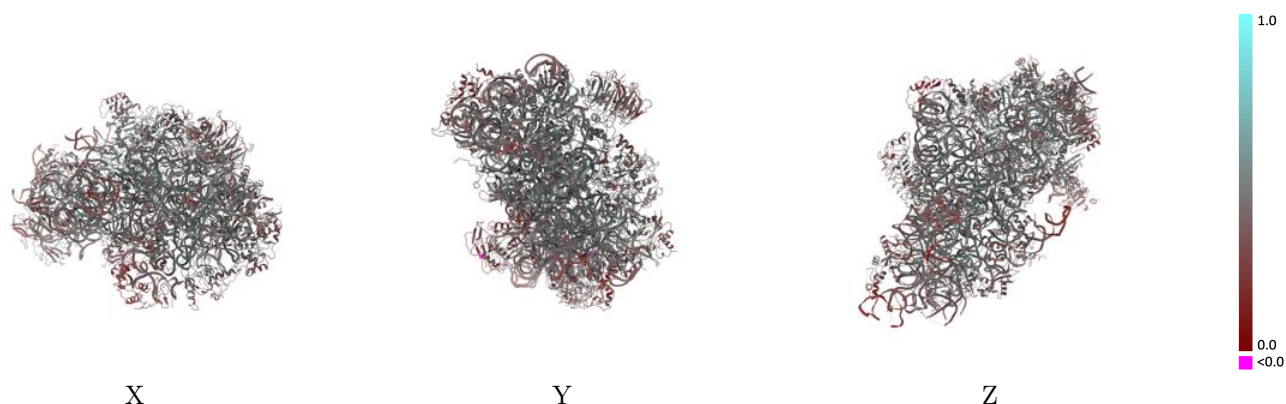
Y



Z

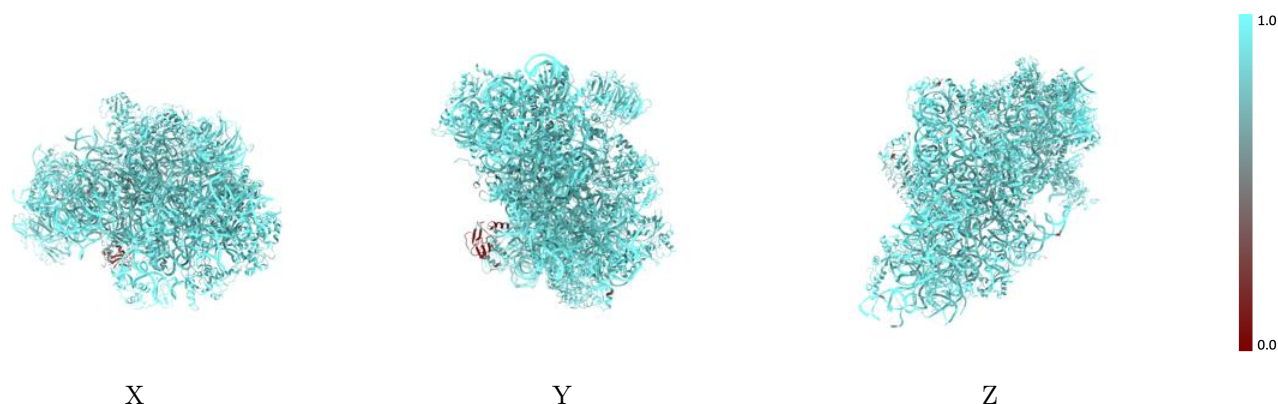
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



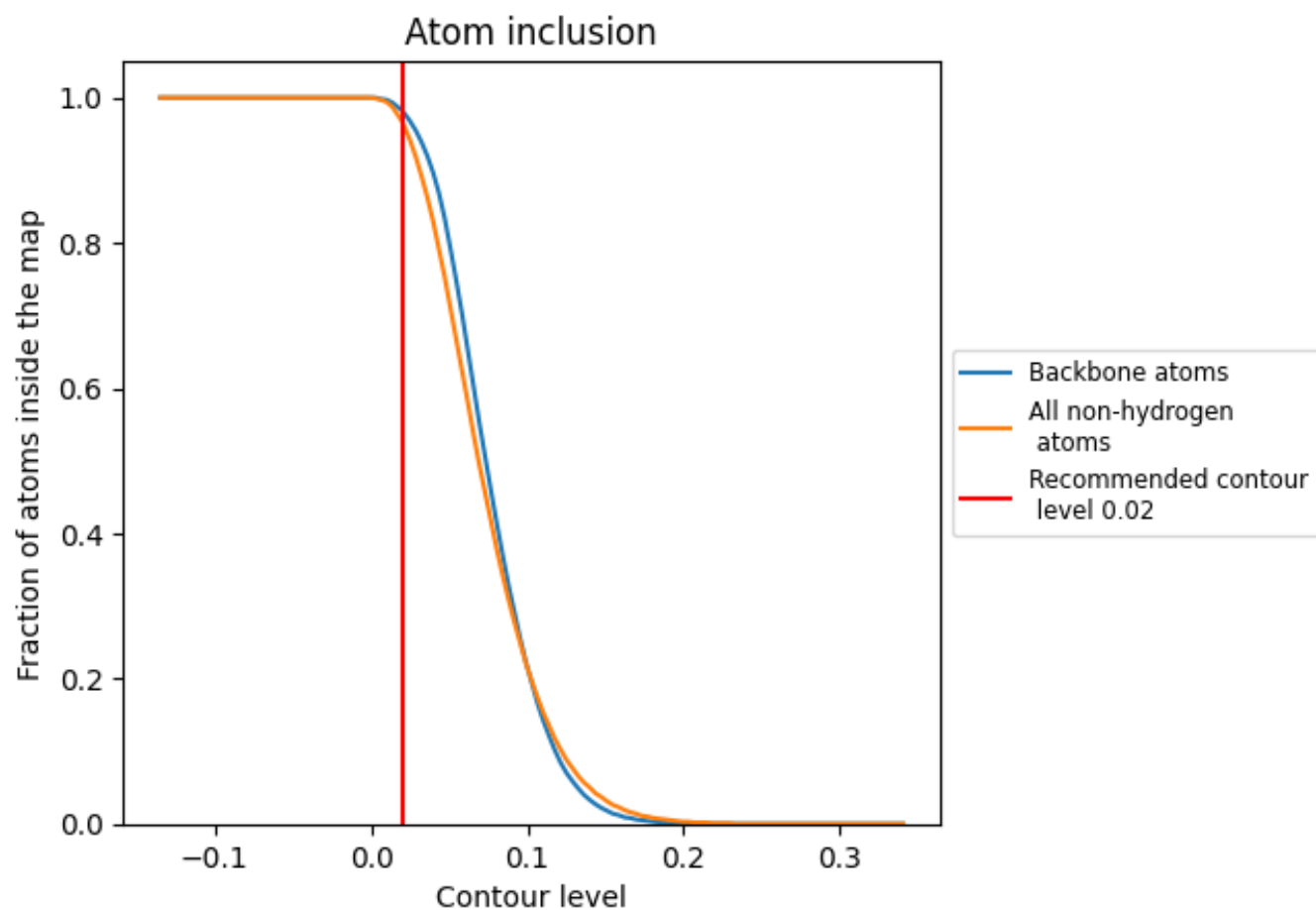
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9670	 0.4370
2	 0.9940	 0.4450
A	 0.9660	 0.4650
B	 0.9340	 0.3750
C	 0.9510	 0.4750
D	 0.9610	 0.4460
E	 0.9580	 0.4510
F	 0.9610	 0.4670
G	 0.9630	 0.3710
H	 0.9580	 0.3880
I	 0.9640	 0.4110
J	 0.9520	 0.4090
K	 0.9730	 0.4240
L	 0.9600	 0.4910
M	 0.9580	 0.2680
N	 0.9610	 0.4650
O	 0.9560	 0.4470
P	 0.9720	 0.4350
Q	 0.9590	 0.4700
R	 0.9560	 0.4430
S	 0.9550	 0.4160
T	 0.9660	 0.4600
U	 0.9630	 0.4410
V	 0.9610	 0.4700
W	 0.9660	 0.5000
X	 0.9780	 0.4980
Y	 0.9780	 0.4030
Z	 0.9450	 0.3820
b	 0.9750	 0.4740
c	 0.9330	 0.4620
d	 0.9820	 0.5090
e	 0.9790	 0.4410
f	 0.9870	 0.3310
g	 0.9690	 0.3990
j	 0.8450	 0.4290



Continued on next page...

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Chain	Atom inclusion	Q-score
k	 0.7000	 0.3540
y	 0.9580	 0.4540
z	 0.9310	 0.4480