Full wwPDB EM Validation Report ⓘ

Apr 8, 2024 – 11:11 am BST

PDB ID	:	8Q7X
EMDB ID	:	EMD-18237
Title	:	Structure of the recycling U5 snRNP bound to chaperone CD2BP2 (State 4)
Authors	:	Riabov Bassat, D.; Plaschka, C.; Vorlaender, M.K.
Deposited on	:	2023-08-17
Resolution	:	4.60 Å(reported)

This is a Full wwPDB EM Validation 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:

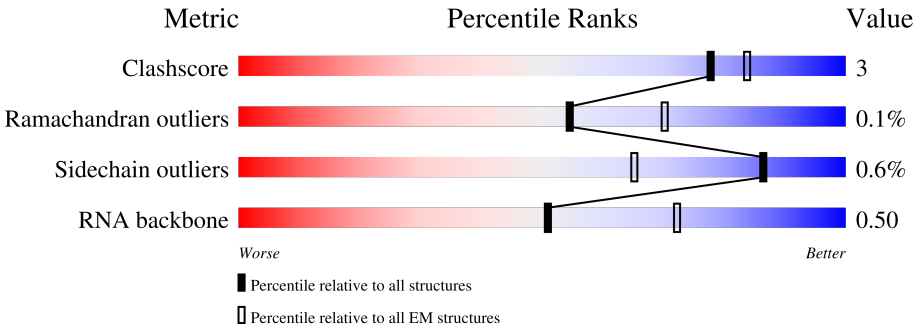
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 >=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 <=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	5	117	46% 33% 8% · 11%
2	A	2335	5% 73% 9% 18%
3	B	2136	27% 80% · 18%
4	C	972	78% 9% 13%
5	D	357	36% 84% · 14%
6	E	820	27% 69% · 30%
7	F	941	· 98%

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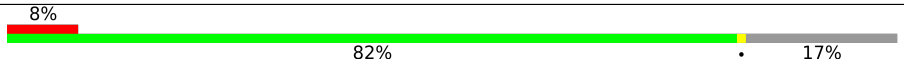
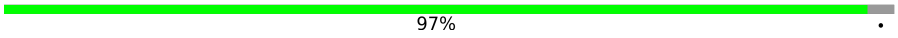
Mol	Chain	Length	Quality of chain
8	G	343	
9	a	119	
10	b	240	
11	c	118	
12	d	126	
13	e	92	
14	f	86	
15	g	76	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 72338 atoms, of which 30983 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 U5 snRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	5	104	3301	983	1109	372	734	103	0	0

- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A	1914	29097	9614	14096	2657	2667	63	0	0

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	B	1749	12700	5211	3966	1760	1761	2	0	0

- Molecule 4 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	C	846	13374	4268	6698	1121	1254	33	0	0

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
5	D	306	2193	894	686	306	307	0	0

- Molecule 6 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	E	575	4815	1871	1713	614	616	1	0	0

- Molecule 7 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	23	Total	C	H	N	O	0	0
			173	69	58	23	23		

- Molecule 8 is a protein called CD2 antigen cytoplasmic tail-binding protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	129	Total	C	H	N	O	S	0	0
			1983	615	983	182	199	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP O95400
G	0	PRO	-	expression tag	UNP O95400

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	81	Total	C	H	N	O	0	0
			567	239	166	81	81		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	73	Total	C	H	N	O	0	0
			511	214	151	73	73		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	98	Total	C	H	N	O	0	0
			688	291	201	98	98		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	d	82	Total	C	H	N	O	S	0	0
			1312	406	666	114	120	6		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	77	Total	C	H	N	O	0	0
			541	227	160	77	77		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	73	Total	C	H	N	O	0	0
			513	210	157	73	73		

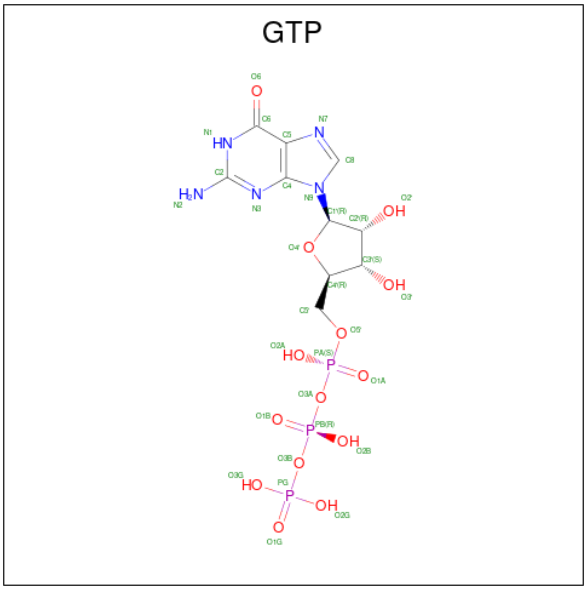
- Molecule 15 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	74	Total	C	H	N	O	0	0
			525	215	161	74	75		

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	C	1	Total	Mg	0
			1	1	

- Molecule 17 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



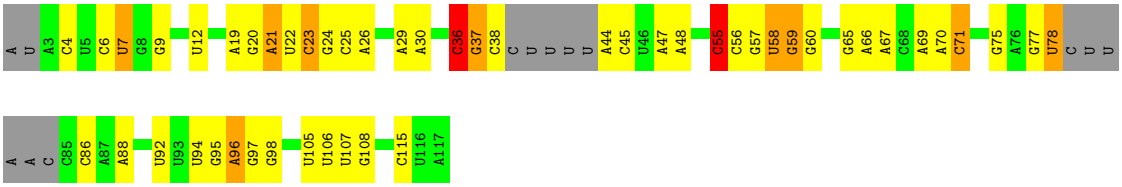
Mol	Chain	Residues	Atoms						AltConf
17	C	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

3 Residue-property plots (i)

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.

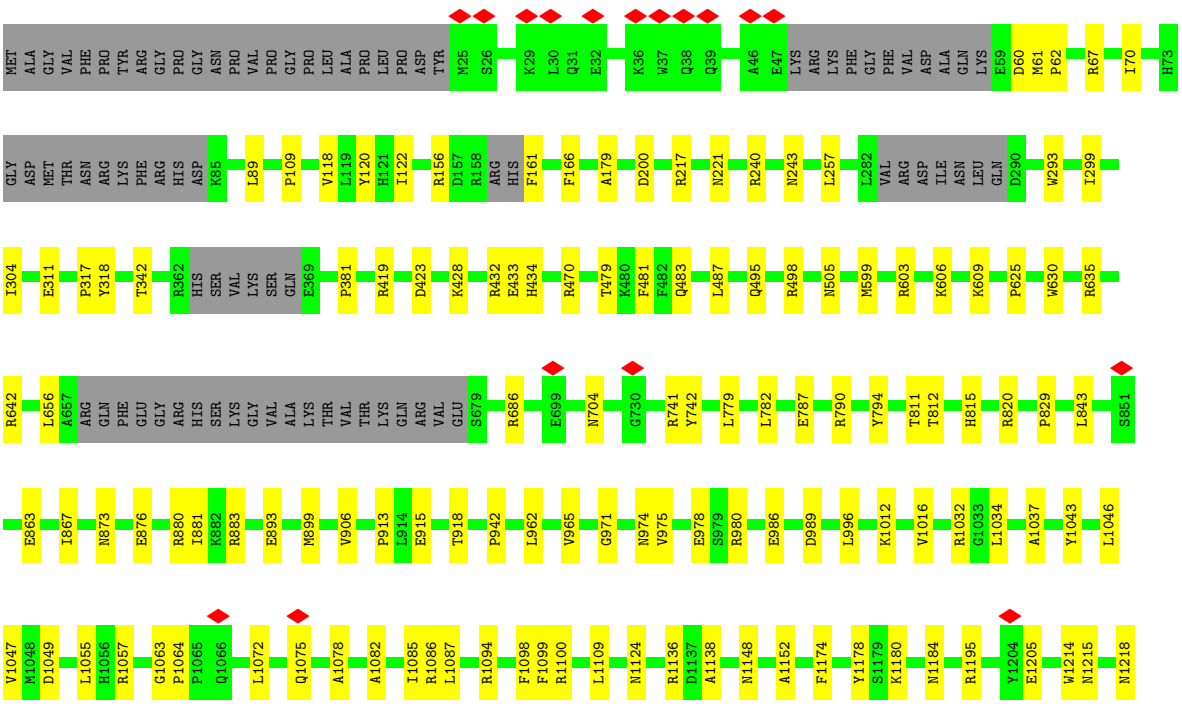
• Molecule 1: U5 snRNA

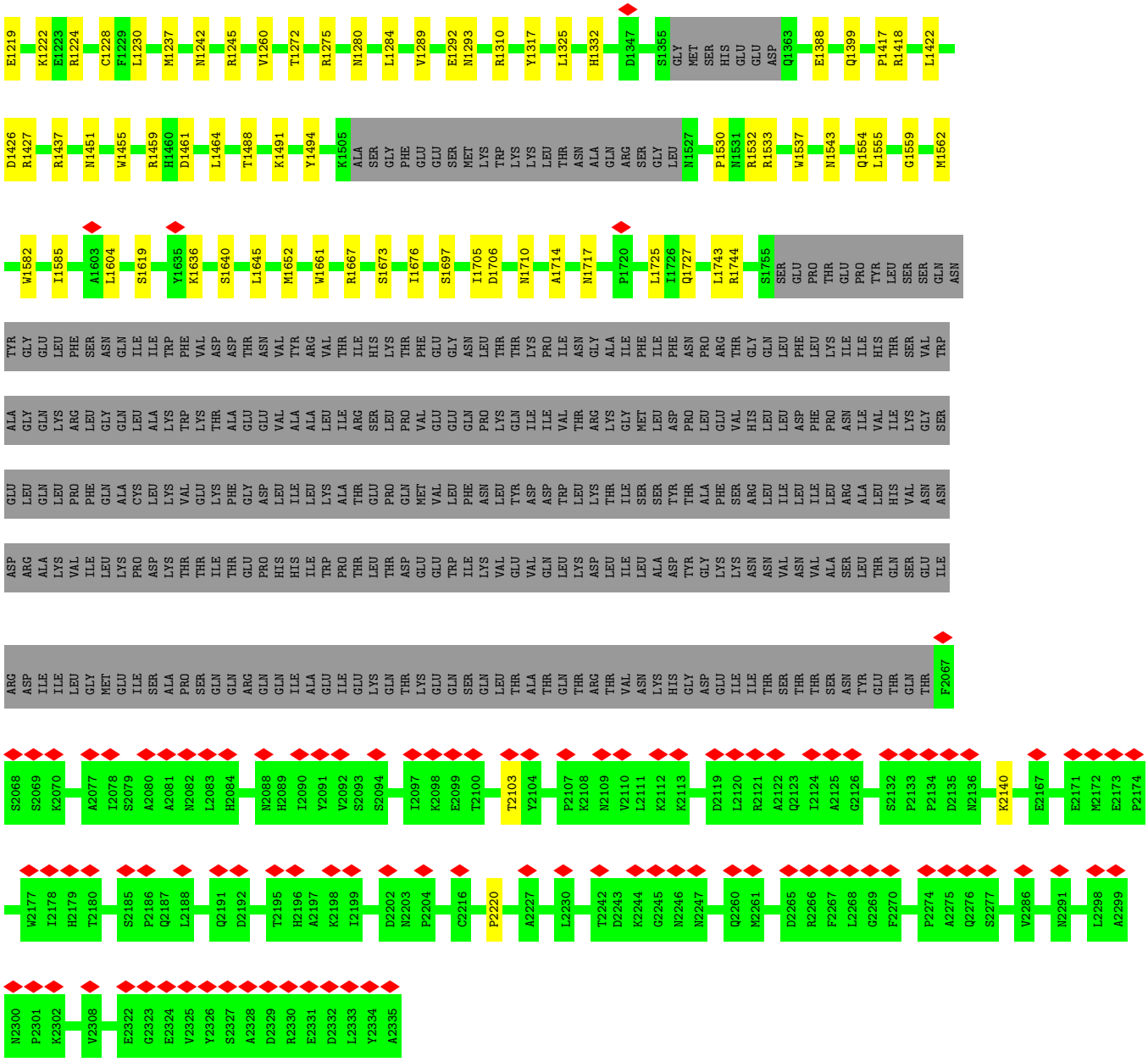
Chain 5: 46% 33% 8% • 11%



• Molecule 2: Pre-mRNA-processing-splicing factor 8

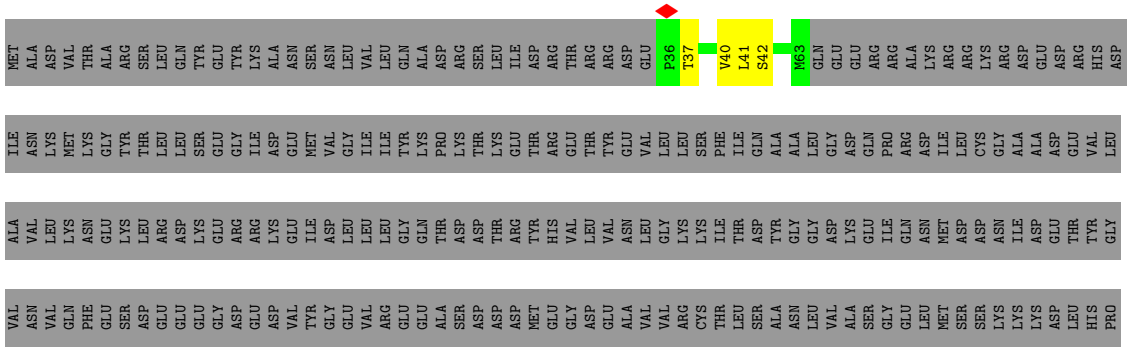
Chain A: 5% 73% 9% 18%

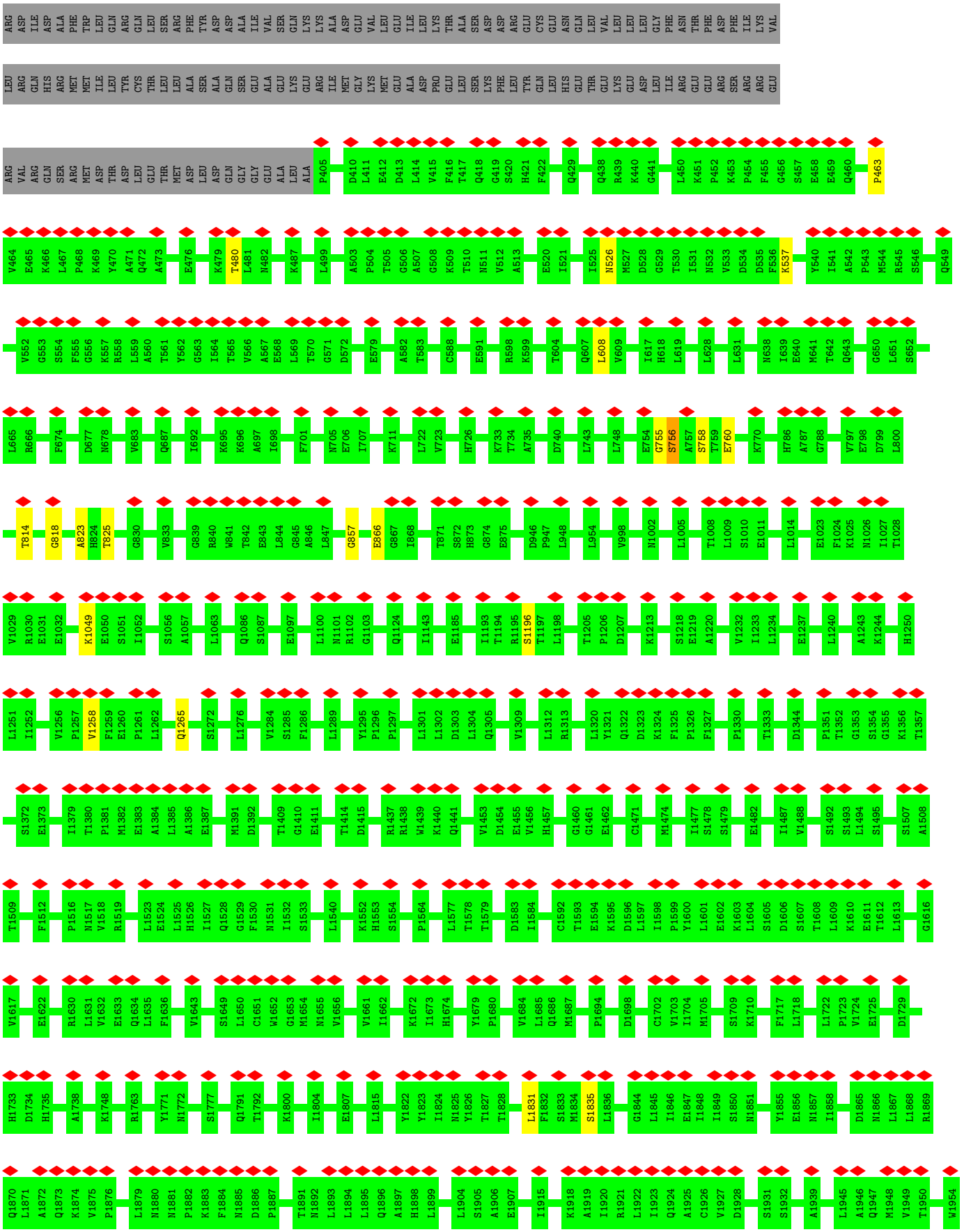


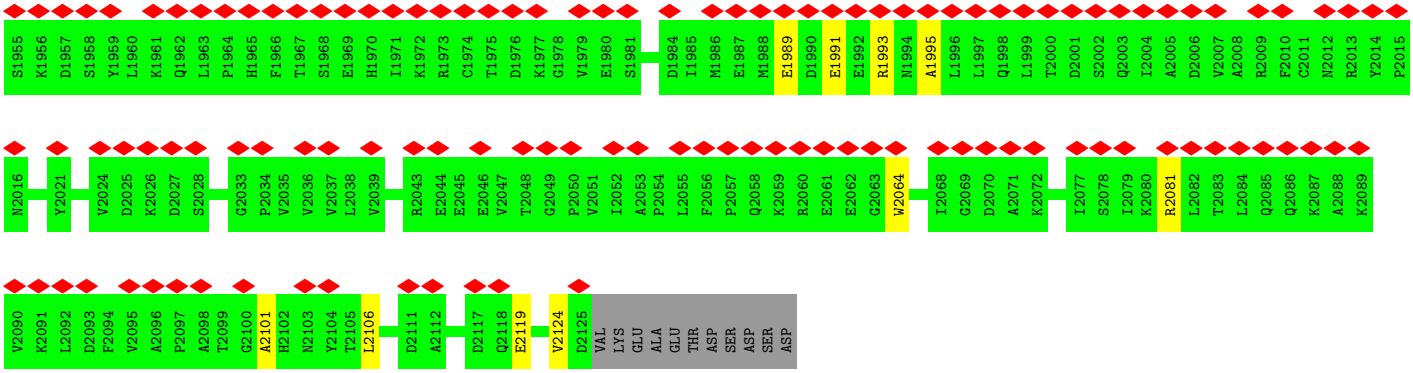


• Molecule 3: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain B:

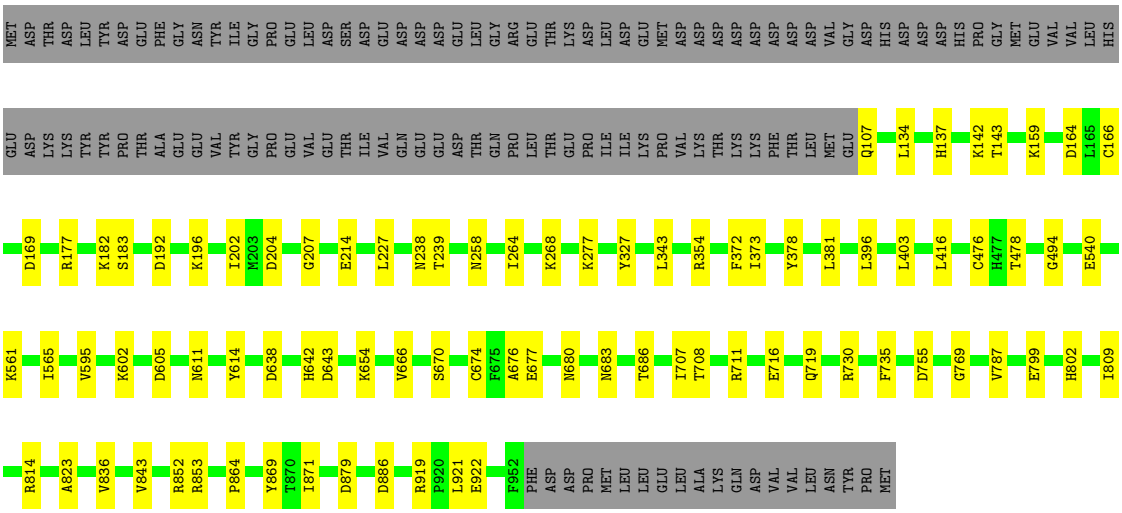



ARG ASP ILE ASP ALA PHE TRP LEU GLN ARG GLN LEU SER ARG PHE TYR ASP ASP ALA ILE VAL SER GLN LYS LYS ALA ASP GLU VAL LEU GLU ILE LEU LYS THR ALA SER ASP ASP ARG GLU CYS GLU ASN GLN LEU VAL LEU LEU LEU GLY PHE ASN THR PHE ASP PHE ILE LYS VAL
LEU ARG GLN HIS ARG MET MET ILE LEU TYR CYS THR LEU LEU ALA SER ALA GLN SER GLU ALA GLU LYS GLU ARG ILE MET GLY LYS MET GLU ALA ASP PRO GLU LEU SER LYS PHE LEU TYR GLN LEU HIS GLU THR GLU LYS GLU ASP LEU ILE ARG GLU GLU ARG SER ARG ARG GLU
ARG VAL ARG GLN SER ARG MET ASP THR ASP LEU GLU THR MET ASP LEU ASP GLN GLY GLY GLU ALA LEU ALA P405 D410 L411 E412 D413 L414 V415 F416 T417 Q418 G419 S420 H421 F422 Q429 Q438 R439 K440 G441 L450 K451 P452 K453 P454 F455 G456 S457 E458 E459 Q460 P463
V464 E465 K466 L467 P468 K469 Y470 A471 Q472 A473 E476 K479 T480 L481 N482 K487 L499 A503 P504 T505 G506 A507 G508 K509 T510 N511 V512 A513 E520 I521 I525 N526 M527 D528 G529 T530 I531 N532 V533 D534 D535 F536 K537 Y540 I541 A542 P543 M544 R545 S546 Q549
V552 G553 S554 F555 G556 K557 R558 L559 A560 T561 Y562 G563 I564 T565 V566 A567 E568 L569 T570 G571 D572 E579 A582 T583 C588 E591 R598 K599 T604 Q607 L608 V609 I617 H618 L619 L628 L631 N638 I639 E640 M641 T642 Q643 G650 L651 S652
L665 R666 F674 D677 N678 V683 Q687 I692 K695 K696 A697 I698 F701 N705 E706 I707 K711 L722 V723 H726 K733 T734 A735 D740 L743 L748 E754 G755 S756 A757 S758 T759 E760 K770 H786 A787 G788 V797 E798 D799 L800
T814 G818 A823 H824 T825 G830 V833 G839 R840 W841 T842 E843 L844 G845 A846 L847 G857 E866 G867 I868 T871 S872 H873 G874 E875 D946 P947 L948 L954 V998 N1002 L1005 T1008 L1009 S1010 E1011 L1014 E1023 F1024 K1025 N1026 I1027 T1028
V1029 R1030 E1031 E1032 K1049 E1050 S1051 I1052 S1056 A1057 L1063 Q1086 S1087 E1097 L1100 N1101 R1102 G1103 Q1124 I1143 E1185 I1193 T1194 R1195 S1196 T1197 L1198 T1205 P1206 D1207 K1213 S1218 E1219 A1220 V1232 I1233 L1234 E1237 L1240 A1243 K1244 H1250
L1251 I1252 V1256 P1257 V1258 F1259 E1260 P1261 L1262 Q1265 S1272 L1276 V1284 S1285 F1286 L1289 Y1295 P1296 P1297 L1301 L1302 D1303 L1304 Q1305 V1309 L1312 R1313 L1320 Y1321 Q1322 D1323 K1324 F1325 P1326 F1327 P1330 T1333 D1344 P1351 T1352 G1353 S1354 G1355 K1356 T1357
S1372 E1373 I1379 T1380 P1381 M1382 E1383 A1384 L1385 A1386 E1387 M1391 D1392 T1409 G1410 E1411 T1414 D1415 R1437 R1438 W1439 K1440 Q1441 V1453 D1454 E1455 V1456 H1457 G1460 C1461 E1462 C1471 M1474 I1477 S1478 S1479 E1482 I1487 V1488 S1492 S1493 L1494 S1495 S1507 A1508
T1509 F1512 P1516 N1517 V1518 R1519 L1523 E1524 L1525 H1526 I1527 Q1528 G1529 F1530 N1531 I1532 S1533 L1540 K1552 H1553 S1554 P1564 L1577 T1578 T1579 D1583 I1584 C1592 T1593 E1594 K1595 D1596 L1597 I1598 P1599 Y1600 L1601 E1602 K1603 L1604 S1605 D1606 S1607 T1608 L1609 K1610 E1611 T1612 L1613 G1616
V1617 E1622 R1630 L1631 V1632 E1633 Q1634 L1635 F1636 V1643 S1649 L1650 C1651 W1652 G1653 M1654 N1655 V1656 V1661 I1662 K1672 I1673 H1674 Y1679 P1680 V1684 L1685 Q1686 M1687 P1694 D1698 C1702 V1703 I1704 M1705 S1709 K1710 F1717 L1718 L1722 P1723 V1724 E1725 D1729
H1733 D1734 H1735 A1738 K1748 R1763 Y1771 N1772 S1777 Q1791 T1792 K1800 I1804 E1807 L1815 Y1822 Y1823 I1824 N1825 Y1826 T1827 T1828 L1831 F1832 S1833 M1834 S1835 L1836 G1844 L1845 I1846 E1847 I1848 I1849 S1850 N1851 Y1855 E1856 N1857 I1858 D1865 N1866 L1867 L1868 R1869
Q1870 L1871 A1872 Q1873 K1874 V1875 P1876 L1879 N1880 N1881 P1882 K1883 F1884 N1885 D1886 P1887 T1891 N1892 L1893 L1894 L1895 Q1896 A1897 H1898 L1899 L1904 S1905 A1906 E1907 I1915 K1918 A1919 I1920 R1921 L1922 I1923 Q1924 A1925 C1926 V1927 D1928 S1931 S1932 A1939 L1945 A1946 Q1947 M1948 V1949 T1950 W1954



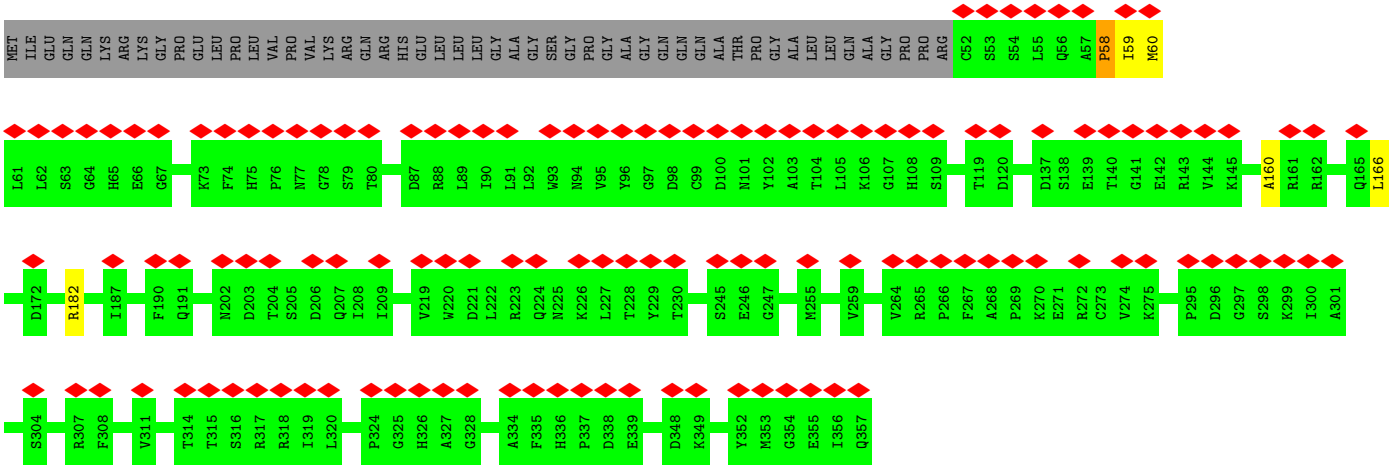
• Molecule 4: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C:



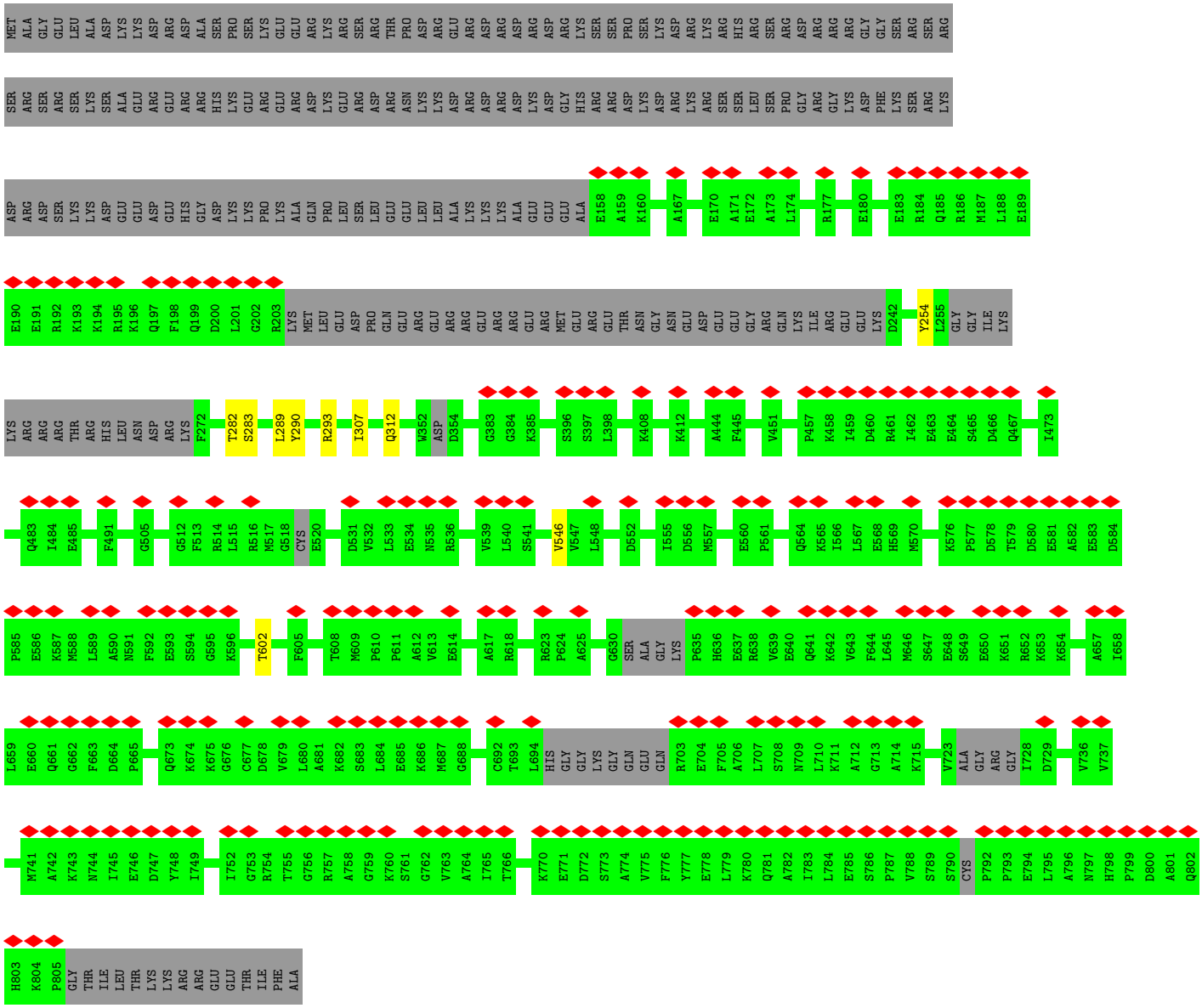
• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain D:



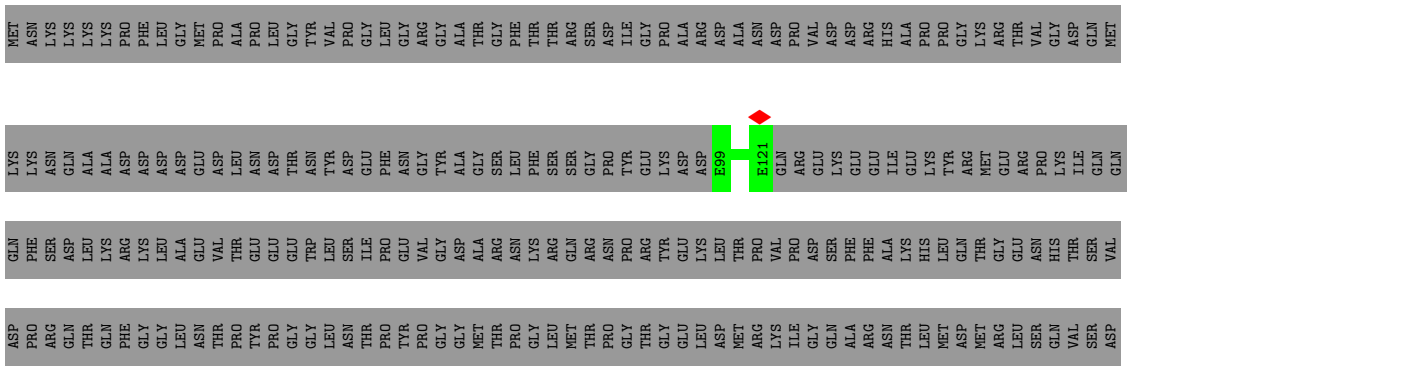
• Molecule 6: Probable ATP-dependent RNA helicase DDX23

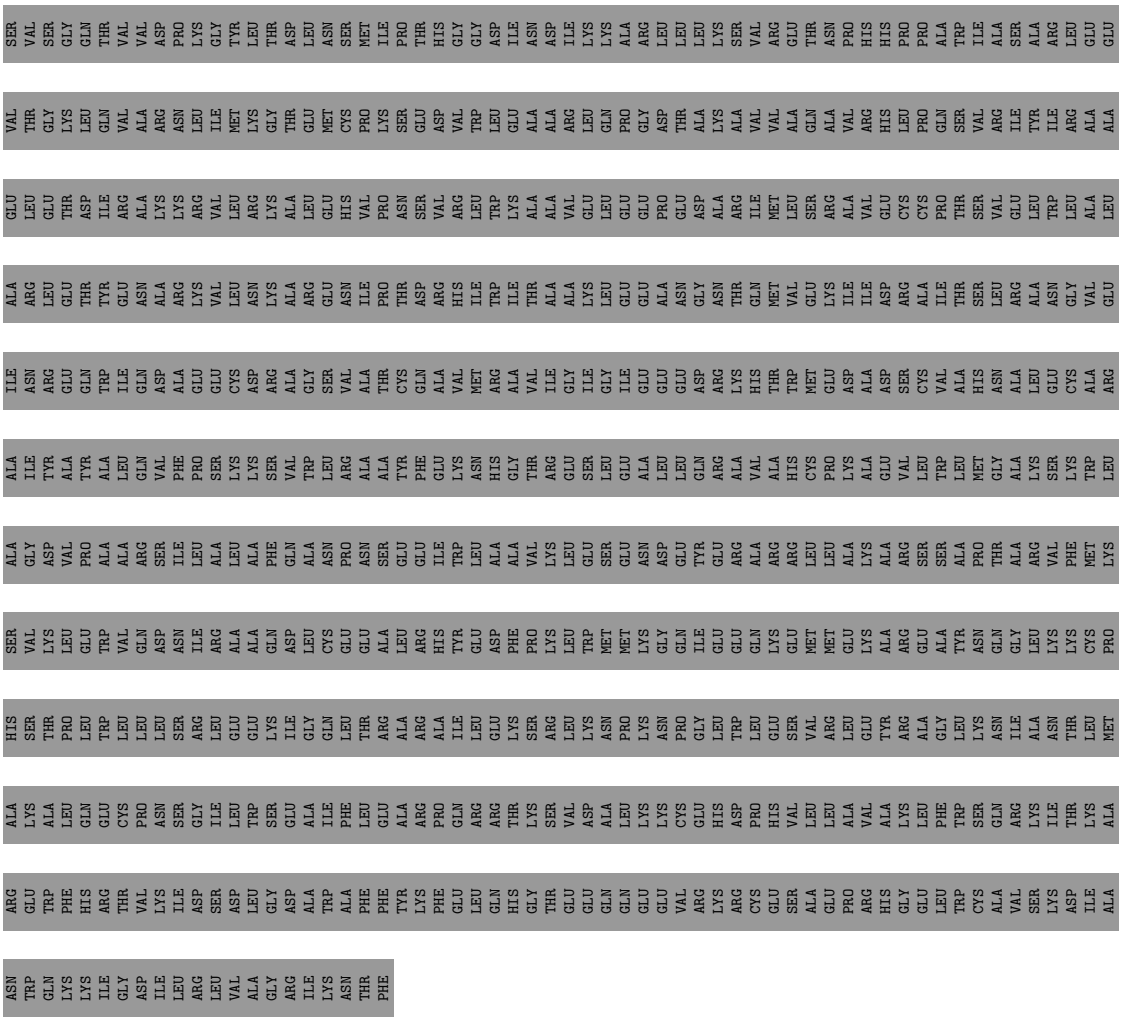
Chain E:



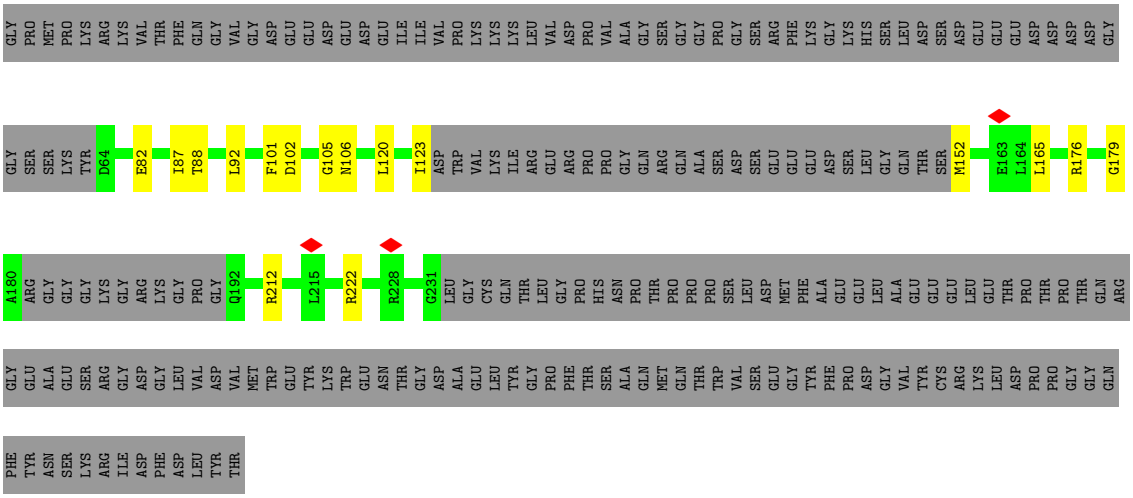
• Molecule 7: Pre-mRNA-processing factor 6

Chain F:



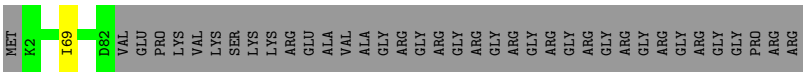


• Molecule 8: CD2 antigen cytoplasmic tail-binding protein 2



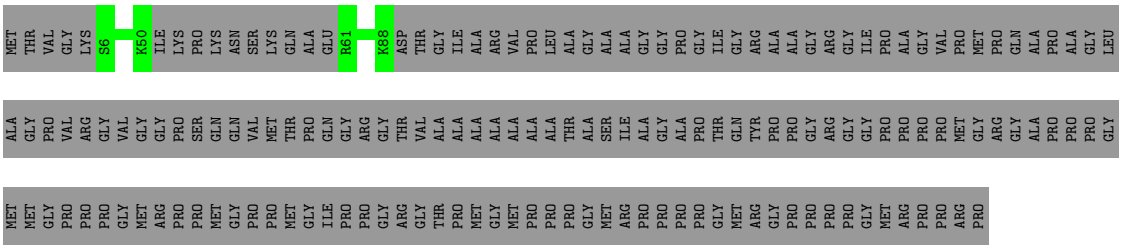
• Molecule 9: Small nuclear ribonucleoprotein Sm D1

Chain a:



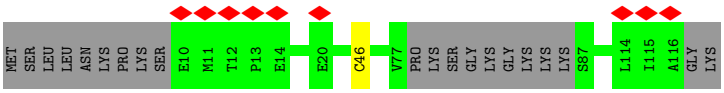
• Molecule 10: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain b:



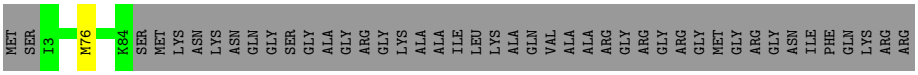
• Molecule 11: Small nuclear ribonucleoprotein Sm D2

Chain c:



• Molecule 12: Small nuclear ribonucleoprotein Sm D3

Chain d:



• Molecule 13: Small nuclear ribonucleoprotein E

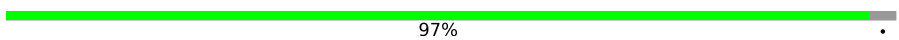
Chain e:

• Molecule 14: Small nuclear ribonucleoprotein F

Chain f:

• Molecule 15: Small nuclear ribonucleoprotein G

Chain g:




MET
SER
K3
V76

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6879	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.684	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	446.4, 446.4, 446.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	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, GTP

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	5	0.31	0/2444	1.15	18/3798 (0.5%)
2	A	0.27	0/15381	0.48	0/20914
3	B	0.32	0/8734	0.55	0/12162
4	C	0.30	0/6826	0.55	0/9272
5	D	0.28	0/1506	0.58	0/2091
6	E	0.31	0/3106	0.52	0/4278
7	F	0.23	0/114	0.39	0/158
8	G	0.25	0/1010	0.52	0/1359
9	a	0.25	0/400	0.59	1/556 (0.2%)
10	b	0.25	0/358	0.53	0/495
11	c	0.25	0/485	0.57	0/674
12	d	0.30	0/654	0.50	0/881
13	e	0.31	0/380	0.57	0/528
14	f	0.28	0/355	0.62	0/490
15	g	0.24	0/363	0.54	0/501
All	All	0.29	0/42116	0.58	19/58157 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
3	B	0	2
11	c	0	1
All	All	0	5

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	23	C	C2-N1-C1'	11.51	131.47	118.80
1	5	23	C	N1-C2-O2	9.22	124.43	118.90
1	5	57	G	O4'-C1'-N9	9.16	115.53	108.20
1	5	23	C	C6-N1-C1'	-8.05	111.14	120.80
1	5	23	C	C6-N1-C2	-7.27	117.39	120.30
1	5	23	C	N3-C2-O2	-7.03	116.98	121.90
1	5	23	C	C5-C6-N1	6.72	124.36	121.00
1	5	36	C	N1-C2-O2	6.62	122.88	118.90
9	a	69	ILE	C-N-CA	6.04	136.79	121.70
1	5	96	A	C2-N3-C4	5.82	113.51	110.60
1	5	36	C	C6-N1-C2	-5.75	118.00	120.30
1	5	55	C	N1-C2-O2	5.54	122.23	118.90
1	5	115	C	C2-N1-C1'	5.54	124.89	118.80
1	5	71	C	C2-N1-C1'	5.43	124.77	118.80
1	5	36	C	N3-C2-O2	-5.34	118.16	121.90
1	5	115	C	N1-C2-O2	5.28	122.07	118.90
1	5	7	U	N1-C2-O2	5.19	126.43	122.80
1	5	96	A	N3-C4-N9	5.06	131.45	127.40
1	5	56	C	N1-C2-O2	5.03	121.92	118.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1205	GLU	Peptide
2	A	166	PHE	Peptide
3	B	1265	GLN	Peptide
3	B	526	ASN	Peptide
11	c	46	CYS	Peptide

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	5	2192	1109	1111	12	0
2	A	15001	14096	14086	114	0
3	B	8734	3966	3966	20	0
4	C	6676	6698	6697	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1507	686	685	4	0
6	E	3102	1713	1706	7	0
7	F	115	58	57	0	0
8	G	1000	983	980	10	0
9	a	401	166	165	0	0
10	b	360	151	149	0	0
11	c	487	201	199	0	0
12	d	646	666	665	0	0
13	e	381	160	159	0	0
14	f	356	157	156	0	0
15	g	364	161	160	0	0
16	C	1	0	0	0	0
17	C	32	12	12	2	0
All	All	41355	30983	30953	193	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 3.

All (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1388:GLU:OE2	2:A:2220:PRO:CB	2.08	1.01
4:C:143:THR:HG22	17:C:1101:GTP:O2B	1.81	0.81
1:5:12:U:H3	1:5:65:G:H1	1.37	0.73
3:B:2106:LEU:O	3:B:2119:GLU:HA	1.91	0.70
2:A:1087:LEU:HB2	2:A:1098:PHE:HB3	1.72	0.70
2:A:1399:GLN:NE2	3:B:1049:LYS:O	2.25	0.70
2:A:1388:GLU:CG	2:A:2220:PRO:CB	2.70	0.69
1:5:36:C:C2	1:5:44:A:N6	2.62	0.68
2:A:974:ASN:HB2	2:A:1178:TYR:HB3	1.77	0.67
2:A:1219:GLU:O	2:A:1222:LYS:HE2	1.94	0.66
2:A:1184:ASN:HD22	2:A:1195:ARG:HH21	1.43	0.65
4:C:142:LYS:HE2	17:C:1101:GTP:O1G	2.01	0.61
4:C:476:CYS:HB2	4:C:565:ILE:HB	1.82	0.60
2:A:428:LYS:O	2:A:432:ARG:HB2	2.03	0.59
2:A:1272:THR:O	2:A:1275:ARG:NH2	2.36	0.58
2:A:1242:ASN:OD1	2:A:1245:ARG:NH1	2.37	0.58
3:B:2101:ALA:HA	3:B:2124:VAL:O	2.03	0.58
2:A:1437:ARG:NH2	2:A:1455:TRP:O	2.36	0.58
2:A:843:LEU:HD22	2:A:867:ILE:HG23	1.86	0.58
2:A:293:TRP:HH2	2:A:299:ILE:HG12	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:980:ARG:HH11	2:A:1094:ARG:HD2	1.68	0.58
2:A:1289:VAL:HG21	3:B:42:SER:HA	1.84	0.58
2:A:606:LYS:O	2:A:609:LYS:HB3	2.05	0.57
6:E:307:ILE:HB	6:E:312:GLN:HE21	1.69	0.57
2:A:60:ASP:O	8:G:176:ARG:NH2	2.38	0.57
2:A:1237:MET:HG2	2:A:1284:LEU:HD13	1.87	0.57
2:A:1214:TRP:HB2	2:A:1228:CYS:HB3	1.86	0.56
1:5:19:A:N3	1:5:21:A:N6	2.53	0.56
2:A:1388:GLU:CD	2:A:2220:PRO:CB	2.74	0.56
2:A:200:ASP:OD1	2:A:240:ARG:NH1	2.40	0.54
2:A:70:ILE:HG21	2:A:495:GLN:HG2	1.89	0.54
2:A:1532:ARG:HD2	8:G:105:GLY:HA3	1.89	0.54
4:C:711:ARG:NH1	4:C:730:ARG:O	2.41	0.54
3:B:463:PRO:HA	3:B:480:THR:HA	1.90	0.54
4:C:159:LYS:HE2	4:C:164:ASP:HA	1.88	0.54
2:A:1667:ARG:NH1	2:A:1673:SER:OG	2.41	0.53
1:5:55:C:OP2	2:A:470:ARG:NH1	2.41	0.53
4:C:614:TYR:OH	4:C:643:ASP:OD2	2.27	0.53
2:A:1676:ILE:HD13	2:A:1706:ASP:HB2	1.90	0.53
2:A:1640:SER:O	2:A:1717:ASN:ND2	2.41	0.53
4:C:177:ARG:NH1	4:C:638:ASP:OD2	2.42	0.53
1:5:77:G:O2'	5:D:182:ARG:O	2.21	0.53
2:A:1543:ASN:HD21	2:A:1562:MET:HA	1.74	0.53
2:A:986:GLU:OE2	2:A:1032:ARG:NH1	2.41	0.53
4:C:277:LYS:NZ	4:C:864:PRO:O	2.38	0.53
4:C:183:SER:HA	4:C:204:ASP:O	2.09	0.53
2:A:975:VAL:HB	2:A:1099:PHE:HB2	1.90	0.52
8:G:152:MET:O	8:G:212:ARG:NH1	2.43	0.52
2:A:812:THR:HG23	2:A:1055:LEU:HD11	1.91	0.52
5:D:160:ALA:HB3	5:D:166:LEU:H	1.74	0.52
2:A:1417:PRO:HB3	2:A:1461:ASP:HA	1.92	0.52
2:A:1124:ASN:ND2	2:A:1148:ASN:OD1	2.40	0.52
2:A:1138:ALA:O	2:A:1184:ASN:ND2	2.42	0.52
2:A:1332:HIS:HB3	3:B:41:LEU:HB2	1.91	0.52
2:A:479:THR:HG22	2:A:481:PHE:H	1.74	0.52
4:C:677:GLU:O	4:C:814:ARG:NH1	2.43	0.52
2:A:1661:TRP:HD1	2:A:1697:SER:HB3	1.75	0.52
4:C:919:ARG:NH2	4:C:922:GLU:OE1	2.42	0.52
8:G:82:GLU:HG2	8:G:87:ILE:HD11	1.92	0.52
4:C:182:LYS:NZ	4:C:214:GLU:OE2	2.39	0.51
2:A:893:GLU:HG2	2:A:1016:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:546:VAL:O	6:E:602:THR:HA	2.11	0.51
2:A:217:ARG:NH2	2:A:221:ASN:O	2.41	0.51
2:A:1332:HIS:HD2	3:B:41:LEU:HD12	1.76	0.51
4:C:853:ARG:NH2	4:C:879:ASP:O	2.43	0.51
2:A:67:ARG:HD3	2:A:179:ALA:HB2	1.92	0.51
4:C:683:ASN:OD1	4:C:683:ASN:N	2.44	0.51
2:A:304:ILE:HD13	4:C:921:LEU:HA	1.93	0.50
2:A:1494:TYR:HB2	2:A:1744:ARG:HD3	1.92	0.50
8:G:120:LEU:HD12	8:G:123:ILE:HD11	1.93	0.50
2:A:118:VAL:HG21	2:A:487:LEU:HD12	1.93	0.50
2:A:1136:ARG:NH1	6:E:254:TYR:O	2.42	0.50
3:B:1991:GLU:O	3:B:1995:ALA:N	2.41	0.50
2:A:381:PRO:O	4:C:354:ARG:NH1	2.45	0.50
4:C:166:CYS:HB3	4:C:169:ASP:HB2	1.92	0.50
4:C:799:GLU:HB2	4:C:802:HIS:HD2	1.77	0.50
2:A:433:GLU:O	2:A:434:HIS:ND1	2.45	0.50
2:A:1554:GLN:HE21	2:A:1559:GLY:HA2	1.77	0.49
2:A:1418:ARG:HH11	2:A:1464:LEU:HA	1.77	0.49
2:A:1422:LEU:O	2:A:1427:ARG:NH2	2.45	0.49
8:G:102:ASP:OD1	8:G:106:ASN:N	2.42	0.49
8:G:92:LEU:HD13	8:G:101:PHE:HE2	1.78	0.49
2:A:899:MET:HB3	2:A:906:VAL:HG13	1.95	0.49
4:C:343:LEU:HD13	4:C:373:ILE:HD11	1.94	0.49
2:A:1310:ARG:HG2	3:B:37:THR:HA	1.95	0.49
4:C:853:ARG:NH1	4:C:886:ASP:OD2	2.42	0.49
4:C:134:LEU:HD13	4:C:202:ILE:HG23	1.94	0.48
2:A:1555:LEU:HA	8:G:88:THR:HB	1.94	0.48
4:C:192:ASP:OD1	4:C:196:LYS:N	2.44	0.48
4:C:107:GLN:HE22	4:C:540:GLU:H	1.62	0.48
4:C:666:VAL:HG22	4:C:787:VAL:HG22	1.95	0.48
4:C:716:GLU:HA	4:C:719:GLN:HG2	1.95	0.48
1:5:78:U:OP1	5:D:182:ARG:O	2.31	0.48
2:A:61:MET:SD	2:A:120:TYR:OH	2.72	0.47
2:A:1230:LEU:O	2:A:1280:ASN:ND2	2.46	0.47
3:B:2064:TRP:O	3:B:2081:ARG:HA	2.14	0.47
4:C:396:LEU:HD13	4:C:403:LEU:HD13	1.96	0.47
8:G:165:LEU:O	8:G:222:ARG:NH2	2.47	0.47
2:A:820:ARG:NH2	2:A:1063:GLY:O	2.47	0.47
3:B:1989:GLU:O	3:B:1993:ARG:N	2.43	0.47
5:D:58:PRO:O	5:D:60:MET:N	2.45	0.47
2:A:419:ARG:NH1	2:A:423:ASP:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1078:ALA:O	2:A:1082:ALA:HB2	2.15	0.47
2:A:1292:GLU:OE2	2:A:1317:TYR:OH	2.31	0.47
2:A:599:MET:HB3	2:A:603:ARG:HH22	1.80	0.47
3:B:756:SER:O	3:B:760:GLU:CB	2.63	0.47
1:5:36:C:O2	1:5:44:A:N6	2.48	0.47
3:B:825:THR:HA	3:B:866:GLU:O	2.15	0.47
4:C:561:LYS:NZ	4:C:614:TYR:O	2.48	0.46
4:C:676:ALA:HB1	4:C:814:ARG:HH11	1.80	0.46
2:A:1426:ASP:OD2	2:A:1459:ARG:NH1	2.44	0.46
2:A:881:ILE:HG12	2:A:918:THR:HG22	1.97	0.46
2:A:62:PRO:HG2	8:G:179:GLY:HA3	1.96	0.46
2:A:257:LEU:HD13	2:A:311:GLU:HB2	1.98	0.46
2:A:779:LEU:HD23	2:A:782:LEU:HD12	1.98	0.46
4:C:207:GLY:O	4:C:238:ASN:ND2	2.44	0.46
2:A:863:GLU:HG3	2:A:913:PRO:HB3	1.98	0.46
2:A:1388:GLU:HG2	2:A:2220:PRO:CB	2.47	0.45
2:A:873:ASN:ND2	2:A:876:GLU:OE1	2.49	0.45
2:A:794:TYR:OH	2:A:989:ASP:OD1	2.33	0.45
4:C:674:CYS:O	4:C:686:THR:HA	2.16	0.45
4:C:755:ASP:OD1	4:C:755:ASP:N	2.49	0.45
1:5:37:G:N2	1:5:44:A:N3	2.64	0.45
3:B:537:LYS:N	3:B:608:LEU:O	2.46	0.45
2:A:161:PHE:HB3	2:A:625:PRO:HG2	1.98	0.45
2:A:962:LEU:HB2	2:A:965:VAL:HB	1.99	0.45
1:5:58:U:H2'	1:5:59:G:C8	2.51	0.45
2:A:1109:LEU:HG	2:A:1152:ALA:HB1	1.99	0.45
3:B:755:GLY:O	3:B:758:SER:N	2.45	0.45
1:5:26:A:O2'	2:A:635:ARG:NH1	2.50	0.45
4:C:602:LYS:O	4:C:605:ASP:HB2	2.16	0.45
2:A:109:PRO:HD3	2:A:630:TRP:HZ2	1.82	0.44
2:A:1046:LEU:O	2:A:1049:ASP:HB2	2.17	0.44
1:5:59:G:H2'	1:5:60:G:H8	1.82	0.44
4:C:836:VAL:HB	4:C:871:ILE:HB	2.00	0.44
2:A:317:PRO:HD2	4:C:177:ARG:HH12	1.82	0.44
2:A:787:GLU:HA	2:A:790:ARG:HG2	2.00	0.44
2:A:880:ARG:HG2	2:A:883:ARG:HH12	1.81	0.44
2:A:1491:LYS:O	2:A:1710:ASN:ND2	2.51	0.44
2:A:122:ILE:HG22	2:A:483:GLN:HE22	1.83	0.44
2:A:318:TYR:HE2	4:C:642:HIS:HD2	1.65	0.44
2:A:971:GLY:HA2	2:A:1180:LYS:HE3	2.00	0.44
1:5:29:A:H2'	1:5:30:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1072:LEU:HD22	2:A:1087:LEU:HD22	2.00	0.43
2:A:1640:SER:HB2	2:A:1652:MET:HG2	2.00	0.43
2:A:1064:PRO:HD3	2:A:1075:GLN:HE21	1.82	0.43
2:A:942:PRO:HB2	2:A:1437:ARG:HD2	1.99	0.43
2:A:1488:THR:HB	2:A:1537:TRP:CE2	2.53	0.43
4:C:670:SER:HB3	4:C:823:ALA:HB2	2.01	0.43
2:A:1260:VAL:HG21	2:A:1325:LEU:HD13	2.00	0.43
2:A:811:THR:O	2:A:815:HIS:ND1	2.38	0.43
2:A:2103:THR:O	2:A:2140:LYS:N	2.45	0.43
4:C:381:LEU:HG	4:C:416:LEU:HD11	2.00	0.43
2:A:1057:ARG:HH11	2:A:1086:ARG:HA	1.84	0.42
2:A:686:ARG:NE	2:A:742:TYR:OH	2.51	0.42
2:A:1582:TRP:NE1	2:A:1619:SER:O	2.38	0.42
4:C:852:ARG:HH22	6:E:289:LEU:HD21	1.83	0.42
2:A:996:LEU:HD23	2:A:1047:VAL:HG21	2.01	0.42
2:A:1640:SER:HA	2:A:1652:MET:HA	2.00	0.42
4:C:264:ILE:HG12	4:C:378:TYR:CE1	2.54	0.42
2:A:915:GLU:OE1	2:A:1012:LYS:NZ	2.52	0.42
2:A:978:GLU:HG3	2:A:1174:PHE:HB3	2.01	0.42
2:A:1218:ASN:O	2:A:1222:LYS:HD3	2.19	0.42
2:A:1085:ILE:HG23	2:A:1099:PHE:HE1	1.85	0.42
2:A:1604:LEU:HD11	2:A:1725:LEU:HD13	2.01	0.42
6:E:290:TYR:HA	6:E:293:ARG:HE	1.84	0.42
2:A:1543:ASN:ND2	2:A:1562:MET:SD	2.93	0.42
2:A:1645:LEU:HD13	2:A:1714:ALA:HB3	2.01	0.42
4:C:843:VAL:HG21	4:C:869:TYR:HD2	1.85	0.41
2:A:89:LEU:HD11	2:A:656:LEU:HD22	2.02	0.41
2:A:109:PRO:HG3	2:A:630:TRP:HE1	1.85	0.41
2:A:1043:TYR:O	2:A:1046:LEU:HB3	2.20	0.41
3:B:1196:SER:O	3:B:1258:VAL:N	2.43	0.41
4:C:478:THR:HA	4:C:494:GLY:HA3	2.01	0.41
4:C:595:VAL:HG22	4:C:654:LYS:HG3	2.02	0.41
2:A:965:VAL:O	2:A:1100:ARG:NH2	2.54	0.41
4:C:769:GLY:HA2	4:C:809:ILE:HG23	2.03	0.41
6:E:282:THR:HG22	6:E:283:SER:H	1.85	0.41
2:A:1215:ASN:OD1	2:A:1224:ARG:NH1	2.54	0.41
2:A:1585:ILE:HD11	2:A:1743:LEU:HB2	2.02	0.41
3:B:1831:LEU:O	3:B:1835:SER:CB	2.69	0.41
6:E:290:TYR:HB3	6:E:293:ARG:HH11	1.86	0.41
2:A:1667:ARG:N	2:A:1705:ILE:O	2.53	0.41
3:B:814:THR:O	3:B:818:GLY:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:823:ALA:O	3:B:857:GLY:N	2.44	0.41
4:C:227:LEU:HD21	4:C:239:THR:HG23	2.03	0.41
4:C:327:TYR:OH	4:C:372:PHE:O	2.36	0.41
2:A:342:THR:OG1	4:C:268:LYS:NZ	2.51	0.41
2:A:1293:ASN:HD21	3:B:40:VAL:H	1.68	0.41
4:C:137:HIS:HD2	4:C:238:ASN:H	1.69	0.40
2:A:1034:LEU:HB2	2:A:1037:ALA:HB2	2.02	0.40
2:A:1530:PRO:HD2	2:A:1533:ARG:HH21	1.87	0.40
2:A:1645:LEU:O	2:A:1727:GLN:NE2	2.52	0.40

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	1894/2335 (81%)	1842 (97%)	51 (3%)	1 (0%)	51 85
3	B	1745/2136 (82%)	1659 (95%)	85 (5%)	1 (0%)	51 85
4	C	844/972 (87%)	817 (97%)	26 (3%)	1 (0%)	51 85
5	D	304/357 (85%)	283 (93%)	19 (6%)	2 (1%)	22 62
6	E	557/820 (68%)	543 (98%)	14 (2%)	0	100 100
7	F	21/941 (2%)	21 (100%)	0	0	100 100
8	G	123/343 (36%)	112 (91%)	11 (9%)	0	100 100
9	a	79/119 (66%)	75 (95%)	4 (5%)	0	100 100
10	b	69/240 (29%)	68 (99%)	1 (1%)	0	100 100
11	c	94/118 (80%)	87 (93%)	7 (7%)	0	100 100
12	d	80/126 (64%)	75 (94%)	5 (6%)	0	100 100
13	e	75/92 (82%)	71 (95%)	4 (5%)	0	100 100
14	f	71/86 (83%)	66 (93%)	5 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	g	72/76 (95%)	69 (96%)	3 (4%)	0	100 100
All	All	6028/8761 (69%)	5788 (96%)	235 (4%)	5 (0%)	54 85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	59	ILE
5	D	58	PRO
3	B	756	SER
2	A	829	PRO
4	C	707	ILE

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
2	A	1471/2108 (70%)	1462 (99%)	9 (1%)	86 92
3	B	23/1908 (1%)	23 (100%)	0	100 100
4	C	748/866 (86%)	743 (99%)	5 (1%)	84 90
6	E	64/721 (9%)	64 (100%)	0	100 100
8	G	104/282 (37%)	104 (100%)	0	100 100
12	d	72/101 (71%)	71 (99%)	1 (1%)	67 81
All	All	2482/5986 (42%)	2467 (99%)	15 (1%)	86 92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	156	ARG
2	A	243	ASN
2	A	498	ARG
2	A	505	ASN
2	A	642	ARG
2	A	704	ASN

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Mol	Chain	Res	Type
2	A	741	ARG
2	A	1451	ASN
2	A	1636	LYS
4	C	258	ASN
4	C	611	ASN
4	C	680	ASN
4	C	708	THR
4	C	735	PHE
12	d	76	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	97	HIS
2	A	210	HIS
2	A	243	ASN
2	A	483	GLN
2	A	505	ASN
2	A	509	HIS
2	A	610	HIS
2	A	704	ASN
2	A	1075	GLN
2	A	1184	ASN
2	A	1261	ASN
2	A	1293	ASN
2	A	1332	HIS
2	A	1451	ASN
2	A	1531	ASN
2	A	1554	GLN
4	C	107	GLN
4	C	137	HIS
4	C	154	HIS
4	C	258	ASN
4	C	611	ASN
4	C	642	HIS
8	G	106	ASN
12	d	16	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	101/117 (86%)	37 (36%)	3 (2%)

All (37) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	4	C
1	5	6	C
1	5	7	U
1	5	9	G
1	5	20	G
1	5	21	A
1	5	22	U
1	5	23	C
1	5	24	G
1	5	25	C
1	5	36	C
1	5	37	G
1	5	38	C
1	5	45	C
1	5	47	A
1	5	48	A
1	5	55	C
1	5	58	U
1	5	59	G
1	5	66	A
1	5	67	A
1	5	69	A
1	5	70	A
1	5	71	C
1	5	75	G
1	5	78	U
1	5	86	C
1	5	88	A
1	5	92	U
1	5	94	U
1	5	95	G
1	5	97	G
1	5	98	G
1	5	105	U
1	5	106	U
1	5	107	U
1	5	108	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	58	U
1	5	96	A
1	5	105	U

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)

Of 2 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
17	GTP	C	1101	16	26,34,34	1.24	4 (15%)	32,54,54	1.61	5 (15%)

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
17	GTP	C	1101	16	-	2/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	1101	GTP	C8-N7	-2.55	1.30	1.35
17	C	1101	GTP	C5-C4	-2.33	1.37	1.43
17	C	1101	GTP	PG-O3G	-2.24	1.46	1.54
17	C	1101	GTP	PG-O2G	-2.09	1.46	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	C	1101	GTP	PA-O3A-PB	-5.00	115.68	132.83
17	C	1101	GTP	PB-O3B-PG	-4.59	117.09	132.83
17	C	1101	GTP	O3G-PG-O2G	3.02	119.19	107.64
17	C	1101	GTP	O6-C6-N1	-2.41	117.80	120.65
17	C	1101	GTP	O6-C6-C5	2.12	128.52	124.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	C	1101	GTP	PB-O3B-PG-O2G
17	C	1101	GTP	PA-O3A-PB-O2B

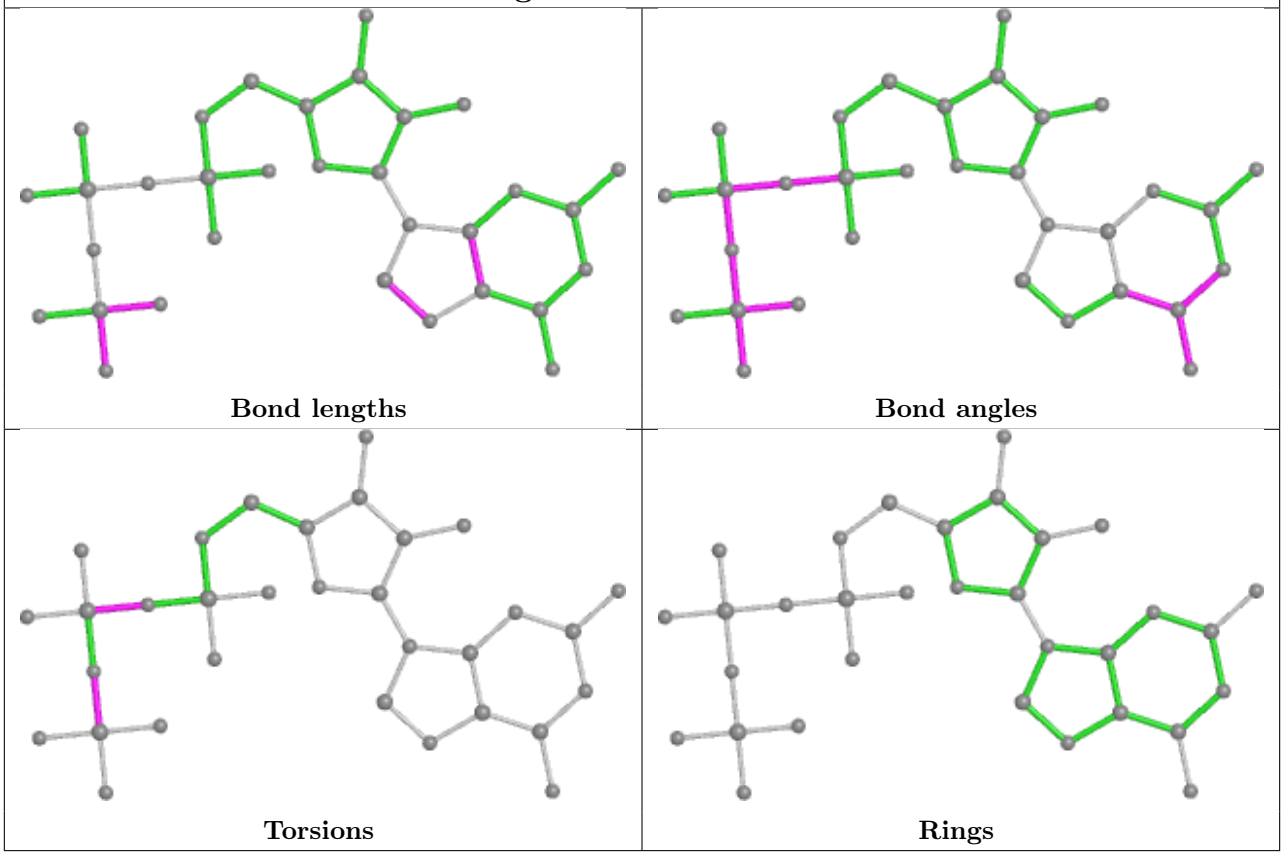
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	1101	GTP	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 then 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.

Ligand GTP C 1101



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

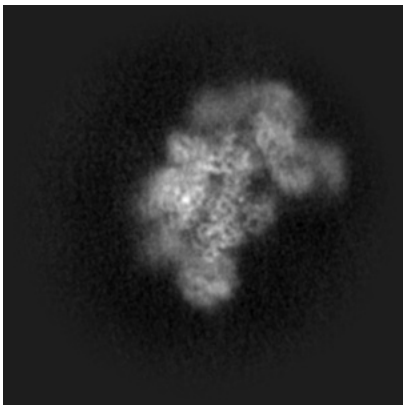
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18237. These allow visual inspection of the internal detail of the map and identification of artifacts.

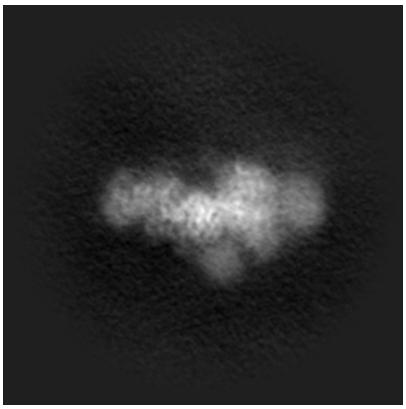
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

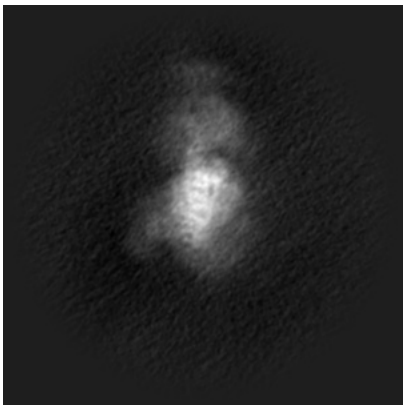
6.1.1 Primary map



X

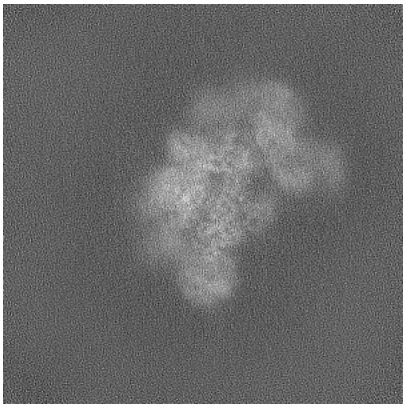


Y

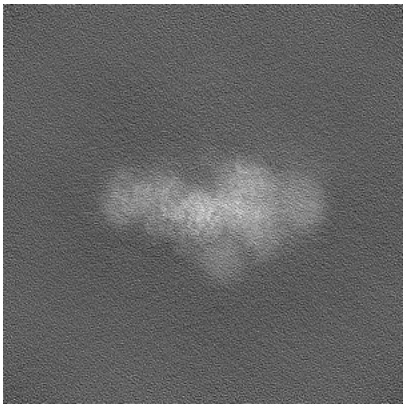


Z

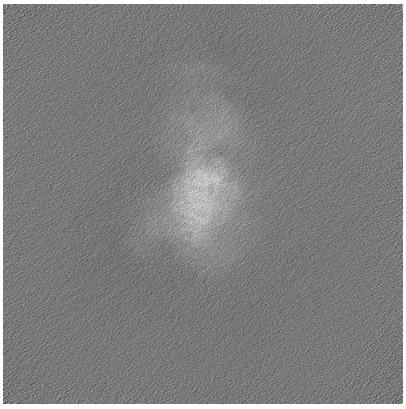
6.1.2 Raw map



X



Y

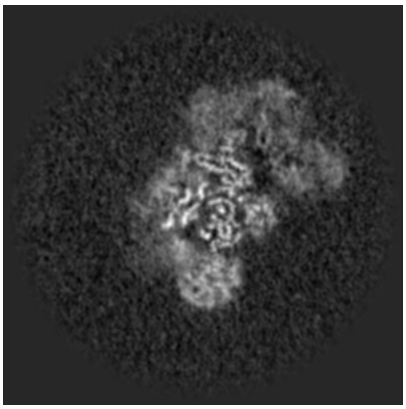


Z

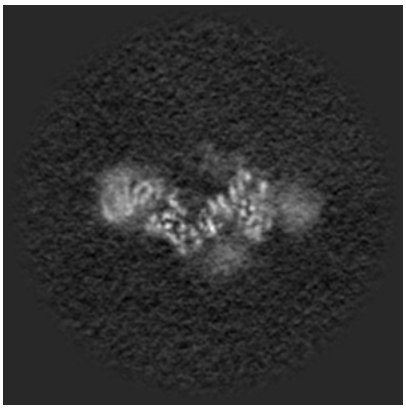
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

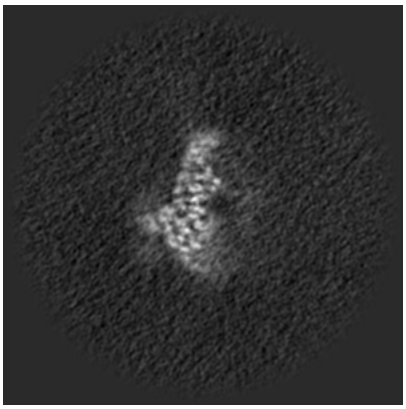
6.2.1 Primary map



X Index: 180

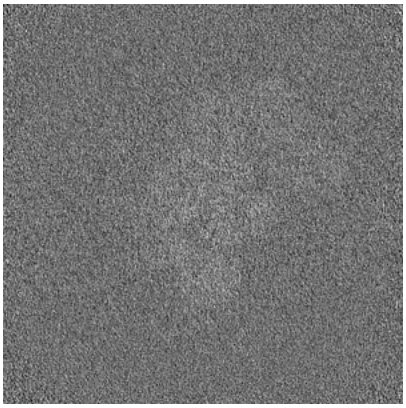


Y Index: 180

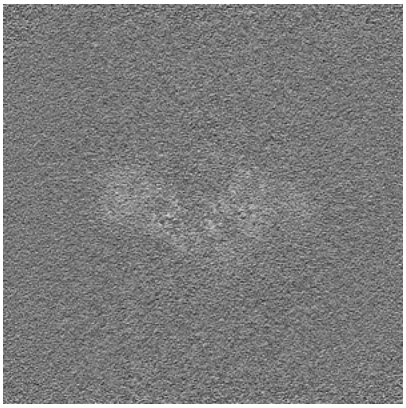


Z Index: 180

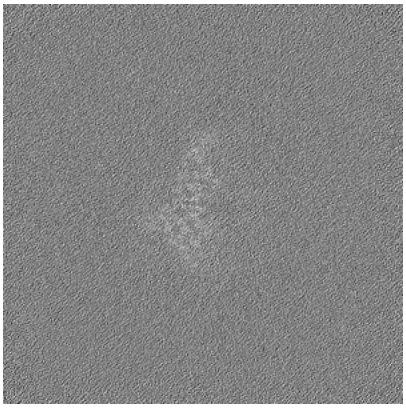
6.2.2 Raw map



X Index: 180



Y Index: 180

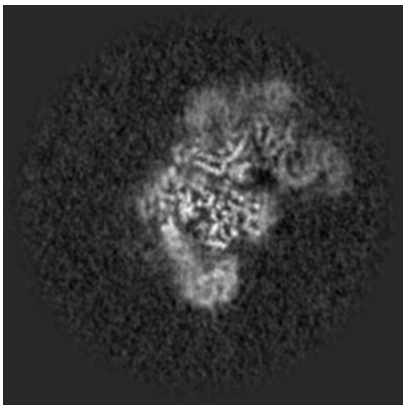


Z Index: 180

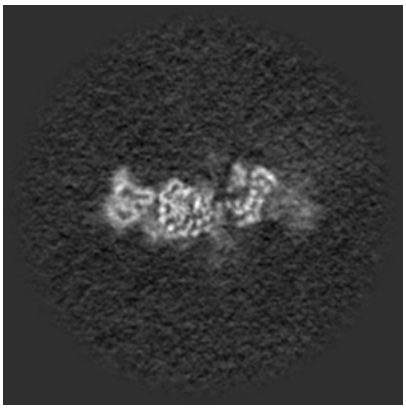
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

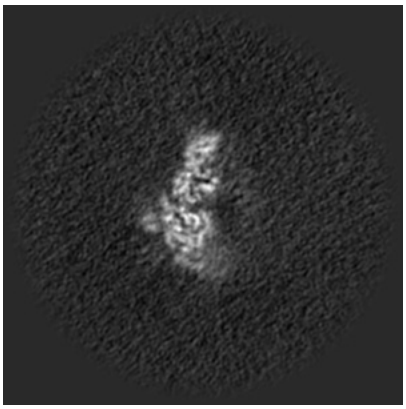
6.3.1 Primary map



X Index: 174

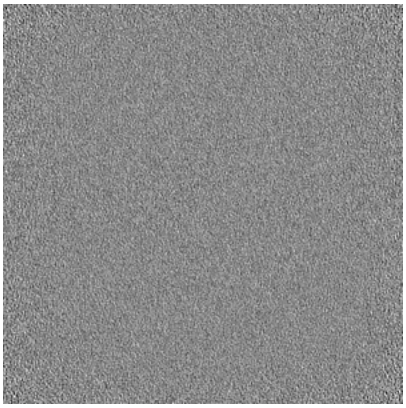


Y Index: 197

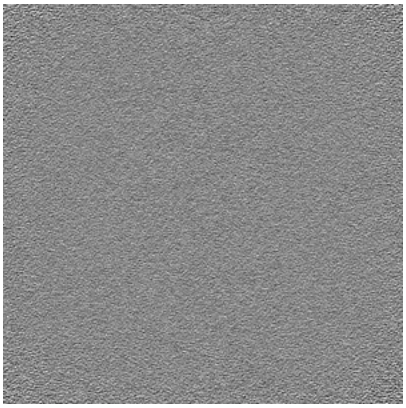


Z Index: 176

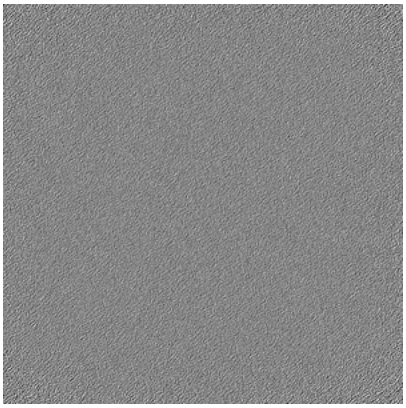
6.3.2 Raw map



X Index: 0



Y Index: 0

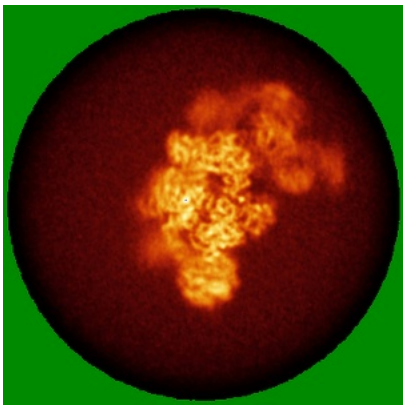


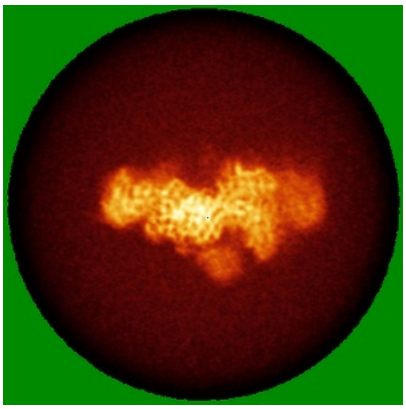
Z Index: 0

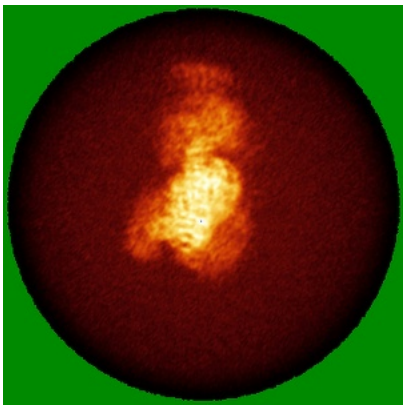
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

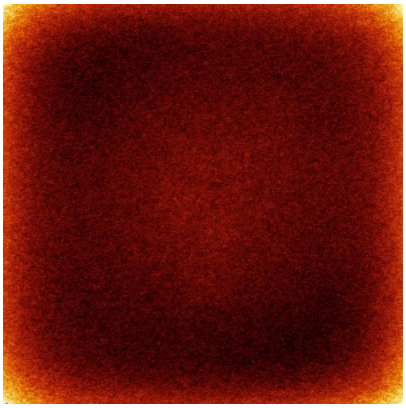
6.4.1 Primary map

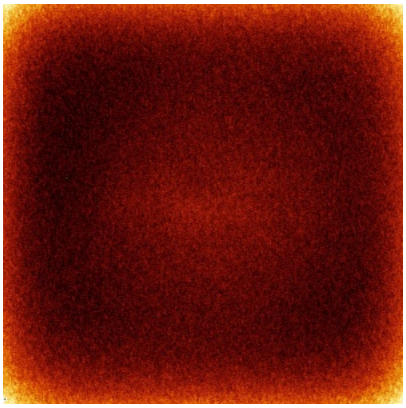

X

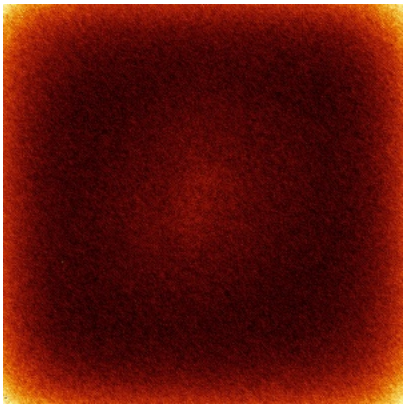

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

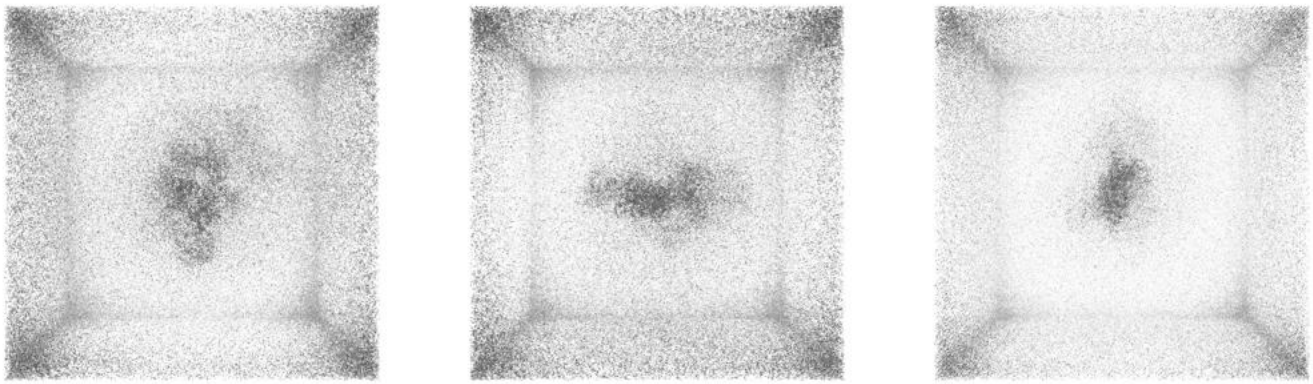
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. 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



X Y Z

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.

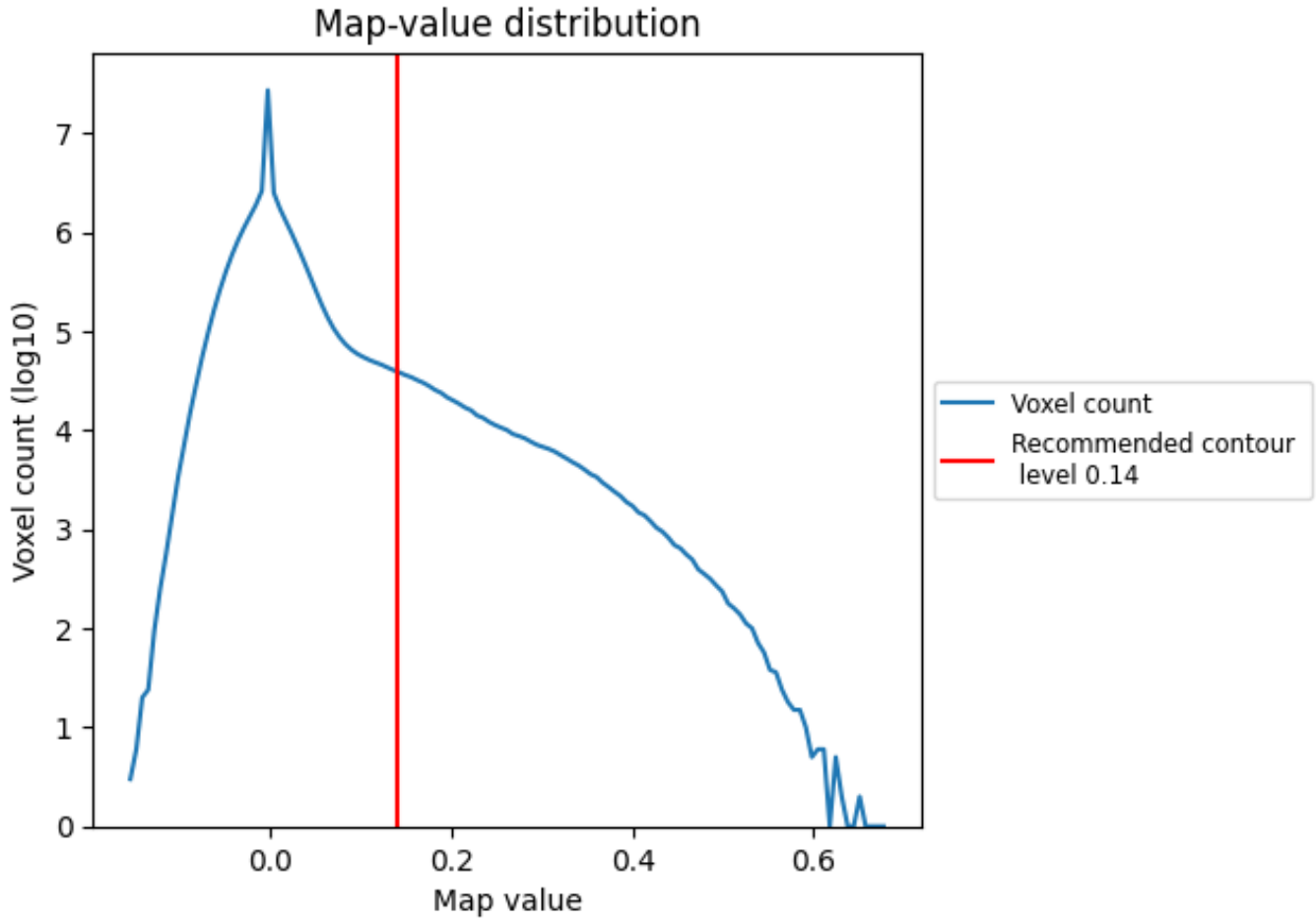
6.6 Mask visualisation (i)

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

7 Map analysis

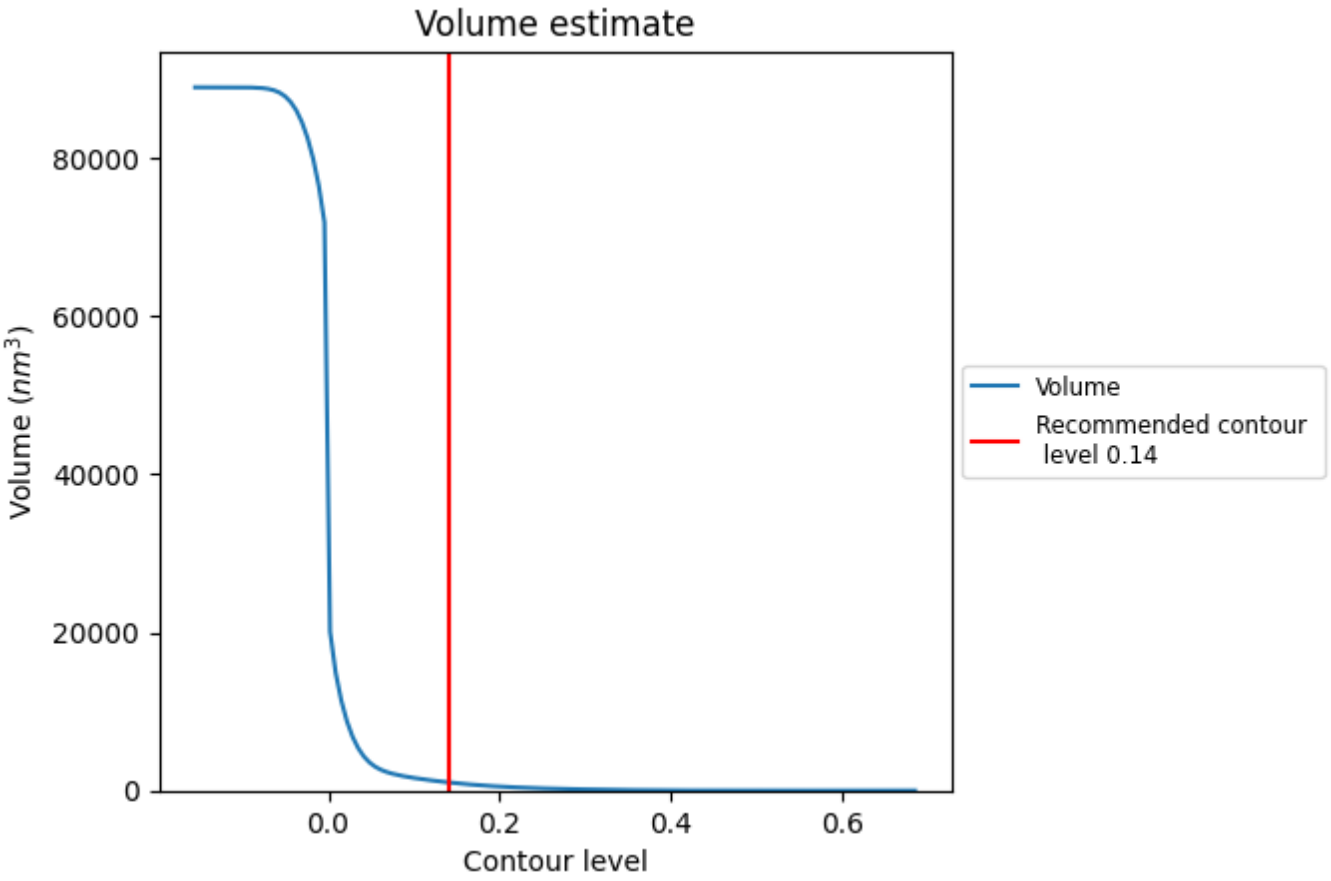
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

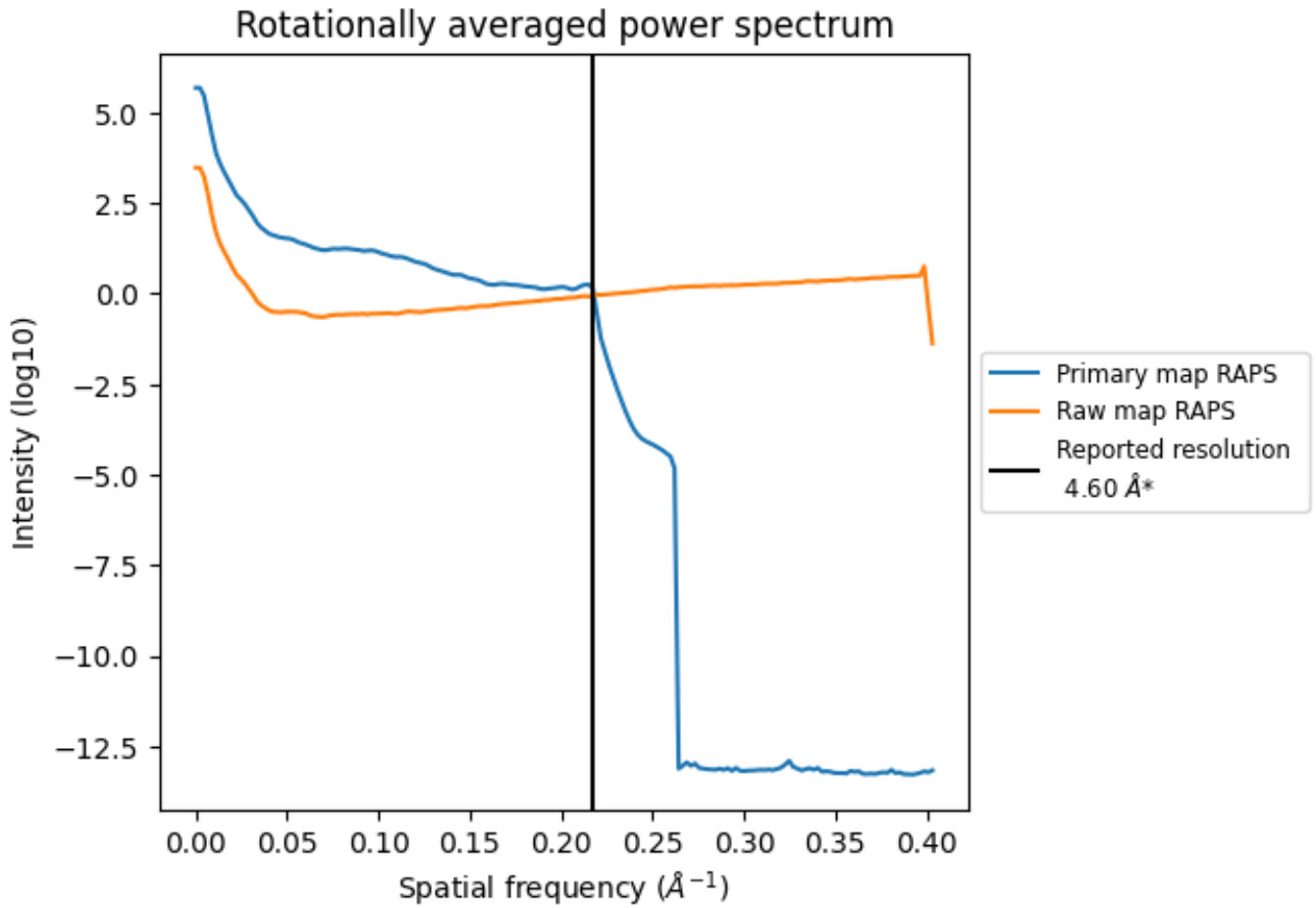
7.2 Volume estimate



The volume at the recommended contour level is 1036 nm^3; this corresponds to an approximate mass of 936 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)

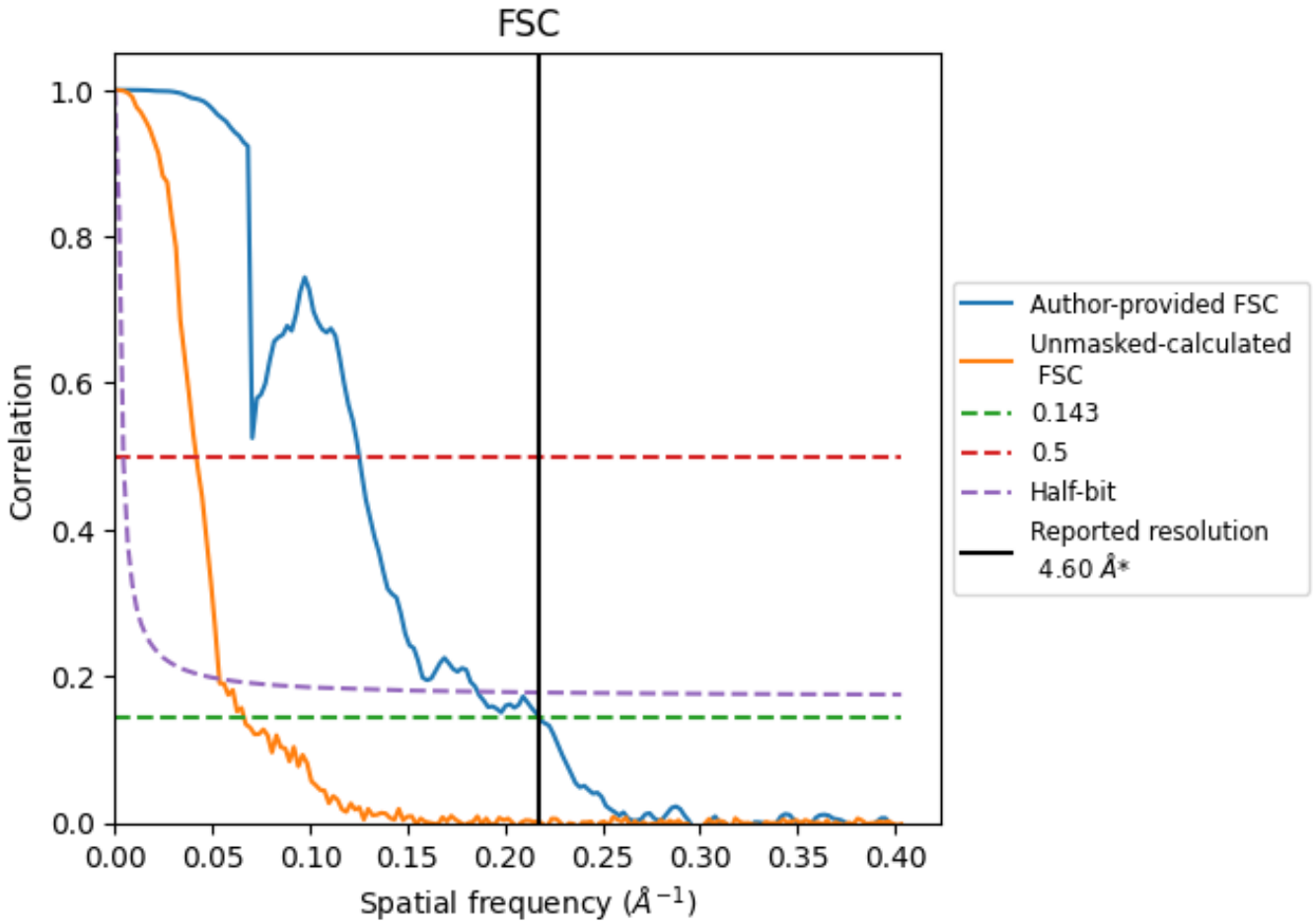


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8.2 Resolution estimates (i)

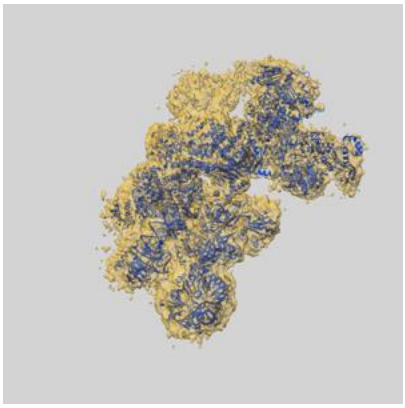
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.60	7.98	5.38
Unmasked-calculated*	15.08	23.92	18.66

*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 15.08 differs from the reported value 4.6 by more than 10 %

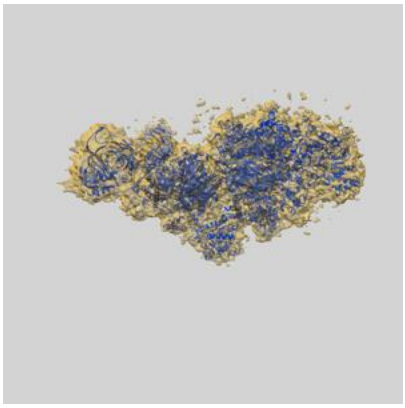
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18237 and PDB model 8Q7X. Per-residue inclusion information can be found in section 3 on page 8.

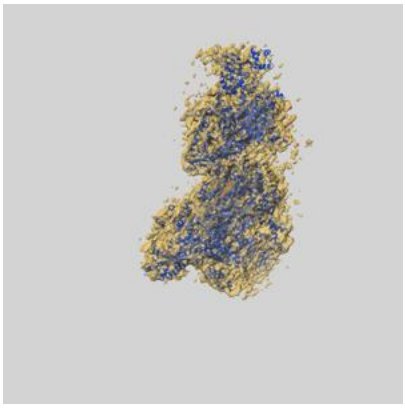
9.1 Map-model overlay



X



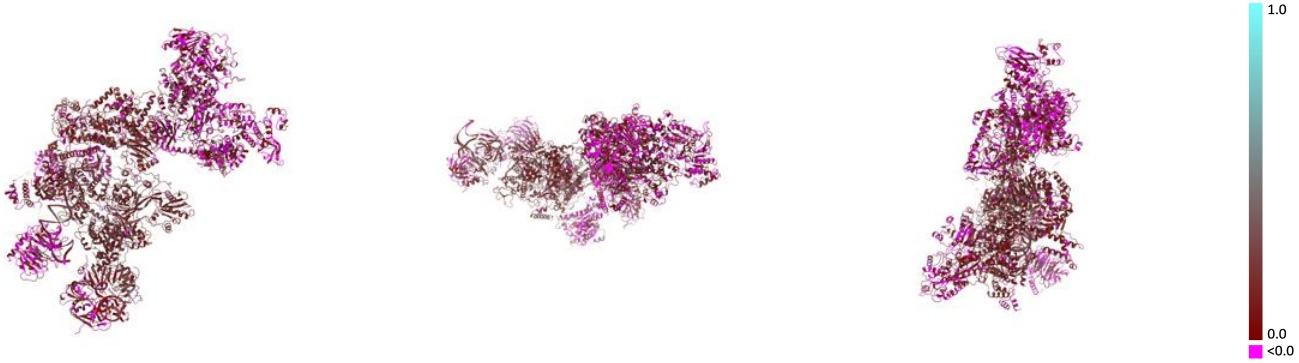
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14 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.

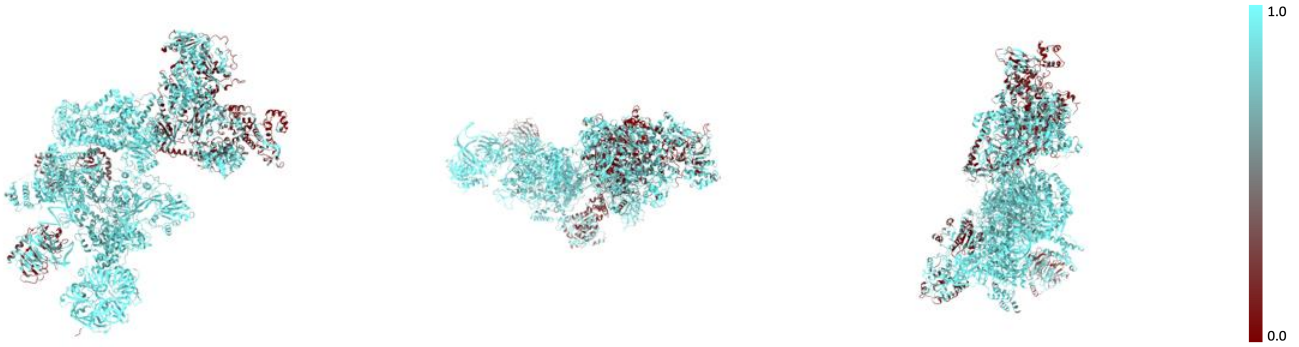
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

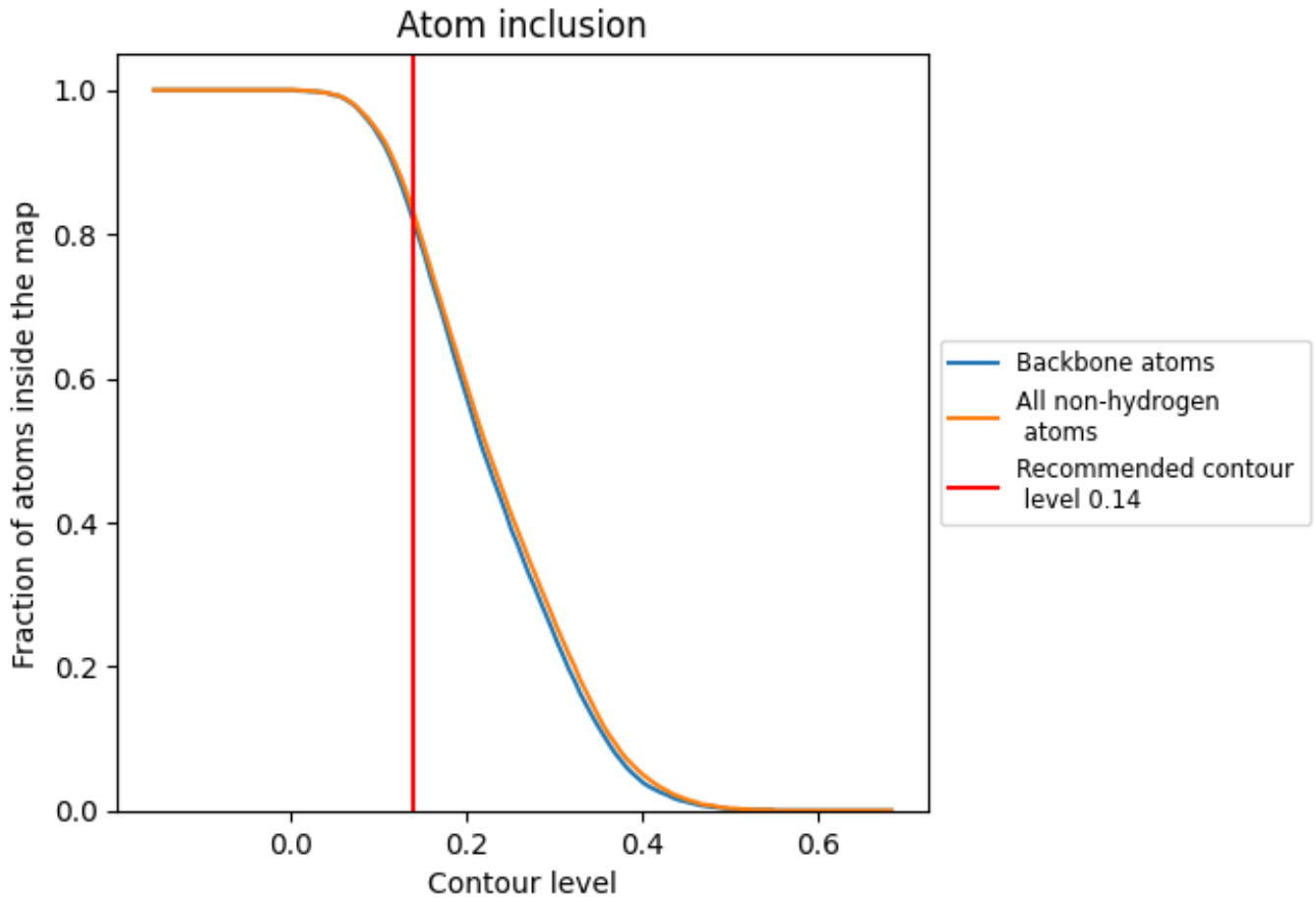
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.14).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 83% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.1480
5	0.9910	0.1970
A	0.8960	0.1690
B	0.6470	0.0850
C	0.9340	0.2150
D	0.5830	0.0340
E	0.6150	0.0890
F	0.9040	0.1740
G	0.9040	0.1430
a	0.9980	0.1390
b	0.9940	0.1810
c	0.9220	0.0930
d	0.9670	0.2030
e	0.9970	0.1520
f	0.9860	0.0660
g	0.9890	0.2420