



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 12:03 am GMT

PDB ID : 5LJ5
EMDB ID : EMD-4057
Title : Overall structure of the yeast spliceosome immediately after branching.
Authors : Galej, W.P.; Wilkinson, M.F.; Fica, S.M.; Oubridge, C.; Newman, A.J.; Nagai, K.
Deposited on : 2016-07-17
Resolution : 10.00 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

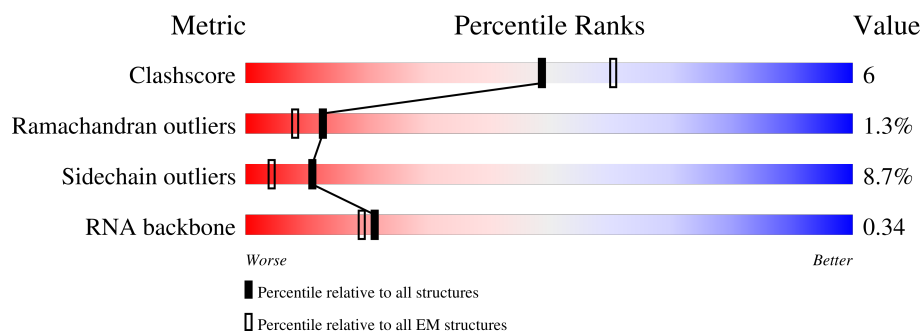
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	U	179	<div> <div>33%</div> <div>36%</div> <div>9%</div> <div>•</div> <div>21%</div> </div>
2	E	16	<div> <div>25%</div> <div>62%</div> <div>12%</div> </div>
3	I	76	<div> <div>22%</div> <div>20%</div> <div>•</div> <div>57%</div> </div>
4	Z	1175	<div> <div>9%</div> <div>5%</div> <div>85%</div> </div>
5	V	112	<div> <div>42%</div> <div>31%</div> <div>12%</div> <div>•</div> <div>13%</div> </div>
6	A	2413	<div> <div>73%</div> <div>15%</div> <div>•</div> <div>10%</div> </div>
7	B	2163	<div> <div>77%</div> <div>•</div> <div>21%</div> </div>






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Mol	Chain	Length	Quality of chain
8	D	278	
9	F	179	
10	C	1008	
11	G	235	
12	H	591	
13	J	451	
14	K	379	
15	L	157	
16	M	339	
17	N	364	
18	O	590	
19	P	175	
20	R	135	
21	S	687	
22	T	859	
23	b	196	
23	k	196	
24	d	101	
24	n	101	
25	e	94	
25	p	94	
26	f	86	
26	q	86	
27	g	77	
27	r	77	

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Mol	Chain	Length	Quality of chain
28	h	146	
28	l	146	
29	j	110	
29	m	110	
30	W	238	
31	Y	111	
32	Q	1071	
33	t	503	
33	u	503	
33	v	503	
33	w	503	
34	s	175	
35	x	188	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	ZN	N	401	-	-	X	-
37	ZN	N	402	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 85476 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 U5 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	141	Total	C	N	O	P	0	0
			2999	1342	530	986	141		

- Molecule 2 is a RNA chain called Exon 1 (5' exon) of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	16	Total	C	N	O	P	0	0
			346	155	66	109	16		

- Molecule 3 is a RNA chain called Intron of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	33	Total	C	N	O	P	0	0
			693	312	116	232	33		

- Molecule 4 is a RNA chain called U2 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	171	Total	C	N	O	P	0	0
			3610	1614	604	1221	171		

- Molecule 5 is a RNA chain called U6 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	97	Total	C	N	O	P	0	0
			2066	925	368	676	97		

- Molecule 6 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	2168	Total	C	N	O	S	0	0
			16919	10835	2966	3060	58		

- Molecule 7 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	1707	Total	C	N	O	1	0
			8462	5048	1707	1707		

- Molecule 8 is a protein called Protein CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	114	Total	C	N	O	S	0	0
			912	577	165	162	8		

- Molecule 9 is a protein called Pre-mRNA-splicing factor CWC25.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	F	46	Total	C	N	O	0	0
			321	203	61	57		

- Molecule 10 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	882	Total	C	N	O	S	0	0
			6756	4393	1133	1203	27		

- Molecule 11 is a protein called Pre-mRNA-splicing factor ISY1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	97	Total	C	N	O	S	0	0
			823	513	154	155	1		

- Molecule 12 is a protein called CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	399	Total	C	N	O	S	0	0
			2639	1657	468	506	8		

- Molecule 13 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	326	Total	C	N	O	S	0	0
			2556	1616	454	476	10		

- Molecule 14 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	163	Total	C	N	O	S	0	0
			1289	808	236	240	5		

- Molecule 15 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1270	797	238	225	10		

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	252	Total	C	N	O	S	0	0
			2012	1277	354	370	11		

- Molecule 17 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	209	Total	C	N	O	S	0	0
			1658	1055	287	301	15		

- Molecule 18 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	283	Total	C	N	O	S	0	0
			2068	1285	385	392	6		

- Molecule 19 is a protein called CWC15.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	P	36	Total	C	N	O	0	0
			275	176	53	46		

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	97	Total	C	N	O	0	0
			544	325	106	113		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	464	Total	C	N	O	S	0	0
			3121	1949	581	584	7		

- Molecule 22 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	T	592	Total	C	N	O	0	0
			2946	1762	592	592		

- Molecule 23 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
23	k	80	Total	C	N	O		0	0
			396	236	80	80			

- Molecule 24 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
24	n	82	Total	C	N	O		0	0
			404	240	82	82			

- Molecule 25 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
25	p	75	Total	C	N	O		0	0
			369	219	75	75			

- Molecule 26 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
26	q	72	Total	C	N	O		0	0
			354	210	72	72			

- Molecule 27 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
27	r	69	Total	C	N	O		0	0
			340	202	69	69			

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
28	l	79	Total	C	N	O		0	0
			392	234	79	79			

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
29	m	94	Total	C	N	O		0	0
			467	279	94	94			

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	W	164	Total	C	N	O	0	0
			816	488	164	164		

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Y	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 32 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Q	619	Total	C	N	O	0	0
			3066	1828	619	619		

- Molecule 33 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	t	438	Total	C	N	O	0	0
			2171	1295	438	438		
33	u	437	Total	C	N	O	0	0
			2166	1292	437	437		
33	v	426	Total	C	N	O	0	0
			2111	1259	426	426		
33	w	435	Total	C	N	O	0	0
			2156	1286	435	435		

- Molecule 34 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	110	Total	C	N	O	0	0
			548	328	110	110		

- Molecule 35 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	x	132	Total	C	N	O	0	0
			660	396	132	132		

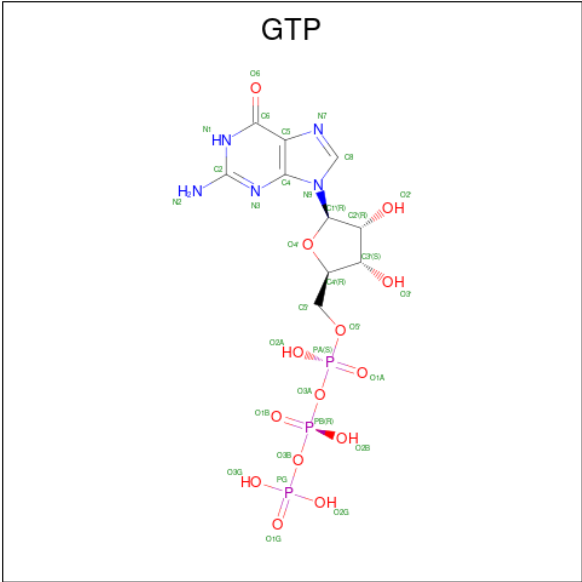
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	E	1	Total	Mg	0
			1	1	
36	V	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

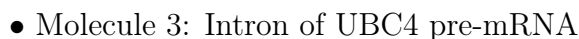
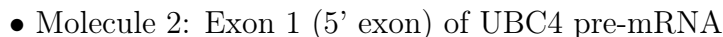
Mol	Chain	Residues	Atoms		AltConf
37	D	1	Total	Zn	0
			1	1	
37	L	3	Total	Zn	0
			3	3	
37	M	1	Total	Zn	0
			1	1	
37	N	2	Total	Zn	0
			2	2	

- Molecule 38 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
38	C	1	Total	C	N	O	P	0
			32	10	5	14	3	


- Molecule 1: U5 snRNA (small nuclear RNA)





-
- | Amino Acid | Percentage (%) |
|------------|----------------|
| C84 | ~10 |
| C85 | ~10 |
| G86 | ~10 |
| U87 | ~10 |
| U88 | ~10 |
| U89 | ~10 |
| U90 | ~10 |
| A91 | ~10 |
| C92 | ~10 |
| A93 | ~10 |
| A99 | ~10 |
| U102 | ~10 |
| A | ~10 |
| U | ~10 |
| U | ~10 |
| U | ~10 |
| U | ~10 |
| C | ~10 |
| G | ~10 |
| U | ~10 |
| U | ~10 |
| U | ~10 |
| U | ~10 |

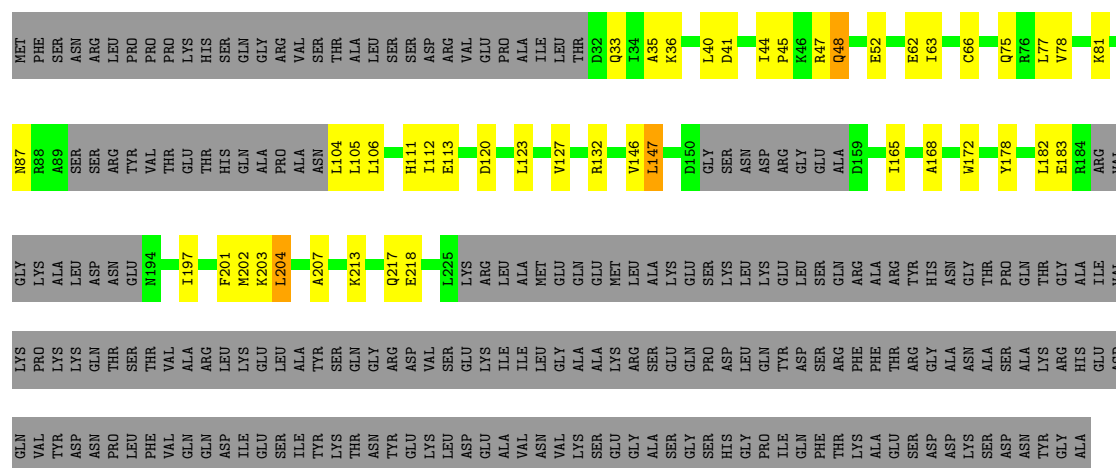
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Chain A:  73% 15% 10%


MET	TLE	LYS	W221		Q648	L752	I882	A1047	V1248	I1367	Y1542	Q1737	V1977
SER	ASN	ALA	R225		L649	Y753	W889	V1048	Y1251	Q1368	R1543	L1738	V1978
GLY	ALA	ARG	R376		I656	Y754	L1049	L1049	Y1251	R1369	V1546	D1742	W2048
LEU	GLU	SER	K228		L507	L756	R893	L1054	N1255	V1370	L1557	S1749	L2060
PRO	LEU	ASN	F239		Q508	E757	L912	T1064	L1258	K1372	T1560	V1752	E2078
PRO	VAL	LEU	Y126		Y514	L758	L919	L1066	E1277	L1373	L1561	F1756	G2085
PRO	ASP	Y126	D244		S521	R759	V922	N1067	D1282	G1374	F1562	T1760	G2085
PRO	PHE	THR	P395		Y522	N760	L929	L1068	W1286	L1375	T1565	N1763	G2085
GLY	LEU	THR	V398		Y522	I766	L937	L1068	D1287	K1378	W1570	L1779	ILE
PRO	PRO	THR	Y403		L526	M770	Y944	V1088	L1288	M1379	F1574	K1795	ILE
GLU	GLU	PRO	Y405		V673	M770	L937	V1089	W1286	R1382	F1574	P1796	LYS
ASP	PRO	PRO	Y405		H675	R775	Y944	V1090	D1287	F1383	F1574	L1779	LYS
SER	PRO	PRO	I141		D682	K778	H948	I1099	L1302	V1387	K1589	K1796	VAL
ASP	PRO	PRO	I142		I686	I782	L951	V1099	I1309	K1388	L1590	S1801	ARG
LEU	GLY	LEU	T145		I687	L783	N952	V1100	K1310	E1393	A1593	M1802	GLN
ALA	LEU	LEU	M149		K690	H785	I954	I1099	R1315	L1394	L1598	R1803	LYS
PRO	LEU	LEU	M153		Y565	H785	I954	I1099	I1316	L1397	Q1599	M1806	ALA
PRO	GLY	LEU	F161		L571	W793	D988	L1103	R1317	I1400	Q1600	M1806	GLU
PRO	THR	THR	L165		C572	W793	I969	I1104	I1317	I1400	I1601	L1815	LEU
PRO	ALA	ALA	K277		I583	N796	T970	I1113	S1323	I1407	P1602	L1815	GLU
GLY	GLU	GLY	D282		P706	I808	N971	I1113	G1324	A1407	M1603	L1815	GLU
TRP	LYS	LYS	S283		A707	I808	M971	I1121	S1324	A1408	R1604	R1820	ALA
GLU	LYS	GLU	R284		W708	I811	M972	I1121	T1326	A1409	L1598	M1803	ALA
ILE	VAL	VAL	P285		ASP	I811	Q976	F1144	T1327	Q1417	W1609	L1823	SER
GLU	GLU	GLU	L286		ASN	W711	Q976	F1144	F1328	T1418	W1610	Q1824	GLU
LEU	LEU	LEU	K174		ASN	L712	N977	F1144	T1329	T1418	I1614	Q1824	LYS
LEU	HIS	GLY	L175		SER	D821	I978	T1162	W1335	H1424	I1614	Q1827	GLN
ASP	LYS	LYS	P182		LEU	N713	I978	T1162	M1336	W1429	Y1620	SER	ASN
ASN	ARG	ARG	Y189		LEU	L715	Y982	L1165	T1337	L1435	V1621	VAL	ASP
MET	LYS	LYS	L305		VAL	R716	T991	R1167	S1338	D1433	I1632	GLN	GLU
VAL	LEU	LEU	K308		SER	T718	W1000	I1168	L1339	E1434	P1639	PRO	ALA
PRO	ASP	ASP	N309		THR	I719	P1015	I1168	L1342	K1435	Y1644	PHE	GLY
SER	GLY	GLY	N310		LEU	K842	K1014	L1171	F1343	L1436	I1643	LEU	ALA
VAL	LYS	LYS	L311		GLU	V845	D1004	W1207	Y1344	Y1436	I1643	ASN	SER
ASN	ASP	ASP	A198		ASN	K945	N1011	P1208	Y1345	Y1447	S1837	THR	THR
GLU	THR	THR	V202		GLY	K947	K1014	K1209	F1346	E1448	I1644	VAL	VAL
ASP	PHE	PHE	W203		ASP	N948	P1015	L1212	R1347	Y1461	I1645	MET	MET
THR	THR	THR	T205		THR	L849	V1015	R1212	I1347	Y1461	Q1647	LYS	LYS
PHE	ARG	ARG	T205		LEU	L852	E1019	M1213	I1350	I1491	W1654	I1893	LYS
LEU	LYS	LYS	E210		PRO	T853	I1020	R1214	E1354	L1494	W1654	L1920	THR
PRO	SER	SER	F211		PRO	T857	P1021	R1217	P1355	L1494	I1657	V1921	ILE
PRO	ARG	ARG	V212		THR	K958	P1022	R1217	L1356	I1510	I1668	L1944	ASN
PRO	LYS	LYS	T213		PHE	K958	L1023	L1222	L1357	L1510	L1669	L1944	ALA
PRO	ARG	ARG	T214		ASP	L849	L1024	L1223	D1358	K1515	M1948	M1948	GLN
PRO	ALA	ALA	Q215		THR	P876	V1025	V1226	L1360	K1515	V1681	GLY	GLY
PRO	LYS	LYS	A216		LEU	E877	W1028	V1226	L1360	E1520	V1681	GLU	GLU
SER	LYS	LYS	W217		THR	E878	W1028	V1226	L1360	E1520	V1681	GLU	GLU
ASN	MET	MET	A218		THR	A879	W1028	V1226	L1360	E1520	V1681	GLU	GLU
PHE	THR	THR	P354		THR	A879	W1028	V1226	L1360	E1520	V1681	GLU	GLU
LYS	LYS	LYS	T220		THR	T881	I1032	T1239	E1364	W1537	L1974	VAL	VAL



Chain K:  31% 11% 57%



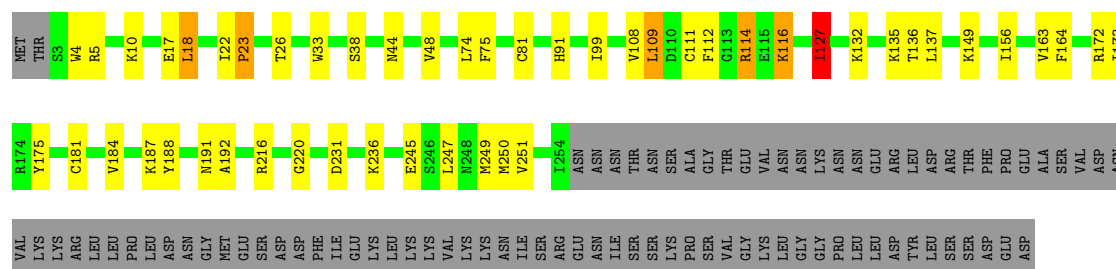
• Molecule 15: Pre-mRNA-splicing factor BUD31

Chain L:  83% 15%



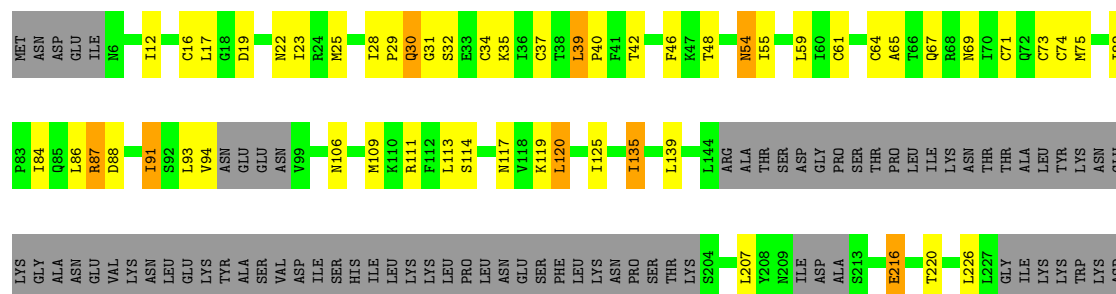
• Molecule 16: Pre-mRNA-splicing factor CWC2

Chain M:  60% 13% 26%

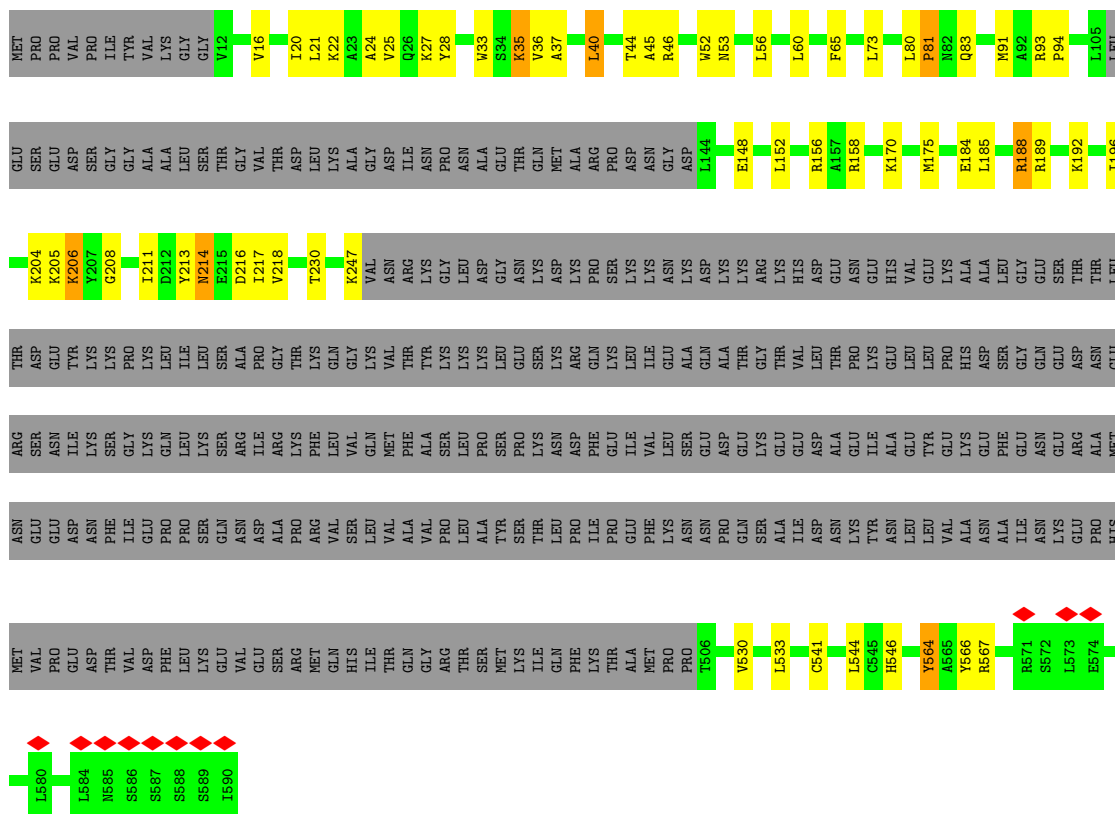
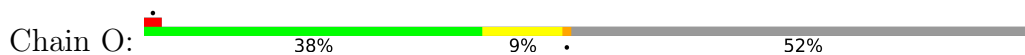


• Molecule 17: Pre-mRNA-splicing factor SLT11

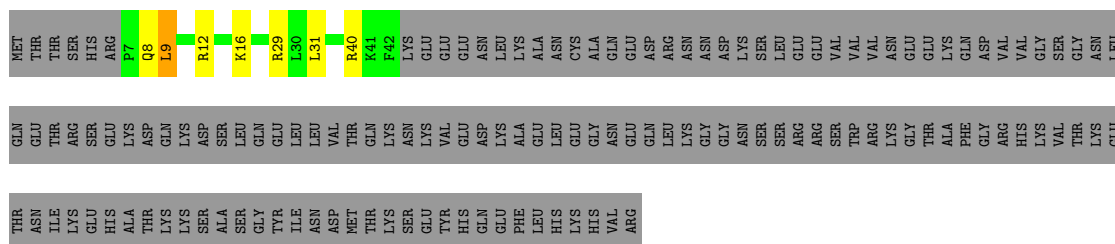
Chain N:  40% 15% 43%



- Molecule 18: Pre-mRNA-splicing factor CEF1



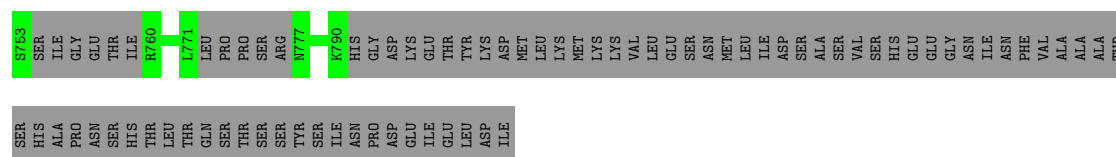
- Molecule 19: CWC15



- Molecule 20: Pre-mRNA-splicing factor CWC21

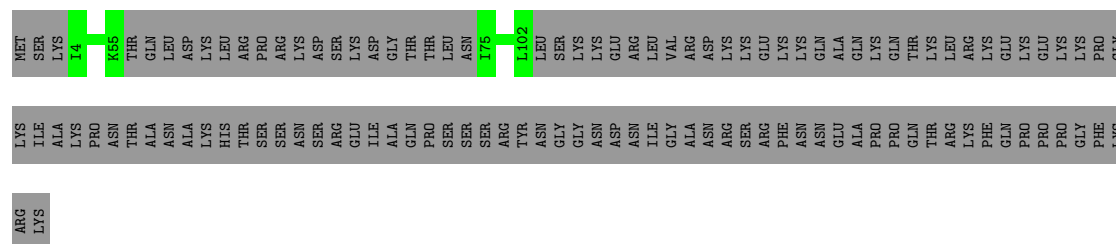






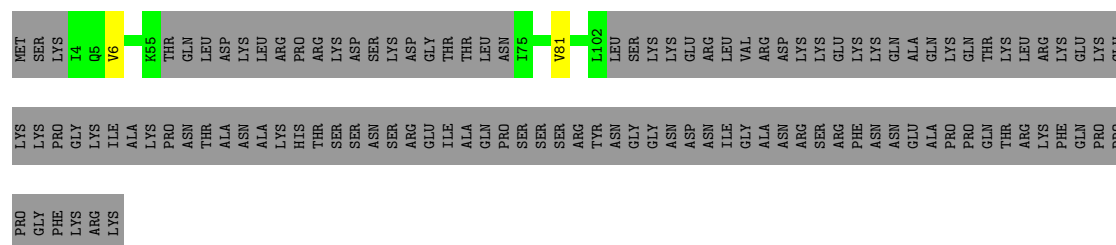
- Molecule 23: Small nuclear ribonucleoprotein-associated protein B

Chain b: 41% 59%



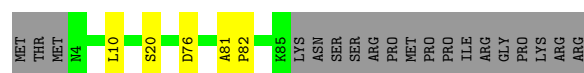
- Molecule 23: Small nuclear ribonucleoprotein-associated protein B

Chain k: 40% 59%



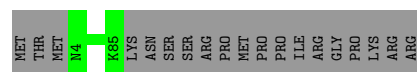
- Molecule 24: Small nuclear ribonucleoprotein Sm D3

Chain d: 76% 5% 19%



- Molecule 24: Small nuclear ribonucleoprotein Sm D3

Chain n: 81% 19%




- Molecule 25: Small nuclear ribonucleoprotein E

Chain e: 74% 5% 20%




- Molecule 25: Small nuclear ribonucleoprotein E

Chain p:  79% 20%




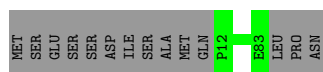
- Molecule 26: Small nuclear ribonucleoprotein F

Chain f:  80% 16%




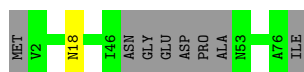
- Molecule 26: Small nuclear ribonucleoprotein F

Chain q:  84% 16%




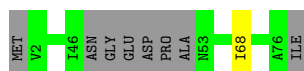
- Molecule 27: Small nuclear ribonucleoprotein G

Chain g:  88% 10%



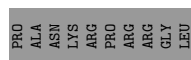
- Molecule 27: Small nuclear ribonucleoprotein G

Chain r:  88% 10%



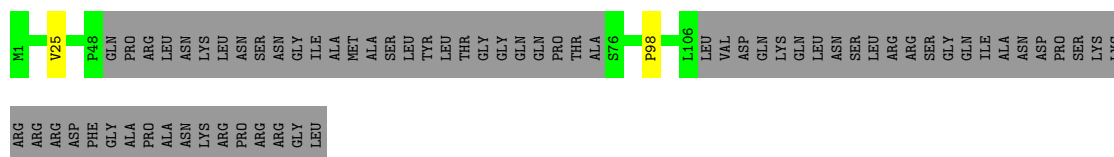
- Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain h:  56% 44%



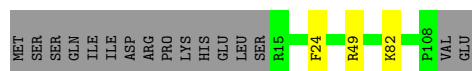
- Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain l:  53% 46%



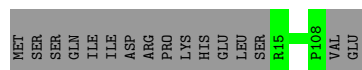
- Molecule 29: Small nuclear ribonucleoprotein Sm D2

Chain j: 83% 15%



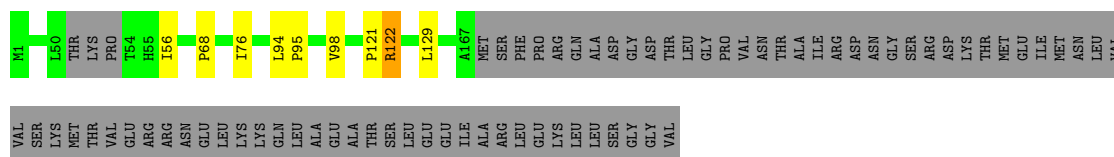
- Molecule 29: Small nuclear ribonucleoprotein Sm D2

Chain m: 85% 15%



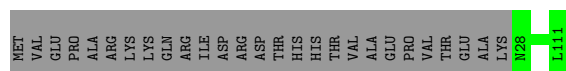
- Molecule 30: U2 small nuclear ribonucleoprotein A'

Chain W: 65% 31%



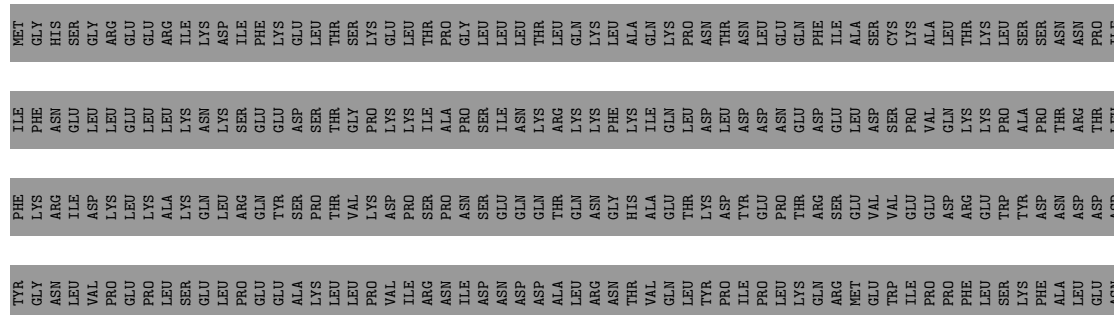
- Molecule 31: U2 small nuclear ribonucleoprotein B''

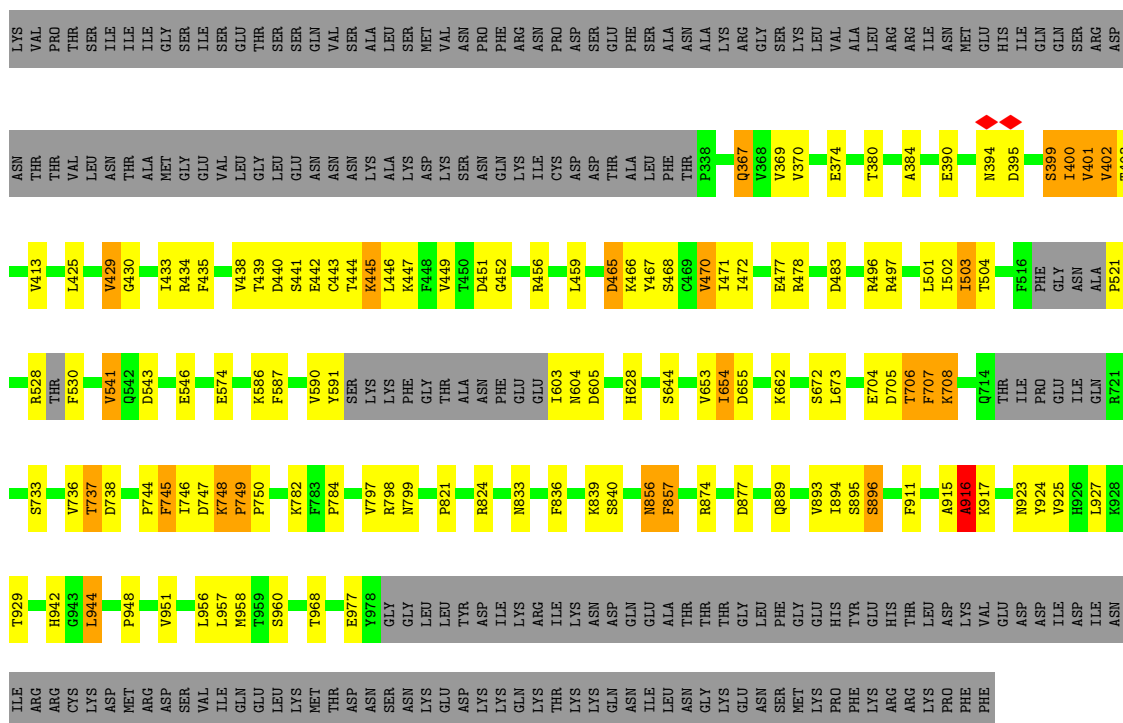
Chain Y: 76% 24%



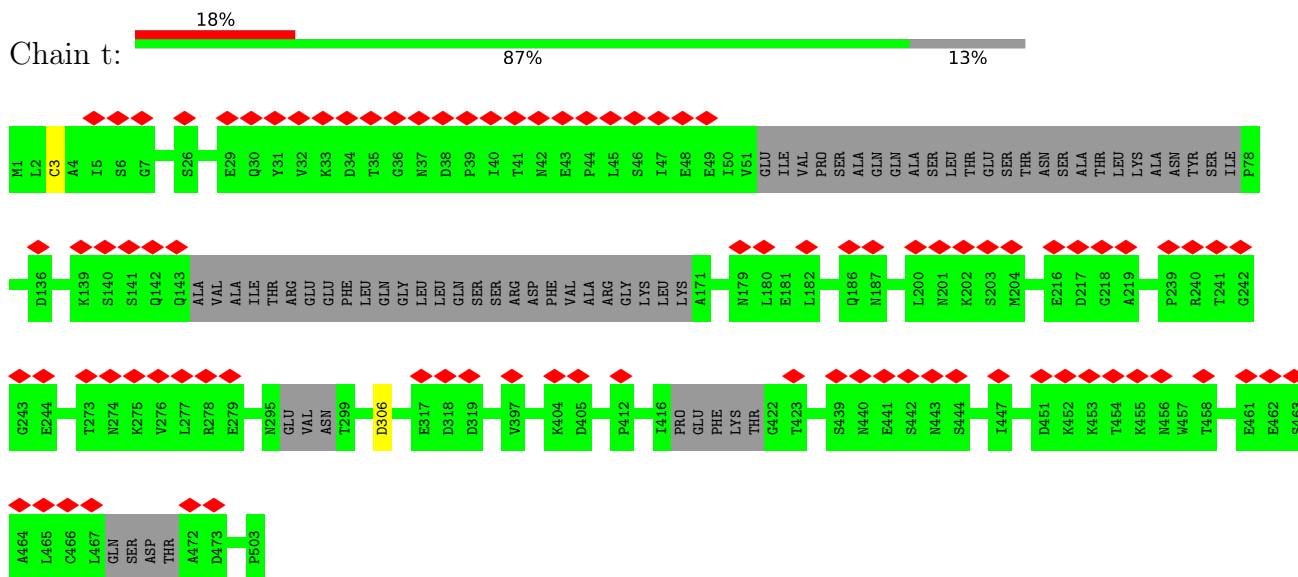
- Molecule 32: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16

Chain Q: 46% 10% 42%

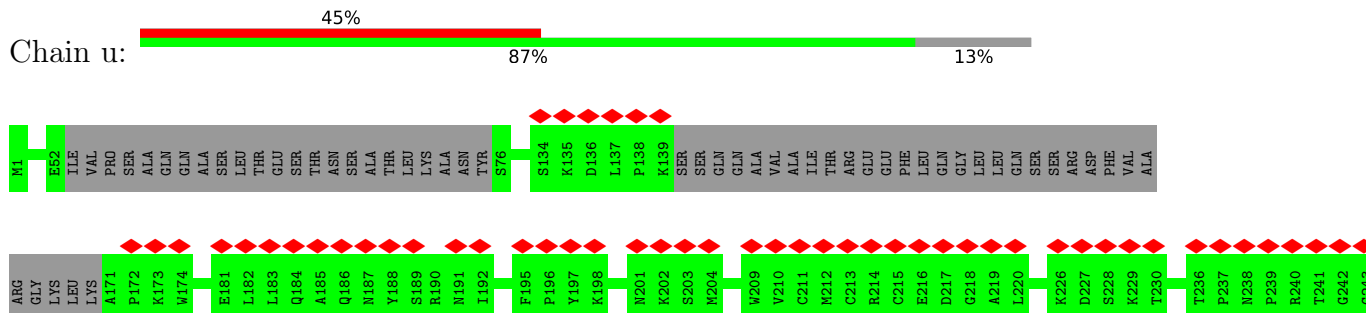


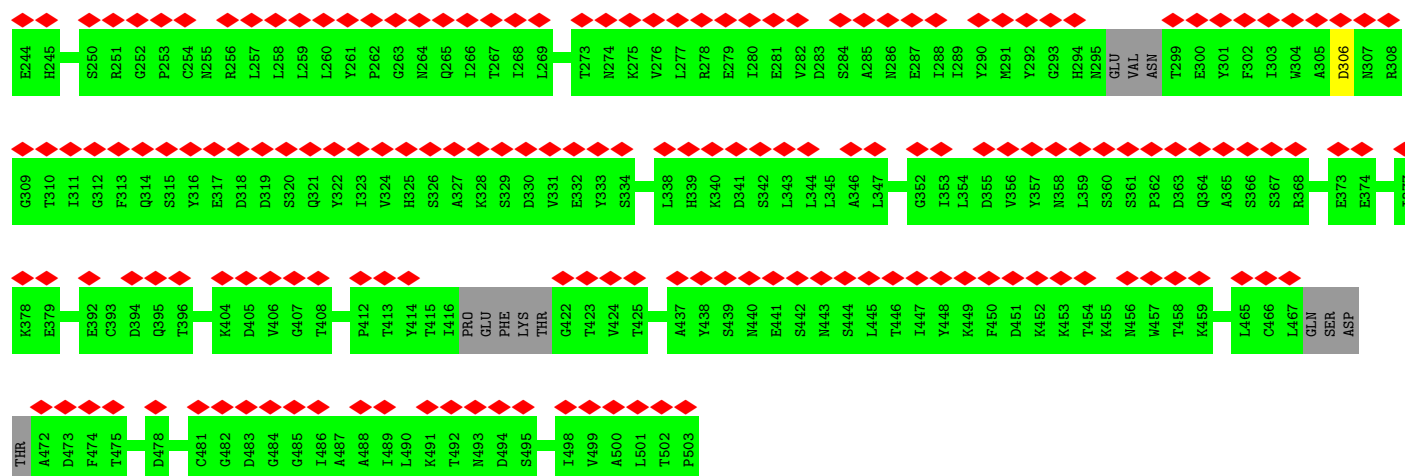


- Molecule 33: Pre-mRNA-processing factor 19

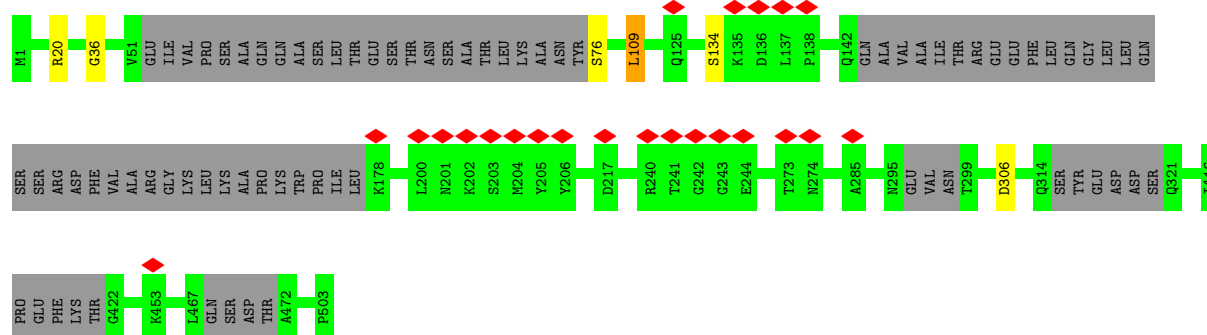
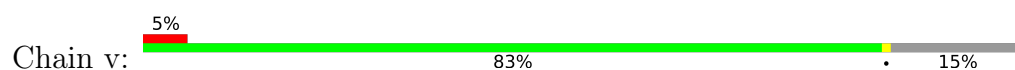


- Molecule 33: Pre-mRNA-processing factor 19

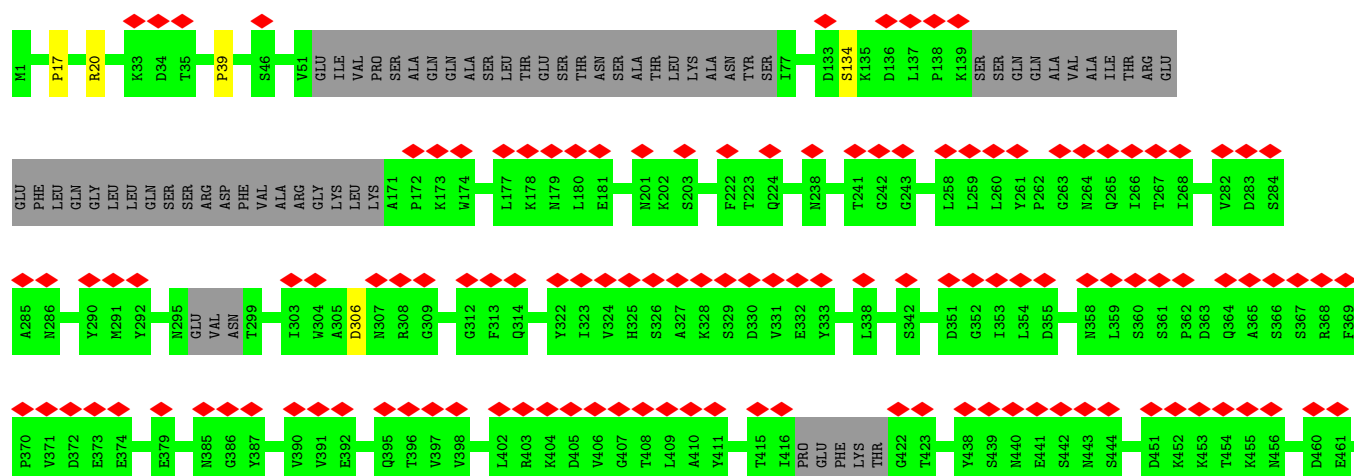
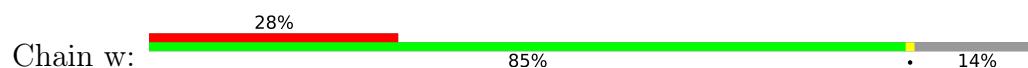


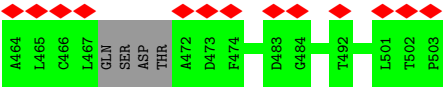


• Molecule 33: Pre-mRNA-processing factor 19

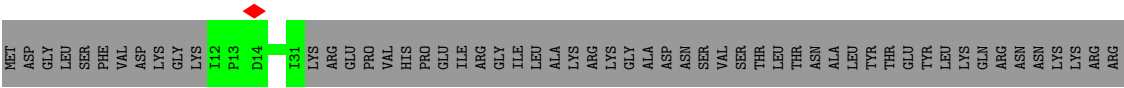


• Molecule 33: Pre-mRNA-processing factor 19





• Molecule 34: Pre-mRNA-splicing factor SNT309



• Molecule 35: unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15872	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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	589.16, 589.16, 589.16	wwPDB
Map dimensions	412, 412, 412	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	Depositor

5 Model quality

5.1 Standard geometry

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

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	U	0.31	0/3351	0.75	1/5213 (0.0%)
2	E	0.36	0/388	0.69	0/603
3	I	0.28	0/772	0.71	0/1195
4	Z	0.26	0/4018	0.72	0/6233
5	V	0.32	0/2310	0.77	3/3594 (0.1%)
6	A	0.44	0/17321	0.75	0/23534
7	B	0.52	0/8463	0.72	0/11800
8	D	0.37	0/929	0.67	0/1243
9	F	0.42	0/325	0.74	0/442
10	C	0.41	0/6902	0.73	0/9386
11	G	0.42	0/839	0.74	0/1126
12	H	0.43	0/2667	0.80	1/3630 (0.0%)
13	J	0.45	0/2613	0.74	0/3551
14	K	0.40	0/1308	0.72	0/1765
15	L	0.40	0/1294	0.75	0/1732
16	M	0.42	0/2058	0.70	0/2769
17	N	0.41	0/1680	0.76	0/2258
18	O	0.49	0/2091	0.86	2/2824 (0.1%)
19	P	0.43	0/282	0.69	0/380
20	R	0.40	0/545	0.77	0/748
21	S	0.44	0/3155	0.83	0/4298
22	T	0.38	0/2918	0.74	0/4032
23	b	0.34	0/636	0.59	0/856
23	k	0.28	0/394	0.50	0/546
24	d	0.36	0/634	0.62	1/859 (0.1%)
24	n	0.29	0/403	0.53	0/559
25	e	0.40	0/585	0.56	0/795
25	p	0.30	0/367	0.55	0/507
26	f	0.39	0/585	0.59	0/791
26	q	0.30	0/353	0.53	0/489
27	g	0.36	0/532	0.55	0/715
27	r	0.28	0/338	0.45	0/467

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	h	0.35	0/649	0.54	0/880
28	l	0.30	0/390	0.53	0/541
29	j	0.38	0/753	0.61	0/1013
29	m	0.31	0/466	0.54	0/649
30	W	0.31	0/814	0.53	0/1134
31	Y	0.32	0/415	0.55	0/577
32	Q	0.51	0/3061	1.22	18/4260 (0.4%)
33	t	0.46	0/2165	0.67	1/3010 (0.0%)
33	u	0.50	0/2160	0.69	1/3003 (0.0%)
33	v	0.51	0/2104	0.74	4/2923 (0.1%)
33	w	0.47	0/2150	0.68	2/2989 (0.1%)
34	s	0.57	0/546	0.80	0/760
All	All	0.43	0/86729	0.75	34/120679 (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
6	A	0	2
11	G	0	1
16	M	0	1
18	O	0	2
21	S	0	1
32	Q	0	45
33	t	0	1
33	v	0	1
33	w	0	1
34	s	0	2
All	All	0	57

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Q	384	ALA	CB-CA-C	8.22	122.43	110.10
1	U	39	U	C2'-C3'-O3'	8.13	127.38	109.50
32	Q	745	PHE	C-N-CA	7.85	141.32	121.70
32	Q	413	VAL	CB-CA-C	7.51	125.67	111.40
32	Q	745	PHE	O-C-N	-6.99	111.52	122.70

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	403	TYR	Peptide
11	G	3	ARG	Peptide
16	M	231	ASP	Peptide
18	O	83	GLN	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	U	2999	0	1515	24	0
2	E	346	0	173	5	0
3	I	693	0	351	3	0
4	Z	3610	0	1831	10	0
5	V	2066	0	1042	23	0
6	A	16919	0	16184	233	0
7	B	8462	0	3706	27	0
8	D	912	0	936	11	0
9	F	321	0	282	3	0
10	C	6756	0	6801	117	0
11	G	823	0	808	10	0
12	H	2639	0	2073	25	0
13	J	2556	0	2551	54	0
14	K	1289	0	1309	17	0
15	L	1270	0	1294	12	0
16	M	2012	0	1968	32	0
17	N	1658	0	1712	59	0
18	O	2068	0	1853	39	0
19	P	275	0	283	4	0
20	R	544	0	345	17	0
21	S	3121	0	2399	55	0
22	T	2946	0	1252	11	0
23	b	631	0	670	0	0
23	k	396	0	169	0	0
24	d	625	0	647	0	0
24	n	404	0	180	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	e	575	0	597	0	0
25	p	369	0	152	0	0
26	f	573	0	572	0	0
26	q	354	0	153	0	0
27	g	529	0	557	0	0
27	r	340	0	152	0	0
28	h	644	0	686	0	0
28	l	392	0	165	0	0
29	j	741	0	778	0	0
29	m	467	0	199	0	0
30	W	816	0	341	1	0
31	Y	416	0	182	0	0
32	Q	3066	0	1345	52	0
33	t	2171	0	945	0	0
33	u	2166	0	942	0	0
33	v	2111	0	917	0	0
33	w	2156	0	938	0	0
34	s	548	0	219	0	0
35	x	660	0	142	0	0
36	E	1	0	0	0	0
36	V	1	0	0	0	0
37	D	1	0	0	1	0
37	L	3	0	0	0	0
37	M	1	0	0	0	0
37	N	2	0	0	5	0
38	C	32	0	12	0	0
All	All	85476	0	62328	741	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 6.

The worst 5 of 741 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)
32:Q:434:ARG:O	32:Q:874:ARG:HA	1.26	1.35
17:N:34:CYS:SG	17:N:37:CYS:SG	1.35	1.34
20:R:36:GLN:O	20:R:40:GLN:N	1.60	1.32
1:U:45:A:N1	1:U:74:U:O4	1.65	1.30
21:S:467:GLN:CA	21:S:471:LEU:HA	1.65	1.24

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	2160/2413 (90%)	1997 (92%)	152 (7%)	11 (0%)	25	64
7	B	1704/2163 (79%)	1585 (93%)	111 (6%)	8 (0%)	25	64
8	D	112/278 (40%)	93 (83%)	17 (15%)	2 (2%)	7	35
9	F	44/179 (25%)	41 (93%)	3 (7%)	0	100	100
10	C	872/1008 (86%)	777 (89%)	82 (9%)	13 (2%)	8	40
11	G	95/235 (40%)	89 (94%)	5 (5%)	1 (1%)	12	47
12	H	389/591 (66%)	362 (93%)	23 (6%)	4 (1%)	13	49
13	J	322/451 (71%)	263 (82%)	47 (15%)	12 (4%)	2	20
14	K	155/379 (41%)	146 (94%)	8 (5%)	1 (1%)	22	60
15	L	153/157 (98%)	136 (89%)	15 (10%)	2 (1%)	10	43
16	M	250/339 (74%)	228 (91%)	19 (8%)	3 (1%)	11	44
17	N	195/364 (54%)	178 (91%)	14 (7%)	3 (2%)	8	40
18	O	277/590 (47%)	248 (90%)	24 (9%)	5 (2%)	7	35
19	P	34/175 (19%)	28 (82%)	5 (15%)	1 (3%)	3	23
20	R	93/135 (69%)	81 (87%)	11 (12%)	1 (1%)	12	47
21	S	432/687 (63%)	416 (96%)	14 (3%)	2 (0%)	25	64
22	T	536/859 (62%)	506 (94%)	21 (4%)	9 (2%)	7	37
23	b	76/196 (39%)	70 (92%)	6 (8%)	0	100	100
23	k	76/196 (39%)	65 (86%)	9 (12%)	2 (3%)	4	26
24	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	10	43
24	n	80/101 (79%)	66 (82%)	14 (18%)	0	100	100
25	e	71/94 (76%)	68 (96%)	3 (4%)	0	100	100
25	p	71/94 (76%)	63 (89%)	7 (10%)	1 (1%)	9	41
26	f	70/86 (81%)	66 (94%)	3 (4%)	1 (1%)	9	41
26	q	70/86 (81%)	61 (87%)	9 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	g	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
27	r	65/77 (84%)	55 (85%)	9 (14%)	1 (2%)	8	40
28	h	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
28	l	75/146 (51%)	63 (84%)	10 (13%)	2 (3%)	4	25
29	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
29	m	92/110 (84%)	84 (91%)	8 (9%)	0	100	100
30	W	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	1	16
31	Y	82/111 (74%)	77 (94%)	5 (6%)	0	100	100
32	Q	609/1071 (57%)	486 (80%)	73 (12%)	50 (8%)	1	9
33	t	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
33	u	425/503 (84%)	413 (97%)	12 (3%)	0	100	100
33	v	412/503 (82%)	403 (98%)	6 (2%)	3 (1%)	19	57
33	w	423/503 (84%)	414 (98%)	7 (2%)	2 (0%)	25	64
34	s	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	1	14
All	All	11527/16230 (71%)	10551 (92%)	821 (7%)	155 (1%)	13	43

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	320	ASP
6	A	737	ARG
7	B	766	ILE
12	H	414	PRO
16	M	127	ILE

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	
6	A	1701/2182 (78%)	1580 (93%)	121 (7%)	12	32
8	D	100/256 (39%)	91 (91%)	9 (9%)	8	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	F	26/163 (16%)	25 (96%)	1 (4%)	28	49
10	C	722/910 (79%)	659 (91%)	63 (9%)	8	25
11	G	89/216 (41%)	81 (91%)	8 (9%)	8	24
12	H	185/552 (34%)	164 (89%)	21 (11%)	4	16
13	J	283/397 (71%)	250 (88%)	33 (12%)	4	16
14	K	143/328 (44%)	115 (80%)	28 (20%)	1	7
15	L	138/141 (98%)	129 (94%)	9 (6%)	14	35
16	M	213/296 (72%)	189 (89%)	24 (11%)	4	17
17	N	194/332 (58%)	175 (90%)	19 (10%)	6	21
18	O	174/525 (33%)	152 (87%)	22 (13%)	3	14
19	P	26/152 (17%)	21 (81%)	5 (19%)	1	7
20	R	23/121 (19%)	19 (83%)	4 (17%)	1	9
21	S	208/633 (33%)	181 (87%)	27 (13%)	3	14
23	b	70/176 (40%)	70 (100%)	0	100	100
24	d	69/89 (78%)	66 (96%)	3 (4%)	25	46
25	e	65/83 (78%)	60 (92%)	5 (8%)	10	30
26	f	63/77 (82%)	61 (97%)	2 (3%)	34	53
27	g	58/66 (88%)	57 (98%)	1 (2%)	56	72
28	h	77/129 (60%)	77 (100%)	0	100	100
29	j	79/103 (77%)	76 (96%)	3 (4%)	28	49
All	All	4706/7927 (59%)	4298 (91%)	408 (9%)	11	25

5 of 408 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	J	202	GLU
15	L	54	GLN
25	e	25	THR
13	J	269	ILE
14	K	48	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
14	K	33	GLN
21	S	61	ASN
14	K	174	ASN
16	M	44	ASN
21	S	79	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	138/179 (77%)	66 (47%)	13 (9%)
2	E	15/16 (93%)	10 (66%)	2 (13%)
3	I	31/76 (40%)	15 (48%)	0
4	Z	162/1175 (13%)	58 (35%)	11 (6%)
5	V	96/112 (85%)	35 (36%)	6 (6%)
All	All	442/1558 (28%)	184 (41%)	32 (7%)

5 of 184 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	13	A
1	U	14	G
1	U	15	A
1	U	16	U
1	U	18	A

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	V	60	G
5	V	74	U
1	U	172	U
1	U	96	U
5	V	84	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 9 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
38	GTP	C	1101	-	26,34,34	0.88	1 (3%)	32,54,54	1.64	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
38	GTP	C	1101	-	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	C	1101	GTP	C6-N1	-2.35	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	C	1101	GTP	PB-O3B-PG	-4.90	116.03	132.83
38	C	1101	GTP	PA-O3A-PB	-3.58	120.56	132.83
38	C	1101	GTP	C5-C6-N1	2.89	119.06	113.95
38	C	1101	GTP	O6-C6-C5	-2.72	119.07	124.37
38	C	1101	GTP	C8-N7-C5	2.53	107.81	102.99

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	C	1101	GTP	C5'-O5'-PA-O3A
38	C	1101	GTP	C5'-O5'-PA-O1A

Continued on next page...

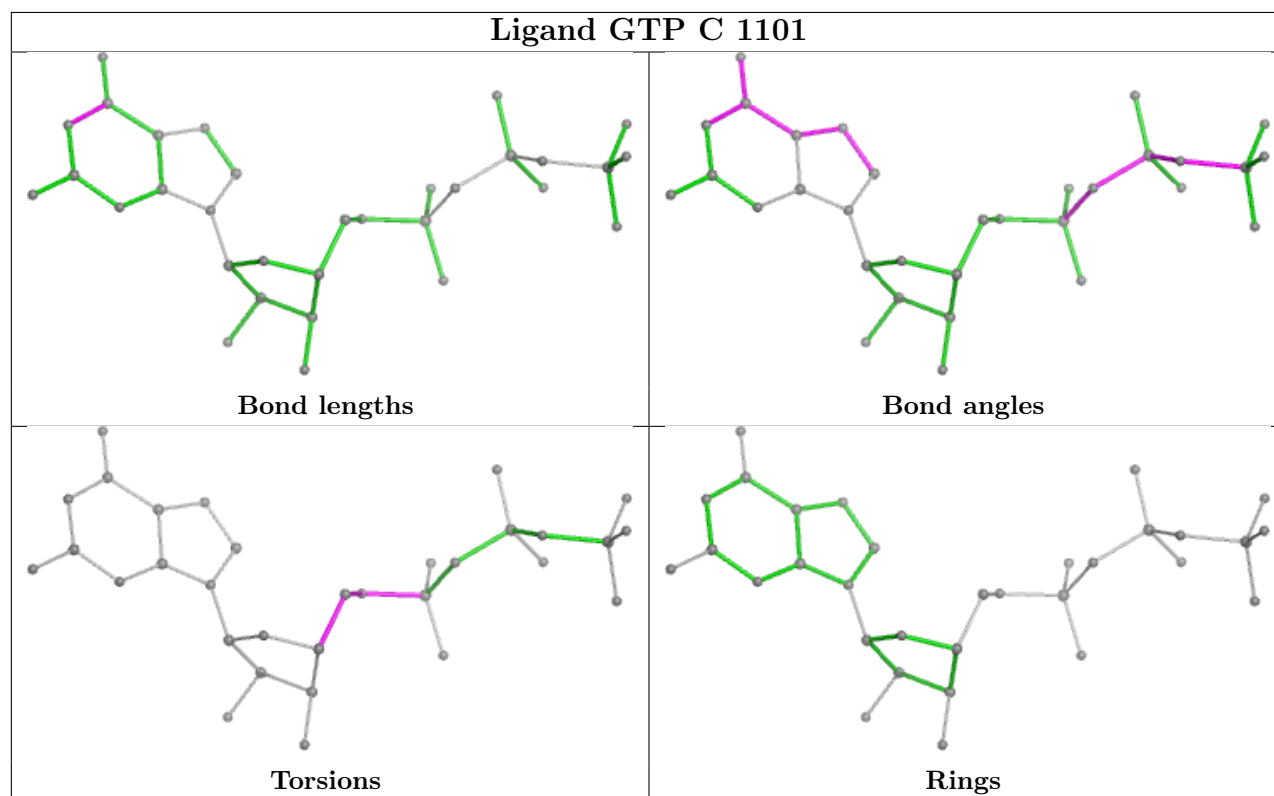
Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	C	1101	GTP	C3'-C4'-C5'-O5'
38	C	1101	GTP	O4'-C4'-C5'-O5'
38	C	1101	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	x	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	54:UNK	C	55:UNK	N	111.76
1	x	110:UNK	C	111:UNK	N	53.94
1	x	36:UNK	C	37:UNK	N	49.39
1	x	87:UNK	C	88:UNK	N	31.03

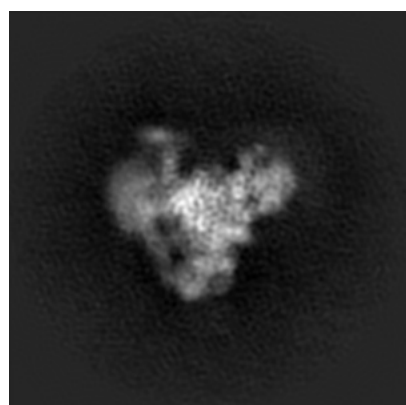
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4057. These allow visual inspection of the internal detail of the map and identification of artifacts.

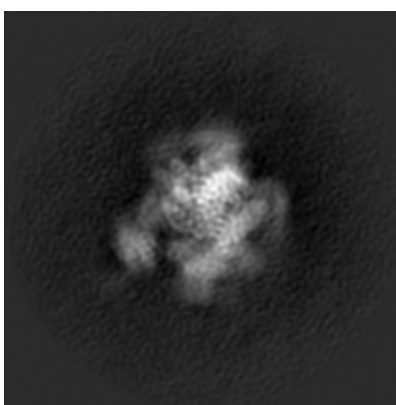
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

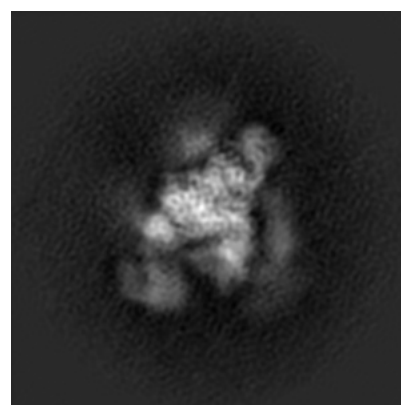
6.1.1 Primary map



X



Y

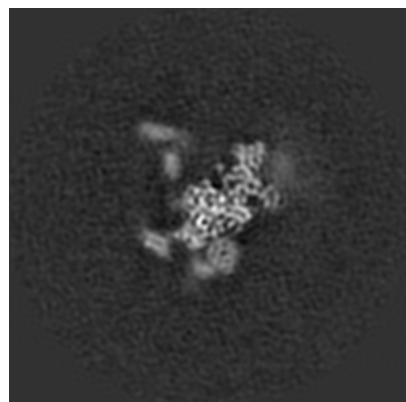


Z

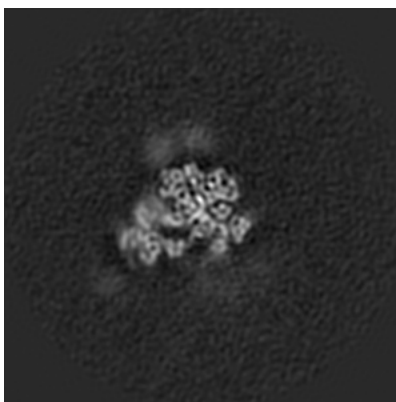
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

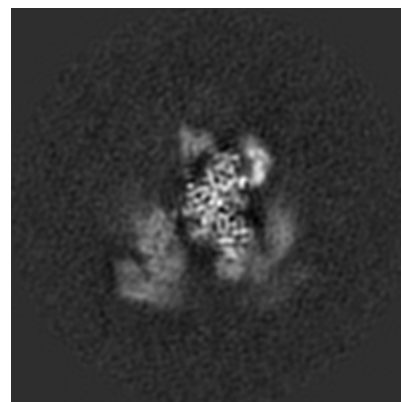
6.2.1 Primary map



X Index: 206



Y Index: 206

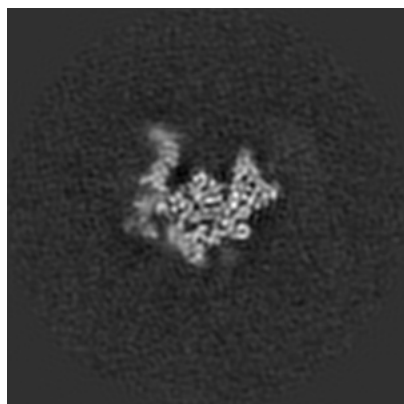


Z Index: 206

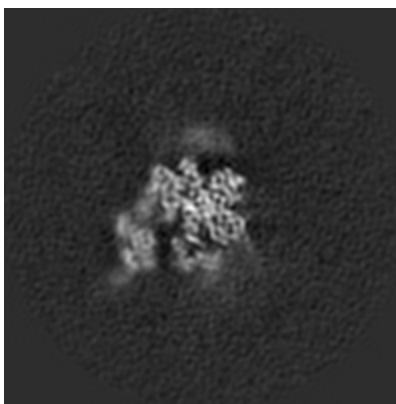
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

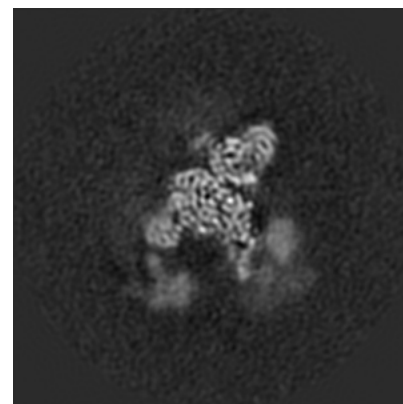
6.3.1 Primary map



X Index: 228



Y Index: 196

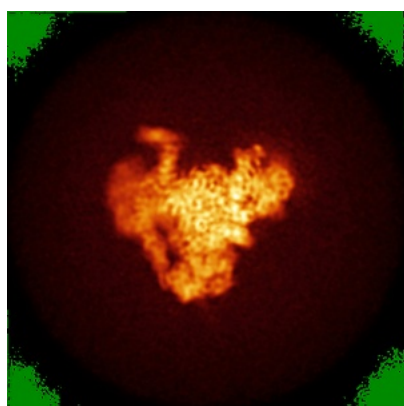


Z Index: 221

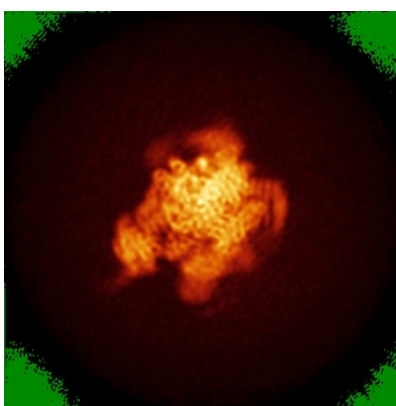
The images above show the largest variance slices of the map in three orthogonal directions.

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

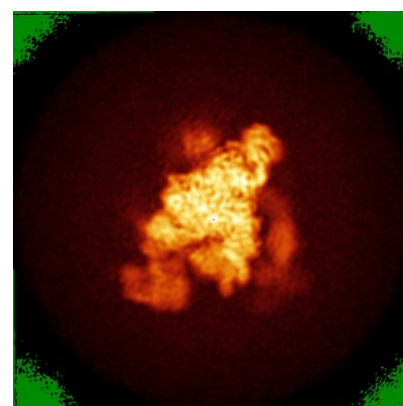
6.4.1 Primary map



X



Y



Z

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 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

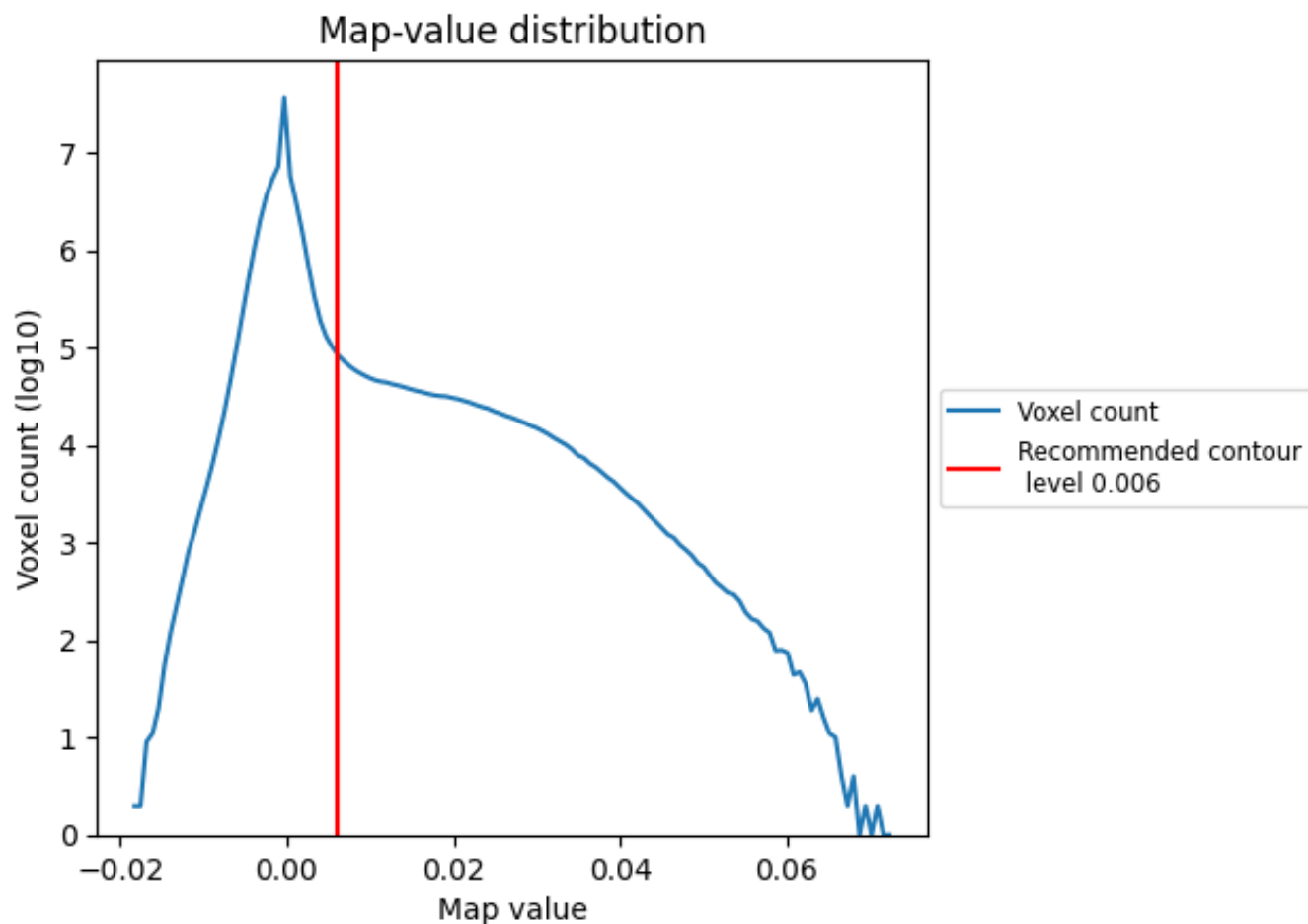
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

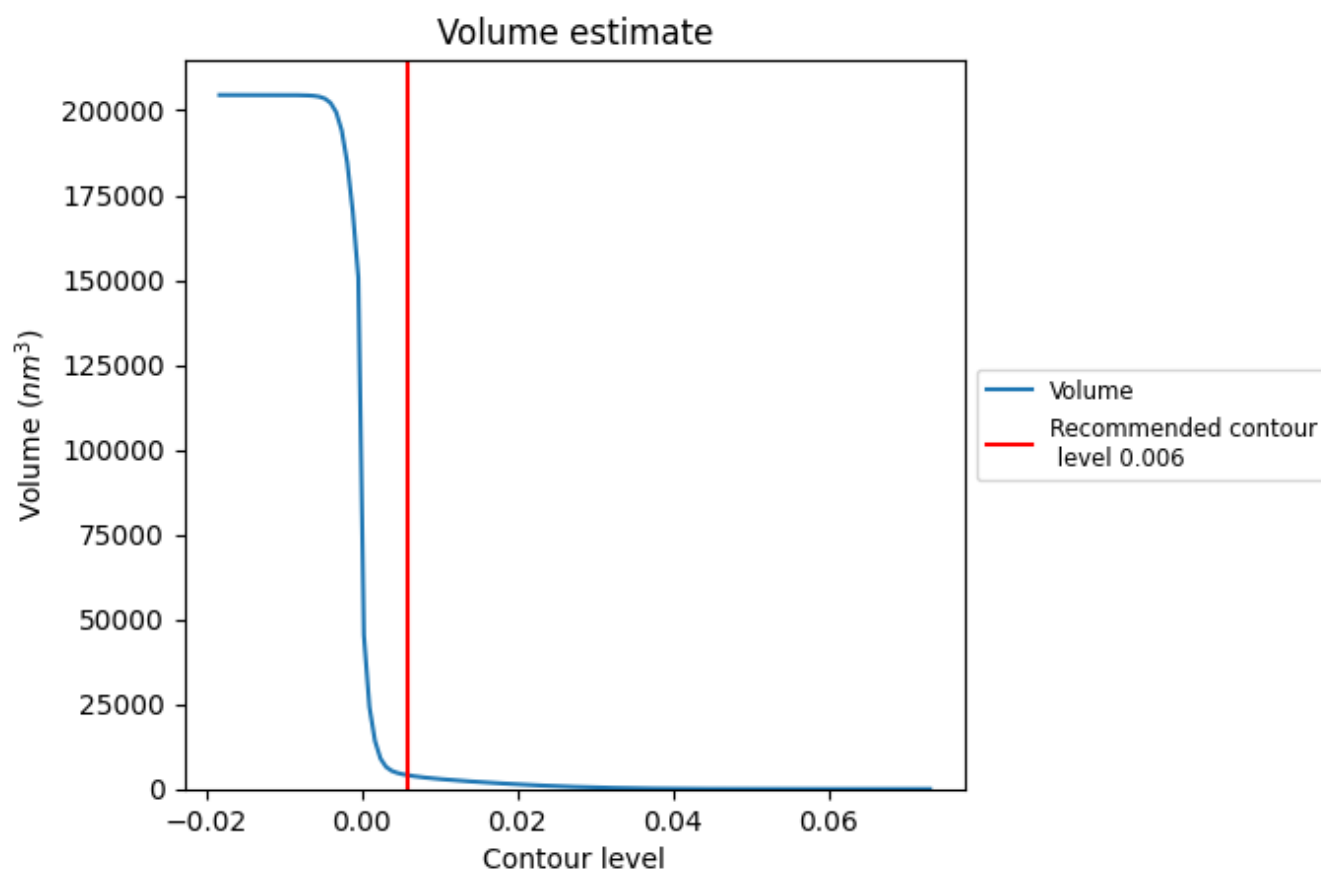
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

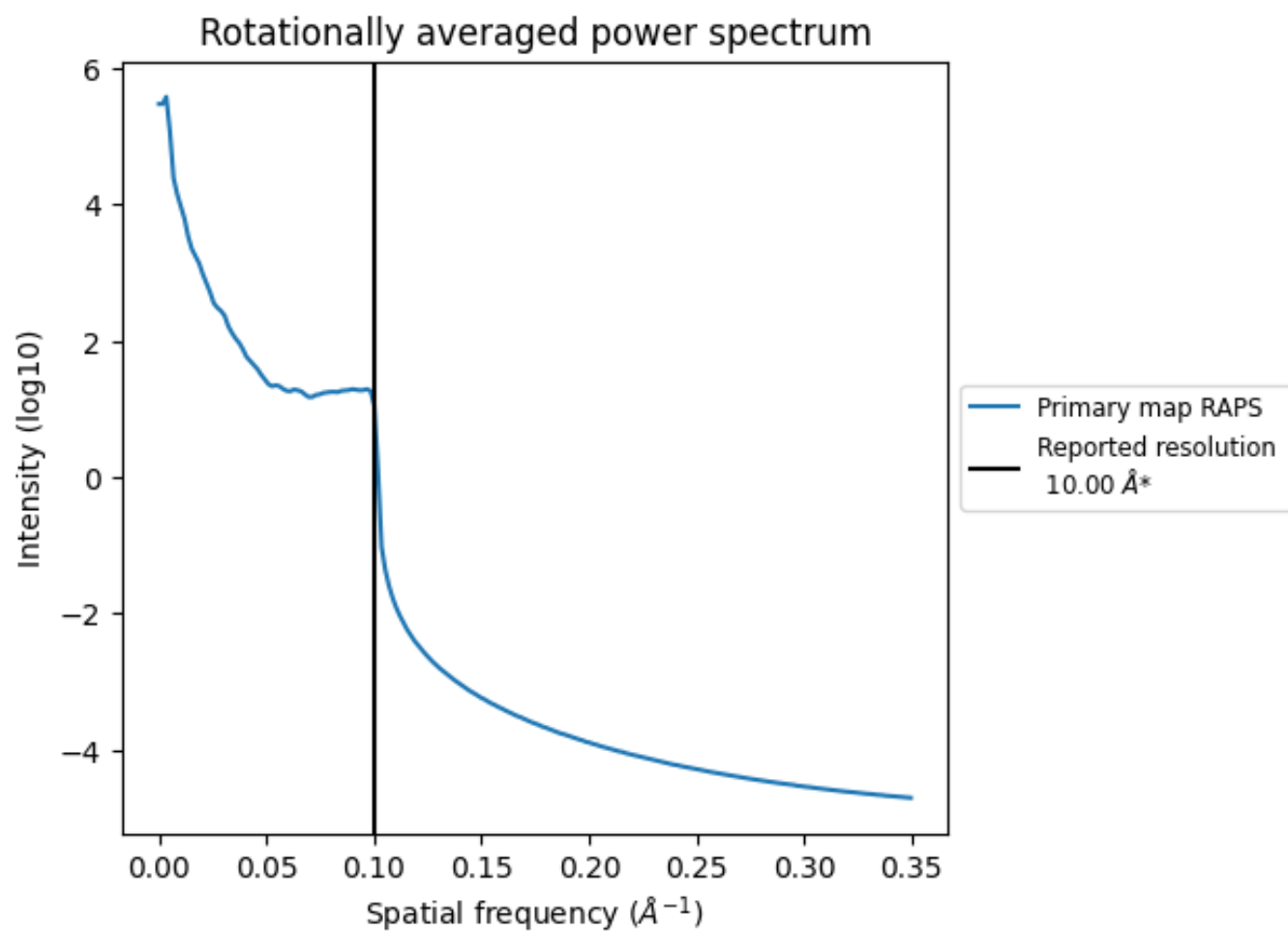
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4018 nm^3 ; this corresponds to an approximate mass of 3629 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 ⓘ

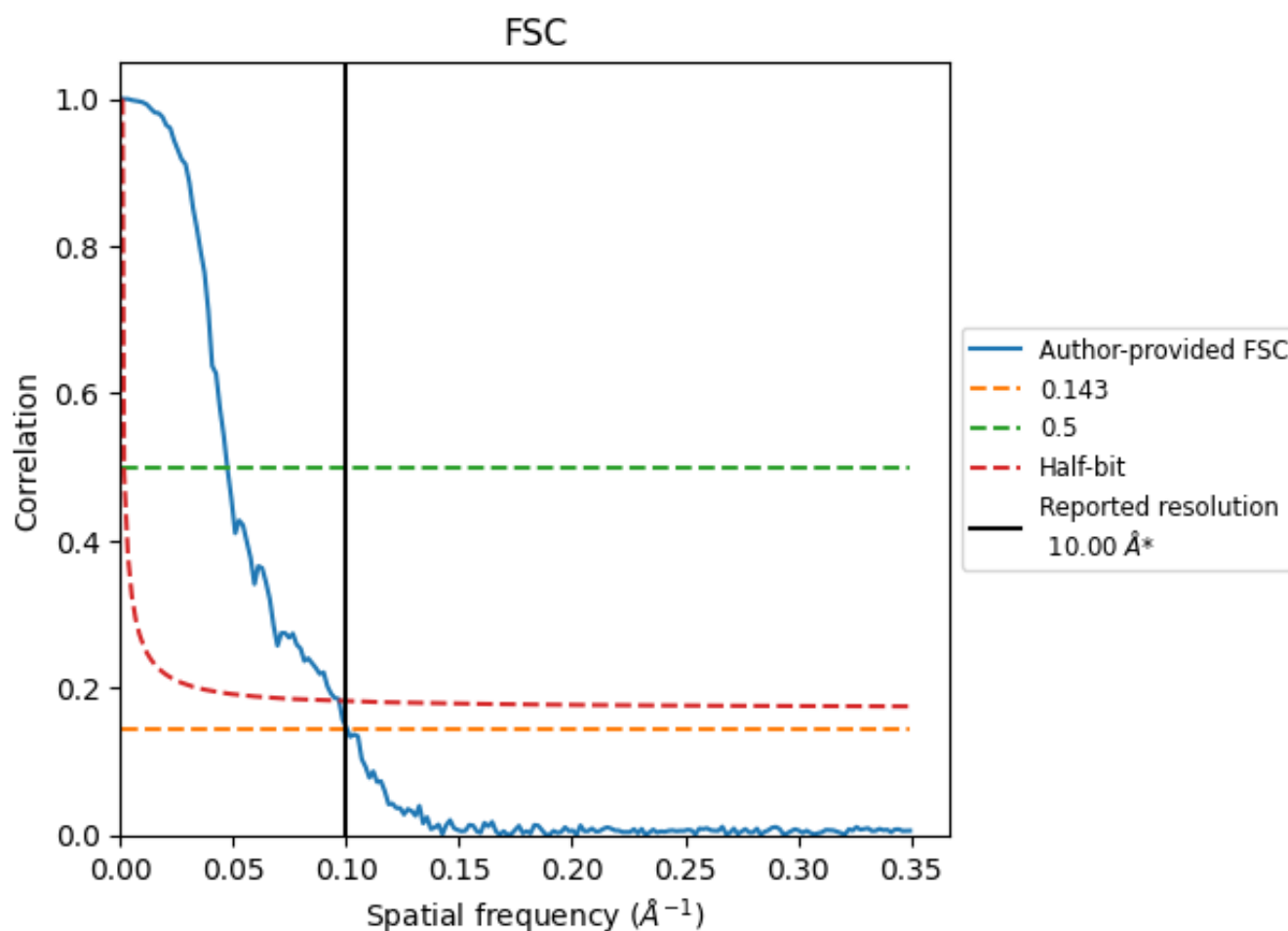


*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

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 0.100 Å⁻¹

8.2 Resolution estimates [i](#)

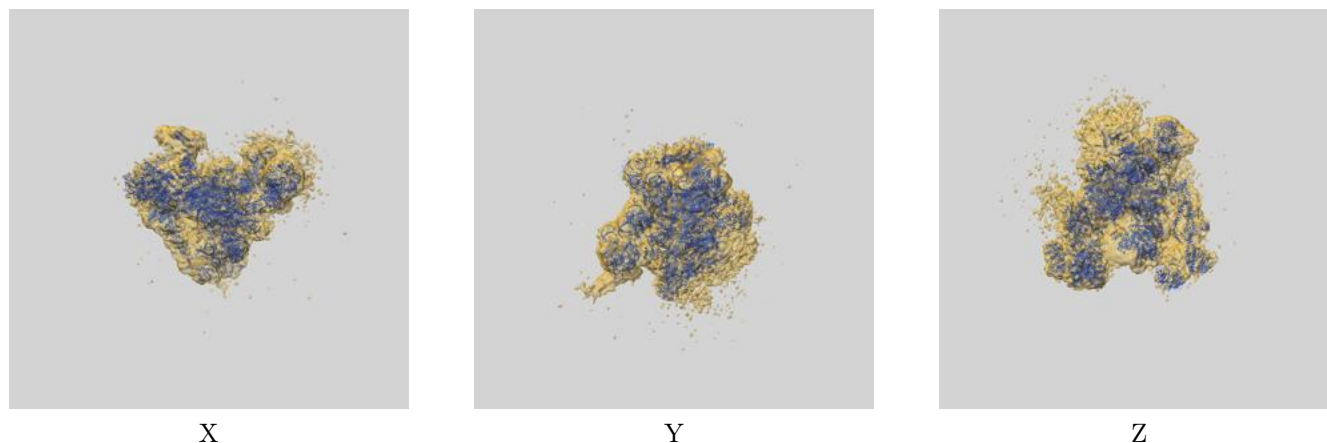
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	9.95	21.10	10.32
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

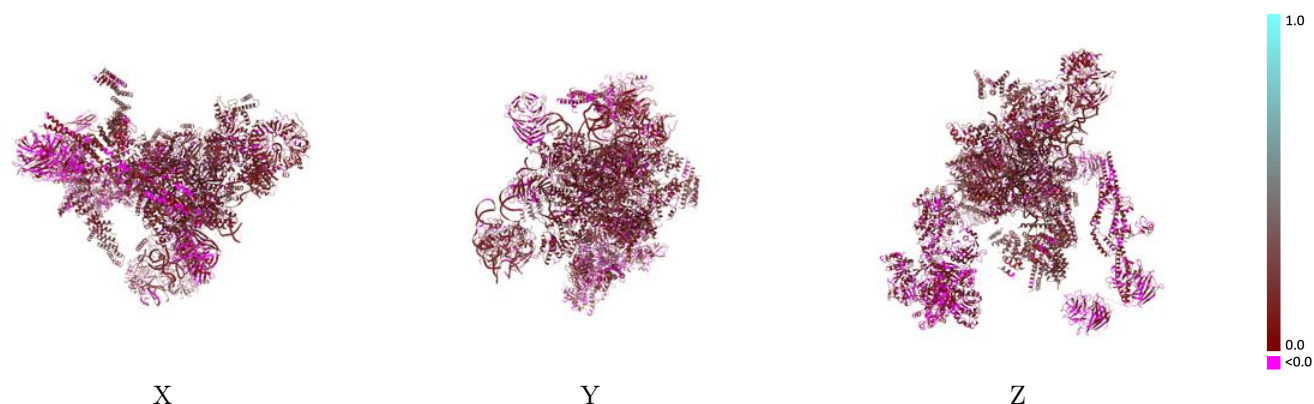
This section contains information regarding the fit between EMDB map EMD-4057 and PDB model 5LJ5. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



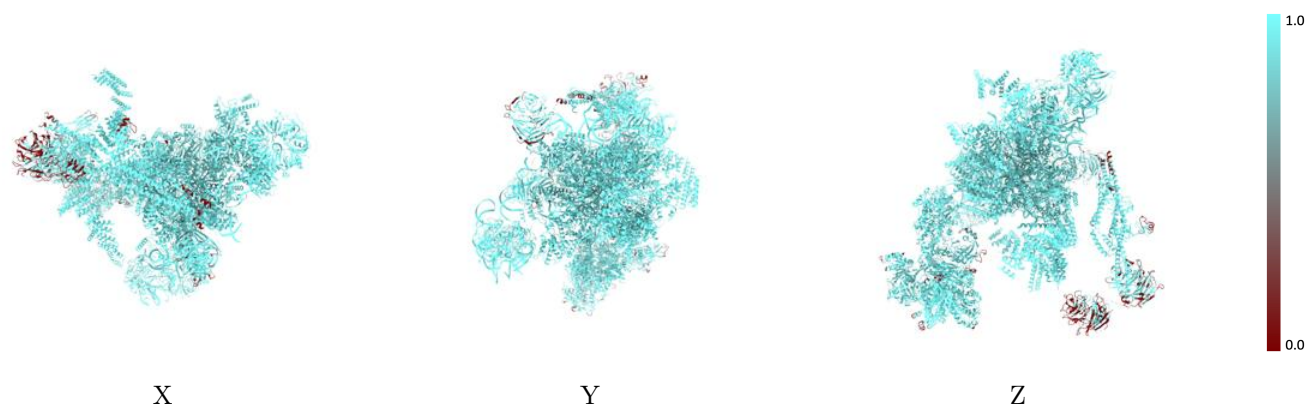
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



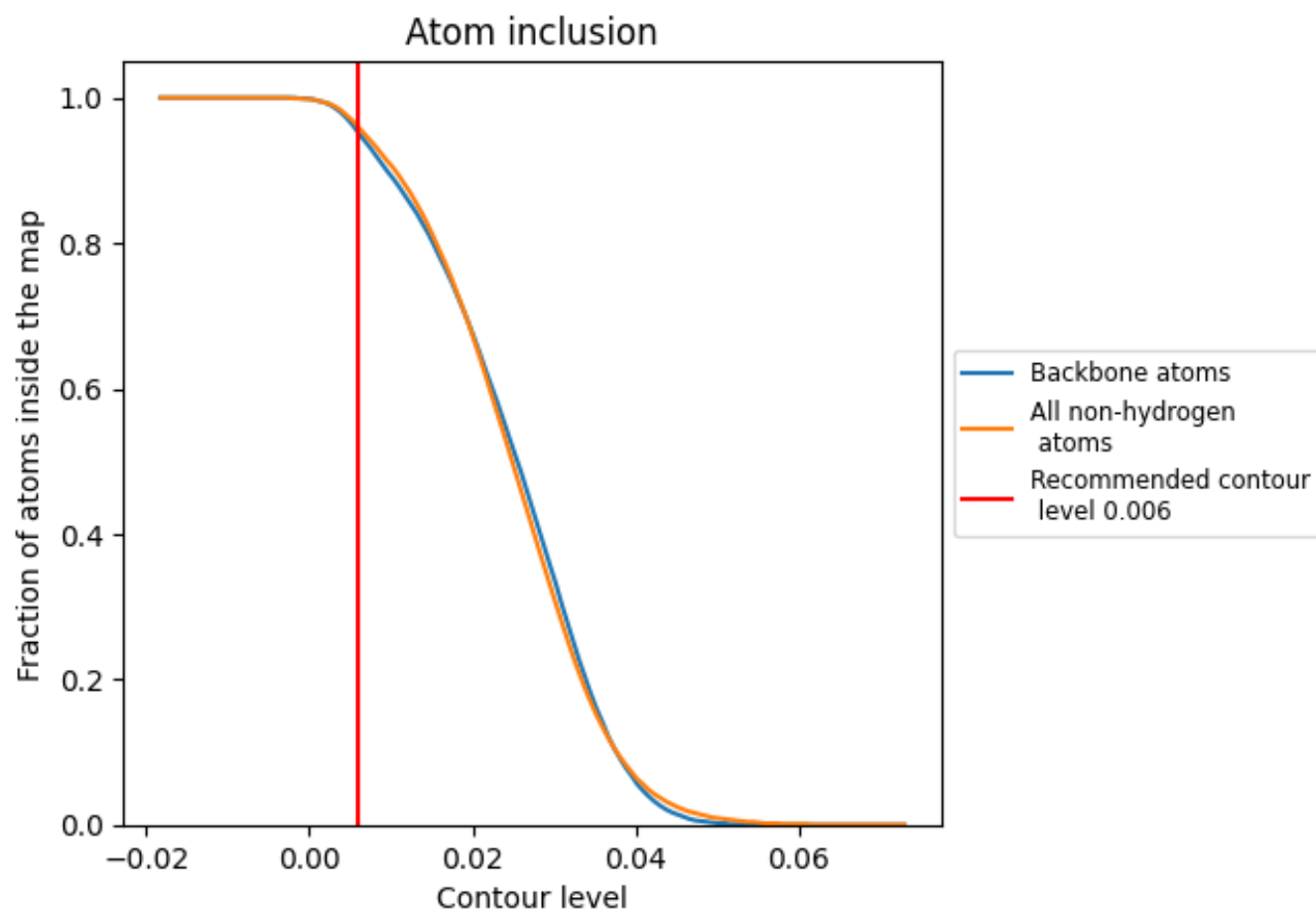
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.1140
A	 0.9820	 0.1130
B	 0.9520	 0.0430
C	 0.9890	 0.1230
D	 0.9820	 0.1110
E	 1.0000	 0.1490
F	 0.9910	 0.1550
G	 0.9910	 0.1270
H	 0.9960	 0.1600
I	 1.0000	 0.1410
J	 0.9900	 0.1030
K	 0.9870	 0.1390
L	 0.9990	 0.1210
M	 0.9880	 0.1220
N	 0.9910	 0.1370
O	 0.9600	 0.1170
P	 0.9890	 0.0910
Q	 0.9970	 0.0980
R	 0.9980	 0.2170
S	 0.9940	 0.1570
T	 1.0000	 0.2110
U	 1.0000	 0.1590
V	 1.0000	 0.1670
W	 0.9990	 0.1180
Y	 1.0000	 0.1230
Z	 1.0000	 0.1350
b	 1.0000	 0.1000
d	 1.0000	 0.1240
e	 1.0000	 0.1180
f	 0.9980	 0.1080
g	 0.9940	 0.1040
h	 0.9980	 0.1150
j	 0.9990	 0.1240
k	 1.0000	 0.1330
l	 1.0000	 0.1610



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Chain	Atom inclusion	Q-score
m	 1.0000	 0.1750
n	 1.0000	 0.1600
p	 1.0000	 0.1770
q	 1.0000	 0.1890
r	 0.9970	 0.1630
s	 0.9640	 0.0670
t	 0.7890	 0.0310
u	 0.4930	 0.0330
v	 0.9440	 0.0720
w	 0.6830	 0.0100
x	 1.0000	 0.2770