



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 08:38 PM UTC

PDB ID : 5MQ0 / pdb_00005mq0
EMDB ID : EMD-3541
Title : Structure of a spliceosome remodeled for exon ligation
Authors : Fica, S.M.; Oubridge, C.; Galej, W.P.; Wilkinson, M.E.; Newman, A.J.; Bai, X.-C.; Nagai, K.
Deposited on : 2016-12-19
Resolution : 4.17 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

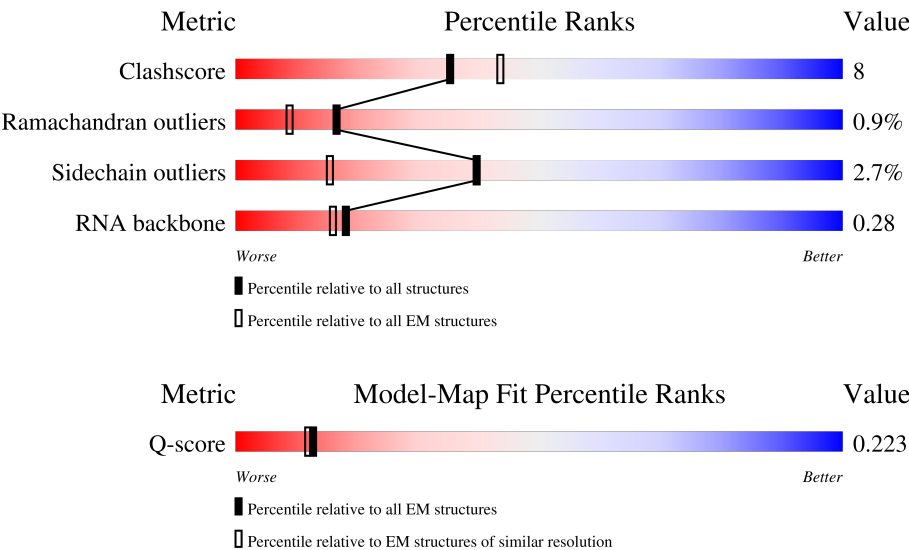
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.17 Å.

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



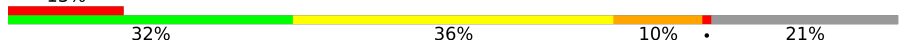
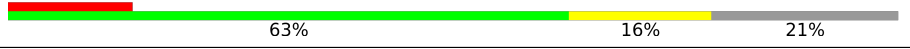
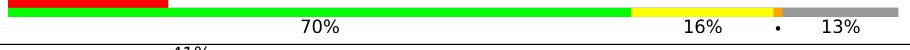
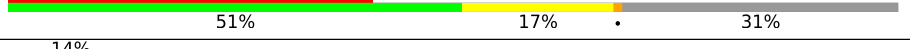
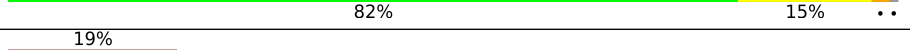
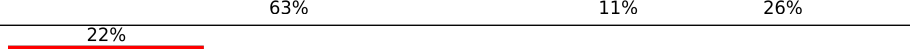
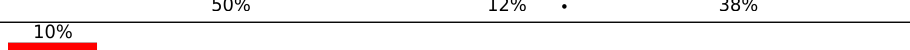
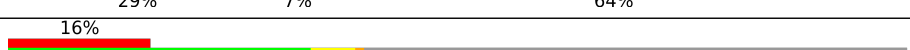
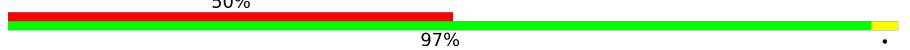
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5438 (3.67 - 4.67)

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	I	95	11% 13% 18% 5% 64%
2	E	20	20% 15% 50% 15% 20%
3	2	1175	10% 8% 87%

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Mol	Chain	Length	Quality of chain
4	6	112	
5	5	179	
6	A	2413	
7	C	1008	
8	H	577	
9	J	451	
10	K	379	
11	L	157	
12	M	339	
13	N	364	
14	O	590	
15	P	175	
16	R	135	
17	S	687	
18	T	877	
19	a	251	
20	c	382	
21	o	455	
22	X	68	
23	y	215	
24	b	196	
24	k	196	
25	d	101	
25	n	101	
26	e	94	

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Mol	Chain	Length	Quality of chain
26	p	94	
27	f	86	
27	q	86	
28	g	77	
28	r	77	
29	h	146	
29	l	146	
30	j	110	
30	m	110	
31	V	1145	
32	W	238	
33	Y	111	
34	3	3	
35	s	175	
36	t	503	
36	u	503	
36	v	503	
36	w	503	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 77441 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 Yeast UBC4 gene for ubiquitin-conjugating enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	34	Total	C	N	O	P	0	0
			714	321	118	241	34		

- Molecule 2 is a RNA chain called 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 S.cerevisiae chromosome II reading frame ORF YBR230c.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	155	Total	C	N	O	P	0	0
			3271	1462	547	1107	155		

- Molecule 4 is a RNA chain called Saccharomyces cerevisiae strain T.52_2H chromosome XII sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	99	Total	C	N	O	P	0	0
			2108	944	375	690	99		

- Molecule 5 is a RNA chain called Saccharomyces cerevisiae strain WI_C_MBSP_4 chromosome VII sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	141	Total	C	N	O	P	0	0
			2999	1342	530	986	141		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1914	Total	C	N	O	S	0	0
			15199	9832	2669	2645	53		

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	874	Total	C	N	O	S	0	0
			6562	4265	1104	1168	25		

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	401	Total	C	N	O	S	0	0
			3261	2104	544	595	18		

- Molecule 9 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	342	Total	C	N	O	S	0	0
			2690	1699	475	506	10		

- Molecule 10 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	187	Total	C	N	O	S	0	0
			1458	908	269	276	5		

- Molecule 11 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	155	Total	C	N	O	S	0	0
			1162	737	217	198	10		

- Molecule 12 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	252	Total	C	N	O	S	0	0
			2016	1281	356	368	11		

- Molecule 13 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	227	Total	C	N	O	S	0	0
			1798	1139	309	335	15		

- Molecule 14 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	211	Total	C	N	O	S	0	0
			1755	1102	320	327	6		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	69	Total	C	N	O	S	0	0
			565	358	112	94	1		

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	108	Total	C	N	O		0	0
			614	369	121	124			

- Molecule 17 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	468	Total	C	N	O	S	0	0
			3229	2025	599	598	7		

- Molecule 18 is a protein called Pre-mRNA-splicing factor SYF1,PRE-MRNA-SPLICING FACTOR SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	633	Total	C	N	O		0	0
			3154	1888	633	633			

- Molecule 19 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	137	Total	C	N	O	S	0	0
			1119	726	194	196	3		

- Molecule 20 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	103	Total	C	N	O	S	0	0
			786	498	142	144	2		

- Molecule 21 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	o	313	Total	C	N	O	S	0	0
			2425	1537	429	451	8		

- Molecule 22 is a protein called UNKNOWN PROTEIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	68	Total	C	N	O	0	0
			338	202	68	68		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	y	83	Total	C	N	O	S	0	0
			679	420	125	133	1		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated protein B.

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

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	p	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

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

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

- Molecule 28 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
28	r	69	Total	C	N	O	S	0	0
			526	336	93	95	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
29	l	79	Total	C	N	O	S	0	0
			618	393	107	116	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
30	m	93	Total	C	N	O	S	0	0
			726	468	136	118	4		

- Molecule 31 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	V	645	Total	C	N	O	0	0
			3189	1899	645	645		

- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 33 is a protein called U2 small nuclear ribonucleoprotein B'.

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

- Molecule 34 is a RNA chain called 3'-EXON OF UBC4 PRE-MRNA, BOUND BY PRP22 HELICASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	3	3	Total	C	N	O	P	0	0
			60	27	6	24	3		

- Molecule 35 is a protein called Pre-mRNA-splicing factor SNT309.

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

- Molecule 36 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	t	438	Total	C	N	O	0	0
			2171	1295	438	438		
36	u	116	Total	C	N	O	0	0
			578	346	116	116		
36	v	118	Total	C	N	O	0	0
			588	352	118	118		
36	w	435	Total	C	N	O	0	0
			2156	1286	435	435		

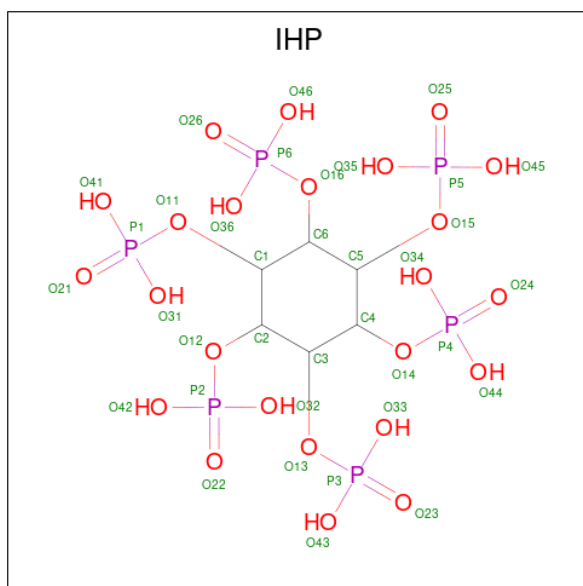
- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	6	3	Total	Mg	0
			3	3	

- Molecule 38 is POTASSIUM ION (CCD ID: K) (formula: K).

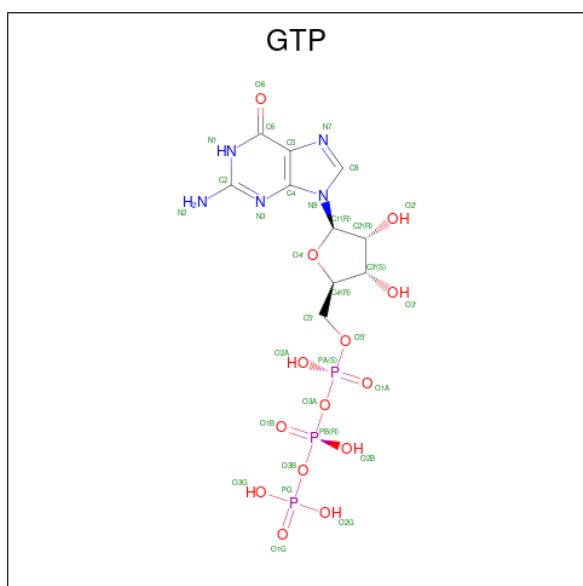
Mol	Chain	Residues	Atoms		AltConf
38	6	2	Total	K	0
			2	2	

- Molecule 39 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

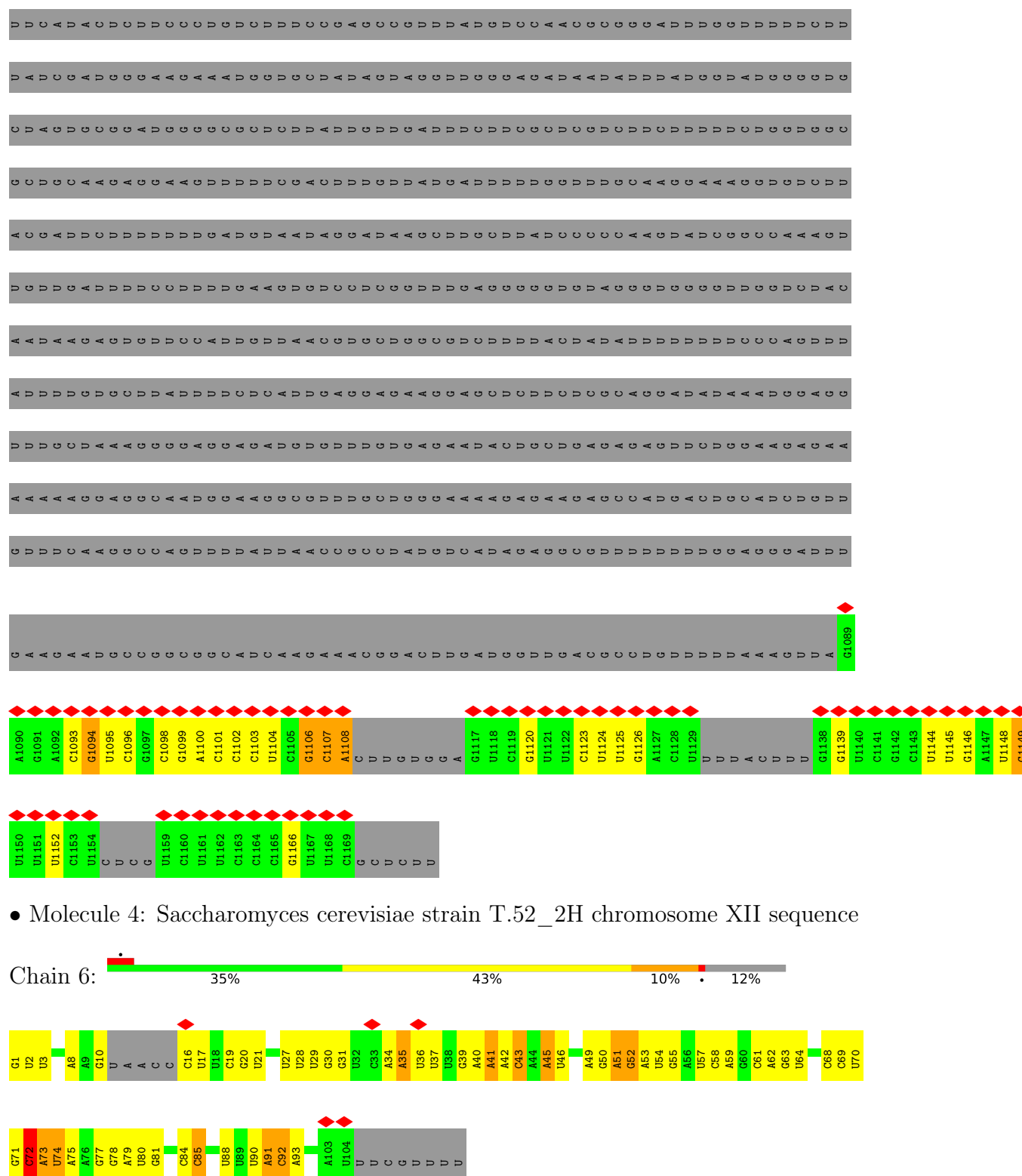
- Molecule 40 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

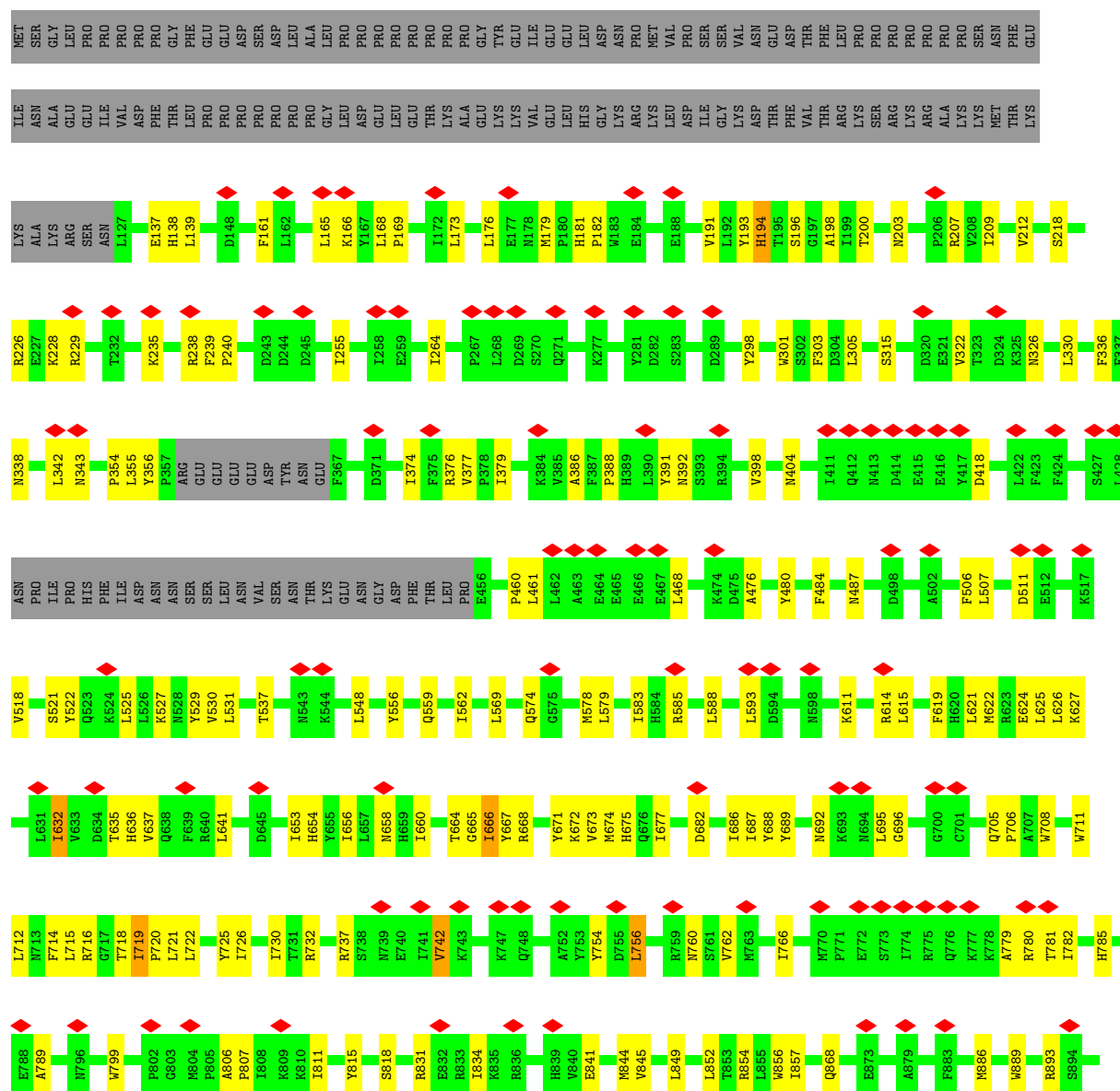


- Molecule 4: *Saccharomyces cerevisiae* strain T.52_2H chromosome XII sequence

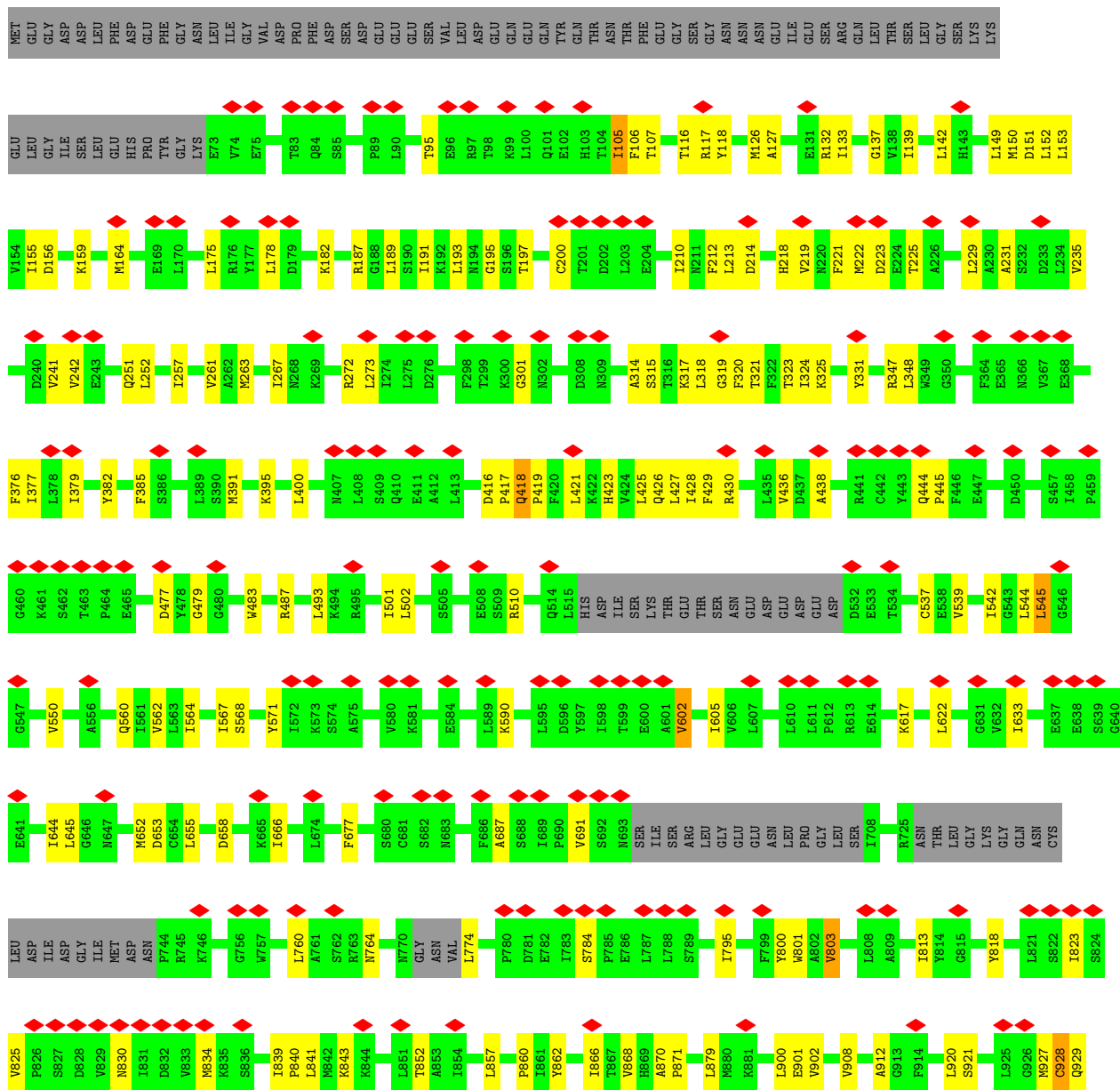
Chain 6: 35% 43% 10% 12%

- Molecule 5: *Saccharomyces cerevisiae* strain WI_C_MBSP_4 chromosome VII sequence

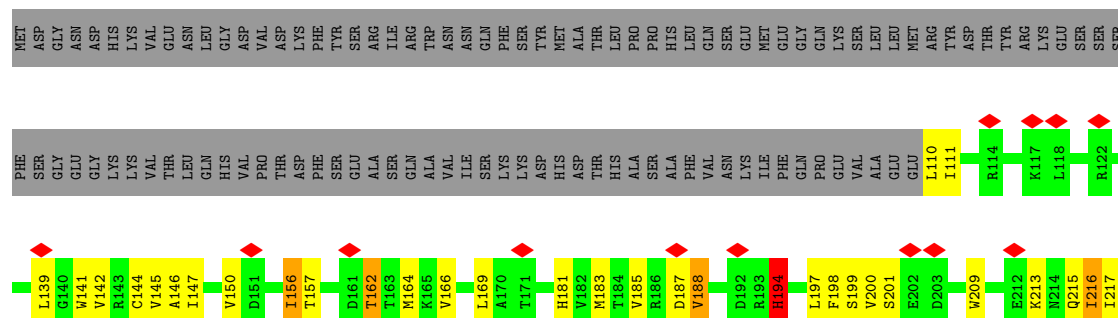
Chain 5: 13% 32% 36% 10% 21%

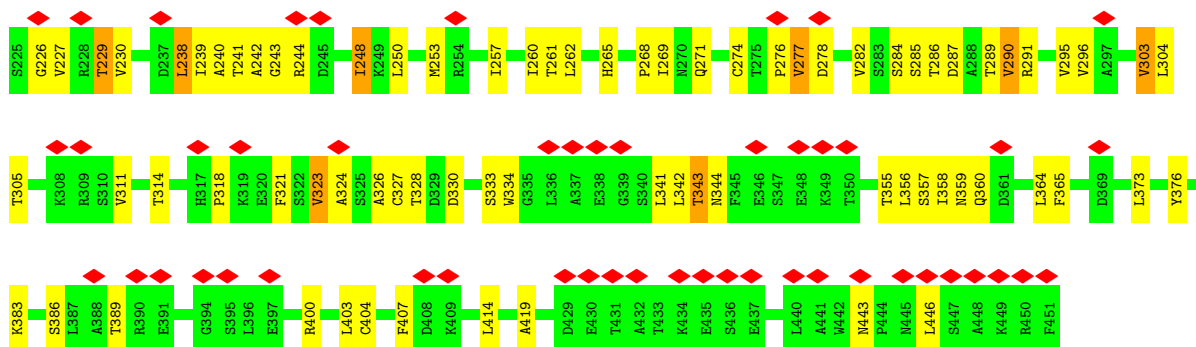




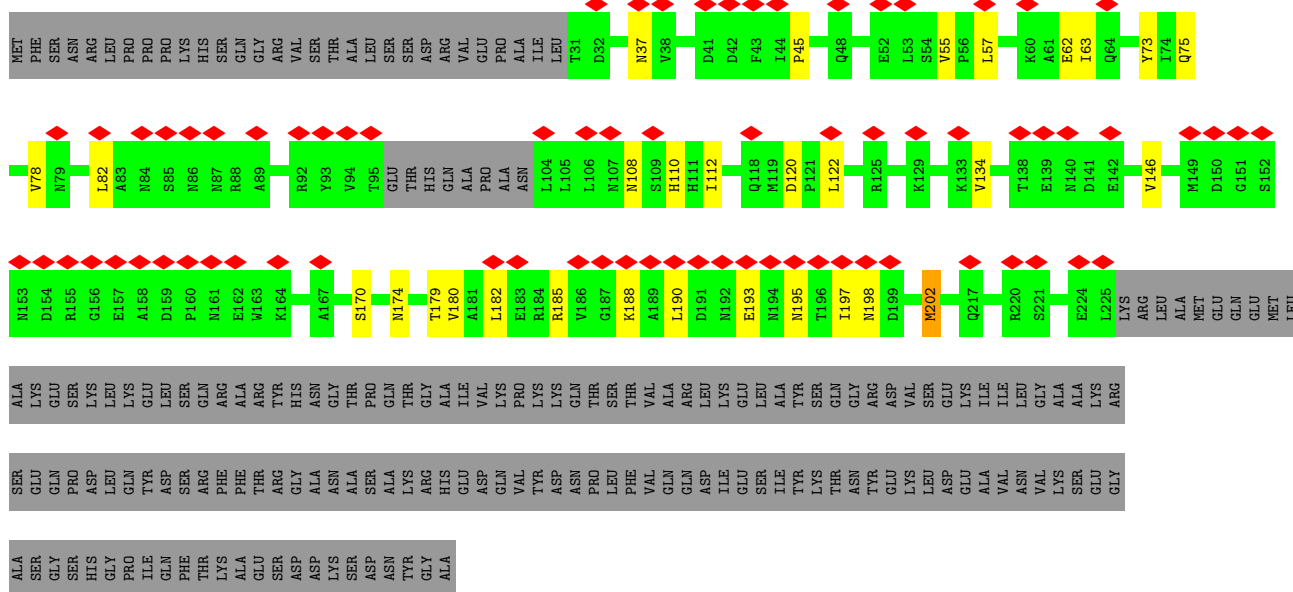
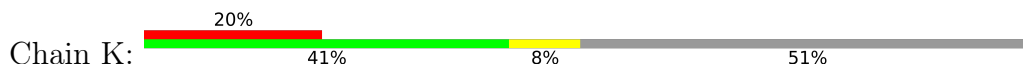


Chain H:

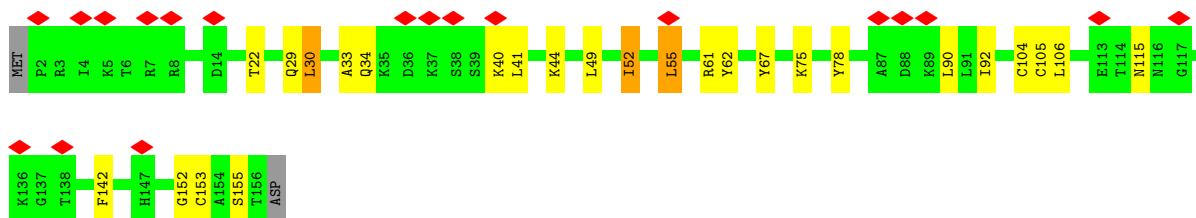
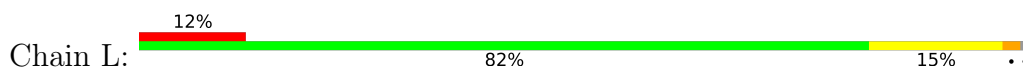




• Molecule 10: Pre-mRNA-processing protein 45

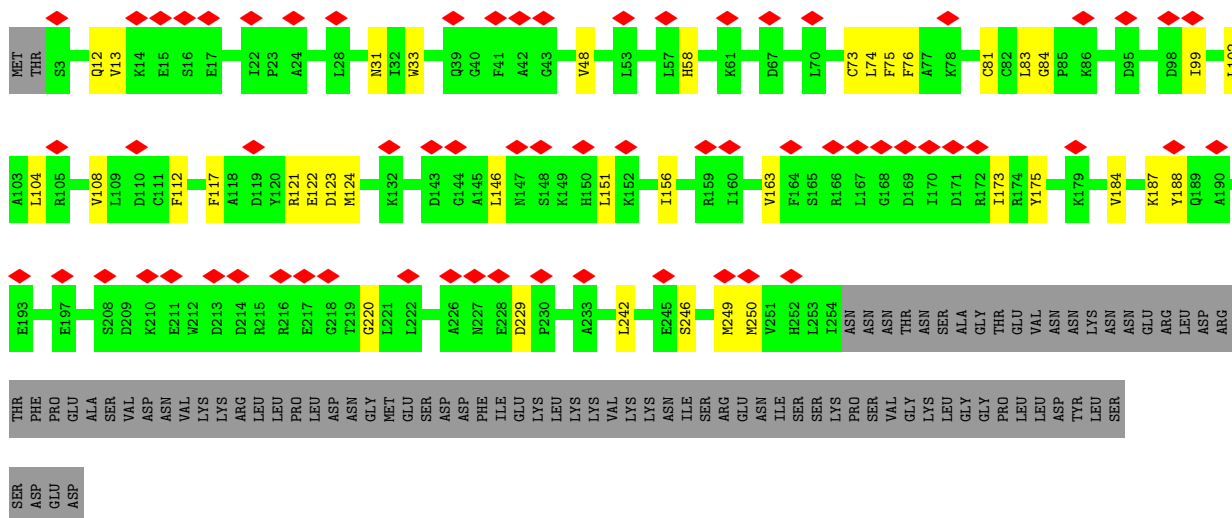


• Molecule 11: Pre-mRNA-splicing factor BUD31

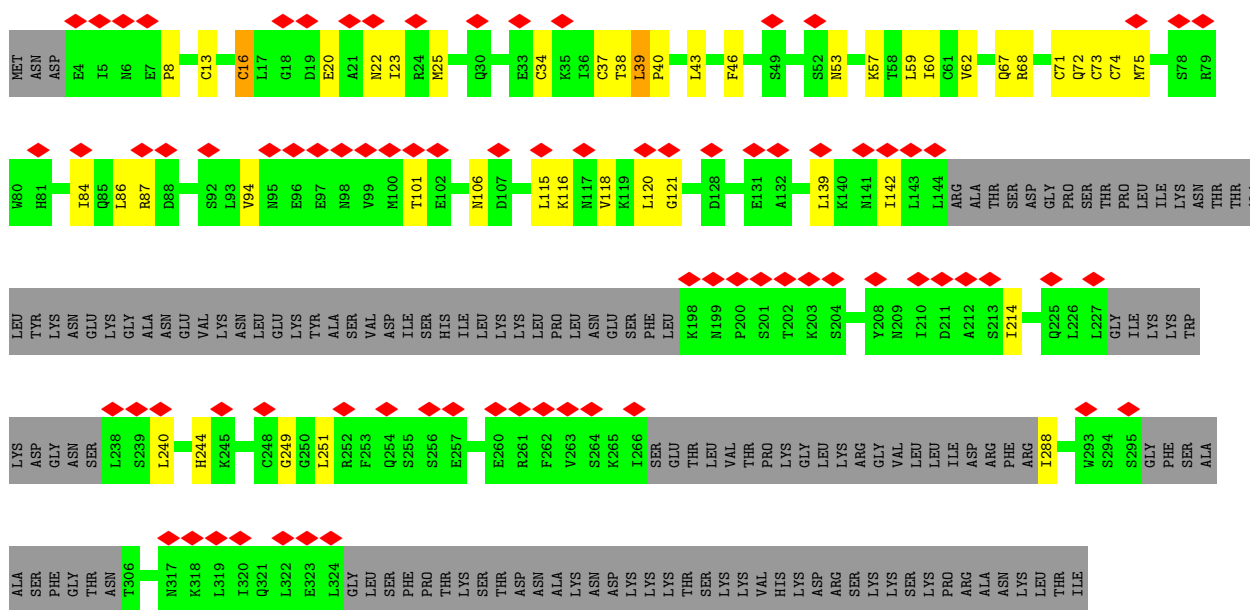


• Molecule 12: Pre-mRNA-splicing factor CWC2

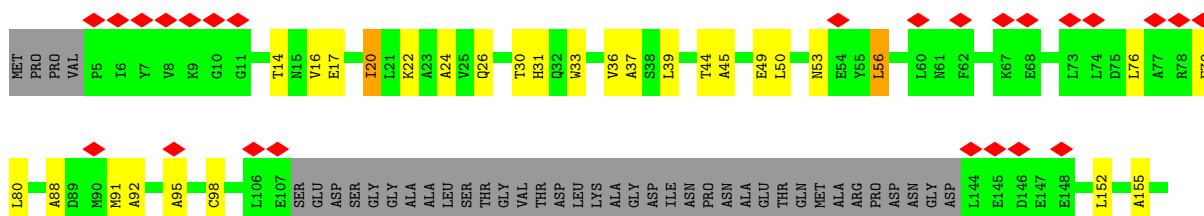


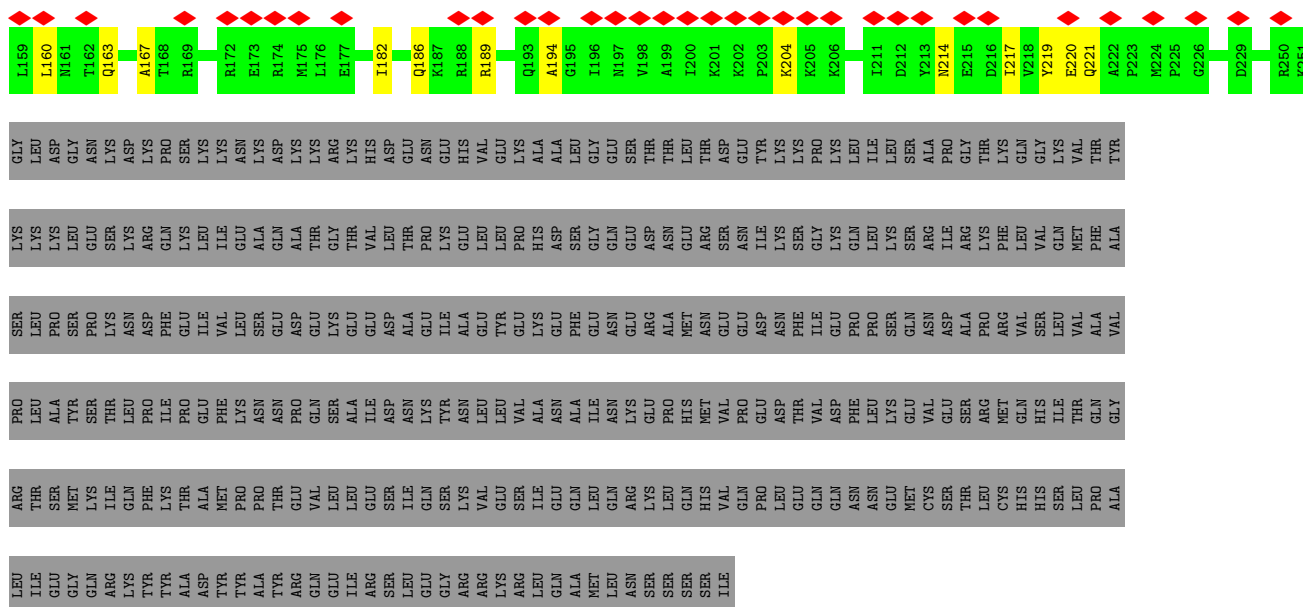


• Molecule 13: Pre-mRNA-splicing factor SLT11

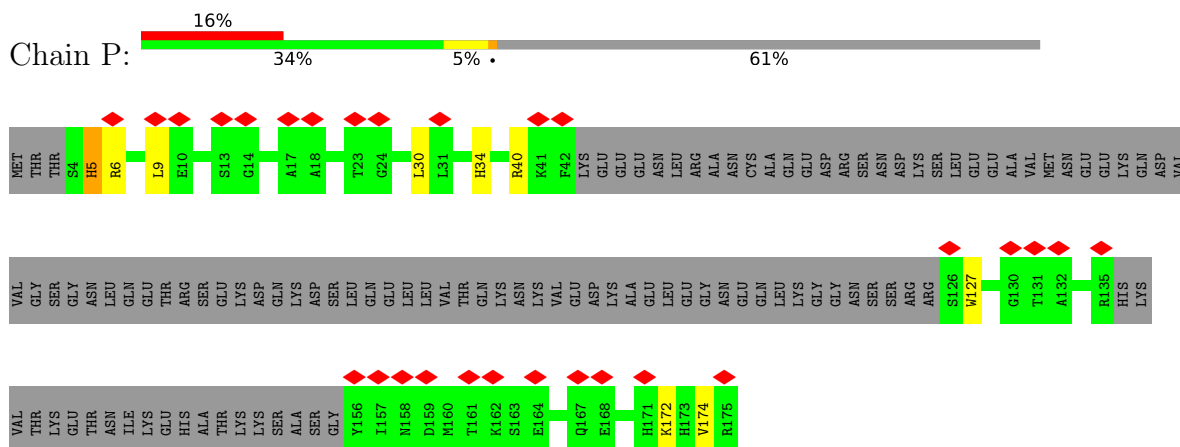


• Molecule 14: Pre-mRNA-splicing factor CEF1

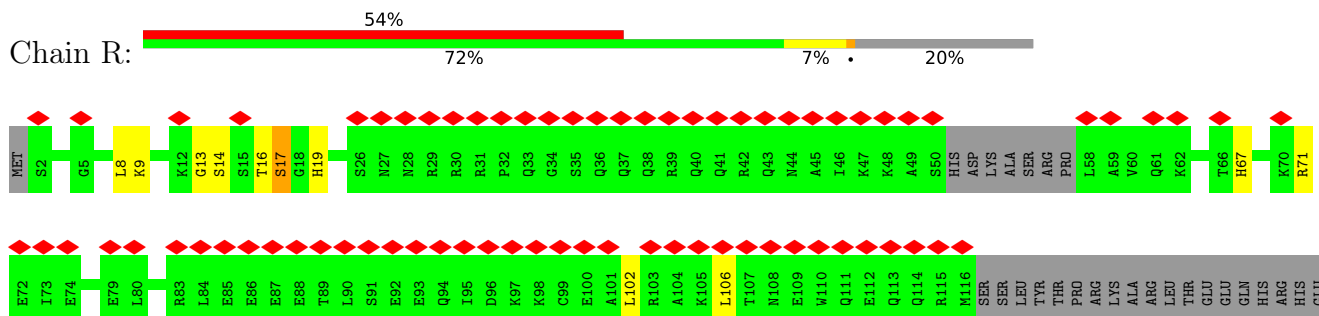




- Molecule 15: Pre-mRNA-splicing factor CWC15

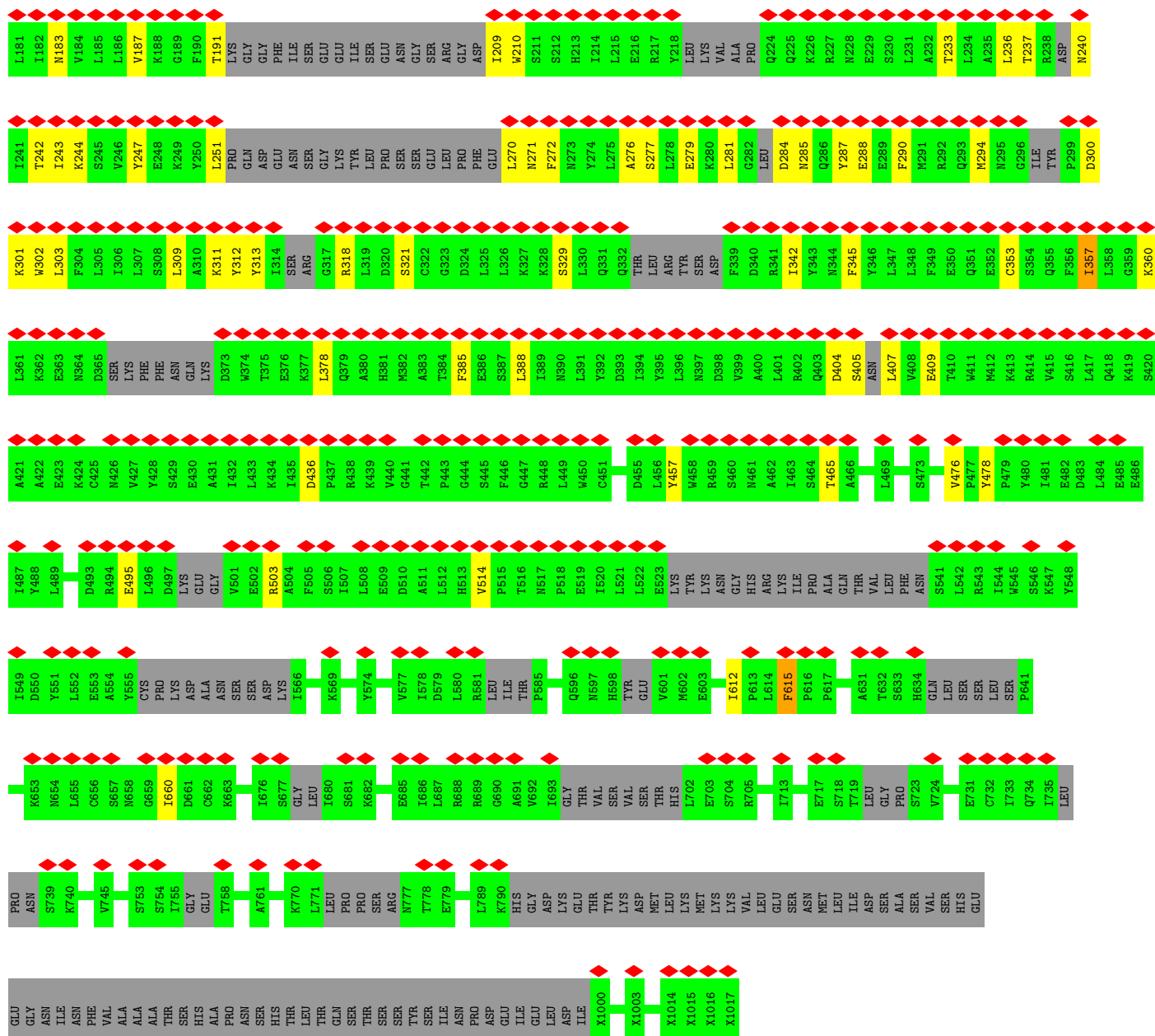


- Molecule 16: Pre-mRNA-splicing factor CWC21

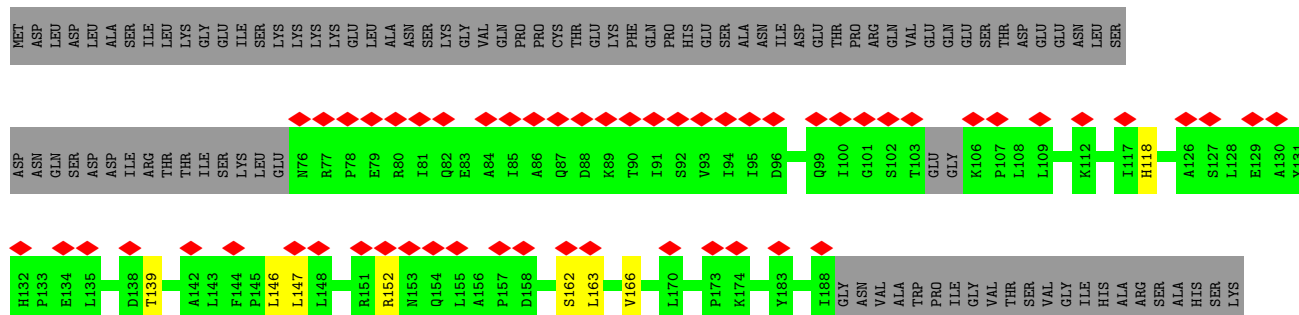


- Molecule 17: Pre-mRNA-splicing factor CLF1

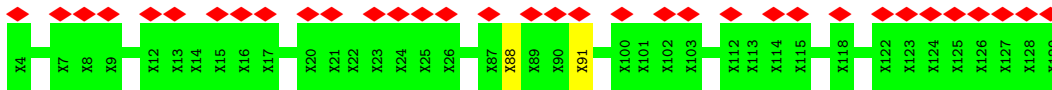




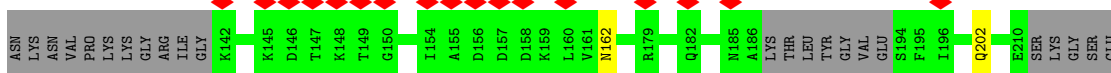
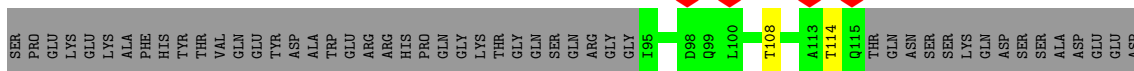
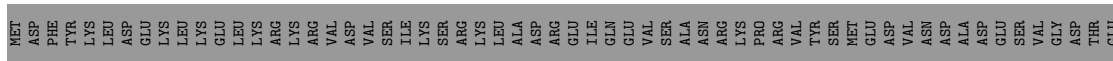
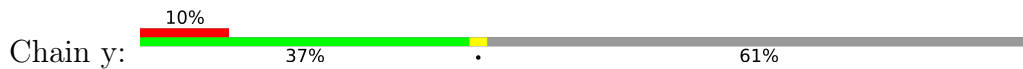
• Molecule 19: Pre-mRNA-splicing factor 18



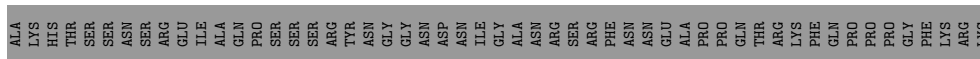
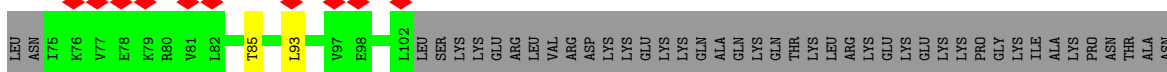
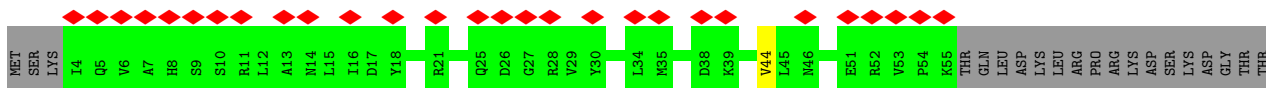
● Molecule 22: UNKNOWN PROTEIN



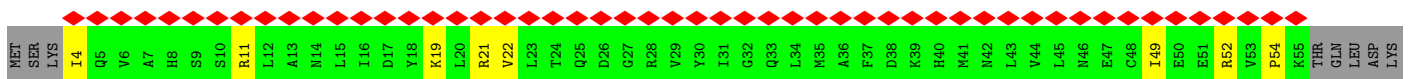
- Molecule 23: Pre-mRNA-splicing factor SYF2



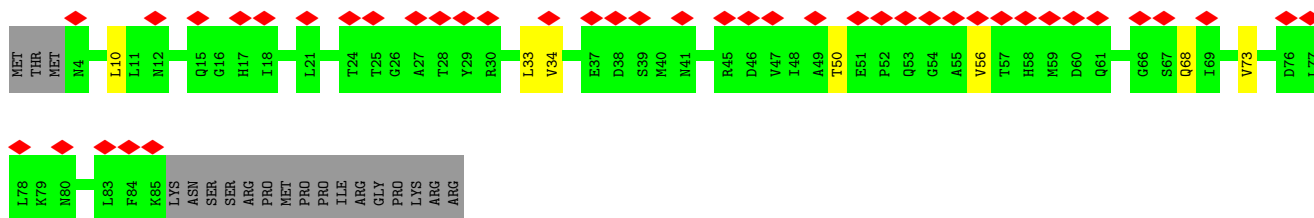
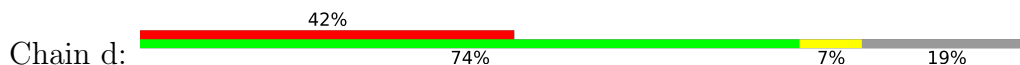
- Molecule 24: Small nuclear ribonucleoprotein-associated protein B



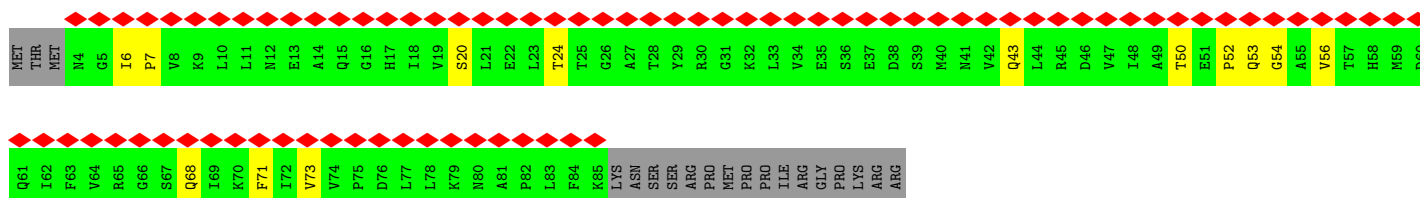
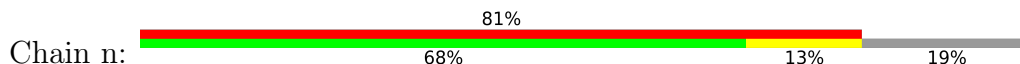
- Molecule 24: Small nuclear ribonucleoprotein-associated protein B



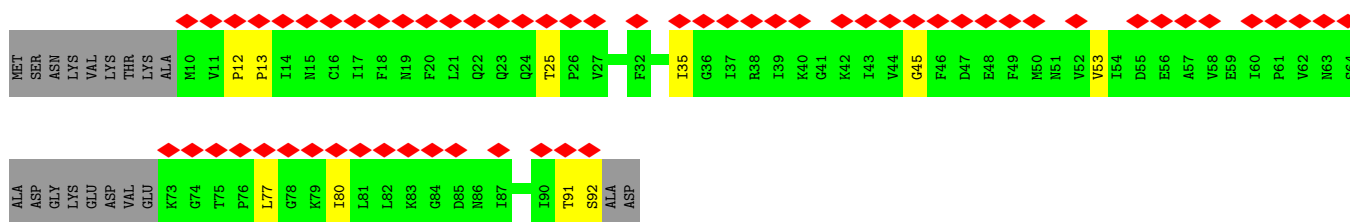
- Molecule 25: Small nuclear ribonucleoprotein Sm D3



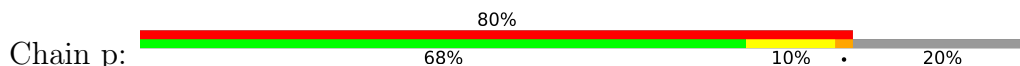
- Molecule 25: Small nuclear ribonucleoprotein Sm D3



- Molecule 26: Small nuclear ribonucleoprotein E

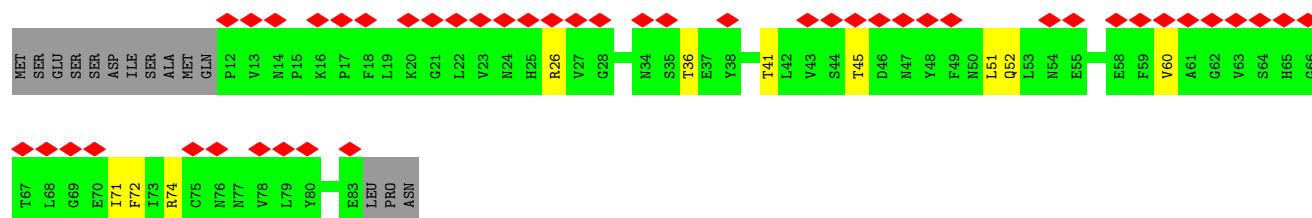


- Molecule 26: Small nuclear ribonucleoprotein E

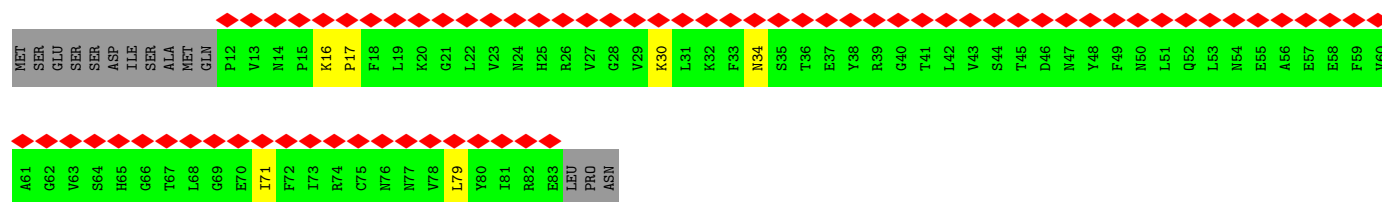
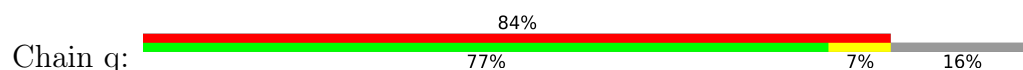




• Molecule 27: Small nuclear ribonucleoprotein F



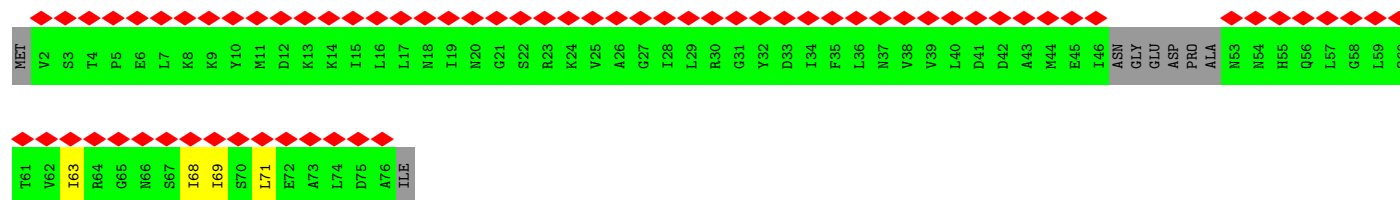
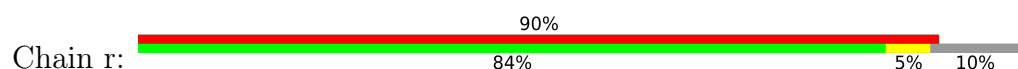
• Molecule 27: Small nuclear ribonucleoprotein F



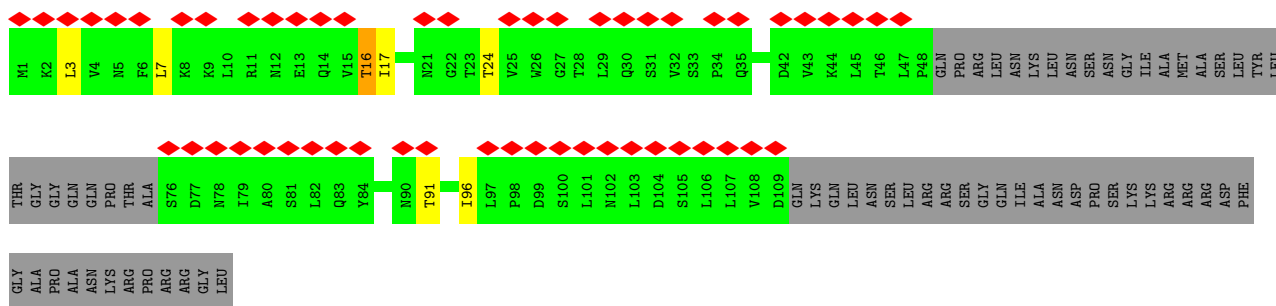
• Molecule 28: Small nuclear ribonucleoprotein G



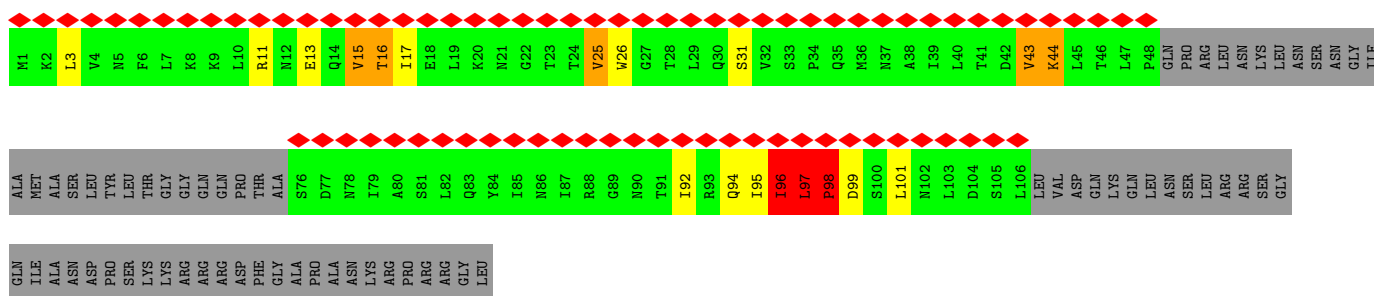
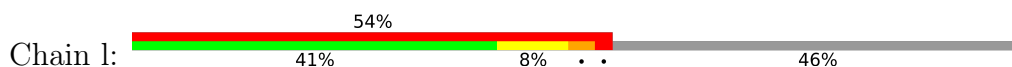
• Molecule 28: Small nuclear ribonucleoprotein G



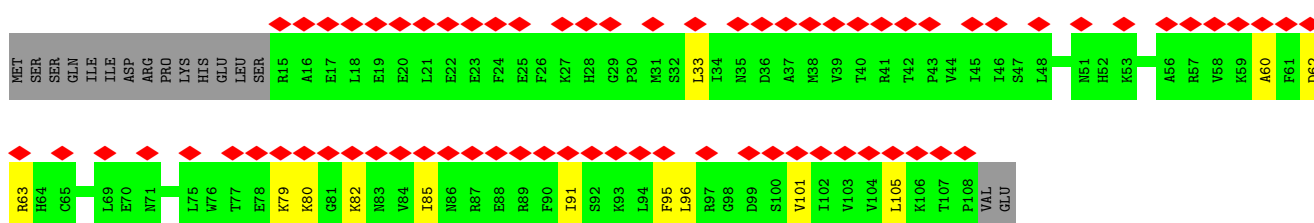
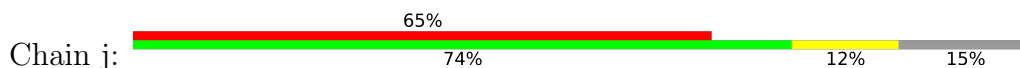
• Molecule 29: Small nuclear ribonucleoprotein Sm D1



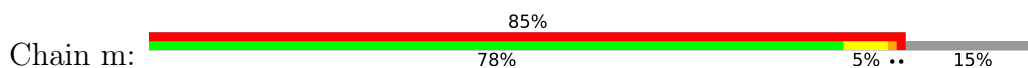
- Molecule 29: Small nuclear ribonucleoprotein Sm D1



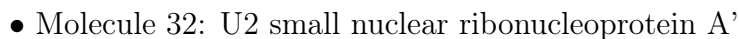
- Molecule 30: Small nuclear ribonucleoprotein Sm D2

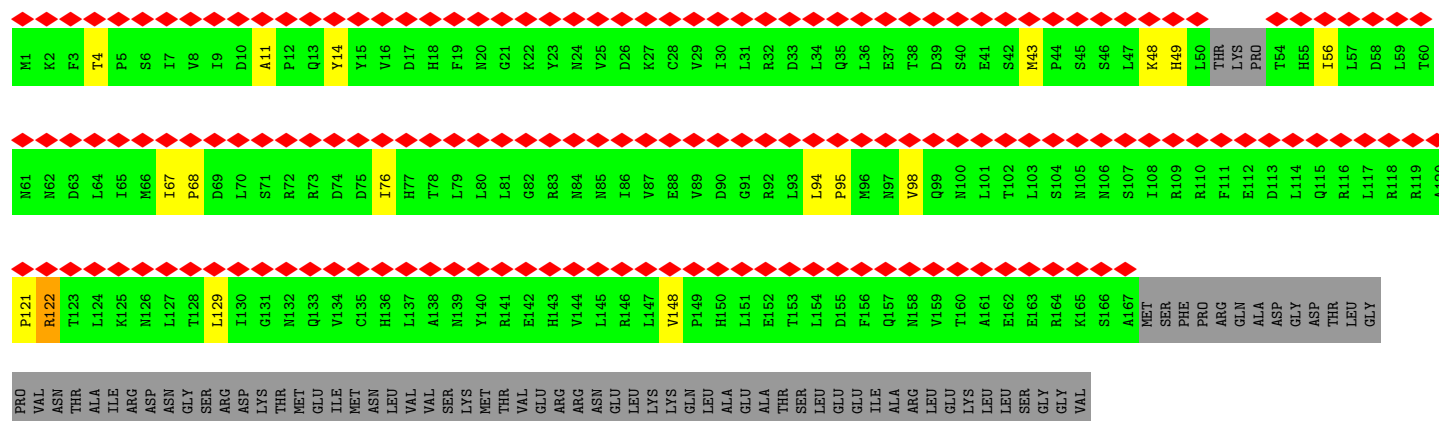


- Molecule 30: Small nuclear ribonucleoprotein Sm D2

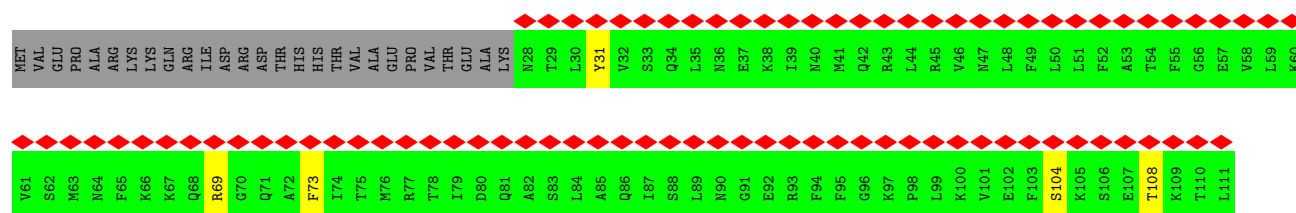
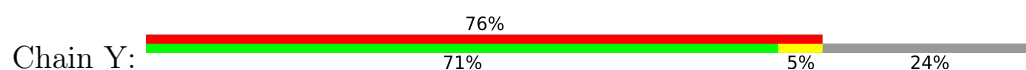


- Molecule 31: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22





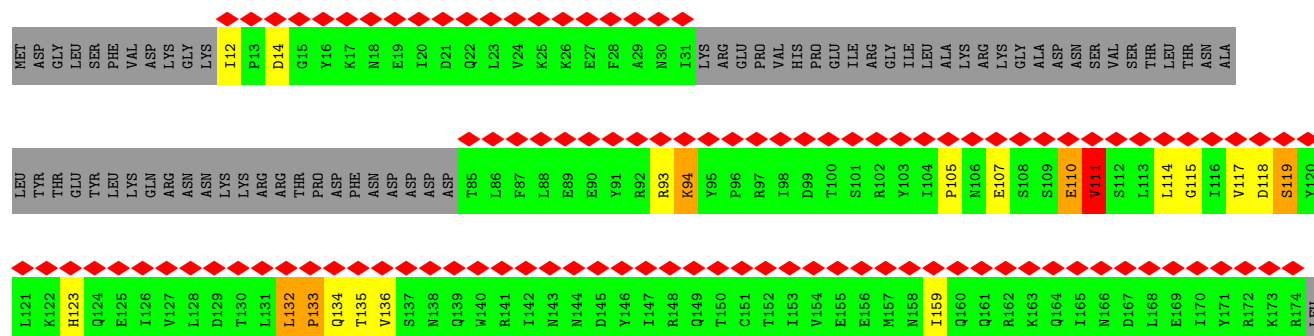
• Molecule 33: U2 small nuclear ribonucleoprotein B''



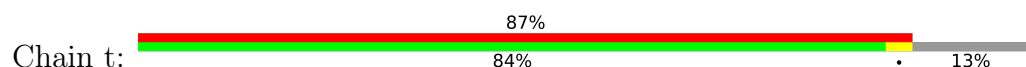
• Molecule 34: 3'-EXON OF UBC4 PRE-MRNA, BOUND BY PRP22 HELICASE

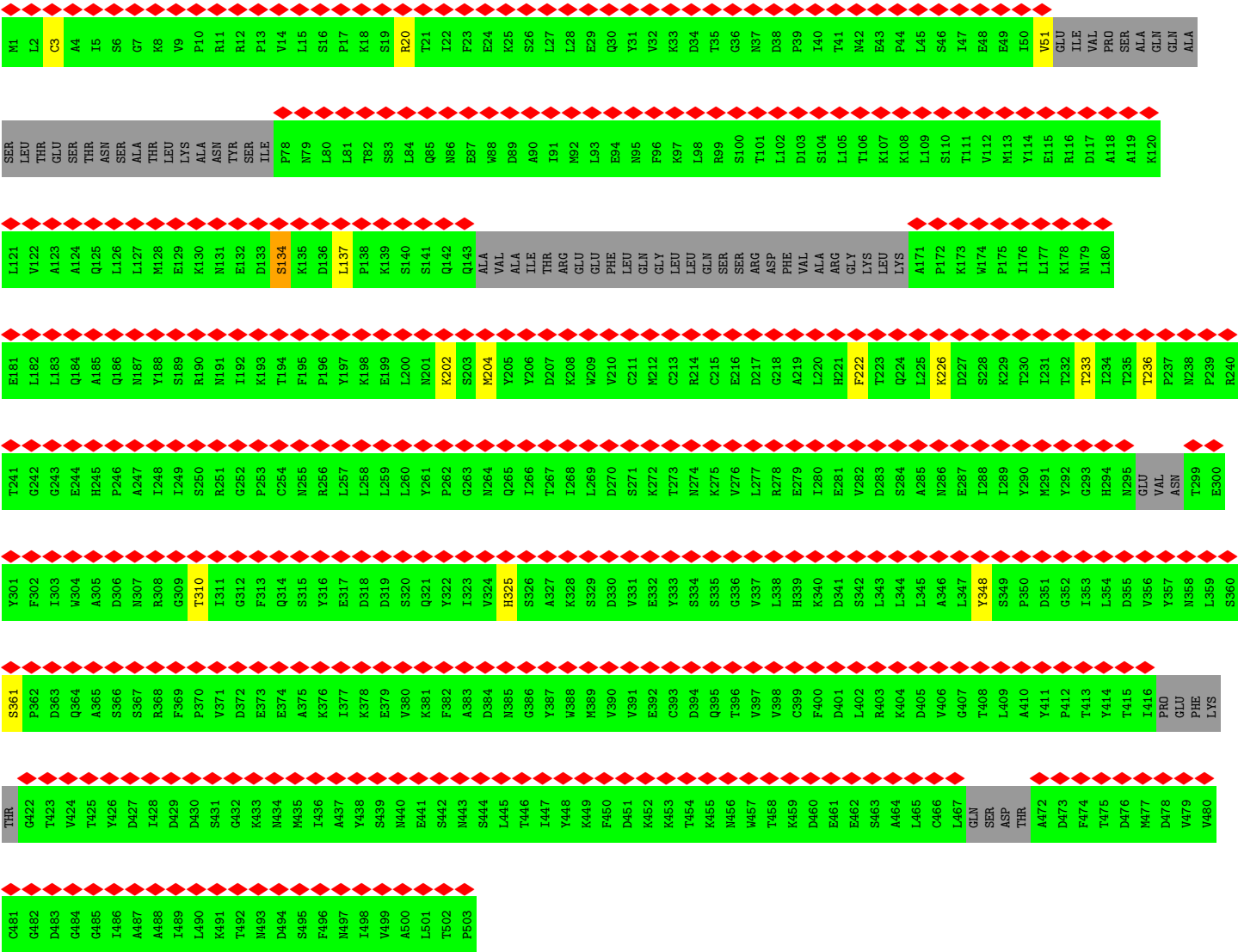


• Molecule 35: Pre-mRNA-splicing factor SNT309

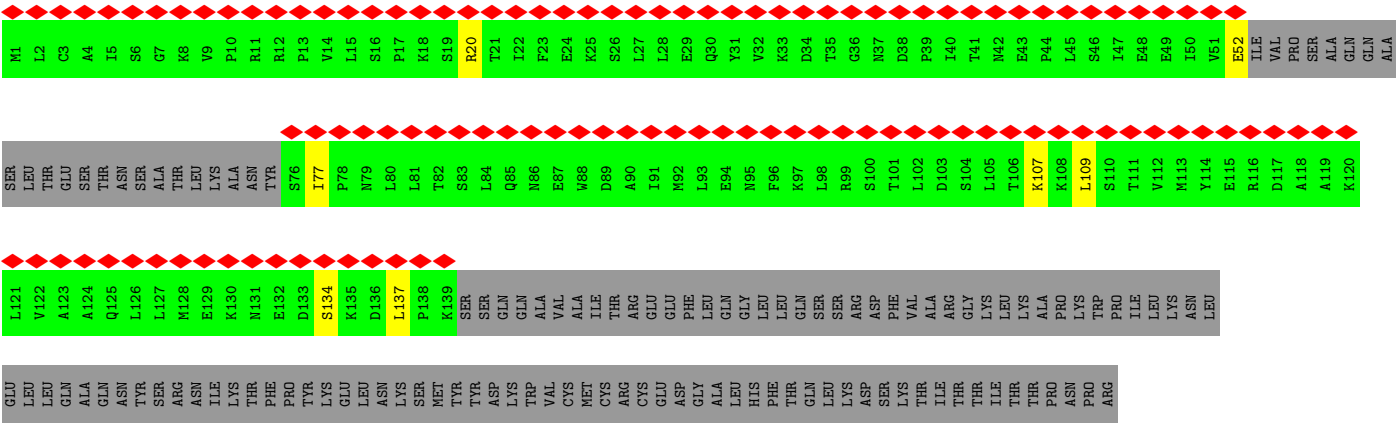


• Molecule 36: Pre-mRNA-processing factor 19





● Molecule 36: Pre-mRNA-processing factor 19



C481	G482	D483	G484	G485	I486	A487	A488	L489	L490	K491	T492	N493	D494	S495	F496	I498	A500	L501	T502	P503																																							
THR	G422	T423	V424	T425	V426	D427	D428	D429	D430	S431	G432	K433	M434	M435	T436	A437	V438	S439	E441	S442	M443	S444	L445	T446	I447	V448	K449	F450	D451	K452	K453	T454	K455	M456	M457	T458	K459	D460	E461	E462	S463	A464	L465	C466	L467	GLN	SER	ASP	THR	A472	D473	F474	T475	D476	M477	D478	V479	V480	
S361	P362	D363	Q364	A365	S366	S367	R368	F369	P370	V371	D372	E373	E374	S375	K376	I377	K378	E379	B380	K381	F382	A383	D384	N385	G386	Y387	W388	N389	V390	V391	E392	C393	D394	Q395	T396	V397	V398	C399	F400	D401	L402	R403	K404	D405	V406	G407	T408	L409	A410	Y411	P412	T413	V414	T415	I416	PRO	GLU	PHE	LYS
Y301	F302	I303	W304	A305	D306	N307	R308	G309	T310	I311	G312	F313	Q314	S315	V316	E317	D318	D319	S320	Q321	Y322	I323	V324	H325	S326	A327	K328	S329	D330	V331	E332	Y333	S334	G335	G336	V337	L338	H339	K340	D341	S342	S342	D343	L344	L345	A346	L347	Y348	S349	P350	D351	G352	I353	L354	D355	V356	Y357	N358	S359
T241	G242	G243	E244	H245	P246	A247	T248	I249	S250	R251	G252	P253	C254	N255	R256	L257	L258	L259	T260	Y261	P262	G263	N264	Q265	T266	T267	L268	L269	D270	S271	K272	T273	N274	K275	V276	L277	R278	E279	T280	E281	V282	D283	S284	A285	N286	E287	T288	L289	Y290	M291	V292	G293	H294	N295	GLU	VAL	ASN	T299	E300
E181	L182	I183	Q184	A185	Q186	N187	Y188	S189	R190	N191	I192	K193	T194	F195	P196	Y197	K198	E199	L200	N201	K202	S203	N204	Y205	Y206	D207	K208	W209	V210	C211	M212	C213	R214	E215	C216	D217	G218	A219	L220	H221	F222	T223	Q224	L225	K226	D227	S228	K229	T230	I231	K178	T232	T233	L234	T235	T236	P237	N238	P239
L121	V122	A123	A124	Q125	L126	L127	M128	E129	K130	N131	E132	D133	S134	K135	D136	L137	P138	K139	SER	SER	GLN	ALA	VAL	ILE	THR	ARG	GLU	PHE	GLU	LEU	GLN	SER	ARG	ASP	PHE	VAL	ALA	ARG	GLY	LYS	LEU	LYS	A171	P172	K173	M174	P175	I176	L177	N179	L180								
SER	LEU	THR	GLU	SER	THR	ASN	SER	THR	LEU	LYS	ALA	ASN	TYR	SER	I77	P78	N79	L80	T81	T82	S83	L84	Q85	N86	E87	W88	D89	I91	M92	L93	E94	N95	F96	K97	L98	R99	S100	T101	L102	D103	S104	L105	T106	K107	K108	L109	T111	M112	M113	Y114	E115	R116	D117	A118	A119	K120			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29527	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)	4500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.03	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, MG, IHP, GTP, K

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	I	0.41	0/795	0.87	3/1231 (0.2%)
2	E	0.40	0/388	0.84	0/603
3	2	0.41	0/3639	0.75	0/5643
4	6	0.41	0/2357	0.83	6/3667 (0.2%)
5	5	0.41	0/3351	0.83	3/5213 (0.1%)
6	A	0.61	5/15598 (0.0%)	1.02	6/21212 (0.0%)
7	C	0.57	1/6703 (0.0%)	0.98	7/9138 (0.1%)
8	H	0.66	0/3314	1.16	3/4463 (0.1%)
9	J	0.61	0/2749	0.86	3/3735 (0.1%)
10	K	0.61	0/1480	1.01	1/2000 (0.1%)
11	L	0.61	0/1186	1.04	0/1606
12	M	0.54	0/2062	0.93	2/2772 (0.1%)
13	N	0.58	0/1823	0.98	0/2456
14	O	0.60	0/1781	1.11	1/2385 (0.0%)
15	P	0.50	0/580	0.82	0/776
16	R	0.57	0/617	1.24	0/848
17	S	0.63	0/3269	1.25	4/4446 (0.1%)
18	T	0.58	0/3036	1.47	12/4197 (0.3%)
19	a	0.55	0/1141	0.87	0/1546
20	c	0.60	1/798 (0.1%)	0.92	1/1074 (0.1%)
21	o	0.57	0/2491	0.82	1/3384 (0.0%)
23	y	0.45	0/681	0.76	0/902
24	b	0.54	0/636	0.75	0/856
24	k	0.56	0/636	0.67	0/856
25	d	0.54	0/634	0.78	0/859
25	n	0.54	0/634	0.76	0/859
26	e	0.68	1/585 (0.2%)	0.84	0/795
26	p	0.61	0/585	0.79	0/795
27	f	0.59	0/585	0.75	0/791
27	q	0.56	0/585	0.83	0/791
28	g	0.70	2/532 (0.4%)	0.80	0/715
28	r	0.54	0/529	0.68	0/711

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	h	0.57	0/649	0.77	0/880
29	l	0.62	0/623	0.88	4/844 (0.5%)
30	j	0.54	0/753	0.80	0/1013
30	m	0.57	0/738	0.87	1/995 (0.1%)
31	V	0.95	4/3186 (0.1%)	2.33	24/4434 (0.5%)
32	W	0.50	0/814	1.18	10/1134 (0.9%)
33	Y	0.49	0/415	1.08	0/577
34	3	0.39	0/65	0.68	0/98
35	s	0.98	1/546 (0.2%)	1.45	11/760 (1.4%)
36	t	0.77	0/2165	1.20	14/3010 (0.5%)
36	u	0.96	1/576 (0.2%)	1.34	3/802 (0.4%)
36	v	1.02	2/586 (0.3%)	1.56	7/816 (0.9%)
36	w	0.76	0/2150	1.12	9/2989 (0.3%)
All	All	0.61	18/79046 (0.0%)	1.09	136/109677 (0.1%)

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
7	C	0	1
9	J	0	1
15	P	0	1
21	o	0	1
24	k	0	1
31	V	0	3
35	s	0	2
36	t	0	2
36	v	0	1
36	w	0	1
All	All	0	14

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	1009	LEU	C-N	12.59	1.50	1.33
31	V	834	THR	C-N	-10.13	1.22	1.33
36	v	109	LEU	C-N	8.04	1.44	1.33
31	V	1112	ALA	C-O	7.39	1.32	1.24
31	V	1112	ALA	CA-C	-6.99	1.44	1.52

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	V	834	THR	CA-C-N	-63.26	5.11	122.13
31	V	834	THR	C-N-CA	-63.26	5.11	122.13
31	V	1009	LEU	O-C-N	37.73	166.52	123.13
31	V	1009	LEU	CA-C-N	-33.31	74.32	120.95
31	V	1009	LEU	C-N-CA	-33.31	74.32	120.95

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	C	105	ILE	Peptide
9	J	194	HIS	Peptide
15	P	5	HIS	Peptide
31	V	659	THR	Mainchain
21	o	239	LYS	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	I	714	0	361	6	0
2	E	346	0	173	11	0
3	2	3271	0	1660	57	0
4	6	2108	0	1063	27	0
5	5	2999	0	1515	35	0
6	A	15199	0	14954	277	0
7	C	6562	0	6486	109	0
8	H	3261	0	3323	95	0
9	J	2690	0	2690	89	0
10	K	1458	0	1468	24	0
11	L	1162	0	1111	19	0
12	M	2016	0	1985	34	0
13	N	1798	0	1842	40	0
14	O	1755	0	1794	30	0
15	P	565	0	555	7	0
16	R	614	0	390	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	S	3229	0	2573	43	0
18	T	3154	0	1331	95	0
19	a	1119	0	1164	10	0
20	c	786	0	719	9	0
21	o	2425	0	2253	41	0
22	X	338	0	70	1	0
23	y	679	0	706	4	0
24	b	631	0	670	3	0
24	k	631	0	665	33	0
25	d	625	0	647	5	0
25	n	625	0	647	15	0
26	e	575	0	597	8	0
26	p	575	0	597	4	0
27	f	573	0	572	7	0
27	q	573	0	572	2	0
28	g	529	0	557	10	0
28	r	526	0	555	2	0
29	h	644	0	686	10	0
29	l	618	0	660	44	0
30	j	741	0	778	16	0
30	m	726	0	754	5	0
31	V	3189	0	1412	13	0
32	W	816	0	340	8	0
33	Y	416	0	182	14	0
34	3	60	0	31	10	0
35	s	548	0	219	17	0
36	t	2171	0	945	4	0
36	u	578	0	246	3	0
36	v	588	0	250	12	0
36	w	2156	0	938	3	0
37	6	3	0	0	0	0
38	6	2	0	0	0	0
39	A	36	0	6	1	0
40	C	32	0	12	0	0
41	L	3	0	0	0	0
41	M	1	0	0	0	0
41	N	2	0	0	0	0
All	All	77441	0	63724	1112	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 8.

The worst 5 of 1112 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)
18:T:119:ALA:HB2	18:T:131:ALA:CB	1.25	1.63
18:T:119:ALA:CB	18:T:131:ALA:HB3	1.40	1.48
18:T:237:THR:N	18:T:240:ASN:N	1.73	1.34
18:T:300:ASP:CB	18:T:303:LEU:CB	2.06	1.33
18:T:119:ALA:HB1	18:T:128:ILE:CA	1.58	1.33

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	
6	A	1906/2413 (79%)	1733 (91%)	161 (8%)	12 (1%)	21	58
7	C	864/1008 (86%)	771 (89%)	87 (10%)	6 (1%)	18	55
8	H	393/577 (68%)	353 (90%)	36 (9%)	4 (1%)	12	47
9	J	340/451 (75%)	295 (87%)	39 (12%)	6 (2%)	6	34
10	K	183/379 (48%)	163 (89%)	17 (9%)	3 (2%)	7	37
11	L	153/157 (98%)	136 (89%)	16 (10%)	1 (1%)	18	55
12	M	250/339 (74%)	236 (94%)	12 (5%)	2 (1%)	16	52
13	N	217/364 (60%)	191 (88%)	22 (10%)	4 (2%)	6	34
14	O	207/590 (35%)	193 (93%)	11 (5%)	3 (1%)	9	39
15	P	63/175 (36%)	56 (89%)	7 (11%)	0	100	100
16	R	104/135 (77%)	91 (88%)	12 (12%)	1 (1%)	12	47
17	S	438/687 (64%)	415 (95%)	20 (5%)	3 (1%)	18	55
18	T	557/877 (64%)	532 (96%)	22 (4%)	3 (0%)	24	62
19	a	131/251 (52%)	123 (94%)	8 (6%)	0	100	100
20	c	97/382 (25%)	87 (90%)	8 (8%)	2 (2%)	5	30
21	o	305/455 (67%)	251 (82%)	46 (15%)	8 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	y	77/215 (36%)	76 (99%)	1 (1%)	0	100	100
24	b	76/196 (39%)	74 (97%)	2 (3%)	0	100	100
24	k	76/196 (39%)	68 (90%)	7 (9%)	1 (1%)	9	41
25	d	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
25	n	80/101 (79%)	74 (92%)	6 (8%)	0	100	100
26	e	71/94 (76%)	62 (87%)	9 (13%)	0	100	100
26	p	71/94 (76%)	66 (93%)	4 (6%)	1 (1%)	9	39
27	f	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
27	q	70/86 (81%)	65 (93%)	5 (7%)	0	100	100
28	g	65/77 (84%)	63 (97%)	2 (3%)	0	100	100
28	r	65/77 (84%)	57 (88%)	8 (12%)	0	100	100
29	h	78/146 (53%)	71 (91%)	7 (9%)	0	100	100
29	l	75/146 (51%)	65 (87%)	8 (11%)	2 (3%)	4	26
30	j	92/110 (84%)	83 (90%)	9 (10%)	0	100	100
30	m	91/110 (83%)	84 (92%)	7 (8%)	0	100	100
31	V	639/1145 (56%)	602 (94%)	34 (5%)	3 (0%)	24	62
32	W	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	1	16
33	Y	82/111 (74%)	76 (93%)	6 (7%)	0	100	100
35	s	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	1	15
36	t	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
36	u	112/503 (22%)	104 (93%)	8 (7%)	0	100	100
36	v	114/503 (23%)	108 (95%)	3 (3%)	3 (3%)	4	26
36	w	423/503 (84%)	414 (98%)	7 (2%)	2 (0%)	24	62
All	All	9407/14756 (64%)	8598 (91%)	725 (8%)	84 (1%)	16	49

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	487	ASN
6	A	742	VAL
6	A	1620	TYR
7	C	568	SER
7	C	901	GLU

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	1577/2182 (72%)	1551 (98%)	26 (2%)	55	68
7	C	681/910 (75%)	664 (98%)	17 (2%)	42	62
8	H	366/538 (68%)	356 (97%)	10 (3%)	39	60
9	J	299/397 (75%)	280 (94%)	19 (6%)	16	39
10	K	159/328 (48%)	153 (96%)	6 (4%)	29	51
11	L	112/141 (79%)	106 (95%)	6 (5%)	20	43
12	M	214/296 (72%)	209 (98%)	5 (2%)	44	64
13	N	211/332 (64%)	207 (98%)	4 (2%)	50	66
14	O	187/525 (36%)	180 (96%)	7 (4%)	30	52
15	P	56/151 (37%)	53 (95%)	3 (5%)	20	43
16	R	25/121 (21%)	24 (96%)	1 (4%)	28	50
17	S	230/633 (36%)	223 (97%)	7 (3%)	36	57
18	T	1/786 (0%)	1 (100%)	0	100	100
19	a	125/225 (56%)	124 (99%)	1 (1%)	73	77
20	c	71/346 (20%)	70 (99%)	1 (1%)	59	70
21	o	256/413 (62%)	247 (96%)	9 (4%)	32	54
23	y	76/193 (39%)	75 (99%)	1 (1%)	61	71
24	b	70/176 (40%)	70 (100%)	0	100	100
24	k	70/176 (40%)	69 (99%)	1 (1%)	59	70
25	d	69/89 (78%)	69 (100%)	0	100	100
25	n	69/89 (78%)	67 (97%)	2 (3%)	37	58
26	e	65/83 (78%)	63 (97%)	2 (3%)	35	56
26	p	65/83 (78%)	60 (92%)	5 (8%)	12	33
27	f	63/77 (82%)	63 (100%)	0	100	100
27	q	63/77 (82%)	60 (95%)	3 (5%)	23	46
28	g	58/66 (88%)	57 (98%)	1 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	r	57/66 (86%)	56 (98%)	1 (2%)	51 66
29	h	77/129 (60%)	76 (99%)	1 (1%)	61 71
29	l	73/129 (57%)	63 (86%)	10 (14%)	3 16
30	j	79/103 (77%)	79 (100%)	0	100 100
30	m	77/103 (75%)	73 (95%)	4 (5%)	21 44
All	All	5601/9963 (56%)	5448 (97%)	153 (3%)	40 60

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	o	177	LEU
25	n	43	GLN
21	o	356	MET
29	l	16	THR
27	q	30	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
12	M	31	ASN
19	a	177	ASN
13	N	254	GLN
17	S	79	HIS
21	o	261	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	32/95 (33%)	14 (43%)	4 (12%)
2	E	15/20 (75%)	5 (33%)	1 (6%)
3	2	146/1175 (12%)	49 (33%)	5 (3%)
34	3	2/3 (66%)	2 (100%)	0
4	6	98/112 (87%)	37 (37%)	3 (3%)
5	5	138/179 (77%)	61 (44%)	3 (2%)
All	All	431/1584 (27%)	168 (38%)	16 (3%)

5 of 168 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	2	U
1	I	3	A
1	I	4	U
1	I	10	A
1	I	11	A

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	5	39	U
5	5	27	G
3	2	1124	U
4	6	92	C
3	2	1123	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
40	GTP	C	1101	-	33,34,34	1.10	4 (12%)	50,54,54	1.78	9 (18%)
39	IHP	A	3001	-	36,36,36	0.71	0	60,60,60	1.07	4 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	GTP	C	1101	-	-	7/22/38/38	0/3/3/3
39	IHP	A	3001	-	-	0/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	C	1101	GTP	C5-C4	2.85	1.46	1.38
40	C	1101	GTP	C5-N7	-2.60	1.33	1.39
40	C	1101	GTP	C4-N9	-2.15	1.32	1.38
40	C	1101	GTP	C6-N1	-2.12	1.34	1.38

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	C	1101	GTP	C5-C4-N3	-5.53	119.59	128.39
40	C	1101	GTP	C2-N3-C4	4.96	120.85	112.30
40	C	1101	GTP	N9-C4-N3	3.87	133.69	125.95
40	C	1101	GTP	C6-C5-N7	3.47	136.61	130.29
39	A	3001	IHP	C3-C2-C1	2.85	116.69	110.43

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	C	1101	GTP	C5'-O5'-PA-O1A
40	C	1101	GTP	O4'-C4'-C5'-O5'
40	C	1101	GTP	C3'-C4'-C5'-O5'
40	C	1101	GTP	C4'-C5'-O5'-PA
40	C	1101	GTP	PB-O3A-PA-O2A

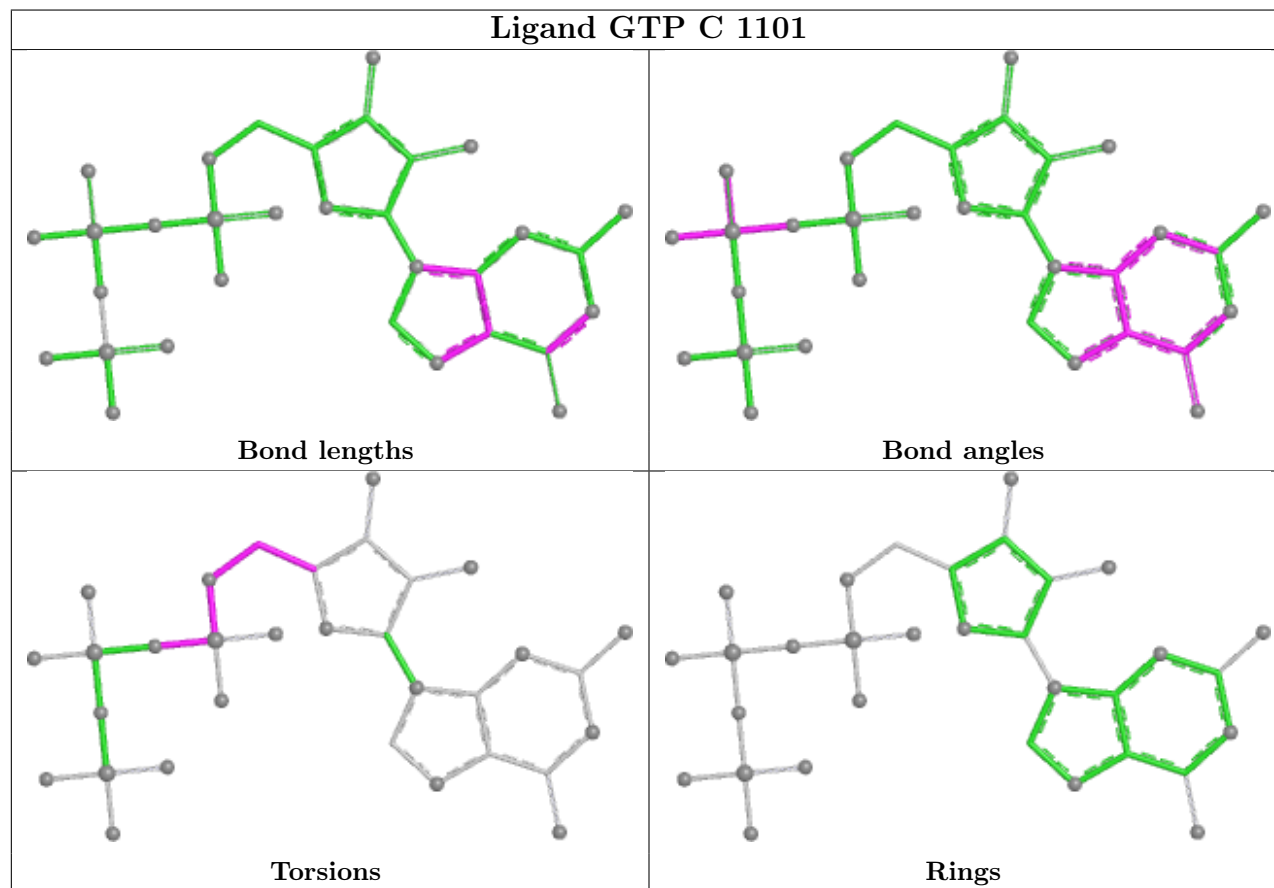
There are no ring outliers.

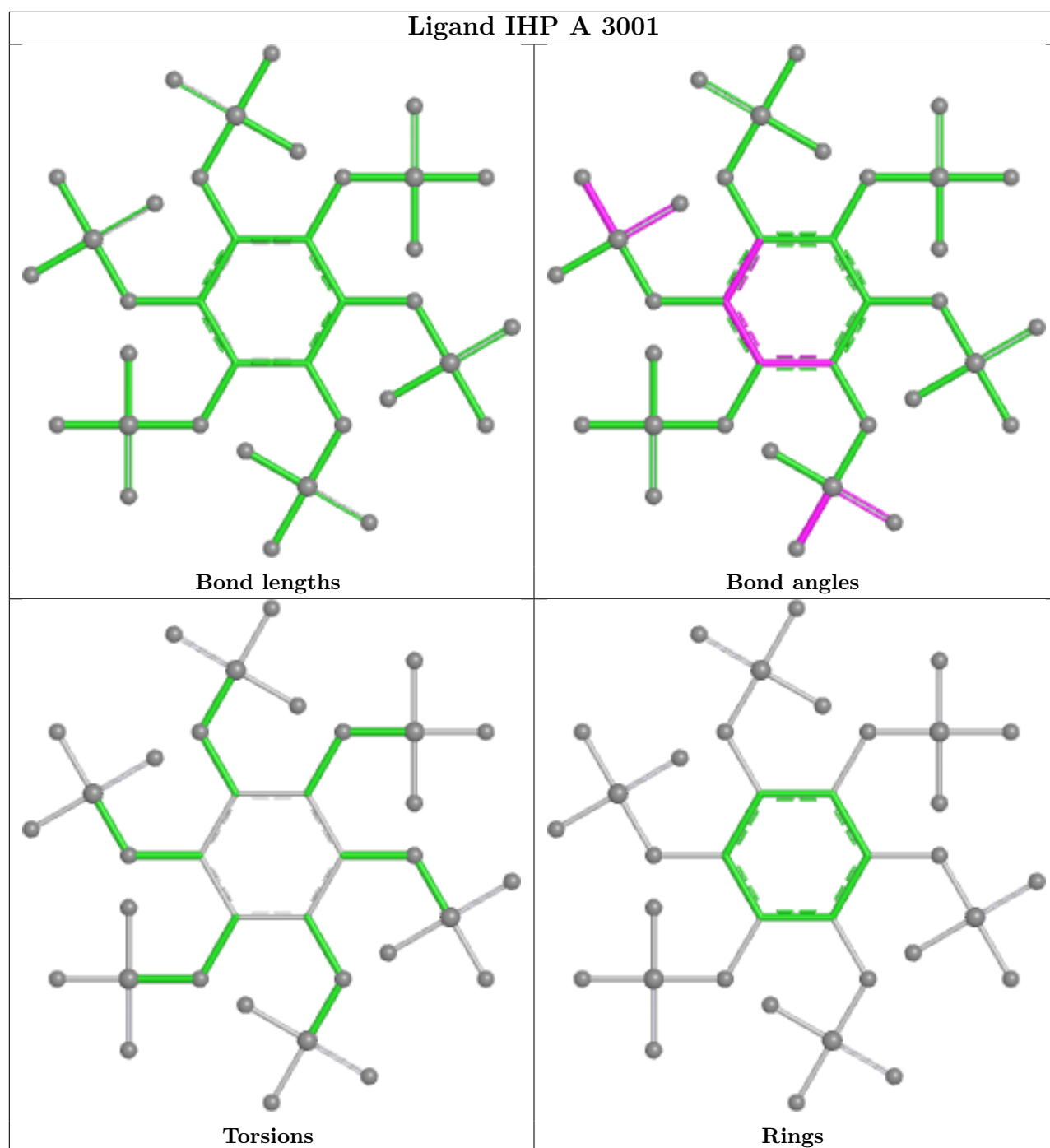
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	A	3001	IHP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	X	1
31	V	1
18	T	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	27:UNK	C	86:UNK	N	8.48
1	V	903:MET	C	904:ASP	N	2.35
1	T	300:ASP	C	301:LYS	N	2.16

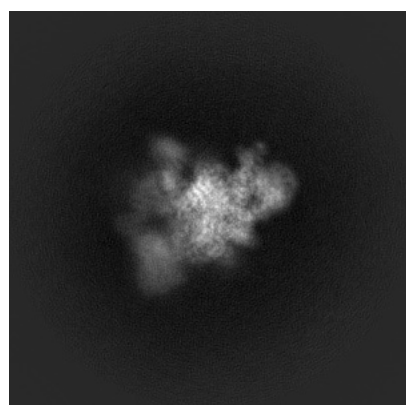
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3541. These allow visual inspection of the internal detail of the map and identification of artifacts.

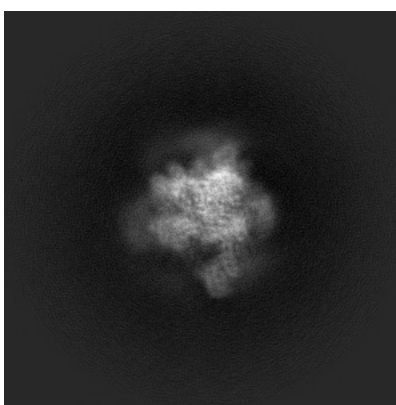
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

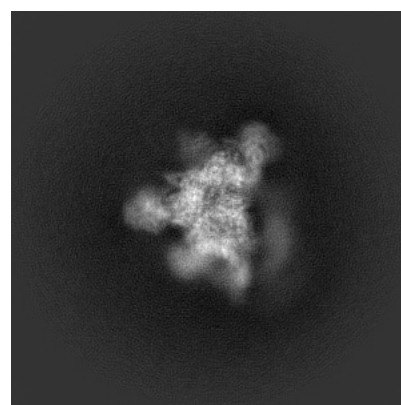
6.1.1 Primary map



X



Y

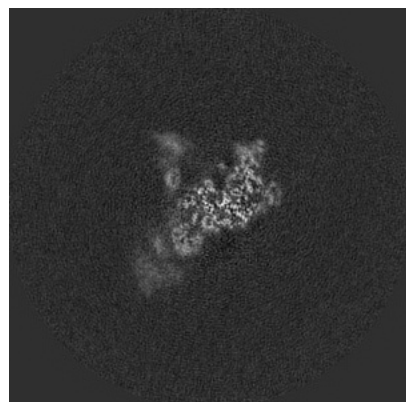


Z

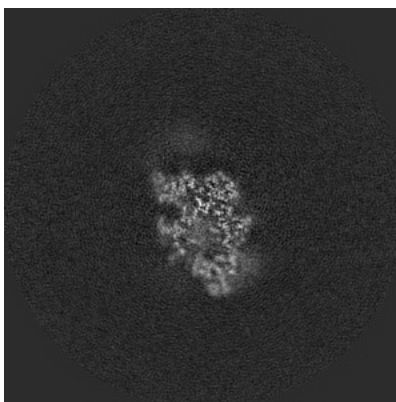
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

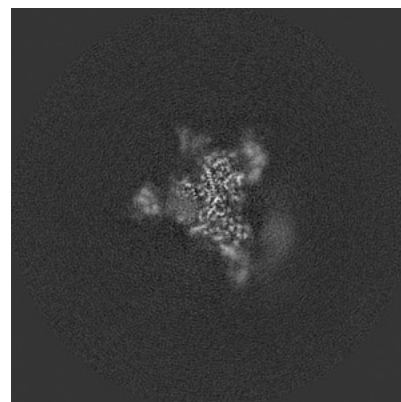
6.2.1 Primary map



X Index: 206



Y Index: 206

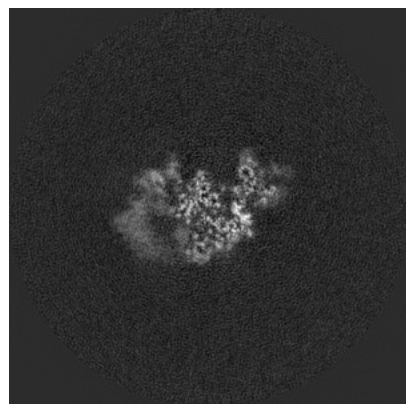


Z Index: 206

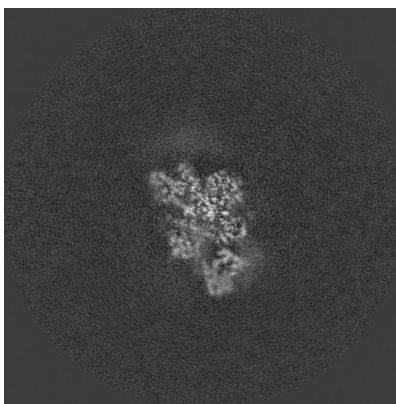
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

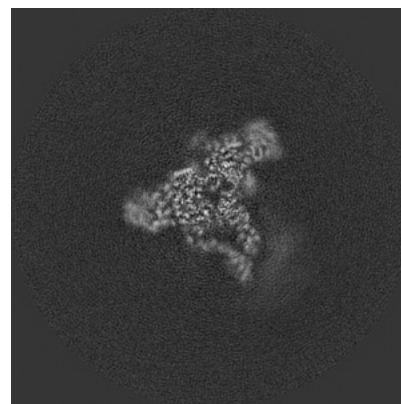
6.3.1 Primary map



X Index: 234



Y Index: 201

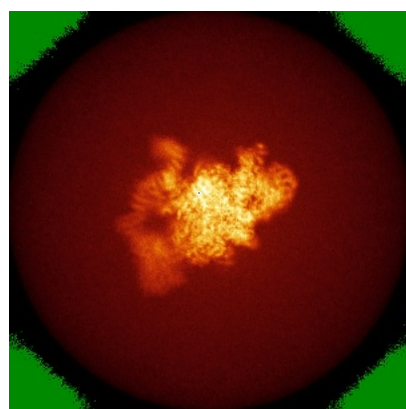


Z Index: 227

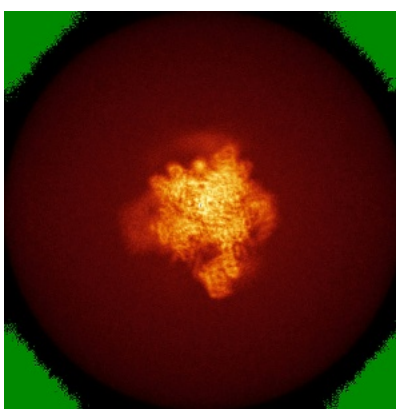
The images above show the largest variance slices of the map in three orthogonal directions.

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

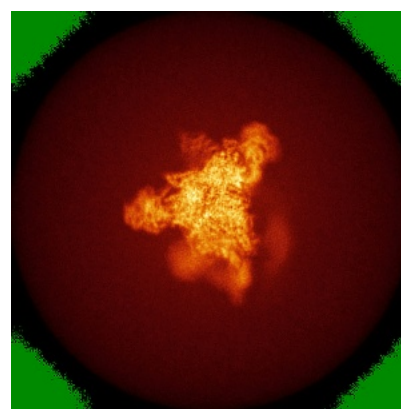
6.4.1 Primary map



X



Y

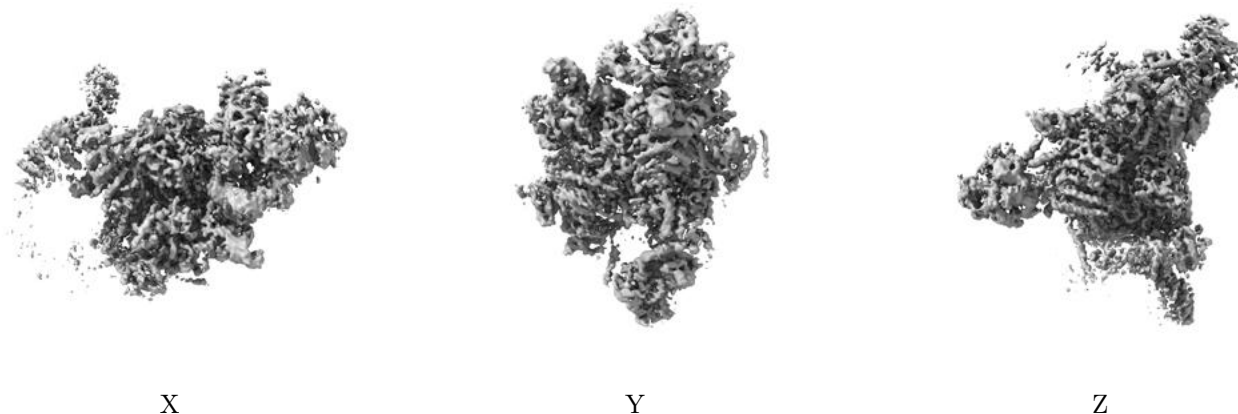


Z

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

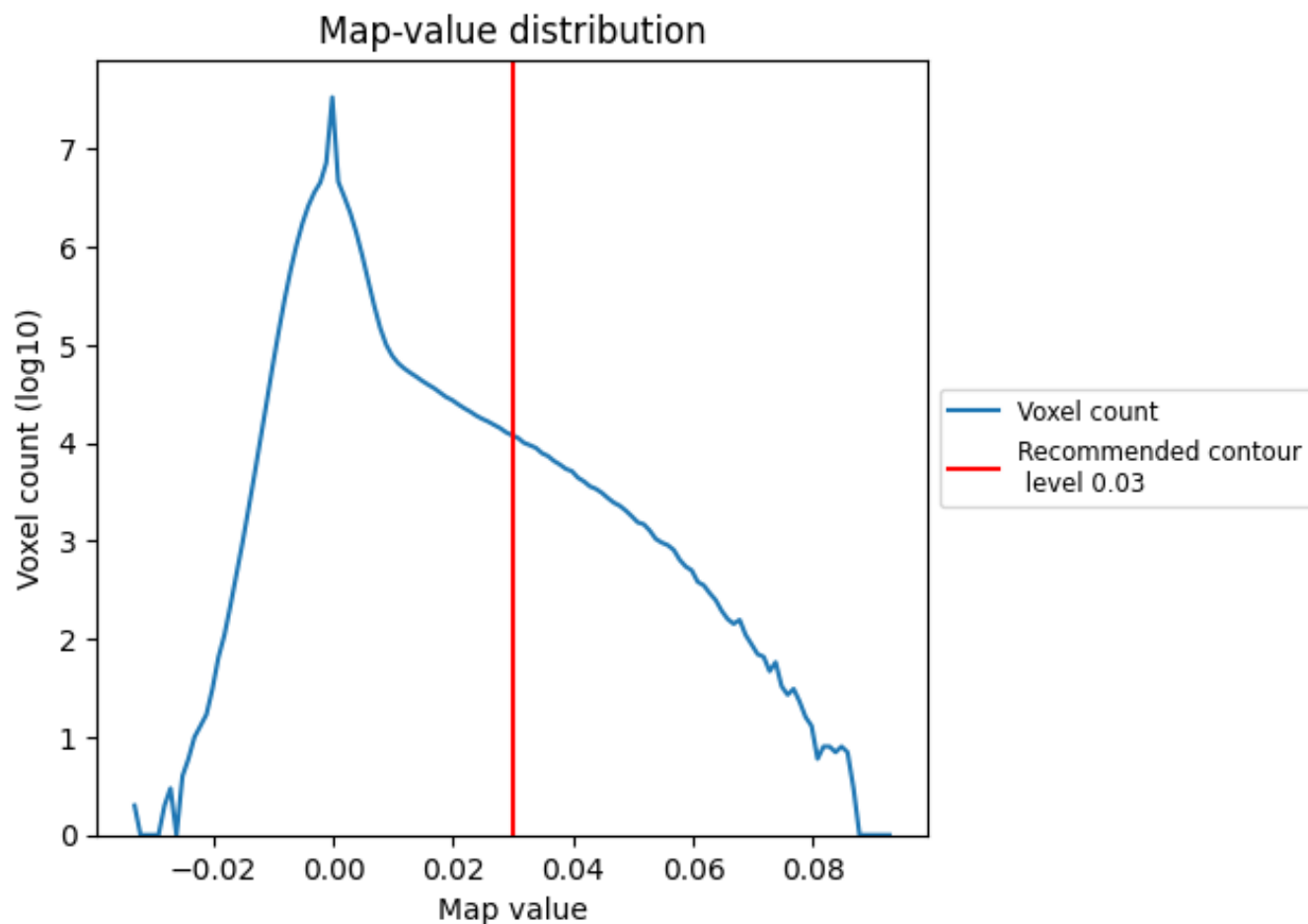
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

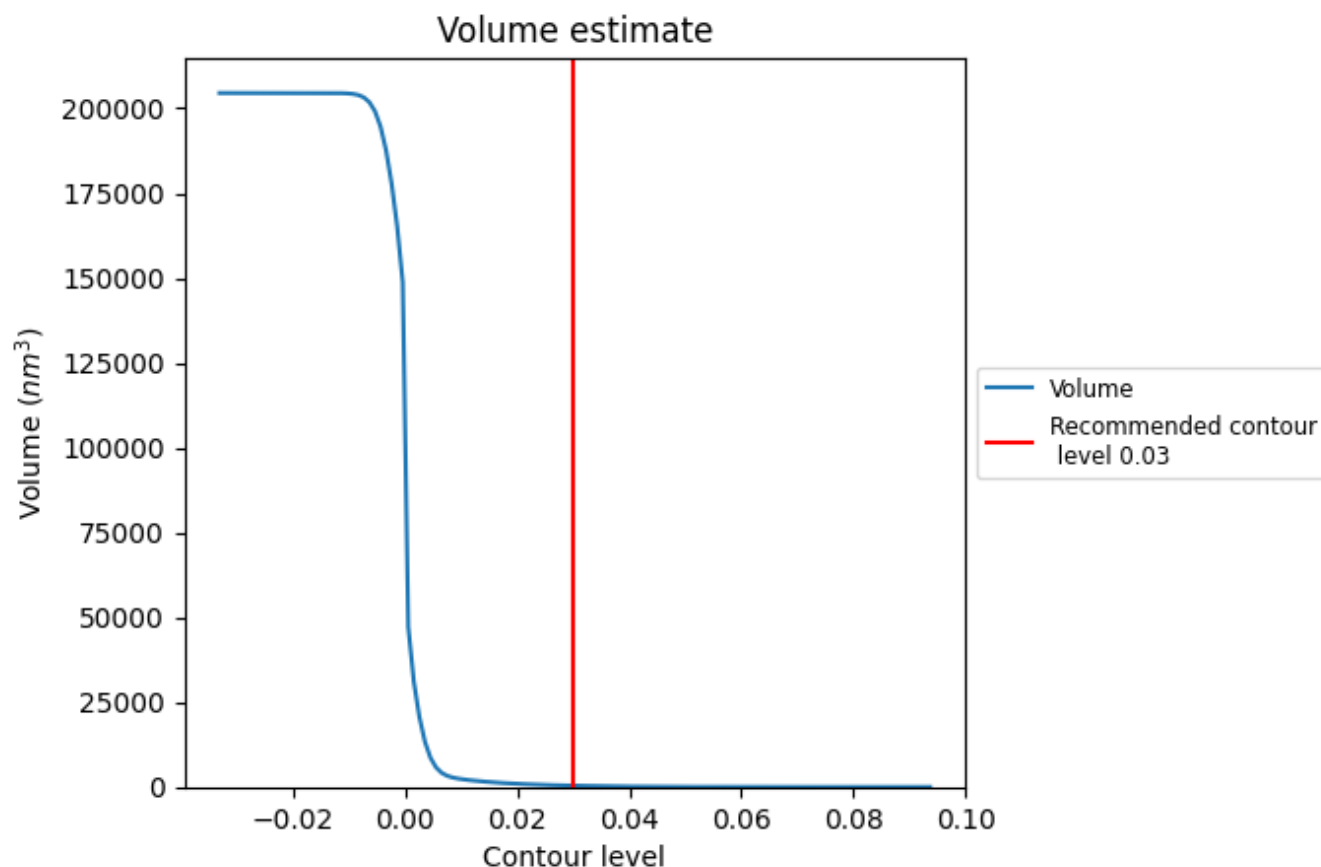
This section contains the results of statistical analysis of the map.

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.

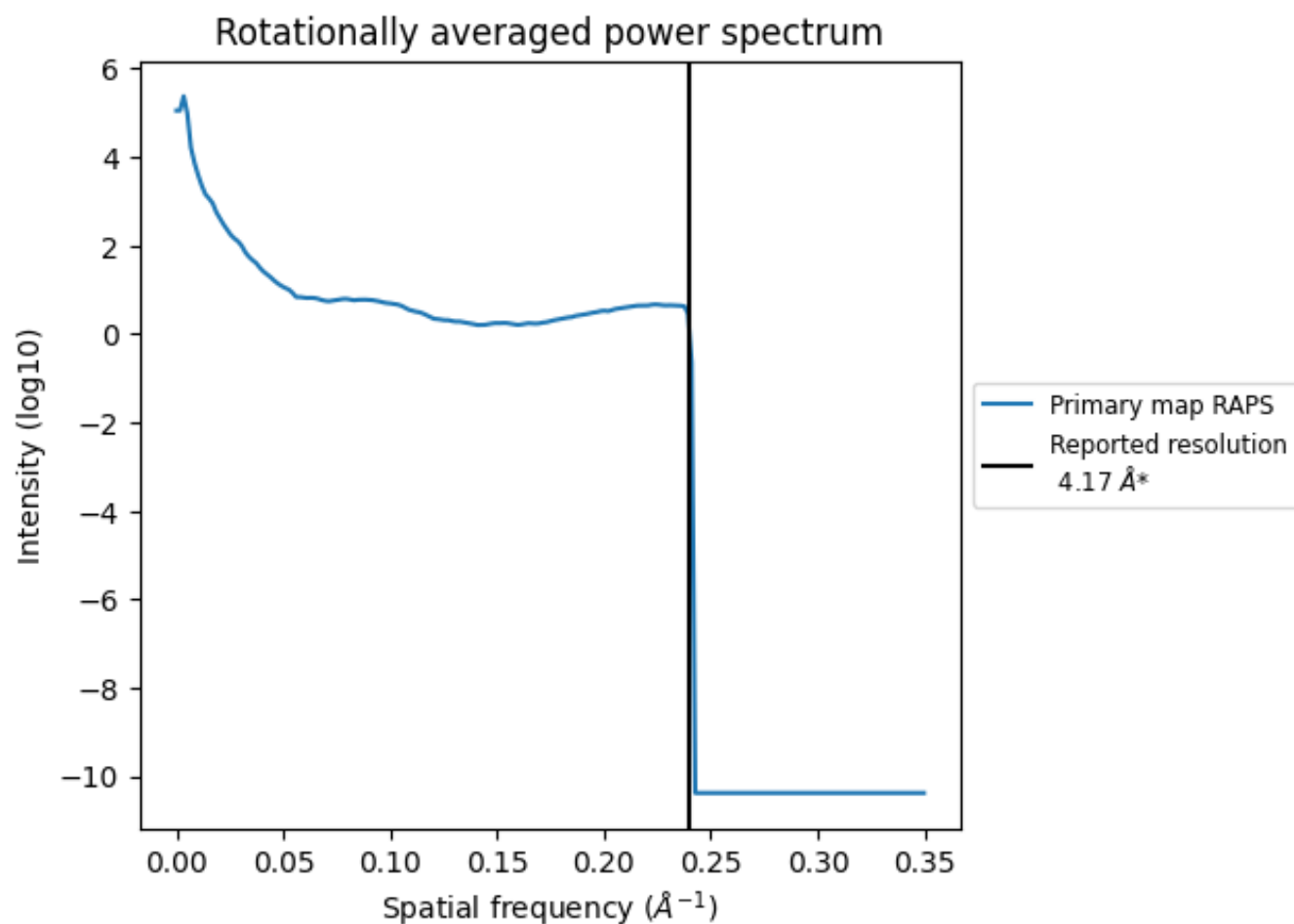
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 380 nm^3 ; this corresponds to an approximate mass of 344 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 0.240 Å⁻¹

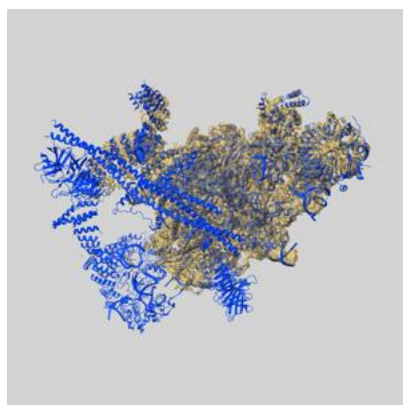
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

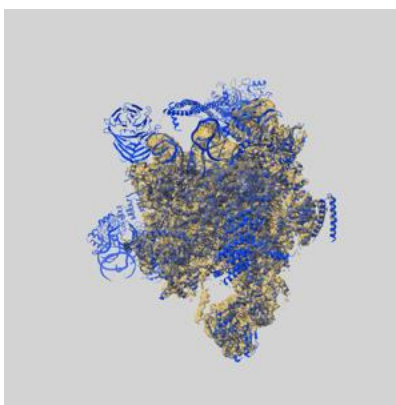
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3541 and PDB model 5MQ0. Per-residue inclusion information can be found in section 3 on page 13.

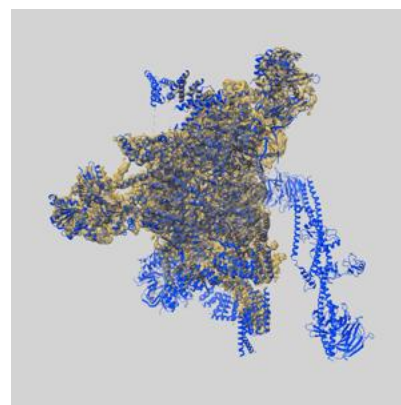
9.1 Map-model overlay [i](#)



X



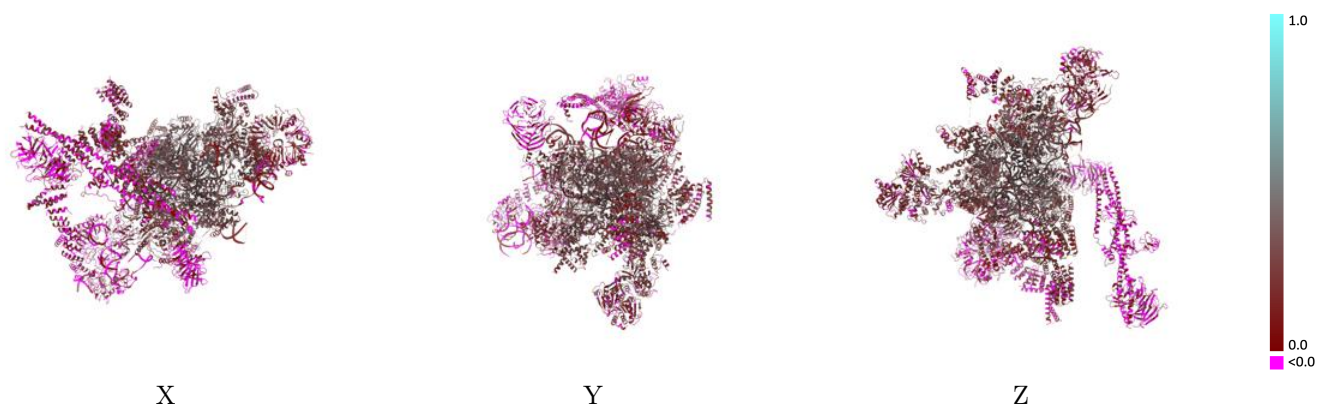
Y



Z

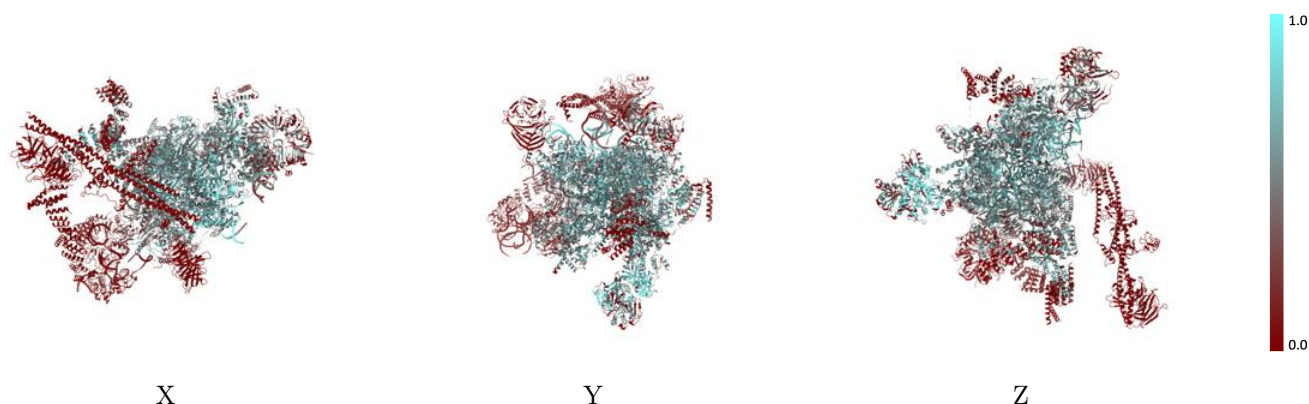
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



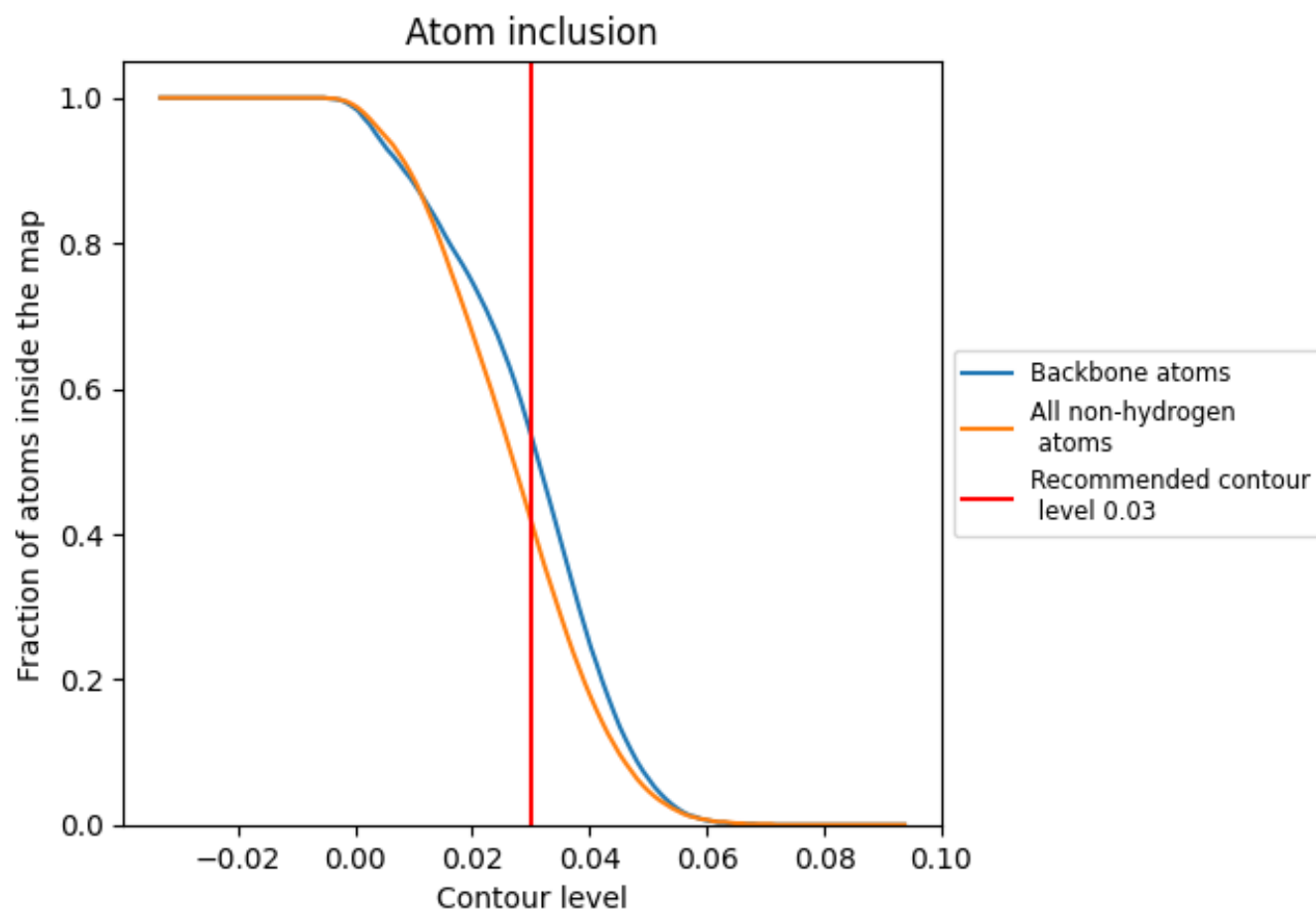
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 42% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4180	 0.2230
2	 0.1850	 0.0890
3	 0.7670	 0.3180
5	 0.6970	 0.2510
6	 0.7630	 0.3180
A	 0.5870	 0.3250
C	 0.5690	 0.3100
E	 0.5950	 0.2930
H	 0.3110	 0.2080
I	 0.5480	 0.2360
J	 0.5830	 0.3480
K	 0.4440	 0.2970
L	 0.6600	 0.3130
M	 0.5570	 0.2870
N	 0.4920	 0.2600
O	 0.5110	 0.2880
P	 0.5000	 0.3400
R	 0.2910	 0.2440
S	 0.4310	 0.2260
T	 0.2500	 0.1360
V	 0.5410	 0.1740
W	 0.0000	 0.0460
X	 0.4820	 0.2650
Y	 0.0000	 0.0360
a	 0.4140	 0.2210
b	 0.3810	 0.2090
c	 0.4480	 0.2410
d	 0.3900	 0.2450
e	 0.2100	 0.1450
f	 0.2990	 0.1120
g	 0.2690	 0.2060
h	 0.2970	 0.1290
j	 0.2220	 0.1380
k	 0.0020	 0.0410
l	 0.0020	 0.0350



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Chain	Atom inclusion	Q-score
m	 0.0010	 0.0390
n	 0.0030	 0.0710
o	 0.3890	 0.2400
p	 0.0000	 0.0120
q	 0.0020	 0.0290
r	 0.0000	 0.0590
s	 0.0000	 0.0560
t	 0.0000	 -0.0010
u	 0.0000	 0.0210
v	 0.0000	 -0.0160
w	 0.0000	 -0.0030
y	 0.4940	 0.2550