wwPDB EM Validation Summary Report

Jul 30, 2024 – 05:13 pm BST

PDB ID	:	8RO1
EMDB ID	:	EMD-19398
Title	:	Structure of the C. elegans Intron Lariat Spliceosome double-primed for disassembly (ILS")
Authors	:	Vorlaender, M.K.; Rothe, P.; Plaschka, C.
Deposited on	:	2024-01-11
Resolution	:	3.00 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:

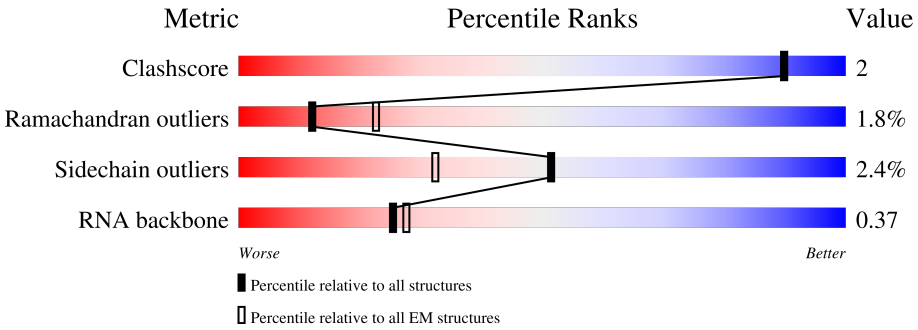
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	228	5% 21% 10% 67%
2	5	112	46% 36% 15%
3	6	101	38% 46% 14%
4	A	2329	74% 9% 15%
5	C	974	82% 9% 8%
6	D	267	21% 70% 26%
7	DX	739	8% 85% 7% 8%

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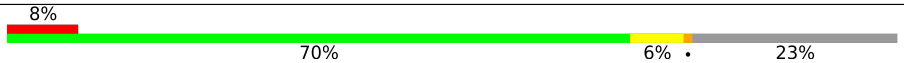
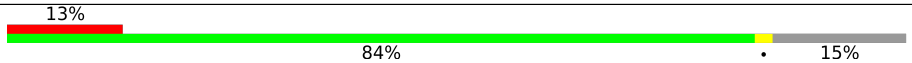
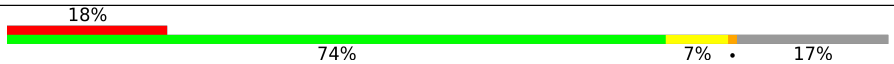
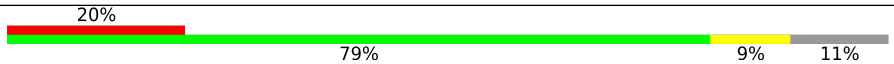
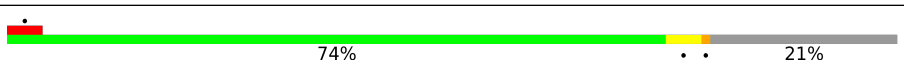
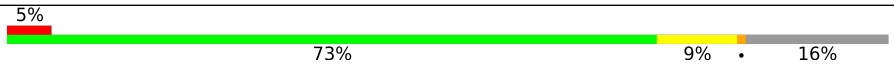
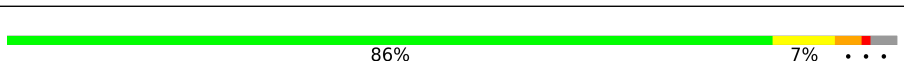
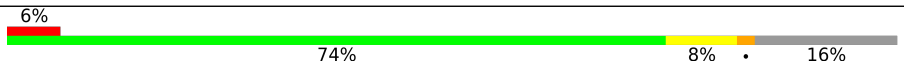
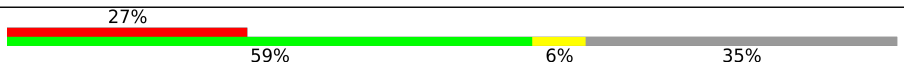
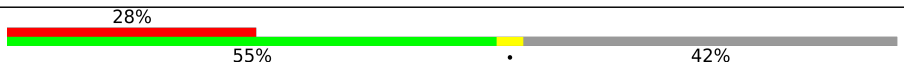
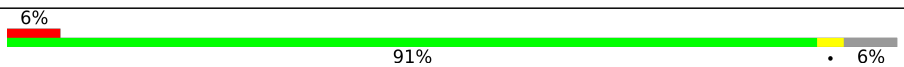
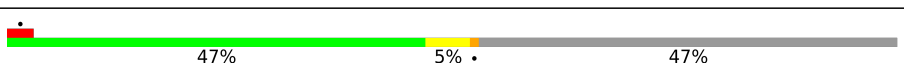
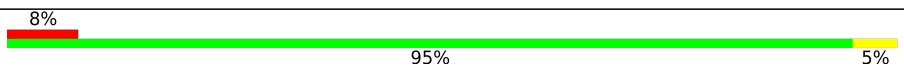
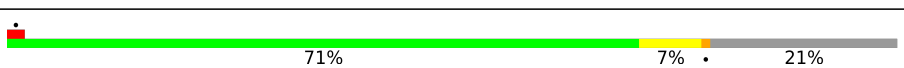
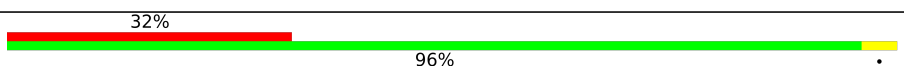
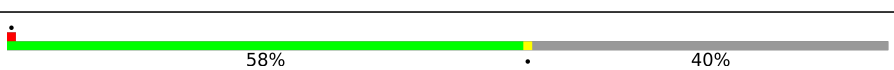
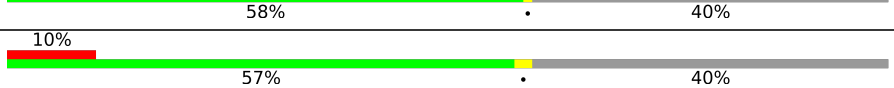
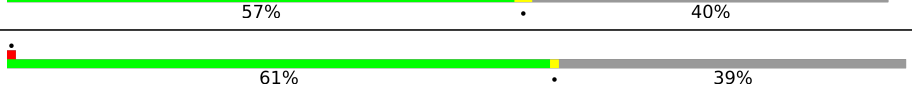
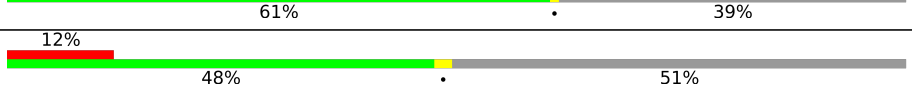
Mol	Chain	Length	Quality of chain
8	E	331	
9	I	855	
10	IN	51	
11	J	744	
12	K	238	
13	L	755	
14	L1	533	
15	L2	460	
16	M	234	
17	N	147	
18	O	408	
19	P	230	
20	PX	809	
21	Q	1467	
22	R	535	
23	S	169	
24	T	494	
25	TF	830	
26	W	567	
27	X	500	
28	Z	69	
29	a	136	
29	h	136	
30	b	160	
30	i	160	

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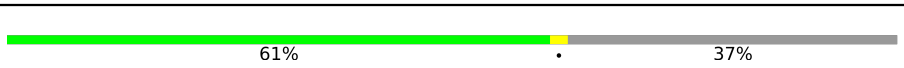
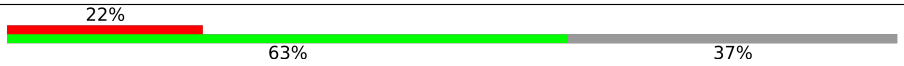
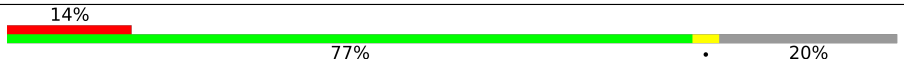
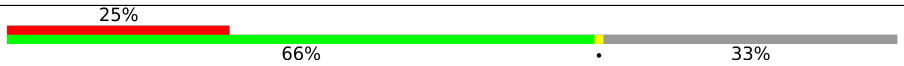
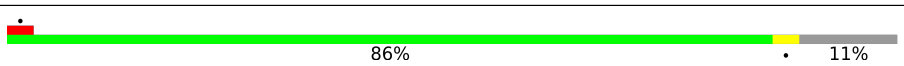
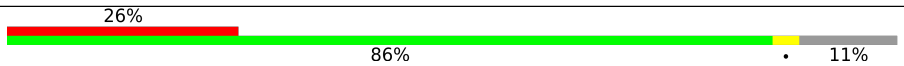
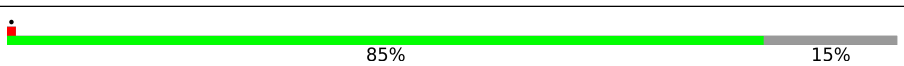
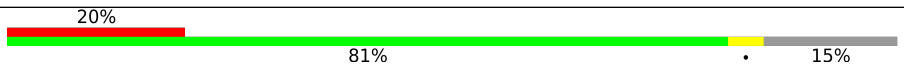
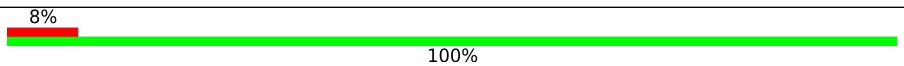
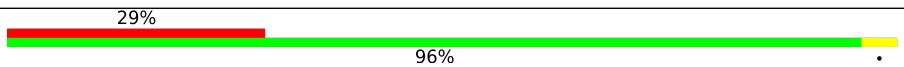
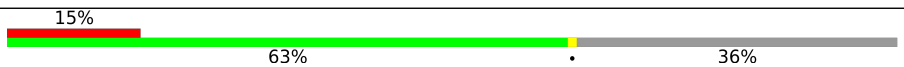
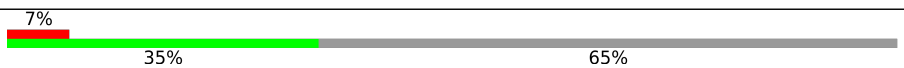
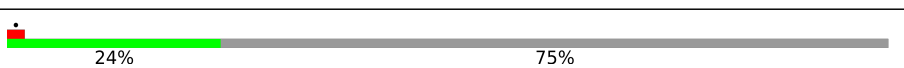
Mol	Chain	Length	Quality of chain
31	c	127	
31	j	127	
32	d	118	
32	k	118	
33	e	90	
33	l	90	
34	f	85	
34	m	85	
35	g	77	
35	n	77	
36	o	253	
37	p	217	
38	q	492	
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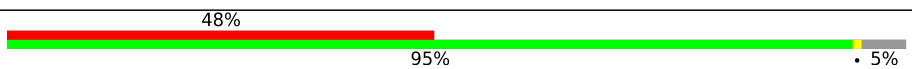
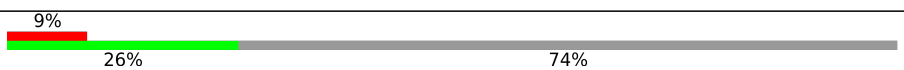
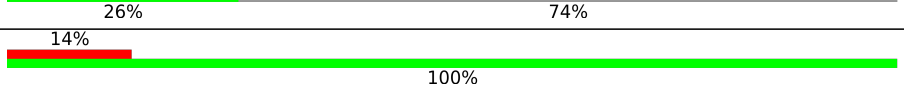
38	s	492	
38	t	492	
39	y	79	

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 120201 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 U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	76	1268	554	140	498	76	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	111	2350	1052	405	782	111	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	101	2153	965	391	696	101	0	0

- Molecule 4 is a protein called Pre-mRNA-splicing factor 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1982	16424	10576	2868	2904	76	0	0

- Molecule 5 is a protein called Tr-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	898	7153	4558	1211	1338	46	0	0

- Molecule 6 is a protein called Protein isy-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	198	1629	1016	293	316	4	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase ddx-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	DX	682	Total	C	N	O	S	0	0
			5465	3464	941	1026	34		

- Molecule 8 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	312	Total	C	N	O	S	0	0
			2445	1528	429	468	20		

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	747	Total	C	N	O	S	0	0
			6169	3916	1081	1128	44		

- Molecule 10 is a RNA chain called Intron lariat RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	IN	33	Total	C	N	O	P	0	0
			425	179	12	201	33		

- Molecule 11 is a protein called TPR_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	574	Total	C	N	O	S	0	0
			4895	3122	855	898	20		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	203	Total	C	N	O	S	0	0
			1666	1041	298	310	17		

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	623	Total	C	N	O	S	0	0
			5030	3115	928	962	25		

- Molecule 14 is a protein called CWF19-like protein 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L1	472	Total	C	N	O	S	0	0
			3683	2345	616	701	21		

- Molecule 15 is a protein called CWF19-like protein 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L2	362	Total	C	N	O	S	0	0
			2974	1846	543	568	17		

- Molecule 16 is a protein called Pre-mRNA-splicing factor syf-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	196	Total	C	N	O	S	0	0
			1654	1021	308	319	6		

- Molecule 17 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	142	Total	C	N	O	S	0	0
			1163	731	212	208	12		

- Molecule 18 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	342	Total	C	N	O	S	0	0
			2721	1703	493	506	19		

- Molecule 19 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	150	Total	C	N	O	S	0	0
			1207	729	232	240	6		

- Molecule 20 is a protein called GCF C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	PX	472	Total	C	N	O	S	0	0
			3838	2396	695	720	27		

- Molecule 21 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	1378	Total	C	N	O	S	0	0
			11293	7218	1964	2064	47		

- Molecule 22 is a protein called Uncharacterized protein T27F2.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	282	Total	C	N	O	S	0	0
			2209	1379	404	416	10		

- Molecule 23 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	169	Total	C	N	O	S	0	0
			1303	818	233	245	7		

- Molecule 24 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	389	Total	C	N	O	S	0	0
			3082	1946	557	560	19		

- Molecule 25 is a protein called Septin and tuftelin-interacting protein 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	TF	559	Total	C	N	O	S	0	0
			4542	2908	769	838	27		

- Molecule 26 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	496	Total	C	N	O	S	0	0
			4072	2584	726	747	15		

- Molecule 27 is a protein called Replication stress response regulator SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	80	Total	C	N	O	S	0	0
			661	407	123	126	5		

- Molecule 28 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	69	Total	C	N	O	S	0	0
			569	356	104	107	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	81	Total	C	N	O	S	0	0
			635	396	113	120	6		
29	h	81	Total	C	N	O	S	0	0
			635	396	113	120	6		

- Molecule 30 is a protein called Probable small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	98	Total	C	N	O	S	0	0
			755	475	141	131	8		
30	i	79	Total	C	N	O	S	0	0
			639	405	117	111	6		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	80	Total	C	N	O	S	0	0
			622	396	109	113	4		
31	j	80	Total	C	N	O	S	0	0
			622	396	109	113	4		

- Molecule 32 is a protein called Probable small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	94	Total	C	N	O	S	0	0
			749	469	135	140	5		
32	k	79	Total	C	N	O	S	0	0
			632	398	118	111	5		

- Molecule 33 is a protein called Probable small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	80	Total	C	N	O	S	0	0
			665	424	118	121	2		
33	l	80	Total	C	N	O	S	0	0
			665	424	118	121	2		

- Molecule 34 is a protein called Probable small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	72	Total	C	N	O	S	0	0
			558	359	93	102	4		
34	m	72	Total	C	N	O	S	0	0
			558	359	93	102	4		

- Molecule 35 is a protein called Probable small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	77	Total	C	N	O	S	0	0
			608	379	107	115	7		
35	n	77	Total	C	N	O	S	0	0
			608	379	107	115	7		

- Molecule 36 is a protein called Probable U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	o	162	Total	C	N	O	S	0	0
			1335	849	236	243	7		

- Molecule 37 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	p	76	Total	C	N	O	S	0	0
			626	402	114	106	4		

- Molecule 38 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	q	121	Total	C	N	O	S	0	0
			941	585	165	186	5		
38	r	131	Total	C	N	O	S	0	0
			1004	621	179	199	5		
38	s	469	Total	C	N	O	S	0	0
			3571	2239	620	703	9		
38	t	128	Total	C	N	O	S	0	0
			993	620	173	195	5		

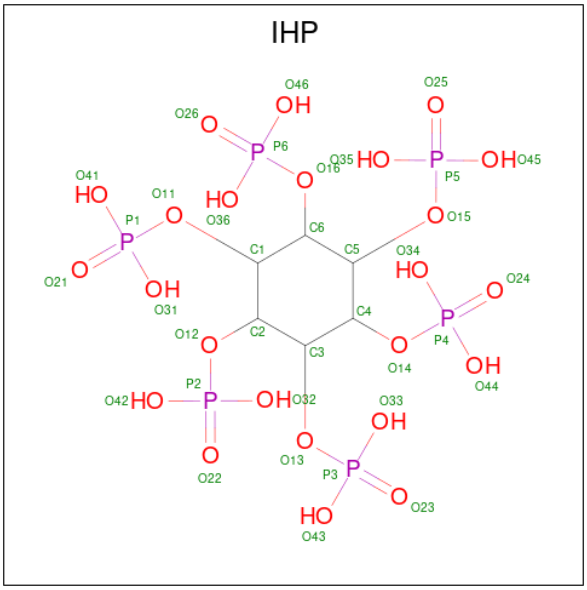
- Molecule 39 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	y	79	Total	C	N	O	S	0	0
			619	396	100	118	5		

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

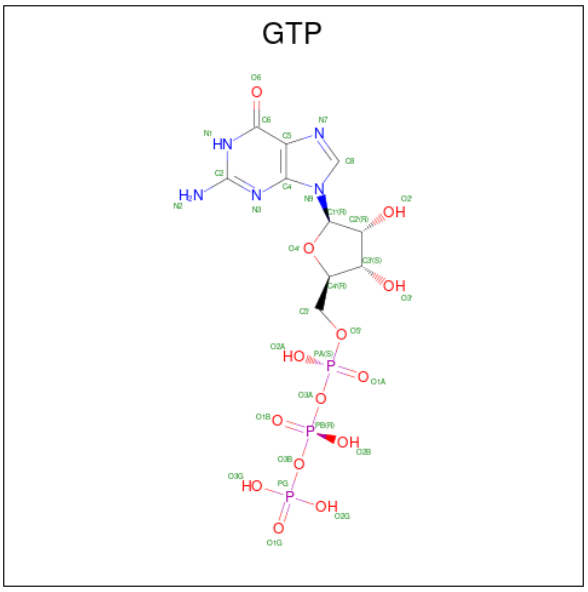
Mol	Chain	Residues	Atoms		AltConf
40	6	6	Total	Mg	0
			6	6	
40	C	1	Total	Mg	0
			1	1	

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 43 is ZINC ION (three-letter code: ZN) (formula: Zn).

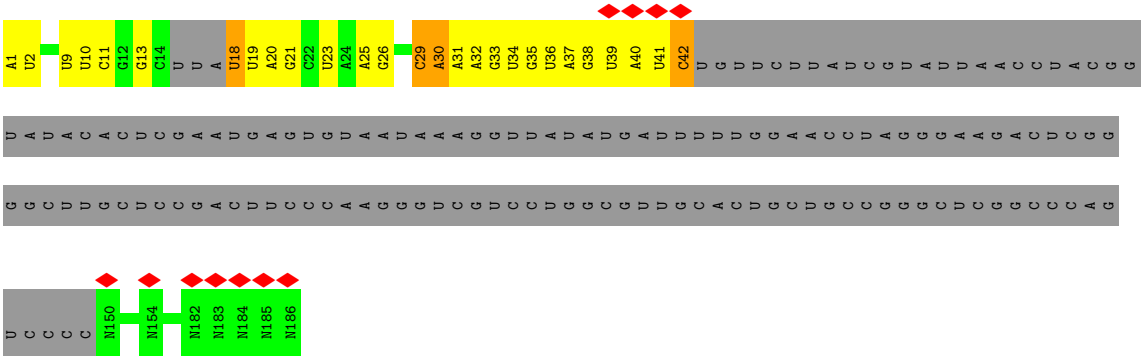
Mol	Chain	Residues	Atoms		AltConf
43	L2	1	Total	Zn	0
			1	1	
43	N	3	Total	Zn	0
			3	3	
43	O	3	Total	Zn	0
			3	3	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

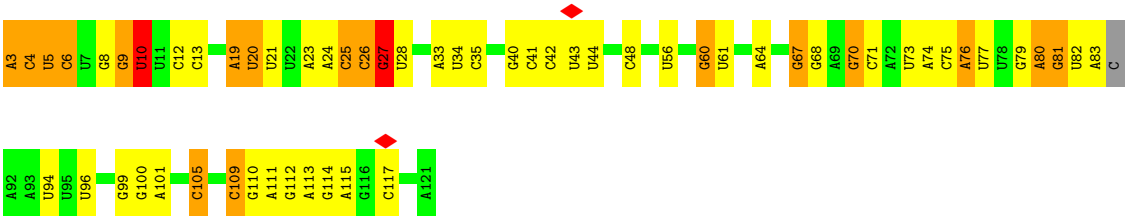
- Molecule 1: U2 snRNA

Chain 2:



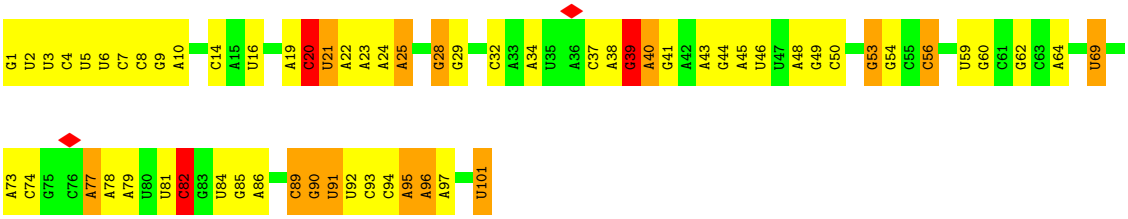
- Molecule 2: U5 snRNA

Chain 5:



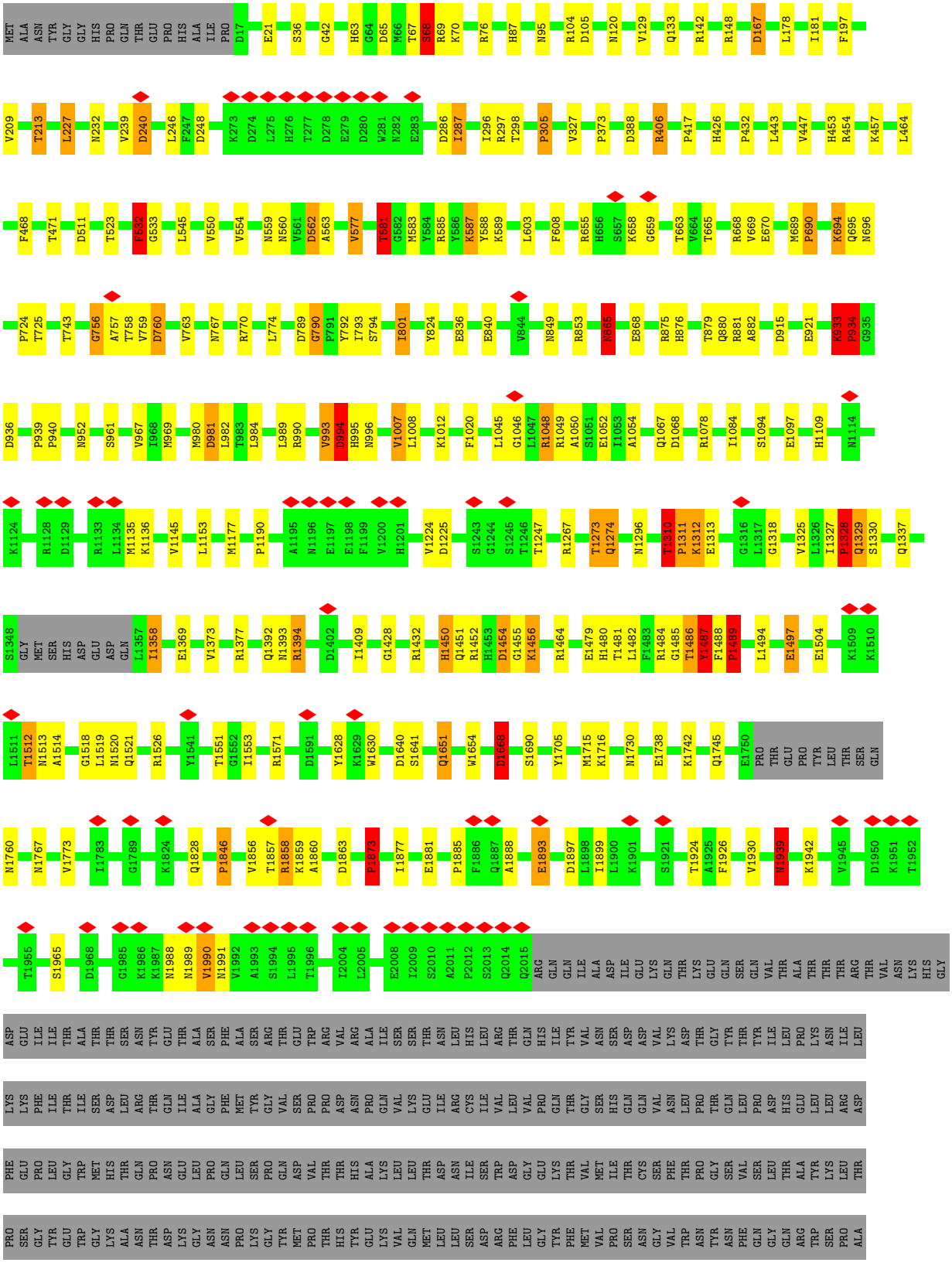
- Molecule 3: U6 snRNA

Chain 6:



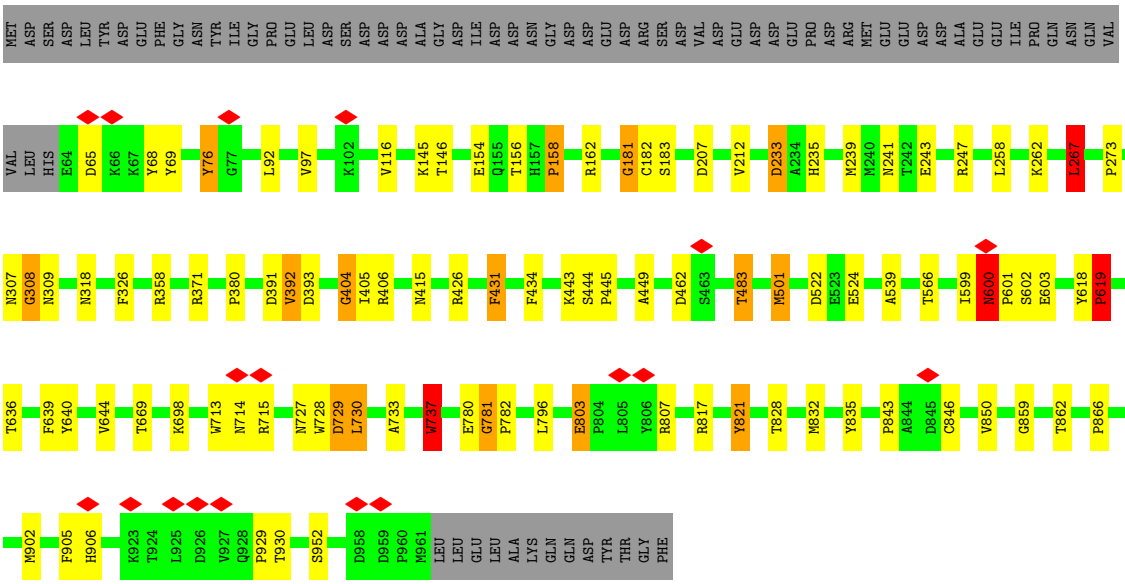
• Molecule 4: Pre-mRNA-splicing factor 8 homolog

Chain A:



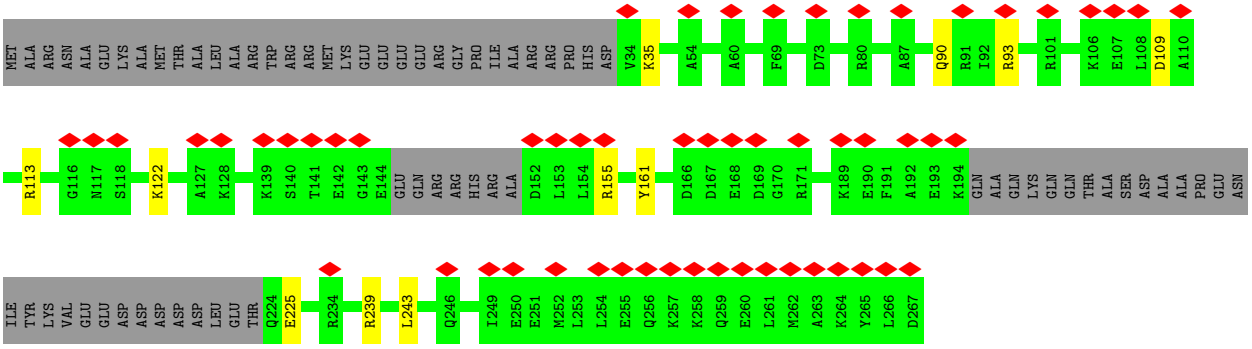
• Molecule 5: Tr-type G domain-containing protein

Chain C:



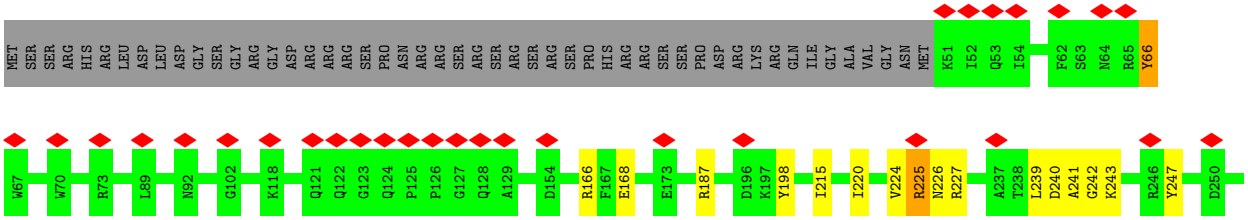
• Molecule 6: Protein isy-1

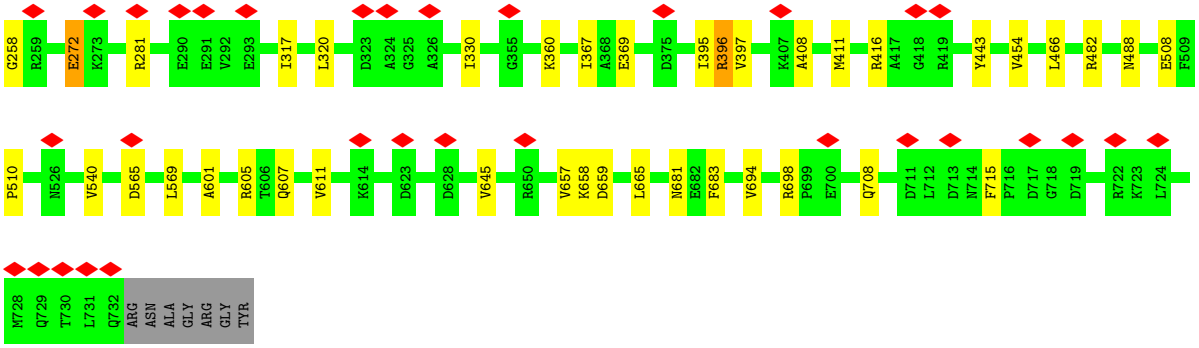
Chain D:



• Molecule 7: Pre-mRNA-splicing factor ATP-dependent RNA helicase ddx-15

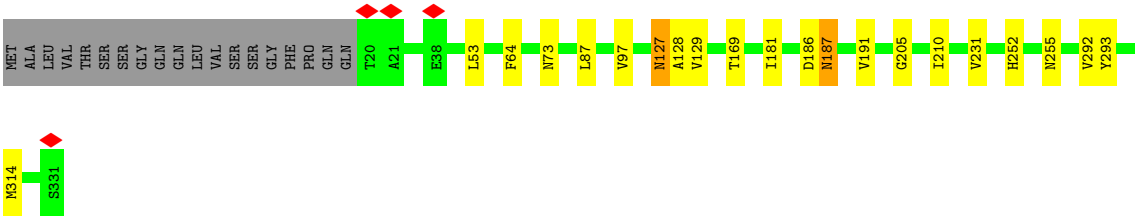
Chain DX:





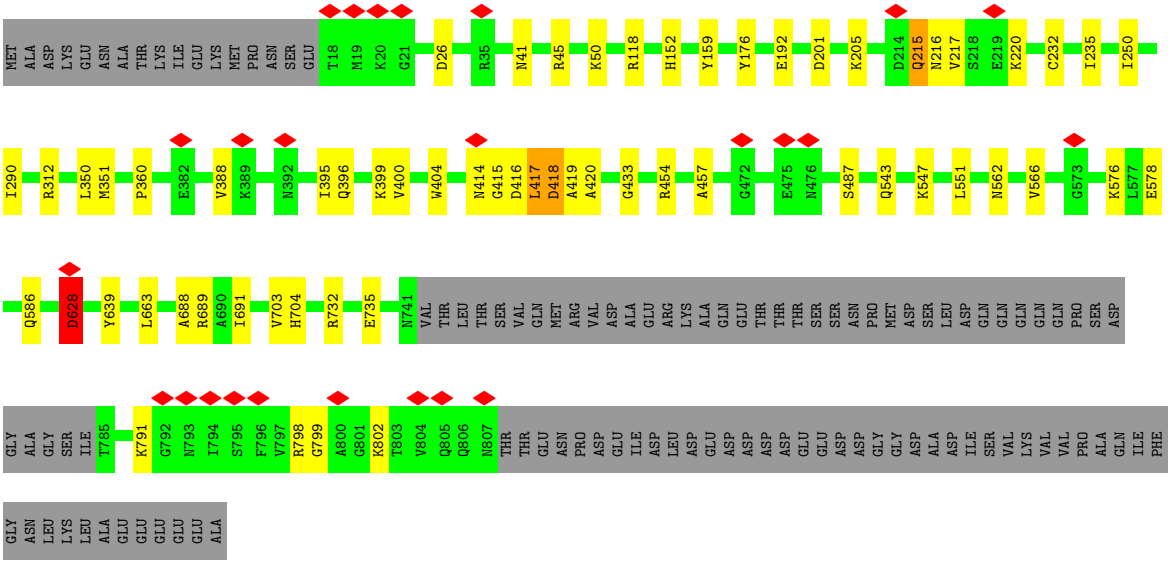
• Molecule 8: WD_REPEATS_REGION domain-containing protein

Chain E:



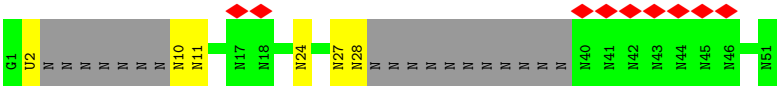
• Molecule 9: Pre-mRNA-splicing factor SYF1

Chain I:



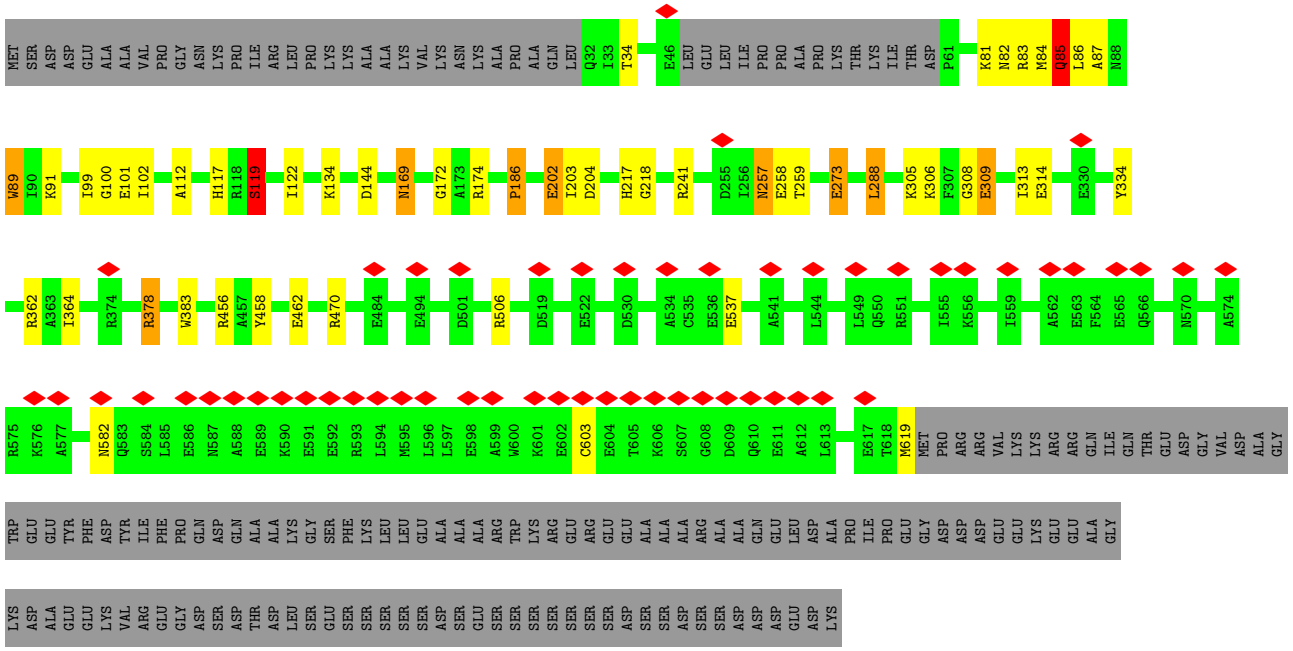
• Molecule 10: Intron lariat RNA

Chain IN:



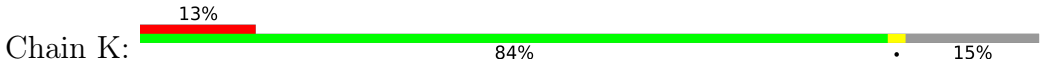
• Molecule 11: TPR_REGION domain-containing protein

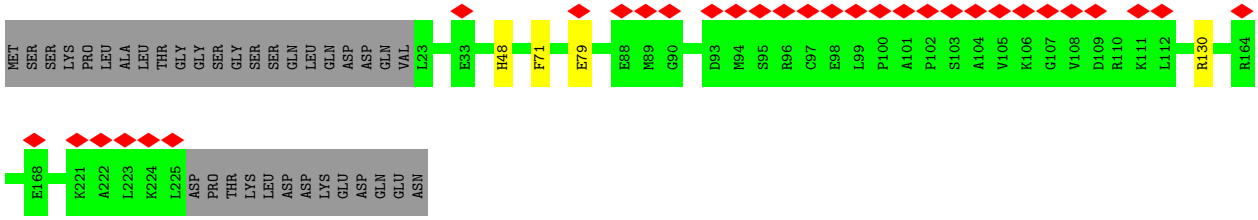
Chain J:



• Molecule 12: Pre-mRNA-splicing factor SPF27

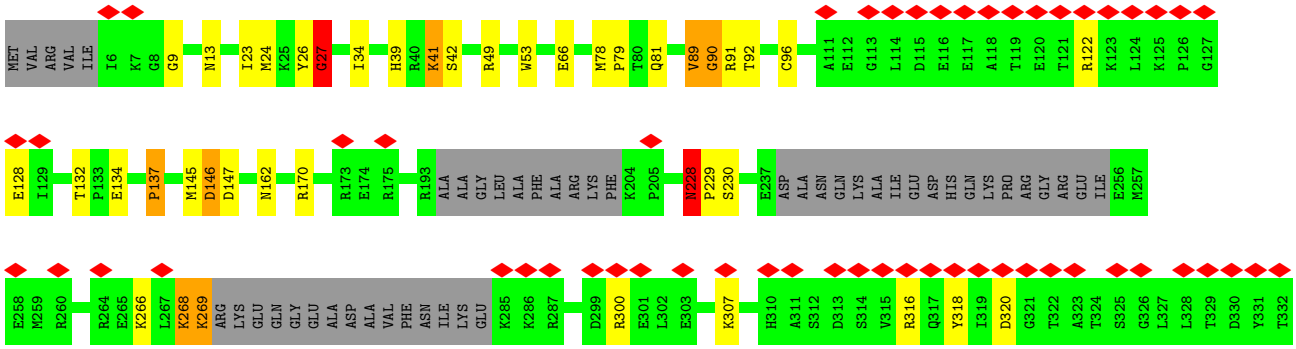
Chain K:

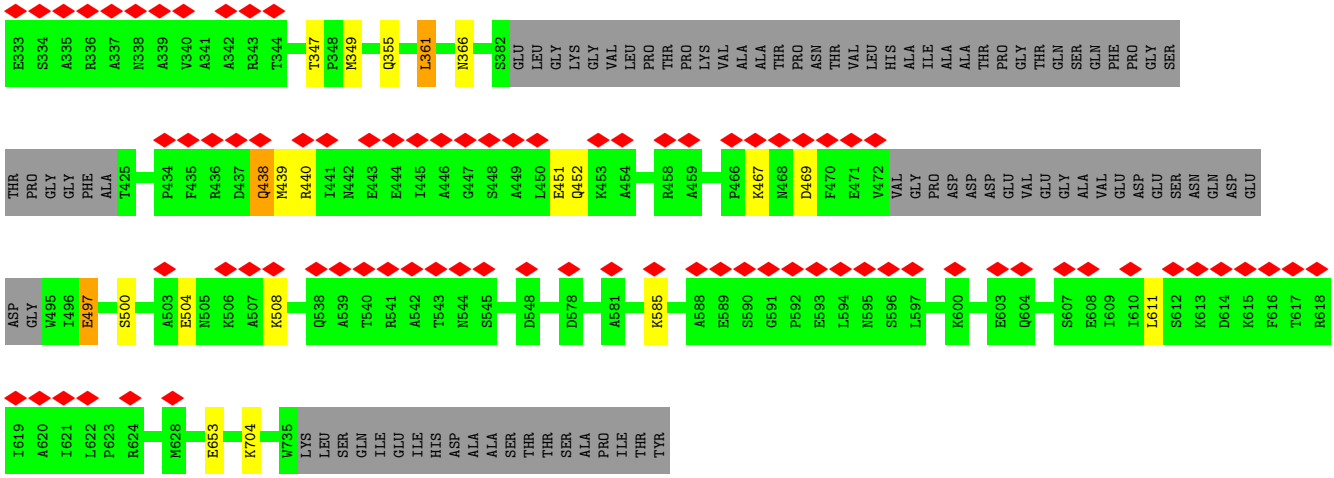




• Molecule 13: Cell division cycle 5-like protein

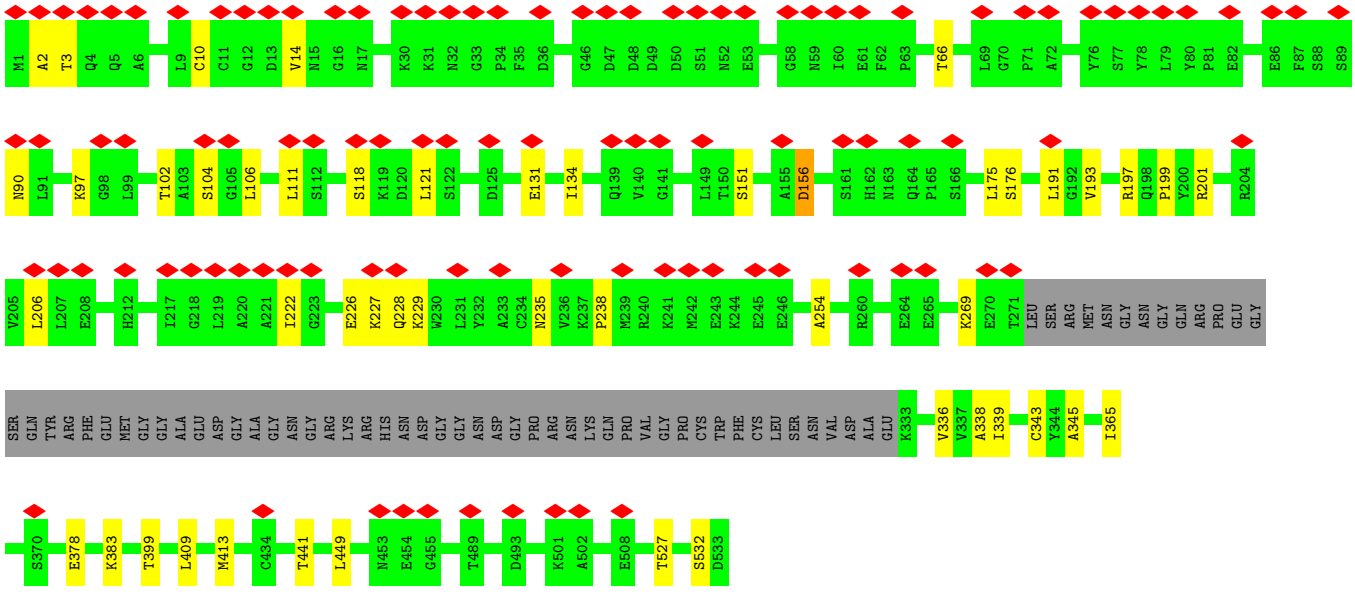
Chain L:





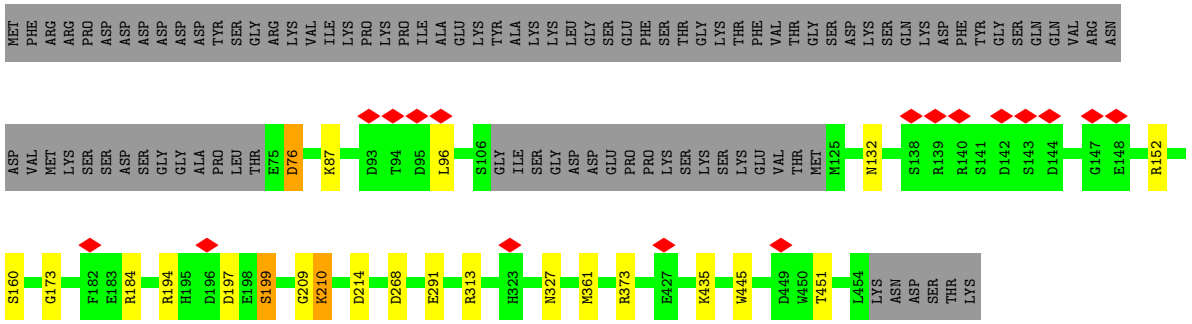
• Molecule 14: CWF19-like protein 1 homolog

Chain L1:



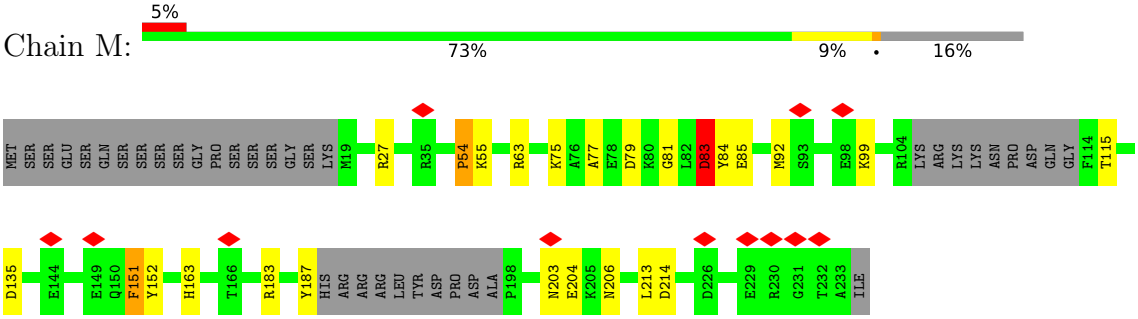
• Molecule 15: CWF19-like protein 2 homolog

Chain L2:



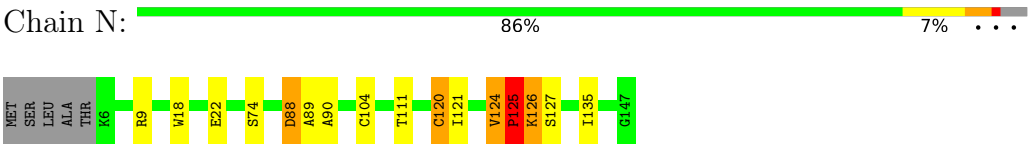
• Molecule 16: Pre-mRNA-splicing factor syf-2

Chain M:



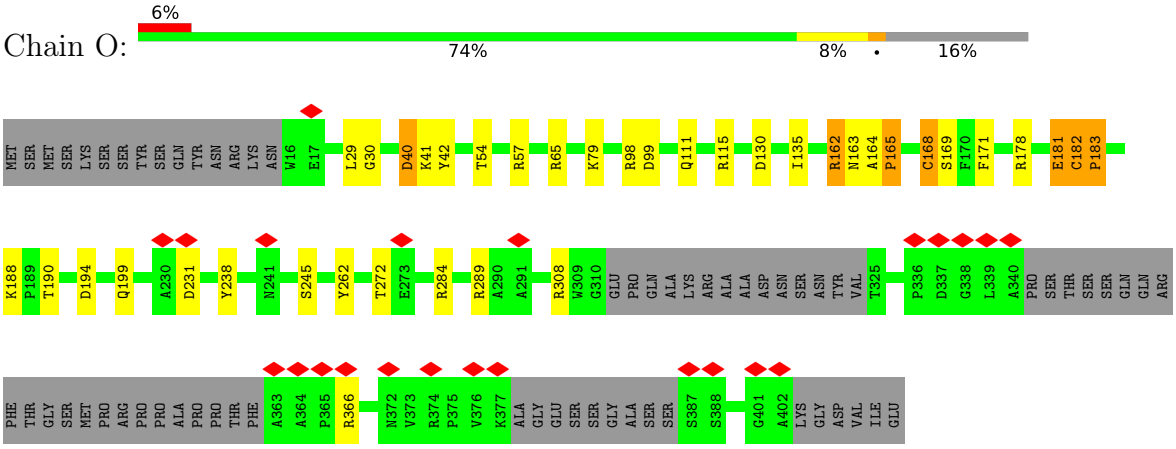
• Molecule 17: Protein BUD31 homolog

Chain N:



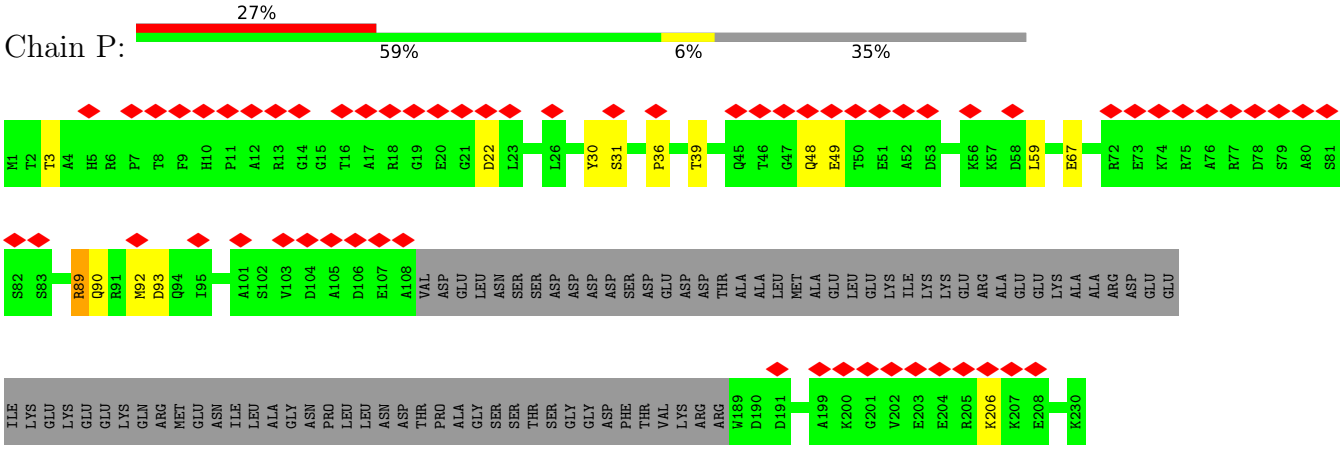
• Molecule 18: Pre-mRNA-splicing factor RBM22

Chain O:



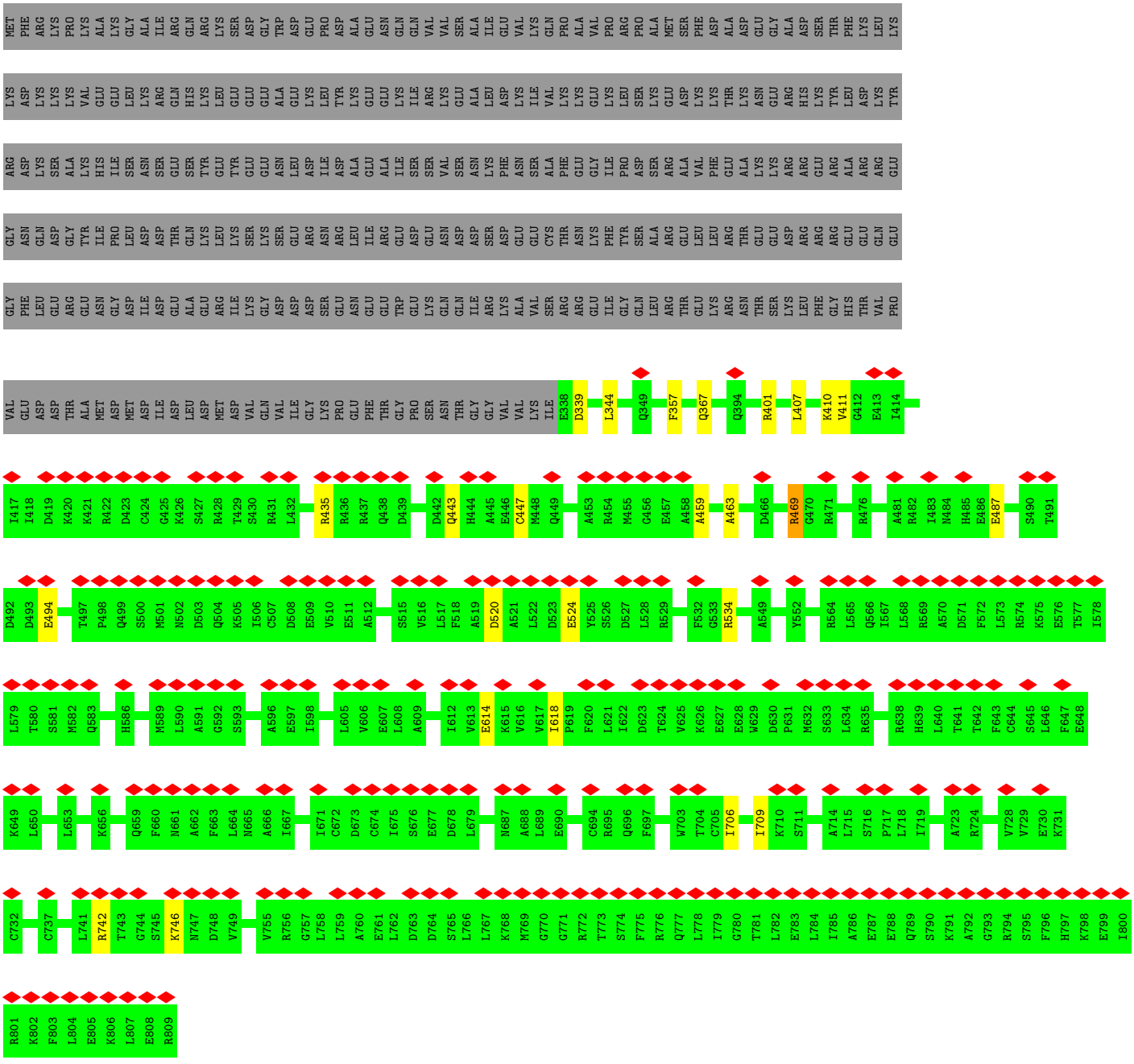
• Molecule 19: Spliceosome-associated protein CWC15 homolog

Chain P:



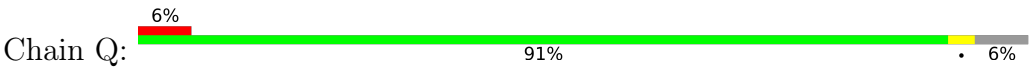
• Molecule 20: GCF C-terminal domain-containing protein

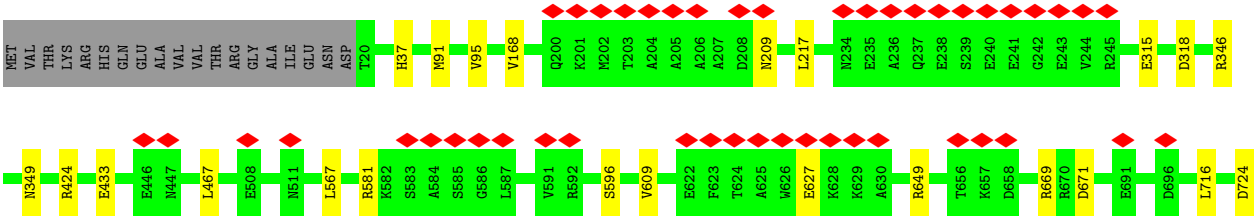
Chain PX:

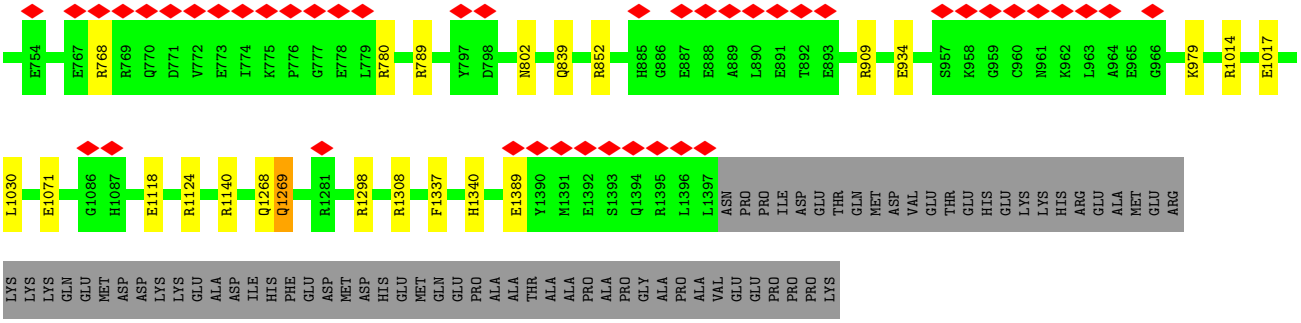


• Molecule 21: Intron-binding protein aquarius

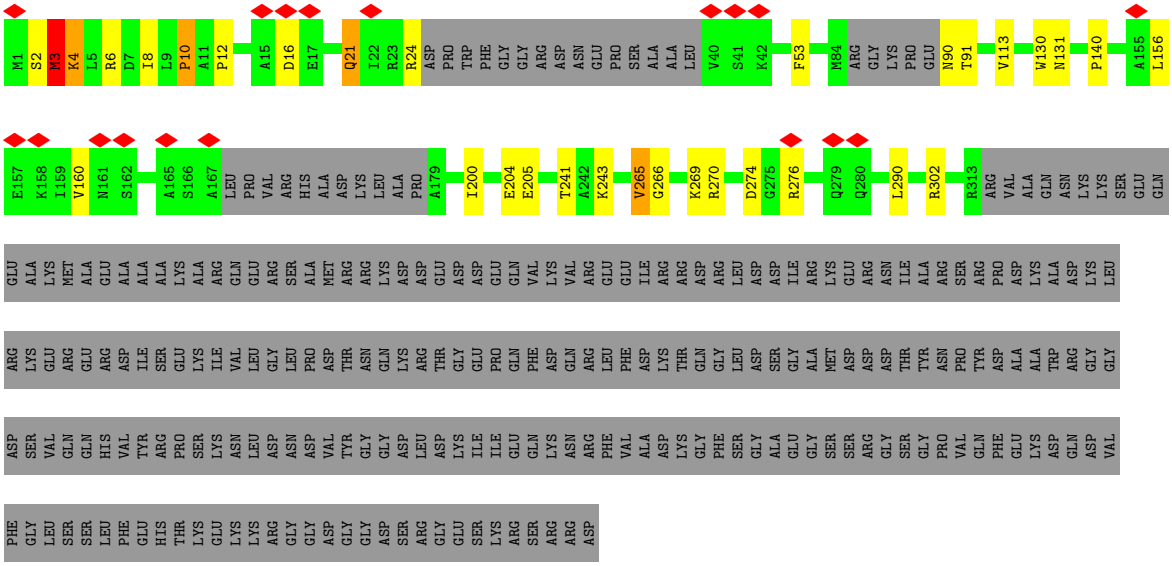
Chain Q:



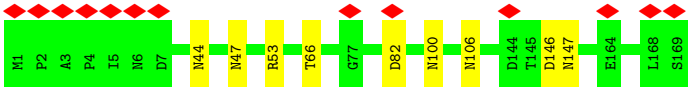




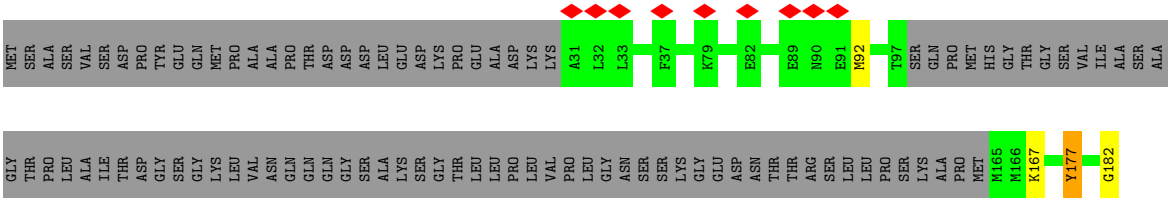
• Molecule 22: Uncharacterized protein T27F2.1

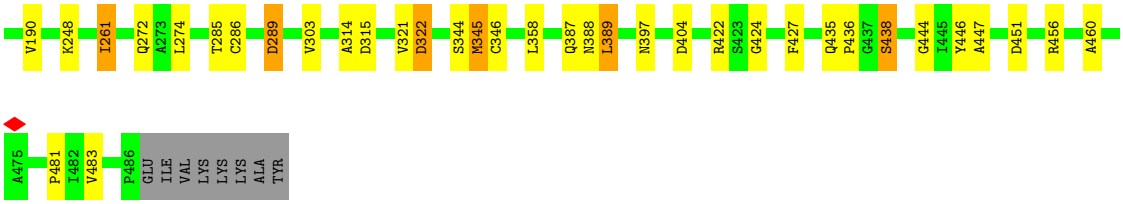


• Molecule 23: Peptidyl-prolyl cis-trans isomerase



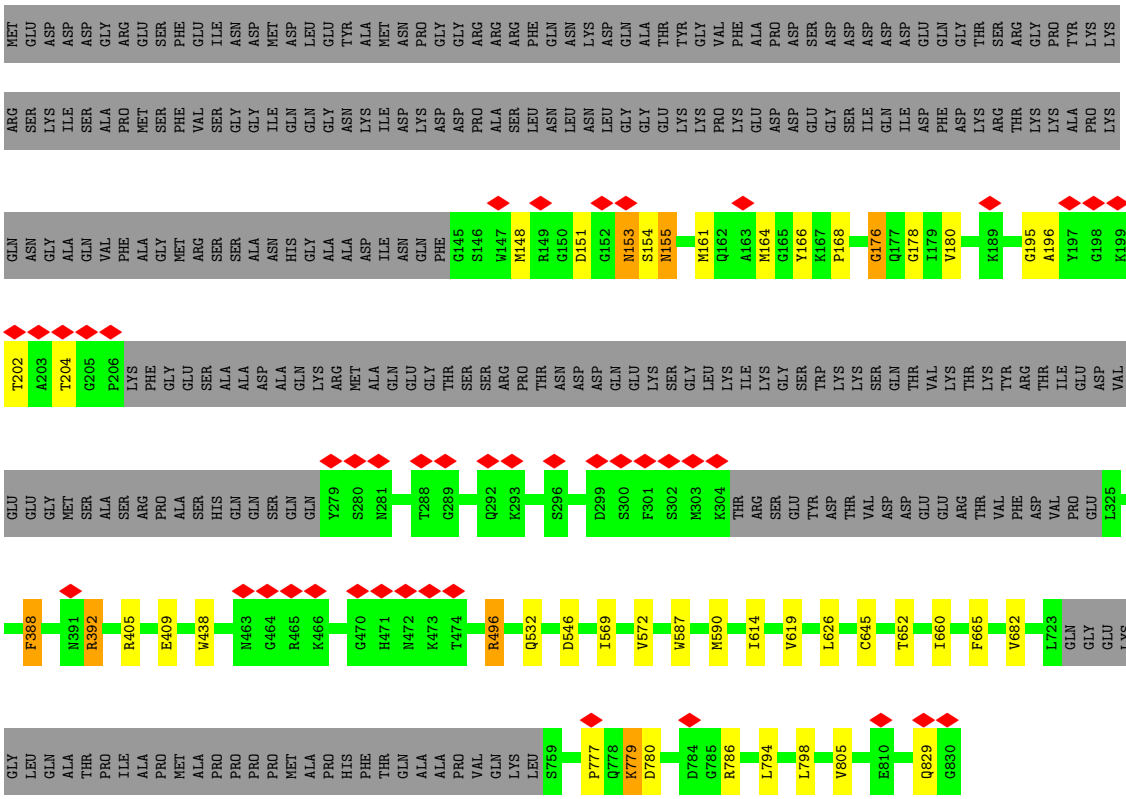
• Molecule 24: WD_REPEATS_REGION domain-containing protein





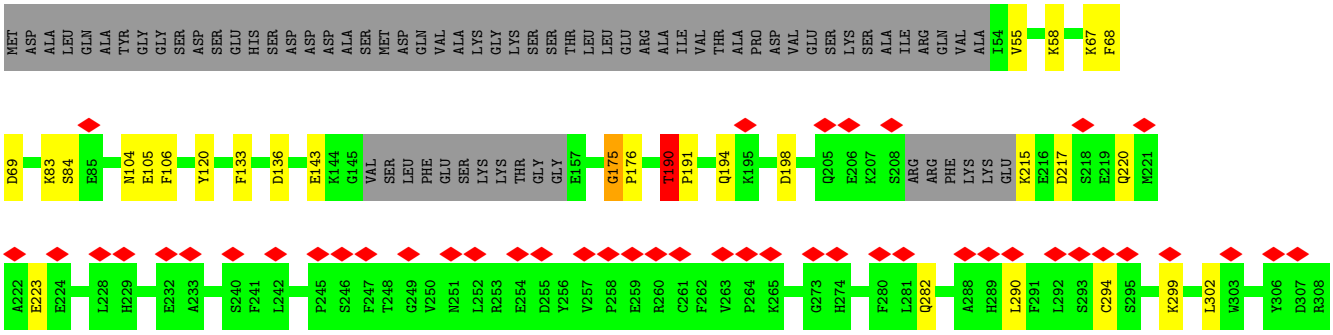
• Molecule 25: Septin and tuftelin-interacting protein 1 homolog

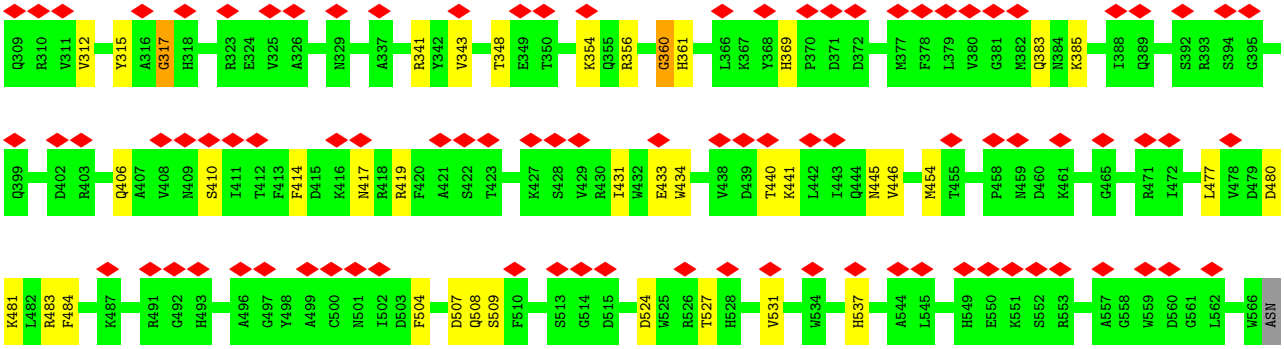
Chain TF:



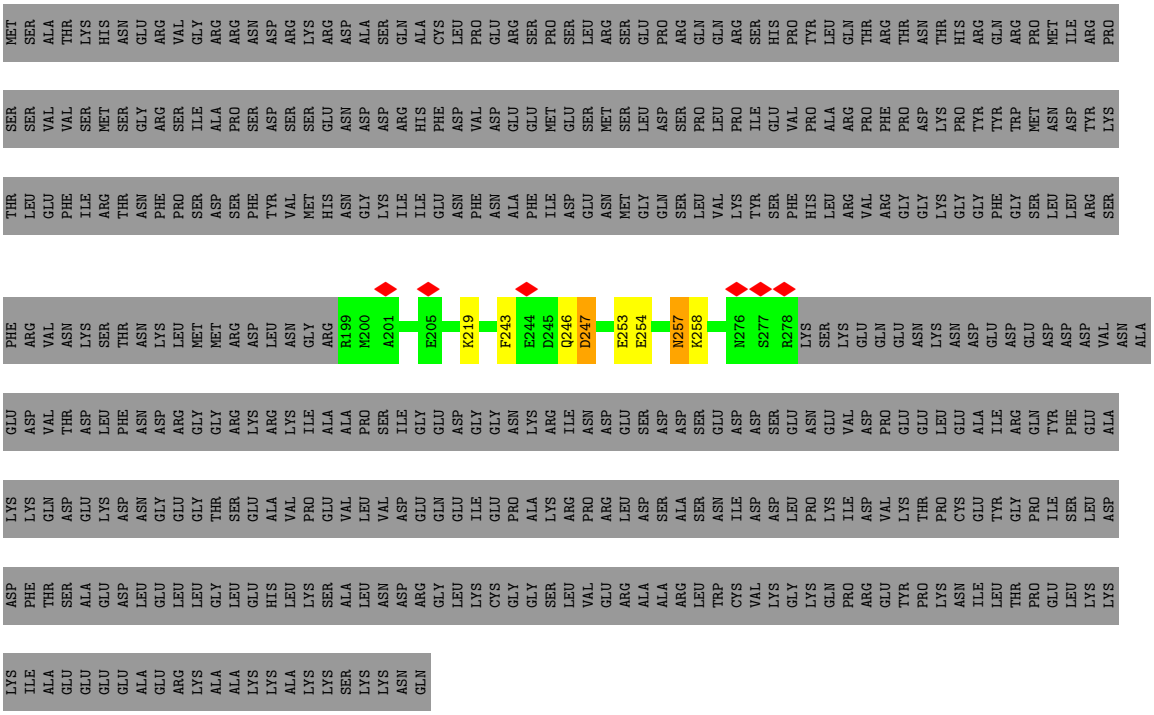
• Molecule 26: WD_REPEATS_REGION domain-containing protein

Chain W:

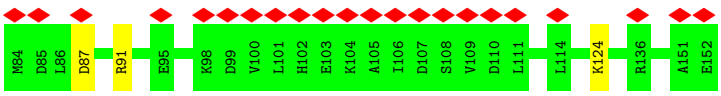




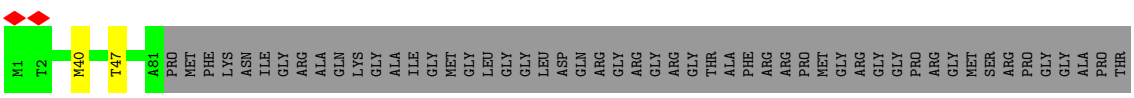
• Molecule 27: Replication stress response regulator SDE2



• Molecule 28: Coiled-coil domain-containing protein 12

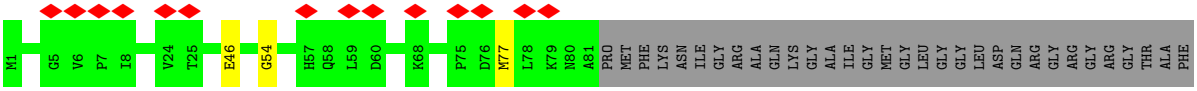


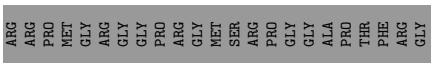
• Molecule 29: Small nuclear ribonucleoprotein Sm D3



• Molecule 29: Small nuclear ribonucleoprotein Sm D3

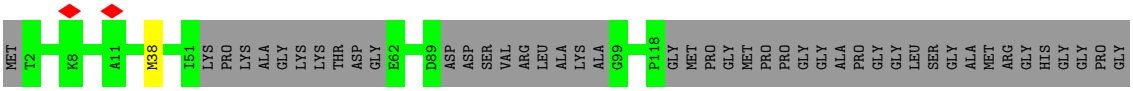
Chain h:

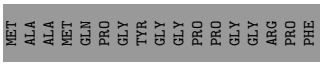




• Molecule 30: Probable small nuclear ribonucleoprotein-associated protein B

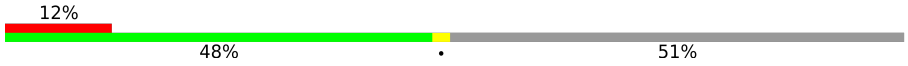
Chain b:

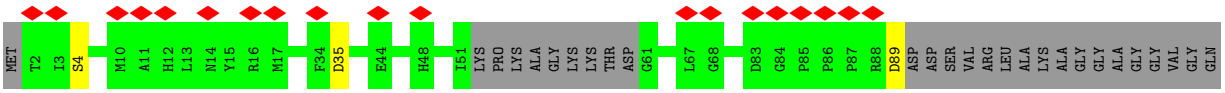


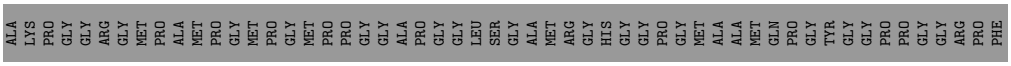


• Molecule 30: Probable small nuclear ribonucleoprotein-associated protein B

Chain i:





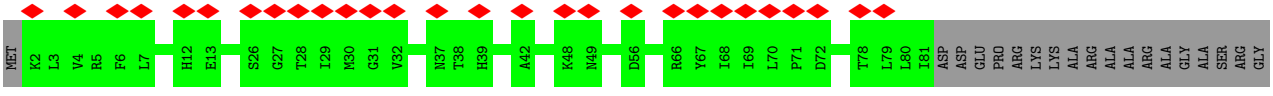


• Molecule 31: Small nuclear ribonucleoprotein Sm D1

Chain c:

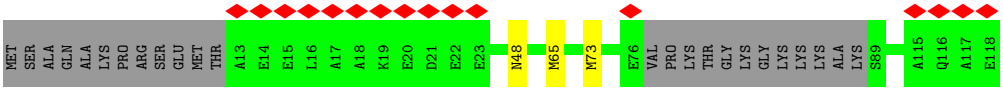
• Molecule 31: Small nuclear ribonucleoprotein Sm D1

Chain j:



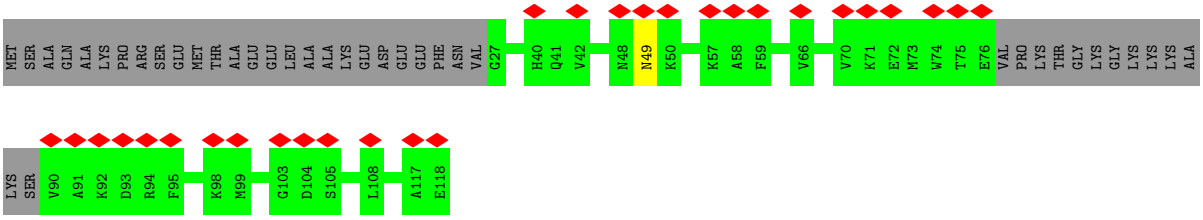
• Molecule 32: Probable small nuclear ribonucleoprotein Sm D2

Chain d:



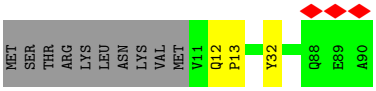
• Molecule 32: Probable small nuclear ribonucleoprotein Sm D2

Chain k:



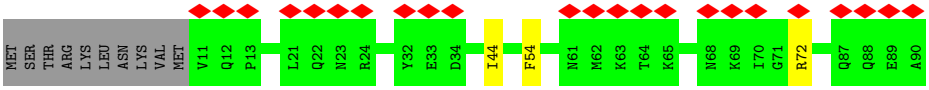
• Molecule 33: Probable small nuclear ribonucleoprotein E

Chain e:



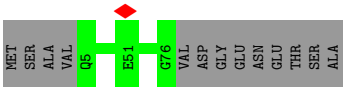
• Molecule 33: Probable small nuclear ribonucleoprotein E

Chain l:



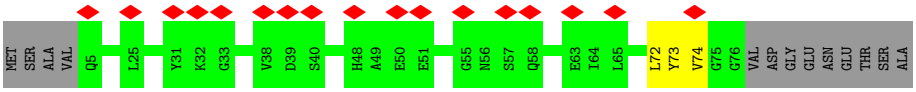
• Molecule 34: Probable small nuclear ribonucleoprotein F

Chain f:



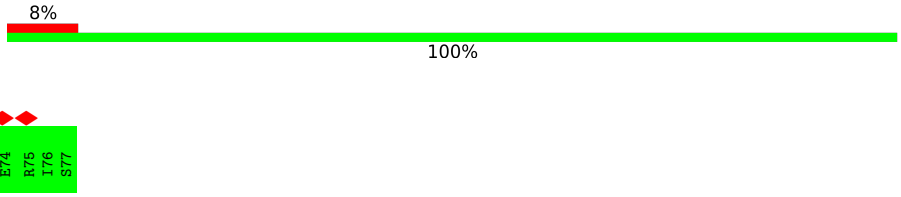
• Molecule 34: Probable small nuclear ribonucleoprotein F

Chain m:



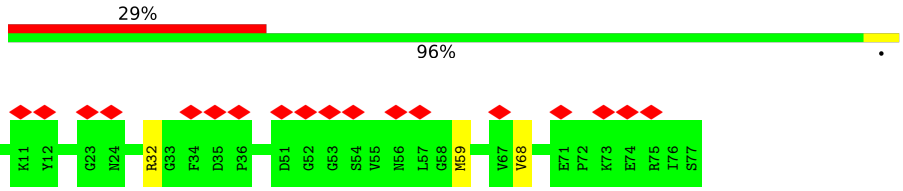
• Molecule 35: Probable small nuclear ribonucleoprotein G

Chain g:



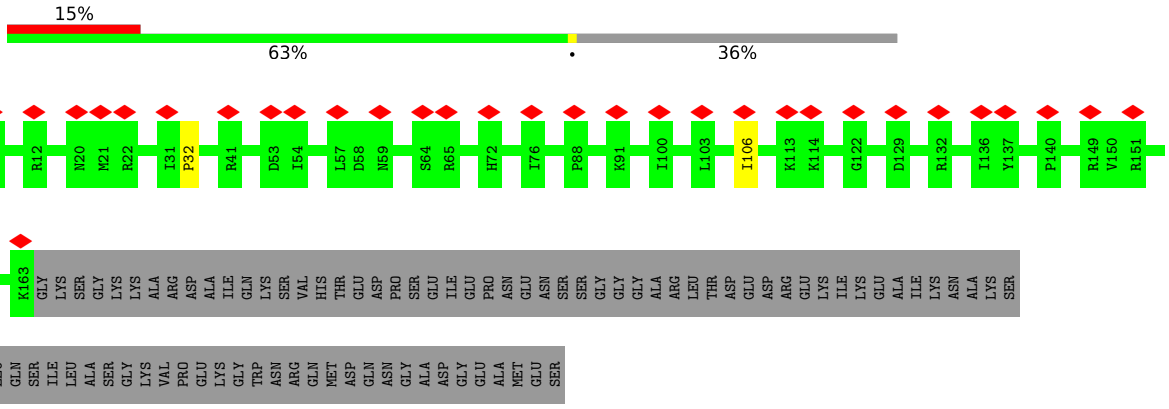
• Molecule 35: Probable small nuclear ribonucleoprotein G

Chain n:



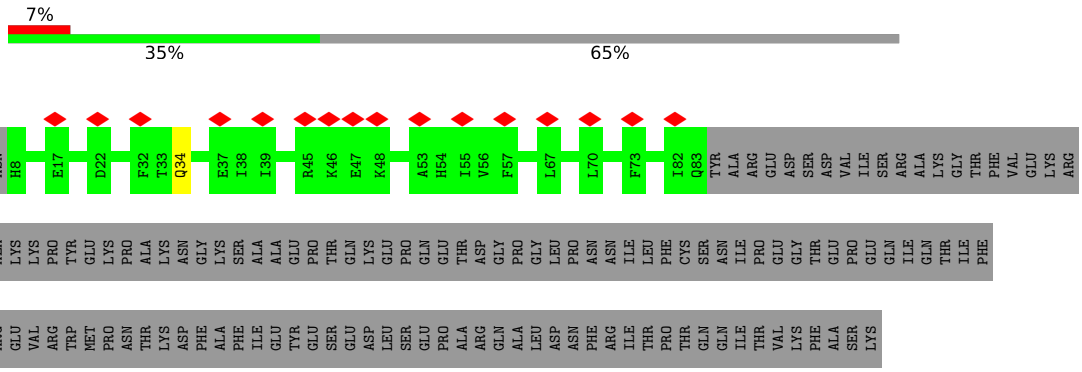
• Molecule 36: Probable U2 small nuclear ribonucleoprotein A'

Chain o:



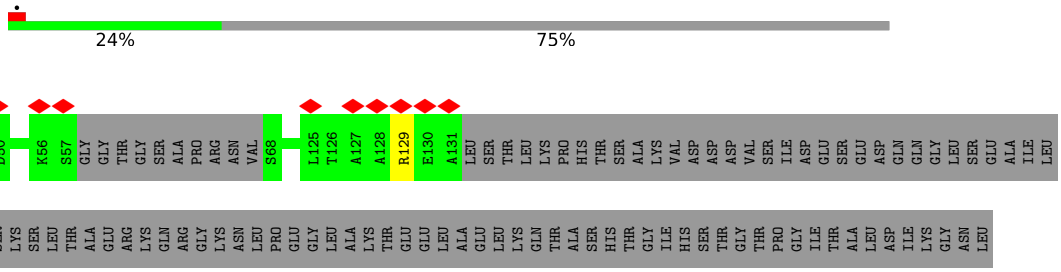
• Molecule 37: RRM domain-containing protein

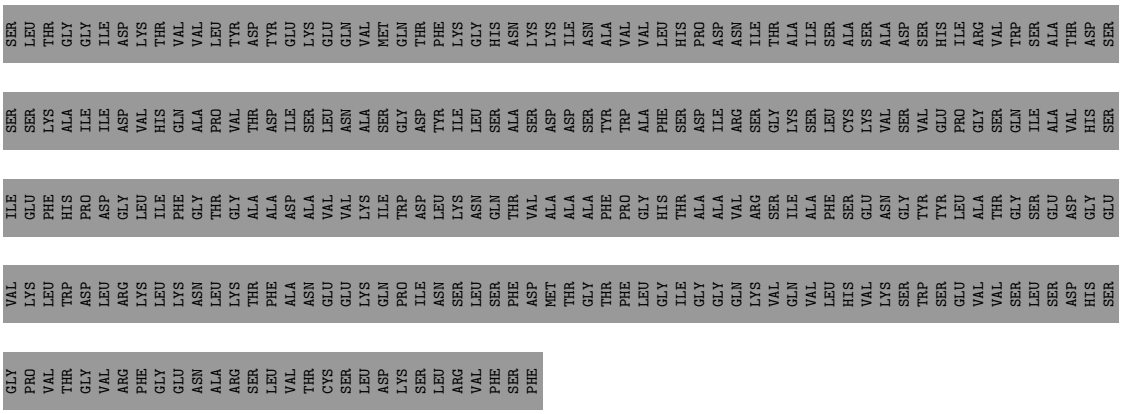
Chain p:



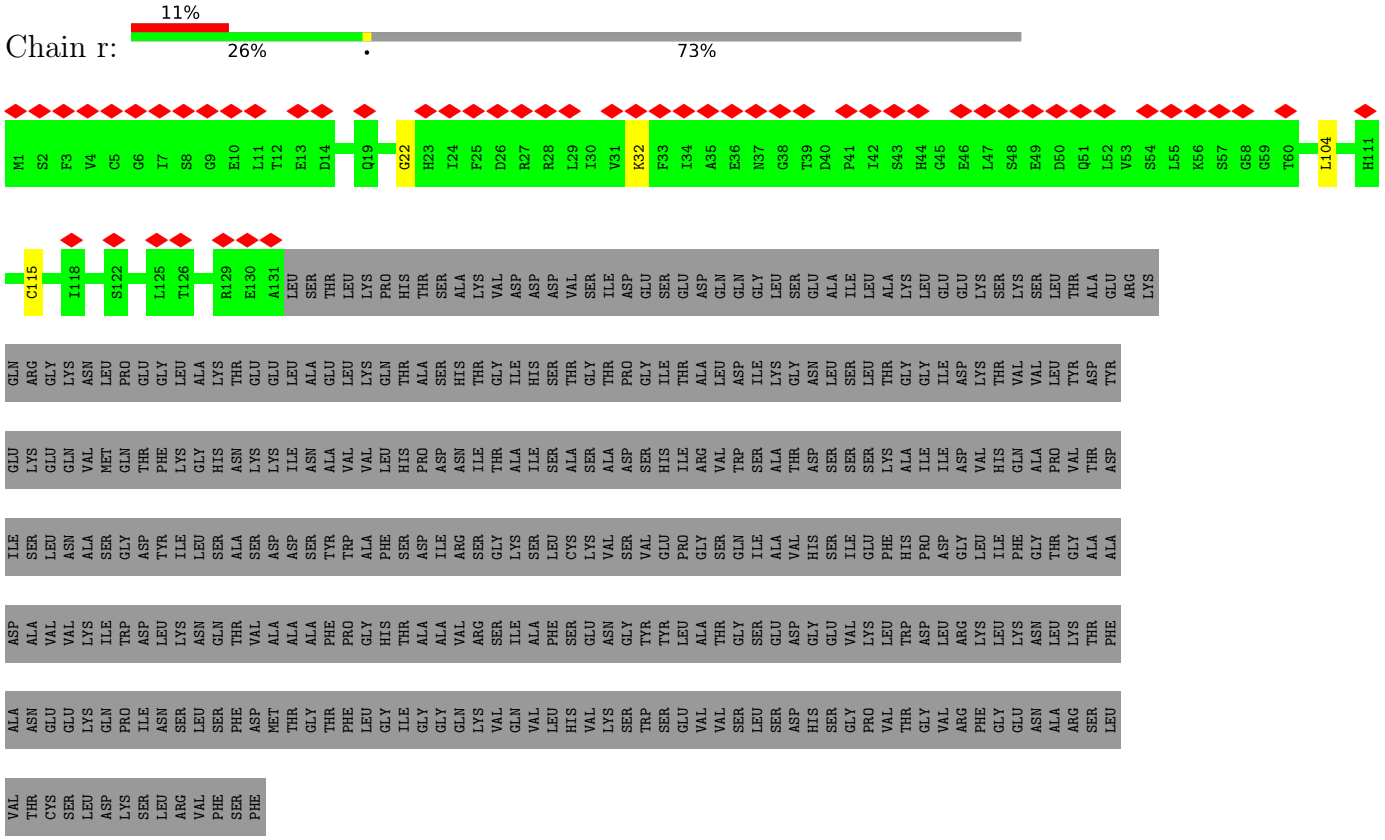
• Molecule 38: Pre-mRNA-processing factor 19

Chain q:

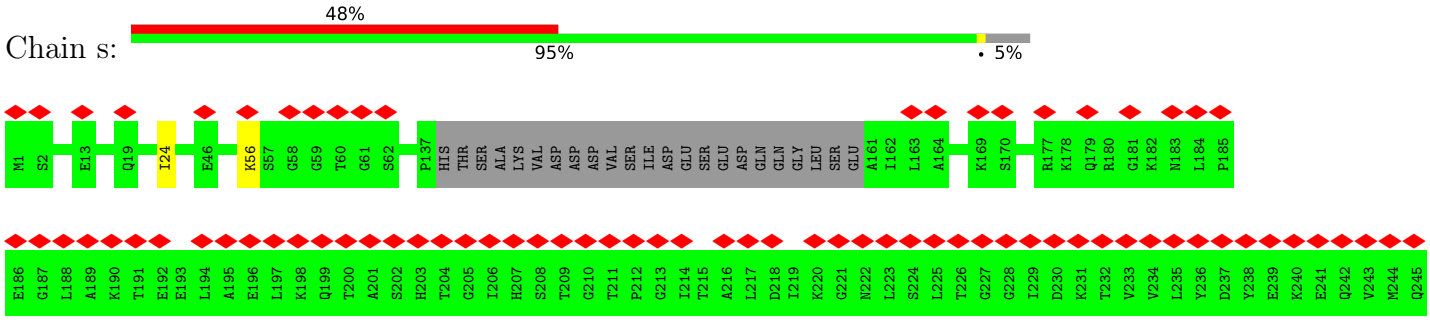


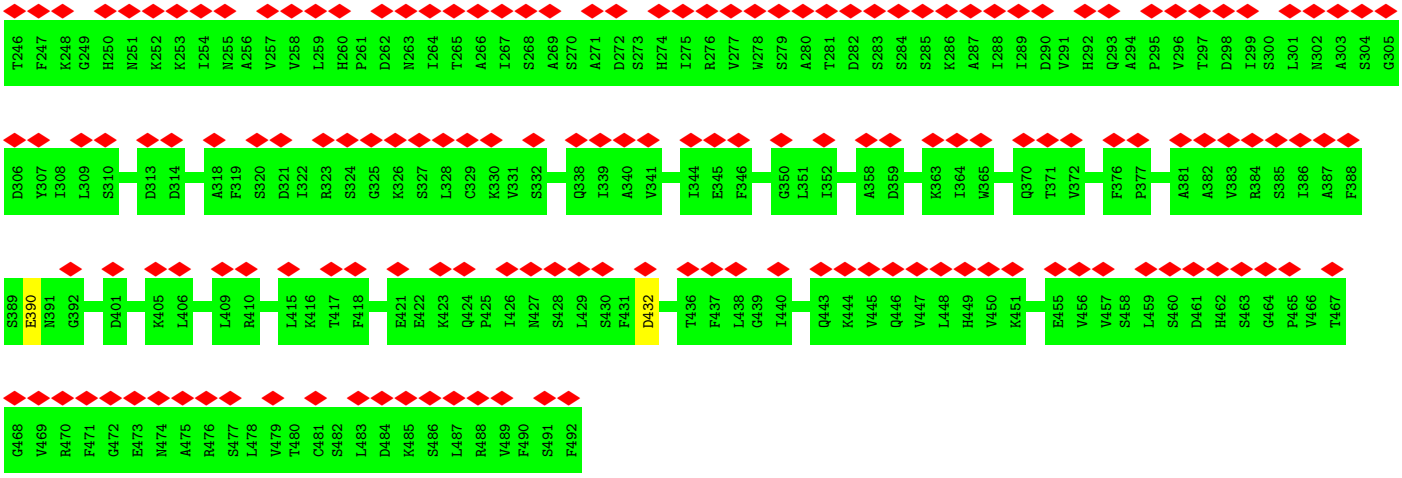


• Molecule 38: Pre-mRNA-processing factor 19



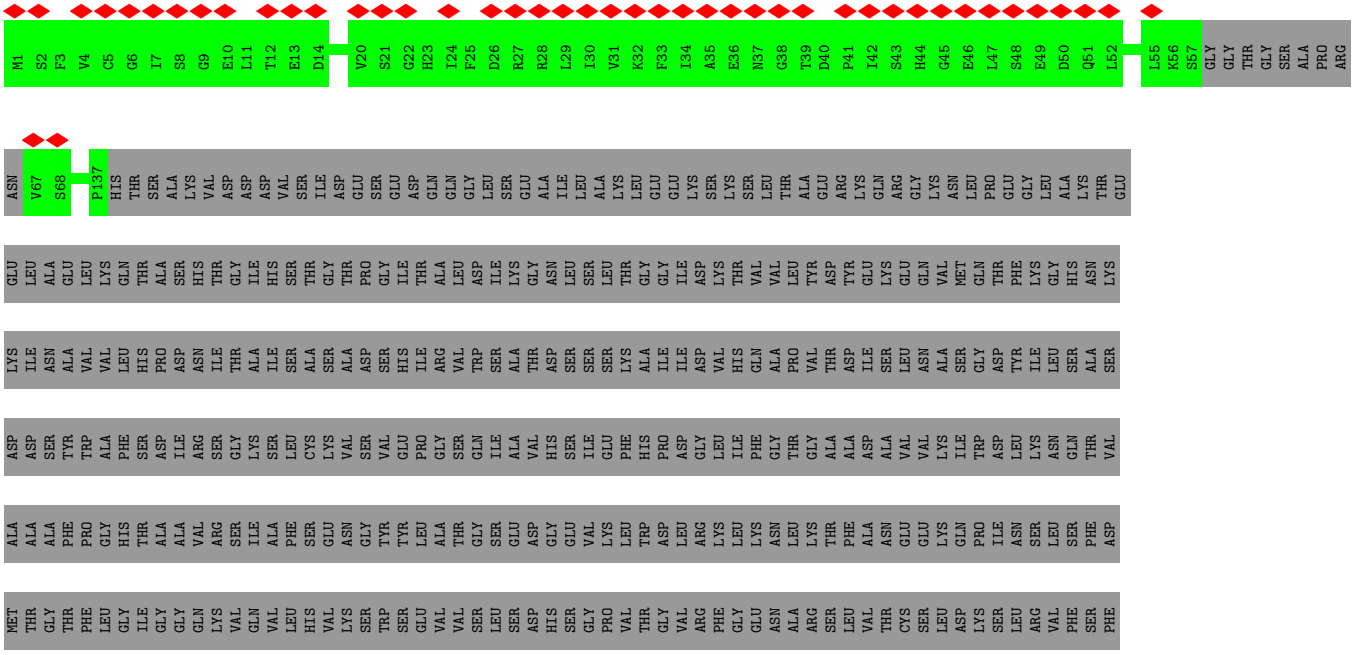
• Molecule 38: Pre-mRNA-processing factor 19





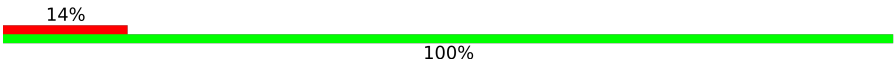
• Molecule 38: Pre-mRNA-processing factor 19

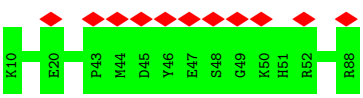
Chain t:



• Molecule 39: Peptidyl-prolyl cis-trans isomerase E

Chain y:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	247908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	10.125	Depositor
Minimum map value	0.000	Depositor
Average map value	0.070	Depositor
Map value standard deviation	0.281	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	258.9587, 300.6003, 307.1068	wwPDB
Map dimensions	199, 231, 236	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3013, 1.3013, 1.3013	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.69	0/918	1.35	3/1424 (0.2%)
2	5	1.08	4/2623 (0.2%)	1.51	35/4079 (0.9%)
3	6	0.84	0/2410	1.39	25/3752 (0.7%)
4	A	0.51	0/16860	0.82	19/22857 (0.1%)
5	C	0.55	1/7310 (0.0%)	0.85	13/9907 (0.1%)
6	D	0.33	0/1649	0.68	0/2202
7	DX	0.53	0/5577	0.76	2/7566 (0.0%)
8	E	0.47	0/2502	0.78	1/3385 (0.0%)
9	I	0.49	0/6307	0.74	3/8518 (0.0%)
10	IN	0.39	0/71	1.37	0/106
11	J	0.50	0/5008	0.80	5/6737 (0.1%)
12	K	0.34	0/1689	0.62	0/2261
13	L	0.37	1/5101 (0.0%)	0.76	4/6840 (0.1%)
14	L1	0.37	0/3765	0.65	0/5090
15	L2	0.39	0/3024	0.73	0/4039
16	M	0.43	0/1680	0.82	1/2241 (0.0%)
17	N	0.67	1/1190 (0.1%)	0.79	0/1597
18	O	0.53	0/2783	0.84	6/3768 (0.2%)
19	P	0.38	0/1223	0.81	0/1626
20	PX	0.34	0/3893	0.69	0/5223
21	Q	0.43	0/11555	0.66	1/15627 (0.0%)
22	R	0.45	0/2254	0.84	2/3042 (0.1%)
23	S	0.34	0/1332	0.71	1/1801 (0.1%)
24	T	0.54	1/3161 (0.0%)	0.85	2/4283 (0.0%)
25	TF	0.41	0/4656	0.72	1/6312 (0.0%)
26	W	0.40	0/4180	0.79	2/5639 (0.0%)
27	X	0.31	0/666	0.69	1/879 (0.1%)
28	Z	0.27	0/573	0.69	0/766
29	a	0.42	0/643	0.78	1/865 (0.1%)
29	h	0.33	0/643	0.73	0/865
30	b	0.43	0/767	0.78	0/1022
30	i	0.31	0/649	0.71	0/866

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	c	0.42	1/628 (0.2%)	0.78	1/849 (0.1%)
31	j	0.34	0/628	0.68	0/849
32	d	0.39	0/757	0.70	0/1014
32	k	0.35	0/639	0.78	0/855
33	e	0.42	0/676	0.73	0/910
33	l	0.34	0/676	0.72	0/910
34	f	0.47	0/569	0.67	0/770
34	m	0.39	0/569	0.73	0/770
35	g	0.36	0/616	0.76	0/821
35	n	0.33	0/616	0.71	0/821
36	o	0.34	0/1358	0.67	0/1837
37	p	0.32	0/638	0.67	0/850
38	q	0.34	0/953	0.63	0/1284
38	r	0.33	0/1018	0.68	0/1374
38	s	0.34	0/3633	0.65	0/4914
38	t	0.32	0/1006	0.62	0/1357
39	y	0.38	0/631	0.66	0/846
All	All	0.48	9/122273 (0.0%)	0.81	129/166216 (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
4	A	0	29
5	C	0	16
7	DX	0	5
8	E	0	3
9	I	0	5
11	J	0	8
13	L	0	9
15	L2	0	2
16	M	0	3
18	O	0	6
19	P	0	1
20	PX	0	1
22	R	0	4
24	T	0	7
25	TF	0	2
26	W	0	3
All	All	0	104

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	96	CYS	CB-SG	-6.74	1.70	1.82
2	5	27	G	C8-N7	-6.08	1.27	1.30
2	5	99	G	N3-C4	-5.59	1.31	1.35
31	c	69	ILE	C-N	-5.52	1.21	1.34
24	T	286	CYS	CB-SG	-5.39	1.73	1.81

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	70	G	O5'-P-OP1	16.43	130.41	110.70
2	5	27	G	O4'-C1'-N9	-11.37	99.11	108.20
9	I	628	ASP	CB-CG-OD1	10.90	128.11	118.30
13	L	27	GLY	N-CA-C	10.79	140.09	113.10
24	T	289	ASP	CB-CG-OD1	10.31	127.58	118.30

There are no chirality outliers.

5 of 104 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	167	ASP	Peptide
4	A	239	VAL	Peptide
4	A	63	HIS	Peptide
4	A	68	SER	Peptide
4	A	76	ARG	Sidechain

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	2	1268	0	715	7	0
2	5	2350	0	1189	13	0
3	6	2153	0	1088	18	0
4	A	16424	0	16438	85	0
5	C	7153	0	7140	32	0
6	D	1629	0	1627	5	0
7	DX	5465	0	5468	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	2445	0	2362	5	0
9	I	6169	0	6076	22	0
10	IN	425	0	274	4	0
11	J	4895	0	4774	21	0
12	K	1666	0	1707	1	0
13	L	5030	0	5111	18	0
14	L1	3683	0	3664	17	0
15	L2	2974	0	2960	11	0
16	M	1654	0	1626	9	0
17	N	1163	0	1142	6	0
18	O	2721	0	2661	13	0
19	P	1207	0	1182	3	0
20	PX	3838	0	3891	12	0
21	Q	11293	0	11206	17	0
22	R	2209	0	2212	10	0
23	S	1303	0	1282	3	0
24	T	3082	0	3042	9	0
25	TF	4542	0	4481	18	0
26	W	4072	0	3967	19	0
27	X	661	0	679	2	0
28	Z	569	0	603	1	0
29	a	635	0	643	0	0
29	h	635	0	643	0	0
30	b	755	0	772	0	0
30	i	639	0	655	0	0
31	c	622	0	672	0	0
31	j	622	0	673	0	0
32	d	749	0	764	0	0
32	k	632	0	662	0	0
33	e	665	0	666	0	0
33	l	665	0	666	0	0
34	f	558	0	560	0	0
34	m	558	0	560	0	0
35	g	608	0	624	0	0
35	n	608	0	624	0	0
36	o	1335	0	1367	0	0
37	p	626	0	646	0	0
38	q	941	0	941	0	0
38	r	1004	0	1003	0	0
38	s	3571	0	3573	0	0
38	t	993	0	1004	0	0
39	y	619	0	598	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	6	6	0	0	0	0
40	C	1	0	0	0	0
41	A	36	0	6	0	0
41	J	36	0	6	2	0
42	C	32	0	12	6	0
43	L2	1	0	0	0	0
43	N	3	0	0	0	0
43	O	3	0	0	0	0
All	All	120201	0	116907	348	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 2.

The worst 5 of 348 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:67:G:O2'	4:A:42:GLY:O	1.97	0.81
5:C:145:LYS:NZ	42:C:1101:GTP:O2G	2.14	0.80
1:2:20:A:OP1	3:6:77:A:N6	2.16	0.78
3:6:59:U:OP2	4:A:655:ARG:NH1	2.18	0.76
9:I:586:GLN:OE1	11:J:305:LYS:NZ	2.19	0.75

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
4	A	1976/2329 (85%)	1789 (90%)	101 (5%)	86 (4%)	2 15
5	C	896/974 (92%)	800 (89%)	66 (7%)	30 (3%)	4 21
6	D	192/267 (72%)	185 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	DX	680/739 (92%)	634 (93%)	36 (5%)	10 (2%)	10 42
8	E	310/331 (94%)	295 (95%)	13 (4%)	2 (1%)	25 64
9	I	743/855 (87%)	702 (94%)	37 (5%)	4 (0%)	29 68
11	J	570/744 (77%)	531 (93%)	22 (4%)	17 (3%)	4 24
12	K	201/238 (84%)	196 (98%)	4 (2%)	1 (0%)	29 68
13	L	611/755 (81%)	570 (93%)	28 (5%)	13 (2%)	7 33
14	L1	468/533 (88%)	435 (93%)	26 (6%)	7 (2%)	10 42
15	L2	358/460 (78%)	336 (94%)	16 (4%)	6 (2%)	9 39
16	M	190/234 (81%)	179 (94%)	6 (3%)	5 (3%)	5 27
17	N	140/147 (95%)	123 (88%)	10 (7%)	7 (5%)	2 12
18	O	334/408 (82%)	302 (90%)	23 (7%)	9 (3%)	5 26
19	P	146/230 (64%)	130 (89%)	10 (7%)	6 (4%)	3 16
20	PX	470/809 (58%)	468 (100%)	2 (0%)	0	100 100
21	Q	1376/1467 (94%)	1336 (97%)	39 (3%)	1 (0%)	51 85
22	R	274/535 (51%)	243 (89%)	26 (10%)	5 (2%)	8 37
23	S	167/169 (99%)	158 (95%)	9 (5%)	0	100 100
24	T	385/494 (78%)	342 (89%)	35 (9%)	8 (2%)	7 33
25	TF	551/830 (66%)	507 (92%)	35 (6%)	9 (2%)	9 40
26	W	490/567 (86%)	435 (89%)	40 (8%)	15 (3%)	4 23
27	X	78/500 (16%)	75 (96%)	2 (3%)	1 (1%)	12 45
28	Z	67/69 (97%)	64 (96%)	3 (4%)	0	100 100
29	a	79/136 (58%)	78 (99%)	1 (1%)	0	100 100
29	h	79/136 (58%)	69 (87%)	8 (10%)	2 (2%)	5 28
30	b	92/160 (58%)	87 (95%)	5 (5%)	0	100 100
30	i	75/160 (47%)	69 (92%)	5 (7%)	1 (1%)	12 45
31	c	78/127 (61%)	76 (97%)	2 (3%)	0	100 100
31	j	78/127 (61%)	72 (92%)	6 (8%)	0	100 100
32	d	90/118 (76%)	86 (96%)	4 (4%)	0	100 100
32	k	75/118 (64%)	72 (96%)	3 (4%)	0	100 100
33	e	78/90 (87%)	74 (95%)	1 (1%)	3 (4%)	3 18
33	l	78/90 (87%)	73 (94%)	3 (4%)	2 (3%)	5 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	f	70/85 (82%)	68 (97%)	2 (3%)	0	100 100
34	m	70/85 (82%)	66 (94%)	3 (4%)	1 (1%)	11 43
35	g	75/77 (97%)	72 (96%)	3 (4%)	0	100 100
35	n	75/77 (97%)	68 (91%)	5 (7%)	2 (3%)	5 26
36	o	160/253 (63%)	154 (96%)	5 (3%)	1 (1%)	25 64
37	p	74/217 (34%)	70 (95%)	4 (5%)	0	100 100
38	q	117/492 (24%)	115 (98%)	2 (2%)	0	100 100
38	r	129/492 (26%)	127 (98%)	1 (1%)	1 (1%)	19 57
38	s	465/492 (94%)	450 (97%)	14 (3%)	1 (0%)	47 82
38	t	124/492 (25%)	121 (98%)	3 (2%)	0	100 100
39	y	77/79 (98%)	76 (99%)	1 (1%)	0	100 100
All	All	13911/18787 (74%)	12978 (93%)	677 (5%)	256 (2%)	12 37

5 of 256 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	68	SER
4	A	69	ARG
4	A	167	ASP
4	A	287	ILE
4	A	305	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	1790/2100 (85%)	1730 (97%)	60 (3%)	37 72
5	C	793/861 (92%)	774 (98%)	19 (2%)	49 79
6	D	173/230 (75%)	170 (98%)	3 (2%)	60 85
7	DX	604/652 (93%)	597 (99%)	7 (1%)	71 90
8	E	275/291 (94%)	268 (98%)	7 (2%)	47 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	660/754 (88%)	641 (97%)	19 (3%)	42	76
11	J	508/650 (78%)	501 (99%)	7 (1%)	67	88
12	K	183/214 (86%)	181 (99%)	2 (1%)	73	90
13	L	543/645 (84%)	523 (96%)	20 (4%)	34	70
14	L1	406/452 (90%)	393 (97%)	13 (3%)	39	74
15	L2	331/417 (79%)	327 (99%)	4 (1%)	71	90
16	M	178/212 (84%)	169 (95%)	9 (5%)	24	60
17	N	125/129 (97%)	121 (97%)	4 (3%)	39	74
18	O	295/351 (84%)	290 (98%)	5 (2%)	60	85
19	P	129/197 (66%)	124 (96%)	5 (4%)	32	69
20	PX	423/724 (58%)	419 (99%)	4 (1%)	78	92
21	Q	1235/1311 (94%)	1222 (99%)	13 (1%)	73	90
22	R	235/447 (53%)	219 (93%)	16 (7%)	16	48
23	S	137/137 (100%)	134 (98%)	3 (2%)	52	81
24	T	335/421 (80%)	319 (95%)	16 (5%)	25	62
25	TF	493/718 (69%)	479 (97%)	14 (3%)	43	77
26	W	444/502 (88%)	427 (96%)	17 (4%)	33	69
27	X	69/443 (16%)	64 (93%)	5 (7%)	14	45
28	Z	63/63 (100%)	62 (98%)	1 (2%)	62	86
29	a	71/106 (67%)	70 (99%)	1 (1%)	67	88
29	h	71/106 (67%)	70 (99%)	1 (1%)	67	88
30	b	79/116 (68%)	78 (99%)	1 (1%)	69	89
30	i	70/116 (60%)	68 (97%)	2 (3%)	42	76
31	c	73/98 (74%)	73 (100%)	0	100	100
31	j	73/98 (74%)	73 (100%)	0	100	100
32	d	84/103 (82%)	81 (96%)	3 (4%)	35	70
32	k	72/103 (70%)	71 (99%)	1 (1%)	67	88
33	e	71/81 (88%)	71 (100%)	0	100	100
33	l	71/81 (88%)	70 (99%)	1 (1%)	67	88
34	f	61/71 (86%)	61 (100%)	0	100	100
34	m	61/71 (86%)	59 (97%)	2 (3%)	38	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	g	69/69 (100%)	69 (100%)	0	100 100
35	n	69/69 (100%)	68 (99%)	1 (1%)	67 88
36	o	151/225 (67%)	150 (99%)	1 (1%)	84 94
37	p	68/192 (35%)	67 (98%)	1 (2%)	65 87
38	q	108/417 (26%)	107 (99%)	1 (1%)	78 92
38	r	114/417 (27%)	111 (97%)	3 (3%)	46 78
38	s	396/417 (95%)	393 (99%)	3 (1%)	81 93
38	t	115/417 (28%)	115 (100%)	0	100 100
39	y	64/64 (100%)	64 (100%)	0	100 100
All	All	12438/16358 (76%)	12143 (98%)	295 (2%)	51 79

5 of 295 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	T	404	ASP
36	o	106	ILE
25	TF	200	GLU
26	W	385	LYS
9	I	159	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
24	T	238	HIS
33	e	37	HIS
32	k	69	ASN
34	f	70	ASN
8	E	252	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	38/228 (16%)	18 (47%)	4 (10%)
10	IN	1/51 (1%)	1 (100%)	0
2	5	110/112 (98%)	32 (29%)	12 (10%)
3	6	100/101 (99%)	45 (45%)	13 (13%)
All	All	249/492 (50%)	96 (38%)	29 (11%)

5 of 96 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	U
1	2	19	U
1	2	21	G
1	2	25	A
1	2	26	G

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	112	G
3	6	85	G
3	6	28	G
3	6	48	A
3	6	23	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 14 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
41	IHP	J	3000	-	36,36,36	2.27	10 (27%)	54,60,60	0.97	3 (5%)
41	IHP	A	3000	-	36,36,36	2.02	6 (16%)	54,60,60	1.22	7 (12%)
42	GTP	C	1101	40	26,34,34	1.49	2 (7%)	32,54,54	2.20	7 (21%)

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
41	IHP	J	3000	-	-	4/30/54/54	0/1/1/1
41	IHP	A	3000	-	-	3/30/54/54	0/1/1/1
42	GTP	C	1101	40	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	J	3000	IHP	C3-C2	-5.48	1.40	1.52
41	A	3000	IHP	P5-O15	5.03	1.68	1.59
41	A	3000	IHP	P4-O14	4.82	1.68	1.59
41	A	3000	IHP	P6-O16	4.76	1.68	1.59
41	J	3000	IHP	P3-O13	4.73	1.68	1.59

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	C	1101	GTP	PB-O3B-PG	-6.27	111.31	132.83
42	C	1101	GTP	C5-C6-N1	5.20	123.14	113.95
42	C	1101	GTP	C2-N1-C6	-4.87	116.14	125.10
42	C	1101	GTP	O6-C6-C5	-3.72	117.10	124.37
42	C	1101	GTP	O3G-PG-O3B	3.35	115.87	104.64

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	A	3000	IHP	C2-O12-P2-O22
41	J	3000	IHP	C5-O15-P5-O25
41	A	3000	IHP	C4-O14-P4-O44
41	A	3000	IHP	C5-O15-P5-O35
41	J	3000	IHP	C4-O14-P4-O34

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	J	3000	IHP	2	0

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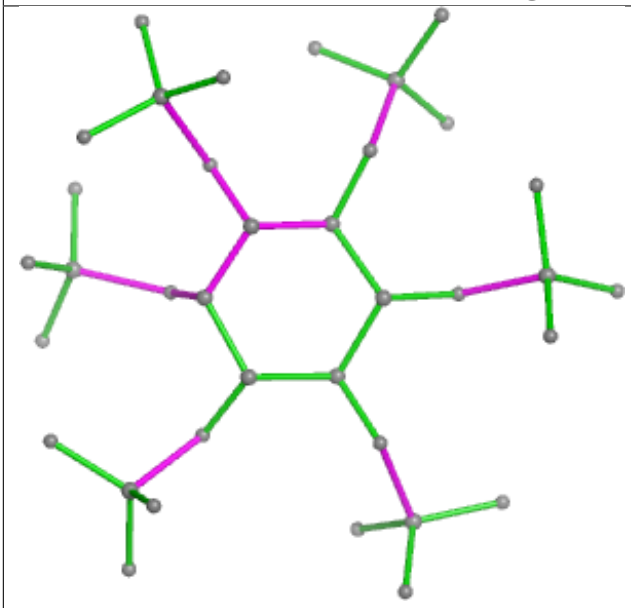
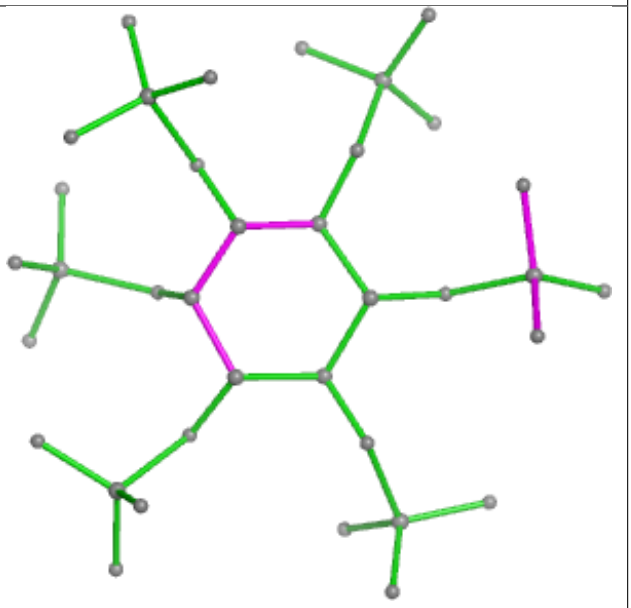
Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	C	1101	GTP	6	0

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

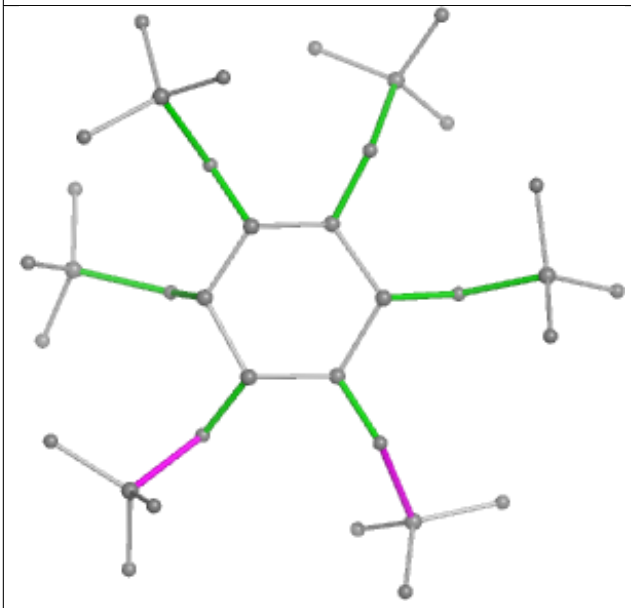
Ligand IHP J 3000



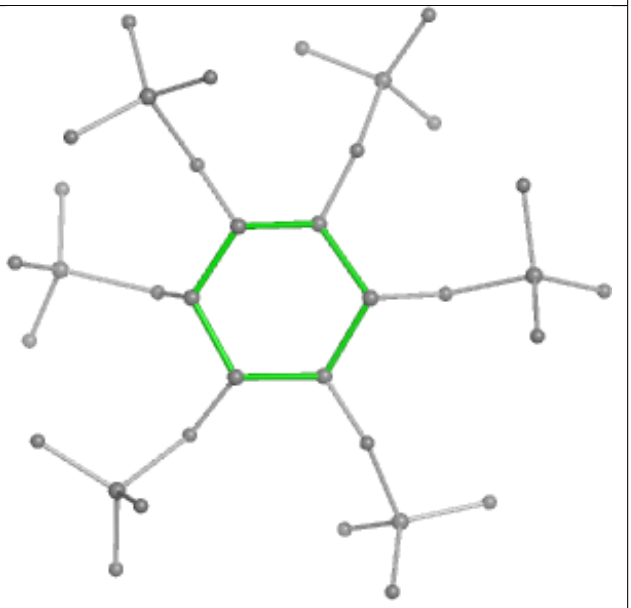
Bond lengths



Bond angles

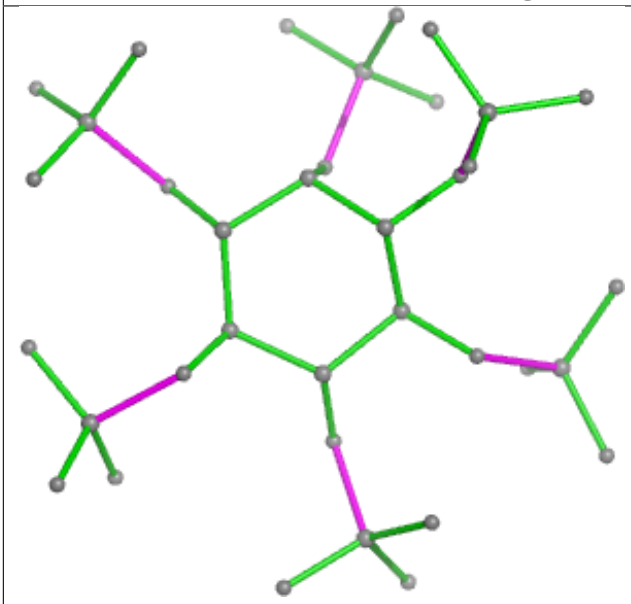


Torsions

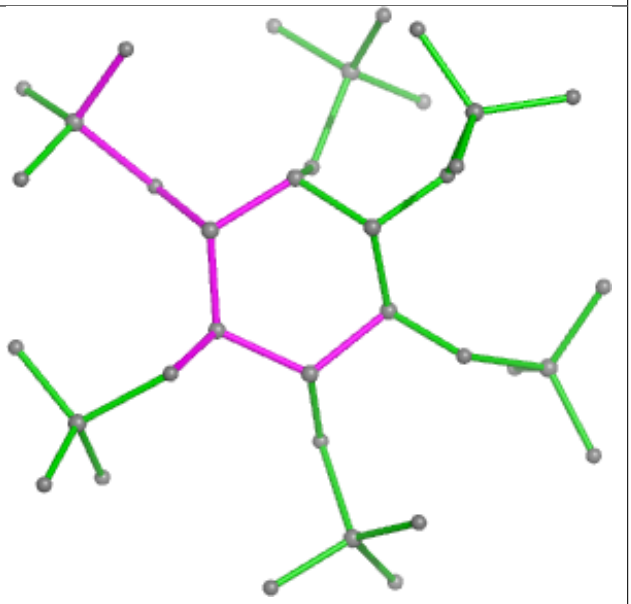


Rings

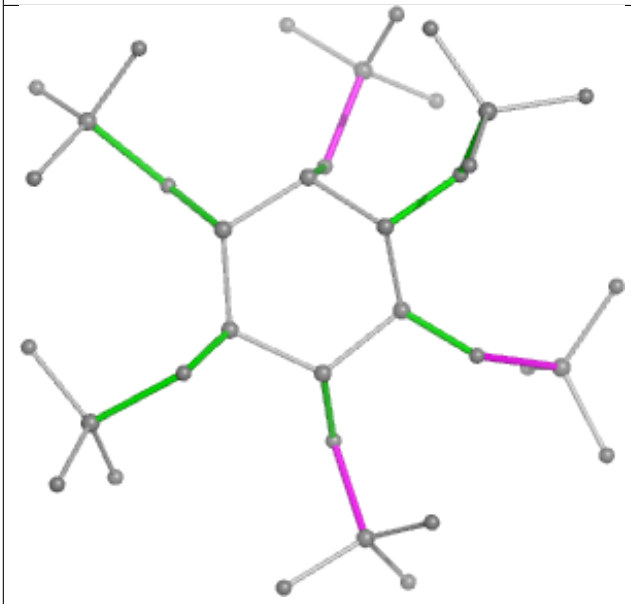
Ligand IHP A 3000



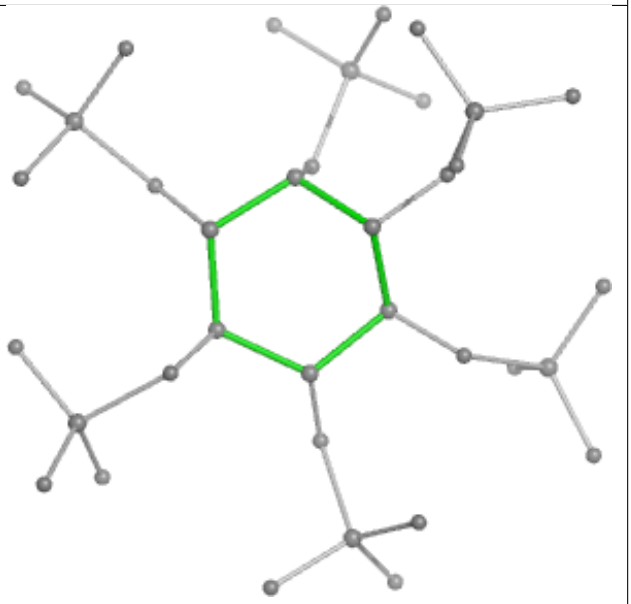
Bond lengths



Bond angles

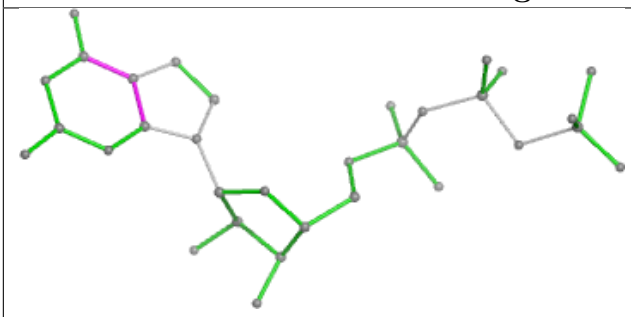


Torsions

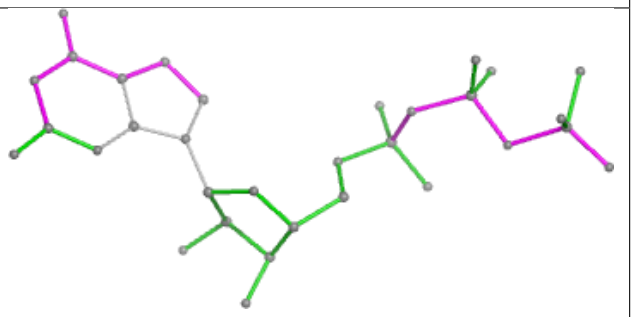


Rings

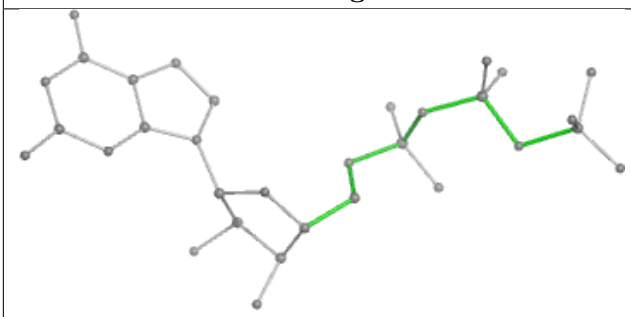
Ligand GTP C 1101



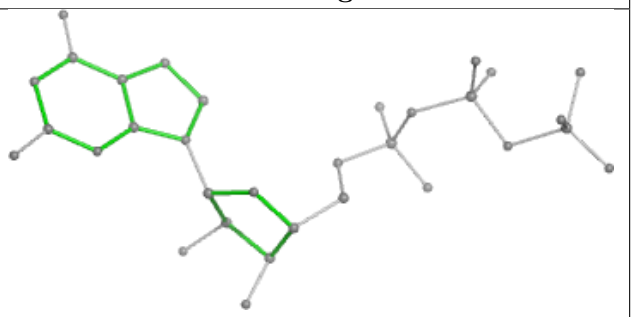
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

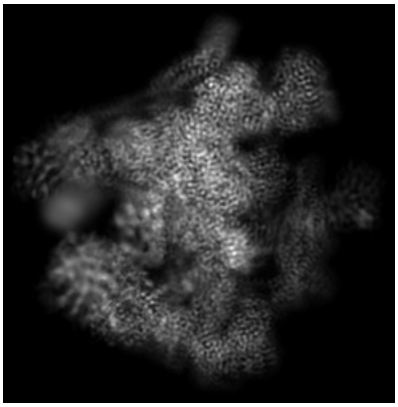
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19398. These allow visual inspection of the internal detail of the map and identification of artifacts.

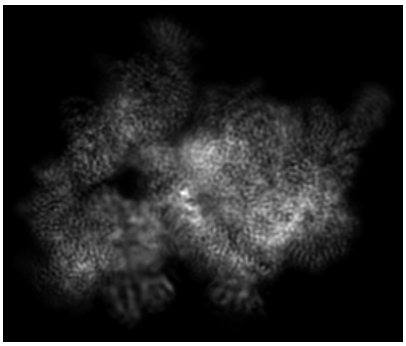
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

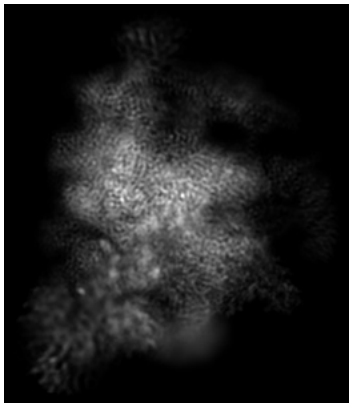
6.1.1 Primary map



X



Y

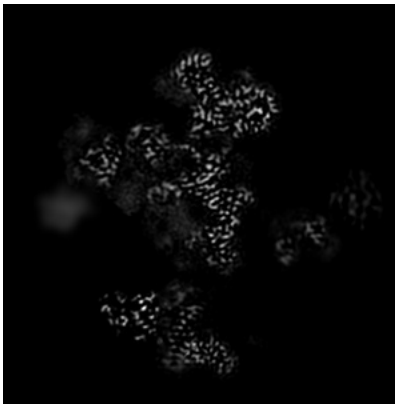


Z

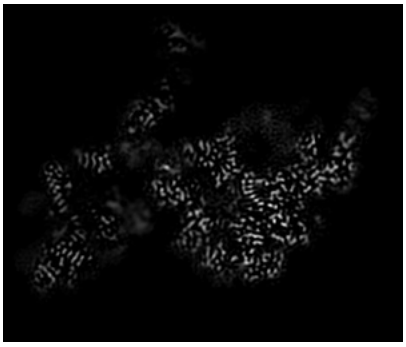
The images above show the map projected in three orthogonal directions.

6.2 Central slices

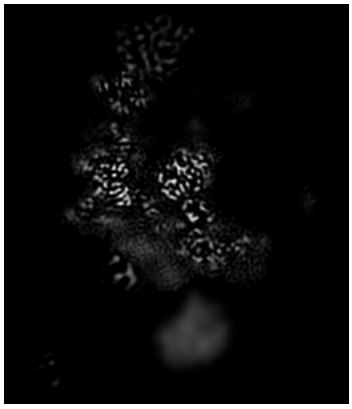
6.2.1 Primary map



X Index: 99



Y Index: 115

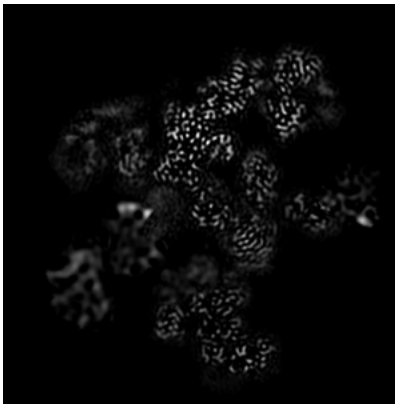


Z Index: 118

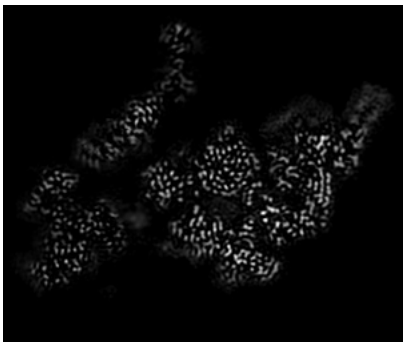
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

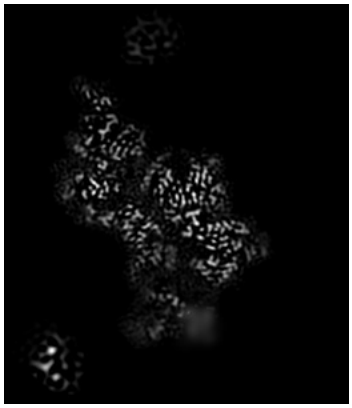
6.3.1 Primary map



X Index: 73



Y Index: 122

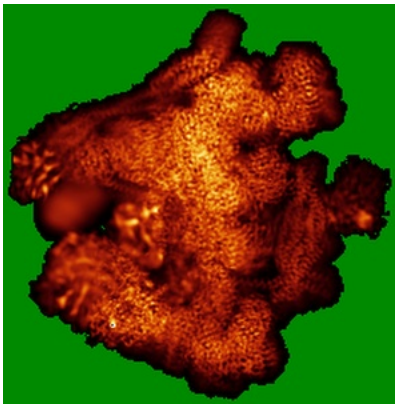


Z Index: 132

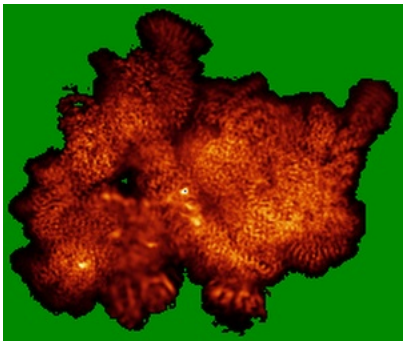
The images above show the largest variance slices of the map in three orthogonal directions.

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

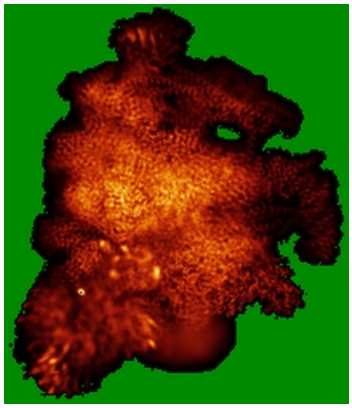
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

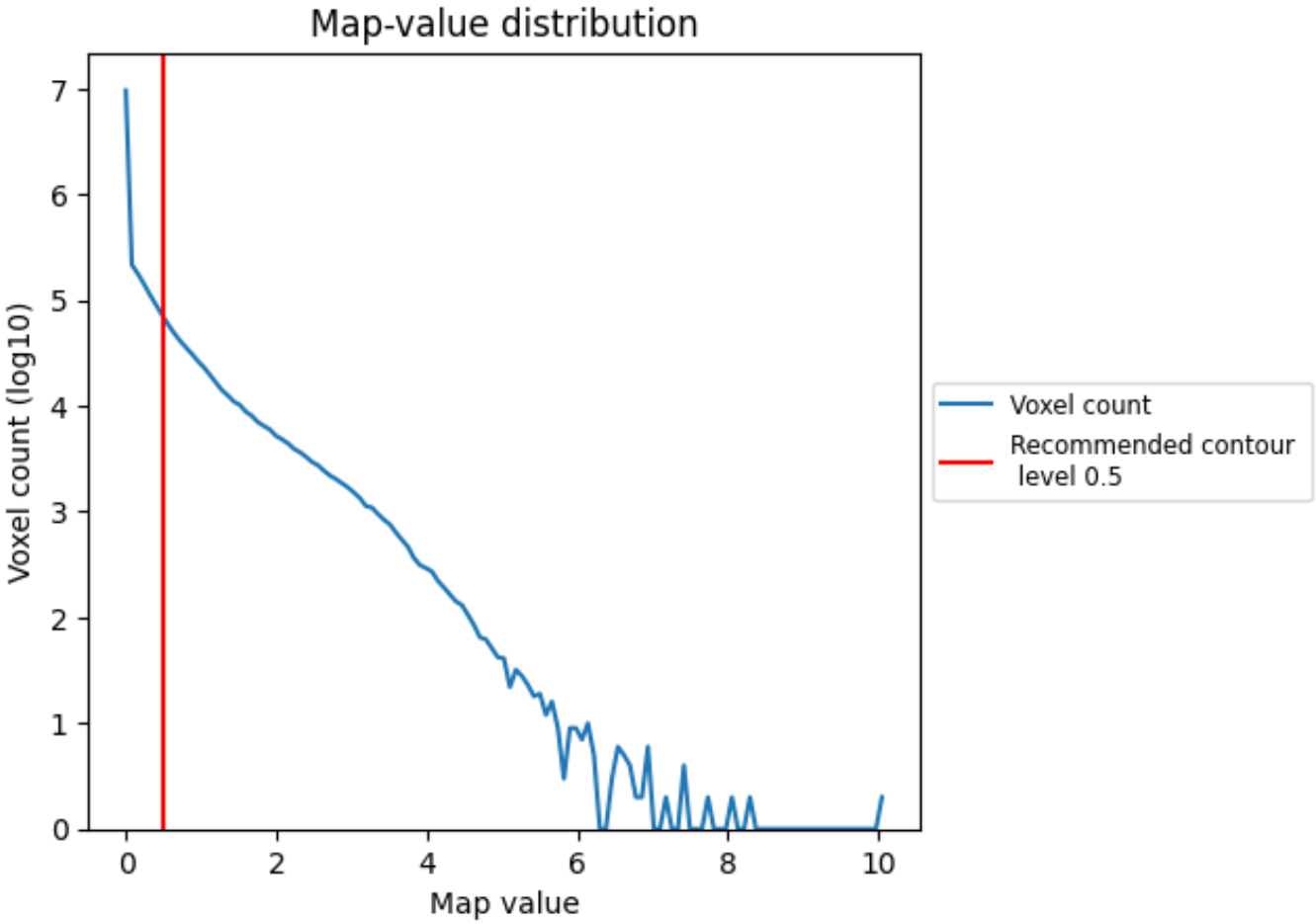
6.6 Mask visualisation (i)

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

7 Map analysis

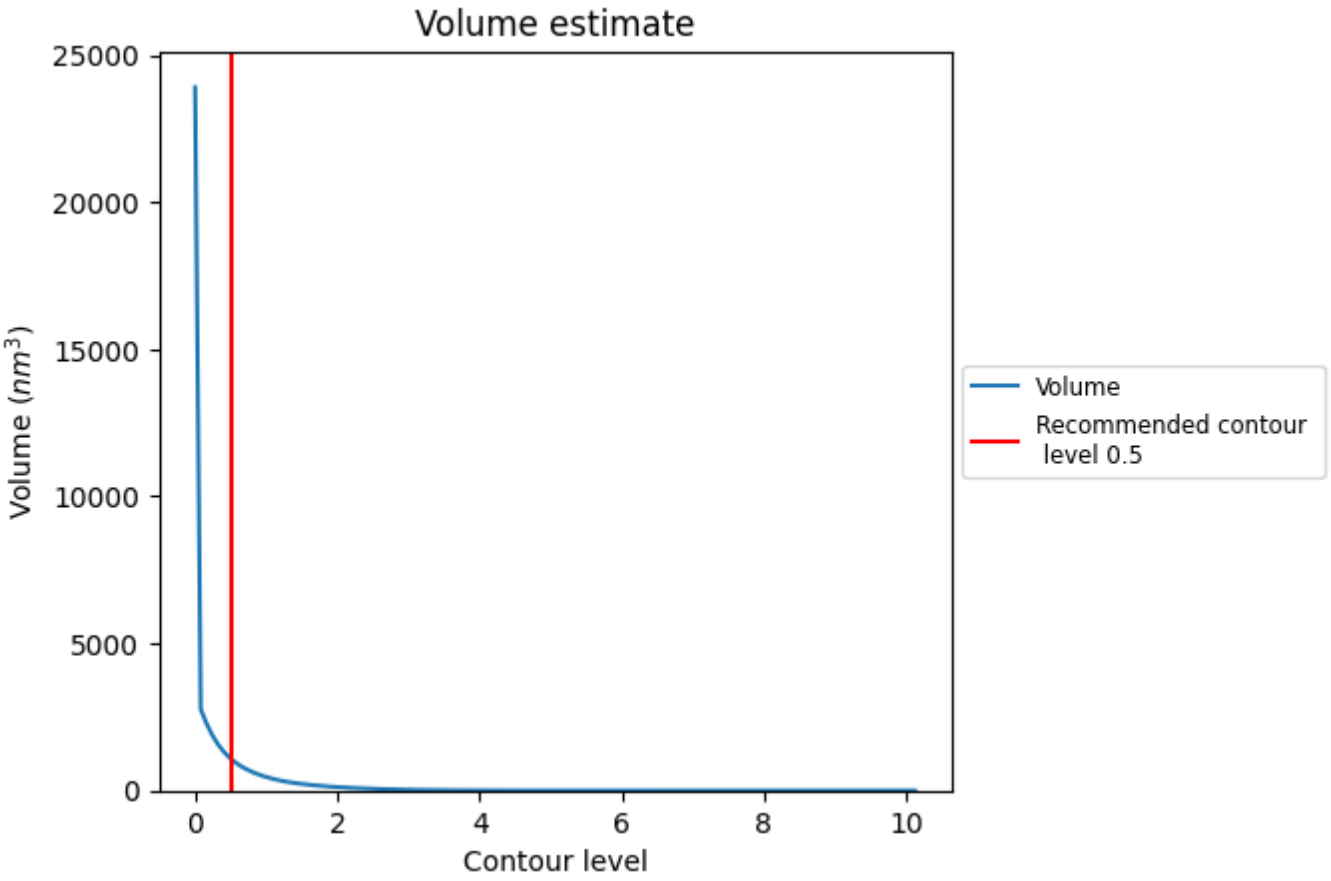
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 1088 nm^3; this corresponds to an approximate mass of 983 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

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

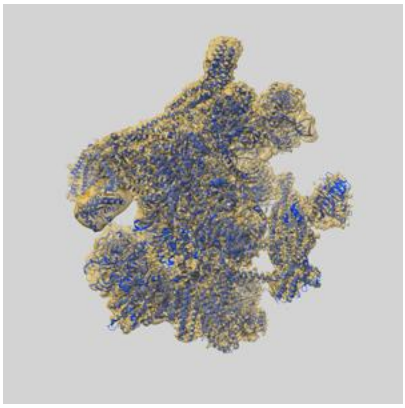
8 Fourier-Shell correlation (i)

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

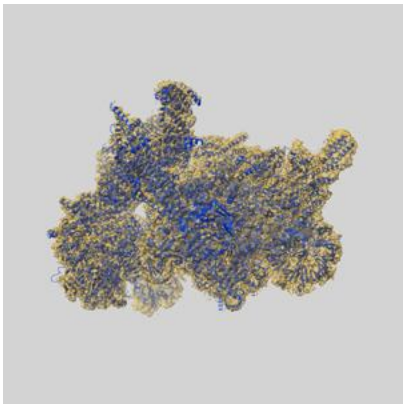
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19398 and PDB model 8RO1. Per-residue inclusion information can be found in section 3 on page 13.

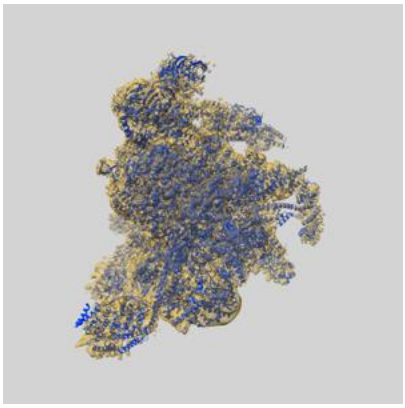
9.1 Map-model overlay



X



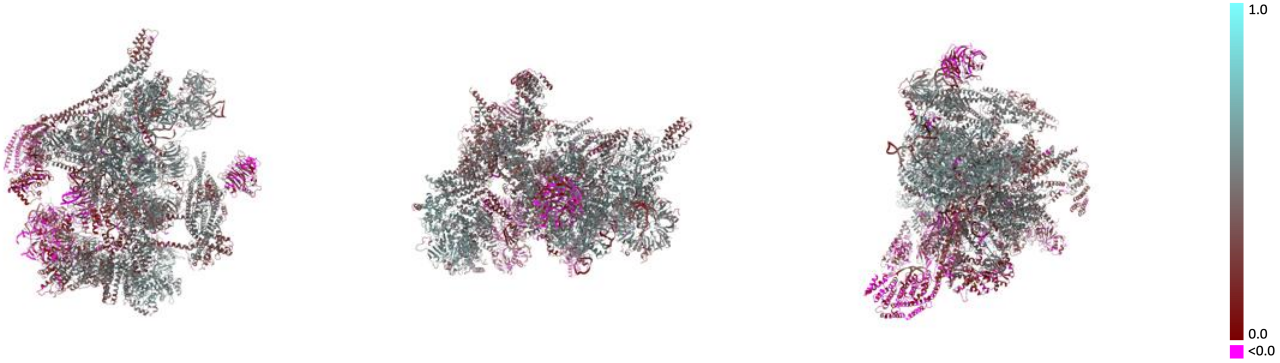
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

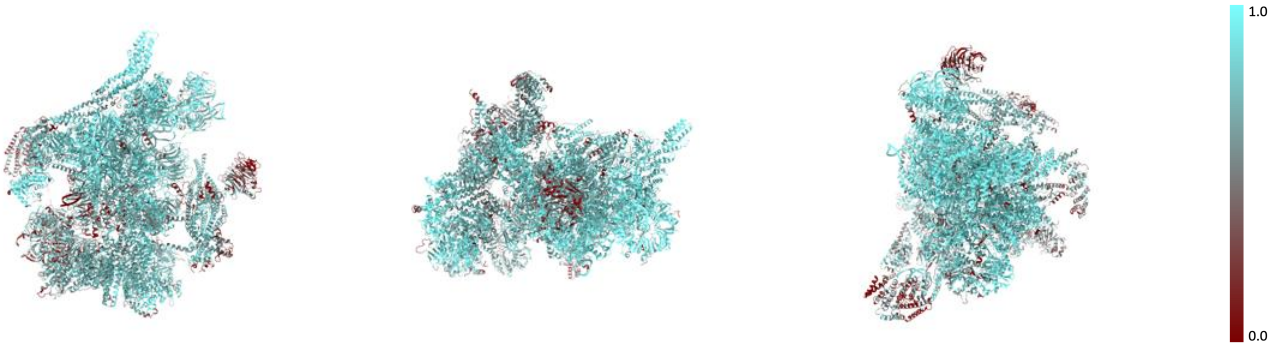
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

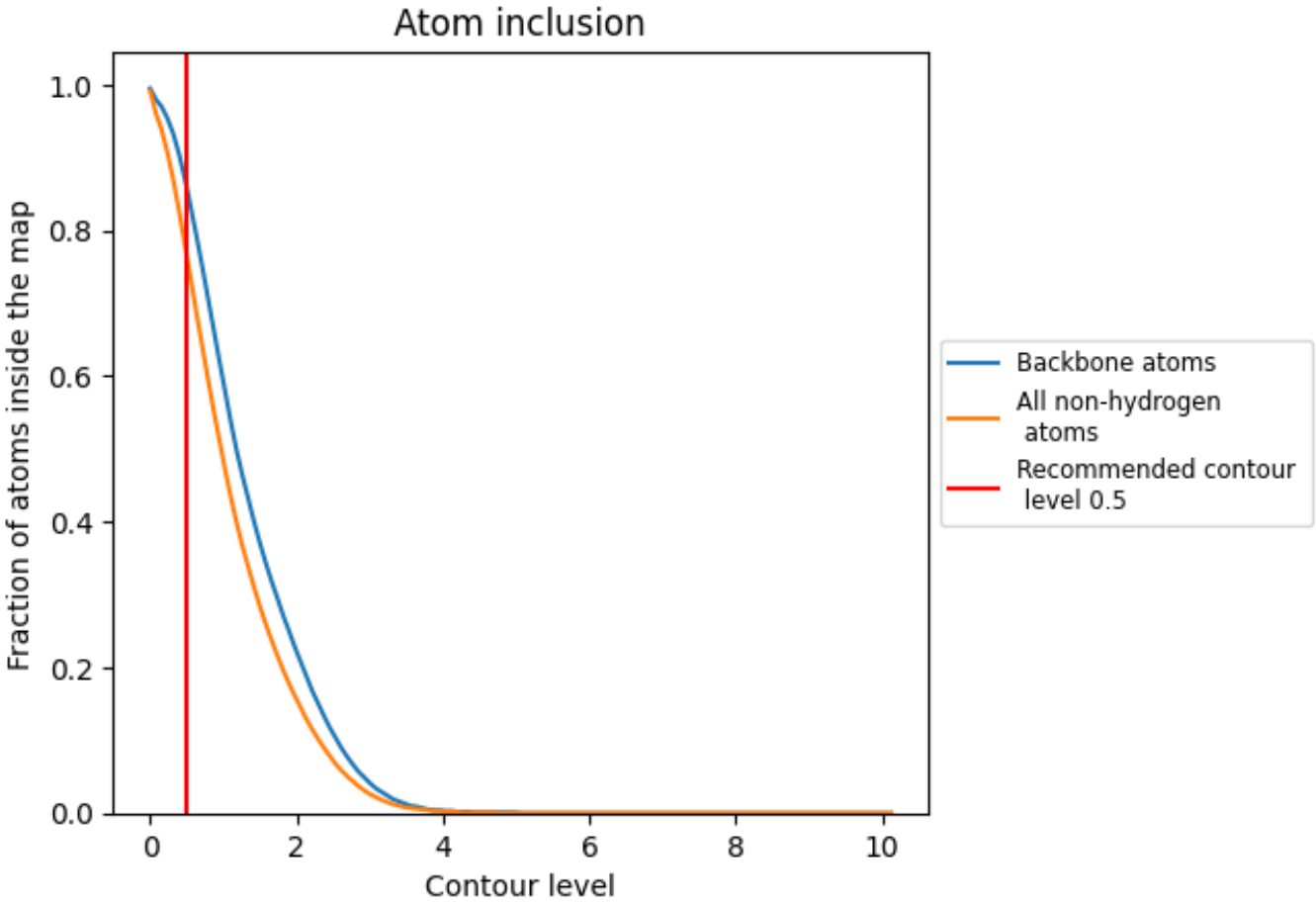
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 77% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.3730
2	0.7910	0.1990
5	0.9250	0.3860
6	0.9140	0.3690
A	0.8850	0.4550
C	0.9180	0.5080
D	0.5890	0.2280
DX	0.6750	0.3620
E	0.8960	0.5150
I	0.8270	0.4520
IN	0.6210	0.1200
J	0.7830	0.4420
K	0.6830	0.4120
L	0.6470	0.3620
L1	0.6700	0.1440
L2	0.8300	0.3910
M	0.7920	0.3580
N	0.9560	0.5340
O	0.8550	0.4330
P	0.5210	0.2890
PX	0.4250	0.0570
Q	0.8260	0.5110
R	0.8360	0.4130
S	0.7870	0.4330
T	0.9160	0.5250
TF	0.8020	0.3470
W	0.6480	0.1480
X	0.6800	0.3030
Z	0.5270	0.3770
a	0.9090	0.4940
b	0.8700	0.4320
c	0.9090	0.4700
d	0.7610	0.3600
e	0.8350	0.4480
f	0.8730	0.4600

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Chain	Atom inclusion	Q-score
g	0.7800	0.4020
h	0.7000	0.0770
i	0.6120	0.0830
j	0.5460	0.0620
k	0.5100	0.0410
l	0.5990	0.0350
m	0.6370	0.0790
n	0.6310	0.0690
o	0.6180	0.0970
p	0.6400	0.0810
q	0.7330	0.4560
r	0.4840	0.3560
s	0.4260	0.1830
t	0.5390	0.3670
y	0.6720	0.4330