wwPDB EM Validation Summary Report (i)

Jul 8, 2024 – 11:31 am BST

PDB ID	:	7QTT
EMDB ID	:	EMD-14146
Title	:	Structural organization of a late activated human spliceosome (Baqr, core region)
Authors	:	Cretu, C.; Pena, V.
Deposited on	:	2022-01-15
Resolution	:	3.10 Å(reported)
Based on initial models	:	6QDV, 6FF4, 6FF7, 5Z57

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 (i) 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 (i)) were used in the production of this report:

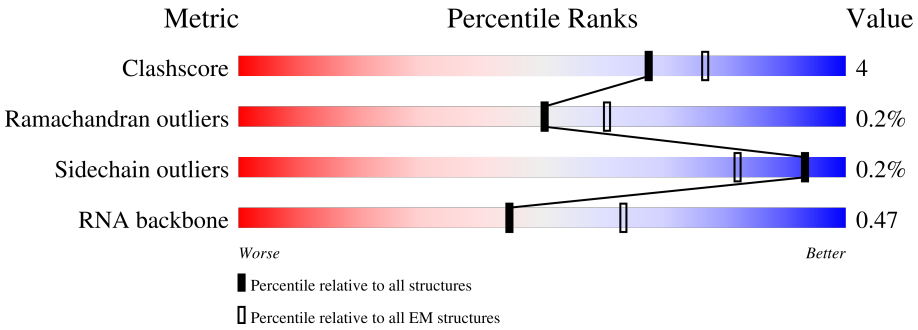
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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	A	1217	32% 92%
2	B	86	80% 19%
3	C	1304	60% 38%
4	D	110	68% 13% 19%
5	E	895	6% 20% 78%
6	F	424	18% 17% 82%
7	G	476	6% 14% 86%

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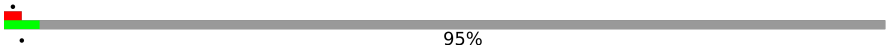
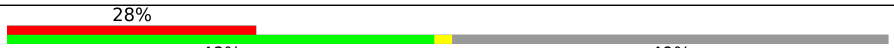
Mol	Chain	Length	Quality of chain
8	I	464	
9	J	501	
10	L	619	
11	N	1041	
12	O	514	
13	P	802	
14	Q	229	
15	T	144	
16	U	420	
17	V	492	
18	W	908	
19	X	848	
20	Y	536	
21	Z	343	
22	a	2335	
23	b	972	
24	d	106	
25	e	117	
26	f	188	
27	g	319	
28	h	86	
29	i	92	
30	j	126	
31	k	119	
32	l	118	

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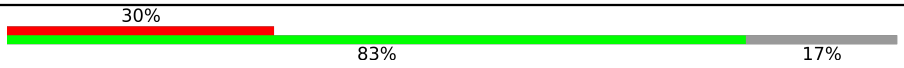
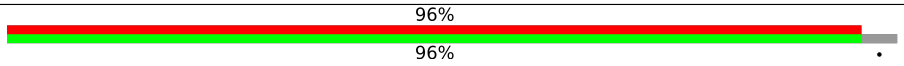
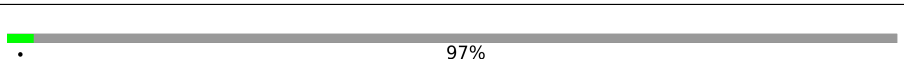
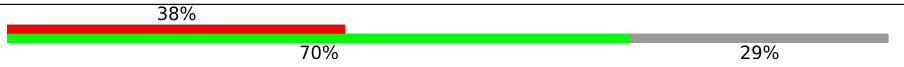
Mol	Chain	Length	Quality of chain
33	m	76	
34	n	240	
35	p	166	
36	q	2752	
37	u	520	

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 73537 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 protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	1164	5744	3416	1164	1164	0	0

- Molecule 2 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	70	350	210	70	70	0	0

- Molecule 3 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	815	5115	3242	928	930	15	0	0

- Molecule 4 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	89	649	399	117	120	13	0	0

- Molecule 5 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	198	1350	855	249	241	5	0	0

- Molecule 6 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	F	78	383	227	78	78	0	0

- Molecule 7 is a protein called G-patch domain and KOW motifs-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	67	Total	C	N	O	0	0
			364	228	68	68		

- Molecule 8 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	84	Total	C	N	O	S	0	0
			533	321	114	96	2		

- Molecule 9 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	72	Total	C	N	O	S	0	0
			510	325	93	88	4		

- Molecule 10 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	28	Total	C	N	O	S	0	0
			177	111	32	32	2		

- Molecule 11 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	792	Total	C	N	O	S	0	0
			6157	3898	1093	1138	28		

- Molecule 12 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	320	Total	C	N	O	S	0	0
			2517	1592	457	460	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	148	Total	C	N	O	S	0	0
			1151	737	202	208	4		

- Molecule 14 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	100	Total	C	N	O	S	0	0
			823	509	161	151	2		

- Molecule 15 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	142	Total	C	N	O	S	0	0
			1176	741	216	208	11		

- Molecule 16 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	295	Total	C	N	O	S	0	0
			2080	1290	380	392	18		

- Molecule 17 is a protein called Peptidyl-prolyl cis-trans isomerase-like 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	285	Total	C	N	O	S	0	0
			1996	1252	338	396	10		

- Molecule 18 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	459	Total	C	N	O	S	0	0
			2921	1817	533	559	12		

- Molecule 19 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	241	Total	C	N	O	S	0	0
			1587	1017	298	270	2		

- Molecule 20 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	306	Total	C	N	O	S	0	0
			2250	1412	411	417	10		

- Molecule 21 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	95	Total	C	N	O	S	0	0
			607	378	109	117	3		

- Molecule 22 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	1936	Total	C	N	O	S	0	0
			15194	9745	2709	2675	65		

- Molecule 23 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	898	Total	C	N	O	S	0	0
			7046	4513	1172	1327	34		

- Molecule 24 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	93	Total	C	N	O	P	0	0
			1989	889	364	643	93		

- Molecule 25 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	e	98	Total	C	N	O	P	0	0
			2070	926	347	699	98		

- Molecule 26 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	f	76	Total	C	N	O	P	0	0
			1600	716	265	543	76		

- Molecule 27 is a RNA chain called MINX.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	g	76	Total	C	N	O	P	0	0
			1559	697	250	536	76		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	h	66	Total 322	C 190	N 66	O 66	0	0

- Molecule 29 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	i	70	Total 346	C 206	N 70	O 70	0	0

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	j	68	Total 335	C 199	N 68	O 68	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
31	k	78	Total 388	C 232	N 78	O 78	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
32	l	68	Total 337	C 201	N 68	O 68	0	0

- Molecule 33 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	m	63	Total 309	C 183	N 63	O 63	0	0

- Molecule 34 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	n	64	Total 315	C 187	N 64	O 64	0	0

- Molecule 35 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	p	159	Total 776	C 457	N 159	O 160	0	0

- Molecule 36 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	74	Total 461	C 285	N 89	O 85	S 2	0	0

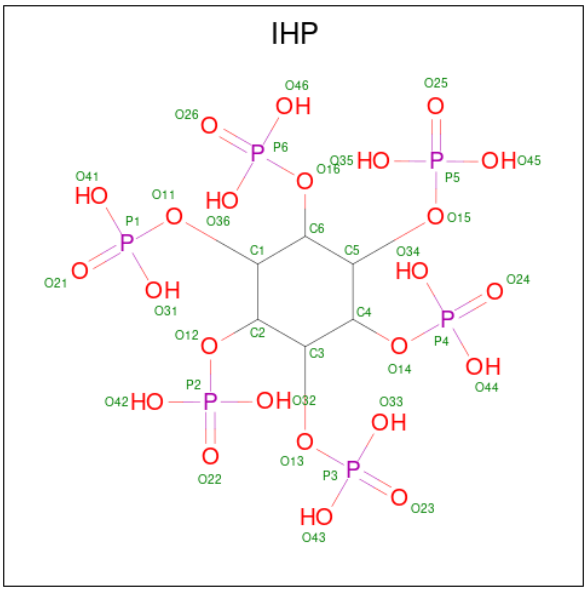
- Molecule 37 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	u	367	Total 1963	C 1181	N 382	O 399	S 1	0	0

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

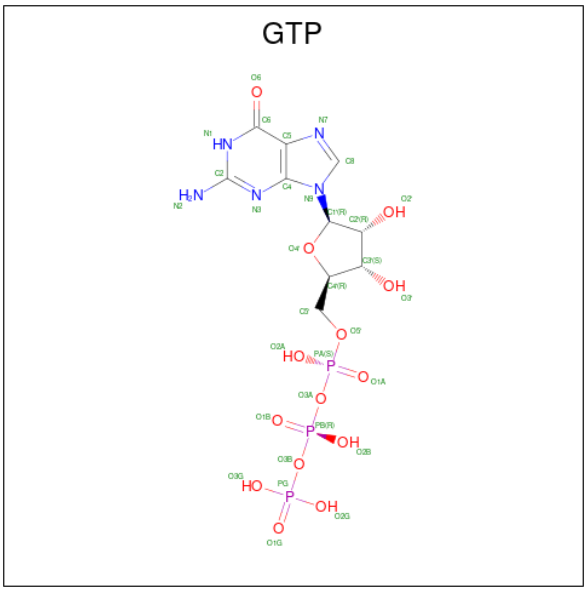
Mol	Chain	Residues	Atoms		AltConf
38	D	3	Total 3	Zn 3	0
38	I	1	Total 1	Zn 1	0
38	J	1	Total 1	Zn 1	0
38	T	3	Total 3	Zn 3	0
38	U	3	Total 3	Zn 3	0
38	Z	1	Total 1	Zn 1	0

- Molecule 39 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 40 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

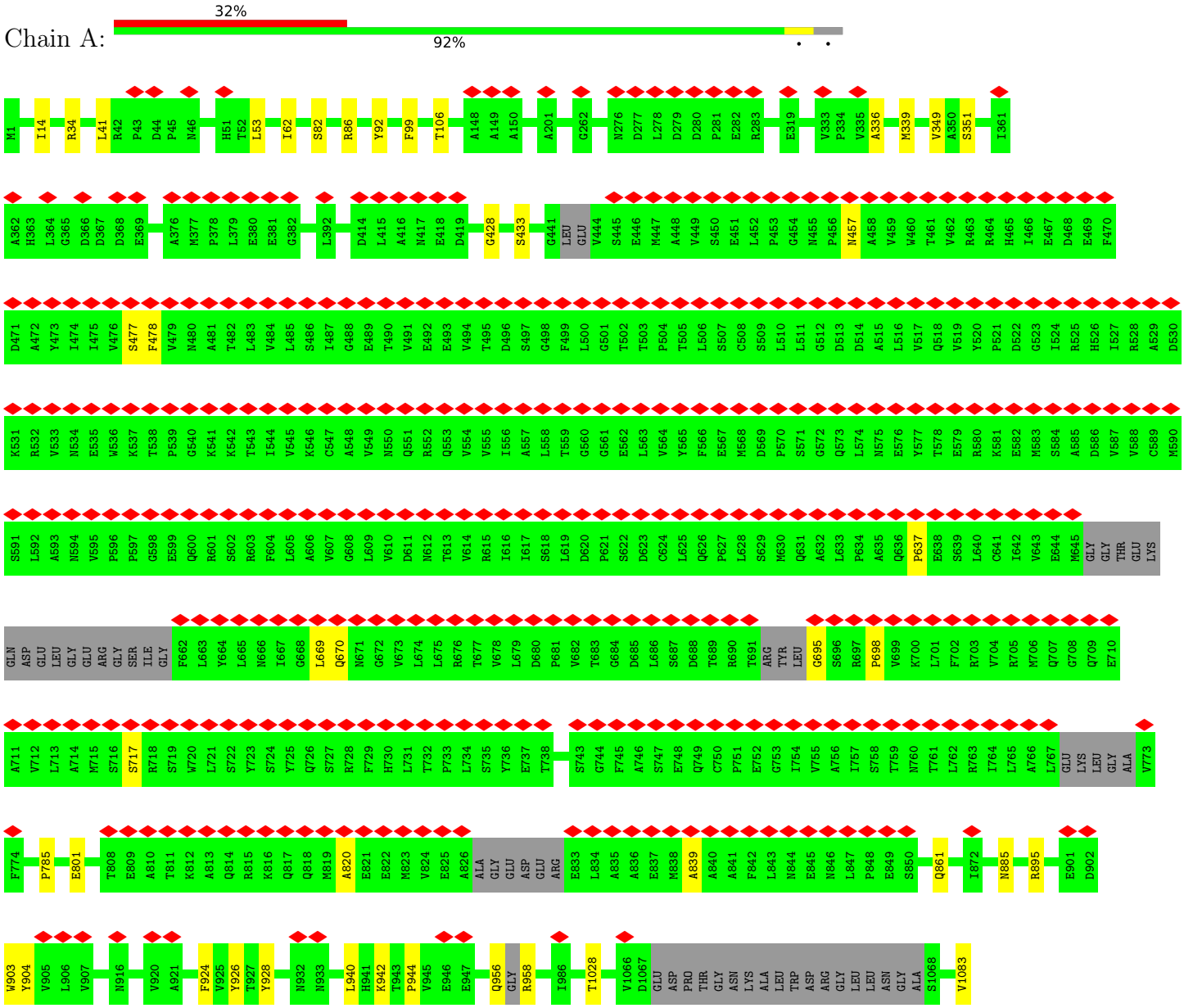
Mol	Chain	Residues	Atoms	AltConf
41	b	1	Total Mg 1 1	0
41	d	6	Total Mg 6 6	0

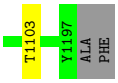
3 Residue-property plots (i)

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

- Molecule 1: Splicing factor 3B subunit 3

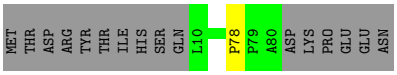
Chain A:





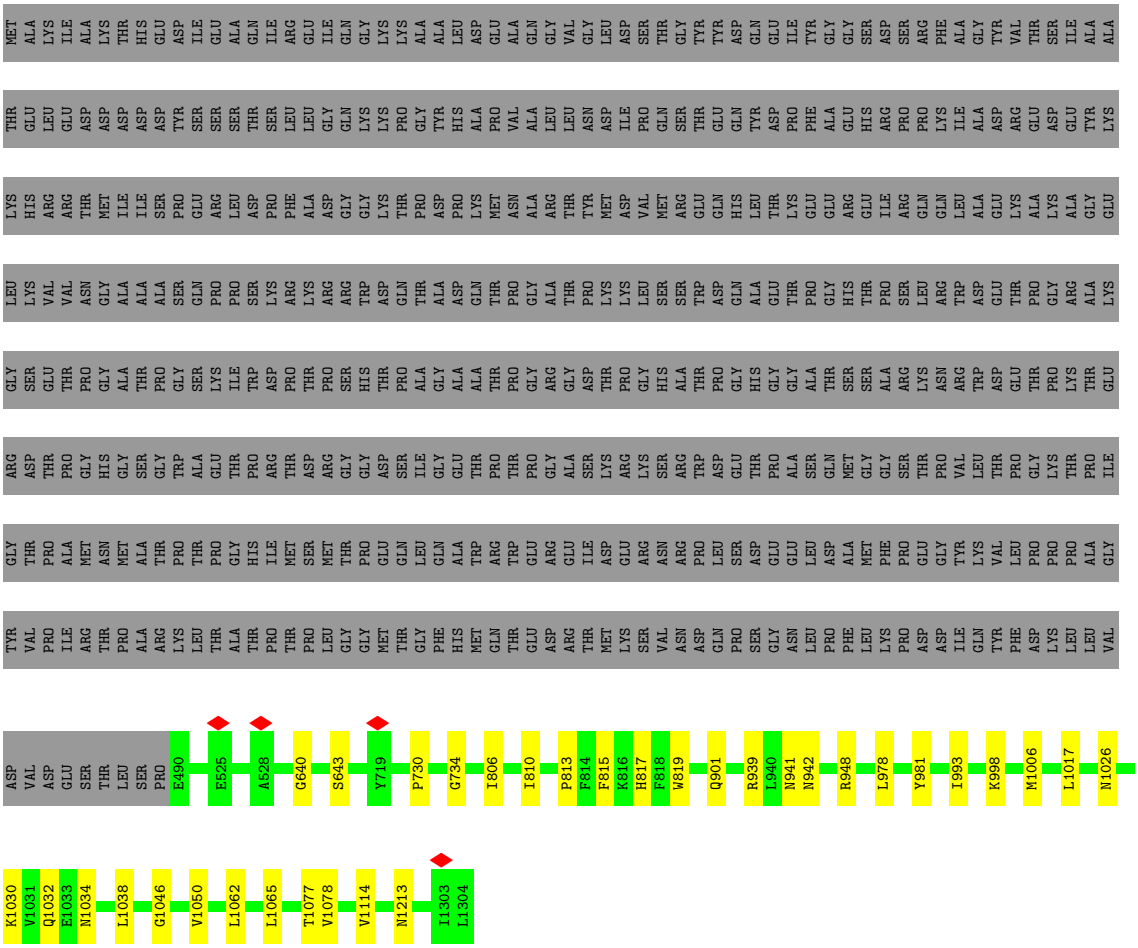
• Molecule 2: Splicing factor 3B subunit 5

Chain B:



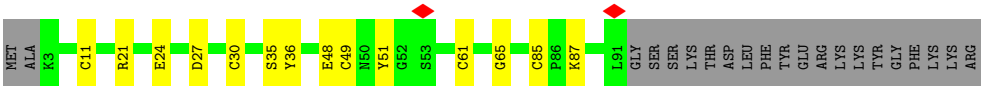
• Molecule 3: Splicing factor 3B subunit 1

Chain C:



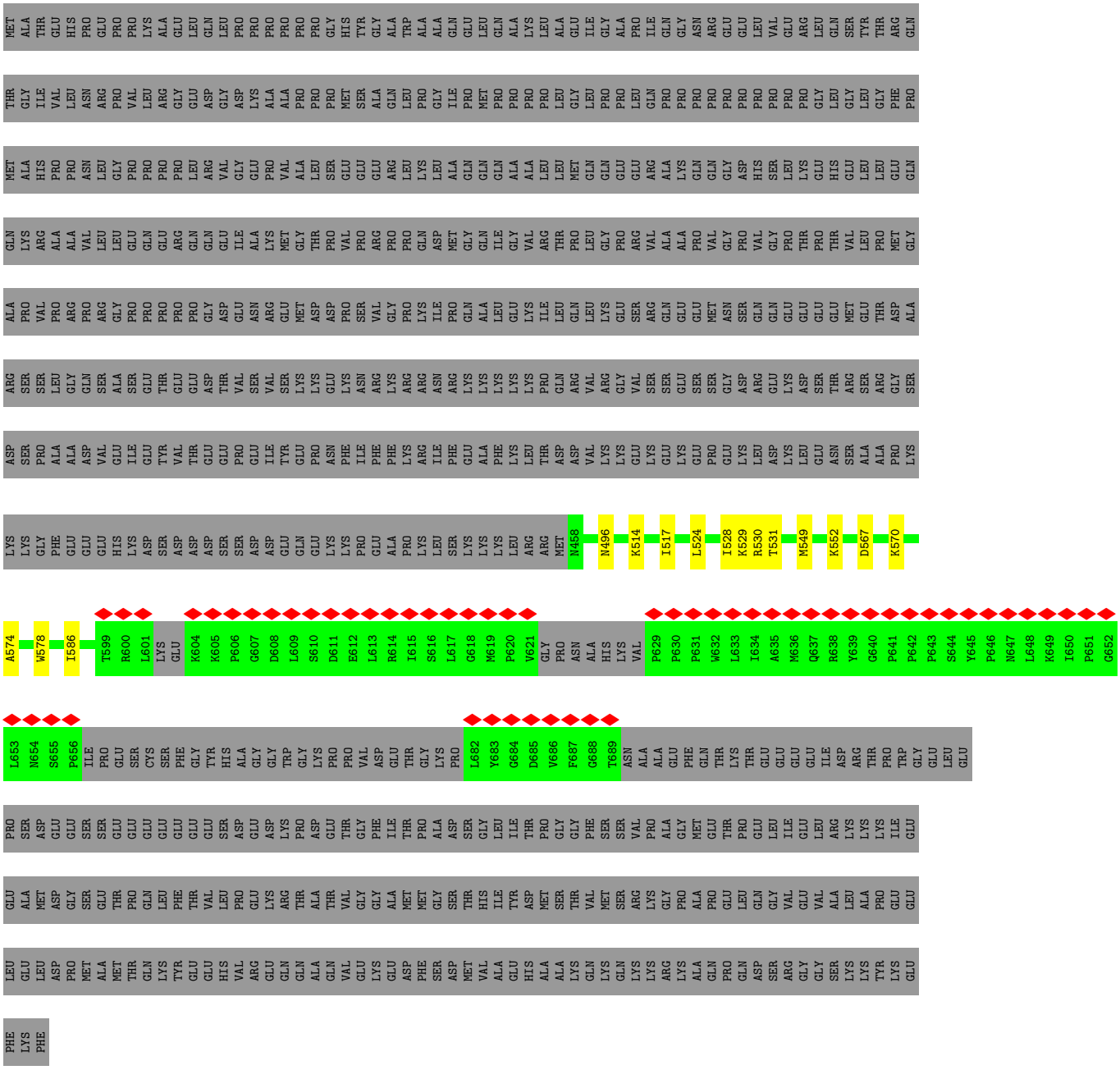
• Molecule 4: PHD finger-like domain-containing protein 5A

Chain D:



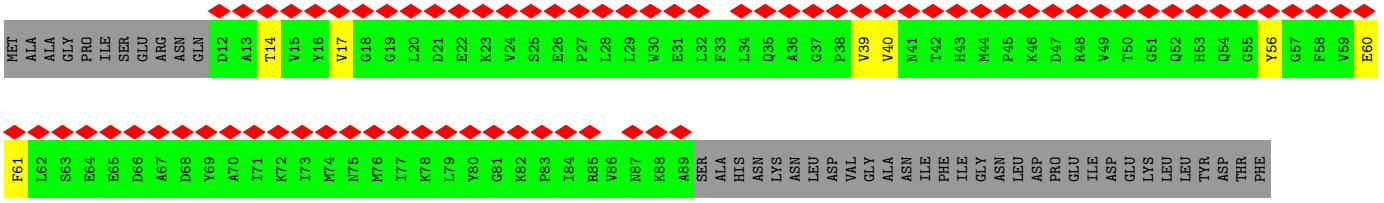
• Molecule 5: Splicing factor 3B subunit 2

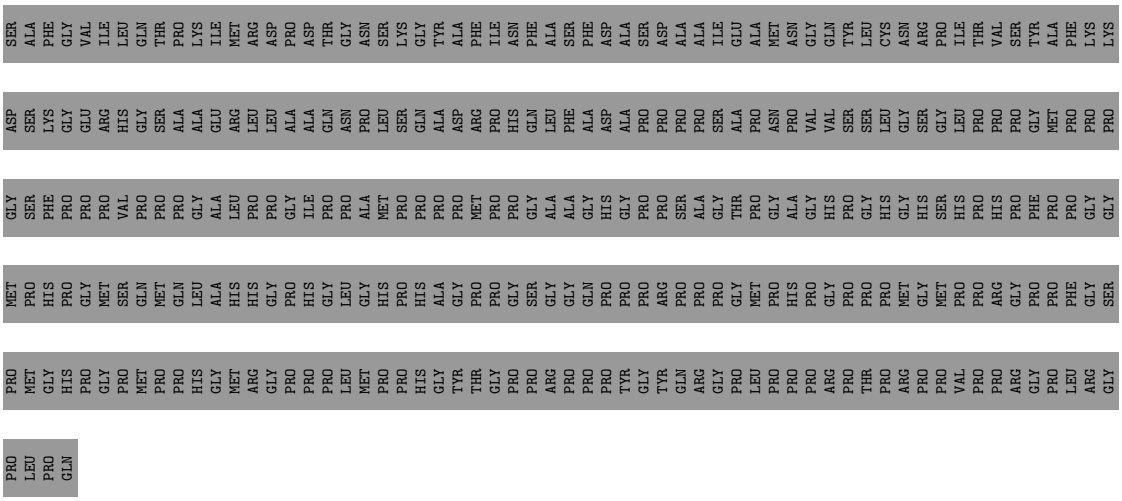
Chain E:



• Molecule 6: Splicing factor 3B subunit 4

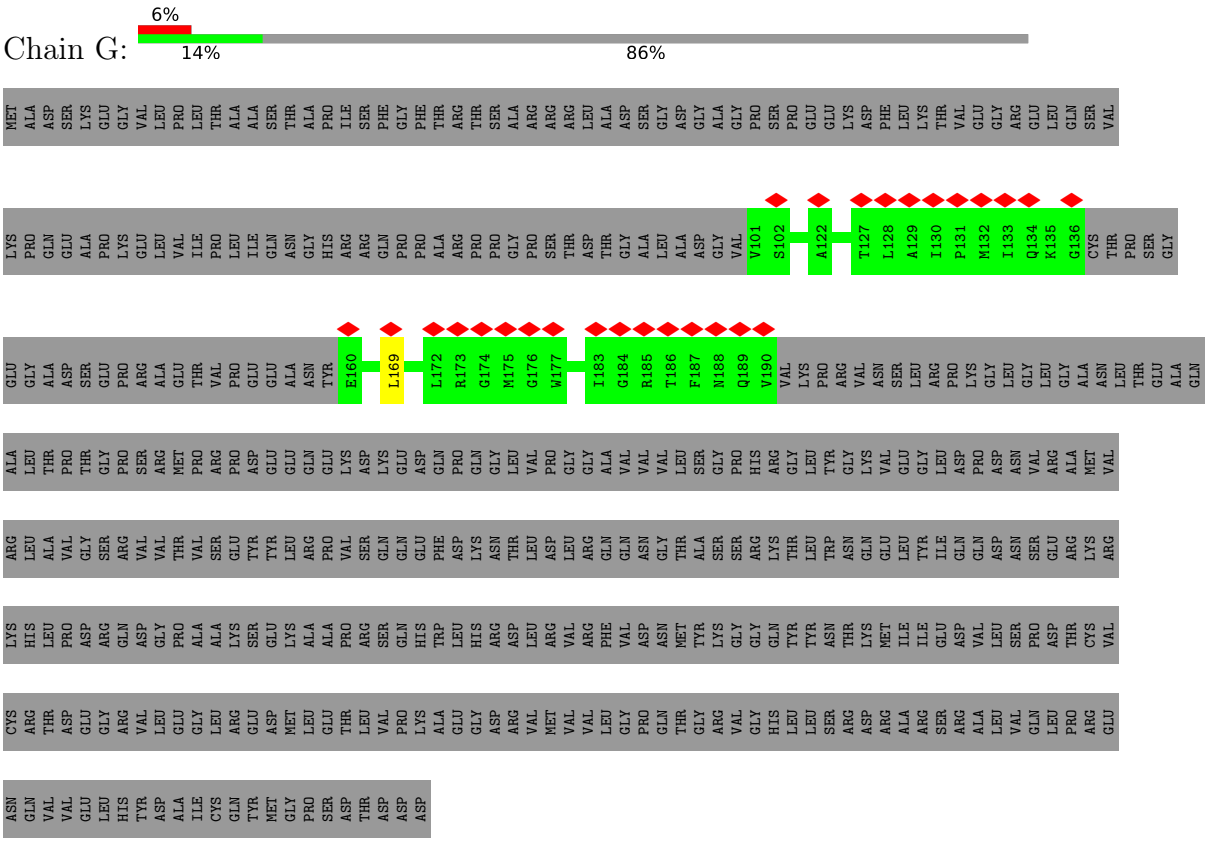
Chain F:





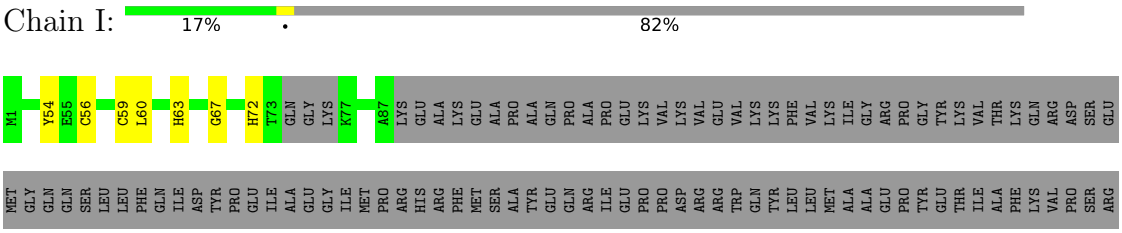
• Molecule 7: G-patch domain and KOW motifs-containing protein

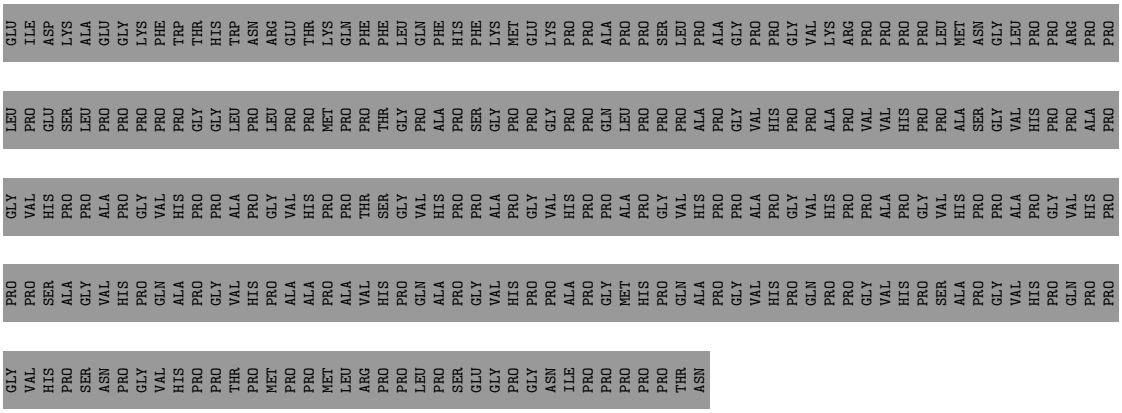
Chain G:



• Molecule 8: Splicing factor 3A subunit 2

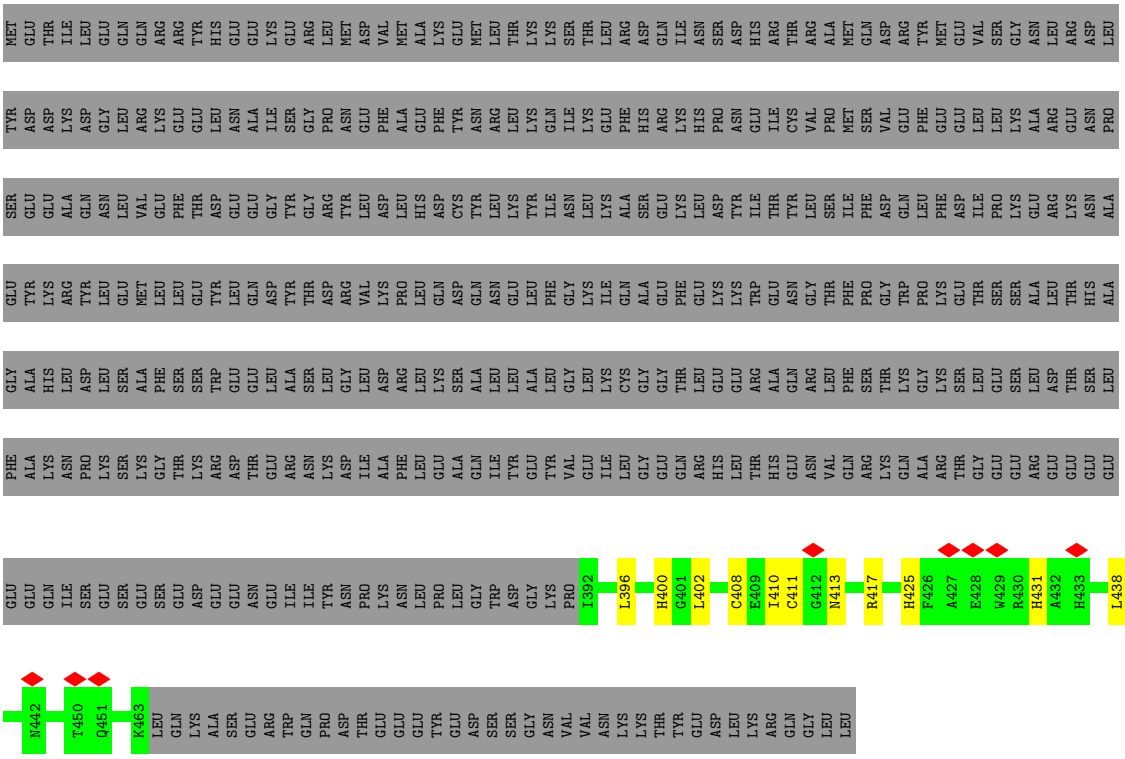
Chain I:





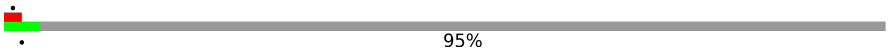
• Molecule 9: Splicing factor 3A subunit 3

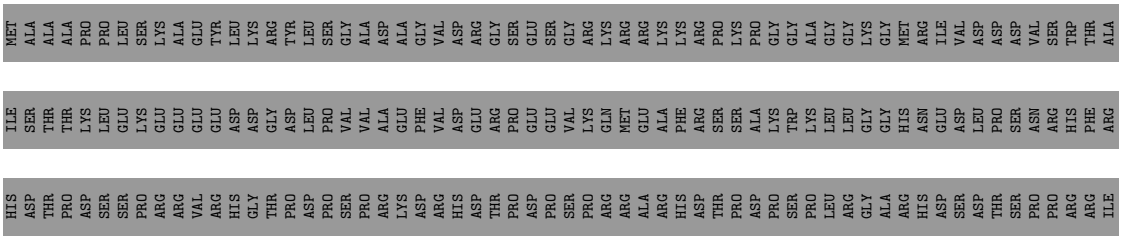
Chain J:

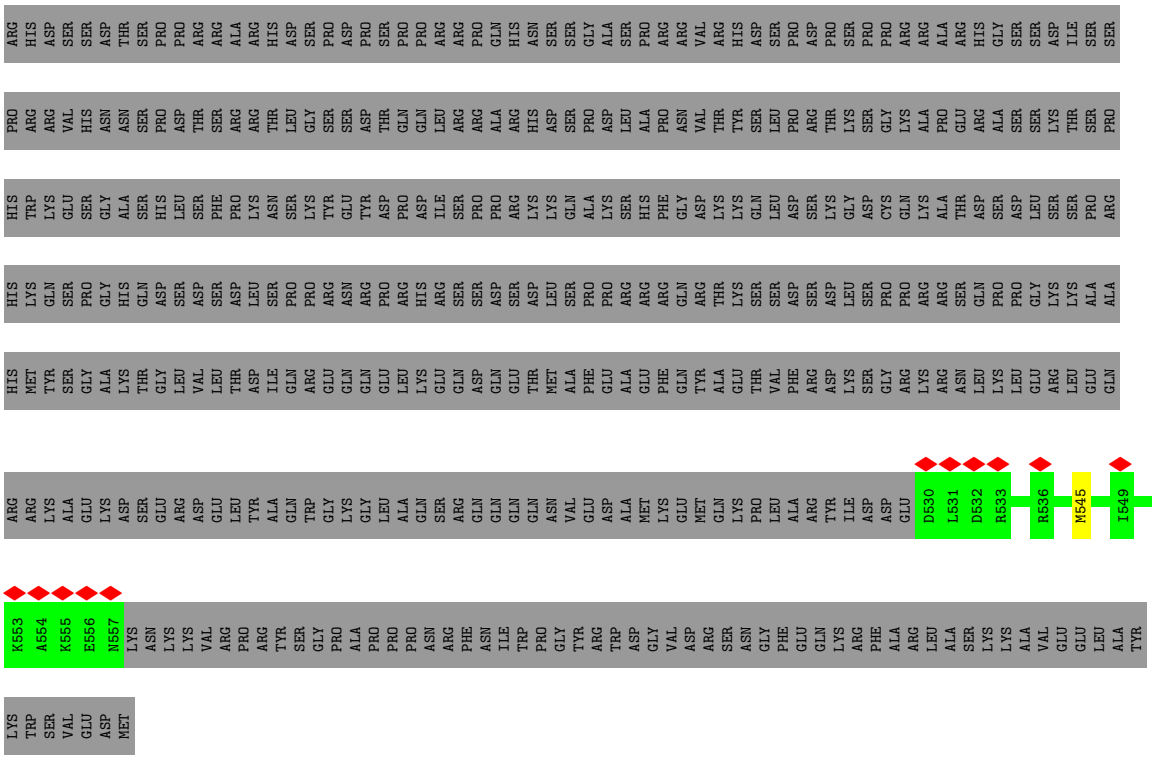


• Molecule 10: BUD13 homolog

Chain L:

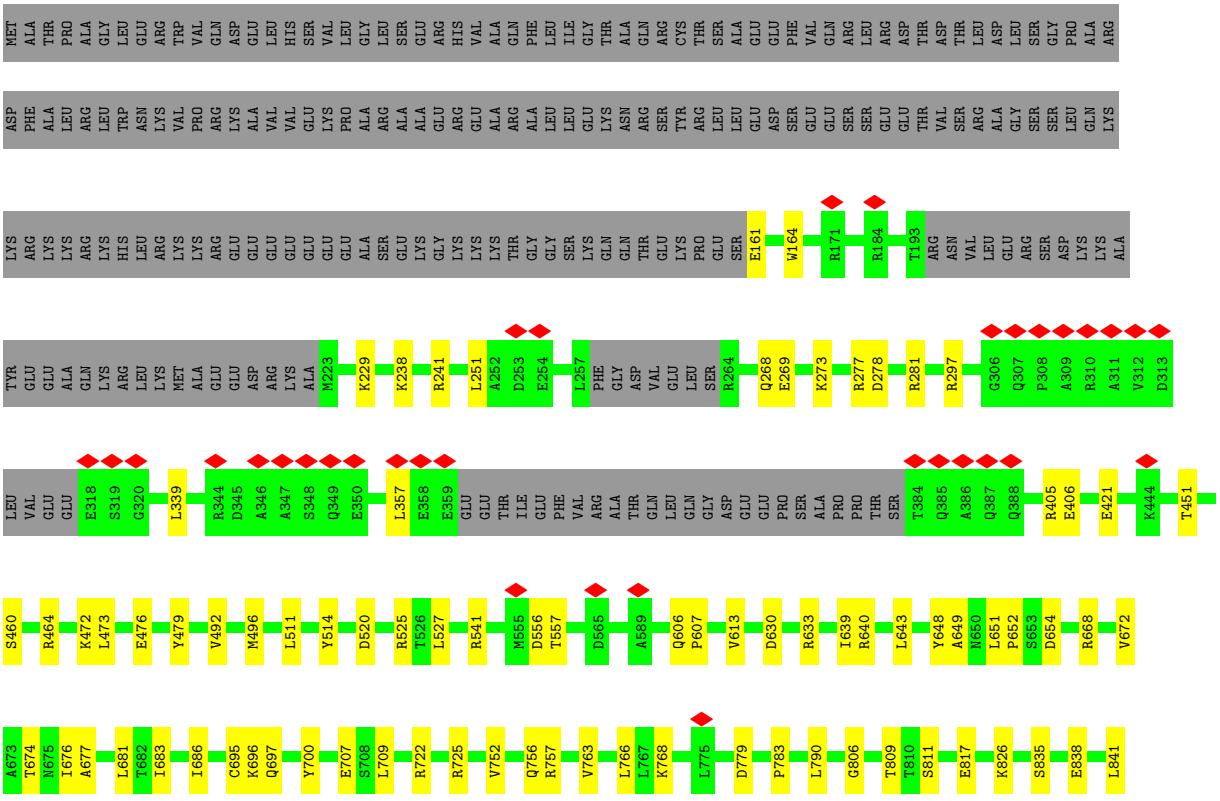


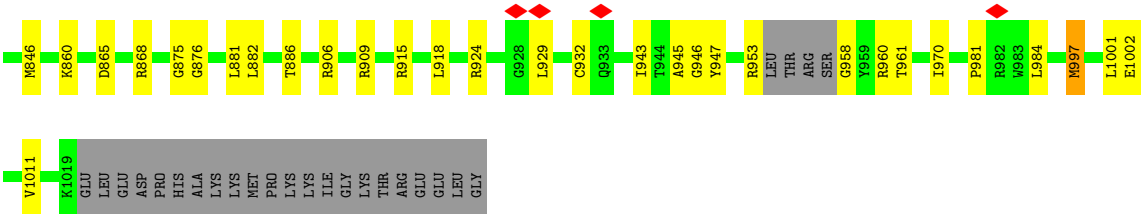




• Molecule 11: Putative pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16

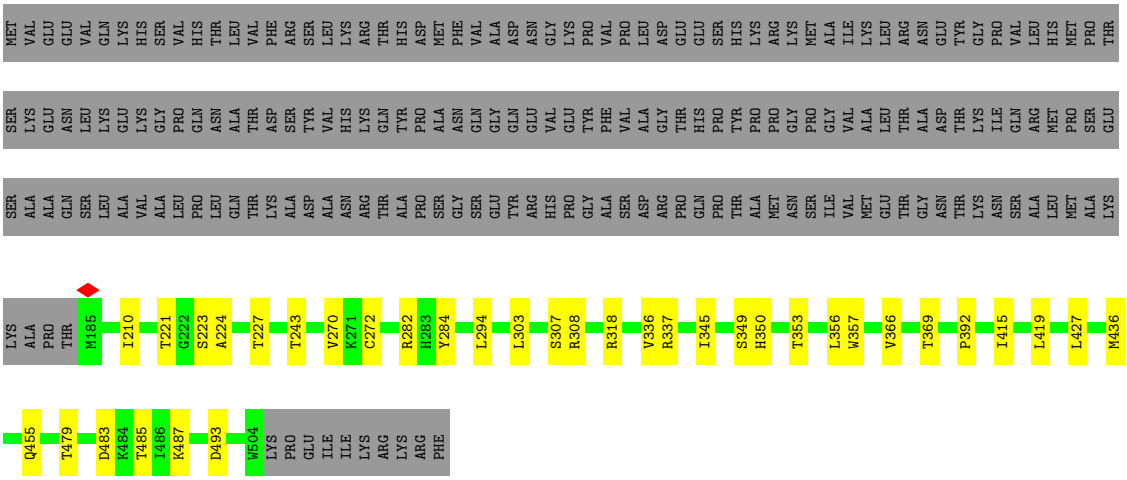
Chain N:





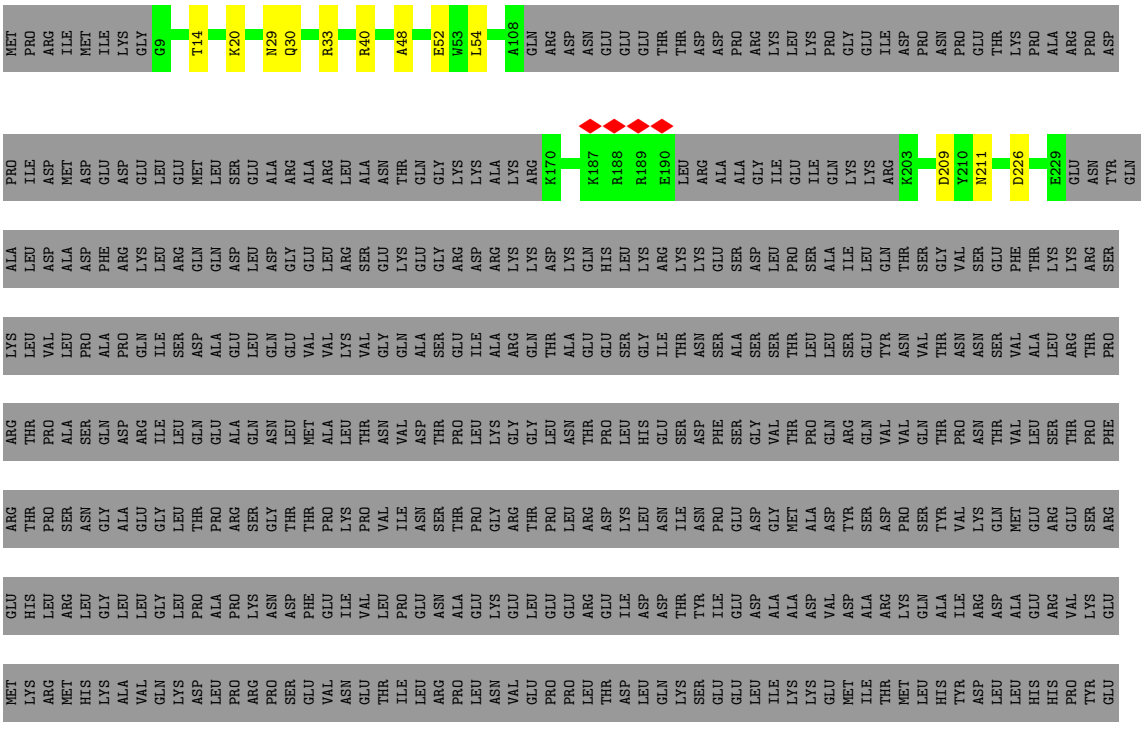
• Molecule 12: Pleiotropic regulator 1

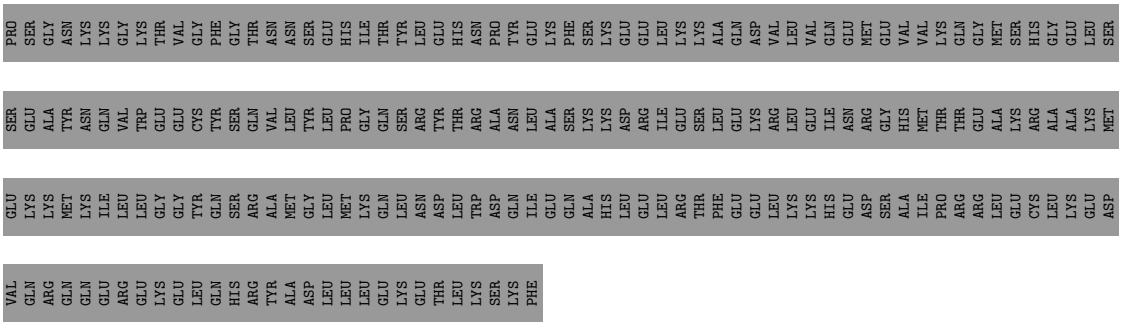
Chain O:



• Molecule 13: Cell division cycle 5-like protein

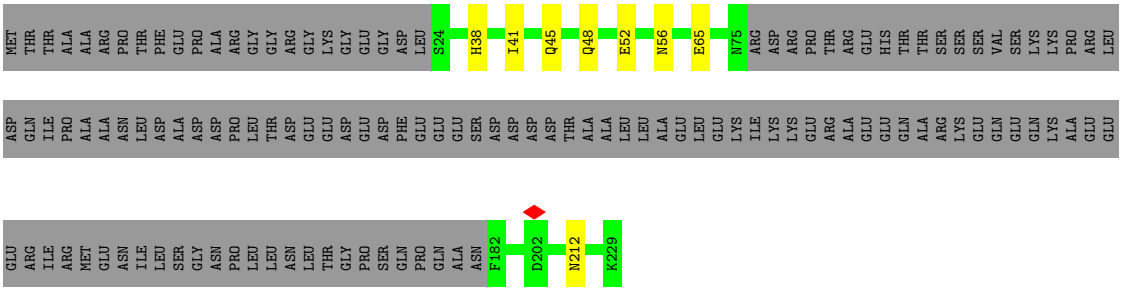
Chain P:





• Molecule 14: Spliceosome-associated protein CWC15 homolog

Chain Q:

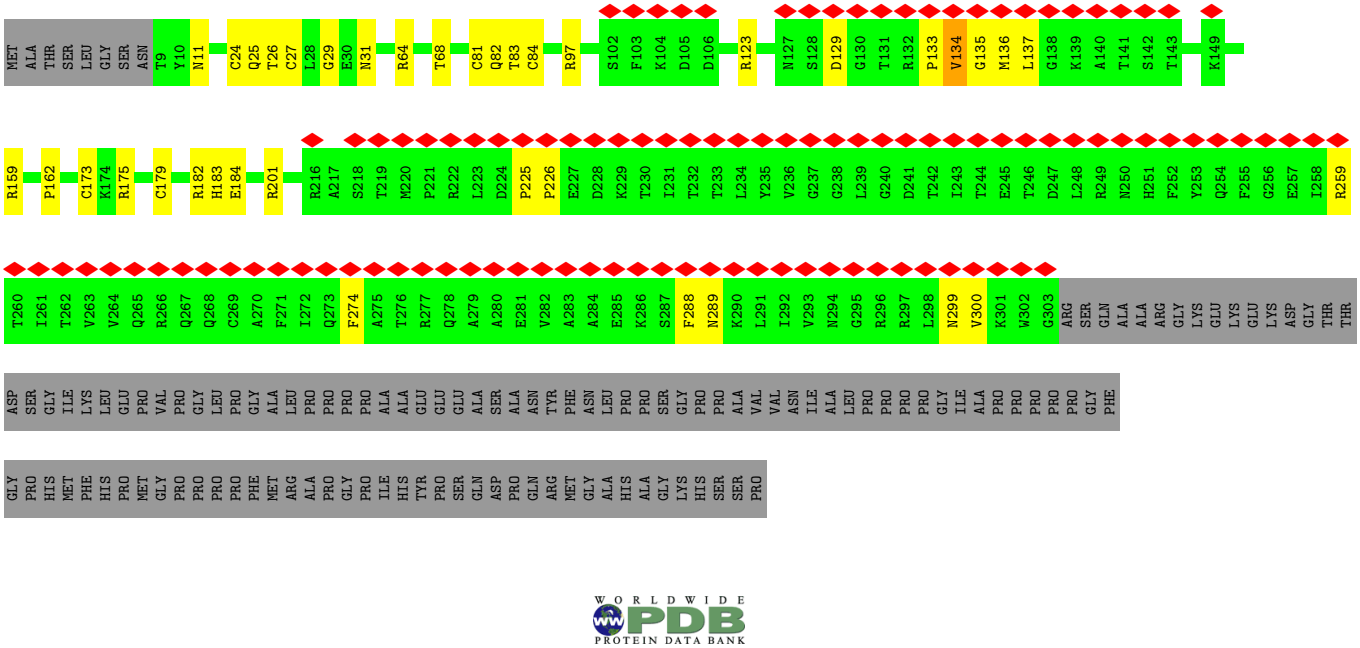


• Molecule 15: Protein BUD31 homolog

Chain T:

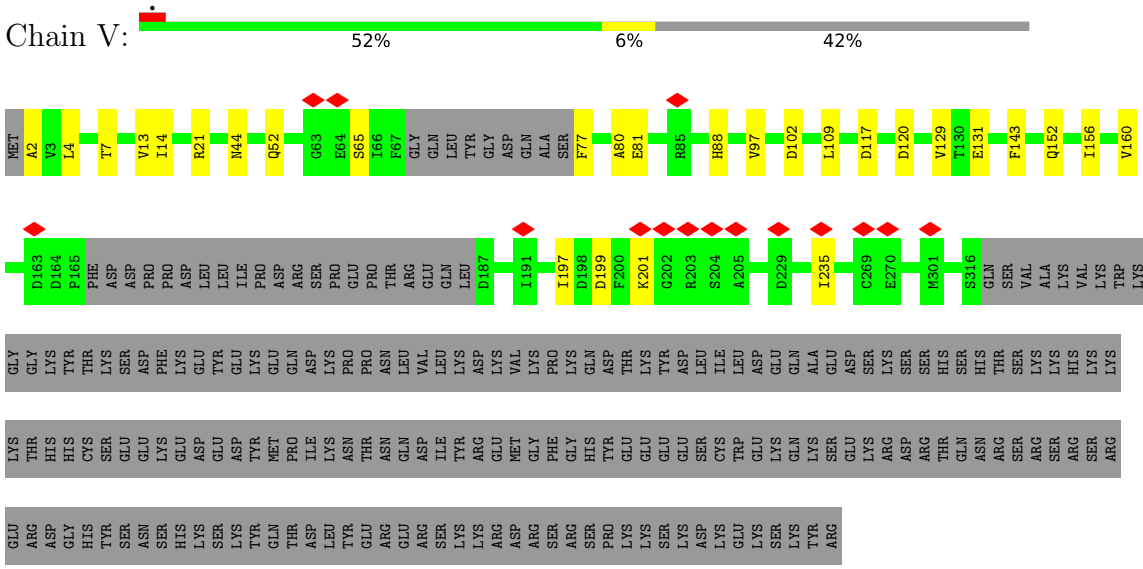
• Molecule 16: Pre-mRNA-splicing factor RBM22

Chain U:



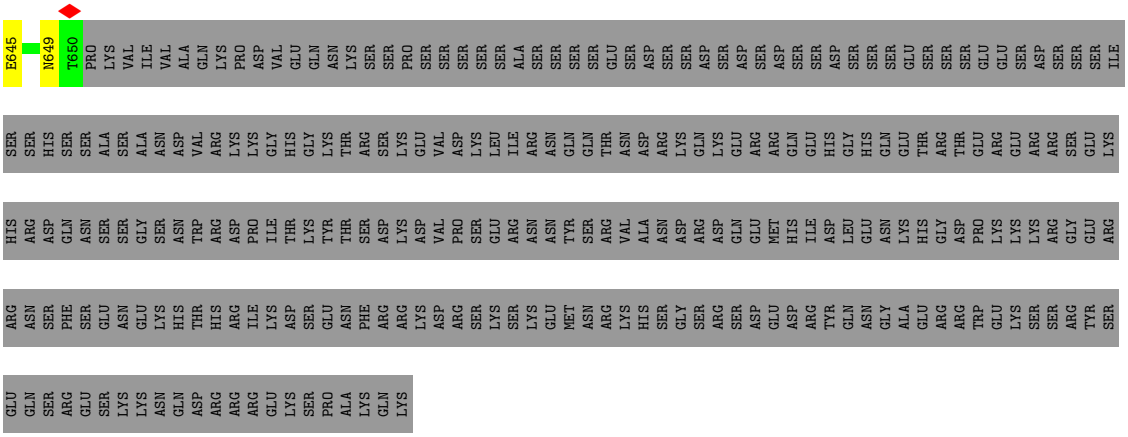
• Molecule 17: Peptidyl-prolyl cis-trans isomerase-like 4

Chain V:

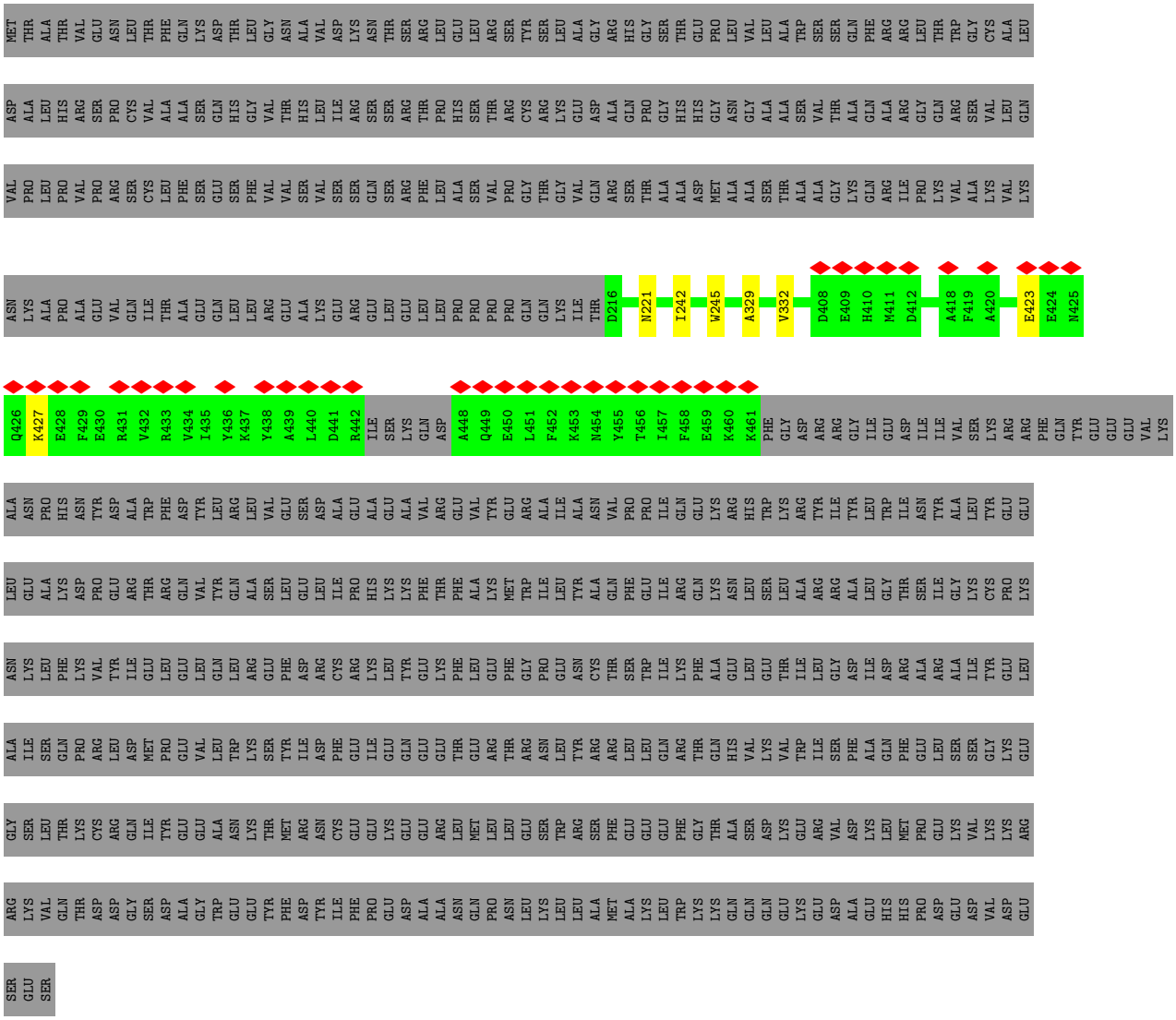


• Molecule 18: Pre-mRNA-splicing factor CWC22 homolog

Chain W:

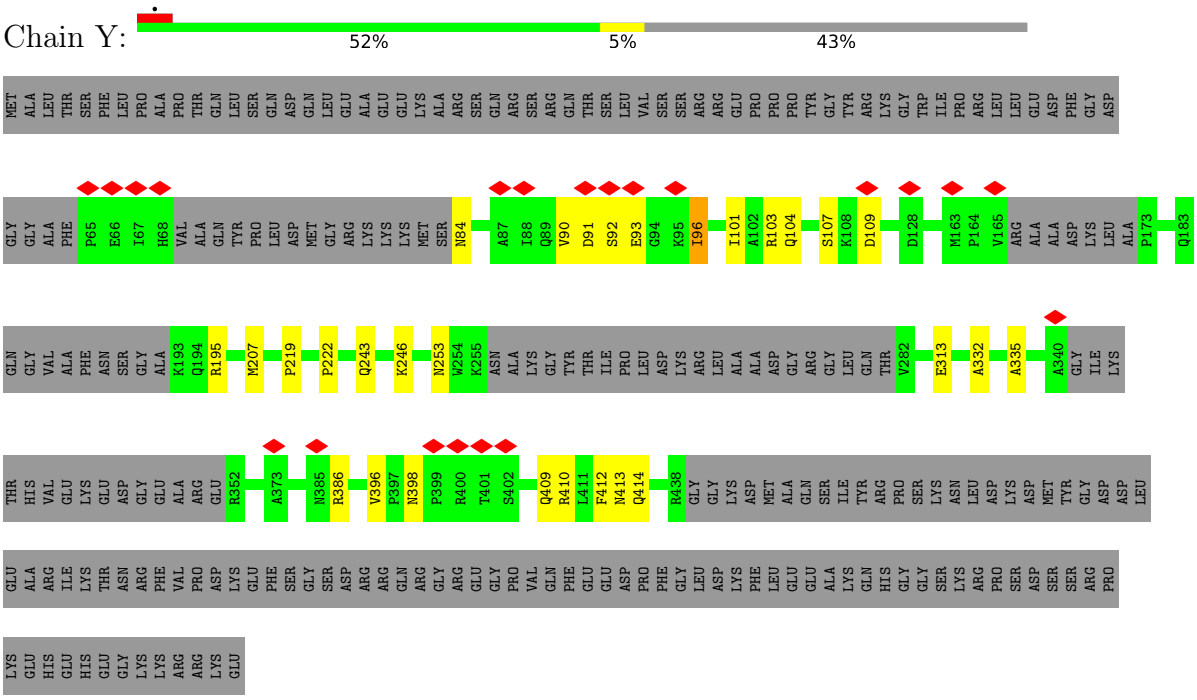


• Molecule 19: Crooked neck-like protein 1



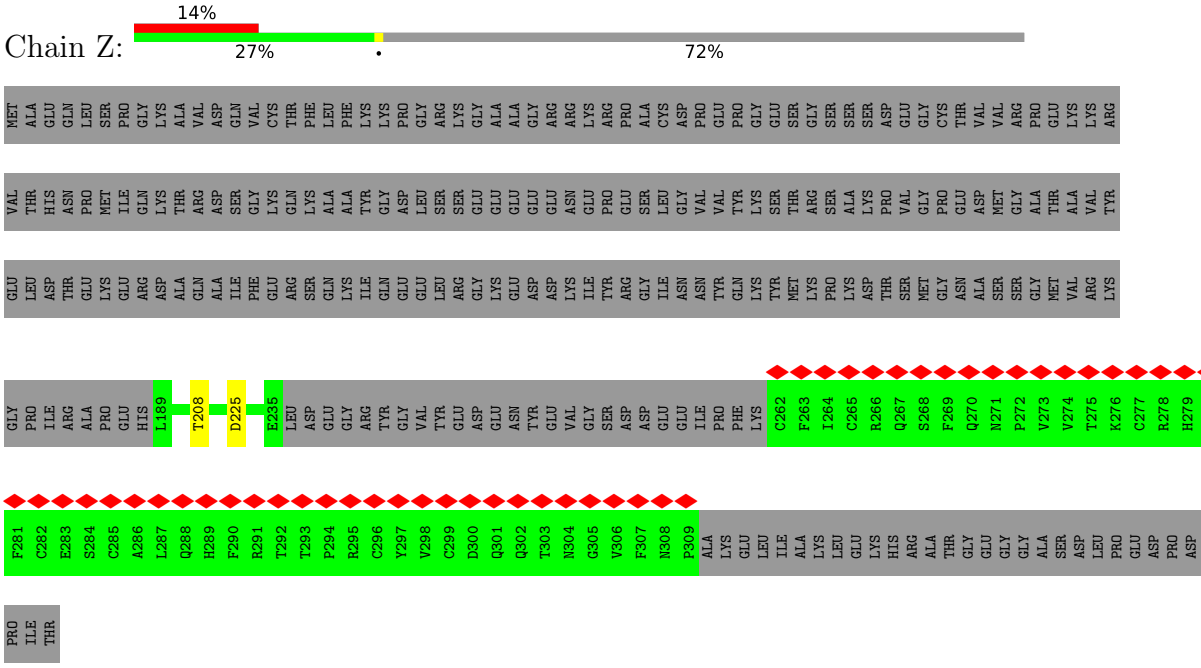
• Molecule 20: SNW domain-containing protein 1

Chain Y:



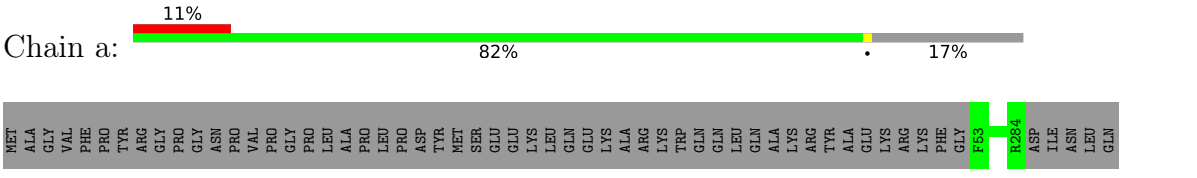
• Molecule 21: RING finger protein 113A

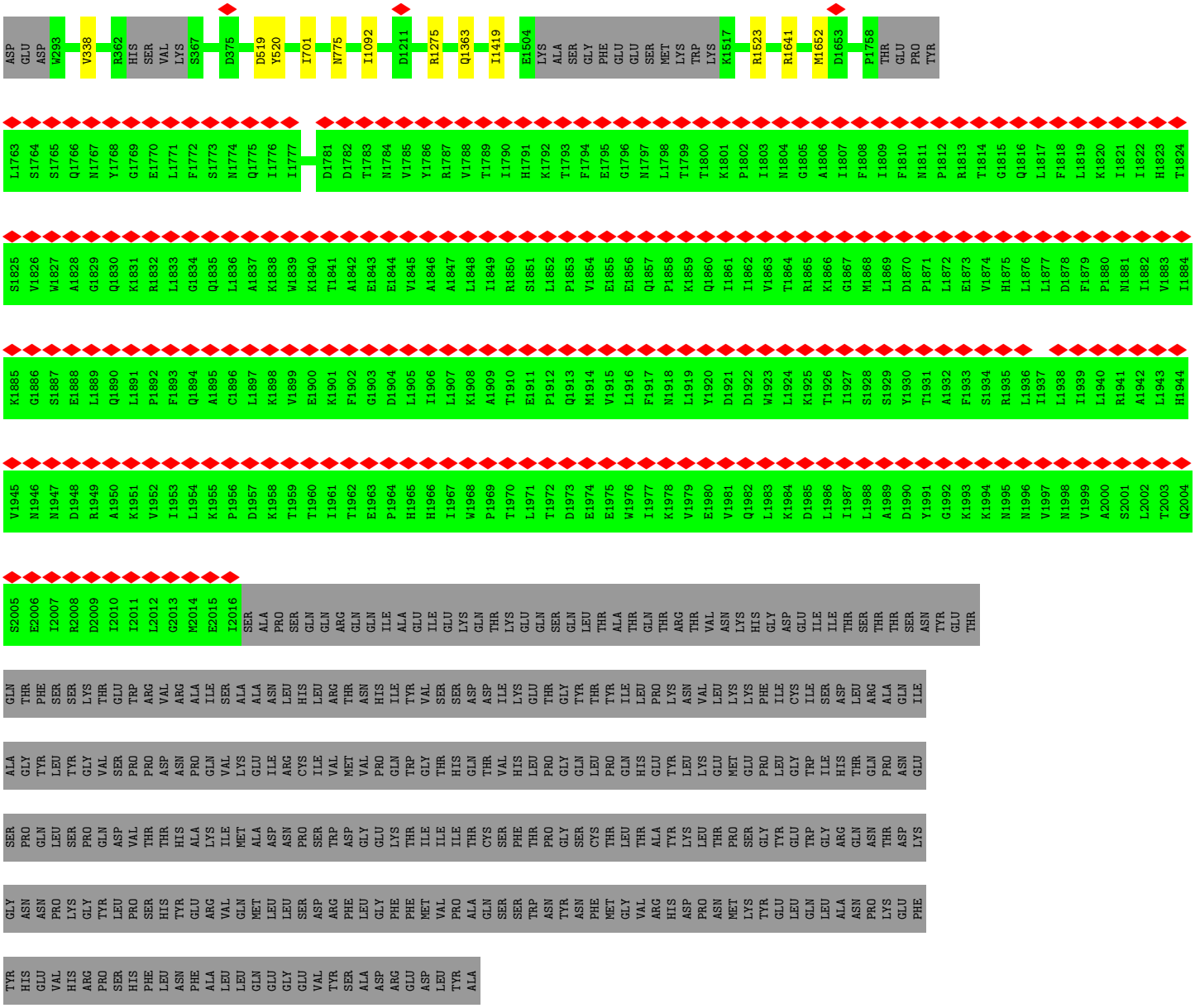
Chain Z:



• Molecule 22: Pre-mRNA-processing-splicing factor 8

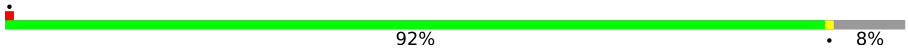
Chain a:

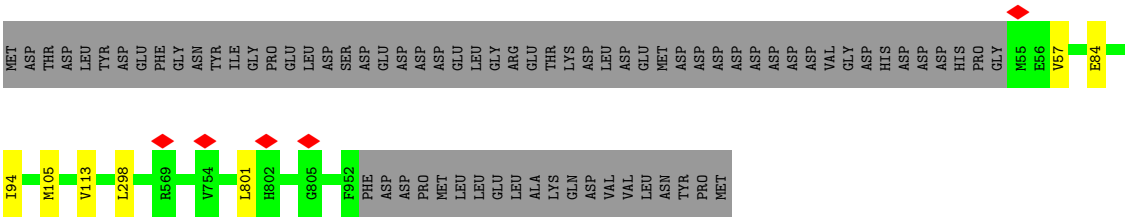




• Molecule 23: 116 kDa U5 small nuclear ribonucleoprotein component

Chain b:



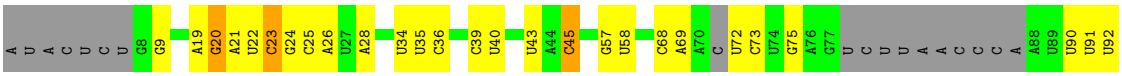


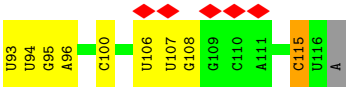
• Molecule 24: U6snRNA

Chain d:

• Molecule 25: U5 snRNA

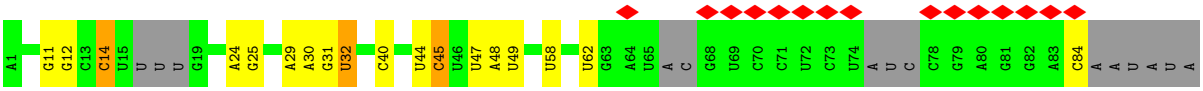
Chain e:





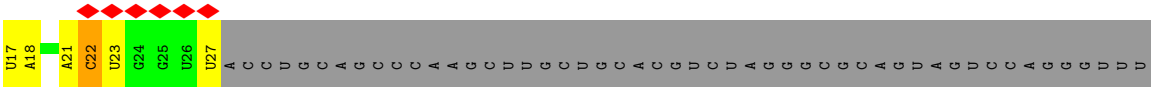
• Molecule 26: U2snRNA

Chain f:



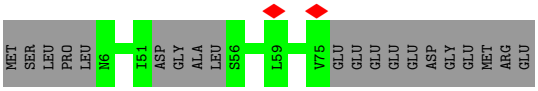
• Molecule 27: MINX

Chain g:

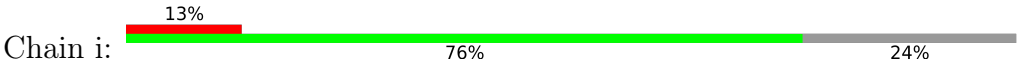


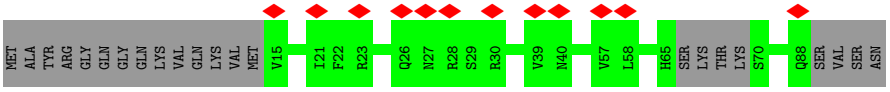
• Molecule 28: Small nuclear ribonucleoprotein F

Chain h:

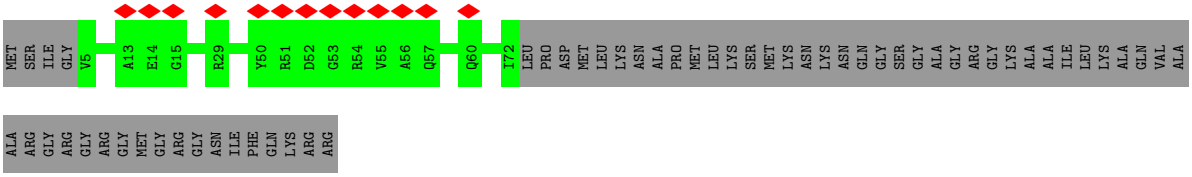


• Molecule 29: Small nuclear ribonucleoprotein E

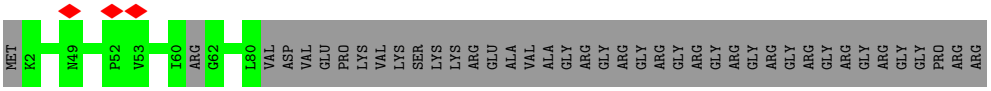




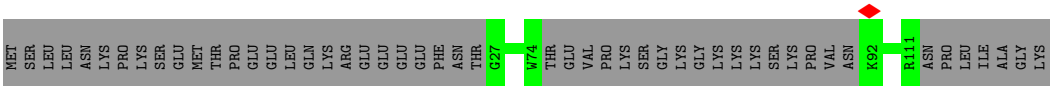
• Molecule 30: Small nuclear ribonucleoprotein Sm D3



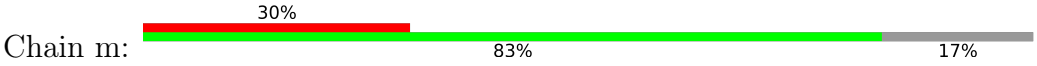
• Molecule 31: Small nuclear ribonucleoprotein Sm D1

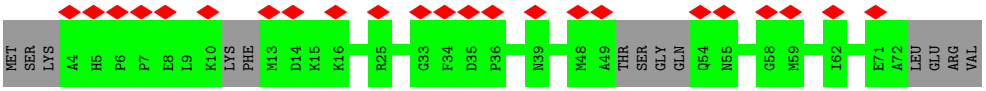


• Molecule 32: Small nuclear ribonucleoprotein Sm D2

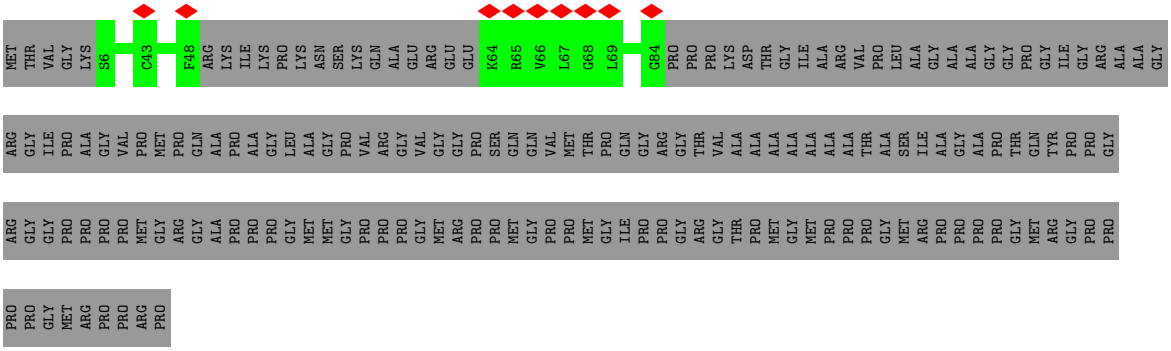


• Molecule 33: Small nuclear ribonucleoprotein G



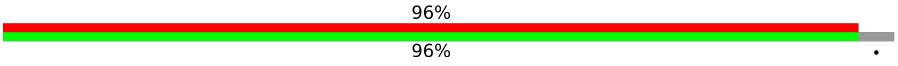


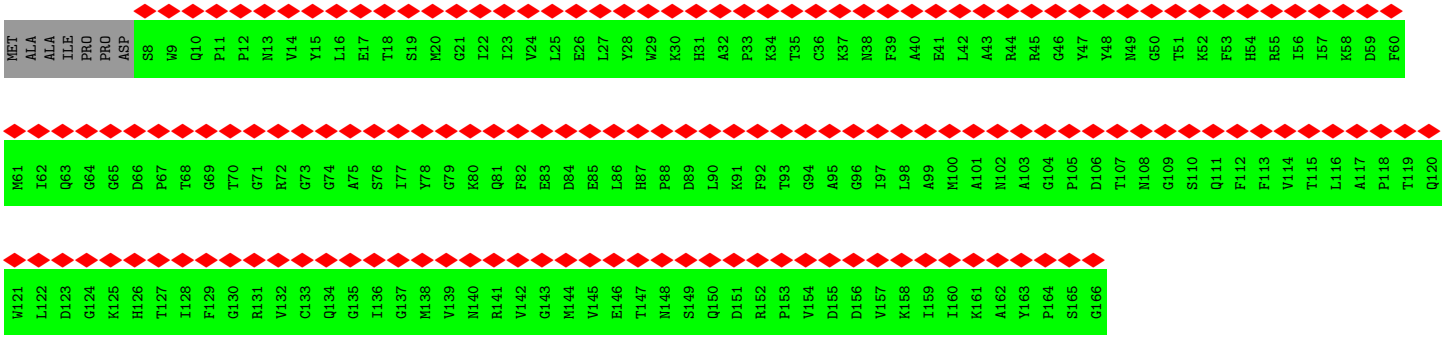
• Molecule 34: Small nuclear ribonucleoprotein-associated proteins B and B'



• Molecule 35: Peptidyl-prolyl cis-trans isomerase-like 1

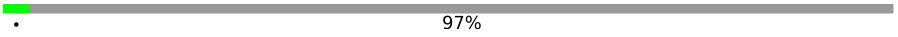
Chain p:

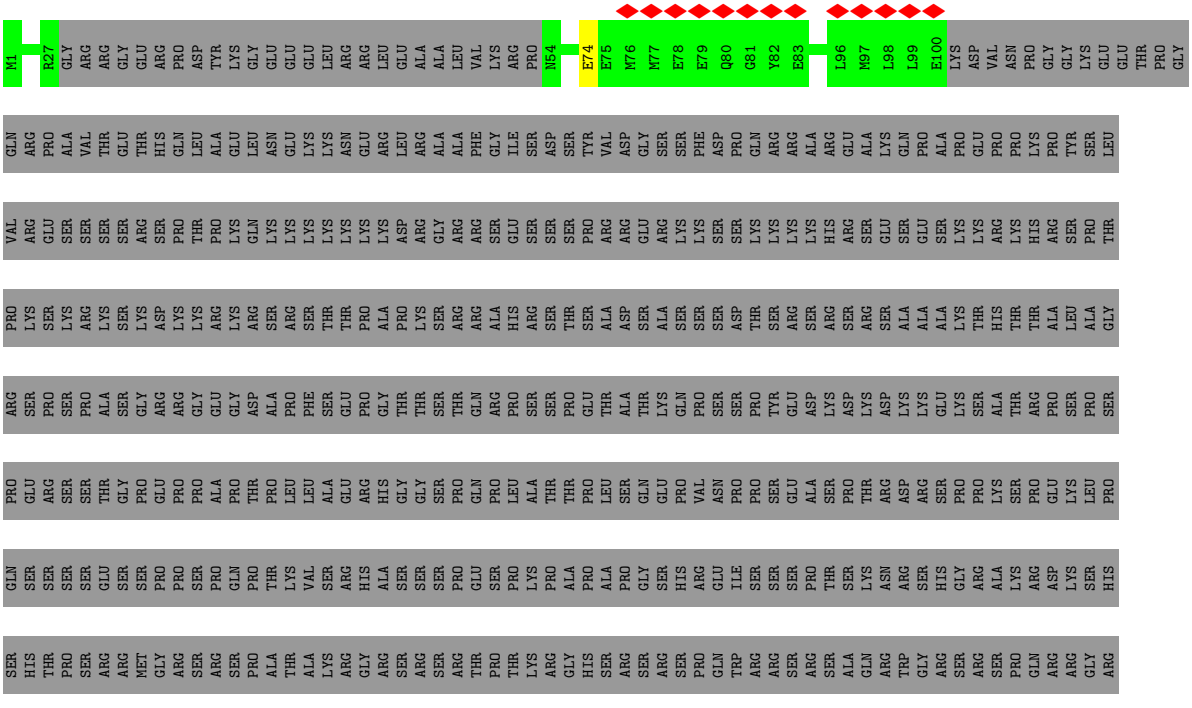


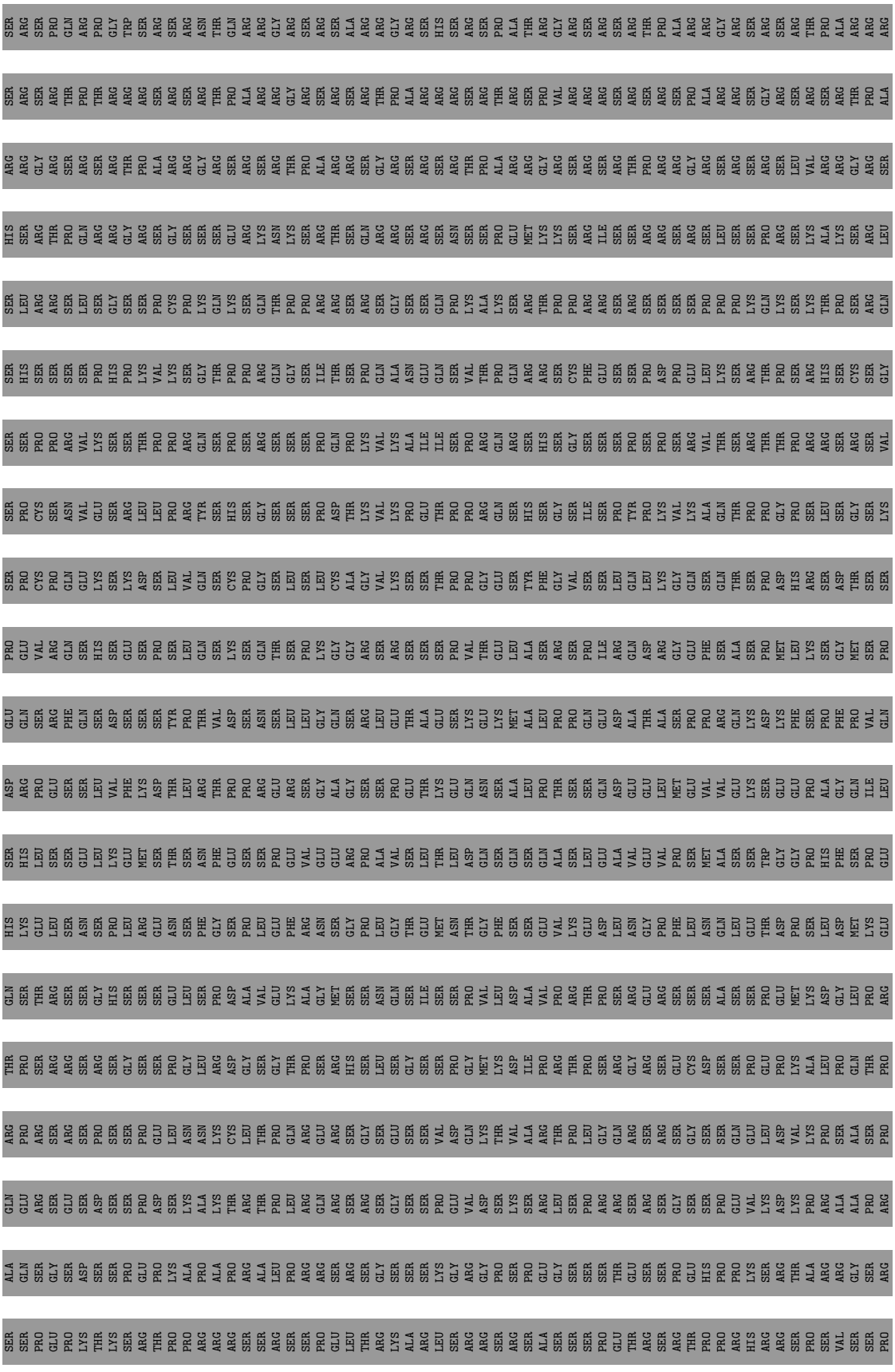


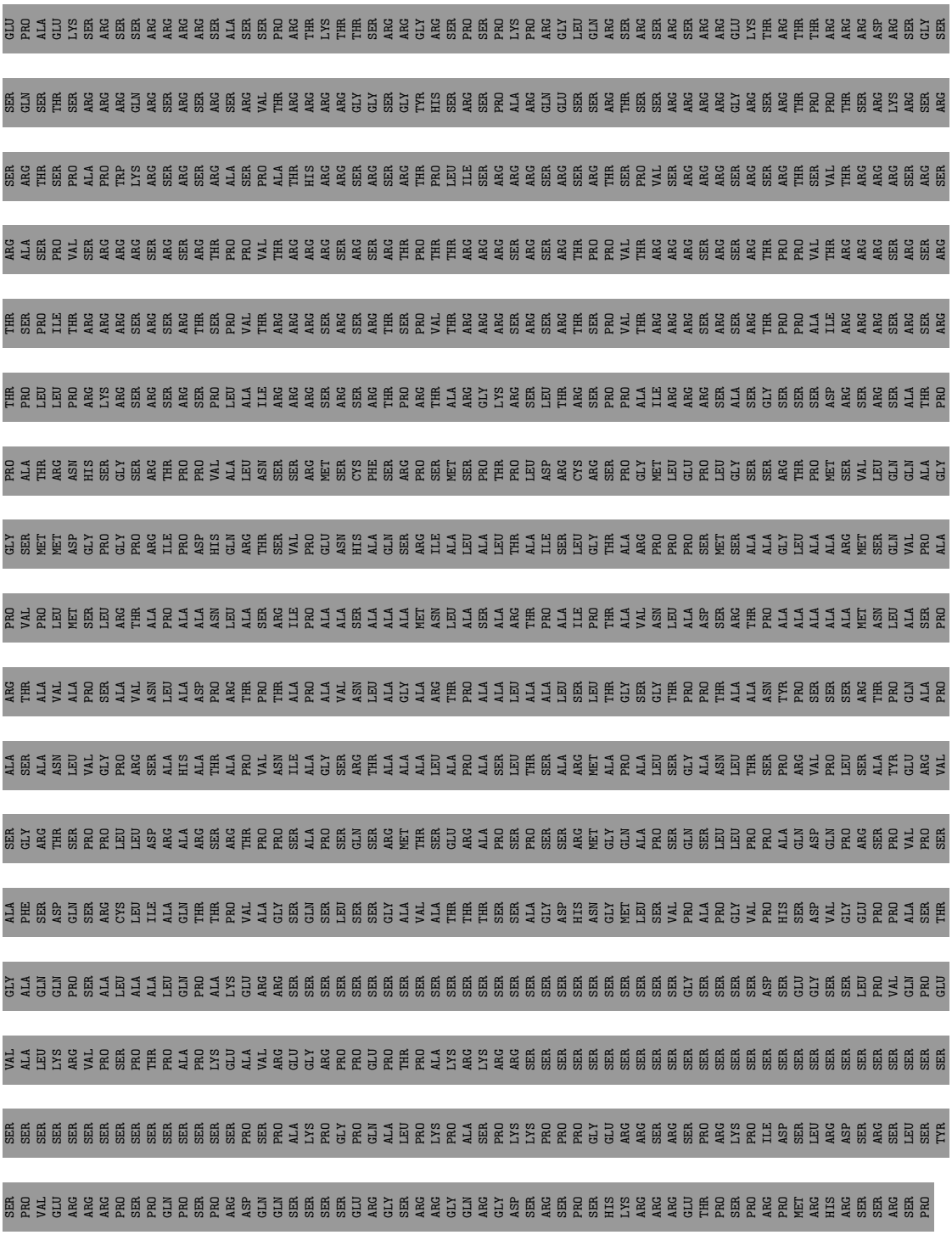
• Molecule 36: Serine/arginine repetitive matrix protein 2

Chain q:



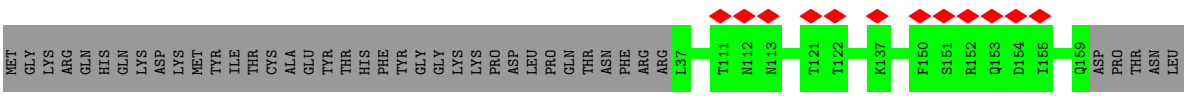


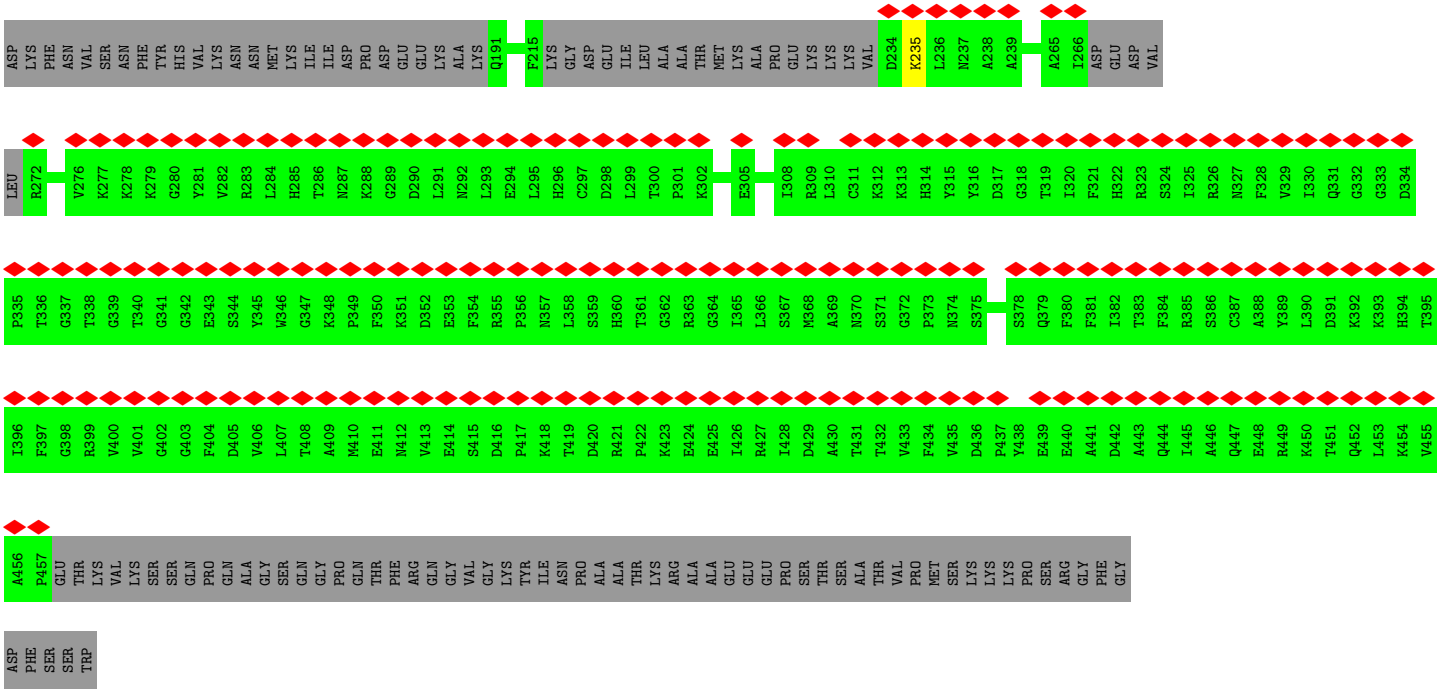




• Molecule 37: RING-type E3 ubiquitin-protein ligase PPIL2

Chain u:




ASP LYS PHE ASN VAL SER ASN PHE TYR HIS VAL LYS ASN ASN MET LYS ILE ILE ASP PRO ASP GLU GLU LYS ALA LYS Q191 F215 LYS GLY ASP GLU ILE LEU ALA ALA THR MET LYS ALA PRO GLU LYS LYS LYS VAL D234 K235 L236 N237 A238 A239 A265 I266 ASP GLU ASP VAL
LEU R272 V276 K277 K278 K279 G280 Y281 V282 R283 L284 H285 T286 N287 K288 G289 D290 L291 N292 L293 E294 L295 H296 C297 D298 L299 T300 P301 K302 E305 I308 R309 L310 C311 K312 K313 H314 Y315 Y316 D317 G318 T319 I320 F321 H322 R323 S324 I325 R326 N327 F328 V329 I330 Q331 G332 G333 D334
P335 T336 G337 T338 G339 T340 G341 G342 E343 S344 Y345 W346 G347 K348 P349 F350 K351 D352 E353 F354 R355 P356 N357 L358 S359 H360 T361 G362 R363 G364 I365 L366 S367 M368 A369 N370 S371 G372 P373 N374 S375 S378 Q379 F380 F381 I382 T383 F384 R385 S386 C387 A388 Y389 L390 D391 K392 K393 H394 T395
I396 F397 G398 R399 V400 V401 G402 G403 F404 D405 V406 L407 T408 A409 M410 E411 N412 V413 E414 S415 D416 P417 K418 T419 D420 R421 P422 K423 E424 E425 I426 R427 I428 D429 A430 T431 T432 V433 F434 V435 D436 P437 Y438 E439 E440 A441 D442 A443 Q444 I445 A446 Q447 E448 R449 K450 T451 Q452 L453 K454 V455
A456 P457 GLU THR LYS VAL LYS SER SER GLN PRO GLN ALA GLY SER GLN GLY PRO GLN THR PHE ARG GLN GLY VAL GLY LYS TYR ILE ASN PRO ALA ALA THR LYS ARG ALA ALA GLU GLU PRO SER THR SER ALA THR VAL PRO MET SER LYS LYS PRO SER ARG GLY PHE GLY
ASP PHE SER SER TRP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146157	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 ($e^-/Å^2$)	45.47	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.033	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: ZN, IHP, GTP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/5737	0.48	0/7975
2	B	0.24	0/351	0.37	0/489
3	C	0.28	0/5209	0.52	0/7211
4	D	0.29	0/660	0.64	0/893
5	E	0.26	0/1383	0.50	0/1887
6	F	0.24	0/382	0.42	0/529
7	G	0.28	0/370	0.53	0/513
8	I	0.26	0/540	0.50	0/733
9	J	0.27	0/525	0.51	0/717
10	L	0.27	0/178	0.51	0/240
11	N	0.30	0/6278	0.66	3/8506 (0.0%)
12	O	0.33	0/2586	0.61	0/3527
13	P	0.28	0/1176	0.54	1/1589 (0.1%)
14	Q	0.34	0/836	0.68	1/1117 (0.1%)
15	T	0.35	0/1202	0.63	1/1611 (0.1%)
16	U	0.29	0/2118	0.57	0/2881
17	V	0.28	0/2026	0.55	0/2760
18	W	0.28	0/2954	0.49	0/4033
19	X	0.27	0/1623	0.48	0/2240
20	Y	0.31	0/2290	0.62	1/3103 (0.0%)
21	Z	0.27	0/618	0.51	0/845
22	a	0.32	0/15587	0.56	3/21197 (0.0%)
23	b	0.31	0/7206	0.58	2/9800 (0.0%)
24	d	0.44	0/2225	1.07	8/3464 (0.2%)
25	e	0.47	0/2307	1.33	39/3584 (1.1%)
26	f	0.38	0/1780	1.21	13/2760 (0.5%)
27	g	0.37	0/1734	1.08	13/2691 (0.5%)
28	h	0.24	0/320	0.48	0/440
29	i	0.25	0/344	0.48	0/476
30	j	0.25	0/334	0.51	0/463
31	k	0.24	0/387	0.46	0/537
32	l	0.24	0/335	0.46	0/464

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	m	0.25	0/306	0.48	0/420
34	n	0.24	0/313	0.47	0/432
35	p	0.26	0/775	0.46	0/1070
36	q	0.31	0/466	0.59	0/639
37	u	0.26	0/1969	0.49	0/2722
All	All	0.31	0/75430	0.66	85/104558 (0.1%)

There are no bond length outliers.

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	f	40	C	N1-C2-O2	11.57	125.84	118.90
25	e	115	C	N1-C2-O2	10.04	124.92	118.90
25	e	23	C	C2-N1-C1'	9.95	129.75	118.80
26	f	40	C	C2-N1-C1'	9.29	129.02	118.80
25	e	36	C	N1-C2-O2	9.28	124.47	118.90

There are no chirality outliers.

There are no planarity outliers.

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	A	5744	0	2562	24	0
2	B	350	0	167	0	0
3	C	5115	0	4128	19	0
4	D	649	0	597	7	0
5	E	1350	0	1111	12	0
6	F	383	0	173	4	0
7	G	364	0	226	1	0
8	I	533	0	410	5	0
9	J	510	0	430	7	0
10	L	177	0	140	1	0
11	N	6157	0	5996	67	0
12	O	2517	0	2466	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	P	1151	0	1096	7	0
14	Q	823	0	779	5	0
15	T	1176	0	1178	6	0
16	U	2080	0	1803	24	0
17	V	1996	0	1727	18	0
18	W	2921	0	2168	9	0
19	X	1587	0	1176	4	0
20	Y	2250	0	2095	21	0
21	Z	607	0	402	1	0
22	a	15194	0	14361	0	0
23	b	7046	0	7031	0	0
24	d	1989	0	1006	0	0
25	e	2070	0	1046	0	0
26	f	1600	0	813	0	0
27	g	1559	0	794	0	0
28	h	322	0	138	0	0
29	i	346	0	144	0	0
30	j	335	0	148	0	0
31	k	388	0	164	0	0
32	l	337	0	139	0	0
33	m	309	0	135	0	0
34	n	315	0	134	0	0
35	p	776	0	358	0	0
36	q	461	0	354	0	0
37	u	1963	0	1065	0	0
38	D	3	0	0	0	0
38	I	1	0	0	0	0
38	J	1	0	0	0	0
38	T	3	0	0	0	0
38	U	3	0	0	0	0
38	Z	1	0	0	0	0
39	a	36	0	6	0	0
40	b	32	0	12	0	0
41	b	1	0	0	0	0
41	d	6	0	0	0	0
All	All	73537	0	58678	245	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 4.

The worst 5 of 245 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)
16:U:24:CYS:SG	16:U:81:CYS:HB2	2.17	0.83
6:F:17:VAL:O	6:F:56:TYR:HA	1.78	0.82
8:I:59:CYS:SG	8:I:72:HIS:CE1	2.79	0.74
9:J:408:CYS:O	9:J:413:ASN:HA	1.95	0.66
20:Y:396:VAL:HG12	20:Y:398:ASN:H	1.62	0.65

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	
1	A	1150/1217 (94%)	1099 (96%)	51 (4%)	0	100	100
2	B	68/86 (79%)	66 (97%)	1 (2%)	1 (2%)	10	39
3	C	813/1304 (62%)	788 (97%)	25 (3%)	0	100	100
4	D	87/110 (79%)	72 (83%)	14 (16%)	1 (1%)	14	46
5	E	190/895 (21%)	179 (94%)	11 (6%)	0	100	100
6	F	76/424 (18%)	71 (93%)	5 (7%)	0	100	100
7	G	63/476 (13%)	62 (98%)	1 (2%)	0	100	100
8	I	80/464 (17%)	80 (100%)	0	0	100	100
9	J	70/501 (14%)	64 (91%)	6 (9%)	0	100	100
10	L	26/619 (4%)	24 (92%)	2 (8%)	0	100	100
11	N	782/1041 (75%)	734 (94%)	46 (6%)	2 (0%)	41	73
12	O	318/514 (62%)	303 (95%)	15 (5%)	0	100	100
13	P	142/802 (18%)	132 (93%)	10 (7%)	0	100	100
14	Q	96/229 (42%)	92 (96%)	4 (4%)	0	100	100
15	T	140/144 (97%)	130 (93%)	10 (7%)	0	100	100
16	U	293/420 (70%)	274 (94%)	16 (6%)	3 (1%)	15	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	V	279/492 (57%)	263 (94%)	15 (5%)	1 (0%)	34	69
18	W	455/908 (50%)	446 (98%)	9 (2%)	0	100	100
19	X	237/848 (28%)	232 (98%)	5 (2%)	0	100	100
20	Y	294/536 (55%)	271 (92%)	22 (8%)	1 (0%)	41	73
21	Z	91/343 (26%)	86 (94%)	4 (4%)	1 (1%)	14	46
22	a	1926/2335 (82%)	1834 (95%)	86 (4%)	6 (0%)	41	73
23	b	896/972 (92%)	861 (96%)	30 (3%)	5 (1%)	25	59
28	h	62/86 (72%)	62 (100%)	0	0	100	100
29	i	66/92 (72%)	65 (98%)	1 (2%)	0	100	100
30	j	66/126 (52%)	64 (97%)	2 (3%)	0	100	100
31	k	74/119 (62%)	70 (95%)	4 (5%)	0	100	100
32	l	64/118 (54%)	62 (97%)	2 (3%)	0	100	100
33	m	57/76 (75%)	56 (98%)	1 (2%)	0	100	100
34	n	60/240 (25%)	59 (98%)	1 (2%)	0	100	100
35	p	157/166 (95%)	152 (97%)	5 (3%)	0	100	100
36	q	70/2752 (2%)	64 (91%)	5 (7%)	1 (1%)	11	40
37	u	359/520 (69%)	332 (92%)	26 (7%)	1 (0%)	41	73
All	All	9607/19975 (48%)	9149 (95%)	435 (4%)	23 (0%)	50	79

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	U	225	PRO
16	U	226	PRO
23	b	57	VAL
11	N	860	LYS
16	U	134	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	2/77 (3%)	2 (100%)	0	100	100
3	C	342/1104 (31%)	342 (100%)	0	100	100
4	D	69/95 (73%)	69 (100%)	0	100	100
5	E	102/776 (13%)	102 (100%)	0	100	100
7	G	10/397 (2%)	10 (100%)	0	100	100
8	I	33/382 (9%)	33 (100%)	0	100	100
9	J	42/446 (9%)	42 (100%)	0	100	100
10	L	11/545 (2%)	11 (100%)	0	100	100
11	N	625/897 (70%)	624 (100%)	1 (0%)	93	97
12	O	274/441 (62%)	274 (100%)	0	100	100
13	P	108/709 (15%)	107 (99%)	1 (1%)	78	91
14	Q	83/203 (41%)	83 (100%)	0	100	100
15	T	129/130 (99%)	129 (100%)	0	100	100
16	U	181/361 (50%)	181 (100%)	0	100	100
17	V	180/451 (40%)	180 (100%)	0	100	100
18	W	180/838 (22%)	177 (98%)	3 (2%)	60	83
19	X	85/751 (11%)	85 (100%)	0	100	100
20	Y	209/459 (46%)	209 (100%)	0	100	100
21	Z	35/294 (12%)	35 (100%)	0	100	100
22	a	1496/2108 (71%)	1493 (100%)	3 (0%)	93	97
23	b	784/866 (90%)	784 (100%)	0	100	100
31	k	1/101 (1%)	1 (100%)	0	100	100
36	q	30/2432 (1%)	30 (100%)	0	100	100
37	u	45/456 (10%)	45 (100%)	0	100	100
All	All	5056/15319 (33%)	5048 (100%)	8 (0%)	93	97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	a	1641	ARG
22	a	1523	ARG
18	W	580	ARG
18	W	575	THR
22	a	775	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
17	V	152	GLN
18	W	629	ASN
22	a	960	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	d	91/106 (85%)	25 (27%)	0
25	e	95/117 (81%)	27 (28%)	0
26	f	72/188 (38%)	16 (22%)	0
27	g	74/319 (23%)	31 (41%)	0
All	All	332/730 (45%)	99 (29%)	0

5 of 99 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
24	d	6	C
24	d	8	C
24	d	9	U
24	d	10	U
24	d	12	G

There are no RNA pucker outliers to report.

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 21 ligands modelled in this entry, 19 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	b	1500	41	26,34,34	1.22	2 (7%)	32,54,54	1.55	7 (21%)
39	IHP	a	3001	-	36,36,36	1.42	6 (16%)	54,60,60	1.34	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	GTP	b	1500	41	-	6/18/38/38	0/3/3/3
39	IHP	a	3001	-	-	4/30/54/54	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	1500	GTP	C5-C6	-4.35	1.38	1.47
39	a	3001	IHP	P5-O15	3.08	1.65	1.59
39	a	3001	IHP	P3-O13	2.96	1.64	1.59
39	a	3001	IHP	P6-O16	2.92	1.64	1.59
39	a	3001	IHP	P1-O11	2.90	1.64	1.59

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	b	1500	GTP	PB-O3B-PG	-3.79	119.82	132.83
39	a	3001	IHP	C6-C1-C2	3.64	118.39	110.41
39	a	3001	IHP	C5-C6-C1	3.30	117.64	110.41
40	b	1500	GTP	C5-C6-N1	3.26	119.70	113.95
40	b	1500	GTP	C8-N7-C5	2.98	108.67	102.99

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	a	3001	IHP	C6-O16-P6-O36

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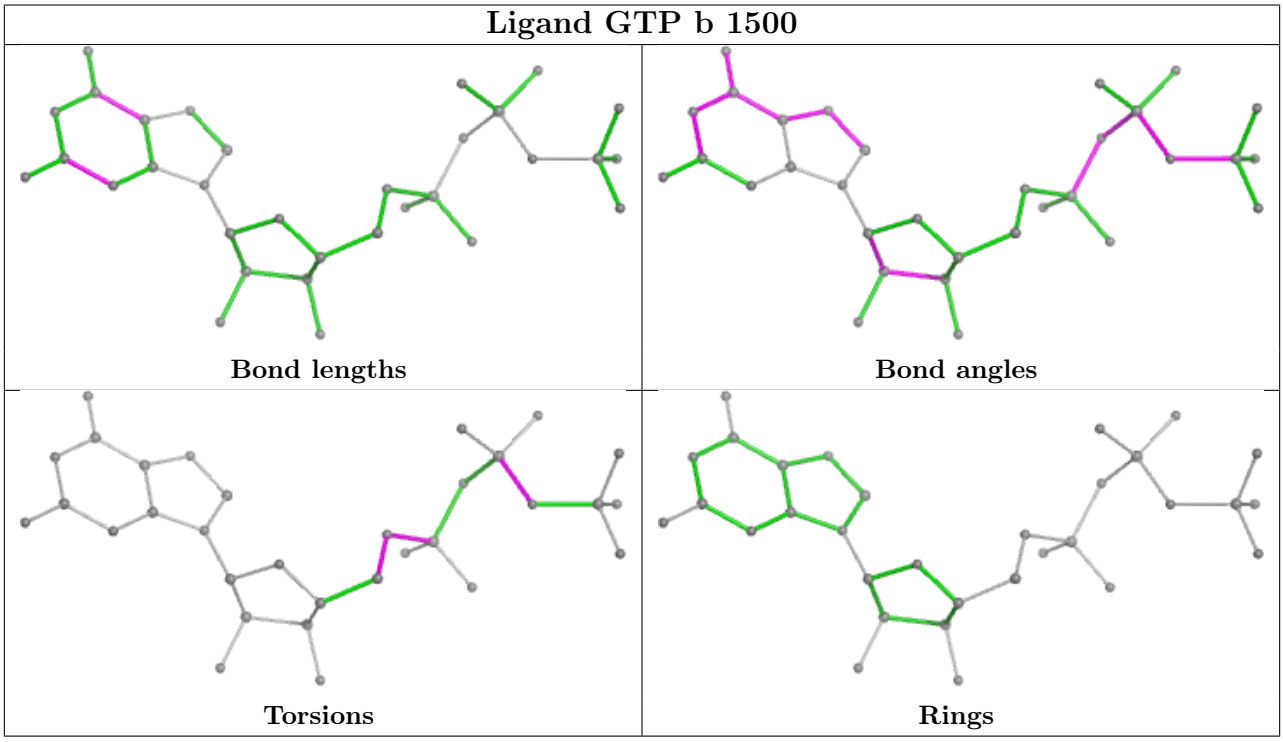
Mol	Chain	Res	Type	Atoms
40	b	1500	GTP	C5'-O5'-PA-O3A
40	b	1500	GTP	C5'-O5'-PA-O2A
39	a	3001	IHP	C2-O12-P2-O22
39	a	3001	IHP	C1-O11-P1-O31

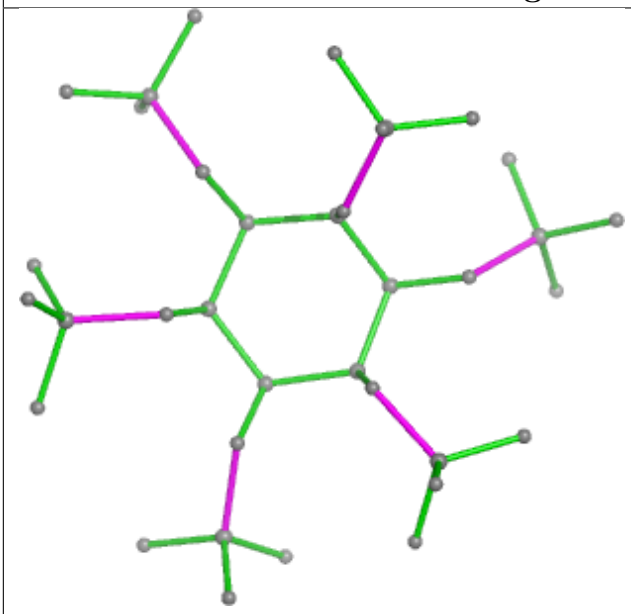
There are no ring outliers.

No monomer is involved in short contacts.

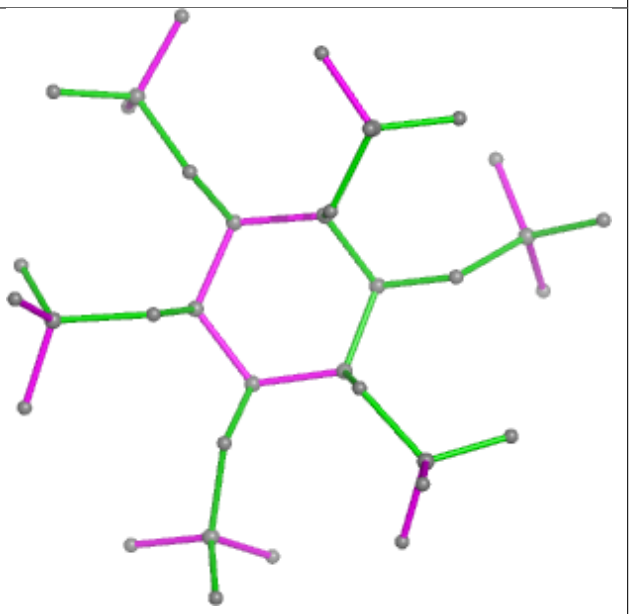
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



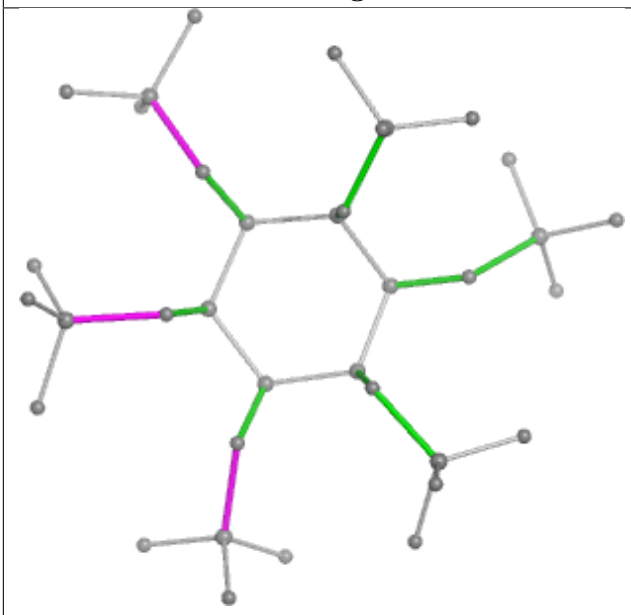
Ligand IHP a 3001



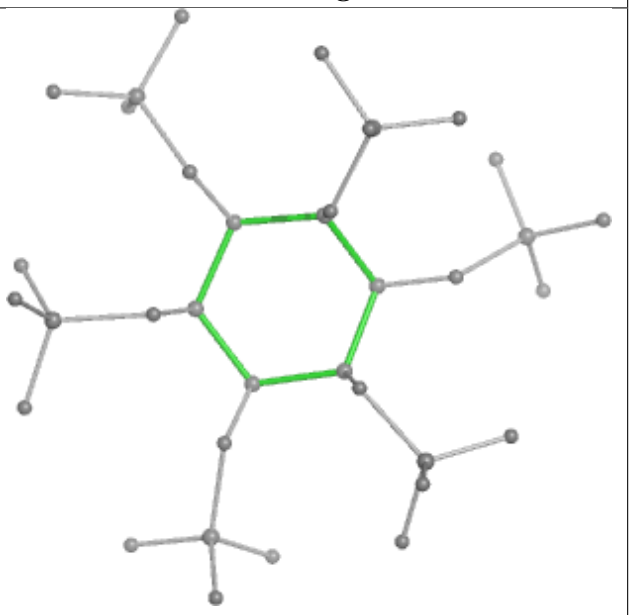
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

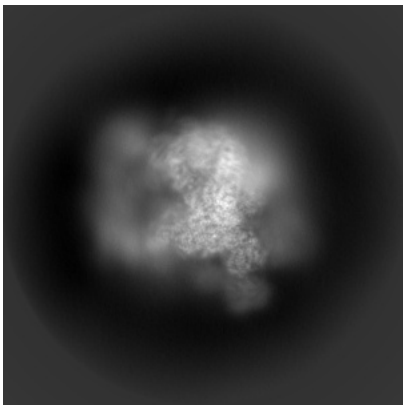
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14146. These allow visual inspection of the internal detail of the map and identification of artifacts.

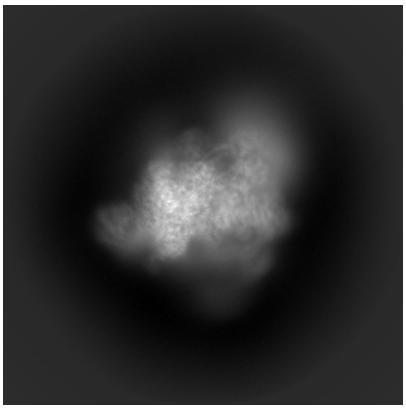
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

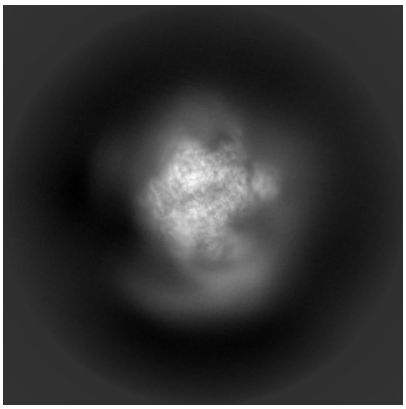
6.1.1 Primary map



X

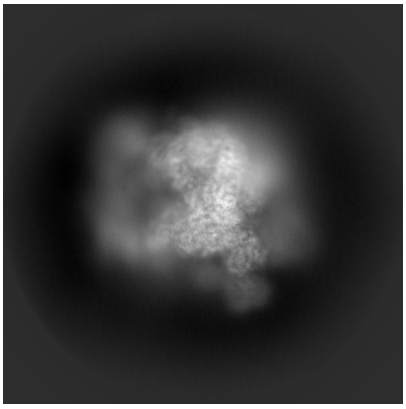


Y

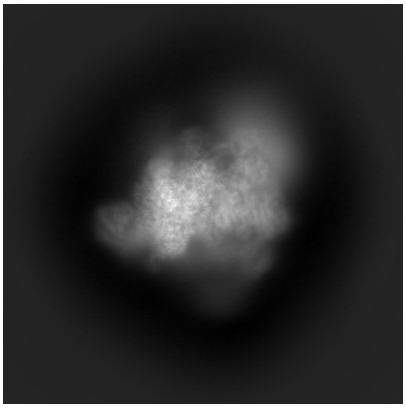


Z

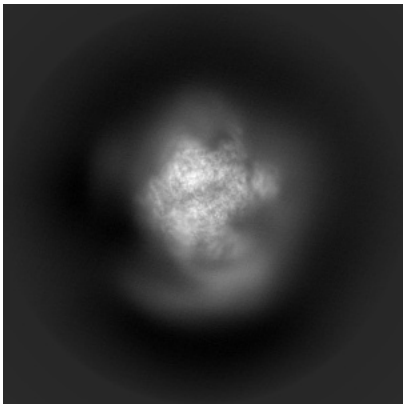
6.1.2 Raw map



X



Y

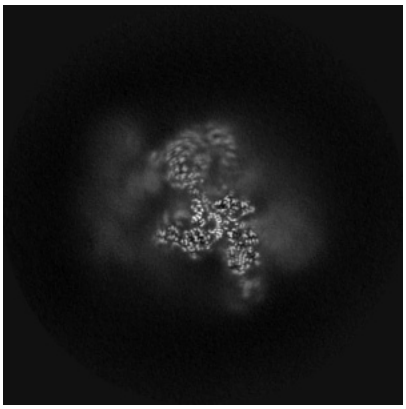


Z

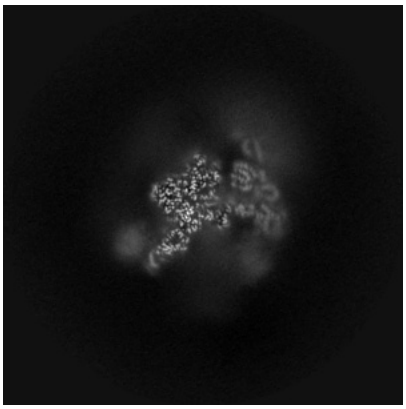
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

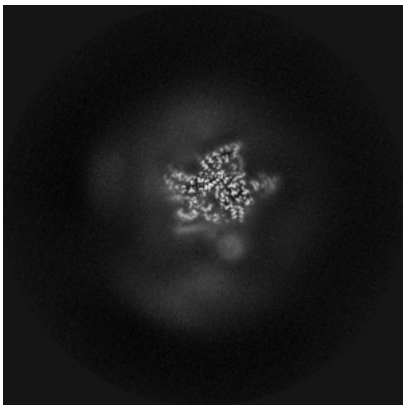
6.2.1 Primary map



X Index: 260

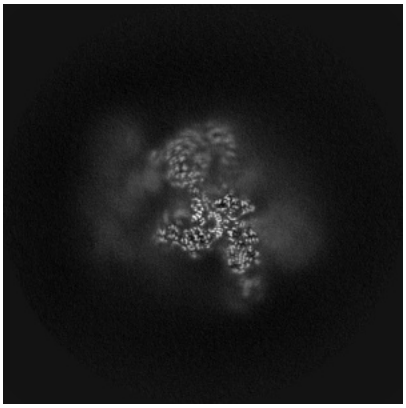


Y Index: 260

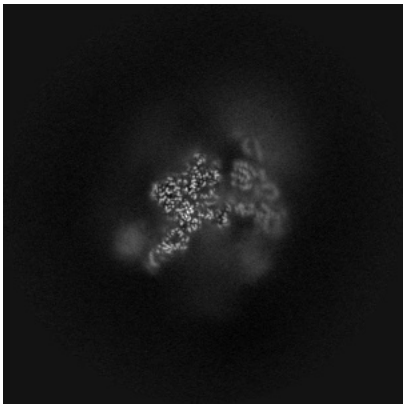


Z Index: 260

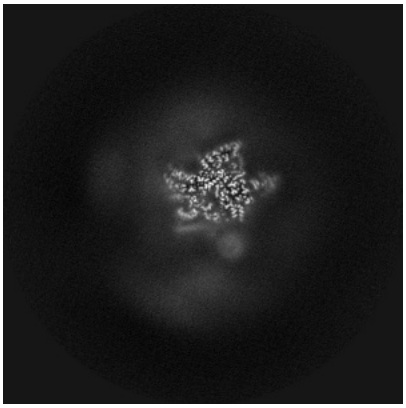
6.2.2 Raw map



X Index: 260



Y Index: 260

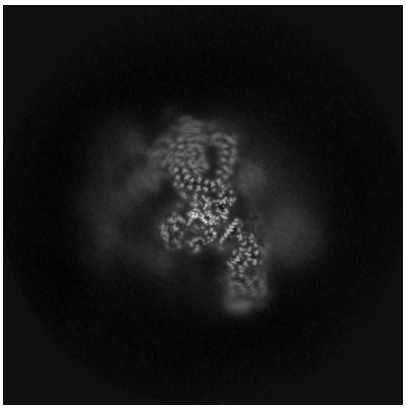


Z Index: 260

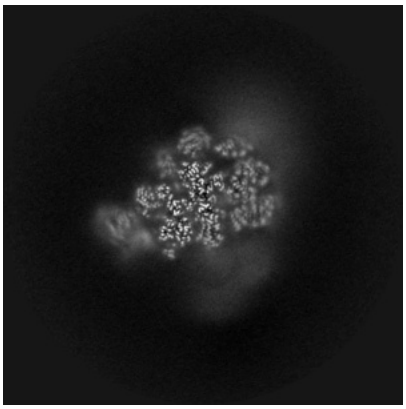
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

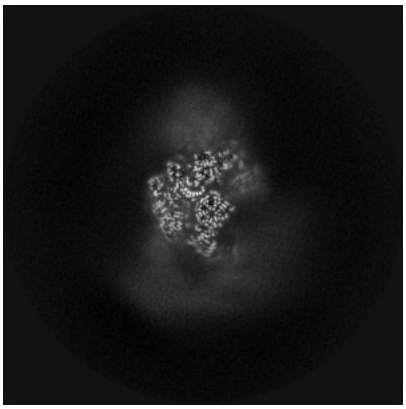
6.3.1 Primary map



X Index: 249

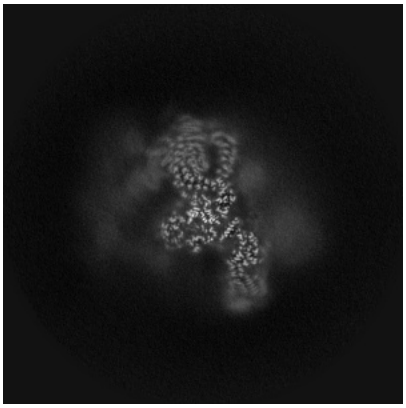


Y Index: 293

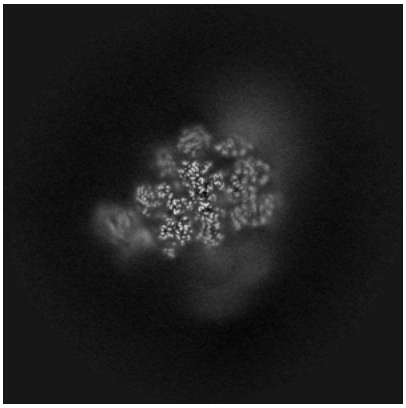


Z Index: 218

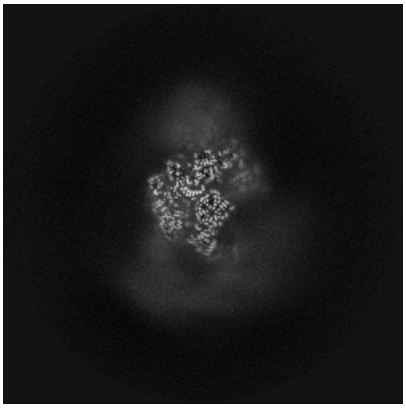
6.3.2 Raw map



X Index: 250



Y Index: 293

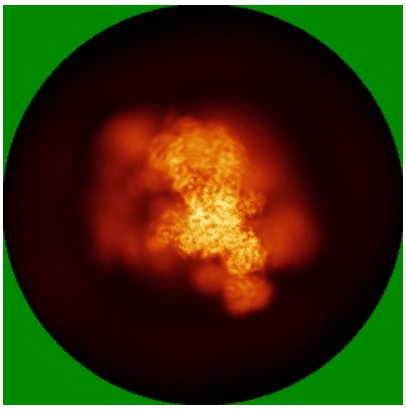


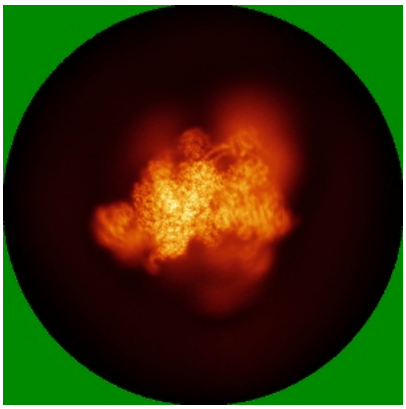
Z Index: 218

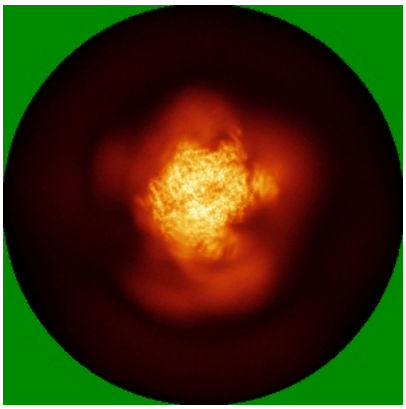
The images above show the largest variance slices of the map in three orthogonal directions.

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

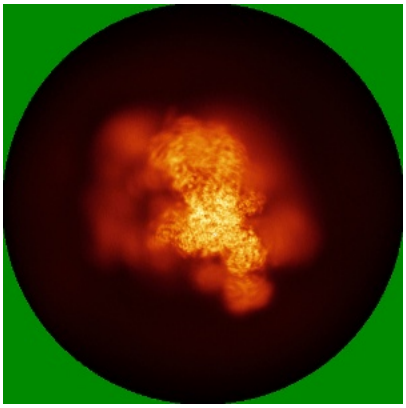
6.4.1 Primary map


X


Y


Z

6.4.2 Raw map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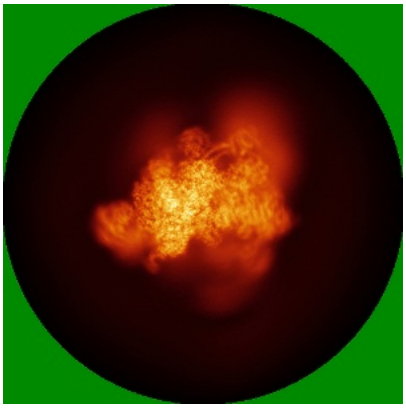
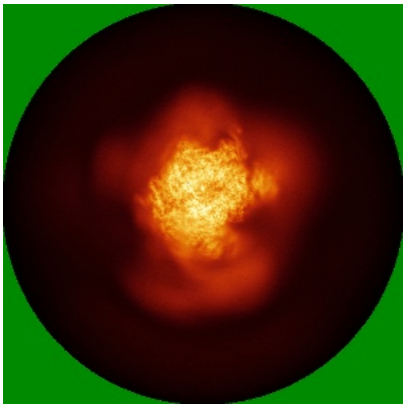

Y


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

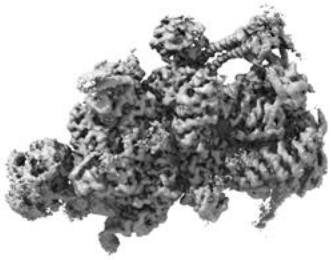
Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X



Y

Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

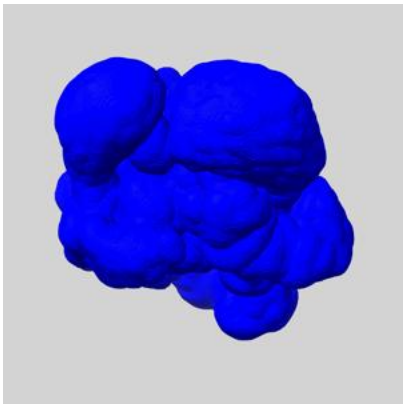
6.6 Mask visualisation (i)

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

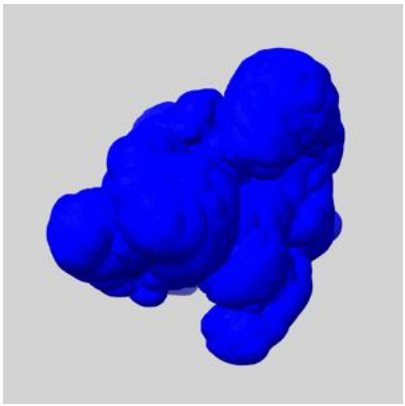
A mask typically either:

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

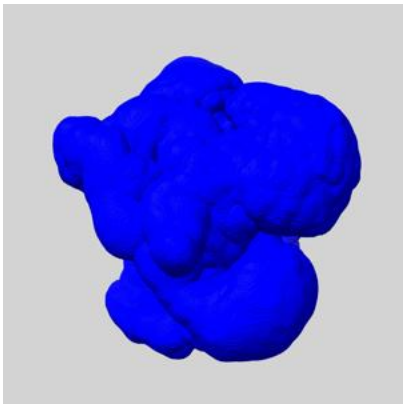
6.6.1 emd_14146_msk_1.map (i)



X



Y

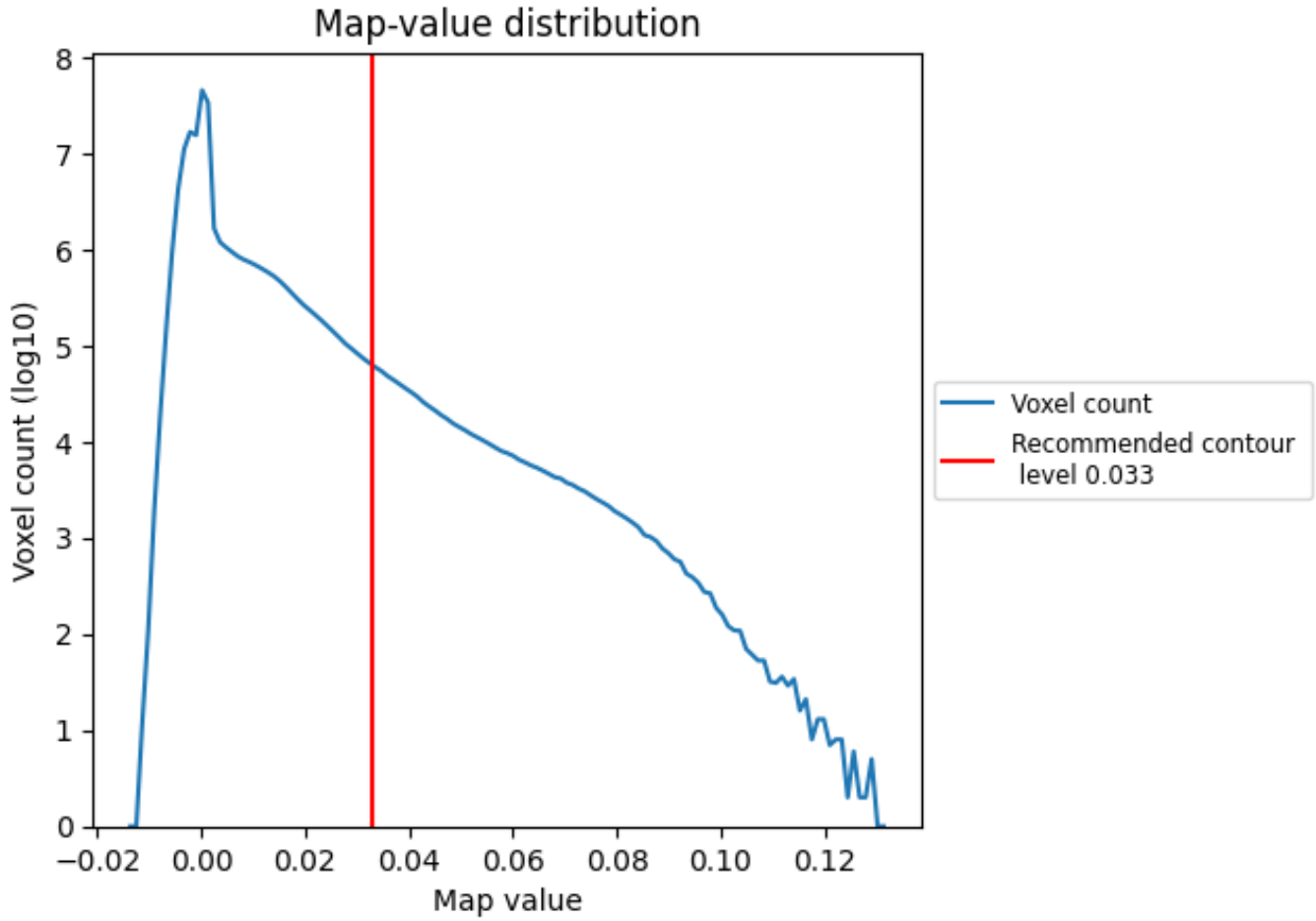


Z

7 Map analysis

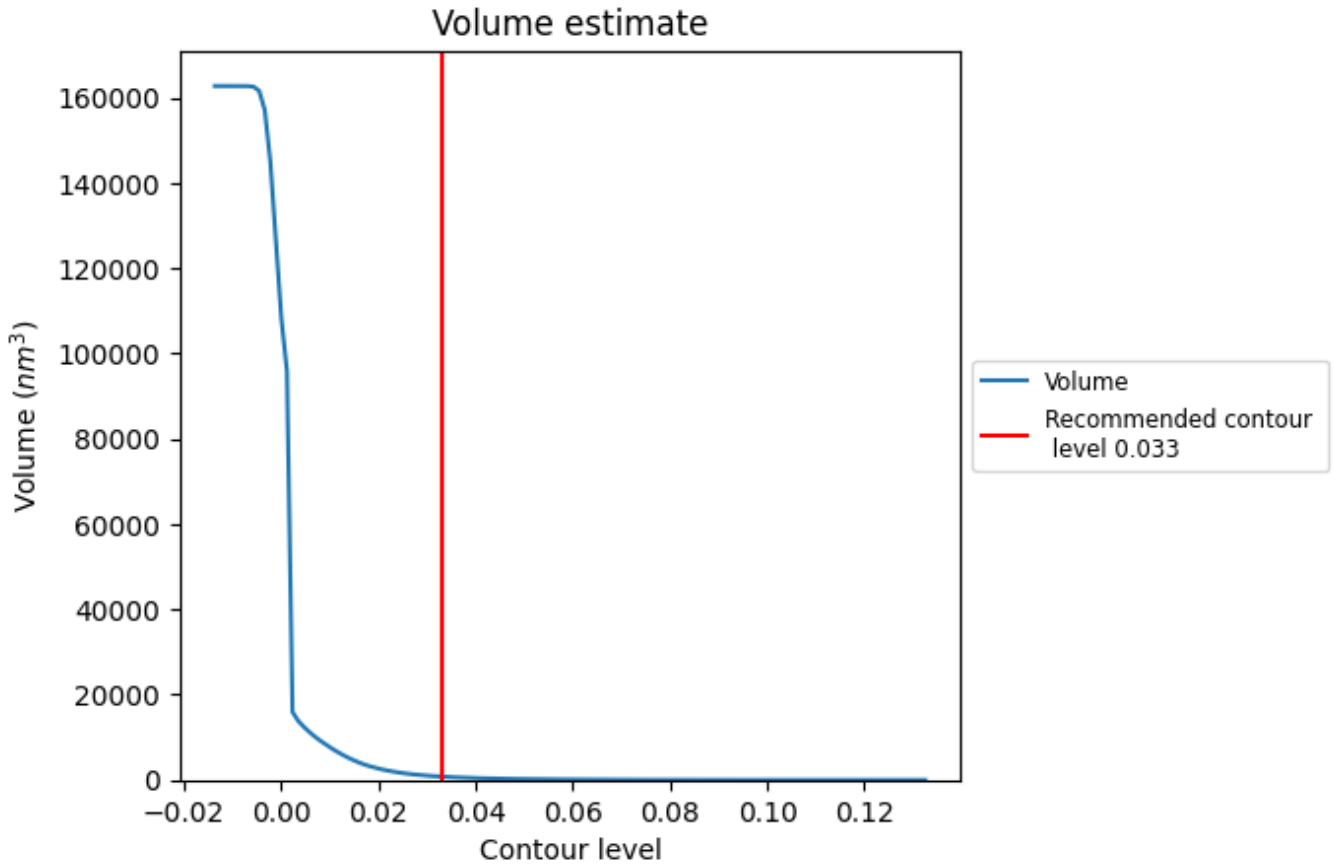
This section contains the results of statistical analysis of the map.

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.

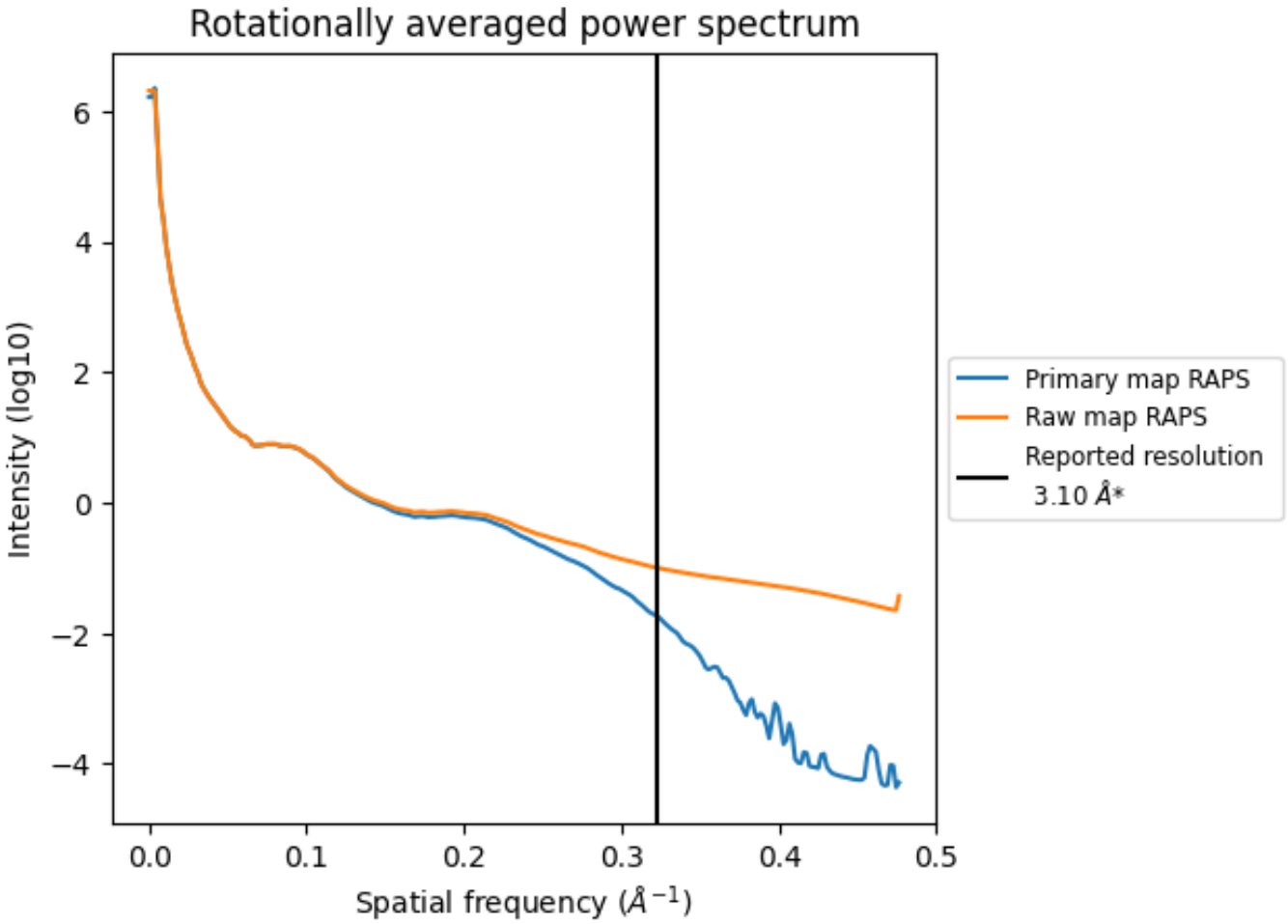
7.2 Volume estimate



The volume at the recommended contour level is 786 nm^3; this corresponds to an approximate mass of 710 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

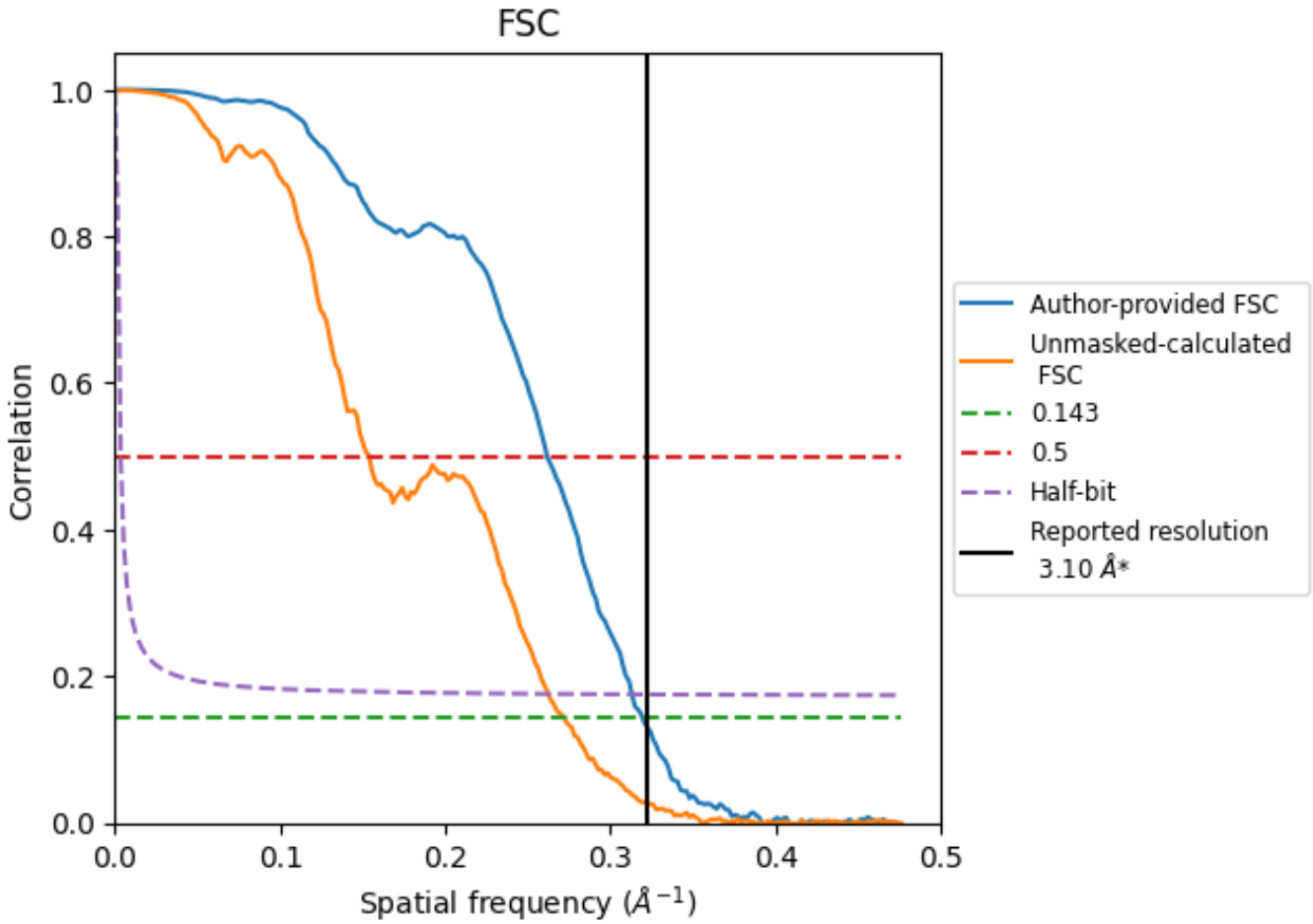


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8.2 Resolution estimates (i)

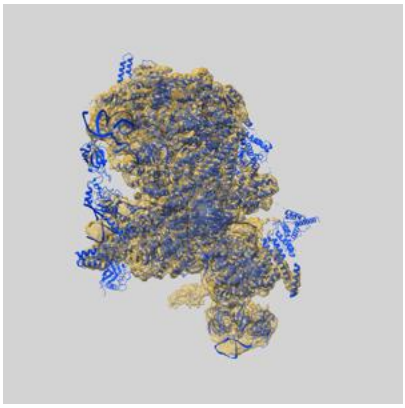
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.82	3.19
Unmasked-calculated*	3.68	6.49	3.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.68 differs from the reported value 3.1 by more than 10 %

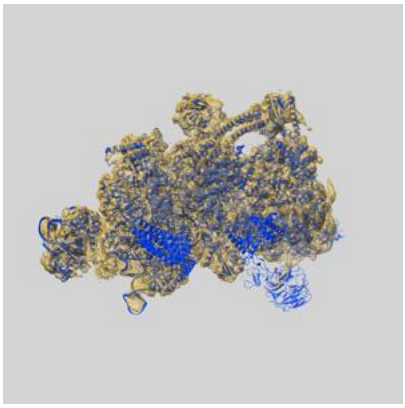
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14146 and PDB model 7QTT. Per-residue inclusion information can be found in section 3 on page 13.

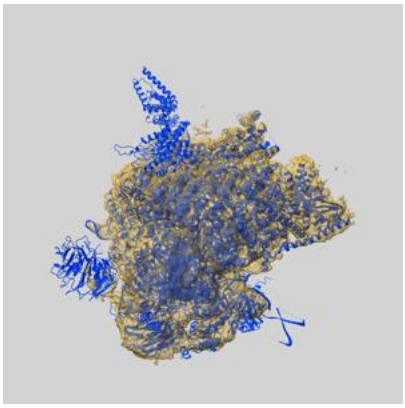
9.1 Map-model overlay



X



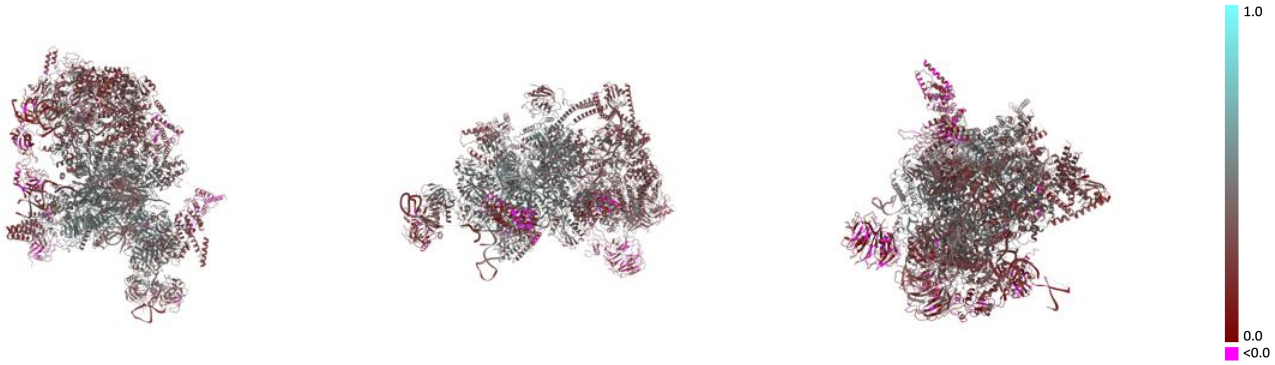
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.033 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.

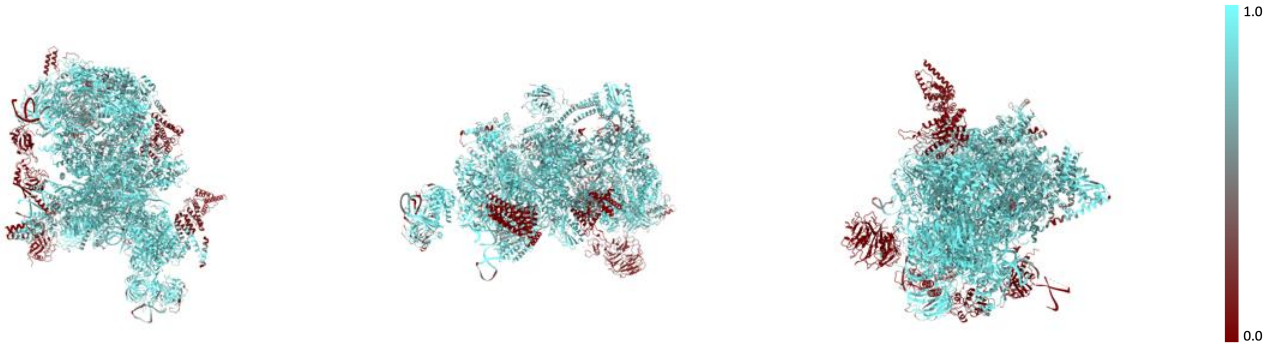
9.2 Q-score mapped to coordinate model (i)



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.

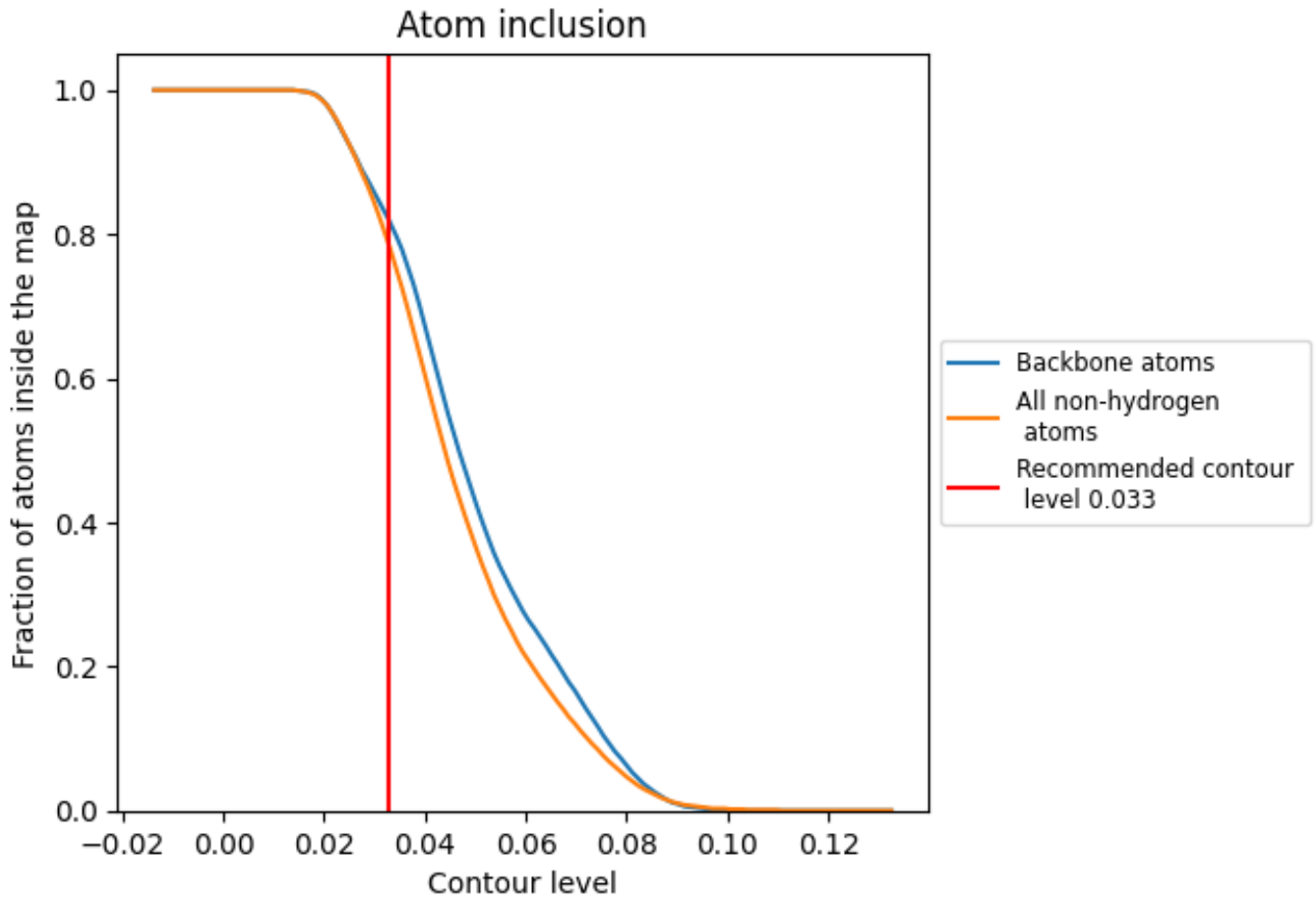
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.033).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.3840
A	0.6410	0.2660
B	0.9770	0.3070
C	0.9050	0.3520
D	0.8210	0.3490
E	0.7010	0.3060
F	0.0500	0.1530
G	0.5660	0.2900
I	0.9560	0.4400
J	0.8020	0.2030
L	0.5250	0.3130
N	0.7800	0.3420
O	0.9470	0.5230
P	0.8580	0.4280
Q	0.8410	0.4580
T	0.9030	0.4560
U	0.6200	0.3610
V	0.7750	0.3290
W	0.4820	0.3160
X	0.8310	0.3970
Y	0.8010	0.4170
Z	0.5490	0.3570
a	0.8460	0.4650
b	0.8810	0.4510
d	0.9200	0.4180
e	0.9020	0.3930
f	0.7480	0.2710
g	0.8880	0.3920
h	0.9470	0.3220
i	0.7600	0.2200
j	0.7640	0.2800
k	0.9330	0.4370
l	0.9590	0.3520
m	0.6150	0.2130
n	0.8220	0.3960

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Continued from previous page...

Chain	Atom inclusion	Q-score
p	0.0000	0.2080
q	0.7730	0.3890
u	0.4500	0.2900