wwPDB EM Validation Summary Report (i)

Dec 4, 2024 – 05:22 am GMT

PDB ID	:	9FMD
EMDB ID	:	EMD-4525
Title	:	Integrative model of the human post-catalytic spliceosome (P-complex)
Authors	:	Rothe, P.; Plaschka, C.; Vorlaender, M.K.
Deposited on	:	2024-06-05
Resolution	:	3.30 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 (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 (1)) were used in the production of this report:

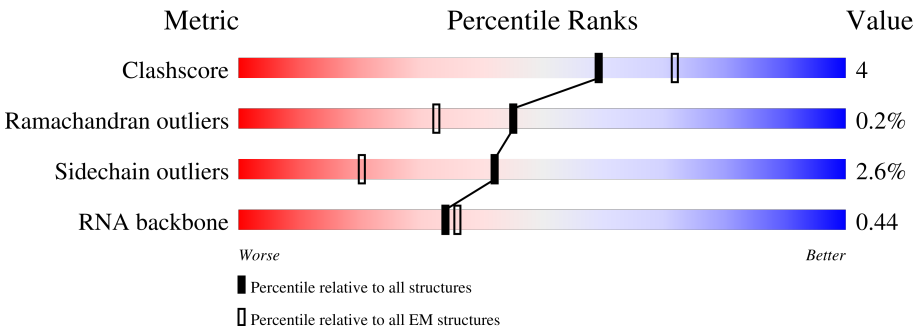
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1	184	35%; 59%; 8%; 33%
2	2	187	36%; 31%; 26%; 6%; •; 36%
3	3	476	16%; 17%; 83%
4	32	112	9%; 44%; 9%; •; 46%
5	5	116	25%; 26%; 37%; 13%; •; 21%
6	50	339	66%; 64%; •; 33%
7	56	222	45%; 45%; 55%

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Mol	Chain	Length	Quality of chain
8	6	106	15% 34% 33% 21% 8%
9	7	411	95% 94% 5%
10	8	174	52% 52% 48%
11	9	146	99% 99%
12	A	2335	15% 81% 15%
13	B	2136	87% 71% 15% 13%
14	C	972	10% 82% 9% 8%
15	D	285	25% 25% 75%
16	E	357	11% 66% 18% 15%
17	EX	14	14% 43% 57%
18	F	758	14% 84%
19	H	908	29% 47% 49%
20	I	855	83% 85% 15%
21	IN	113	11% 11% 12% 12% 63%
22	J	848	39% 70% 29%
23	K	225	78% 84% 16%
24	L	802	41% 63% 6% 31%
25	M	243	41% 92% 8%
26	N	144	7% 83% 16%
27	NO	301	58% 56% 42%
28	O	420	26% 56% 13% 31%
29	P	229	8% 41% 54%
30	Q	1485	89% 89% 11%
31	R	536	21% 50% 11% 39%
32	S	166	22% 82% 16%

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Mol	Chain	Length	Quality of chain
33	SR	2752	97%
34	T	514	9%, 57%, 13%, 29%
35	U	586	13%, 42%, 9%, 50%
36	V	1220	57%, 60%, 40%
37	W	579	11%, 68%, 20%, 11%
38	X	451	14%, 14%, 85%
39	Z	166	32%, 31%, 68%
40	a	126	32%, 67%, 33%
40	h	126	30%, 66%, 34%
41	b	240	23%, 36%, 64%
41	i	240	29%, 34%, 66%
42	c	119	61%, 67%, 33%
42	j	119	62%, 67%, 33%
43	d	118	75%, 75%, 25%
43	k	118	78%, 81%, 19%
44	e	92	86%, 86%, 14%
44	l	92	73%, 88%, 12%
45	f	86	81%, 81%, 16%
45	m	86	76%, 84%, 16%
46	g	76	76%, 93%
46	n	76	54%, 95%
47	o	255	63%, 63%, 36%
48	p	225	40%, 41%, 59%
49	q	504	20%, 20%, 80%
49	r	504	24%, 24%, 76%

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Mol	Chain	Length	Quality of chain
49	s	504	26% 26% 74%
49	t	504	20% 20% 80%
50	w	646	82% 82% 18%
51	x	289	43% 44% 56%
52	y	301	26% 26% 74%
53	z	415	10% 17% 83%

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 120489 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 PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	123	1013	635	193	180	5	0	0

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	120	2535	1135	428	852	120	0	0

- Molecule 3 is a protein called Splicing factor ESS-2 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	3	82	408	244	82	82	0	0

- Molecule 4 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	32	60	504	314	96	92	2	0	0

- Molecule 5 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	5	92	1936	867	322	655	92	0	0

- Molecule 6 is a protein called Protein FAM50A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	50	226	1124	671	226	227	0	0

- Molecule 7 is a protein called STING ER exit protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	56	101	498	296	101	101	0	0

- Molecule 8 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	6	97	2075	928	381	669	97	0	0

- Molecule 9 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	7	390	1928	1147	390	391	0	0

- Molecule 10 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	8	91	445	263	91	91	0	0

- Molecule 11 is a protein called Protein mago nashi homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	9	144	712	423	144	145	0	0

- Molecule 12 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	A	2250	17802	11405	3151	3176	70	0	0

- Molecule 13 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	B	1864	15004	9583	2569	2775	77	0	0

- Molecule 14 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	C	894	7069	4521	1178	1336	34	0	0

- Molecule 15 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	D	72	358	214	72	72	0	0

- Molecule 16 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	E	303	2370	1489	416	452	13	0	0

- Molecule 17 is a RNA chain called Exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	EX	14	296	132	52	98	14	0	0

- Molecule 18 is a protein called Splicing factor Cactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	F	122	1089	714	197	176	2	0	0

- Molecule 19 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	H	459	2932	1827	533	560	12	0	0

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	I	727	3610	2156	727	727	0	0

- Molecule 21 is a RNA chain called INTRON.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	IN	42	893	400	158	293	42	0	0

- Molecule 22 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	J	602	2998	1794	602	602	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	K	189	941	563	189	189	0	0

- Molecule 24 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	L	555	3642	2233	706	695	8	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	M	224	1115	666	224	225	0	0

- Molecule 26 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	N	144	1189	748	218	211	12	0	0

- Molecule 27 is a protein called Nitric oxide synthase-interacting protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	NO	174	864	516	174	174	0	0

- Molecule 28 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	O	289	2327	1459	416	432	20	0	0

- Molecule 29 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	P	106	889	544	174	169	2	0	0

- Molecule 30 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	Q	1322	6554	3910	1322	1322	0	0

- Molecule 31 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
31	R	328	2618	1634	479	489	2	14	0	0

- Molecule 32 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	S	164	1271	810	220	234	7	0	0

- Molecule 33 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	SR	70	412	251	80	80	1	0	0

- Molecule 34 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	T	363	2881	1820	525	526	10	0	0

- Molecule 35 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	U	295	2425	1525	431	461	8	0	0

- Molecule 36 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	V	733	3629	2163	733	733	0	0

- Molecule 37 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	W	513	4158	2643	719	772	24	0	0

- Molecule 38 is a protein called Splicing regulator SDE2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	X	66	328	196	66	66	0	0

- Molecule 39 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	Z	53	265	159	53	53	0	0

- Molecule 40 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	a	84	658	412	116	124	6	0	0
40	h	83	652	409	115	122	6	0	0

- Molecule 41 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	b	87	654	412	120	115	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	i	82	664	419	121	117	7	0	0

- Molecule 42 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	c	80	634	404	111	115	4	0	0
42	j	80	634	404	111	115	4	0	0

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	d	89	723	454	133	131	5	0	0
43	k	95	774	486	141	142	5	0	0

- Molecule 44 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	e	79	651	413	115	118	5	0	0
44	l	81	669	424	119	121	5	0	0

- Molecule 45 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	f	72	562	364	93	100	5	0	0
45	m	72	562	364	93	100	5	0	0

- Molecule 46 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	g	73	568	358	102	102	6	0	0
46	n	73	568	358	102	102	6	0	0

- Molecule 47 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	o	162	1282	820	219	240	3	0	0

- Molecule 48 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	p	92	745	480	130	130	5	0	0

- Molecule 49 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	q	103	514	308	103	103	0	0
49	r	119	594	356	119	119	0	0
49	s	132	659	395	132	132	0	0
49	t	103	514	308	103	103	0	0

- Molecule 50 is a protein called Peptidylprolyl isomerase domain and WD repeat-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	w	528	2605	1548	528	529	0	0

- Molecule 51 is a protein called Splicing factor C9orf78.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	x	128	636	379	128	129	0	0

- Molecule 52 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	y	79	318	160	79	79	0	0

- Molecule 53 is a protein called NF-kappa-B-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	z	70	430	259	83	86	2	0	0

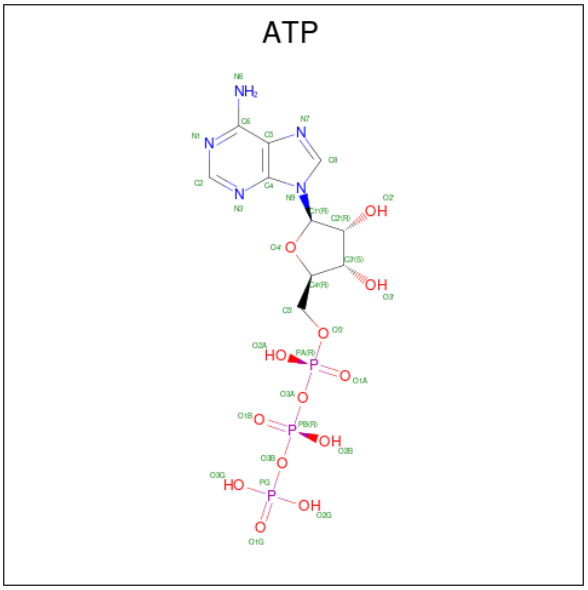
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	6	5	5	5	0
54	7	1	1	1	0

- Molecule 55 is POTASSIUM ION (three-letter code: K) (formula: K).

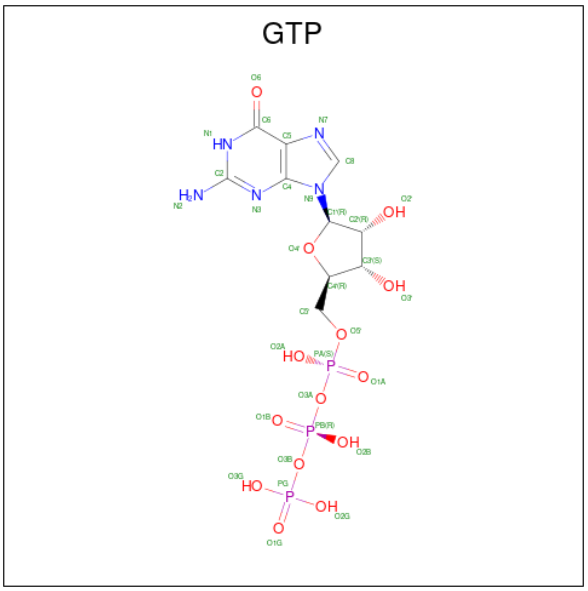
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
55	6	1	1	1	0

- Molecule 56 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	7	1	31	10	5	13	3	0

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

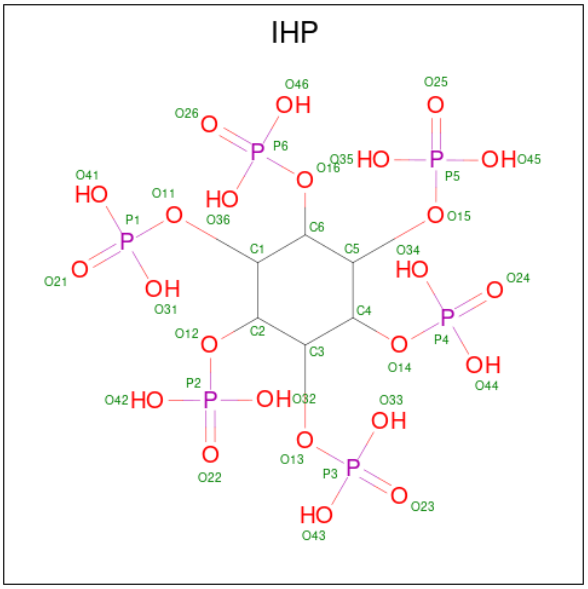


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	C	1	32	10	5	14	3	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
58	N	3	3	3	0
58	O	3	Total	Zn	0
			3	3	

- Molecule 59 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



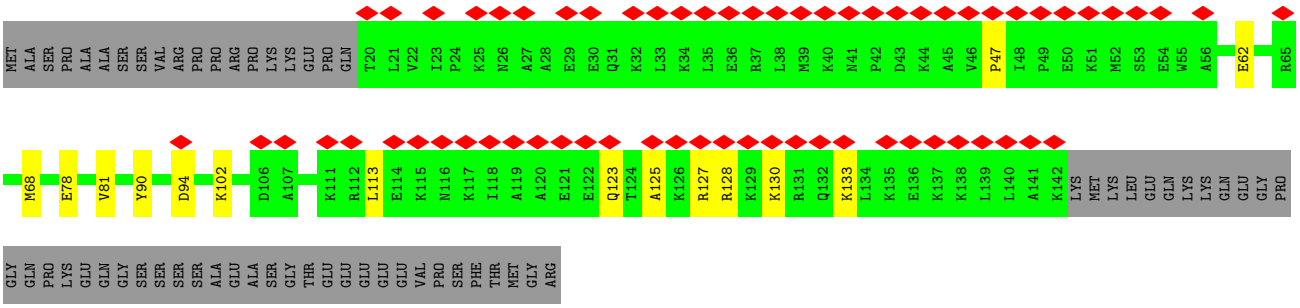
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
59	U	1	36	6	24	6	0

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: PRKR-interacting protein 1

Chain 1:

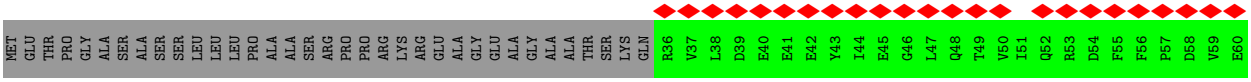


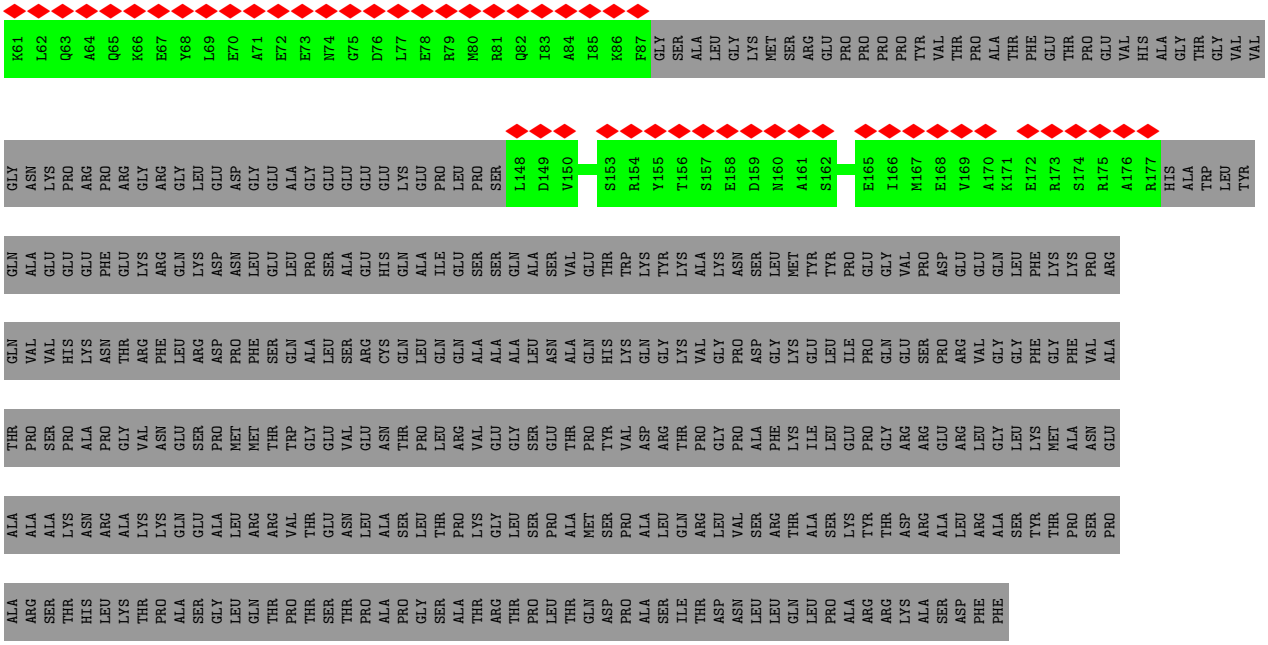
- Molecule 2: U2 snRNA

Chain 2:

- Molecule 3: Splicing factor ESS-2 homolog

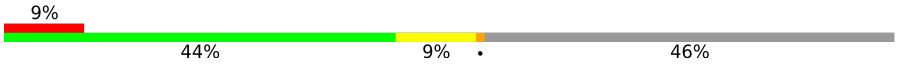
Chain 3:

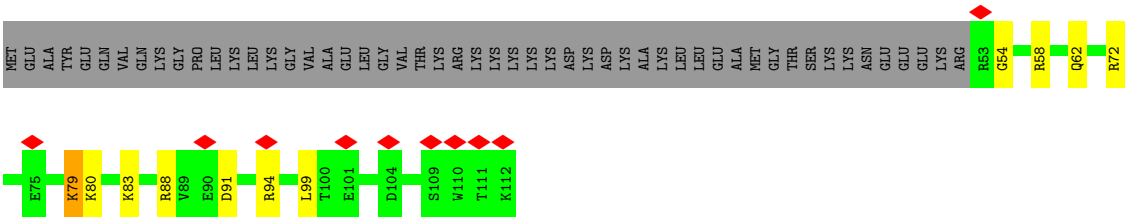




- Molecule 4: Protein FAM32A

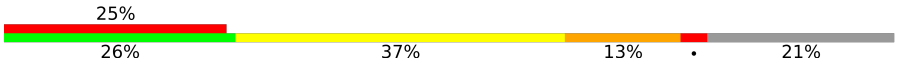
Chain 32:

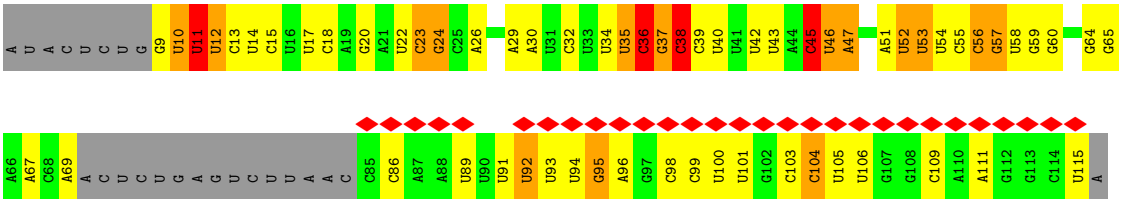




- Molecule 5: U5 snRNA

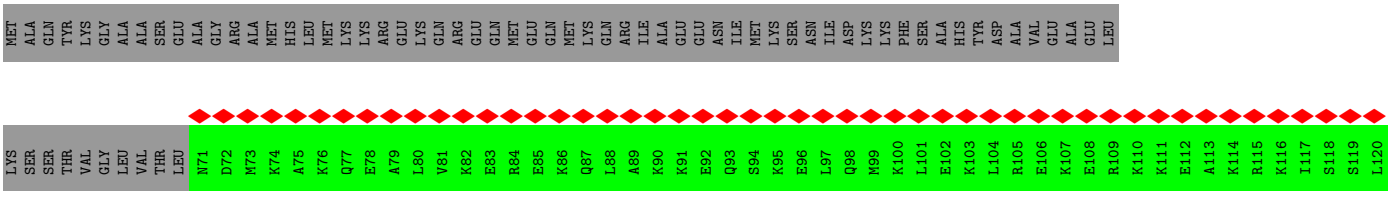
Chain 5:

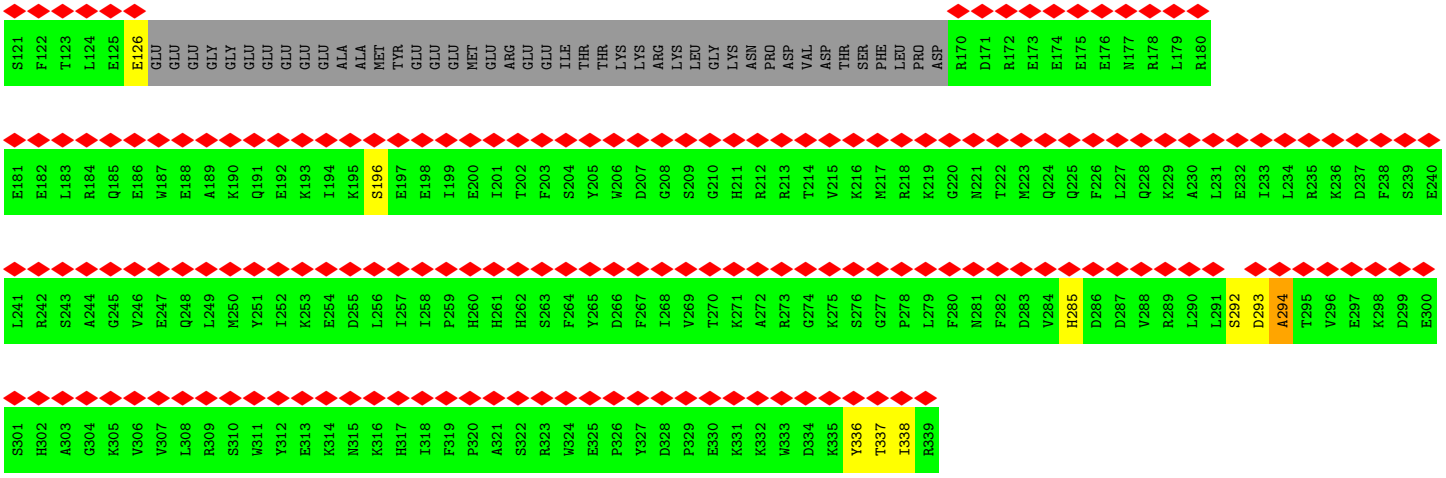




- Molecule 6: Protein FAM50A

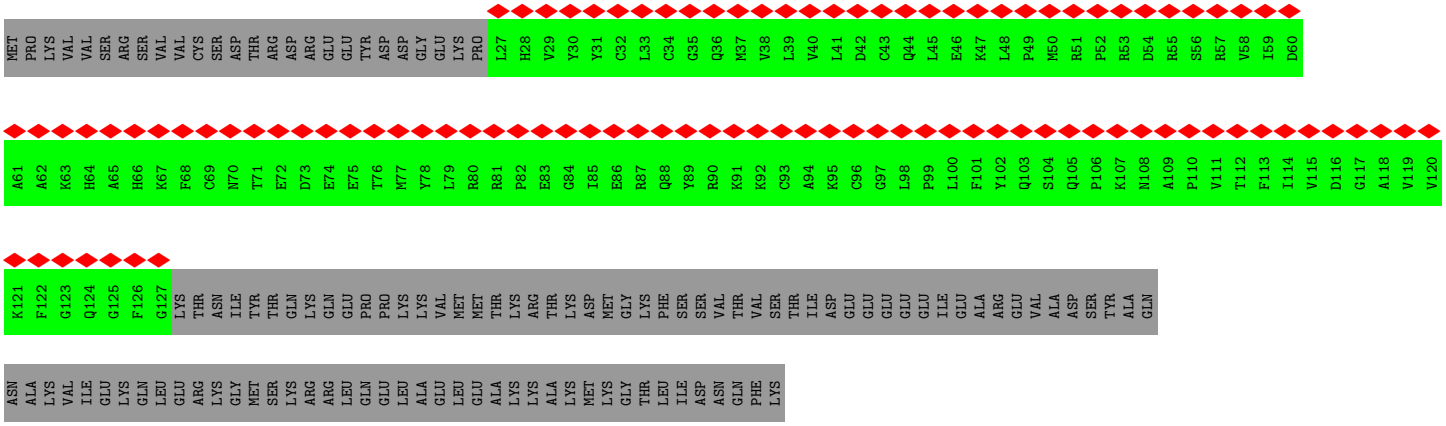
Chain 50:





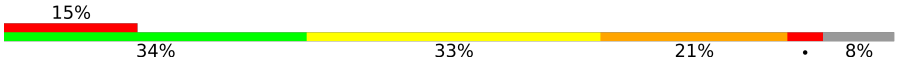
- Molecule 7: STING ER exit protein

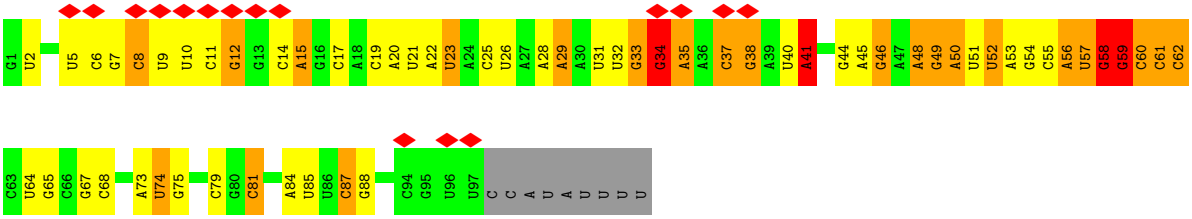
Chain 56:



- Molecule 8: U6 snRNA

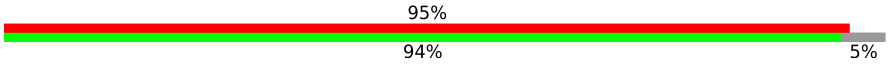
Chain 6:

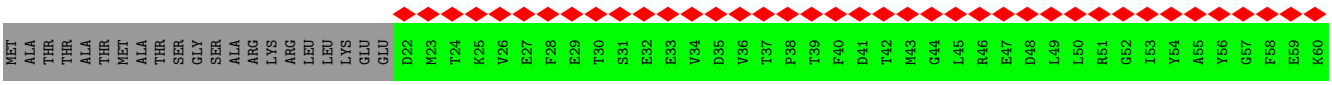




- Molecule 9: Eukaryotic initiation factor 4A-III

Chain 7:





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Q121 I122 Q123 K124 G125 L126 L127 A128 L129 G130 D131 Y132 M133 N134 V135 Q136 C137 H138 A139 C140 I141 G142 G143 T144 N145 V146 G147 E148 D149 I150 R151 K152 L153 D154 Y155 G156 Q157 H158 V159 V160 A161 G162 T163 P164 G165 R166 V167 F168 D169 M170 I171 R172 R173 R174 S175 L176 R177 T178 R179 A180

I181 K182 M183 L184 V185 L186 D187 E188 A189 D190 E191 M192 L193 N194 K195 G196 F197 K198 E199 Q200 I201 Y202 D203 V204 Y205 R206 Y207 L208 P209 P210 A211 T212 Q213 V214 V215 L216 I217 S218 A219 T220 L221 P222 H223 E224 I225 L226 E227 M228 T229 N230 K231 F232 M233 T234 D235 P236 I237 R238 I239 L240

V241 K242 R243 D244 E245 L246 T247 L248 E249 G250 I251 K252 Q253 F254 F255 V256 A257 V258 E259 R260 E261 E262 W263 K264 F265 D266 T267 L268 C269 D270 L271 Y272 D273 T274 L275 T276 I277 T278 Q279 A280 V281 I282 F283 C284 N285 T286 K287 R288 K289 V290 D291 W292 L293 T294 E295 K296 M297 R298 E299 A300

N301 F302 T303 V304 S305 S306 M307 H308 G309 D310 M311 P312 Q313 K314 E315 R316 E317 S318 I319 M320 K321 E322 F323 R324 S325 G326 A327 S328 R329 V330 L331 I332 S333 T334 D335 V336 W337 A338 R339 G340 L341 D342 V343 P344 Q345 V346 S347 L348 I349 I350 N351 Y352 D353 L354 P355 N356 N357 R358 E359 L360

Y361 I362 H363 R364 I365 G366 R367 S368 G369 R370 Y371 G372 R373 K374 G375 V376 A377 I378 S318 N379 F380 V381 K382 N383 D384 D385 I386 R387 I388 L389 R390 D391 I392 E393 Q394 Y395 Y396 S397 T398 Q399 I400 D401 E402 M403 P404 M405 N406 V407 A408 D409 L410 I411

- Molecule 10: RNA-binding protein 8A

Chain 8: 52% 52% 48%

MET ALA ASP VAL LEU ASP LEU HIS GLU ALA GLY GLY GLU ASP PHE ALA MET ASP GLU ASP GLY ASP GLU SER ILE HIS LYS LEU LYS GLU LYS ALA LYS LYS ARG LYS GLY ARG GLY PHE GLY SER GLU GLU GLY SER ARG ALA ARG MET ARG GLU ASP TYR ASP SER VAL GLU GLN ASP

GLY ASP GLU P64 G65 P66 Q67 R68 S69 V70 E71 G72 W73 I74 L75 F76 V77 T78 G79 V80 H81 E82 E83 A84 T85 E86 E87 D88 I89 H90 D91 K92 F93 A94 E95 Y96 G97 E98 I99 K100 N101 I102 H103 L104 N105 L106 D107 R108 R109 T110 G111 Y112 L113 K114 G115 Y116 T117 L118 V119 E120

Y121 E122 T123 Y124 K125 E126 A127 Q128 A129 A130 M131 E132 G133 L134 N135 G136 Q137 D138 L139 M140 G141 Q142 P143 I144 S145 V146 D147 W148 C149 F150 V151 R152 G153 P154 PRO LYS GLY LYS ARG ARG GLY GLY ARG ARG ARG ARG SER ARG SER PRO ASP ARG ARG ARG ARG ARG

- Molecule 11: Protein mago nashi homolog

Chain 9: 99% 99%

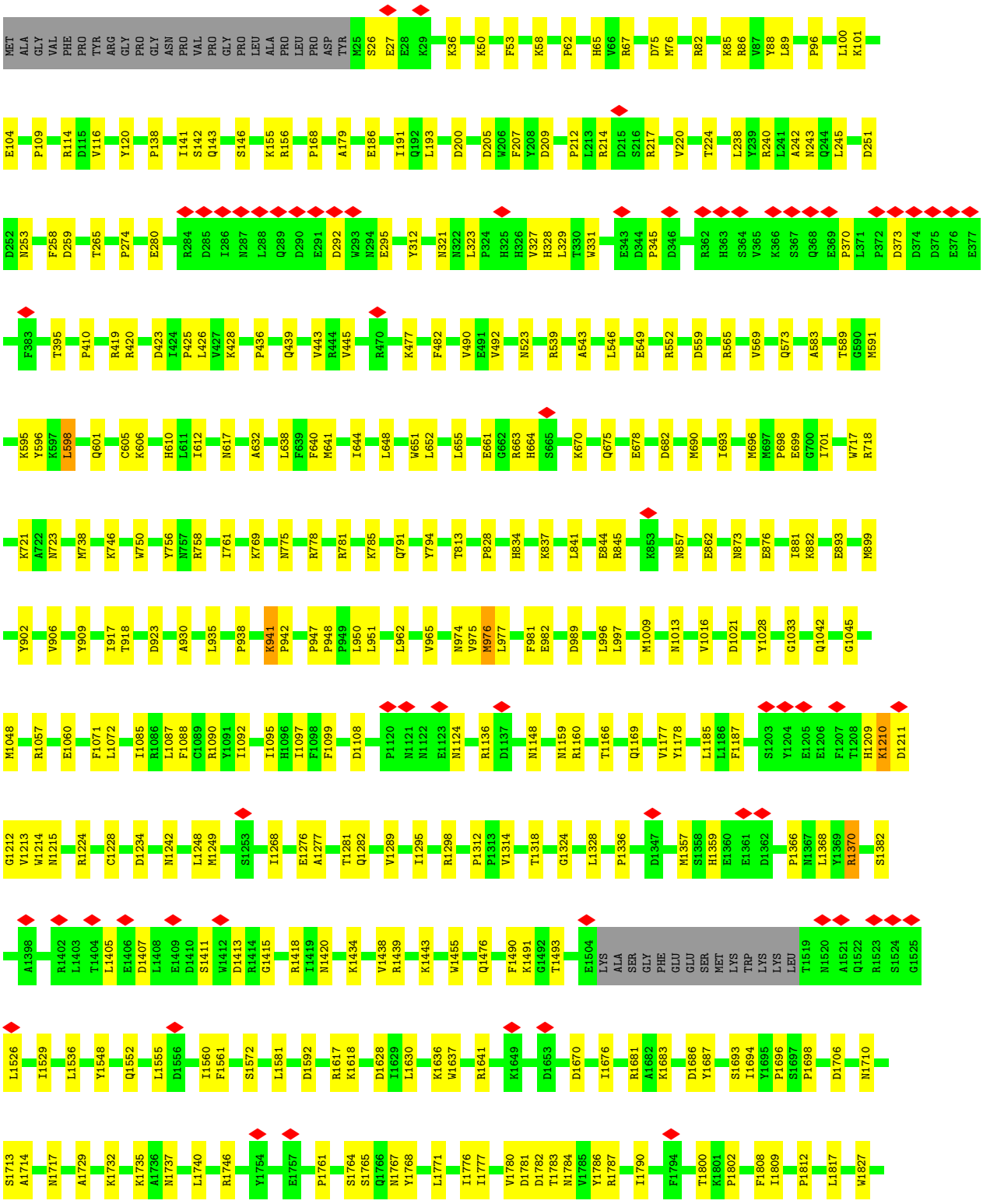
MET GLU S5 D6 F7 Y8 L9 R10 Y11 Y12 V13 G14 H15 K16 G17 K18 F19 G20 H21 E22 F23 L24 E25 F26 E27 F28 R29 P30 D31 G32 K33 L34 R35 Y36 A37 N38 N39 S40 N41 Y42 K43 N44 D45 V46 M47 I48 R49 K50 E51 A52 Y53 V54 H55 K56 S57 V58 M59 E60 E61 L62

K63 R64 I65 I66 D67 D68 S69 E70 I71 T72 K73 E74 D75 D76 A77 L78 W79 P80 P81 P82 D83 R84 V85 G86 R87 Q88 E89 L90 E91 I92 V93 I94 G95 D96 E97 H98 I99 S100 F101 T102 T103 S104 K105 I106 G107 S108 L109 I110 D111 V112 N113 Q114 S115 K116 D117 P118 E119 G120 L121 R122

V123 F124 Y125 Y126 L127 V128 Q129 D130 L131 K132 C133 L134 V135 F136 S137 L138 I139 G140 L141 H142 F143 K144 I145 K146 P147 I148

- Molecule 12: Pre-mRNA-processing-splicing factor 8

Chain A:



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P2019 SER GLN GLN ARG GLN GLN ILE ALA GLU ILE GLU LYS GLN THR LYS GLU GLN SER GLN LEU THR ALA THR GLN THR ARG THR VAL ASN LYS HIS GLY ASP GLU ILE ILE THR SER THR THR SER ASN TYR GLU THR GLN THR F2067 S2068 S2069 K2070 T2071 E2072 W2073 R2074 V2075 R2076 A2077 I2078

S2079 A2080 A2081 N2082 L2083 H2084 L2085 R2086 T2087 N2088 H2089 I2090 Y2091 V2092 S2093 S2094 D2095 D2096 I2097 K2098 E2099 T2100 G2101 Y2102 T2103 Y2104 I2105 L2106 P2107 K2108 N2109 V2110 L2111 K2112 K2113 F2114 I2115 C2116 I2117 S2118 D2119 L2120 R2121 A2122 Q2123 I2124 A2125 G2126 Y2127 L2128 Y2129 G2130 V2131 S2132 P2133 P2134 D2135 N2136 P2137 Q2138

V2139 K2140 E2141 I2142 R2143 C2144 I2145 V2146 M2147 V2148 P2149 Q2150 W2151 G2152 T2153 H2154 Q2155 T2156 V2157 H2158 L2159 P2160 G2161 Q2162 L2163 P2164 Q2165 H2166 E2167 Y2168 L2169 K2170 E2171 M2172 E2173 P2174 L2175 G2176 W2177 I2178 H2179 T2180 Q2181 P2182 N2183 E2184 S2185 P2186 Q2187 L2188 S2189 P2190 Q2191 D2192 V2193 T2194 T2195 H2196 A2197 K2198

I2199 M2200 A2201 D2202 N2203 P2204 S2205 W2206 D2207 G2208 E2209 K2210 T2211 I2212 I2213 I2214 T2215 C2216 S2217 F2218 T2219 P2220 G2221 S2222 C2223 T2224 L2225 T2226 A2227 Y2228 K2229 L2230 T2231 P2232 S2233 G2234 Y2235 E2236 W2237 G2238 R2239 Q2240 N2241 T2242 D2243 K2244 G2245 N2246 N2247 P2248 K2249 G2250 Y2251 L2252 P2253 S2254 H2255 Y2256 E2257 R2258

V2259 Q2260 M2261 L2262 L2263 S2264 D2265 R2266 F2267 L2268 G2269 F2270 F2271 M2272 V2273 P2274 A2275 Q2276 S2277 S2278 W2279 N2280 Y2281 N2282 F2283 M2284 G2285 V2286 R2287 H2288 D2289 P2290 N2291 M2292 K2293 Y2294 E2295 L2296 Q2297 L2298 A2299 N2300 P2301 K2302 E2303 F2304 Y2305 H2306 E2307 V2308 H2309 R2310 P2311 S2312 H2313 F2314 L2315 N2316 F2317 A2318

L2319 L2320 Q2321 E2322 G2323 E2324 V2325 Y2326 S2327 A2328 D2329 R2330 E2331 D2332 L2333 Y2334 A2335

- Molecule 13: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain B:

MET ALA ASP VAL THR ALA ARG SER LEU GLN TYR GLU TYR LYS ALA ASN SER ASN LEU VAL LEU GLN ALA ASP ARG SER LEU ILE ASP ARG THR ARG ARG ASP GLU PRO THR GLY GLU VAL LEU SER LEU VAL GLY LYS LEU GLU GLY THR ARG MET GLY ASP LYS ALA GLN ARG THR LYS

PRO GLN MET GLN GLU GLU ARG ARG ALA LYS ARG ARG LYS ARG ASP GLU ASP ARG HIS ASP ILE ASN LYS MET LYS GLY TYR THR LEU LEU SER GLU GLY ILE ASP GLU MET VAL GLY ILE ILE TYR LYS PRO LYS THR K107 E108 T109 R110 E111 T112 Y113 E114 V115 L116 L117 S118 F119 I120

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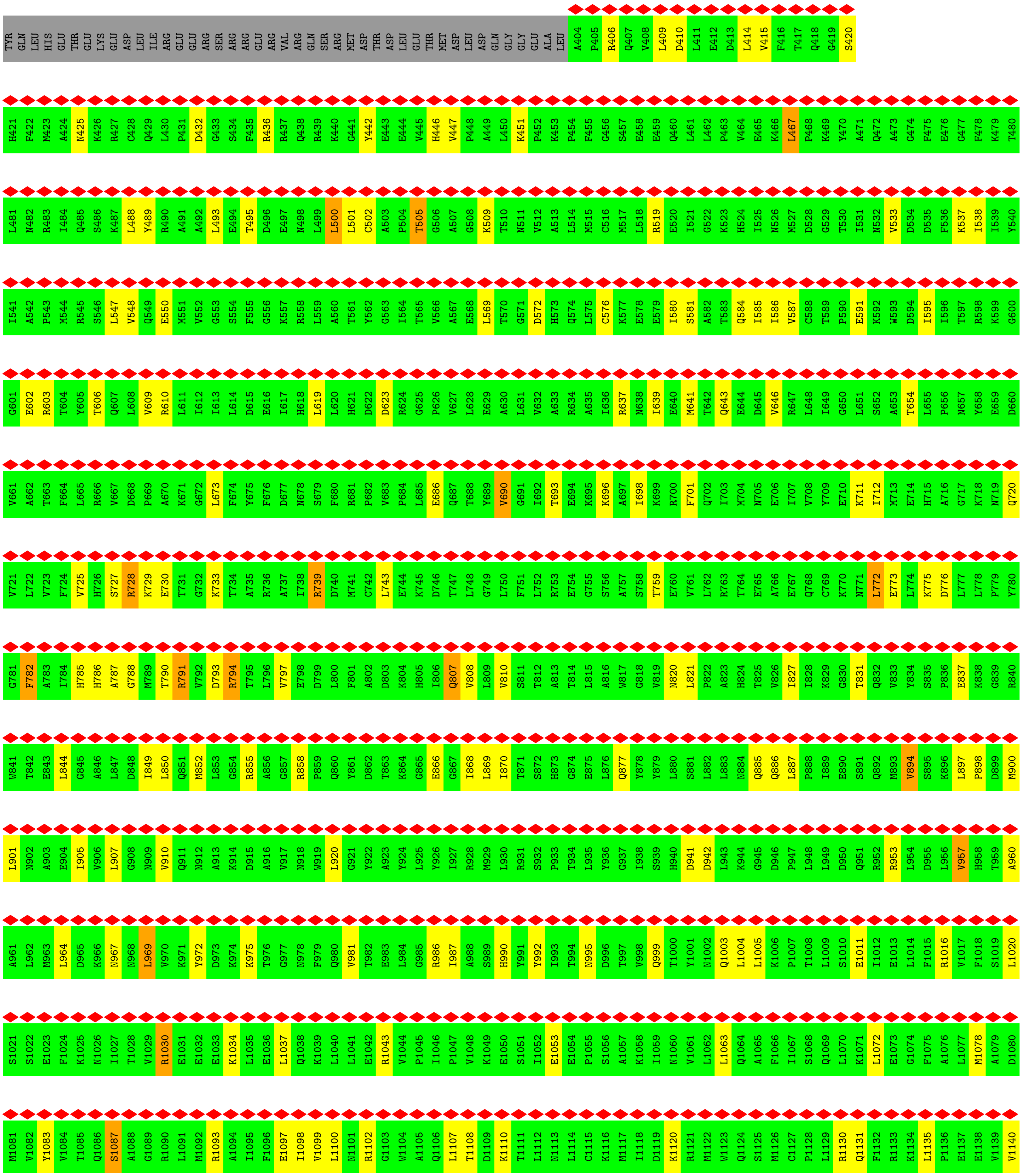
ASP TYR GLY GLY ASP LYS GLU ILE GLN ASN MET ASP ASP ASN ILE ASP GLU THR TYR GLY VAL ASN VAL GLN PHE GLU SER ASP GLU GLU GLU GLY ASP GLU ASP VAL TYR GLY GLU VAL ARG GLU GLU ALA SER ASP ASP ASP MET GLU GLY ASP GLU ALA VAL VAL ARG CYS THR LEU

SER ALA ASN LEU VAL ALA SER GLY GLU LEU MET SER SER LYS LYS LYS ASP LEU HIS P260 R261 D262 I263 D264 A265 F266 W267 L268 Q269 R270 Q271 L272 S273 R274 F275 Y276 D277 D278 A279 I280 V281 S282 Q283 K284 K285 A286 D287 E288 V289 L290 E291 I292 L293 K294 T295 A296 S297 D298 D299 R300

E301 C302 E303 N304 Q305 L306 V307 L308 L309 L310 G311 F312 N313 T314 F315 D316 F317 I318 K319 V320 L321 R322 Q323 H324 R325 M326 M327 I328 L329 Y330 C331 T332 L333 L334 A335 SER ALA GLN SER GLU ALA GLU LYS GLU ARG ILE MET GLY LYS MET GLU ALA ASP PRO GLU LEU SER LYS PHE LEU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Q1441 R1442 K1443 N1444 V1445 Q1446 N1447 I1448 N1449 L1450 F1451 V1452 V1453 D1454 E1455 V1456 H1457 L1458 I1459 G1460 G1461 E1462 N1463 G1464 P1465 V1466 L1467 E1468 V1469 I1470 C1471 S1472 R1473 M1474 R1475 Y1476 I1477 S1478 S1479 Q1480 I1481 E1482 R1483 P1484 I1485 R1486 I1487 V1488 A1489 L1490 S1491 S1492 S1493 L1494 S1495 N1496 A1497 K1498 D1499 V1500

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V1561 F1562 Y1563 P1564 S1565 R1566 K1567 Q1568 T1569 R1570 L1571 T1572 A1573 T1574 D1575 I1576 L1577 T1578 T1579 C1580 A1581 A1582 D1583 I1584 Q1585 R1586 Q1587 R1588 F1589 L1590 H1591 C1592 T1593 E1594 K1595 D1596 L1597 T1598 P1599 Y1600 L1601 E1602 K1603 L1604 S1605 D1606 S1607 T1608 L1609 K1610 E1611 T1612 I1613 L1614 N1615 G1616 V1617 G1618 Y1619 L1620

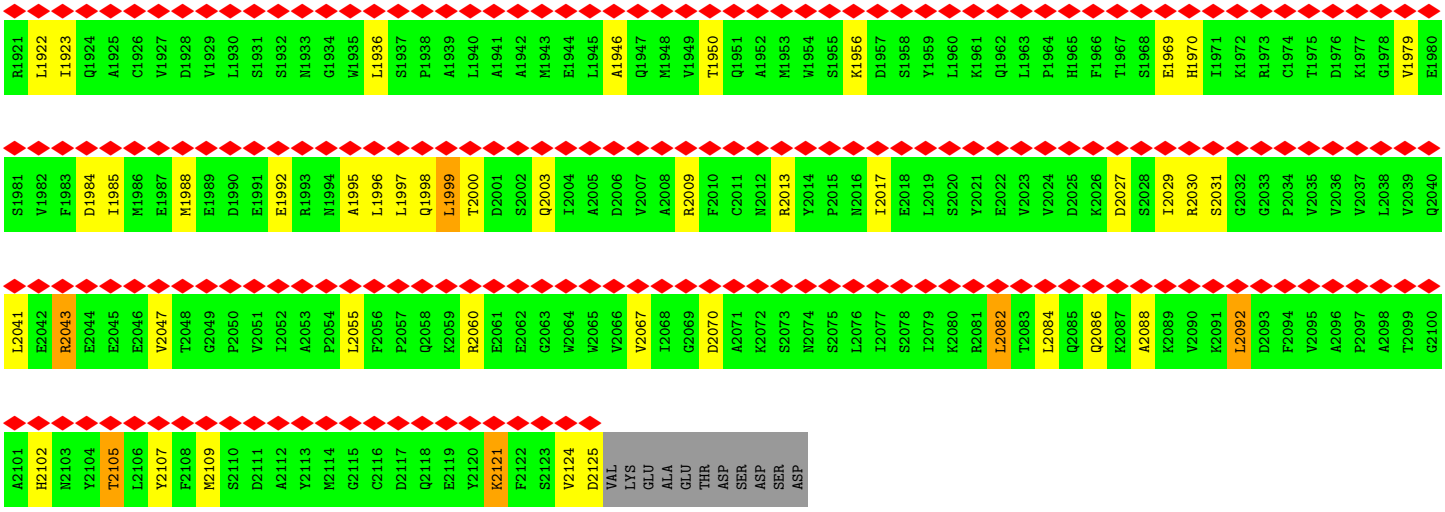
H1621 E1622 G1623 L1624 S1625 P1626 M1627 E1628 R1629 R1630 L1631 V1632 E1633 Q1634 L1635 F1636 S1637 S1638 G1639 A1640 I1641 Q1642 V1643 V1644 V1645 A1646 S1647 R1648 S1649 L1650 C1651 W1652 G1653 M1654 N1655 V1656 A1657 A1658 H1659 E1660 V1661 I1662 I1663 M1664 D1665 T1666 Q1667 Y1668 Y1669 N1670 G1671 K1672 I1673 H1674 A1675 Y1676 V1677 D1678 Y1679 P1680

I1681 Y1682 D1683 V1684 L1685 Q1686 M1687 V1688 G1689 H1690 A1691 N1692 R1693 P1694 L1695 Q1696 D1697 D1698 E1699 G1700 R1701 C1702 V1703 I1704 M1705 C1706 Q1707 G1708 S1709 K1710 K1711 D1712 F1713 F1714 K1715 K1716 F1717 L1718 Y1719 E1720 P1721 L1722 P1723 V1724 E1725 S1726 H1727 L1728 D1729 H1730 C1731 M1732 H1733 D1734 H1735 F1736 N1737 A1738 E1739 I1740

V1741 T1742 K1743 T1744 I1745 E1746 N1747 K1748 Q1749 D1750 A1751 V1752 D1753 Y1754 L1755 T1756 W1757 T1758 F1759 L1760 Y1761 R1762 R1763 M1764 T1765 Q1766 N1767 P1768 N1769 Y1770 Y1771 N1772 L1773 Q1774 G1775 I1776 S1777 H1778 R1779 H1780 L1781 S1782 D1783 H1784 L1785 S1786 E1787 L1788 V1789 E1790 Q1791 T1792 L1793 S1794 D1795 L1796 E1797 Q1798 S1799 K1800

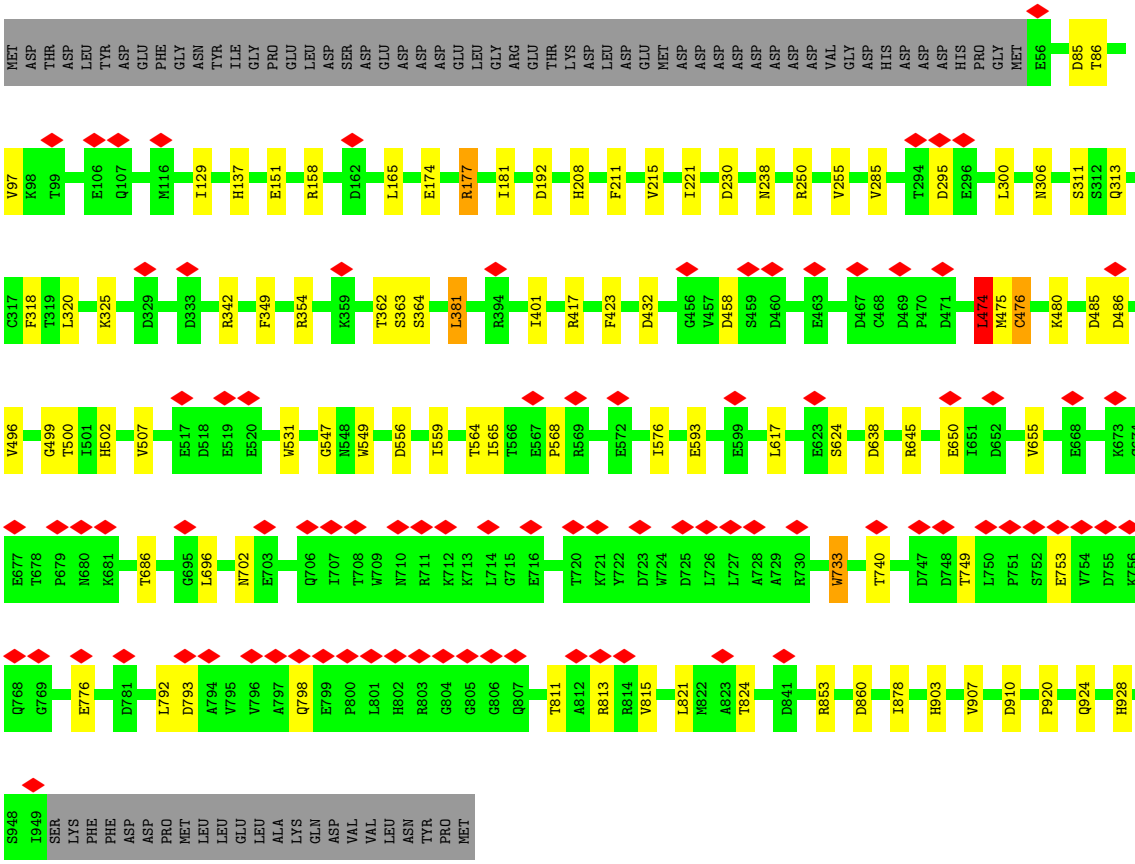
C1801 I1802 S1803 I1804 E1805 D1806 E1807 M1808 D1809 V1810 A1811 P1812 L1813 N1814 L1815 G1816 M1817 I1818 A1819 A1820 Y1821 Y1822 Y1823 I1824 N1825 Y1826 T1827 T1828 I1829 E1830 L1831 F1832 S1833 M1834 S1835 L1836 N1837 A1838 K1839 T1840 K1841 V1842 R1843 G1844 L1845 I1846 E1847 I1848 I1849 S1850 N1851 A1852 A1853 E1854 Y1855 E1856 N1857 I1858 P1859 I1860

R1861 H1862 H1863 E1864 D1865 N1866 L1867 L1868 R1869 Q1870 L1871 A1872 Q1873 K1874 V1875 P1876 H1877 K1878 L1879 N1880 N1881 P1882 K1883 F1884 N1885 D1886 P1887 H1888 V1889 K1890 T1891 N1892 L1893 L1894 L1895 Q1896 A1897 H1898 L1899 S1900 R1901 M1902 Q1903 L1904 S1905 A1906 E1907 L1908 Q1909 S1910 D1911 T1912 E1913 E1914 I1915 L1916 S1917 K1918 A1919 I1920



- Molecule 14: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C:



- Molecule 15: Pre-mRNA-splicing factor ISY1 homolog

Chain D:

GLN ASN ALA GLY LEU GLY GLU PHE ARG ILE ARG ASP LEU ASN ASP GLU ILE ASN LYS LEU LEU ARG GLU LYS GLY HIS TRP GLU VAL ARG ILE LYS GLU LEU GLY GLY PRO ASP TYR GLY LYS VAL GLY PRO LYS MET LEU ASP HIS GLU GLY LYS GLU VAL PRO GLY ASN ARG GLY TYR

LYS TYR PHE GLY ALA ALA LYS ASP LEU PRO GLY VAL ARG GLU LEU PHE GLU LYS GLU PRO LEU PRO PRO PRO ARG LYS THR R148 A149 E150 L151 M152 K153 A154 I155 D156 F157 E158 Y159 Y160 G161 Y162 L163 D164 E165 D166 D167 G168 V169 I170 V171 P172 L173 E174 Q175 E176 Y177 E178 K179 K180

L181 R182 A183 E184 L185 V186 E187 K188 W189 K190 A191 E192 R193 E194 A195 R196 L197 A198 ARG GLY GLU LYS GLU GLU GLU GLU GLU GLU GLU GLU GLU ILE ASN ILE TYR ALA VAL THR GLU GLU GLU GLU SER ASP GLU GLU GLY SER GLN GLU LYS GLY GLY ASP ASP SER GLN GLN LYS PHE ILE

ALA HIS VAL PRO VAL PRO SER GLN Q249 E250 I251 E252 E253 A254 L255 V256 R257 R258 K259 K260 M261 E262 L263 L264 Q265 K266 Y267 A268 S269 GLU THR LEU GLN ALA ALA GLN SER GLU GLU ALA ARG ARG LEU LEU GLY TYR

- Molecule 16: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:

MET ILE GLU GLN GLN LYS ARG LYS GLY PRO GLU LEU PRO LEU VAL PRO VAL LYS ARG GLN ARG HIS GLU LEU LEU LEU LEU GLY ALA GLY SER GLY PRO GLY ALA GLY GLN GLN GLN ALA THR PRO GLY ALA LEU LEU GLN ALA GLY PRO PRO ARG CYS SER SER L55 Q56 A57 P58 I59 H60

L61 L62 E66 G67 E68 V69 H75 P76 N77 L81 A84 D87 I90 L91 G97 D98 N101 L105 K106 A111 H116 D120 G121 S122 A127 D130 V133 D137 S138 E139 T140 G141 E142 L147 K148 G149 H150 N155 S156 C157 Y158 P159

A160 R161 R162 L166 T169 G170 S171 D172 D173 K177 L178 I181 R182 K183 K184 I187 Q188 T189 V196 D203 T204 I208 D214 I217 L222 R223 M231 T239 L243 S244 S245 E246 G247 L251 V259 D263 V264 R265 P266 F267 K270 E271

F277 Q278 G279 N280 R290 C291 D296 D306 R307 F308 V309 Y310 V311 W312 D313 S316 R317 R318 Y321 K322 L323 I330 N331 E332 D338 I343 S346 S347 D348 K349 R350 L351 I356 Q357

- Molecule 17: Exon

Chain EX:

G-12 G-11 C-10 C-9 U-8 C-7 C-6 G-5 A-4 A-3 C-2 G-1 C1 U2

- Molecule 18: Splicing factor Cactin

Chain F:

MET GLY ARG ASP THR ARG SER ARG SER ARG SER ARG SER ALA GLY ARG ARG ARG GLY ARG ARG ARG ARG GLN SER GLN SER GLY SER ARG SER ARG SER ARG SER ARG SER HIS GLY ARG ARG ASN ARG ARG ARG ARG ARG ASP GLU GLY ARG ARG ARG ARG ARG ARG ARG SER ARG GLU ARG ARG SER ASP SER GLU

GLU GLU ARG TRP GLN ARG SER GLY MET ARG SER ARG SER PRO ARG PRO LYS TRP HIS SER ARG ASP GLY SER SER GLN SER ASP SER GLY GLU GLU GLN SER ARG GLY ARG GLN TRP ALA ARG ARG ARG ARG ARG SER TRP SER PRO SER SER SER ALA SER SER SER SER ALA SER

PRO GLY ARG SER GLN SER PRO ARG ALA ALA ALA ALA ALA LEU SER GLN GLN GLN SER LEU GLN GLU ARG LEU ARG LEU ARG GLU GLU ARG LYS GLN GLN GLU GLU LEU MET LYS ALA PHE GLU THR PRO GLU GLU LYS ARG ALA ARG ARG LEU ALA LYS LYS GLU ALA LYS GLU ARG LYS

LYS ARG GLU LYS MET GLY TRP GLY GLU GLU GLU TYR MET GLY TYR THR ASN THR ASP ASN PRO PHE GLY ASP ASN ASN ASN LEU LEU GLY THR PHE ILE TRP ASN LYS ALA LEU GLU LYS LYS GLY ILE SER HIS LEU GLU GLU GLU LYS GLU LEU LYS GLU ARG ASN LYS ARG ILE GLN GLU ASP ASN

ARG LEU GLU LEU GLN LYS VAL LYS GLN LEU ARG LEU GLU ARG GLU ARG GLU LYS ALA MET ARG GLU GLN GLU LEU GLU MET LEU GLN ARG GLU LYS GLU ALA GLU HIS PHE LYS THR TRP GLU GLU GLN GLN GLU ASP ASN PHE HIS LEU GLU GLN GLN ALA LYS LEU ARG SER LYS ILE ARG ILE

ARG ASP GLY ARG ALA LYS PRO ILE ASP LEU LEU ALA LYS TYR ILE SER ALA GLU ASP ASP ASP LEU ALA VAL GLU MET HIS GLU PRO TYR THR PHE LEU ASN GLY LEU THR VAL ALA ASP MET GLU ASP LEU LEU GLU ASP ILE GLN VAL TYR MET GLU LEU GLU GLN GLN GLY LYS ASN ALA

ASP PHE TRP ARG ASP MET THR THR ILE THR GLU ASP GLU ILE SER LYS LEU ARG LYS LEU GLU ALA SER GLY LYS GLY PRO GLY GLU ARG ARG GLU GLY VAL ASN ALA SER VAL SER SER ASP VAL GLN SER VAL PHE LYS GLY LYS THR TYR ASN GLN LEU GLN GLN GLY GLY LYS GLN GLY

ILE GLU GLY LYS ILE ARG ALA GLY GLY PRO ASN LEU ASP MET GLY TYR TRP GLU SER LEU LEU GLU ALA GLY ALA MET ALA ARG ALA ARG LEU ARG HIS GLN ASP VAL LEU ARG GLN LYS LEU TYR LYS LEU LYS GLN GLU GLN GLY VAL GLU SER GLU PRO LEU PHE

PRO ILE LEU LYS GLN GLU PRO GLN SER PRO SER ARG SER LEU GLU PRO GLU ASP ALA ALA PRO THR PRO PRO GLY PRO SER SER GLU GLY GLY PRO ALA GLU ALA GLU VAL ASP GLY ALA THR PRO THR GLU GLY ASP GLY ASP GLY ASP GLY GLU GLU GLY GLU GLU GLU ALA VAL

LEU MET GLU GLU ASP LEU ILE GLN GLN SER LEU ASP ASP TYR ASP ALA GLY ARG TYR SER PRO ARG LEU LEU THR ALA HIS GLU LEU PRO LEU ASP ALA HIS VAL LEU GLU PRO ASP GLU ASP LEU GLN ARG LEU GLN LEU SER ARG GLN GLN LEU GLN VAL THR GLY ASP ALA SER GLU

SER ALA GLU ASP ILE PHE PHE ARG ARG ALA LYS GLU GLY MET GLN ASP GLU ALA GLN PHE SER VAL GLU MET PRO LEU THR GLY LYS ALA TYR LEU TRP ALA ASP K637 Y638 R639 P643 R644 W655 Y658 N659 Q660 Y663 D664 F665 D666 N667 Y682 P683 D684 L685 I686

D687 K688 R689 E697 A698 C699 A700 D701 N702 K703 D704 L708 A712 G713 P714 P715 Y716 E717 D718 I719 K722 H732 R733 Q739 R757 R758

- Molecule 19: Pre-mRNA-splicing factor CWC22 homolog

Chain H: 29% 47% • 49%

MET LYS SER SER VAL ALA GLN ILE LYS PRO SER SER GLY HIS ASP ARG ARG GLU ASN LEU ASN SER TYR GLN ARG ASN SER SER PRO GLU ASP ARG TYR GLU GLU GLN GLU ARG ASP ARG ASP TYR PHE ASP TYR SER ARG SER ASP TYR GLU HIS SER ARG ARG GLY ARG

SER TYR ASP SER SER MET GLU SER ARG ASN ARG ASP ARG GLU LYS ARG ARG GLU ARG GLU ARG ASP THR ASP ARG LYS ARG SER LYS SER PRO SER PRO GLY ARG ARG ASN PRO GLU THR SER VAL THR GLN SER SER SER ALA GLN ASP GLU PRO ALA THR LYS LYS LYS LYS ASP

GLU LEU ASP PRO LEU LEU THR ARG THR GLY GLY ALA TYR ILE PRO PRO ALA LYS LEU ARG MET MET GLN GLU GLN ILE THR ASP K149 N150 S151 L152 A153 Y154 Q155 R156 M157 S158 W159 E160 A161 L162 K163 K164 S165 I166 N167 G168 L169 I170 N171 K172 V173 N174 I175 S176 N177 I178 S179 I180

I181 I182 Q183 E184 L185 L186 Q187 E188 N189 I190 V191 R192 G193 R194 G195 L196 L197 S198 R199 S200 V201 L202 Q203 A204 Q205 S206 A207 S208 P209 I210 F211 T212 H213 V214 Y215 A216 A217 L218 V219 A220 I221 I222 N223 S224 K225 F226 P227 Q228 I229 G230 E231 L232 I233 I234 K235 R236 L237 I238 L239 N240

F241 R242 K243 G244 Y245 R246 R247 N248 D249 K250 Q251 L252 C253 L254 T255 A256 S257 K258 F259 V260 A261 H262 L263 I264 N265 Q266 N267 V268 A269 H270 E271 V272 L273 C274 L275 E276 M277 L278 T279 L280 L281 L282 E283 R284 P285 T286 D287 D288 S289 V290 E291 V292 A293 I294 G295 F296 L297 K298 E299 C300

G301 L302 K303 L304 T305 Q306 V307 S308 P309 R310 G311 I312 N313 A314 I315 F316 E317 R318 N321 I322 L323 H324 E325 S326 E327 I328 D329 K330 R331 V332 Q333 Y334 M335 I336 E337 V338 A341 V342 D345 G346 F347 K348 D349 H350 P351 I352 I353 L354 E355 G356 L357 D358 L359 V360 E361 E362 D363

D364 Q365 F366 T367 H368 M369 L370 P371 L372 E373 D374 D375 Y376 N377 P378 E379 D380 V381 L382 N383 V384 F385 K386 M387 D388 P389 N390 F391 M392 E393 N394 E395 E396 K397 Y398 K399 A400 I401 K402 K403 E404 I405 L406 ASP GLU GLY ASP THR ASP SER ASN THR ASP GLN ASP ALA GLY SER SER GLU

GLU ASP GLU GLU GLU GLU GLU GLU GLU GLY GLU GLU ASP GLU GLU GLY GLN LYS VAL THR ILE HIS ASP LYS T448 E449 T450 S465 D468 H474 F481 L494 R501 E504 L517 F525 I528 I536 H537 R538 L544 R545 N546 V547 L555 L560

E572 E573 T576 S577 S578 S579 K584 I585 L590 L599 E606 E613 R618 D619 R622 N623 T624 R625 I628 N629 I634 G635 L636 L639 T640 D641 R644 K648 ASN THR PRO LYS VAL ILE VAL ALA GLN LYS PRO ASP VAL GLU GLN ASN LYS SER

SER PRO SER SER SER SER SER ALA SER SER SER SER GLU SER ASP SER SER ASP SER ASP SER ASP SER SER SER ASP SER SER SER SER GLU GLU SER SER SER GLU GLU SER ASP SER SER SER ILE SER SER HIS SER SER ALA SER ALA ASN ASP VAL ARG LYS LYS GLY HIS GLY LYS THR ARG

SER LYS GLU VAL ASP LYS LEU ILE ARG ASN GLN GLN THR ASN ASP ARG LYS GLN LYS GLU ARG ARG GLN GLU HIS GLY HIS GLN GLN GLU THR ARG THR GLU ARG GLU ARG ARG SER GLU LYS HIS ARG ASP GLN ASN SER SER GLY SER ASN TRP ARG ASP PRO ILE THR LYS TYR THR SER

ASP LYS ASP VAL PRO SER GLU ARG ASN ASN TYR SER ARG VAL ALA ASN ASP ARG ASP GLN GLU MET HIS ILE ASP LEU GLU ASN LYS HIS GLY ASP PRO LYS LYS LYS ARG GLY GLU ARG ASN SER PHE SER GLU ASN GLU LYS HIS THR HIS ARG ILE LYS ASP SER GLU ASN PHE

ARG ARG LYS ASP ARG SER LYS SER LYS GLU MET ASN ARG LYS HIS SER GLY SER ARG SER ASP GLU ASP ARG TYR GLN ASN GLY ALA GLU ARG ARG TRP GLU LYS SER SER ARG TYR SER GLU GLN SER ARG GLU SER LYS LYS ASN GLN ASP ARG ARG ARG GLU LYS SER PRO ALA LYS

GLN LYS

- Molecule 20: Pre-mRNA-splicing factor SYF1

Chain I: 83% 85% 15%

MET VAL VAL MET ALA ARG LEU SER ARG PRO GLU ARG PRO ASP LEU VAL PHE GLU E19 E20 D21 L22 P23 Y24 E25 E26 E27 I28 M29 R30 N31 Q32 F33 S34 V35 K36 C37 W38 L39 R40 Y41 I42 E43 F44 K45 Q46 G47 A48 P49 K50 P51 R52 L53 N54 Q55 L56 Y57 E58 R59 A60

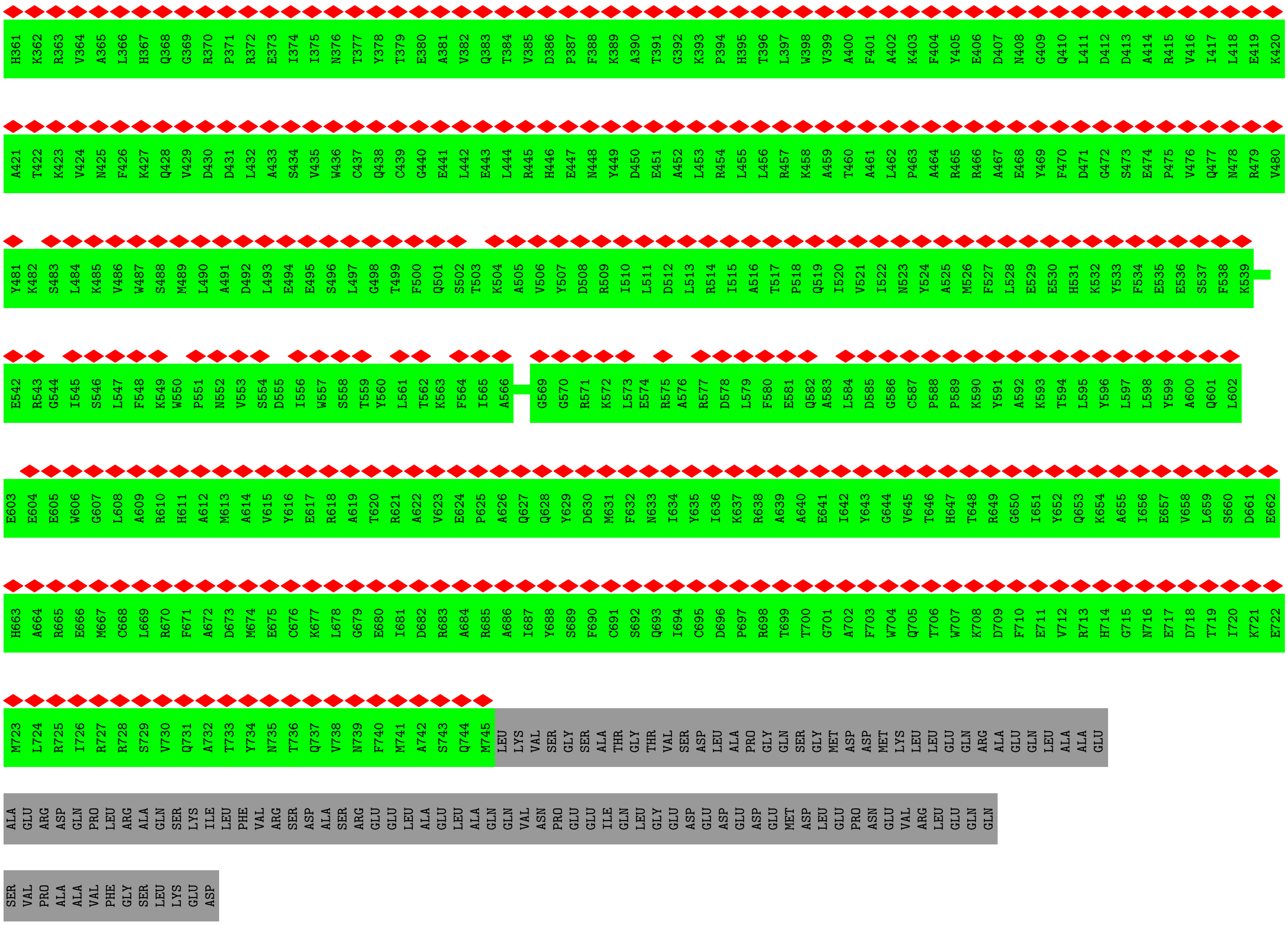
L61 K62 L63 L64 P65 C66 S67 Y68 K69 L70 W71 Y72 R73 Y74 L75 K76 A77 R78 R79 A80 Q81 V82 K83 H84 R85 C86 V87 T88 D89 P90 A91 Y92 E93 D94 V95 N96 N97 C98 H99 E100 R101 A102 F103 V104 F105 M106 H107 K108 M109 P110 R111 L112 W113 L114 D115 Y116 C117 Q118 F119 L120

M121 D122 Q123 G124 R125 V126 T127 H128 T129 R130 R131 T132 F133 D134 R135 A136 L137 R138 A139 L140 P141 I142 T143 Q144 H145 S146 R147 I148 W149 P150 L151 Y152 L153 R154 F155 L156 R157 S158 H159 P160 L161 P162 E163 T164 A165 V166 H167 G168 Y169 R170 R171 F172 L173 K174 L175 S176 P177 E178 S179 A180

E181 E182 Y183 I184 E185 Y186 L187 K188 S189 S190 D191 R192 L193 D194 E195 A196 A197 Q198 R199 L200 A201 T202 V203 V204 N205 D206 E207 R208 F209 V210 S211 K212 A213 G214 K215 S216 N217 Y218 Q219 L220 W221 H222 E223 L224 C225 D226 L227 I228 S229 Q230 N231 P232 D233 K234 V235 Q236 S237 L238 N239 V240

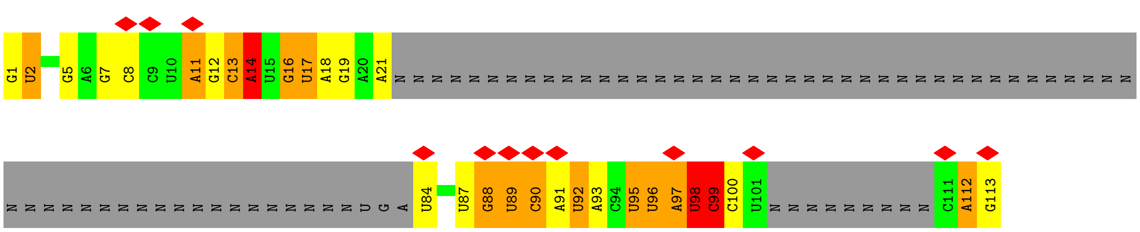
D241 A242 I243 I244 R245 G246 G247 L248 T249 R250 F251 T252 D253 Q254 L255 G256 K257 L258 W259 C260 S261 L262 A263 D264 Y265 Y266 I267 R268 S269 G270 H271 F272 E273 K274 A275 R276 D277 V278 Y279 E280 E281 A282 I283 R284 T285 V286 M287 T288 V289 R290 D291 F292 T293 Q294 V295 F296 D297 S298 Y299 A300

Q301 F302 E303 E304 S305 M306 I307 A308 A309 K310 M311 E312 T313 A314 S315 E316 L317 G318 R319 E320 E321 E322 D323 D324 V325 D326 L327 E328 L329 R330 L331 A332 R333 F334 E335 Q336 L337 I338 S339 R340 R341 P342 L343 L344 L345 N346 S347 V348 L349 L350 R351 Q352 N353 P354 H355 H356 V357 H358 E359 W360



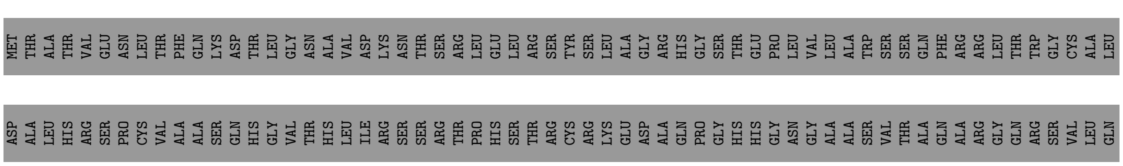
- Molecule 21: INTRON

Chain IN:



- Molecule 22: Crooked neck-like protein 1

Chain J:



VAL PRO LEU PRO VAL PRO ARG SER CYS LEU PHE SER GLU SER PHE VAL VAL SER VAL SER SER GLN SER ARG PHE LEU ALA SER VAL PRO GLY THR GLY VAL GLN ARG SER THR ALA ALA ASP MET ALA ALA SER THR ALA ALA GLY LYS GLN ARG ILE PRO LYS V176 V179 A185

A191 K213 N221 I303 V326 A329 G419 D420 E421 H422 M423 D424 K439 E440 F441 E442 K449 D453 R454 I455 S456 K457 Q458 D459 A460 I469 F470 E471 K472 K473 D476 R477 R478 G479 I480 E481 D482 I483 I484 V485 S486 K487 R488 R489 F490 Q491 Y492 E493

E494 E495 V496 K497 A498 N499 P500 H501 N502 Y503 D504 A505 W506 F507 D508 Y509 L510 R511 L512 V513 E514 S515 D516 A517 E518 A519 E520 A521 V522 R523 E524 V525 Y526 E527 R528 A529 I530 A531 N532 V533 P534 P535 I536 Q537 E538 K539 R540 H541 W542 K543 R544 Y545 I546 Y547 L548 W549 I550 N551 Y552 A553

L554 Y555 E556 E557 L558 E559 A560 K561 D562 P563 E564 R565 T566 R567 Q568 V569 Y570 Q571 A572 S573 L574 E575 L576 I577 P578 H579 K580 K581 F582 T583 F584 A585 K586 M587 W588 I589 L590 Y591 A592 Q593 F594 E595 I596 R597 Q598 K599 N600 L601 S602 L603 A604 R605 R606 A607 L608 G609 T610 S611 I612 G613

K614 C615 P616 K617 N618 K619 L620 F621 K622 V623 Y624 I625 E626 L627 E628 L629 Q630 L631 R632 E633 F634 D635 R636 C637 K638 K639 L640 Y641 E642 K643 F644 L645 E646 F647 G648 P649 E650 N651 C652 T653 S654 W655 I656 K657 F658 A659 E660 L661 E662 T663 I664 L665 G666 D667 I668 D669 R670 A671 R672 A673

I674 Y675 E676 L677 A678 I679 S680 Q681 P682 R683 L684 D685 M686 P687 E688 V689 L690 W691 K692 S693 Y694 I695 D696 F697 E698 I699 E700 Q701 E702 E703 T704 E705 R706 T707 R708 N709 L710 Y711 R712 R713 L714 L715 Q716 R717 T718 Q719 H720 V721 K722 V723 W724 I725 S726 F727 A728 Q729 F730 E731 L732 S733

S734 G735 K736 E737 G738 S739 L740 T741 K742 C743 R744 Q745 I746 Y747 E748 E749 A750 N751 K752 T753 M754 R755 N756 C757 E758 E759 K760 E761 E762 R763 L764 M765 A766 L767 E768 S769 W770 R771 S772 F773 E774 E775 E776 F777 G778 T779 A780 S781 D782 K783 E784 R785 V786 D787 K788 L789 MET PRO GLU LYS

VAL LYS LYS ARG ARG LYS VAL GLN THR ASP ASP GLY SER ASP ALA GLY TRP GLU GLU TYR PHE ASP TYR ILE PHE PRO GLU ASP ALA ALA ASN GLN PRO ASN LEU LYS LEU LEU ALA MET ALA LYS LEU TRP LYS LYS GLN GLN GLN GLU LYS GLU ASP ALA GLU HIS HIS PRO ASP GLU

ASP VAL ASP GLU SER GLU SER

- Molecule 23: Pre-mRNA-splicing factor SPF27

Chain K: 78% 84% 16%

MET ALA GLY THR GLY LEU VAL ALA GLY GLU VAL VAL VAL ASP ALA LEU PRO TYR PHE ASP GLN GLY TYR GLU ALA PRO GLY V28 R29 E30 A31 A32 A33 A34 L35 V36 E37 E38 E39 T40 R41 R42 Y43 R44 P45 T46 K47 N48 Y49 L50 S51 Y52 L53 T54 A55 P56 D57 Y58 S59 A60

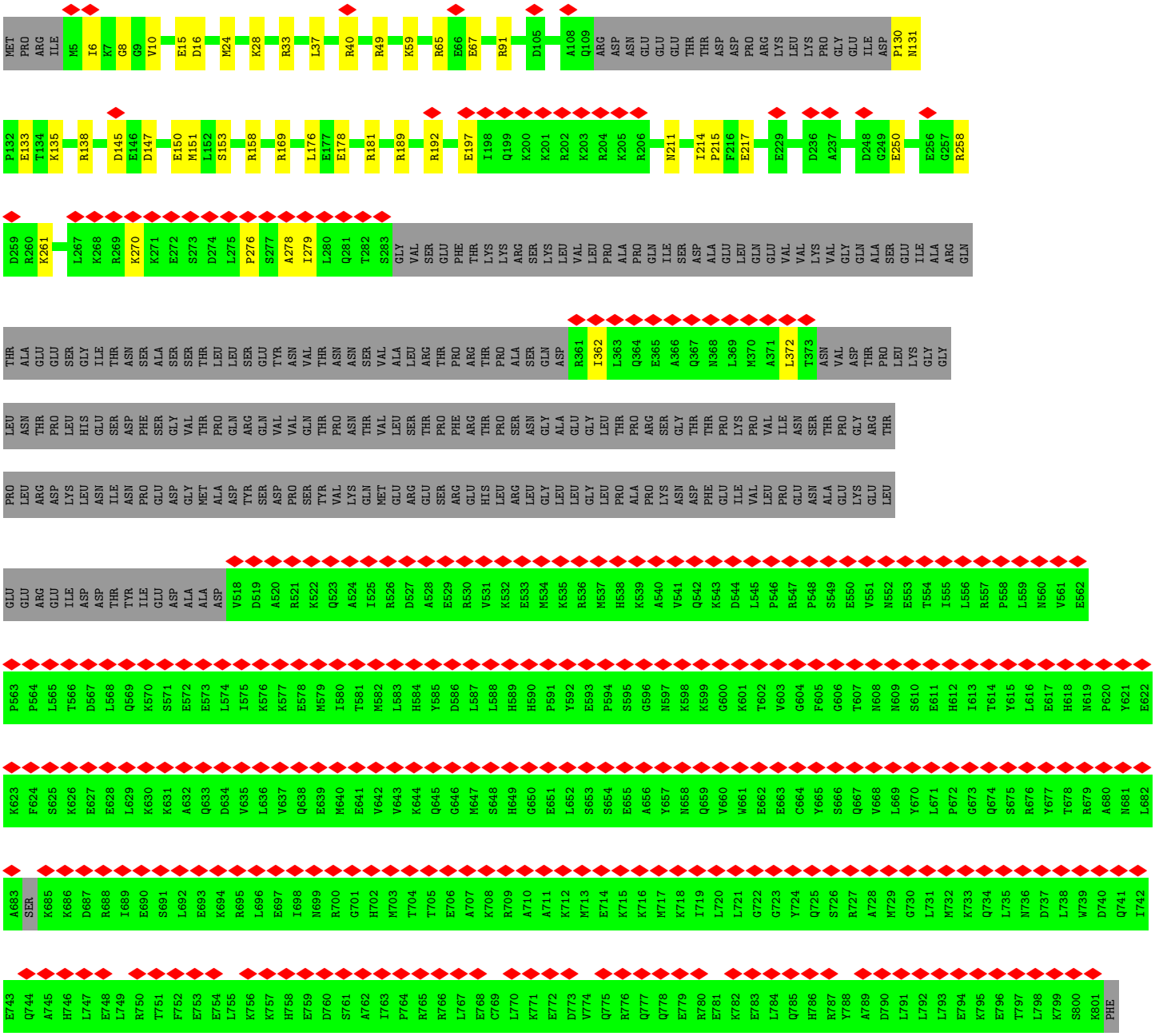
F61 E62 T63 D64 I65 M66 R67 N68 E69 F70 E71 R72 L73 A74 A75 R76 Q77 P78 I79 E80 L81 L82 S83 M84 K85 R86 Y87 E88 L89 P90 A91 P92 S93 S94 G95 Q96 K97 N98 D99 I100 T101 A102 W103 Q104 E105 C106 V107 N108 N109 S110 M111 A112 Q113 L114 E115 H116 Q117 A118 V119 R120

I121 E122 N123 L124 E125 L126 M127 S128 Q129 H130 G131 C132 N133 A134 W135 K136 V137 Y138 N139 E140 N141 L142 V143 H144 M145 I146 E147 H148 A149 Q150 K151 E152 L153 Q154 R157 K158 Q161 D162 L163 N164 W165 Q166 R167 K168 N169 M170 Q171 L172 T173 A174 G175 S176 K177 L178 R179 E180 M181 E182

S183 N184 W185 V186 S187 L188 V189 S190 K191 N192 Y193 E194 I195 E196 R197 T198 I199 V200 Q201 L202 E203 N204 E205 I206 Y207 Q208 I209 K210 Q211 Q212 H213 G214 E215 A216 ASN LYS GLU ASN ILE ARG GLN ASP PHE

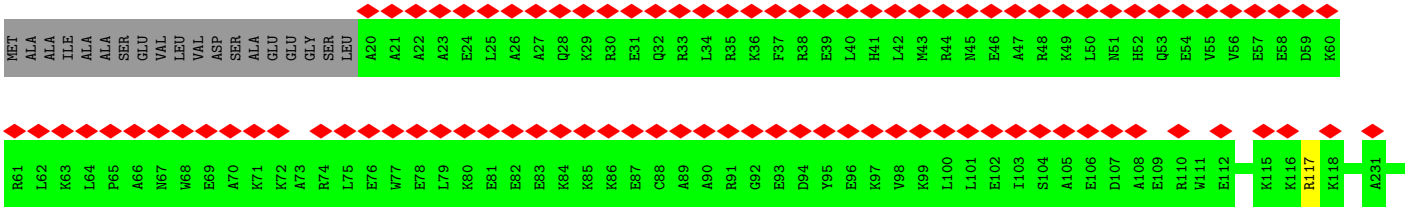
- Molecule 24: Cell division cycle 5-like protein

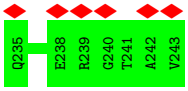
Chain L: 41% 63% 6% 31%



• Molecule 25: Pre-mRNA-splicing factor SYF2

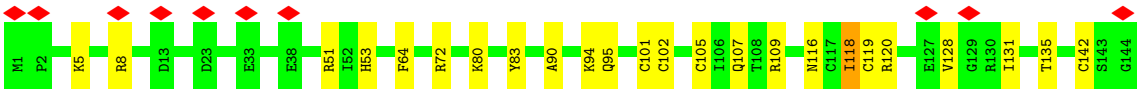
Chain M: 41% 92% 8%





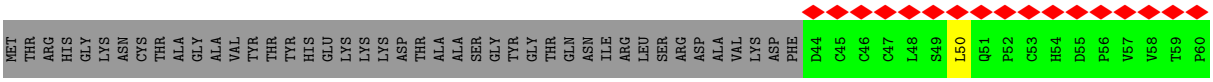
• Molecule 26: Protein BUD31 homolog

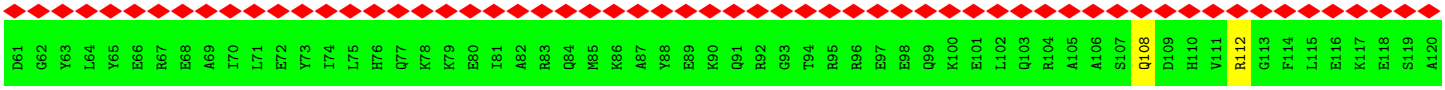
Chain N:

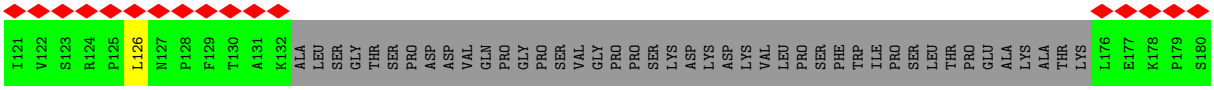


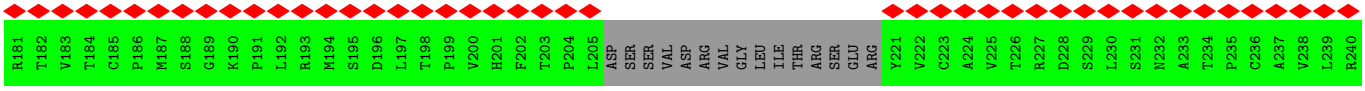
• Molecule 27: Nitric oxide synthase-interacting protein

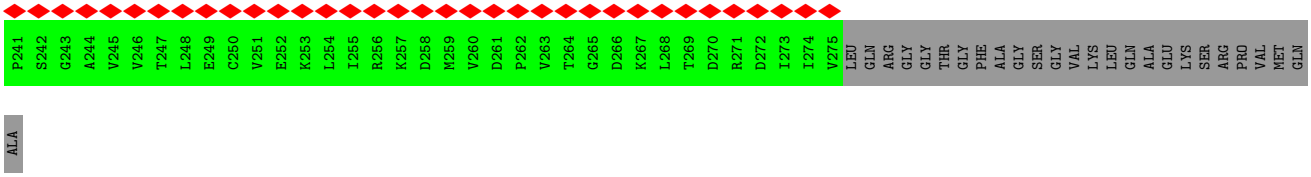
Chain NO:





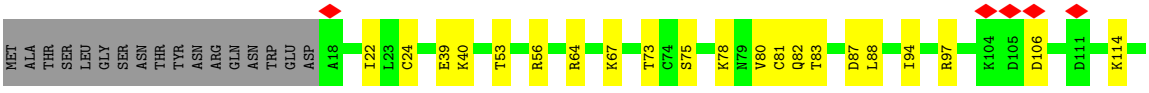


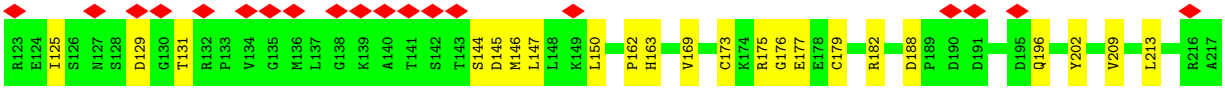


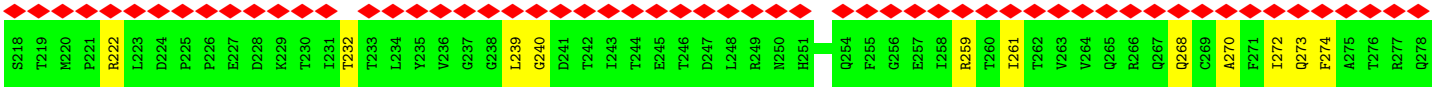


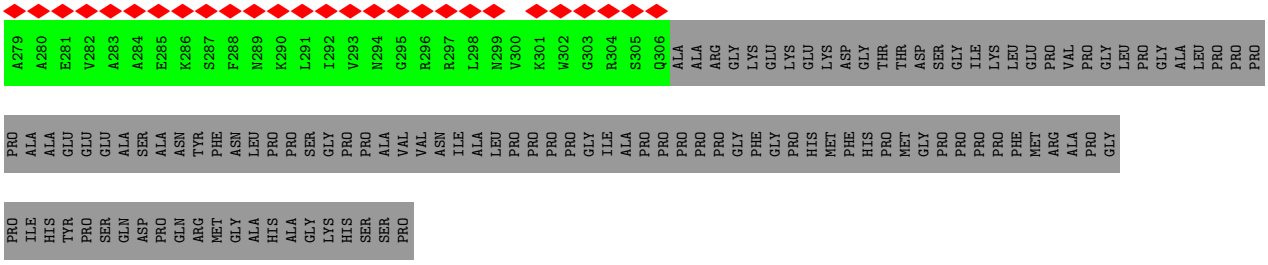
• Molecule 28: Pre-mRNA-splicing factor RBM22

Chain O:



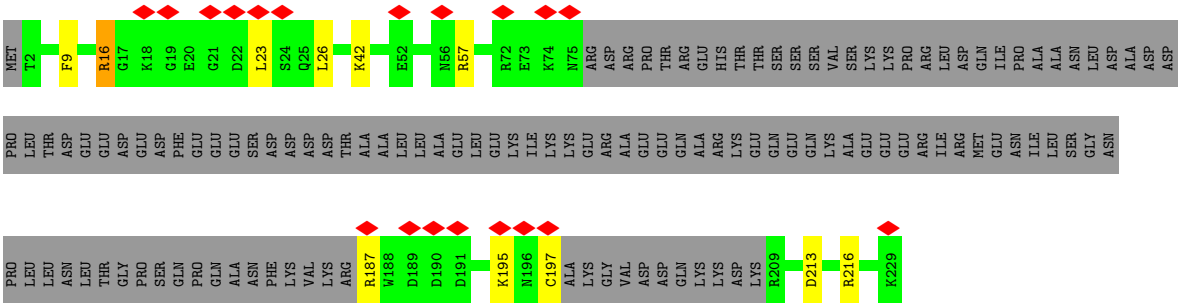






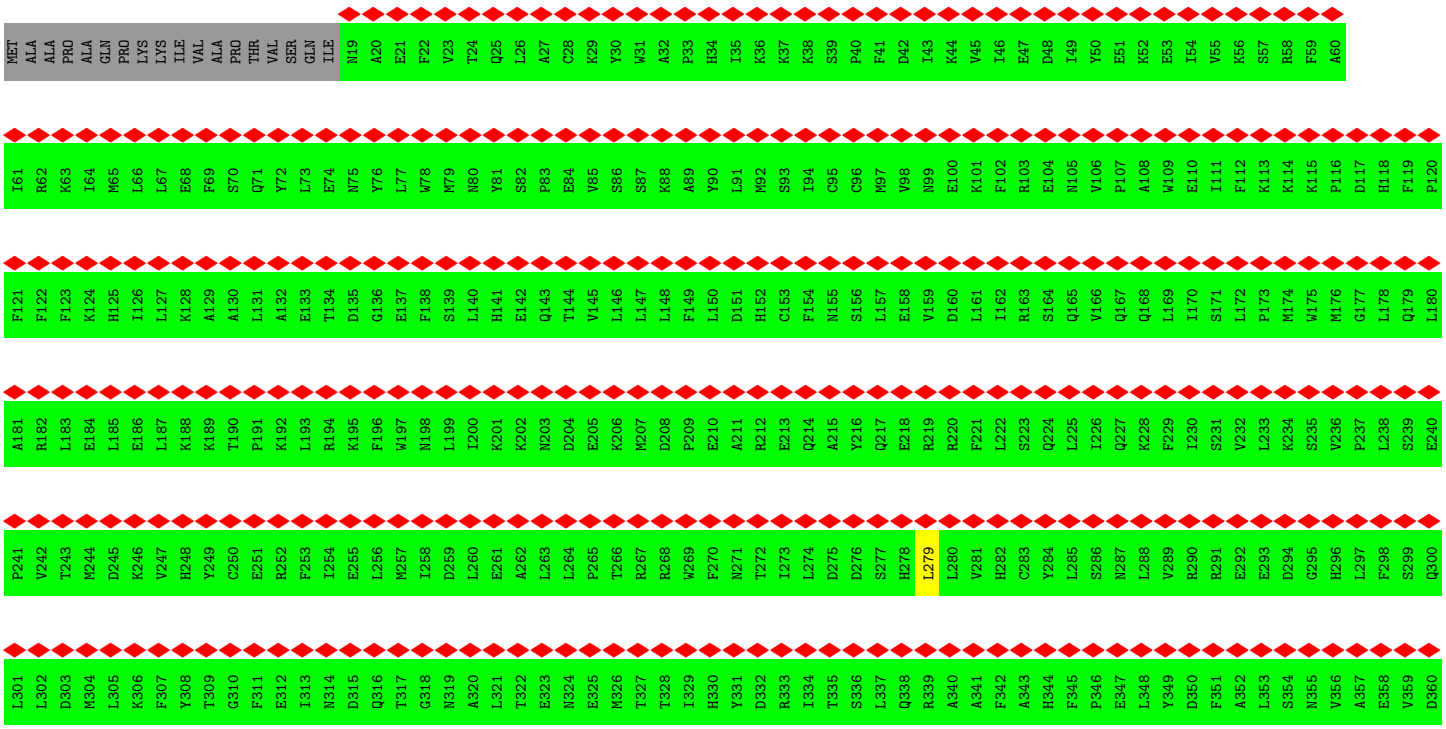
• Molecule 29: Spliceosome-associated protein CWC15 homolog

Chain P:



• Molecule 30: Intron-binding protein aquarius

Chain Q:



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L421 N422 Q423 M424 P425 L426 Y427 P428 T429 E430 K431 I432 I433 W434 D435 E436 N437 I438 V439 P440 T441 E442 V443 Y444 S445 G446 E447 G448 C449 L450 A451 L452 P453 K454 L455 N456 L457 Q458 F459 L460 T461 L462 H463 D464 Y465 L466 L467 R468 N469 F470 N471 L472 F473 R474 L475 E476 S477 T478 Y479 E480

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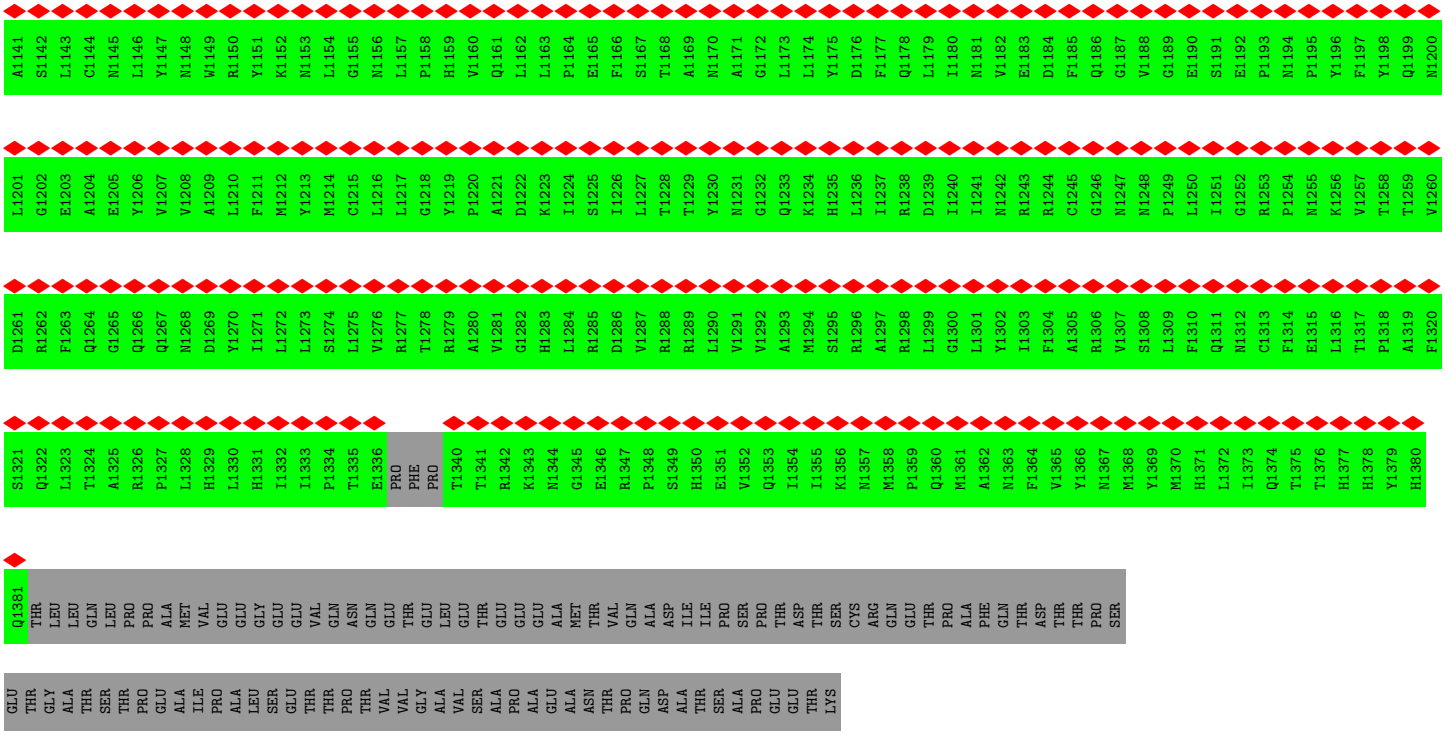
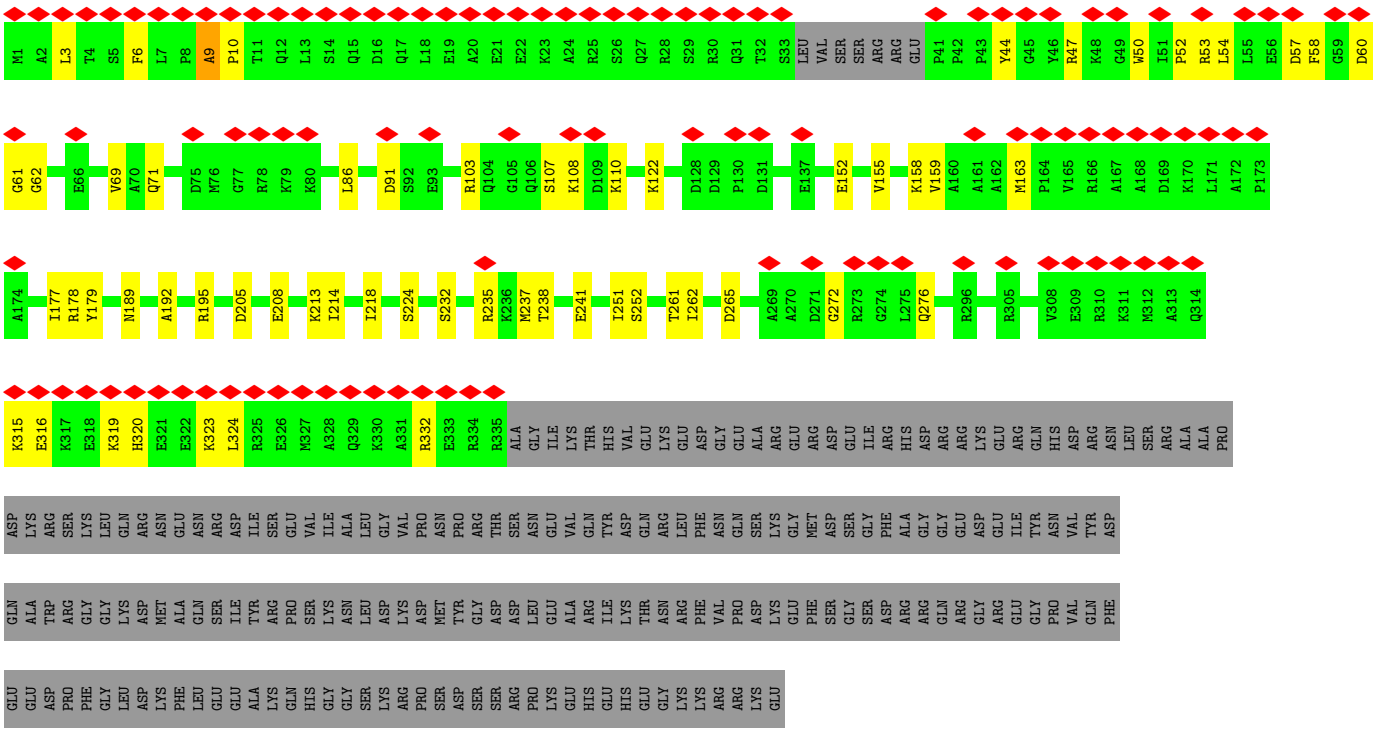
P1081 Q1082 D1083 G1084 F1085 S1086 R1087 L1088 K1089 R1090 W1091 I1092 M1093 I1094 G1095 D1096 H1097 H1098 Q1099 L1100 P1101 P1102 V1103 I1104 K1105 N1106 M1107 A1108 F1109 Q1110 K1111 Y1112 S1113 N1114 M1115 E1116 Q1117 S1118 L1119 F1120 T1121 R1122 F1123 V1124 R1125 V1126 G1127 V1128 P1129 T1130 V1131 D1132 L1133 D1134 A1135 Q1136 G1137 R1138 A1139 R1140



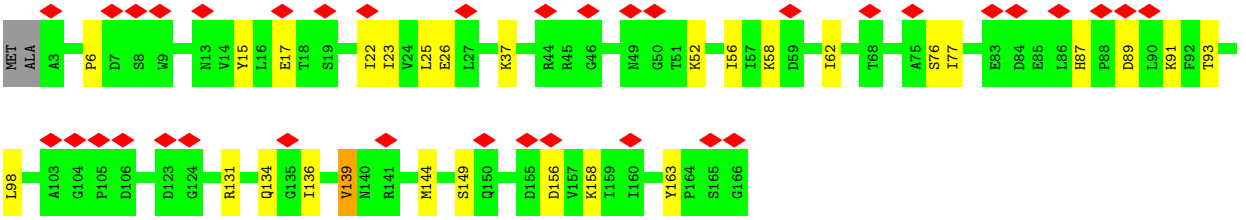
- Molecule 31: SNW domain-containing protein 1

Chain R:



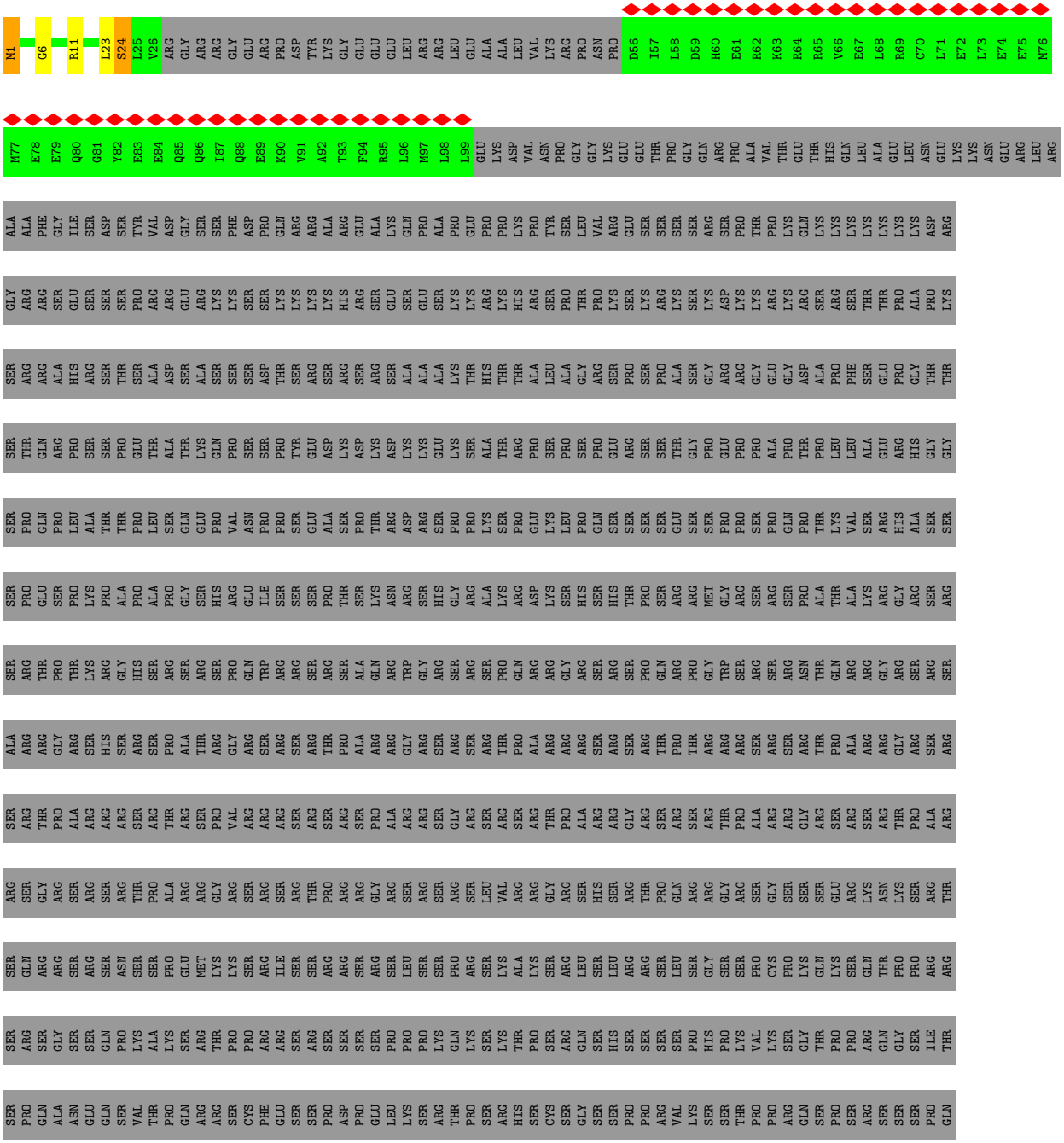
- Molecule 32: Peptidyl-prolyl cis-trans isomerase-like 1

Chain S:



• Molecule 33: Serine/arginine repetitive matrix protein 2

Chain SR: 97%



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THR LYS VAL LYS PRO GLU THR PRO PRO ARG GLN SER HIS SER GLY SER ILE SER PRO TYR PRO LYS VAL LYS ALA GLN THR PRO PRO GLY PRO SER LEU SER GLY SER LYS SER PRO CYS PRO GLN GLU LYS SER LYS ASP SER LEU VAL GLN SER CYS PRO GLY SER LEU SER LEU CYS

ALA GLY VAL LYS SER SER THR PRO PRO GLY GLU SER TYR PHE GLY VAL SER SER LEU GLN LEU LYS GLY GLN SER GLN THR SER PRO ASP HIS ARG SER ASP THR SER SER PRO GLU VAL ARG GLN SER HIS SER GLU SER PRO SER LEU GLN SER LYS SER GLN THR SER PRO LYS GLY

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GLY SER SER PRO GLU THR LYS GLU GLN ASN SER ALA LEU PRO THR SER SER GLN ASP GLU GLU LEU MET GLU VAL VAL GLU LYS SER GLU GLU PRO ALA GLY GLN ILE LEU SER HIS LEU SER SER GLU LEU LYS GLU MET SER THR SER ASN PHE GLU SER SER PRO GLU VAL GLU GLU

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HIS SER LEU SER GLY SER SER PRO GLY MET LYS ASP ILE PRO ARG THR PRO SER ARG GLY ARG SER GLU CYS ASP SER SER PRO GLU PRO LYS ALA LEU PRO GLN THR PRO ARG PRO ARG SER ARG SER PRO SER SER PRO GLU LEU ASN ASN LYS CYS LEU THR PRO GLN ARG GLU ARG

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SER ARG THR PRO THR THR ARG ARG ARG SER ARG SER ARG THR PRO PRO VAL THR ARG ARG ARG SER ARG SER ARG THR PRO PRO VAL THR ARG ARG ARG SER ARG SER ARG THR SER PRO ILE THR ARG ARG ARG SER ARG SER ARG THR SER PRO VAL THR ARG ARG ARG SER ARG SER

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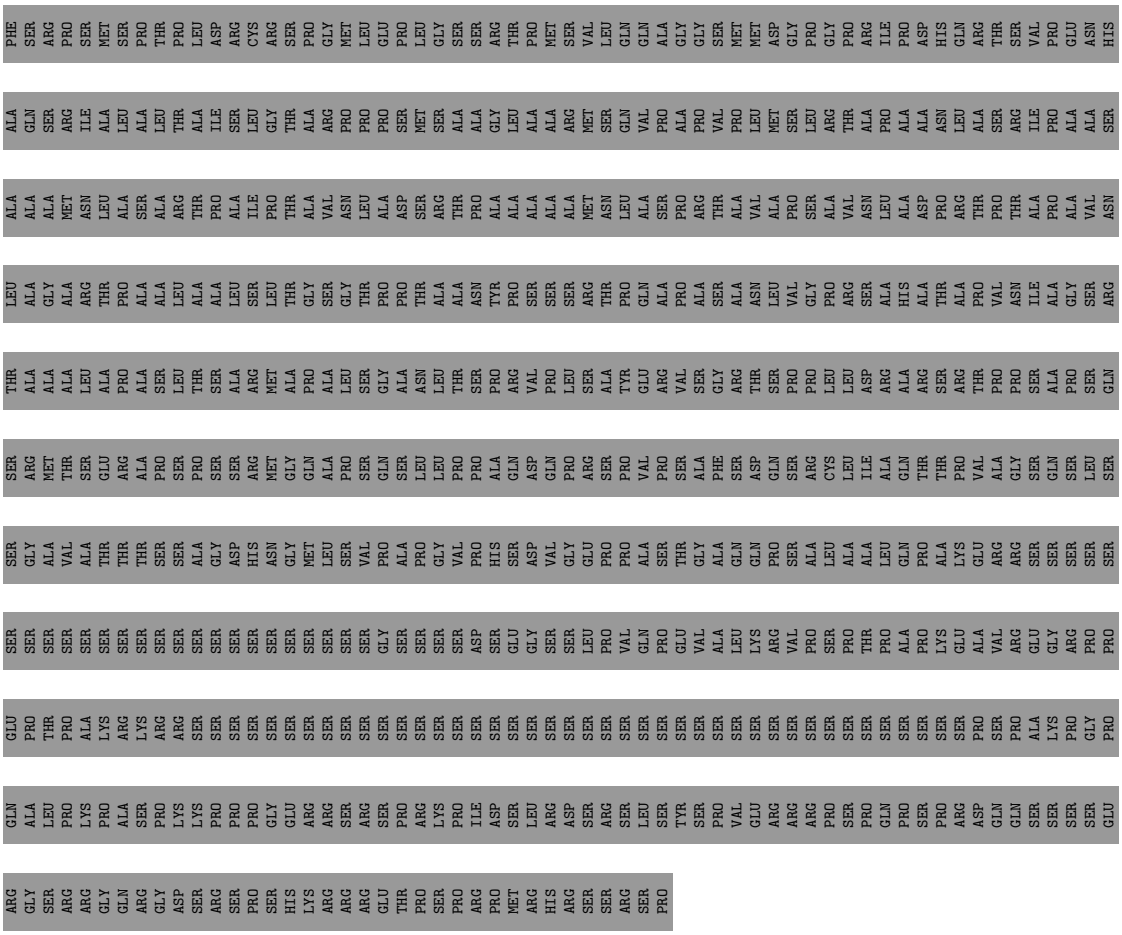
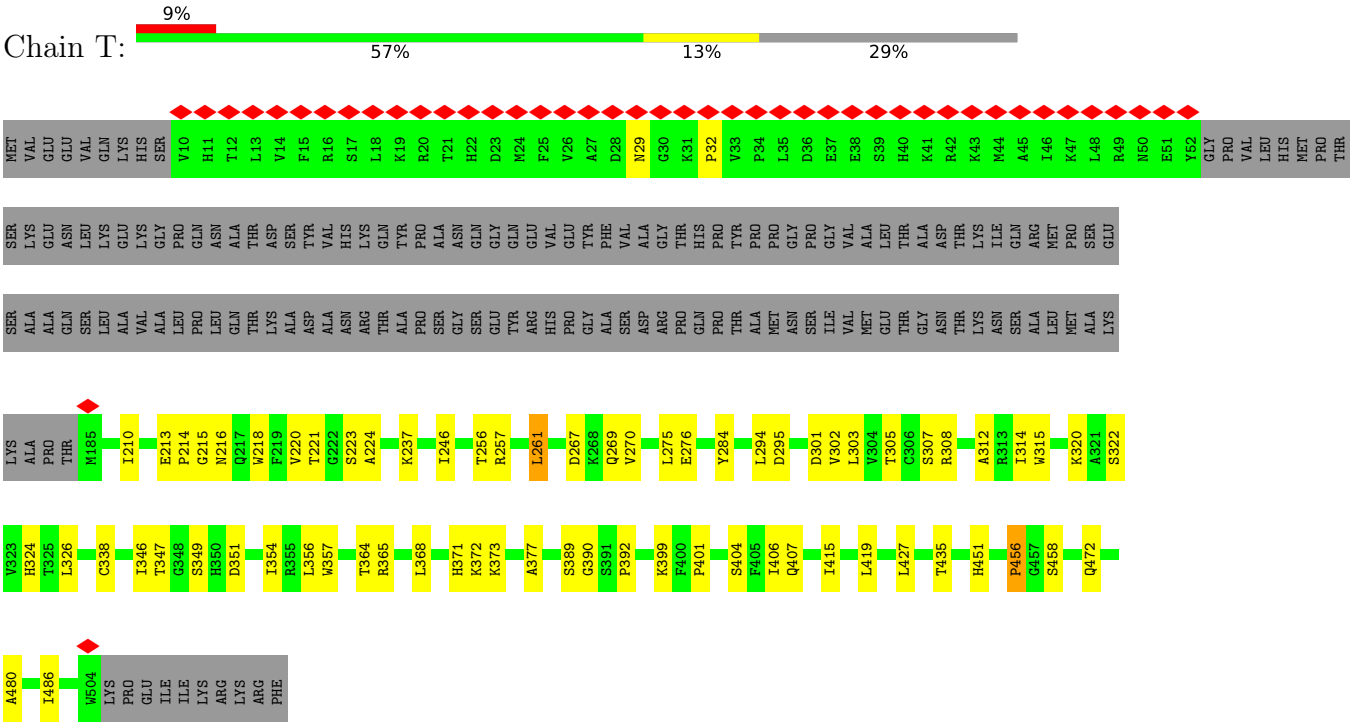
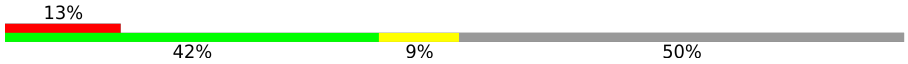


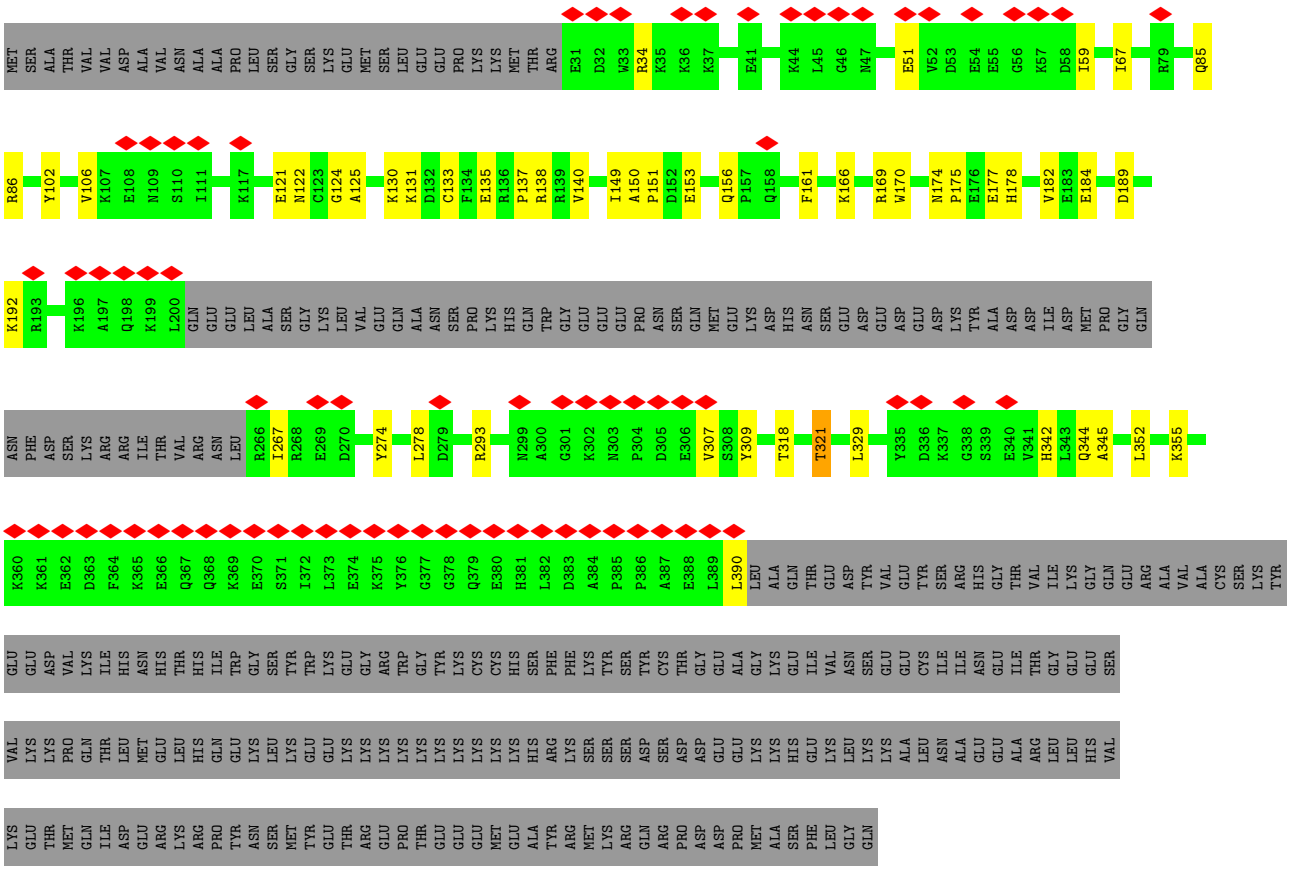
• Molecule 34: Pleiotropic regulator 1



• Molecule 35: Pre-mRNA-splicing factor SLU7

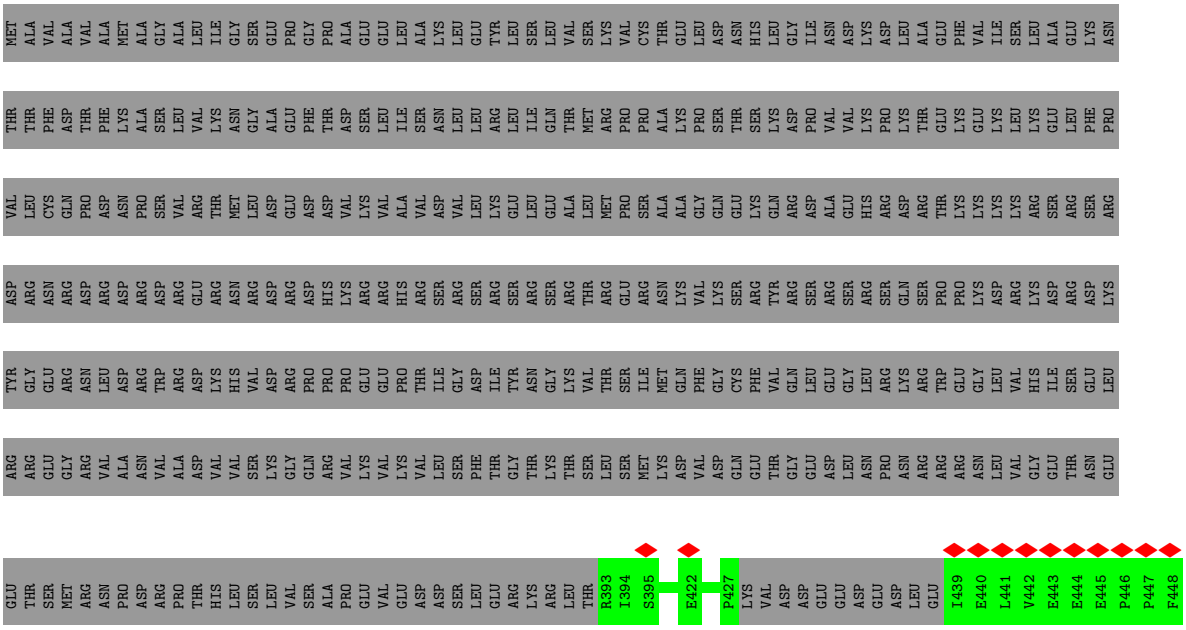
Chain U:





- Molecule 36: ATP-dependent RNA helicase DHX8

Chain V:



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TRP VAL ASP PRO LEU PRO ASP ALA GLU GLY ARG GLN ILE ALA ALA ASN MET ARG GLY ILE GLY MET MET PRO ASN ASP ILE PRO GLU TRP LYS LYS HIS ALA PHE GLY GLY ASN LYS ALA SER TYR GLY LYS LYS THR GLN MET SER ILE L559 E560 Q561 R562 E563 S564 L565 P566 I567 Y568

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T749 K750 E751 P752 E753 T754 D755 Y756 L757 D758 A759 S760 L761 I762 T763 V764 M765 Q766 I767 H768 L769 T770 E771 P772 P773 G774 D775 I776 L777 V778 F779 L780 T781 G782 Q783 E784 E785 I786 D787 T788 A789 C790 E791 I792 L793 Y794 E795 R796 M797 K798 S799 L800 G801 P802 D803 V804 P805 E806 L807 I808

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V929 L930 S931 L932 K933 A934 M935 G936 I937 N938 D939 L940 L941 S942 F943 D944 F945 M946 D947 A948 P949 P950 M951 E952 T953 L954 I955 T956 A957 M958 E959 Q960 L961 Y962 T963 L964 G965 A966 L967 D968 D969 E970 G971 L972 L973 T974 R975 L976 G977 R978 R979 M980 A981 E982 F983 P984 L985 E986 P987 M988

L989 C990 K991 M992 L993 I994 M995 S996 V997 H998 L999 G1000 C1001 S1002 E1003 E1004 M1005 L1006 T1007 I1008 V1009 S1010 M1011 L1012 S1013 V1014 Q1015 N1016 V1017 F1018 Y1019 R1020 P1021 K1022 D1023 K1024 Q1025 A1026 L1027 A1028 D1029 Q1030 K1031 K1032 A1033 K1034 F1035 H1036 Q1037 T1038 E1039 G1040 D1041 H1042 L1043 T1044 L1045 L1046 A1047 V1048

Y1049 N1050 S1051 W1052 K1053 N1054 N1055 K1056 F1057 S1058 N1059 P1060 W1061 C1062 Y1063 E1064 N1065 F1066 I1067 Q1068 A1069 R1070 S1071 L1072 R1073 R1074 A1075 Q1076 D1077 I1078 R1079 K1080 Q1081 M1082 L1083 G1084 I1085 M1086 D1087 A1088 H1089 K1090 L1091 D1092 V1093 V1094 S1095 C1096 G1097 K1098 S1099 T1100 Y1101 H1102 V1103 Q1104 K1105 A1106 I1107 C1108

S1109 G1110 F1111 W1112 R1113 N1114 A1115 A1116 K1117 K1118 D1119 P1120 Q1121 E1122 G1123 Y1124 R1125 P1126 T1127 I1128 D1129 Q1130 Q1131 V1132 V1133 Y1134 I1135 H1136 P1137 S1138 S1139 A1140 L1141 F1142 N1143 R1144 Q1145 P1146 E1147 W1148 V1149 V1150 Y1151 H1152 E1153 L1154 V1155 L1156 T1157 T1158 K1159 E1160 Y1161 M1162 R1163 E1164 V1165 T1166 T1167 I1168

D1169 P1170 R1171 W1172 L1173 V1174 E1175 F1176 A1177 P1178 A1179 F1180 F1181 K1182 V1183 S1184 D1185 P1186 T1187 K1188 L1189 S1190 K1191 Q1192 K1193 K1194 Q1195 GLN ARG LEU GLU PRO LEU TYR ASN ARG TYR GLU GLU PRO ASN ALA TRP ARG ILE SER ARG ALA PHE ARG ARG ARG

- Molecule 37: Pre-mRNA-processing factor 17

Chain W: 11% 68% 20% • 11%

MET SER ALA ALA ILE ALA ALA LEU ALA ALA SER TYR GLY SER GLY SER GLY SER GLU SER ASP SER ASP SER GLU SER SER ARG CYS PRO LEU PRO ALA ALA ASP SER LEU MET HIS LEU THR LYS SER PRO SER SER LYS PRO SER LEU ALA VAL ALA VAL ASP SER ALA PRO GLU VAL

ALA VAL LYS GLU ASP LEU E67 T68 G69 L72 A75 V76 K77 Q80 Y81 N82 E92 E96 R100 Q103 R108 L111 S112 P117 A118 N121 M124 F125 E126 R129 R130 Y137 S142 L143 D144 N145 H146 Q147 V148 S149 A150 S155 V156 E157

Q163 G164 L165 Q172 K173 K174 T175 E176 K177 N188 I189 D190 G191 F192 L193 K203 D204 V205 A206 K207 P208 S209 E210 E211 E212 Q213 K214 E215 L216 D217 E218 A221 K222 R223 Q224 K225 K226 G227 K228 Q229 E230 E231 E232 K233 P234 G235 E236 T239 K244 E245 M246 G251

L255 H256 I257 P258 Q259 D260 V261 G262 V263 N264 L265 R266 P270 P271 E272 L276 Q280 I281 H282 V283 W284 S285 G286 L296 F297 P298 L299 S300 G301 H302 L303 L304 L305 S306 C307 I313 W316 E317 E321 R322 F328 K333 A334 V335 R336 A343 D353

L358 E362 T363 G364 I367 R373 D384 E385 D386 K387 Q388 N389 L390 F391 V392 D397 K398 K399 I400 V401 Q402 W403 D404 I405 R406 S407 G408 E409 L418 N422 D428 R431 R432 F433 V434 S435 T436 K440 S441 L442 R443 V444 W445 E446 D452 F453 K454 Y455 I456

M464 L476 A477 C478 Q479 Q484 I487 A490 R493 K503 G504 H505 M506 Q513 V514 D515 P518 D519 I524 S525 G526 D527 K531 I534 S544 D550 K551 V552 V557 W558 H559 I567 W571 D572 D579

• Molecule 38: Splicing regulator SDE2

Chain X: 14% 14% 85%

MET ALA GLU ALA ALA ALA LEU VAL TRP ILE ARG GLY PRO GLY PHE GLY CYS LYS ALA VAL ARG CYS ALA SER GLY ARG CYS THR VAL ARG ASP PHE ILE HIS ARG HIS CYS GLN ASP GLN ASN VAL PRO VAL GLU ASN PHE PHE VAL LYS CYS ASN GLY ALA LEU ILE ASN THR SER ASP

THR VAL GLN HIS GLY ALA VAL TYR SER LEU GLU PRO ARG LEU CYS GLY GLY LYS GLY GLY PHE GLY SER MET LEU ARG ALA LEU GLY ALA GLN ILE GLU LYS THR THR N97 R98 E99 A100 C101 R102 D103 L104 S105 G106 R107 R108 L109 R110 D111 V112 N113 H114 E115 K116 A117 M118 A119 E120

W121 V122 K123 Q124 Q125 A126 E127 R128 E129 A130 E131 K132 GLU GLN LYS ARG LEU GLU ARG LEU GLN ARG LYS LEU VAL GLU PRO LYS HIS CYS PHE THR SER P154 D155 Y156 Q157 Q158 Q159 C160 H161 E162 M163 A164 E165 R166 L167 E168 D169 S170 V171 L172 K173 G174 M175 Q176 A177 A178 S179 S180

K181 M182 V183 SER ALA GLU ILE SER GLU ASN ARG LYS ARG GLN TRP PRO THR LYS SER GLN THR ASP ARG GLY ALA SER ALA GLY LYS ARG ARG CYS PHE TRP LEU GLY MET GLU GLY LEU GLU THR ALA GLU GLY SER ASN SER GLU SER SER ASP ASP SER GLU GLU ALA PRO SER

THR SER GLY MET GLY PHE HIS ALA PRO LYS ILE GLY SER ASN GLY VAL GLU MET ALA ALA LYS PHE PRO SER GLY SER GLN ARG ALA ARG VAL VAL ASN THR ASP HIS GLY SER PRO GLU GLN LEU GLN ILE PRO VAL THR ASP SER GLY ARG HIS ILE LEU GLU ASP SER CYS ALA GLU

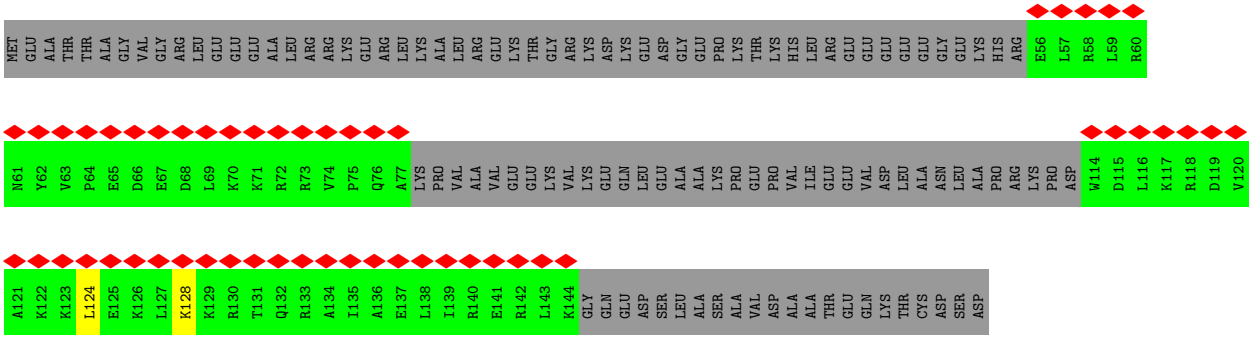
LEU GLY GLU SER LYS GLU HIS MET GLU SER ARG MET VAL THR GLU THR GLU GLU THR GLN GLU LYS LYS ALA GLU SER LYS GLU PRO ILE GLU GLU GLU PRO THR GLY ALA GLY LEU ASN LYS ASP LYS GLU THR GLU GLU ARG THR ASP GLY ARG HIS ILE LEU GLU ASP SER CYS ALA PRO GLU

GLU ARG GLU ASN VAL ALA VAL ALA LYS LEU GLN GLU SER GLN PRO GLY ASN ALA VAL ILE ASP LYS GLU THR ILE ASP LEU LEU ALA PHE THR SER VAL ALA GLU LEU GLU LEU LEU GLY LEU GLU LYS LEU LYS CYS GLU LEU MET ALA LEU GLY LEU LYS CYS GLY GLY THR LEU GLN

GLU ARG ALA ALA ARG LEU PHE SER VAL ARG GLY LEU ALA LYS GLU GLN ILE ASP PRO ALA LEU PHE ALA LYS PRO LEU LYS GLY LYS LYS LYS

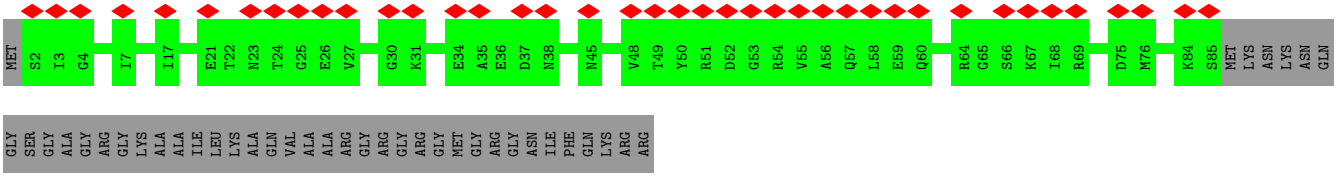
• Molecule 39: Coiled-coil domain-containing protein 12

Chain Z:



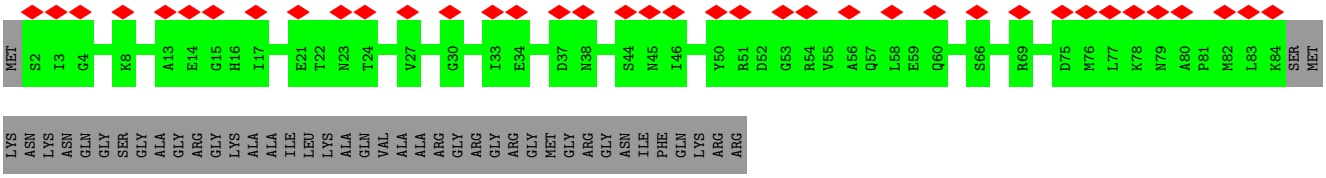
• Molecule 40: Small nuclear ribonucleoprotein Sm D3

Chain a:



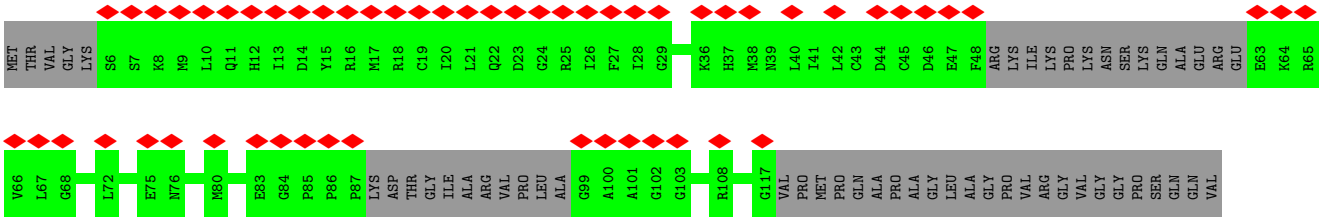
• Molecule 40: Small nuclear ribonucleoprotein Sm D3

Chain h:



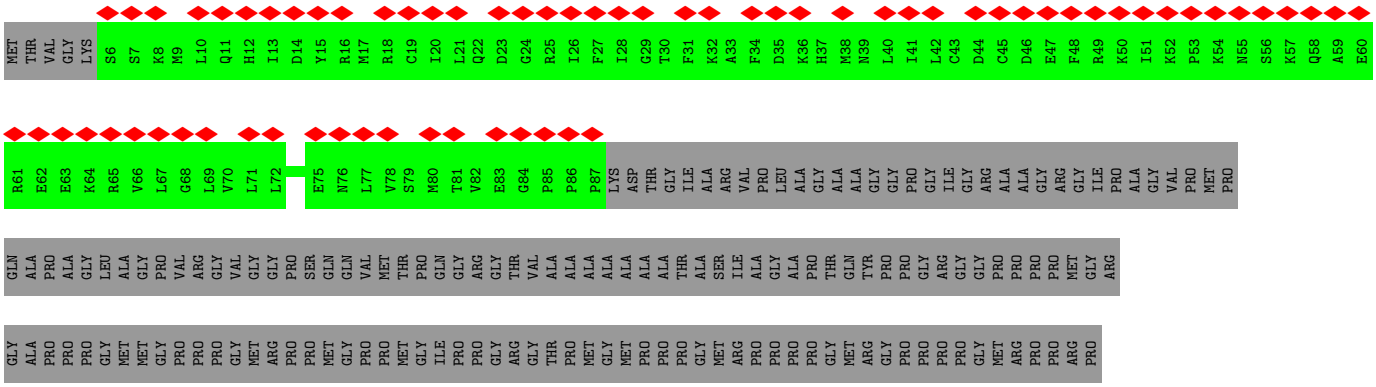
• Molecule 41: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain b:



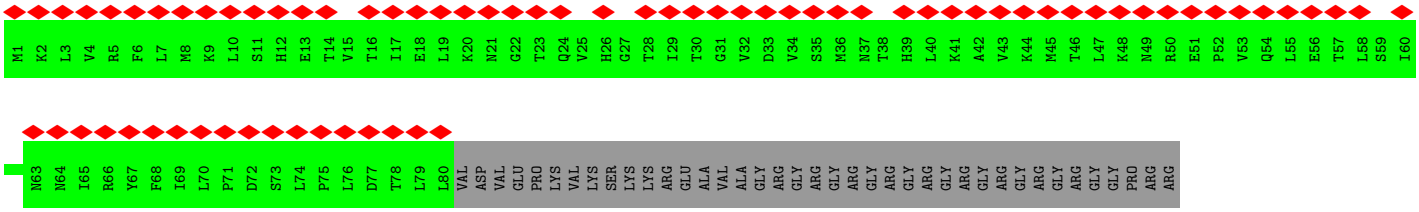
- Molecule 41: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain i:



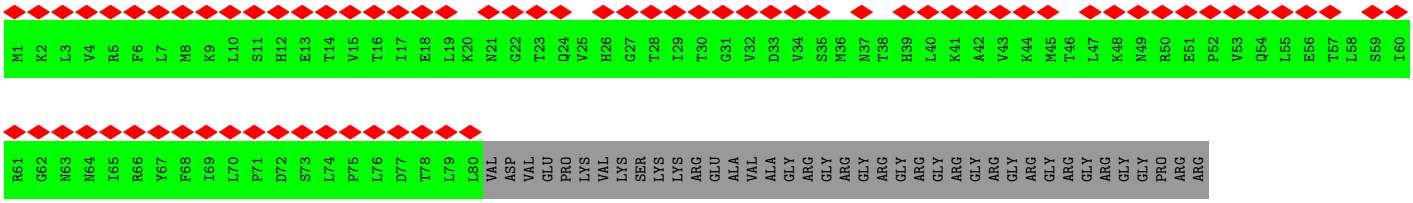
- Molecule 42: Small nuclear ribonucleoprotein Sm D1

Chain c:



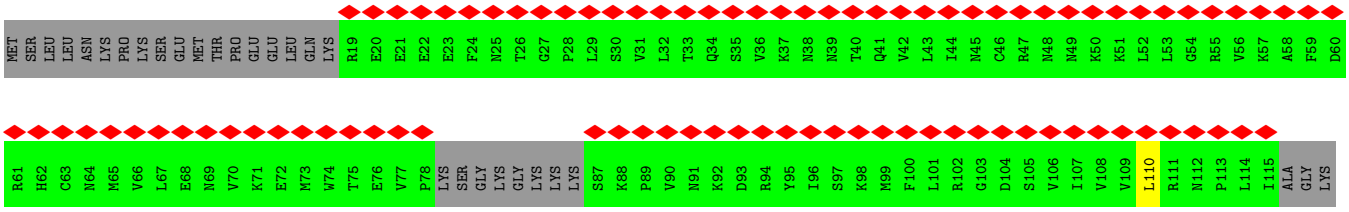
- Molecule 42: Small nuclear ribonucleoprotein Sm D1

Chain j:



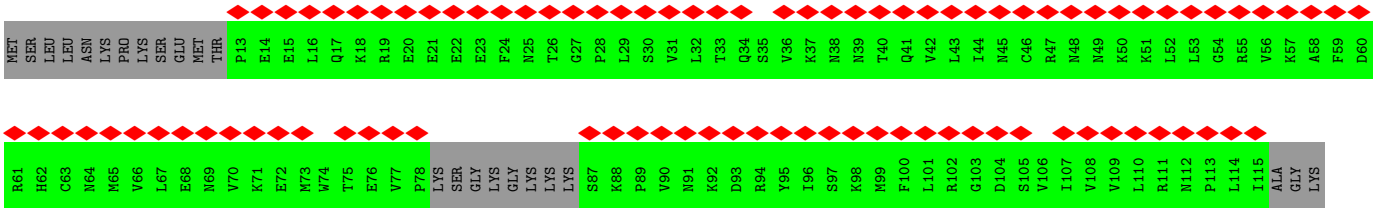
- Molecule 43: Small nuclear ribonucleoprotein Sm D2

Chain d:



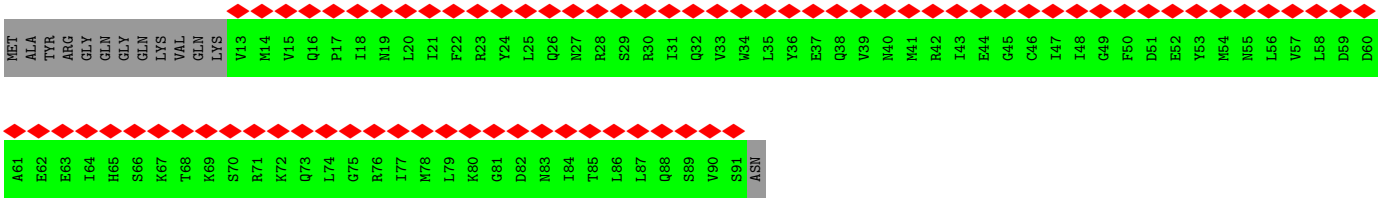
- Molecule 43: Small nuclear ribonucleoprotein Sm D2

Chain k:



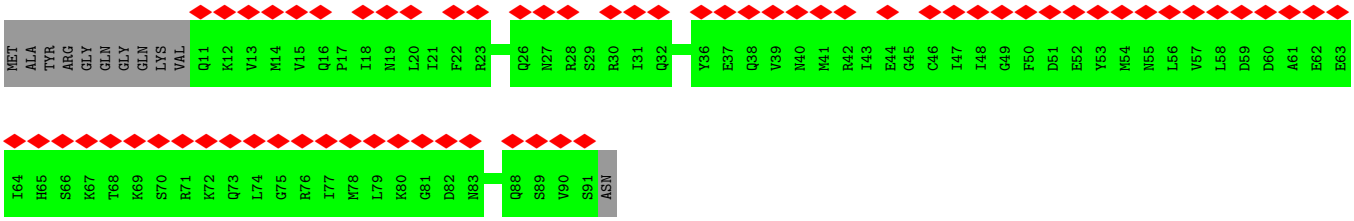
• Molecule 44: Small nuclear ribonucleoprotein E

Chain e:



• Molecule 44: Small nuclear ribonucleoprotein E

Chain l:

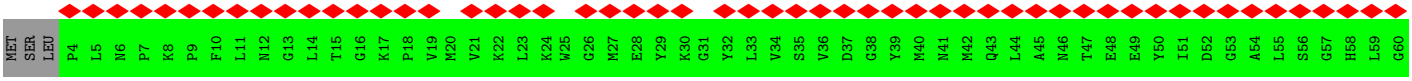


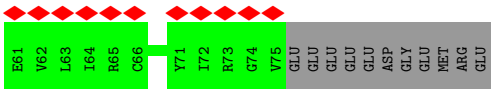
• Molecule 45: Small nuclear ribonucleoprotein F

Chain f:

• Molecule 45: Small nuclear ribonucleoprotein F

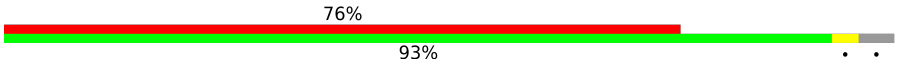
Chain m:

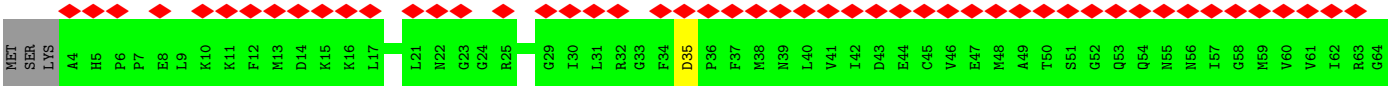


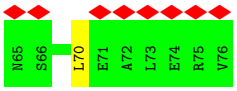


- Molecule 46: Small nuclear ribonucleoprotein G

Chain g:

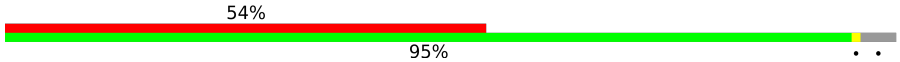


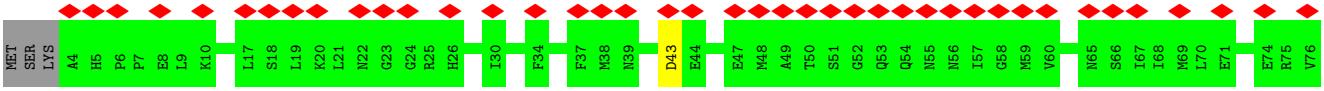




- Molecule 46: Small nuclear ribonucleoprotein G

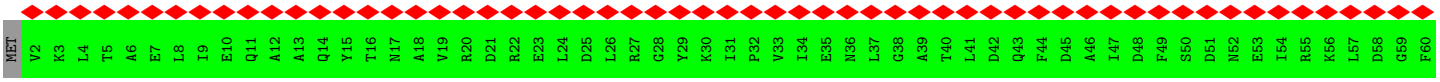
Chain n:

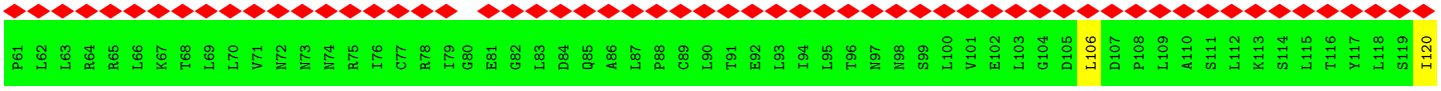


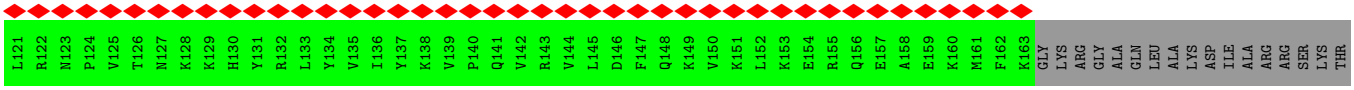


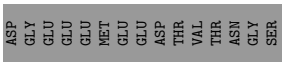
- Molecule 47: U2 small nuclear ribonucleoprotein A'

Chain o:



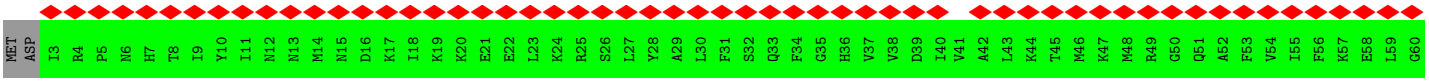






- Molecule 48: U2 small nuclear ribonucleoprotein B"

Chain p:



S61 S62 T63 N64 A65 L66 R67 Q68 L69 Q70 G71 F72 P73 F74 Y75 G76 K77 P78 M79 R80 I81 Q82 Y83 A84 K85 T86 D87 S88 D89 I90 I91 S92 K93 M94 ARG GLY THR PHE ALA ASP LYS GLU LYS LYS LYS GLU LYS LYS LYS LYS ALA LYS THR VAL GLU GLN THR ALA THR THR THR

ASN LYS LYS PRO GLY GLN GLY THR PRO ASN SER ALA ASN THR GLN GLY ASN SER THR PRO ASN PRO GLN VAL PRO ASP TYR PRO PRO ASN TYR ILE LEU PHE LEU ASN ASN LEU PRO GLU GLU THR ASN GLU MET MET LEU SER MET LEU PHE ASN GLN PHE PRO GLY PHE LYS GLU VAL

ARG LEU VAL PRO GLY ARG HIS ASP ILE ALA PHE VAL GLU PHE GLU ASN ASP GLY GLN ALA GLY ALA ALA ALA ARG ASP ALA LEU GLN GLY PHE LYS ILE THR PRO SER HIS ALA MET LYS ILE THR TYR ALA LYS LYS

- Molecule 49: Pre-mRNA-processing factor 19

Chain q: 20% 20% 80%

MET SER LEU ILE CYS SER ILE SER ASN GLU VAL PRO E13 H14 P15 C16 V17 S18 P19 V20 S21 N22 H23 V24 Y25 E26 R27 R28 L29 I30 E31 K32 Y33 I34 A35 E36 N37 G38 T39 D40 P41 I42 N43 N44 Q45 P46 L47 S48 E49 E50 Q51 LEU ILE ASP ILE LYS VAL ALA HIS PRO

ILE ARG PRO LYS PRO PRO SER ALA THR SER I71 P72 A73 I74 L75 K76 A77 L78 Q79 D80 E81 W82 D83 A84 V85 M86 L87 H88 S89 F90 T91 L92 R93 Q94 Q95 L96 Q97 T98 T99 R100 Q101 E102 L103 S104 H105 A106 L107 Y108 Q109 H110 D111 A112 A113 C114 R115 V116 I117 A118 R119 L120

T121 K122 E123 V124 T125 A126 A127 R128 E129 A130 L131 A132 T133 L134 LYS PRO GLN ALA GLY LEU ILE VAL PRO GLN ALA VAL PRO SER SER GLN PRO SER VAL VAL GLY ALA GLY GLU PRO MET ASP LEU GLY GLU LEU VAL GLY MET THR PRO GLU ILE ILE GLN LYS LEU GLN ASP LYS ALA

THR VAL LEU THR THR GLU ARG LYS LYS ARG GLY LYS THR VAL PRO GLU GLU LEU VAL LYS PRO GLU GLU LEU SER LYS LYS TYR ARG GLN VAL ALA SER HIS VAL GLY LEU HIS SER ALA SER ILE PRO GLY ILE LEU ALA LEU ASP LEU CYS PRO SER ASP THR ASN LYS ILE LEU THR GLY

GLY ALA ASP LYS ASN VAL VAL VAL PHE ASP LYS SER SER GLU GLN ILE LEU ALA THR LEU LYS GLY HIS THR LYS LYS VAL THR SER VAL VAL PHE HIS PRO SER GLN ASP LEU VAL PHE SER ALA SER PRO ASP ALA THR ILE ARG ILE TRP SER VAL PRO ASN ALA SER CYS VAL GLN

VAL VAL ARG ALA HIS GLU SER ALA VAL THR GLY LEU SER LEU HIS ALA THR GLY ASP TYR LEU LEU SER SER SER ASP ASP GLN TYR TRP ALA PHE SER ASP ILE GLN THR GLY ARG VAL LEU THR LYS VAL THR ASP GLU THR SER GLY CYS SER LEU THR CYS ALA GLN PHE HIS PRO

ASP GLY LEU ILE PHE GLY THR GLY THR MET ASP SER GLN ILE LYS ILE TRP ASP LEU LYS GLU ARG THR ASN VAL ALA ASN PHE PRO GLY HIS SER GLY PRO ILE THR SER ILE ALA PHE SER GLU ASN GLY TYR TYR LEU ALA THR ALA ALA ASP ASP SER SER VAL LYS LEU TRP ASP

LEU ARG LYS LEU LYS ASN PHE LYS THR LEU GLN LEU ASP ASN ASN PHE GLU VAL LYS SER LEU ILE PHE ASP GLN SER GLY THR TYR LEU ALA LEU GLY GLY THR ASP VAL GLN ILE TYR ILE CYS LYS GLN TRP THR GLU ILE LEU HIS PHE THR GLU HIS SER GLY LEU THR THR GLY

VAL ALA PHE GLY HIS HIS ALA LYS PHE ILE ALA SER THR GLY MET ASP ARG SER LEU LYS PHE TYR SER LEU

- Molecule 49: Pre-mRNA-processing factor 19

Chain r: 24% 24% 76%

M1 S2 L3 I4 C5 S6 I7 S8 N9 E10 V11 P12 E13 H14 P15 C16 V17 S18 P19 V20 S21 N22 H23 V24 Y25 E26 R27 R28 L29 I30 E31 K32 Y33 I34 A35 E36 N37 G38 T39 D40 P41 I42 N43 N44 Q45 P46 L47 S48 E49 E50 Q51 L52 I53 D54 I55 LYS VAL ALA HIS PRO

ILE ARG PRO LYS PRO PRO SER ALA THR SER I71 P72 A73 I74 L75 K76 A77 L78 Q79 D80 E81 W82 D83 A84 V85 M86 L87 H88 S89 F90 T91 L92 R93 Q94 Q95 L96 Q97 T98 T99 R100 Q101 E102 L103 S104 H105 A106 L107 Y108 Q109 H110 D111 A112 A113 C114 R115 V116 I117 A118 R119 L120

T121 K122 E123 V124 T125 A126 A127 R128 E129 A130 L131 A132 T133 L134 LYS PRO GLN ALA GLY LEU ILE VAL PRO GLN ALA VAL PRO SER SER GLN PRO SER VAL VAL GLY ALA GLY GLU PRO MET ASP LEU GLY GLU LEU VAL GLY MET THR PRO GLU ILE ILE GLN LYS LEU GLN ASP LYS ALA

THR VAL LEU THR THR GLU ARG LYS LYS ARG GLY LYS THR VAL PRO GLU GLU LEU VAL LYS PRO GLU GLU LEU SER LYS TYR ARG GLN VAL ALA SER HIS VAL GLY LEU HIS SER ALA SER ILE PRO GLY ILE LEU ALA LEU ASP LEU CYS PRO SER ASP THR ASN LYS ILE LEU THR GLY

GLY ALA ASP LYS ASN VAL VAL VAL PHE ASP LYS SER SER GLU GLN ILE LEU ALA THR LEU LYS GLY HIS THR LYS LYS VAL THR SER VAL VAL PHE HIS PRO SER GLN ASP LEU VAL PHE SER ALA SER PRO ASP ALA THR ILE ARG ILE TRP SER VAL PRO ASN ALA SER CYS VAL GLN

VAL VAL ARG ALA HIS GLU SER ALA VAL THR GLY LEU SER LEU HIS ALA THR GLY ASP TYR TYR LEU LEU SER SER SER SER ASP ASP GLN TYR TRP ALA PHE SER ASP ILE GLN THR GLY ARG VAL LEU THR LYS VAL THR ASP GLU THR SER GLY CYS SER LEU THR CYS ALA GLN PHE HIS PRO

ASP GLY LEU ILE PHE GLY THR GLY THR MET ASP SER GLN ILE LYS ILE TRP ASP LEU LYS GLU ARG THR ASN VAL ALA ASN PHE PRO GLY HIS SER GLY PRO ILE THR SER ILE ALA PHE SER GLU ASN GLY TYR TYR LEU ALA THR ALA ALA ASP SER SER VAL LYS LEU TRP ASP

LEU ARG LYS LEU LYS ASN PHE LYS THR LEU GLN LEU ASP ASN ASN PHE GLU VAL LYS SER LEU ILE PHE ASP GLN SER GLY THR TYR LEU ALA LEU GLY GLY THR ASP VAL GLN ILE TYR ILE CYS LYS GLN TRP THR GLU ILE LEU HIS PHE THR GLU HIS SER GLY LEU THR THR GLY

VAL ALA PHE GLY HIS HIS ALA LYS PHE ILE ALA SER THR GLY MET ASP ARG SER LEU LYS PHE TYR SER LEU

- Molecule 49: Pre-mRNA-processing factor 19

Chain s: 26% 26% 74%

M1 S2 L3 I4 C5 S6 I7 S8 N9 E10 V11 P12 E13 H14 P15 C16 V17 S18 P19 V20 S21 N22 H23 V24 Y25 E26 R27 R28 L29 I30 E31 K32 Y33 I34 A35 E36 N37 G38 T39 D40 P41 I42 N43 N44 Q45 P46 L47 S48 E49 E50 Q51 L52 I53 D54 I55 K56 V57 A58 H59 P60

I61 R62 P63 K64 P65 P66 S67 A68 T69 S70 I71 P72 A73 I74 L75 K76 A77 L78 Q79 D80 E81 W82 D83 A84 V85 M86 L87 H88 S89 F90 T91 L92 R93 Q94 Q95 L96 Q97 T98 T99 R100 Q101 E102 L103 S104 H105 A106 L107 Y108 Q109 H110 D111 A112 A113 C114 R115 V116 I117 A118 R119 L120

T121 K122 E123 V124 T125 A126 A127 R128 E129 A130 L131 A132 THR LEU LYS PRO GLN ALA GLY LEU ILE VAL PRO GLN ALA VAL PRO SER SER GLN PRO SER VAL VAL GLY ALA GLY GLU PRO MET ASP LEU GLY GLU LEU VAL GLY MET THR PRO GLU ILE ILE GLN LYS LEU GLN ASP LYS ALA

THR VAL LEU THR THR GLU ARG LYS LYS ARG GLY LYS THR VAL PRO GLU GLU LEU VAL LYS PRO GLU GLU LEU SER LYS TYR ARG GLN VAL ALA SER HIS VAL GLY LEU HIS SER ALA SER ILE PRO GLY ILE LEU ALA LEU ASP LEU CYS PRO SER ASP THR ASN LYS ILE LEU THR GLY

GLY ALA ASP LYS ASN VAL VAL VAL PHE ASP LYS SER SER GLU GLN ILE LEU ALA THR LEU LYS GLY HIS THR LYS LYS VAL THR SER VAL VAL PHE HIS PRO SER GLN ASP LEU VAL PHE SER ALA SER PRO ASP ALA THR ILE ARG ILE TRP SER VAL PRO ASN ALA SER CYS VAL GLN

VAL VAL ARG ALA HIS GLU SER ALA VAL THR GLY LEU SER LEU HIS ALA THR GLY ASP TYR TYR LEU LEU SER SER SER SER ASP ASP GLN TYR TRP ALA PHE SER ASP ILE GLN THR GLY ARG VAL LEU THR LYS VAL THR ASP GLU THR SER GLY CYS SER LEU THR CYS ALA GLN PHE HIS PRO

ASP GLY LEU ILE PHE GLY THR GLY THR MET ASP SER GLN ILE LYS ILE TRP ASP LEU LYS GLU ARG THR ASN VAL ALA ASN PHE PRO GLY HIS SER GLY PRO ILE THR SER ILE ALA PHE SER GLU ASN GLY TYR TYR LEU ALA THR ALA ALA ASP SER SER VAL LYS LEU TRP ASP

LEU ARG LYS LEU LYS ASN PHE LYS THR LEU GLN LEU ASP ASN ASN PHE GLU VAL LYS SER LEU ILE PHE ASP GLN SER GLY THR TYR LEU ALA LEU GLY GLY THR ASP VAL GLN ILE TYR ILE CYS LYS GLN TRP THR GLU ILE LEU HIS PHE THR GLU HIS SER GLY LEU THR THR GLY

VAL ALA PHE GLY HIS HIS ALA LYS PHE ILE ALA SER THR GLY MET ASP ARG SER LEU LYS PHE TYR SER LEU

- Molecule 49: Pre-mRNA-processing factor 19

Chain t: 20% 20% 80%

MET SER LEU ILE CYS SER ILE SER ASN GLU VAL PRO E13 H14 P15 C16 V17 S18 P19 V20 S21 N22 H23 V24 Y25 E26 R27 R28 L29 I30 E31 K32 Y33 I34 A35 E36 N37 G38 T39 D40 P41 I42 N43 N44 Q45 P46 L47 S48 E49 E50 Q51 LEU ILE ASP ILE LYS VAL ALA HIS PRO

ILE ARG PRO LYS PRO PRO SER ALA THR SER I71 P72 A73 I74 L75 K76 A77 L78 Q79 D80 E81 W82 D83 A84 V85 M86 L87 H88 S89 F90 T91 L92 R93 Q94 Q95 L96 Q97 T98 T99 R100 Q101 E102 L103 S104 H105 A106 L107 Y108 Q109 H110 D111 A112 A113 C114 R115 V116 I117 A118 R119 L120

T121 K122 E123 V124 T125 A126 A127 R128 E129 A130 L131 A132 T133 L134 LYS PRO GLN ALA GLY LEU ILE VAL PRO GLN ALA VAL PRO SER SER GLN PRO SER VAL VAL GLY ALA GLY GLU PRO MET ASP LEU GLY GLU LEU VAL GLY MET THR PRO GLU ILE ILE GLN LYS LEU GLN ASP LYS ALA

THR VAL LEU THR THR GLU ARG LYS LYS ARG GLY LYS THR VAL PRO GLU GLU LEU VAL LYS PRO GLU GLU LEU SER LYS TYR ARG GLN VAL ALA SER HIS VAL GLY LEU HIS SER ALA SER ILE PRO GLY ILE LEU ALA LEU ASP LEU CYS PRO SER ASP THR ASN LYS ILE LEU THR GLY

GLY ALA ASP LYS ASN VAL VAL VAL PHE ASP LYS SER SER GLU GLN ILE LEU ALA THR LEU LYS GLY HIS THR LYS LYS VAL THR SER VAL VAL PHE HIS PRO SER GLN ASP LEU VAL PHE SER ALA SER PRO ASP ALA THR ILE ARG ILE TRP SER VAL PRO ASN ALA SER CYS VAL GLN

VAL VAL ARG ALA HIS GLU SER ALA VAL THR GLY LEU SER LEU HIS ALA THR GLY ASP TYR LEU LEU SER SER SER ASP ASP GLN TYR TRP ALA PHE SER ASP ILE GLN THR GLY ARG VAL LEU THR LYS VAL THR ASP GLU THR SER GLY CYS SER LEU THR CYS ALA GLN PHE HIS PRO

ASP GLY LEU ILE PHE GLY THR GLY THR MET ASP SER GLN ILE LYS ILE TRP ASP LEU LYS GLU ARG THR ASN VAL ALA ASN PHE PRO GLY HIS SER GLY PRO ILE THR SER ILE ALA PHE SER GLU ASN GLY TYR TYR LEU ALA THR ALA ALA ASP ASP SER SER VAL LYS LEU TRP ASP

LEU ARG LYS LEU LYS ASN PHE LYS THR LEU GLN LEU ASP ASN ASN PHE GLU VAL LYS SER LEU ILE PHE ASP GLN SER GLY THR TYR LEU ALA LEU GLY GLY THR ASP VAL GLN ILE TYR ILE CYS LYS GLN TRP THR GLU ILE LEU HIS PHE THR GLU HIS SER GLY LEU THR THR GLY

VAL ALA PHE GLY HIS HIS ALA LYS PHE ILE ALA SER THR GLY MET ASP ARG SER LEU LYS PHE TYR SER LEU

- Molecule 50: Peptidylprolyl isomerase domain and WD repeat-containing protein 1

Chain w: 82% 82% 18%

MET ALA ALA GLU SER GLY SER ASP PHE GLN GLN ARG ARG ARG ARG ARG ARG ASP PRO GLU GLU PRO GLU LYS THR GLU LEU SER GLU ARG GLU LEU ALA VAL ALA VAL ALA VAL SER GLN GLU ASN ASP GLU GLU ASN GLU GLU ARG TRP VAL GLY PRO LEU PRO VAL GLU ALA THR LEU

ALA LYS LYS ARG LYS VAL LEU GLU PHE E70 R71 V72 Y73 L74 D75 N76 L77 P78 S79 A80 S81 M82 Y83 E84 R85 S86 Y87 M88 H89 R90 D91 V92 I93 T94 H95 V96 V97 C98 T99 K100 T101 D102 F103 I104 I105 T106 A107 S108 H109 D110 G111 H112 V113 K114 F115 W116 K117 K118 I119 E120

E121 G122 I123 E124 F125 V126 K127 H128 F129 R130 S131 H132 L133 G134 V135 I136 E137 S138 I139 A140 V141 S142 S143 E144 G145 A146 L147 F148 C149 S150 V151 G152 D153 D154 K155 A156 M157 K158 V159 F160 D161 V162 V163 N164 F165 D166 M167 I168 N169 M170 L171 K172 L173 G174 Y175 F176 P177 G178 Q179 C180

E181 W182 I183 Y184 C185 P186 G187 D188 A189 I190 S191 S192 V193 A194 A195 S196 E197 K198 S199 T200 G201 K202 I203 F204 I205 Y206 D207 G208 R209 G210 D211 N212 Q213 P214 L215 H216 I217 F218 D219 K220 A281 Y282 P283 T284 S285 V286 C287 F288 S289 P290 D291 G292 K293 K294 I295 A296 T297 I298 G299 S300

S241 D242 K243 S244 G245 M246 I247 E248 Y249 W250 T251 G252 P253 P254 H255 E256 Y257 K258 F259 P260 K261 N262 V263 N264 W265 E266 Y267 K268 T269 D270 T271 D272 L273 Y274 E275 F276 A277 K278 C279 K280 L221 H222 T223 S224 P225 L226 T227 Q228 I229 R230 L231 N232 P233 V234 Y235 K236 A237 V238 V239 S240

D301 R302 K303 V304 R305 I306 F307 R308 F309 V310 T311 G312 K313 L314 M315 R316 V317 F318 D319 E320 S321 L322 S323 M324 F325 T326 E327 L328 Q329 Q330 M331 R332 Q333 Q334 L335 P336 D337 M338 E339 F340 G341 R342 R343 M344 A345 V346 E347 R348 E349 L350 E351 K352 V353 D354 A355 V356 R357 L358 I359 N360

I361 V362 F363 D364 E365 T366 G367 H368 F369 V370 L371 Y372 G373 T374 M375 L376 G377 I378 K379 V380 I381 N382 V383 E384 T385 N386 R387 C388 V389 R390 I391 L392 G393 K394 Q395 E396 N397 T398 R399 V400 M401 Q402 L403 A404 L405 F406 GLN GLY ILE ALA LYS HIS ARG ALA ALA THR THR ILE GLU

MET LYS ALA SER GLU ASN PRO VAL LEU GLN ASN ILE GLN ALA ASP PRO T437 I438 V439 C440 T441 S442 F443 K444 K445 N446 R447 F448 Y449 M450 F451 T452 K453 R454 E455 P456 E457 D458 T459 K460 S461 A462 D463 S464 D465 R466 D467 V468 F469 N470 E471 K472 P473 SER LYS GLU GLU VAL MET ALA

ALA THR GLN ALA GLU GLY PRO LYS ARG VAL SER ASP S493 A494 I495 I496 H497 T498 S499 M500 G501 D502 I503 H504 T505 K506 L507 F508 P509 V510 E511 C512 P513 K514 T515 V516 E517 N518 F519 C520 V521 H522 S523 R524 N525 G526 Y527 Y528 N529 G530 H531 T532 F533 H534 R535 I536 I537 K538 G539 F540

M541 I542 Q543 T544 G545 D546 P547 T548 G549 T550 G551 M552 G553 G554 E555 S556 I557 W558 G559 G560 E561 F562 E563 D564 E565 F566 H567 S568 T569 L570 R571 H572 D573 R574 P575 Y576 T577 L578 S579 M580 A581 N582 A583 G584 S585 N586 T587 N588 G589 S590 Q591 F592 R593 I594 T595 V596 V597 P598 T599 P600

W601 L602 D603 N604 K605 H606 T607 V608 F609 G610 R611 V612 T613 K614 G615 M616 E617 V618 V619 Q620 R621 I622 S623 N624 V625 K626 V627 N628 P629 K630 T631 D632 K633 P634 Y635 E636 D637 V638 S639 I640 I641 N642 I643 T644 V645 K646

- Molecule 51: Splicing factor C9orf78

Chain x: 43% 44% 56%

MET PRO VAL VAL R5 K6 I7 F8 R9 R10 R11 R12 G13 D14 S15 E16 S17 E18 E19 D20 E21 Q22 D23 S24 E25 E26 V27 R28 L29 K30 L31 E32 E33 T34 R35 E36 V37 Q38 N39 L40 R41 K42 R43 P44 N45 G46 V47 S48 A49 V50 A51 L52 L53 V54 G55 GLU LYS VAL GLN GLU

GLU THR THR LEU VAL ASP ASP PRO PHE GLN MET LYS THR GLY GLY MET VAL ASP MET LYS LYS LEU LYS GLU ARG GLY LYS ASP LYS ILE SER GLU GLU GLU GLU ASP LEU HIS LEU GLY THR SER PHE SER ALA GLU THR ASN ARG ARG ASP E111 D112 A113 D114 M115 M116 K117 Y118 I119 E120

T121 E122 L123 K124 K125 R126 LYS GLY ILE VAL GLU HIS GLU GLU GLN LYS VAL LYS PRO LYS ASN ALA GLU ASP CYS LEU TYR GLU LEU PRO GLU ASN ILE ARG VAL SER SER ALA LYS LYS THR E162 E163 M164 L165 S166 N167 Q168 M169 L170 S171 G172 D177 L178 G179 I180 D181 A182 K183

I184 K185 N186 I187 I188 S189 T190 E191 D192 A193 K194 A195 R196 L197 L198 A199 E200 Q201 Q202 N203 K204 K205 K206 D207 SER GLU THR SER PHE VAL PRO THR ASN MET ALA VAL ASN TYR VAL GLN HIS ASN ARG PHE TYR HIS GLU GLU LEU ASN ALA PRO ILE ARG ARG ASN LYS GLU GLU PRO

LYS ALA ARG PRO LEU ARG VAL GLY ASP THR GLU LYS PRO GLU PRO GLU ARG SER PRO PRO ASN ARG LYS ARG PRO ALA ASN GLU LYS ALA THR D275 D276 Y277 H278 Y279 E280 K281 F282 K283 K284 M285 N286 R287 R288 Y289

- Molecule 52: Peptidyl-prolyl cis-trans isomerase E

Chain y: 26% 26% 74%

MET ALA THR THR K5 R6 V7 L8 Y9 V10 G11 G12 L13 A14 E15 E16 V17 D18 D19 K20 V21 L22 H23 A24 A25 F26 I27 P28 F29 G30 D31 I32 T33 D34 I35 Q36 I37 P38 L39 D40 Y41 E42 T43 E44 K45 H46 R47 G48 F49 A50 F51 V52 E53 F54 E55 L56 A57 E58 D59 A60

A61 A62 A63 I64 D65 N66 M67 N68 E69 S70 E71 L72 F73 G74 R75 T76 I77 R78 V79 M80 L81 A82 K83 PRO MET ARG ILE LYS GLU GLY SER SER ARG PRO VAL TRP SER ASP ASP ASP TRP LEU LYS LYS PHE SER GLY LYS THR LEU GLU GLU ASN LYS GLU GLU GLU GLY SER GLU

PRO PRO LYS ALA GLU THR GLN GLU GLY GLU PRO ILE ALA LYS LYS ALA ARG SER ASN PRO GLN VAL TYR MET ASP ILE LYS ILE GLY ASN LYS PRO ALA GLY ARG ILE GLN MET LEU LEU ARG SER ASP VAL VAL PRO MET THR ALA GLU ASN PHE ARG CYS LEU CYS THR HIS GLU LYS

GLY PHE GLY PHE LYS GLY SER SER PHE HIS ARG ILE ILE PRO GLN PHE MET CYS GLN GLY GLY ASP PHE THR ASN HIS ASN GLY THR GLY GLY LYS SER ILE TYR GLY LYS LYS PHE ASP GLU ASN PHE ILE LEU LYS HIS THR GLY PRO GLY LEU LEU SER MET ALA ASN SER GLY

PRO ASN THR ASN GLY SER GLN PHE PHE LEU THR CYS ASP LYS THR ASP TRP LEU ASP GLY LYS HIS VAL VAL PHE GLY GLU VAL THR GLU GLY LEU ASP VAL LEU LEU ARG GLN ILE GLU ALA GLN GLY SER LYS ASP GLY LYS PRO LYS GLN LYS VAL ILE ILE ALA ASP CYS GLY GLU TYR

VAL

- Molecule 53: NF-kappa-B-activating protein

Chain z: 10% 17% 83%

MET ALA PRO VAL SER GLY SER ARG SER PRO ASP ARG GLU ALA SER GLY SER GLY GLY ARG ARG ARG SER SER SER LYS SER PRO LYS PRO SER LYS SER ALA ARG SER PRO ARG GLY ARG ARG SER ARG SER HIS SER CYS SER ARG SER GLY ASP ARG ASN GLY LEU THR HIS GLN LEU

GLY GLY LEU SER GLN GLY SER ARG ASN GLN SER TYR ARG SER ARG SER ARG SER ARG SER ARG GLU ARG PRO SER ALA PRO ARG GLY ILE PRO PHE ALA SER ALA ARG SER PRO ARG GLY ARG ARG SER ARG SER HIS SER ARG PRO TYR GLY SER ASP LYS PRO TRP PRO SER LEU LEU ASP LYS

GLU ARG GLU GLU SER LEU ARG GLN LYS ARG LEU SER GLU ARG GLU ARG ILE GLY GLU LEU GLY ALA PRO GLU VAL TRP GLY LEU SER PRO LYS ASN PRO GLU PRO ASP SER ASP GLU HIS THR PRO VAL GLU ASP GLU GLU PRO LYS LYS SER THR THR SER ALA SER THR SER GLU GLU

GLU LYS LYS LYS SER SER ARG SER LYS GLU ARG SER LYS LYS ARG ARG LYS LYS LYS SER SER LYS ARG LYS HIS LYS LYS TYR SER GLU ASP SER ASP SER ASP SER GLU THR ASP SER SER ASP ASP ASN LYS ARG ARG ALA LYS LYS ALA LYS LYS LYS LYS GLU LYS

LYS LYS LYS HIS ARG SER LYS TYR LYS LYS LYS ARG SER LYS LYS SER ARG LYS GLU SER SER LYS GLU SER GLN GLU GLU PHE LEU GLU GLU ASN PRO TRP LYS ASP ARG THR LYS ALA GLU GLU PRO SER ASP LEU ILE GLY PRO GLU ALA PRO LYS THR LEU THR

SER GLN ASP ASP LYS PRO LEU ASN TYR GLY HIS ALA LEU LEU PRO GLY GLU GLY ALA ALA MET ALA GLU TYR VAL LYS ALA GLY K329 R330 R358 HIS ARG ARG MET GLU ALA VAL ARG LEU ARG LYS GLU ASN GLN ILE TYR SER A376 D377 E378 K379 R380 A381 L382 A383 S384 F385 N386

Q387 E388 E389 R390 R391 K392 R393 E394 N395 K396 I397 L398 A399 S400 F401 R402 E403 M404 V405 Y406 R407 K408 T409 K410 G411 K412 D413 D414 K415

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103860	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 ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	492.00003, 492.00003, 492.00003	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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: GTP, IHP, SEP, ZN, MG, K, ATP

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	1	0.38	0/1030	0.74	1/1371 (0.1%)
2	2	0.73	1/2827 (0.0%)	1.40	46/4393 (1.0%)
3	3	0.28	0/406	0.43	0/564
4	32	0.37	0/513	0.66	0/683
5	5	1.01	2/2157 (0.1%)	1.78	82/3351 (2.4%)
6	50	0.37	0/1122	0.86	3/1562 (0.2%)
7	56	0.28	0/497	0.57	0/690
8	6	1.06	2/2323 (0.1%)	1.44	36/3619 (1.0%)
9	7	0.31	0/1927	0.65	1/2681 (0.0%)
10	8	0.29	0/444	0.67	0/614
11	9	0.31	0/711	0.62	0/987
12	A	0.61	1/18250 (0.0%)	0.71	9/24798 (0.0%)
13	B	0.36	0/15311	0.76	17/20733 (0.1%)
14	C	0.58	0/7228	0.87	15/9822 (0.2%)
15	D	0.30	0/356	0.52	0/494
16	E	0.45	1/2424 (0.0%)	0.75	4/3285 (0.1%)
17	EX	1.43	0/329	2.62	36/510 (7.1%)
18	F	0.46	0/1134	0.69	1/1530 (0.1%)
19	H	0.40	0/2965	0.65	1/4049 (0.0%)
20	I	0.31	0/3609	0.57	0/5036
21	IN	0.73	0/996	1.71	36/1544 (2.3%)
22	J	0.34	1/2997 (0.0%)	0.63	0/4187
23	K	0.31	0/940	0.53	0/1312
24	L	0.41	0/3674	0.64	1/4988 (0.0%)
25	M	0.29	0/1114	0.53	0/1553
26	N	0.58	1/1215 (0.1%)	0.75	1/1627 (0.1%)
27	NO	0.31	0/861	0.58	0/1197
28	O	0.50	0/2375	0.67	0/3204
29	P	0.47	0/903	0.70	0/1201
30	Q	0.30	0/6545	0.57	0/9115
31	R	0.48	1/2647 (0.0%)	0.73	4/3554 (0.1%)
32	S	0.38	0/1305	0.65	0/1767

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	SR	0.60	2/414 (0.5%)	0.56	0/568
34	T	0.70	1/2957 (0.0%)	0.77	1/4023 (0.0%)
35	U	0.50	0/2483	0.68	0/3341
36	V	0.30	0/3626	0.58	0/5050
37	W	0.53	1/4266 (0.0%)	0.71	4/5761 (0.1%)
38	X	0.28	0/326	0.49	0/452
39	Z	0.28	0/263	0.53	0/365
40	a	0.34	0/666	0.68	0/897
40	h	0.36	0/660	0.68	0/889
41	b	0.31	0/663	0.65	0/885
41	i	0.31	0/674	0.61	0/899
42	c	0.29	0/642	0.59	0/867
42	j	0.28	0/642	0.60	0/867
43	d	0.29	0/732	0.66	0/984
43	k	0.32	0/784	0.64	0/1053
44	e	0.28	0/659	0.67	0/885
44	l	0.31	0/677	0.68	0/908
45	f	0.35	0/574	0.74	1/775 (0.1%)
45	m	0.34	0/574	0.65	0/775
46	g	0.34	0/575	0.72	2/768 (0.3%)
46	n	0.32	0/575	0.66	0/768
47	o	0.30	0/1299	0.71	1/1761 (0.1%)
48	p	0.30	0/759	0.57	0/1016
49	q	0.30	0/512	0.48	0/713
49	r	0.35	0/592	0.56	0/825
49	s	0.36	0/658	0.58	0/919
49	t	0.32	0/512	0.54	0/713
50	w	0.30	0/2602	0.65	0/3615
51	x	0.30	0/632	0.50	0/874
52	y	0.28	0/317	0.62	0/396
53	z	0.37	0/431	0.56	0/582
All	All	0.50	14/122881 (0.0%)	0.80	303/169215 (0.2%)

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
12	A	0	2
13	B	0	20
14	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	E	0	1
29	P	0	1
31	R	0	2
All	All	0	29

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	58	PRO	C-N	8.75	1.54	1.34
37	W	307	CYS	CB-SG	-7.03	1.70	1.82
34	T	220	VAL	CB-CG2	-6.66	1.38	1.52
8	6	58	G	N7-C5	-6.19	1.35	1.39
5	5	57	G	C2-N3	-5.78	1.28	1.32

The worst 5 of 303 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	IN	98	U	O4'-C1'-N1	14.52	119.82	108.20
17	EX	-2	C	O4'-C1'-N1	14.41	119.73	108.20
5	5	24	G	O4'-C1'-N9	-12.84	97.93	108.20
5	5	86	C	N1-C2-O2	12.79	126.57	118.90
2	2	50	C	N1-C2-O2	11.92	126.05	118.90

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	1418	ARG	Sidechain
12	A	941	LYS	Peptide
13	B	129	ARG	Sidechain
13	B	728	ARG	Sidechain
13	B	739	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	1	1013	0	1058	9	0
2	2	2535	0	1281	19	0
3	3	408	0	181	0	0
4	32	504	0	509	11	0
5	5	1936	0	982	22	0
6	50	1124	0	485	22	0
7	56	498	0	220	0	0
8	6	2075	0	1048	28	0
9	7	1928	0	855	0	0
10	8	445	0	203	0	0
11	9	712	0	299	0	0
12	A	17802	0	17006	233	0
13	B	15004	0	15162	103	0
14	C	7069	0	7089	32	0
15	D	358	0	167	0	0
16	E	2370	0	2306	43	0
17	EX	296	0	153	2	0
18	F	1089	0	1023	25	0
19	H	2932	0	2204	17	0
20	I	3610	0	1639	0	0
21	IN	893	0	453	13	0
22	J	2998	0	1333	3	0
23	K	941	0	424	0	0
24	L	3642	0	2904	31	0
25	M	1115	0	513	0	0
26	N	1189	0	1192	17	0
27	NO	864	0	371	1	0
28	O	2327	0	2315	41	0
29	P	889	0	865	9	0
30	Q	6554	0	2828	1	0
31	R	2618	0	2663	35	0
32	S	1271	0	1244	18	0
33	SR	412	0	287	6	0
34	T	2881	0	2836	41	0
35	U	2425	0	2370	38	0
36	V	3629	0	1603	0	0
37	W	4158	0	4060	78	0
38	X	328	0	156	1	0
39	Z	265	0	114	1	0
40	a	658	0	675	0	0
40	h	652	0	670	0	0
41	b	654	0	667	0	0
41	i	664	0	690	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	c	634	0	680	0	0
42	j	634	0	680	0	0
43	d	723	0	750	0	0
43	k	774	0	802	0	0
44	e	651	0	671	0	0
44	l	669	0	692	0	0
45	f	562	0	574	0	0
45	m	562	0	574	0	0
46	g	568	0	590	0	0
46	n	568	0	590	0	0
47	o	1282	0	1305	0	0
48	p	745	0	767	0	0
49	q	514	0	236	0	0
49	r	594	0	270	0	0
49	s	659	0	299	0	0
49	t	514	0	236	0	0
50	w	2605	0	1124	0	0
51	x	636	0	276	0	0
52	y	318	0	88	0	0
53	z	430	0	321	0	0
54	6	5	0	0	0	0
54	7	1	0	0	0	0
55	6	1	0	0	0	0
56	7	31	0	12	0	0
57	C	32	0	12	0	0
58	N	3	0	0	0	0
58	O	3	0	0	0	0
59	U	36	0	6	1	0
All	All	120489	0	96658	760	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 760 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)
6:50:336:TYR:O	18:F:667:ASN:HB2	1.14	1.30
28:O:144:SER:OG	28:O:147:LEU:HB2	1.42	1.17
6:50:336:TYR:O	18:F:667:ASN:CB	2.07	1.01
6:50:294:ALA:HA	18:F:663:TYR:OH	1.62	0.99
6:50:293:ASP:O	12:A:2001:SER:OG	1.81	0.98

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	1	121/184 (66%)	114 (94%)	6 (5%)	1 (1%)	16	46
3	3	78/476 (16%)	78 (100%)	0	0	100	100
4	32	58/112 (52%)	56 (97%)	2 (3%)	0	100	100
6	50	222/339 (66%)	214 (96%)	6 (3%)	2 (1%)	14	44
7	56	99/222 (45%)	98 (99%)	1 (1%)	0	100	100
9	7	388/411 (94%)	377 (97%)	10 (3%)	1 (0%)	37	66
10	8	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	12	40
11	9	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
12	A	2244/2335 (96%)	2107 (94%)	134 (6%)	3 (0%)	48	76
13	B	1856/2136 (87%)	1785 (96%)	68 (4%)	3 (0%)	44	71
14	C	892/972 (92%)	816 (92%)	72 (8%)	4 (0%)	30	61
15	D	68/285 (24%)	67 (98%)	1 (2%)	0	100	100
16	E	301/357 (84%)	281 (93%)	20 (7%)	0	100	100
18	F	120/758 (16%)	109 (91%)	11 (9%)	0	100	100
19	H	455/908 (50%)	439 (96%)	15 (3%)	1 (0%)	44	71
20	I	725/855 (85%)	710 (98%)	15 (2%)	0	100	100
22	J	600/848 (71%)	572 (95%)	26 (4%)	2 (0%)	37	66
23	K	187/225 (83%)	174 (93%)	12 (6%)	1 (0%)	25	56
24	L	545/802 (68%)	524 (96%)	20 (4%)	1 (0%)	44	71
25	M	222/243 (91%)	215 (97%)	6 (3%)	1 (0%)	25	56
26	N	142/144 (99%)	131 (92%)	9 (6%)	2 (1%)	9	34
27	NO	168/301 (56%)	158 (94%)	8 (5%)	2 (1%)	11	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	O	287/420 (68%)	271 (94%)	16 (6%)	0	100	100
29	P	100/229 (44%)	94 (94%)	6 (6%)	0	100	100
30	Q	1304/1485 (88%)	1267 (97%)	34 (3%)	3 (0%)	44	71
31	R	322/536 (60%)	296 (92%)	25 (8%)	1 (0%)	37	66
32	S	162/166 (98%)	148 (91%)	14 (9%)	0	100	100
33	SR	66/2752 (2%)	59 (89%)	7 (11%)	0	100	100
34	T	359/514 (70%)	340 (95%)	16 (4%)	3 (1%)	16	46
35	U	291/586 (50%)	272 (94%)	18 (6%)	1 (0%)	37	66
36	V	727/1220 (60%)	708 (97%)	18 (2%)	1 (0%)	48	76
37	W	511/579 (88%)	462 (90%)	49 (10%)	0	100	100
38	X	62/451 (14%)	59 (95%)	3 (5%)	0	100	100
39	Z	49/166 (30%)	49 (100%)	0	0	100	100
40	a	82/126 (65%)	77 (94%)	5 (6%)	0	100	100
40	h	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
41	b	81/240 (34%)	80 (99%)	1 (1%)	0	100	100
41	i	80/240 (33%)	74 (92%)	6 (8%)	0	100	100
42	c	78/119 (66%)	73 (94%)	5 (6%)	0	100	100
42	j	78/119 (66%)	76 (97%)	2 (3%)	0	100	100
43	d	85/118 (72%)	82 (96%)	3 (4%)	0	100	100
43	k	91/118 (77%)	88 (97%)	3 (3%)	0	100	100
44	e	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
44	l	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
45	f	70/86 (81%)	70 (100%)	0	0	100	100
45	m	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
46	g	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
46	n	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
47	o	160/255 (63%)	146 (91%)	14 (9%)	0	100	100
48	p	90/225 (40%)	88 (98%)	2 (2%)	0	100	100
49	q	99/504 (20%)	98 (99%)	1 (1%)	0	100	100
49	r	115/504 (23%)	111 (96%)	4 (4%)	0	100	100
49	s	130/504 (26%)	125 (96%)	4 (3%)	1 (1%)	16	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	t	99/504 (20%)	96 (97%)	2 (2%)	1 (1%)	13	42
50	w	522/646 (81%)	504 (97%)	18 (3%)	0	100	100
51	x	120/289 (42%)	118 (98%)	2 (2%)	0	100	100
52	y	77/301 (26%)	75 (97%)	2 (3%)	0	100	100
53	z	66/415 (16%)	64 (97%)	1 (2%)	1 (2%)	8	33
All	All	16534/28198 (59%)	15754 (95%)	743 (4%)	37 (0%)	45	71

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	50	285	HIS
13	B	1584	ILE
30	Q	1078	LEU
49	s	65	PRO
9	7	340	GLY

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	
1	1	106/157 (68%)	105 (99%)	1 (1%)	75	85
4	32	54/99 (54%)	53 (98%)	1 (2%)	52	72
12	A	1792/2108 (85%)	1783 (100%)	9 (0%)	86	91
13	B	1668/1908 (87%)	1514 (91%)	154 (9%)	7	26
14	C	794/866 (92%)	767 (97%)	27 (3%)	32	59
16	E	259/300 (86%)	258 (100%)	1 (0%)	89	93
18	F	111/655 (17%)	110 (99%)	1 (1%)	75	85
19	H	182/838 (22%)	180 (99%)	2 (1%)	70	82
24	L	233/709 (33%)	232 (100%)	1 (0%)	89	93
26	N	130/130 (100%)	129 (99%)	1 (1%)	79	87
28	O	258/361 (72%)	257 (100%)	1 (0%)	89	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	P	94/203 (46%)	94 (100%)	0	100	100
31	R	275/457 (60%)	274 (100%)	1 (0%)	89	93
32	S	133/134 (99%)	132 (99%)	1 (1%)	79	87
33	SR	21/2432 (1%)	20 (95%)	1 (5%)	21	50
34	T	316/441 (72%)	312 (99%)	4 (1%)	65	79
35	U	258/520 (50%)	253 (98%)	5 (2%)	52	72
37	W	451/502 (90%)	445 (99%)	6 (1%)	65	79
40	a	74/101 (73%)	74 (100%)	0	100	100
40	h	73/101 (72%)	73 (100%)	0	100	100
41	b	68/177 (38%)	68 (100%)	0	100	100
41	i	75/177 (42%)	75 (100%)	0	100	100
42	c	75/101 (74%)	75 (100%)	0	100	100
42	j	75/101 (74%)	75 (100%)	0	100	100
43	d	85/110 (77%)	84 (99%)	1 (1%)	67	80
43	k	91/110 (83%)	91 (100%)	0	100	100
44	e	74/84 (88%)	74 (100%)	0	100	100
44	l	76/84 (90%)	76 (100%)	0	100	100
45	f	61/74 (82%)	60 (98%)	1 (2%)	58	76
45	m	61/74 (82%)	61 (100%)	0	100	100
46	g	63/66 (96%)	63 (100%)	0	100	100
46	n	63/66 (96%)	62 (98%)	1 (2%)	58	76
47	o	139/218 (64%)	138 (99%)	1 (1%)	81	88
48	p	81/195 (42%)	81 (100%)	0	100	100
53	z	25/366 (7%)	25 (100%)	0	100	100
All	All	8394/15025 (56%)	8173 (97%)	221 (3%)	42	66

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	B	1443	LYS
13	B	1969	GLU
46	n	43	ASP
31	R	315	LYS
13	B	1477	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
34	T	216	ASN
37	W	250	GLN
34	T	417	ASN
35	U	122	ASN
40	a	42	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	EX	14/14 (100%)	5 (35%)	1 (7%)
2	2	117/187 (62%)	30 (25%)	5 (4%)
21	IN	39/113 (34%)	19 (48%)	3 (7%)
5	5	90/116 (77%)	23 (25%)	2 (2%)
8	6	96/106 (90%)	37 (38%)	5 (5%)
All	All	356/536 (66%)	114 (32%)	16 (4%)

5 of 114 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	16	U
2	2	17	U
2	2	19	G
2	2	20	G
2	2	24	A

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	IN	95	U
21	IN	90	C
8	6	33	G
17	EX	-12	G
8	6	5	U

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
31	SEP	R	224	31	8,9,10	1.46	1 (12%)	8,12,14	1.87	1 (12%)
31	SEP	R	232	31	8,9,10	1.57	1 (12%)	8,12,14	1.38	1 (12%)

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
31	SEP	R	224	31	-	1/5/8/10	-
31	SEP	R	232	31	-	3/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	232	SEP	P-O1P	3.37	1.61	1.50
31	R	224	SEP	P-O1P	3.07	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	224	SEP	P-OG-CB	-4.76	105.18	118.30
31	R	232	SEP	P-OG-CB	-2.75	110.73	118.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	R	232	SEP	CB-OG-P-O1P
31	R	232	SEP	CB-OG-P-O2P
31	R	232	SEP	CB-OG-P-O3P
31	R	224	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 13 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	$\#\|Z\| > 2$
57	GTP	C	1500	-	26,34,34	1.43	2 (7%)	32,54,54	1.68	8 (25%)
56	ATP	7	501	54	26,33,33	0.63	0	31,52,52	1.06	2 (6%)
59	IHP	U	601	-	36,36,36	1.34	6 (16%)	54,60,60	0.95	3 (5%)

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
57	GTP	C	1500	-	-	0/18/38/38	0/3/3/3
56	ATP	7	501	54	-	0/18/38/38	0/3/3/3
59	IHP	U	601	-	-	6/30/54/54	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)
57	C	1500	GTP	C5-C6	-4.99	1.37	1.47
59	U	601	IHP	P3-O13	2.68	1.64	1.59
59	U	601	IHP	P6-O16	2.57	1.64	1.59
59	U	601	IHP	P2-O12	2.35	1.63	1.59
57	C	1500	GTP	C5-C4	-2.31	1.37	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	C	1500	GTP	C5-C6-N1	3.65	120.40	113.95
57	C	1500	GTP	PA-O3A-PB	-3.43	121.06	132.83
57	C	1500	GTP	C2-N1-C6	-3.25	119.11	125.10
57	C	1500	GTP	C8-N7-C5	3.07	108.84	102.99
59	U	601	IHP	C6-C1-C2	-3.04	103.75	110.41

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	U	601	IHP	C2-O12-P2-O42
59	U	601	IHP	C5-O15-P5-O25
59	U	601	IHP	C6-O16-P6-O26
59	U	601	IHP	C1-O11-P1-O31
59	U	601	IHP	C1-O11-P1-O41

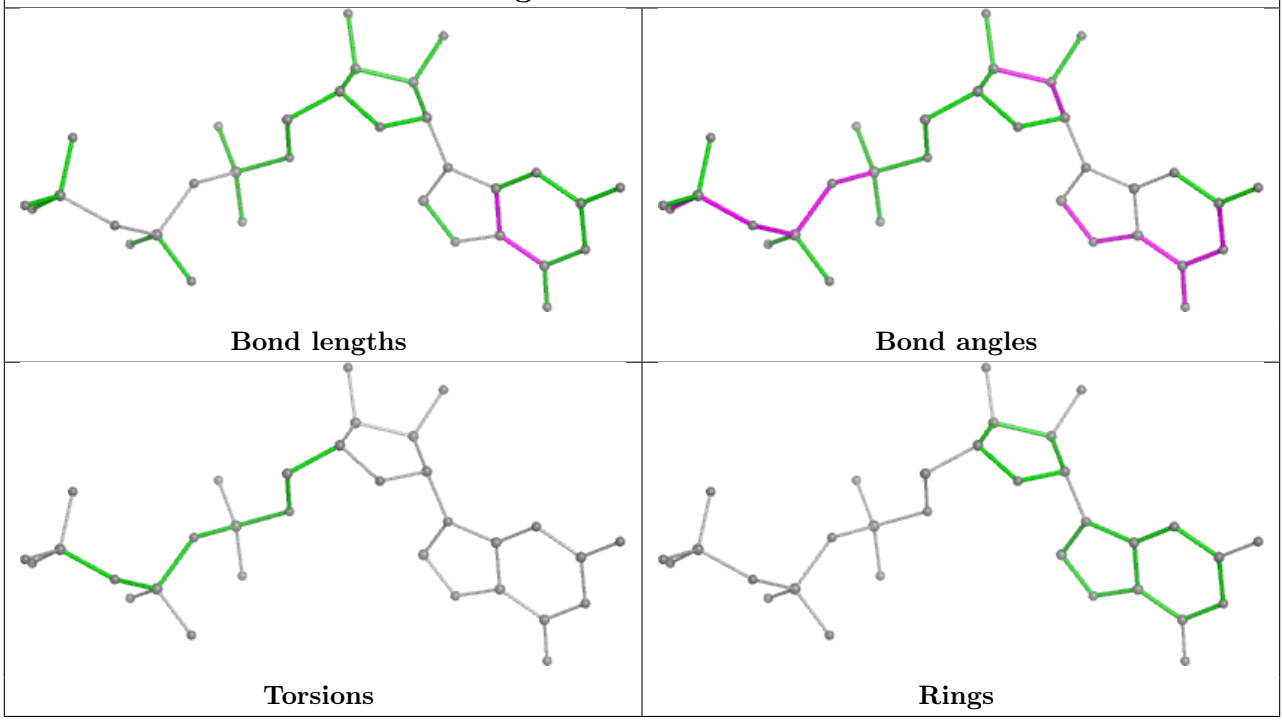
There are no ring outliers.

1 monomer is involved in 1 short contact:

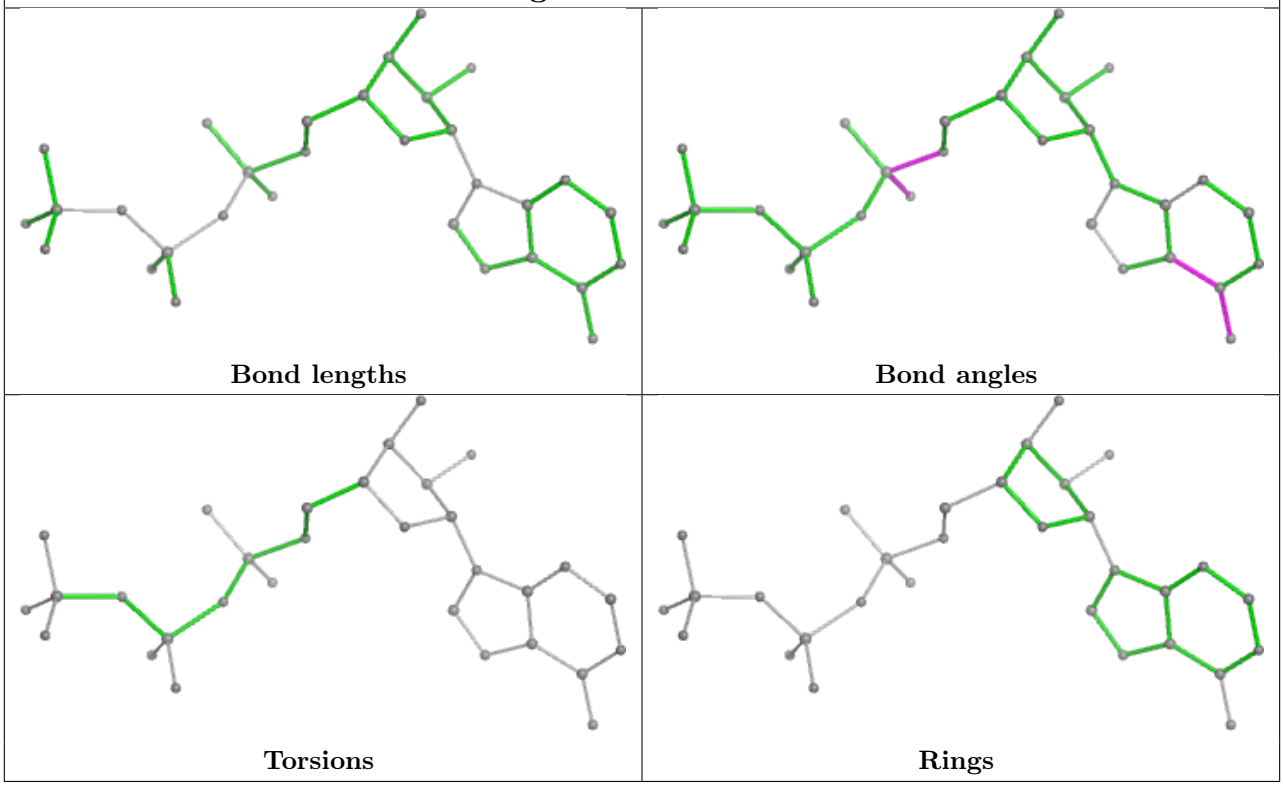
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	U	601	IHP	1	0

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

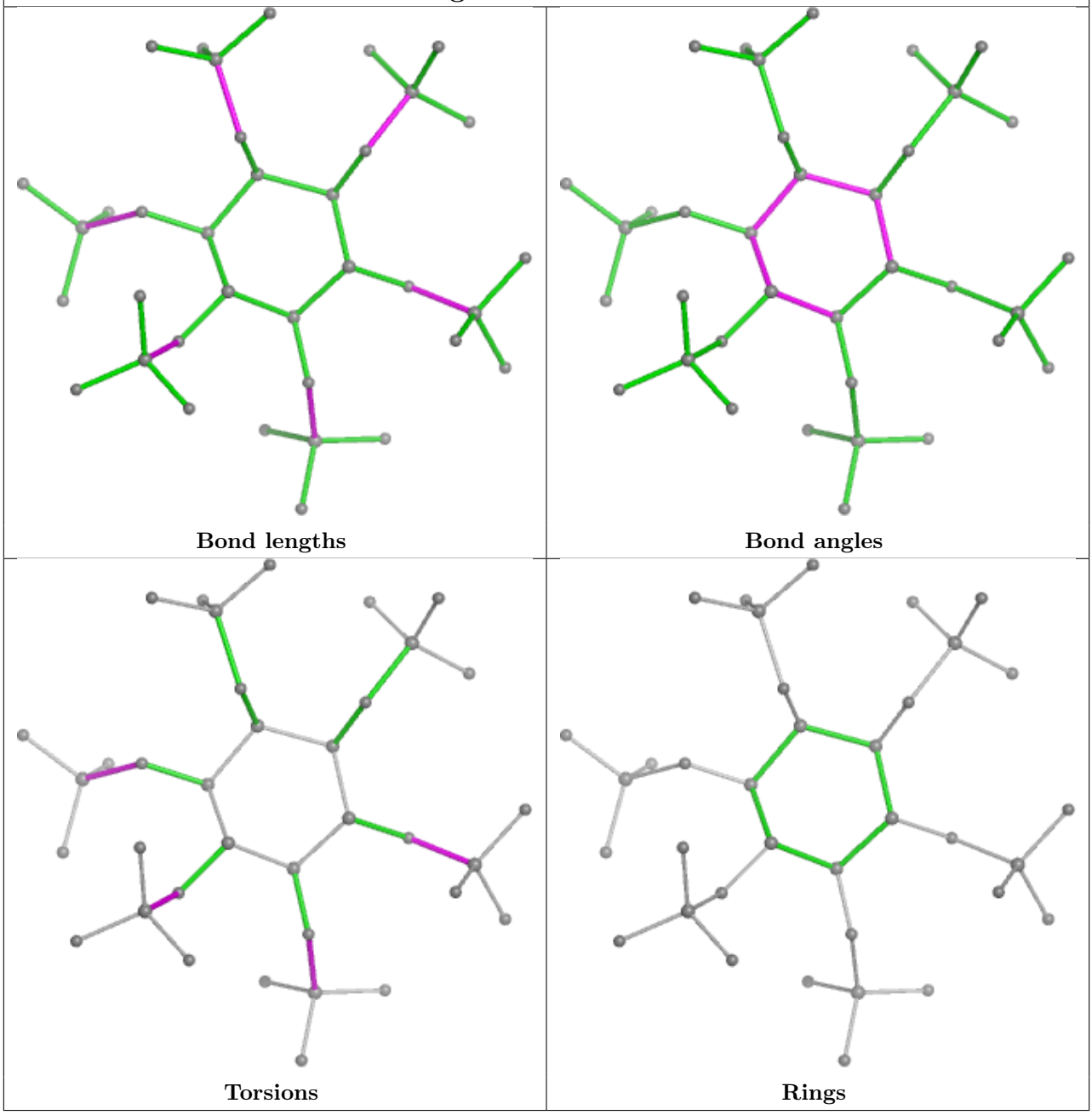
Ligand GTP C 1500



Ligand ATP 7 501



Ligand IHP U 601



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.

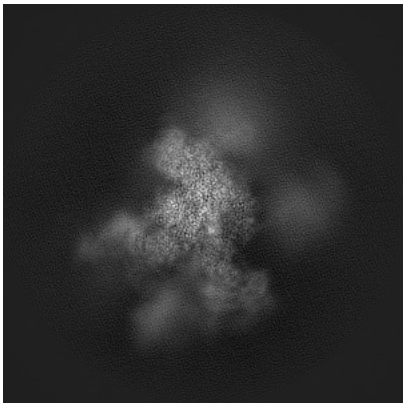
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4525. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



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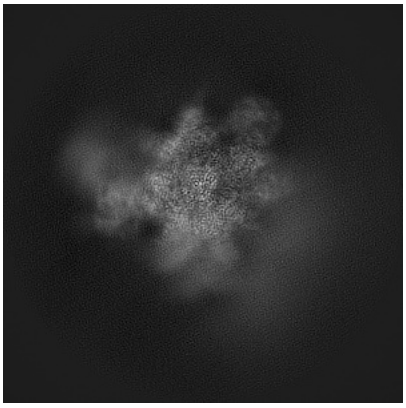
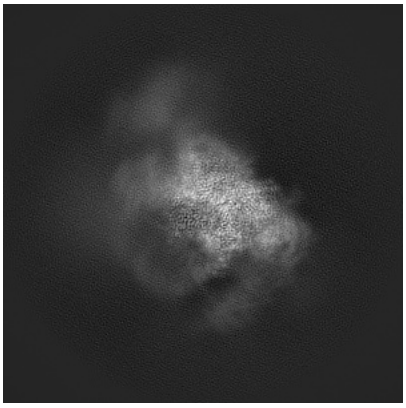


Y

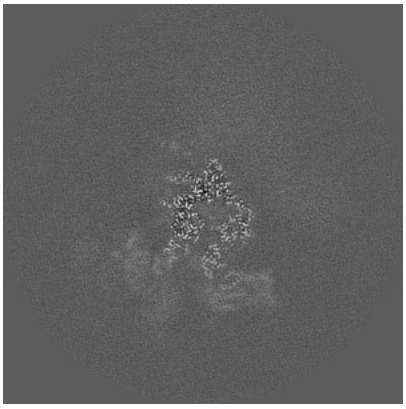


Z

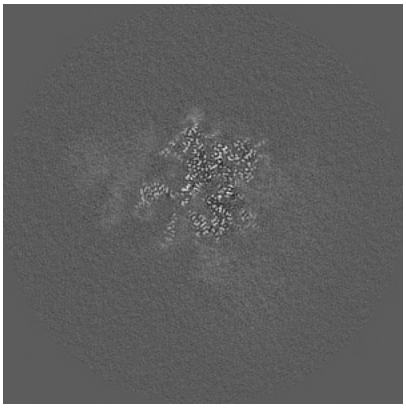
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

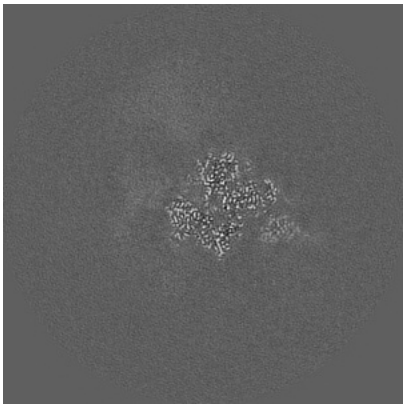
6.2.1 Primary map



X Index: 205



Y Index: 205

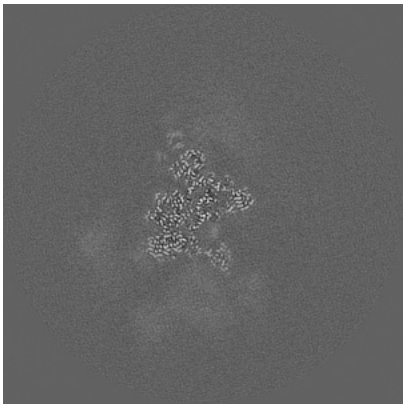


Z Index: 205

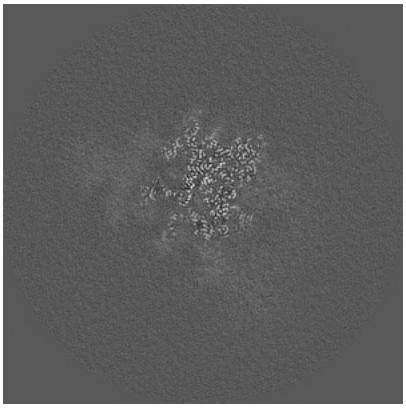
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

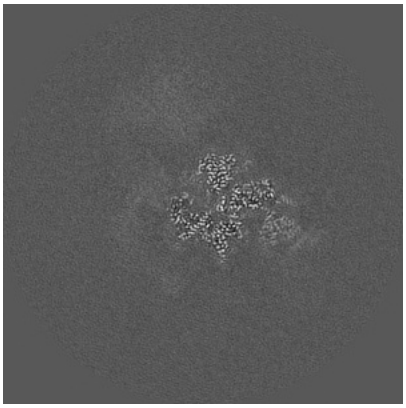
6.3.1 Primary map



X Index: 231



Y Index: 203

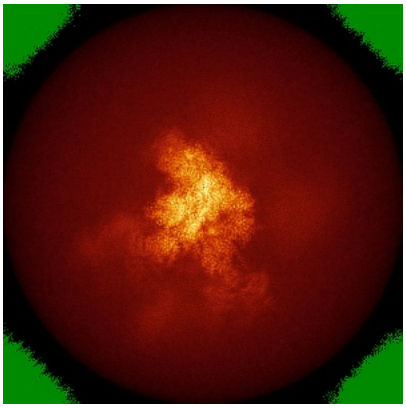


Z Index: 202

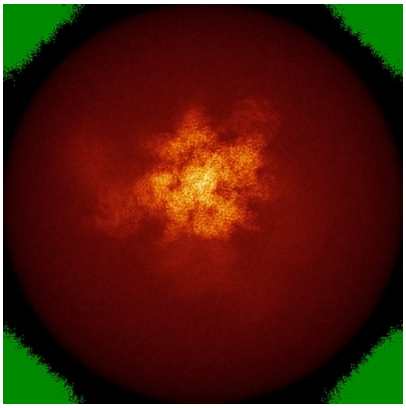
The images above show the largest variance slices of the map in three orthogonal directions.

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

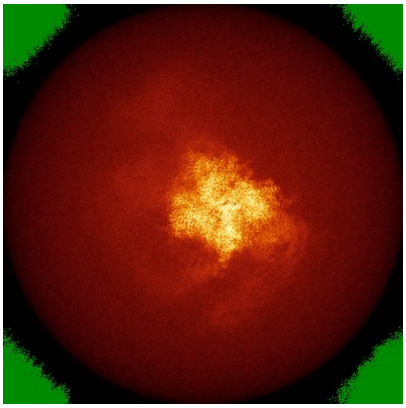
6.4.1 Primary map



X



Y

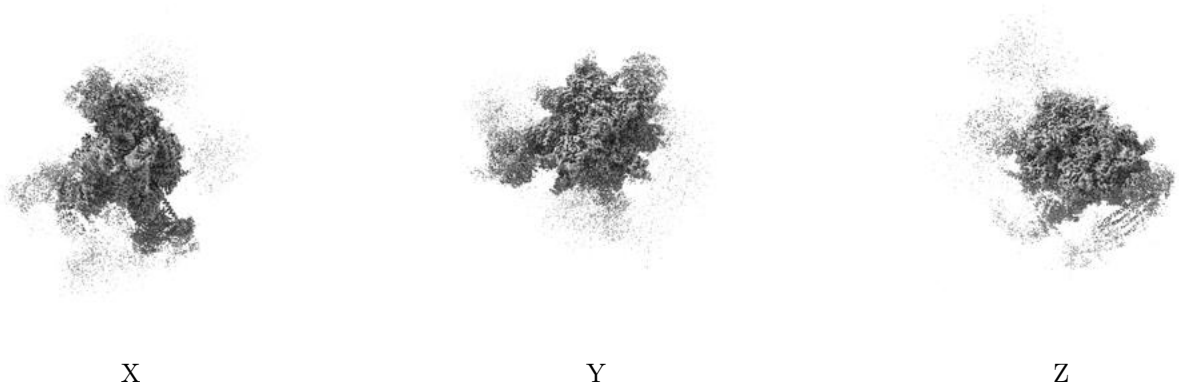


Z

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

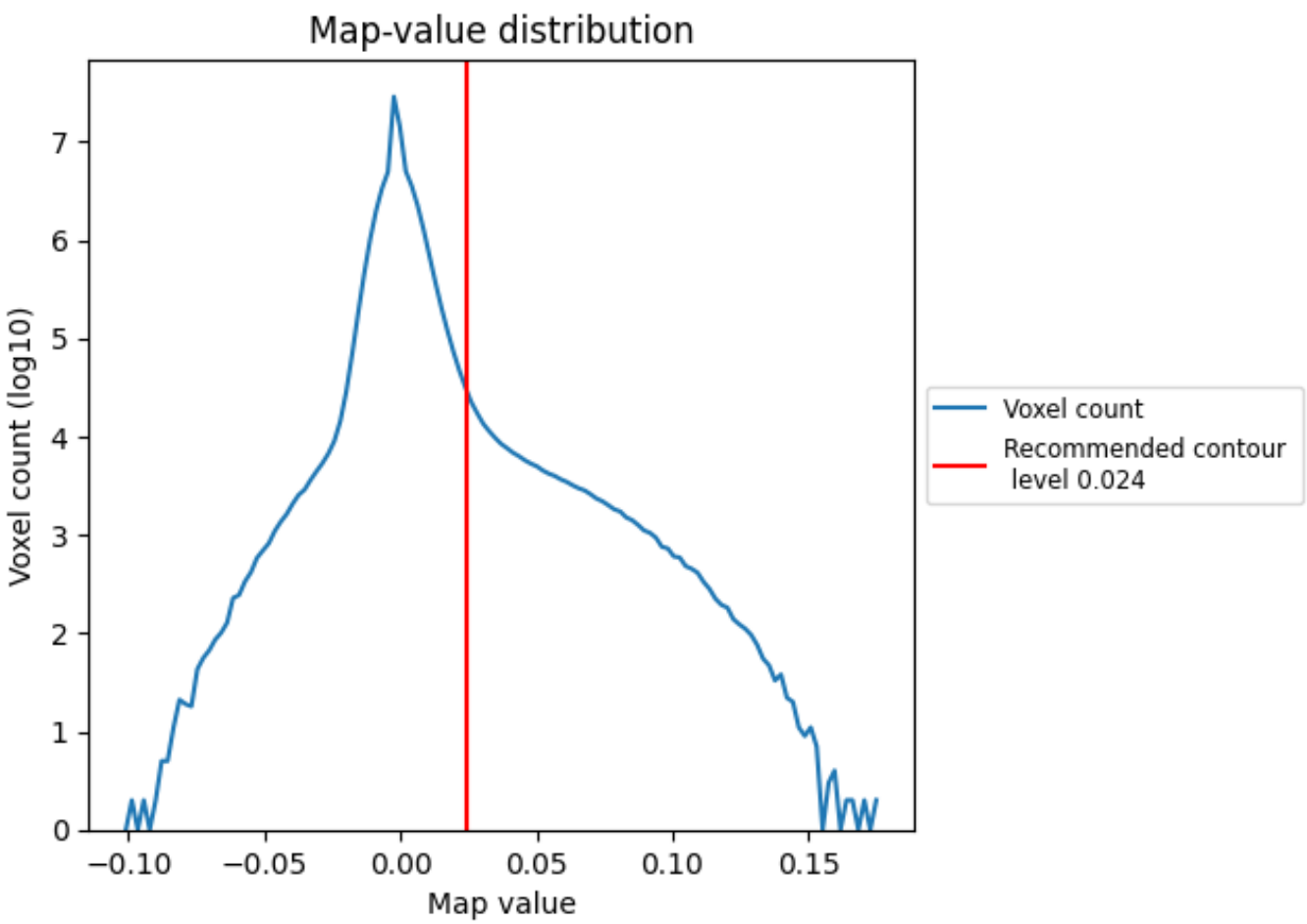
6.6 Mask visualisation (i)

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

7 Map analysis (i)

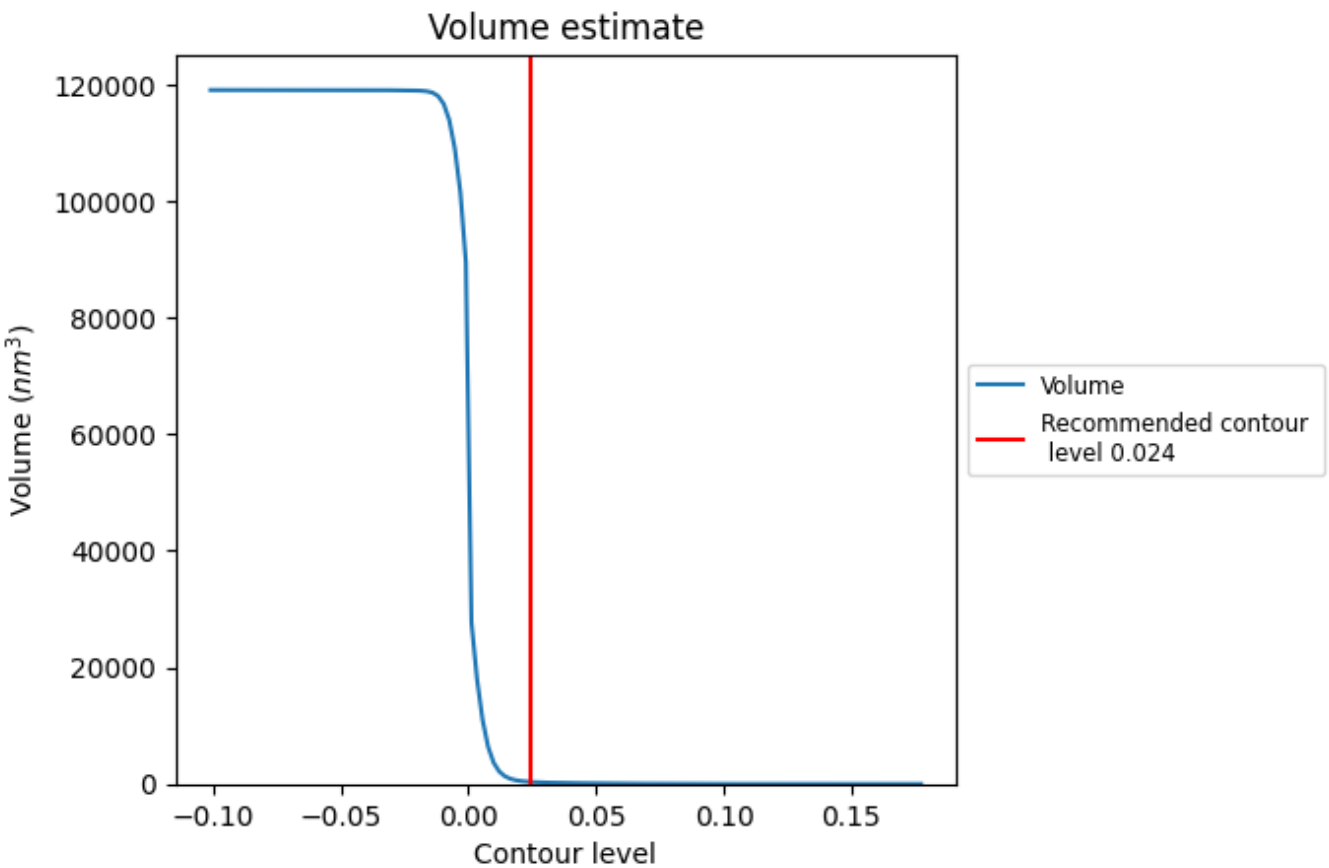
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

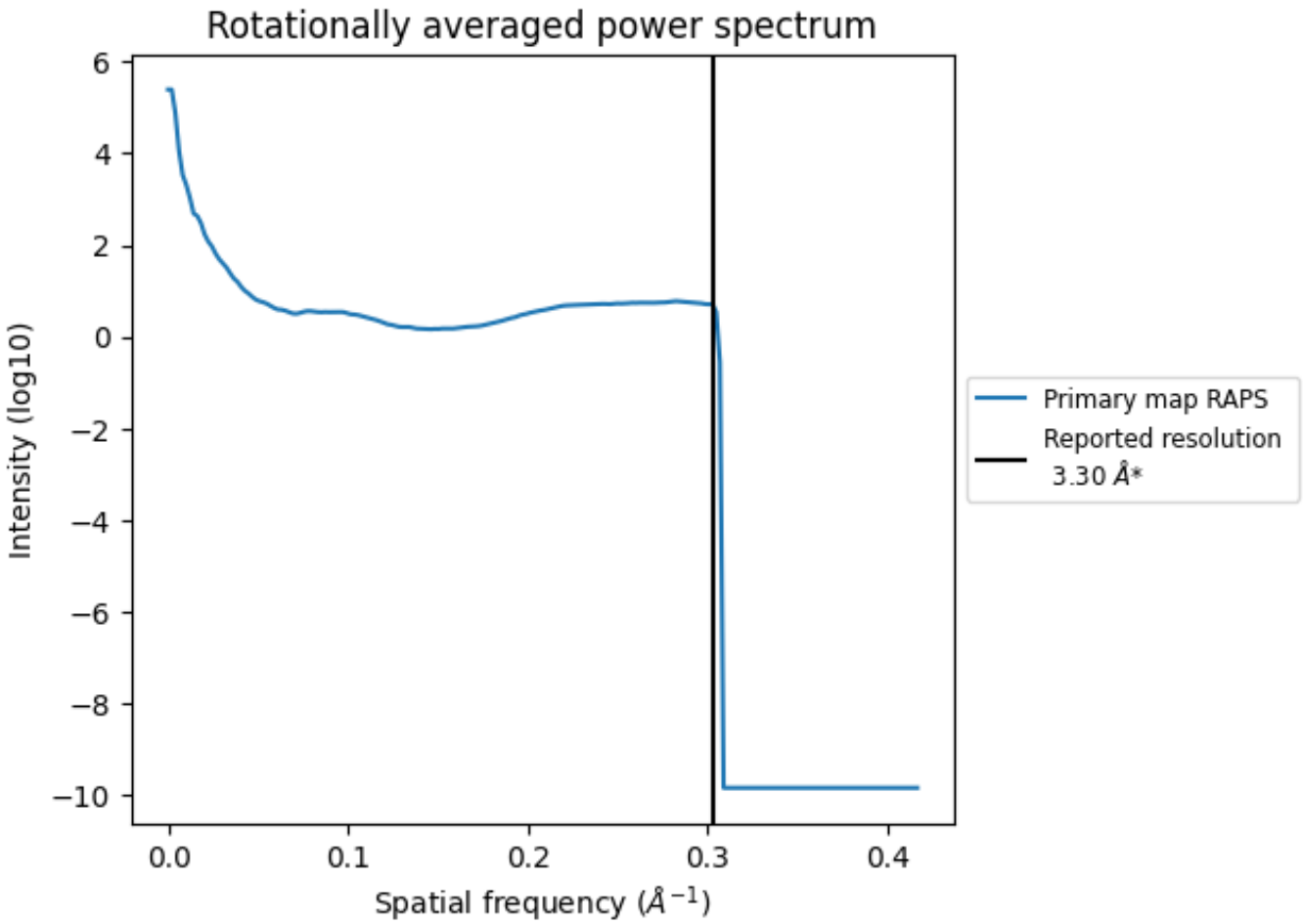
7.2 Volume estimate (i)



The volume at the recommended contour level is 356 nm^3; this corresponds to an approximate mass of 321 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)

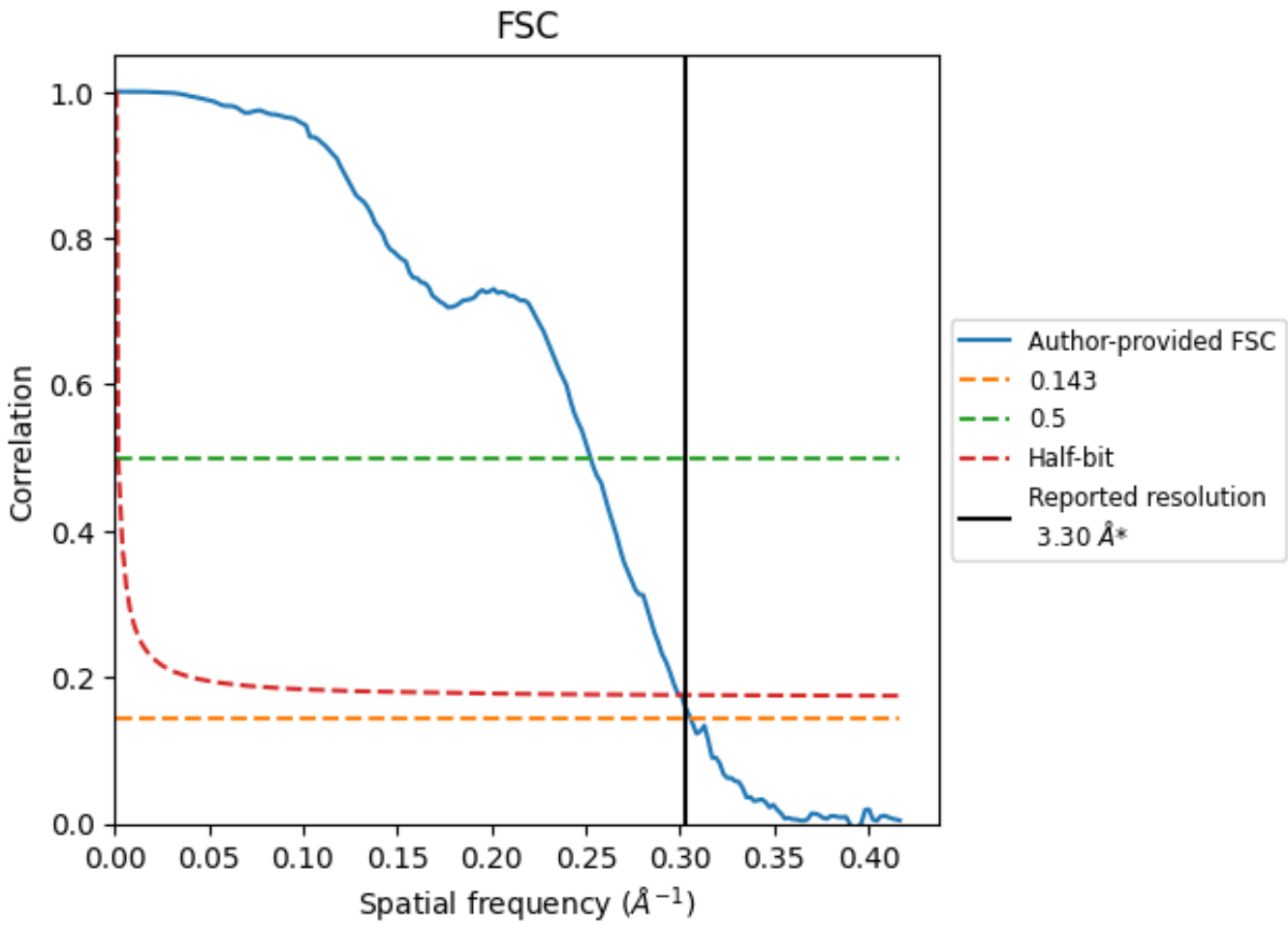


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

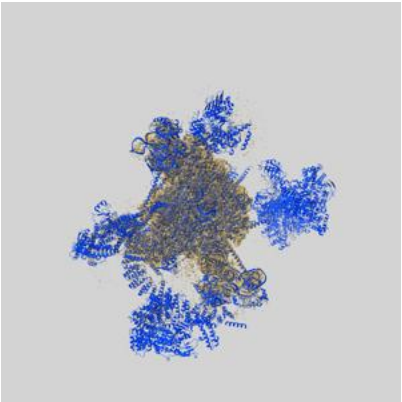
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.96	3.33
Unmasked-calculated*	-	-	-

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

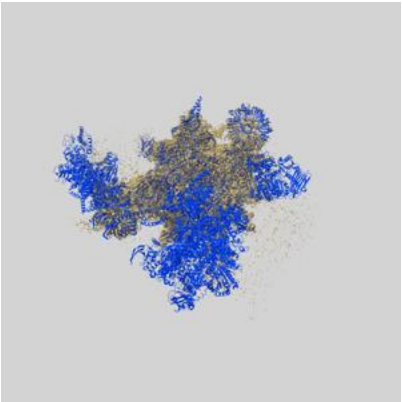
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4525 and PDB model 9FMD. Per-residue inclusion information can be found in section 3 on page 17.

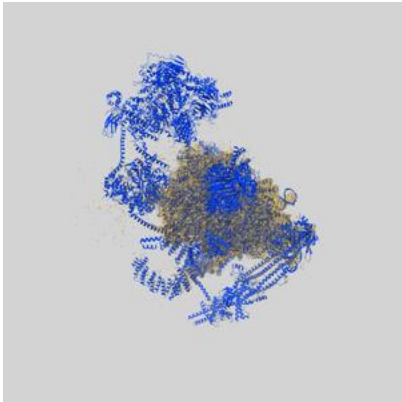
9.1 Map-model overlay (i)



X



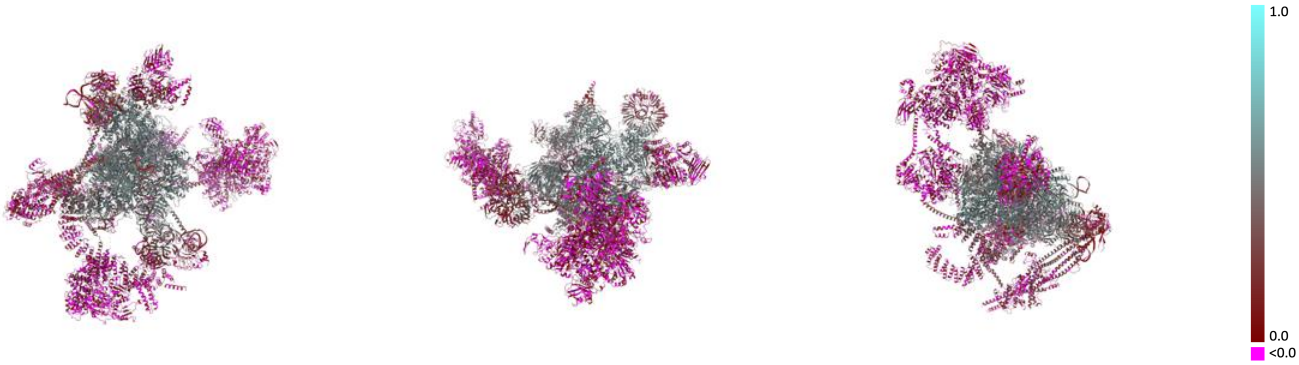
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024 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.

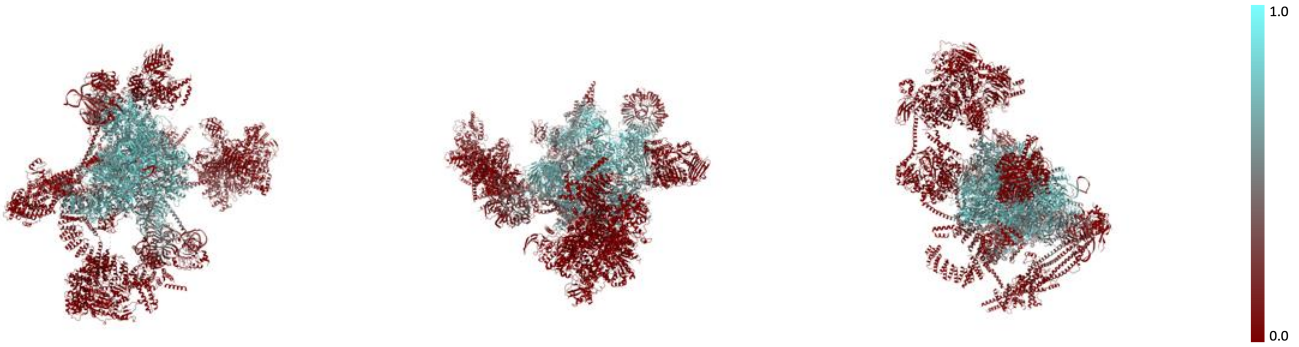
9.2 Q-score mapped to coordinate model (i)



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.

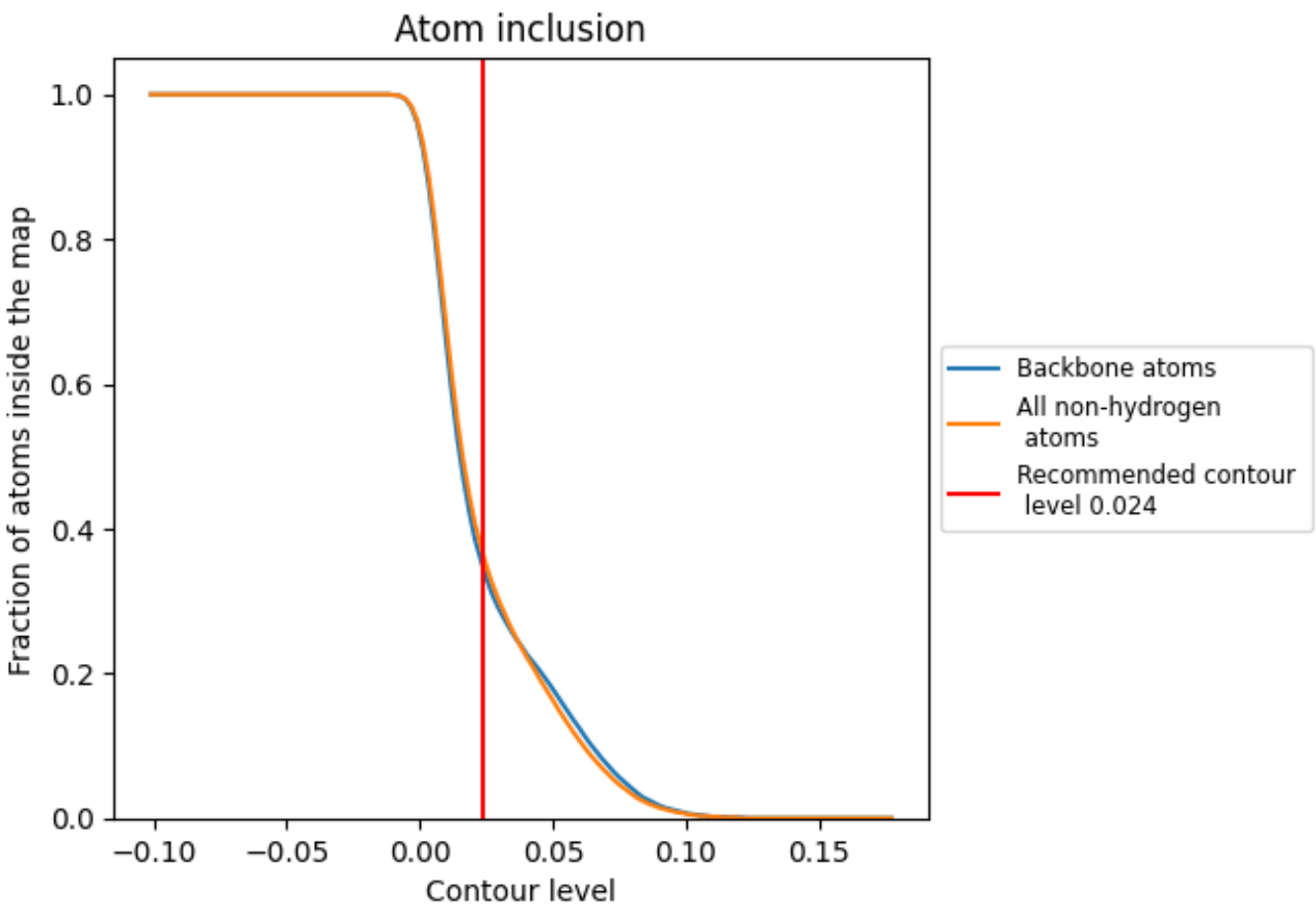
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.024).

9.4 Atom inclusion (i)



At the recommended contour level, 34% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3610	0.2970
1	0.4060	0.3790
2	0.4230	0.3010
3	0.1450	0.2540
32	0.5850	0.5090
5	0.6140	0.3800
50	0.0160	0.0940
56	0.0000	-0.0080
6	0.7320	0.4560
7	0.0070	0.1120
8	0.0000	0.0520
9	0.0000	0.0410
A	0.7230	0.5070
B	0.0010	0.0490
C	0.6930	0.4900
D	0.0000	0.0980
E	0.6300	0.4760
EX	0.8110	0.5290
F	0.6270	0.4680
H	0.4160	0.3540
I	0.0520	0.1010
IN	0.5690	0.3790
J	0.3950	0.2850
K	0.1140	0.1850
L	0.4040	0.3650
M	0.4950	0.3800
N	0.7540	0.5330
NO	0.0010	0.1280
O	0.5190	0.4460
P	0.6500	0.5200
Q	0.0020	0.0540
R	0.5290	0.4400
S	0.5720	0.4560
SR	0.4090	0.3340
T	0.7370	0.5080

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Chain	Atom inclusion	Q-score
U	0.5840	0.4550
V	0.0500	0.0800
W	0.6700	0.5010
X	0.0150	0.1510
Z	0.0150	0.0570
a	0.4280	0.4140
b	0.3330	0.3340
c	0.1390	0.2060
d	0.0680	0.1490
e	0.0870	0.1940
f	0.0470	0.1550
g	0.2180	0.3330
h	0.3940	0.3510
i	0.2460	0.2900
j	0.1200	0.2020
k	0.0810	0.1590
l	0.2390	0.2770
m	0.1380	0.1770
n	0.3620	0.3680
o	0.0250	0.1130
p	0.0560	0.1370
q	0.0430	0.1160
r	0.0180	0.0870
s	0.0290	0.1440
t	0.0120	0.0880
w	0.0000	0.0340
x	0.0270	0.1330
y	0.0060	0.1250
z	0.3540	0.2970