wwPDB EM Validation Summary Report ⓘ

Nov 9, 2022 – 03:47 AM JST

PDB ID	:	6ID0
EMDB ID	:	EMD-9646
Title	:	Cryo-EM structure of a human intron lariat spliceosome prior to Prp43 loaded (ILS1 complex) at 2.9 angstrom resolution
Authors	:	Zhang, X.; Zhan, X.; Yan, C.; Shi, Y.
Deposited on	:	2018-09-07
Resolution	:	2.90 Å(reported)

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

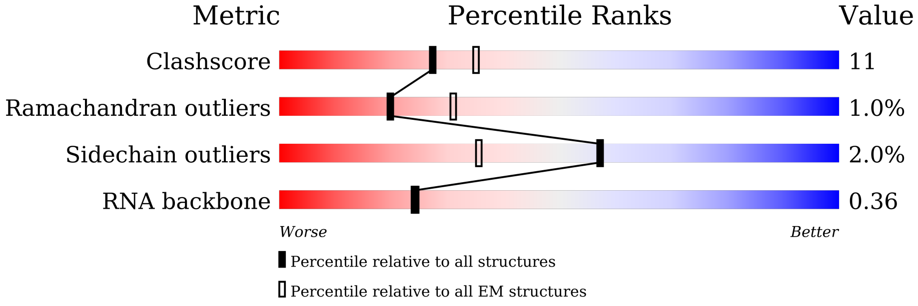
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

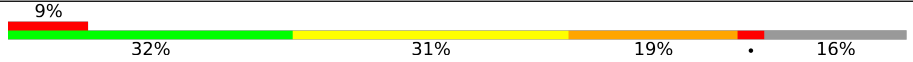
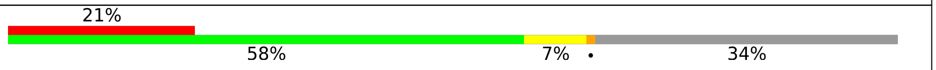
The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	2335	
2	B	117	
3	C	972	
4	E	357	
5	F	107	
6	J	848	
7	L	802	

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Mol	Chain	Length	Quality of chain
8	M	243	45% 8% 47%
9	N	144	• 85% 11% • •
10	O	420	5% 54% 14% 31%
11	P	229	• 44% 7% 48%
12	R	536	• 40% 10% • 49%
13	S	166	• 70% 25% • •
14	T	514	47% 13% • 38%
15	W	579	6% 72% 15% • 12%
16	G	272	7% • 7% 10% 6% 74%
17	H	188	37% 12% 25% 33% 5% 26%
18	U	894	• 29% 8% • 61%
19	I	855	30% 56% 10% • 34%
20	a	126	13% 64% 36%
20	h	126	35% 64% 36%
21	b	231	19% 37% 63%
21	i	231	23% 37% 63%
22	c	119	17% 69% 31%
22	j	119	48% 69% 31%
23	d	118	22% 81% • 18%
23	k	118	53% 71% • 28%
24	f	86	40% 86% 14%
24	m	86	64% 86% 14%
25	e	92	43% 86% 14%
25	l	92	68% 86% 14%
26	g	76	49% 97% •

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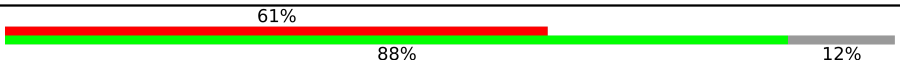
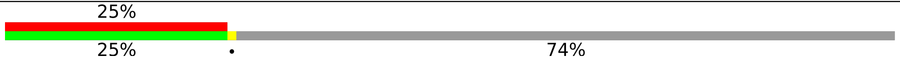
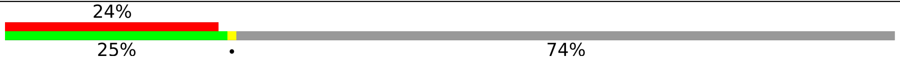
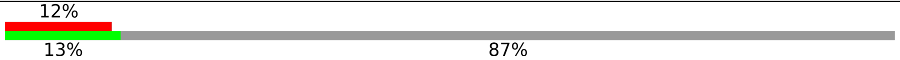
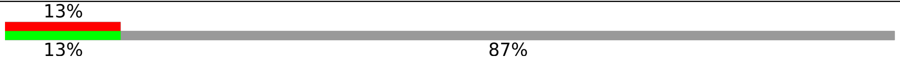
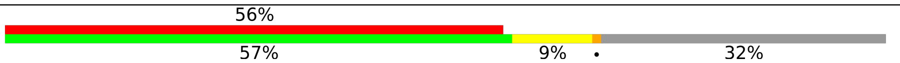
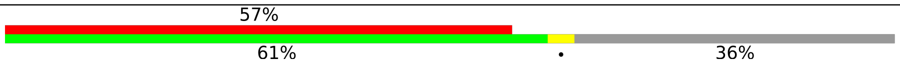
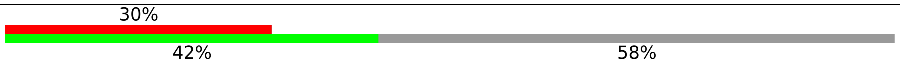
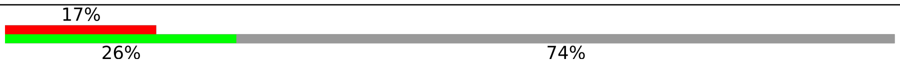
Mol	Chain	Length	Quality of chain
26	n	76	
27	q	504	
27	r	504	
27	s	504	
27	t	504	
28	K	225	
29	o	255	
30	p	225	
31	Q	1485	
32	y	301	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	GTP	C	1500	-	-	X	-

2 Entry composition ⓘ

There are 36 unique types of molecules in this entry. The entry contains 78004 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 Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1981	16477	10621	2883	2902	71	0	0

- Molecule 2 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	98	2060	923	341	698	98	0	0

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	888	7022	4494	1172	1322	34	0	0

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	303	2366	1487	415	451	13	0	0

- Molecule 5 is a RNA chain called U6snRNA.

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

- Molecule 6 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	556	3758	2344	705	703	6	0	0

- Molecule 7 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	L	475	3237	1985	627	619	6	0	0

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	M	130	1098	684	204	208	2	0	0

- Molecule 9 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	N	143	1184	746	217	209	12	0	0

- Molecule 10 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	O	290	2340	1469	415	436	20	0	0

- Molecule 11 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	P	118	985	601	194	188	2	0	0

- Molecule 12 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
12	R	272	2165	1357	393	401	2	12	0	0

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	S	159	1236	787	215	227	7	0	0

- Molecule 14 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	T	317	2496	1574	453	461	8	0	0

- Molecule 15 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	W	509	3008	1833	568	603	4	0	0

- Molecule 16 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	G	70	1246	549	158	469	70	0	0

- Molecule 17 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	H	140	2968	1327	511	990	140	0	0

- Molecule 18 is a protein called CWF19-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	U	347	2864	1817	496	529	22	0	0

- Molecule 19 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	I	568	2822	1683	569	569	1	0	0

- Molecule 20 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	a	81	399	237	81	81	0	0
			Total	C	N	O		
20	h	81	398	236	81	81	0	0

- Molecule 21 is a protein called Small nuclear ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
21	b	86	Total C N O 424 252 86 86	0	0
21	i	86	Total C N O 424 252 86 86	0	0

- Molecule 22 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms	AltConf	Trace
22	c	82	Total C N O 406 242 82 82	0	0
22	j	82	Total C N O 406 242 82 82	0	0

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms	AltConf	Trace
23	d	97	Total C N O 480 286 97 97	0	0
23	k	85	Total C N O 422 252 85 85	0	0

- Molecule 24 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms	AltConf	Trace
24	f	74	Total C N O 361 213 74 74	0	0
24	m	74	Total C N O 361 213 74 74	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
25	e	79	Total C N O 391 233 79 79	0	0
25	l	79	Total C N O 391 233 79 79	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
26	g	74	Total C N O 363 215 74 74	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
26	n	67	Total C N O 329 195 67 67	0	0

- Molecule 27 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms	AltConf	Trace
27	q	132	Total C N O 659 395 132 132	0	0
27	r	131	Total C N O 654 392 131 131	0	0
27	s	67	Total C N O 335 201 67 67	0	0
27	t	67	Total C N O 335 201 67 67	0	0

- Molecule 28 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms	AltConf	Trace
28	K	152	Total C N O 757 453 152 152	0	0

- Molecule 29 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms	AltConf	Trace
29	o	162	Total C N O 804 480 162 162	0	0

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms	AltConf	Trace
30	p	94	Total C N O 464 276 94 94	0	0

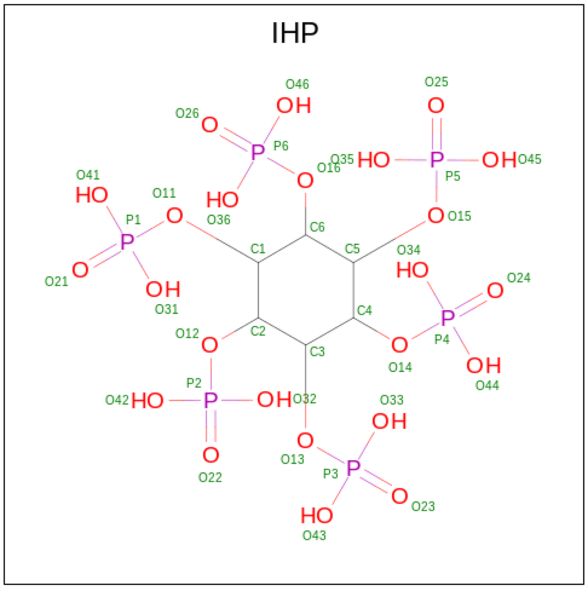
- Molecule 31 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms	AltConf	Trace
31	Q	1322	Total C N O 6562 3918 1322 1322	4	0

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

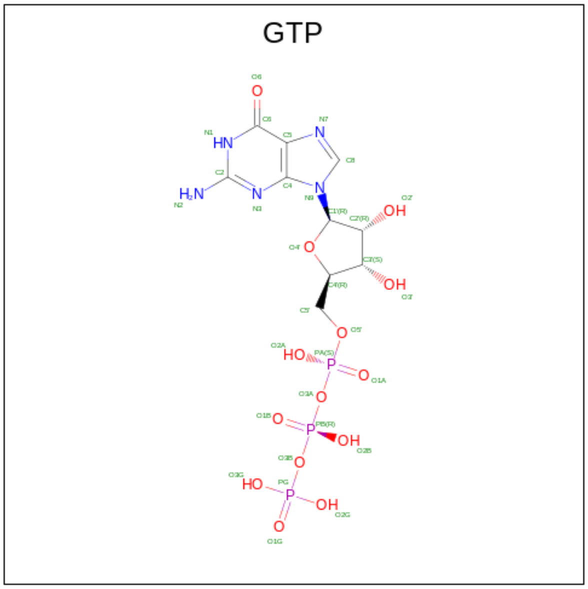
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	y	79	390	232	79	79	0	0

- Molecule 33 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 34 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	
34	C	1	32	10	5	14	3	0

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
35	C	1	1	1	0
35	F	6	6	6	0

- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

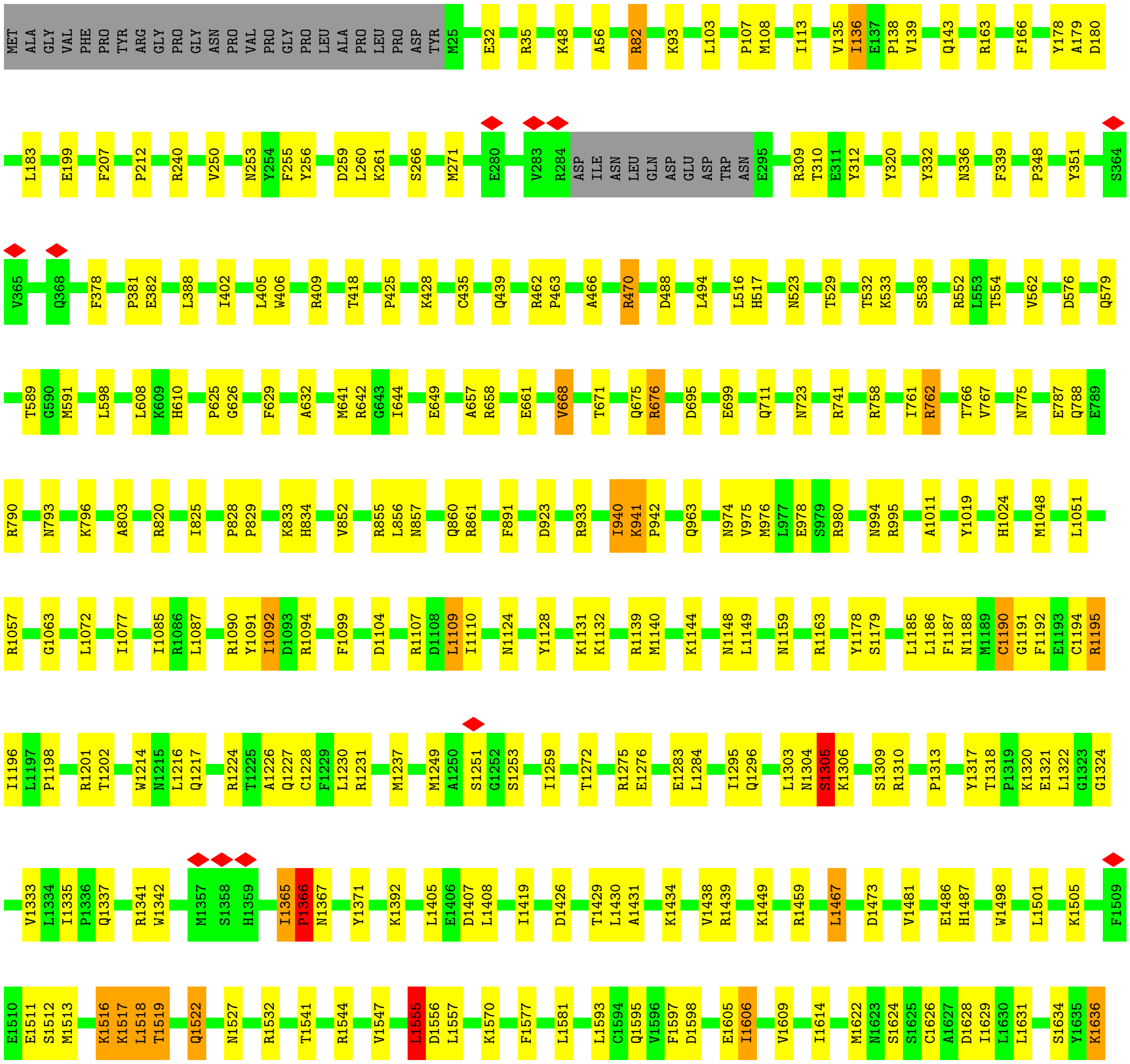
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
36	N	3	3	3	0
36	O	3	3	3	0
36	U	1	1	1	0

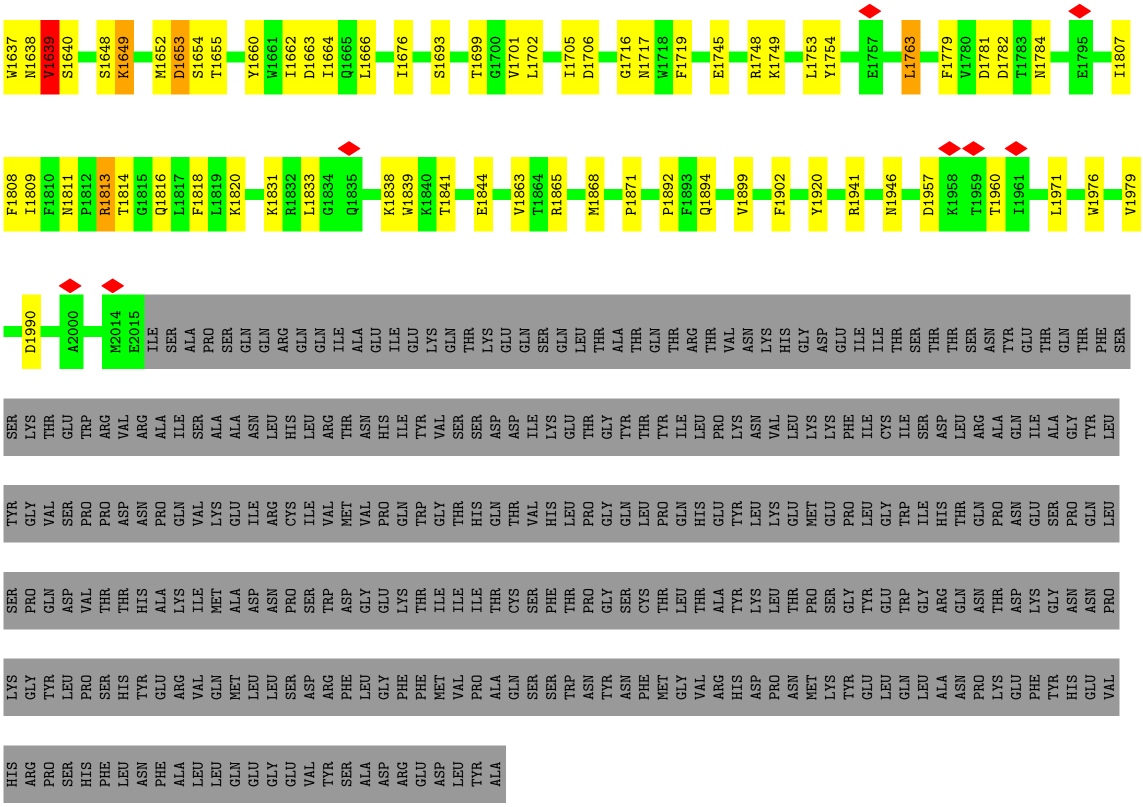
3 Residue-property plots ⓘ

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

- Molecule 1: Pre-mRNA-processing-splicing factor 8

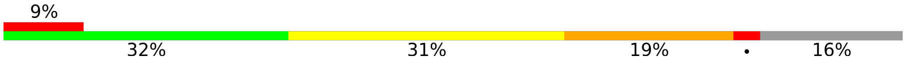
Chain A:

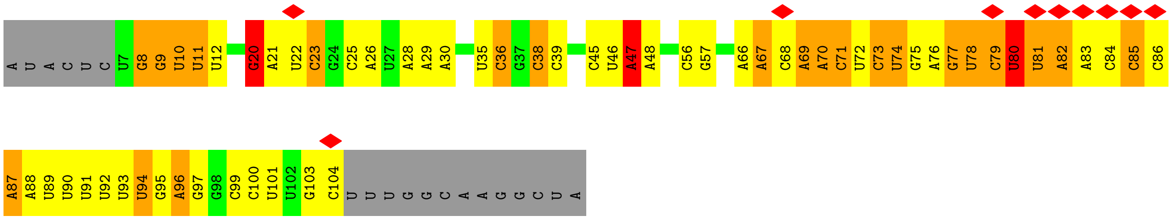




- Molecule 2: U5snRNA

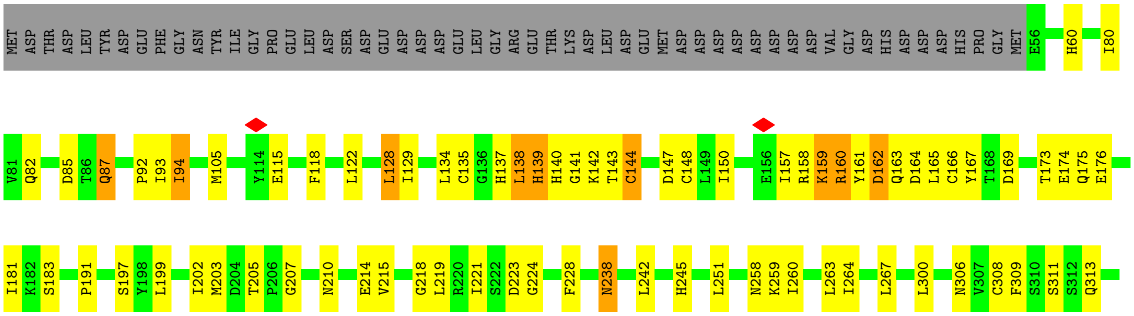
Chain B:

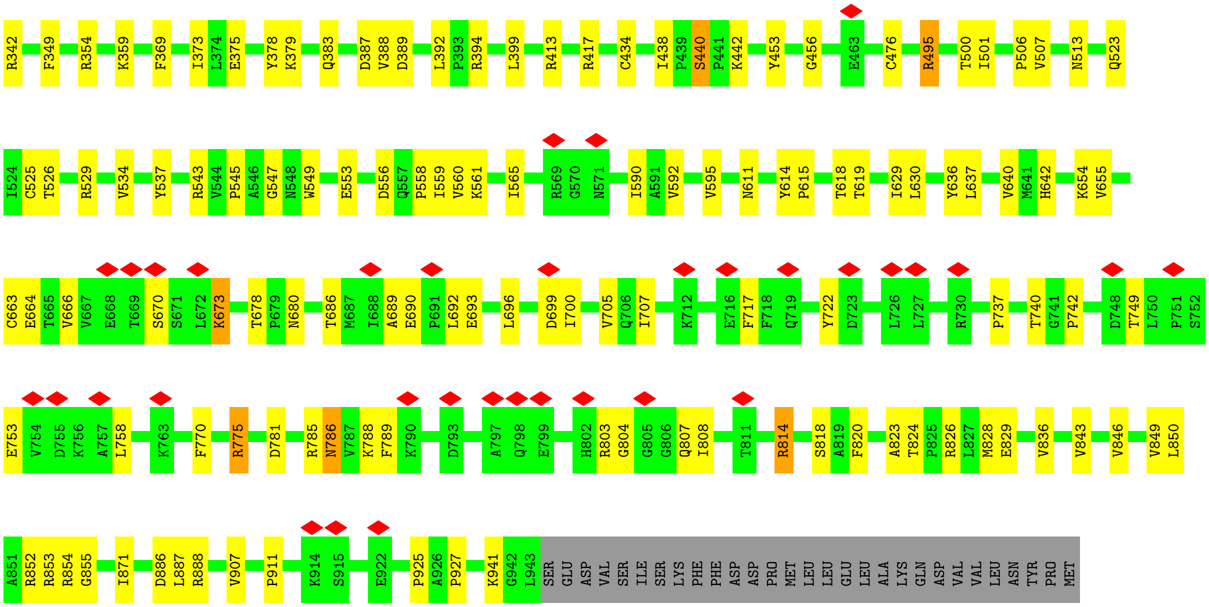




- Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

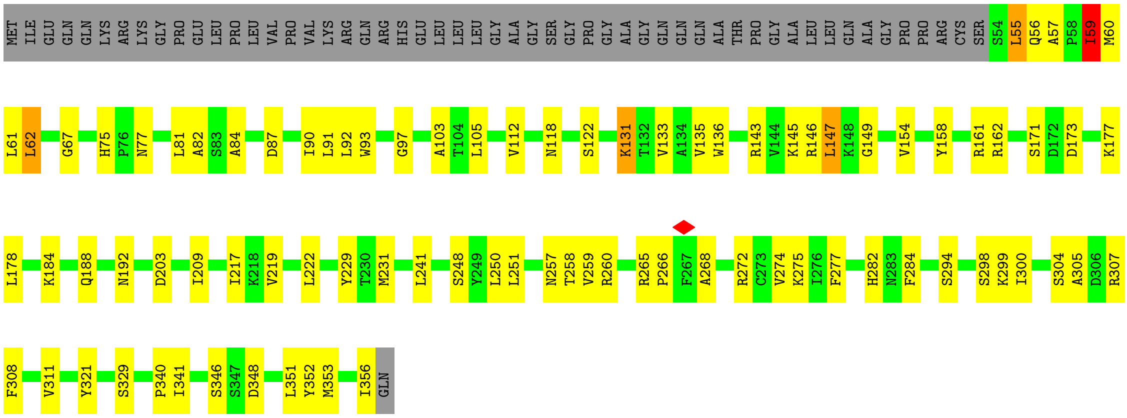
Chain C:





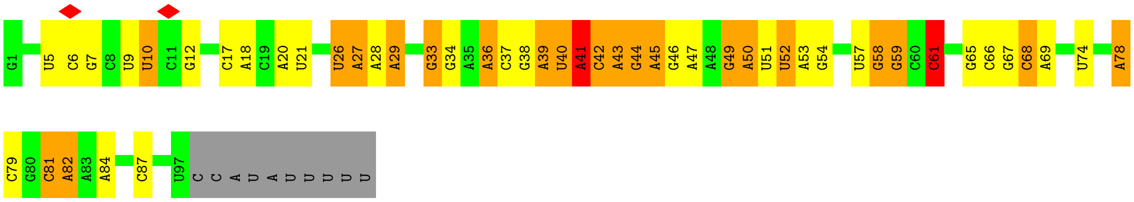
- Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:



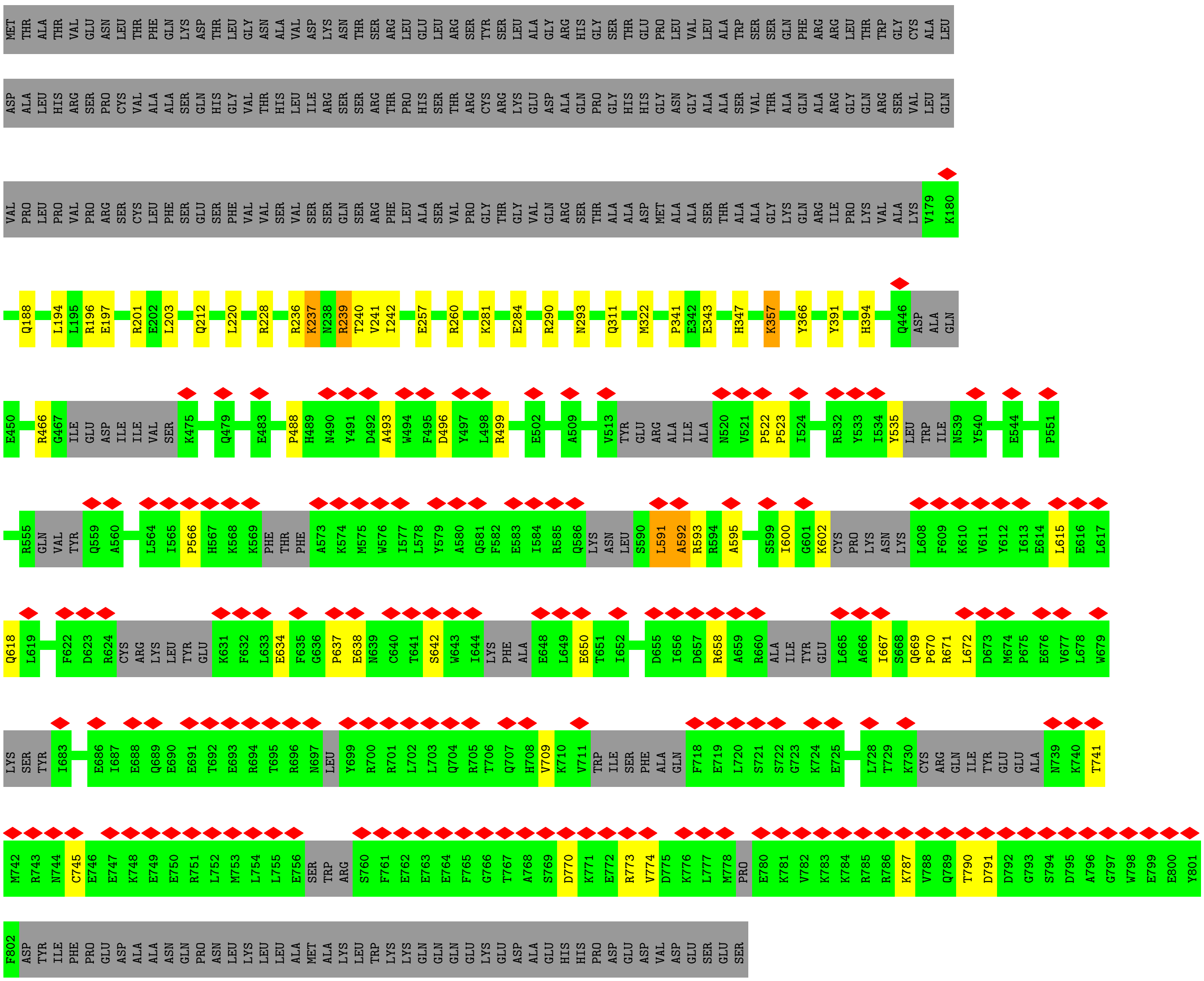
- Molecule 5: U6snRNA

Chain F:

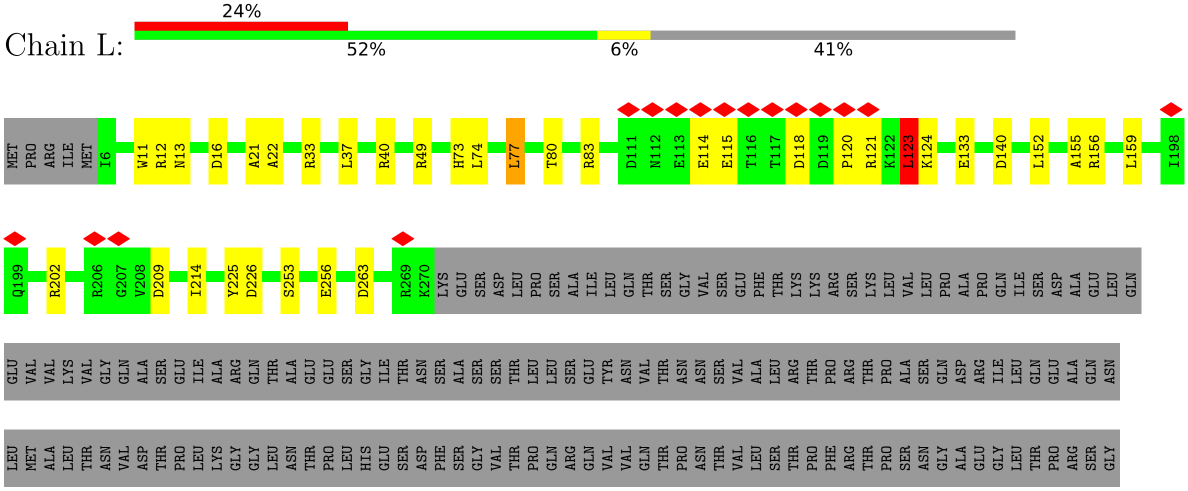


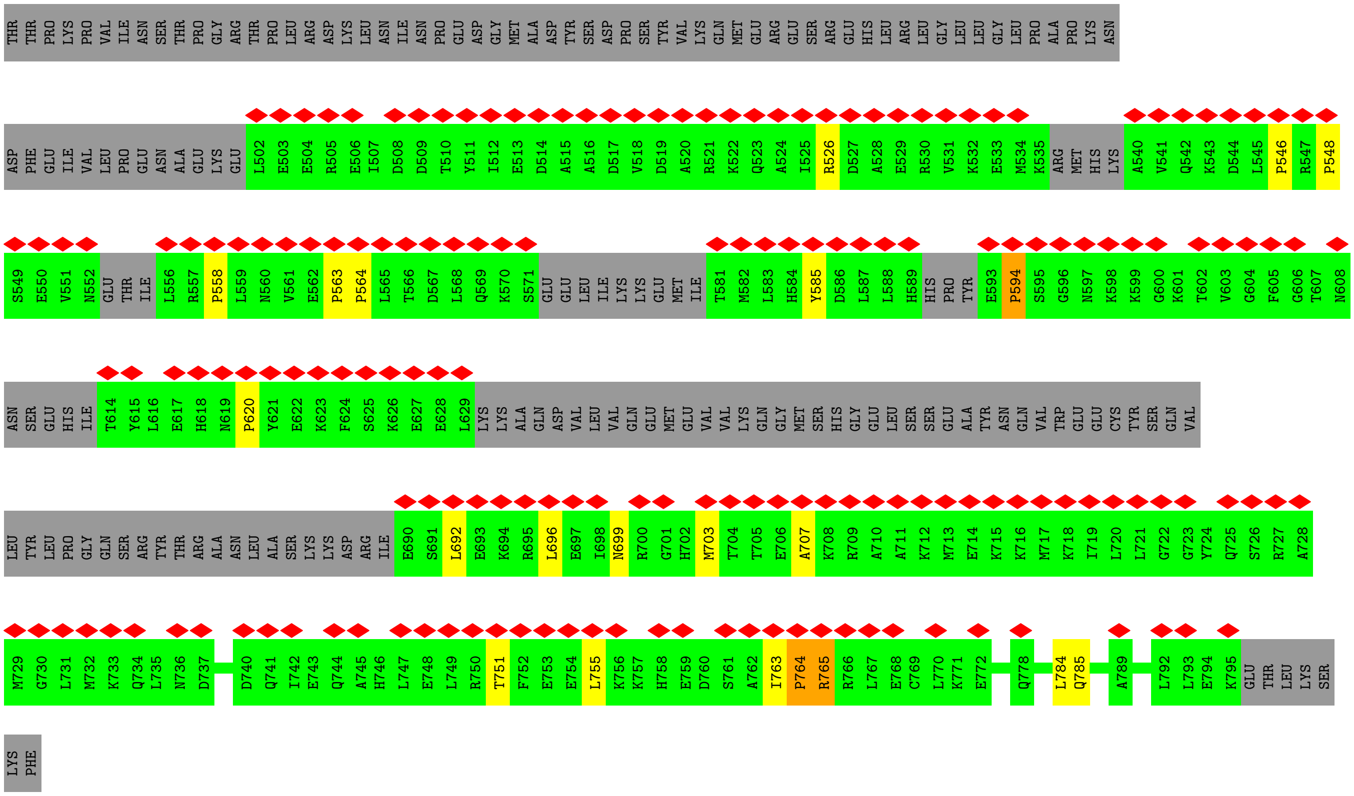
- Molecule 6: Crooked neck-like protein 1

Chain J:



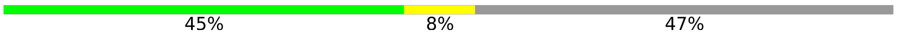
- Molecule 7: Cell division cycle 5-like protein

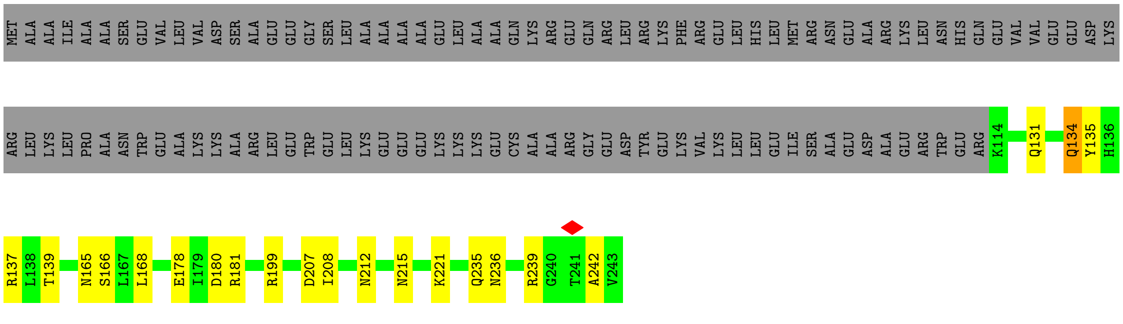




- Molecule 8: Pre-mRNA-splicing factor SYF2

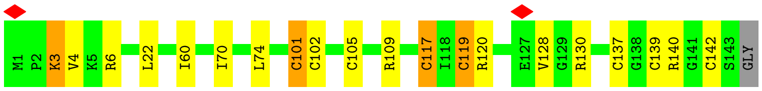
Chain M:





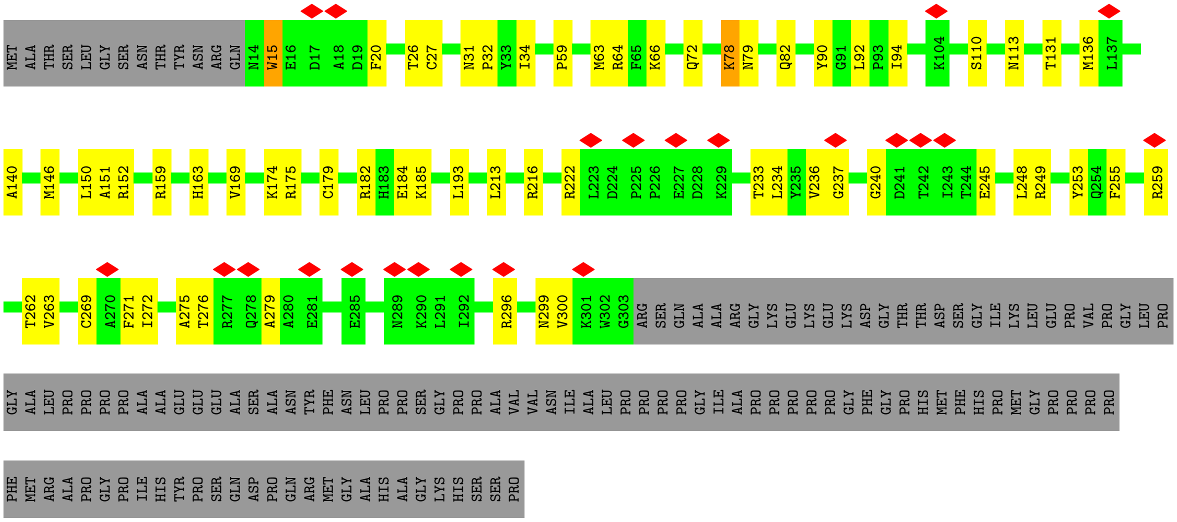
- Molecule 9: Protein BUD31 homolog

Chain N:



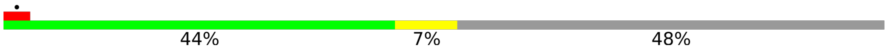
- Molecule 10: Pre-mRNA-splicing factor RBM22

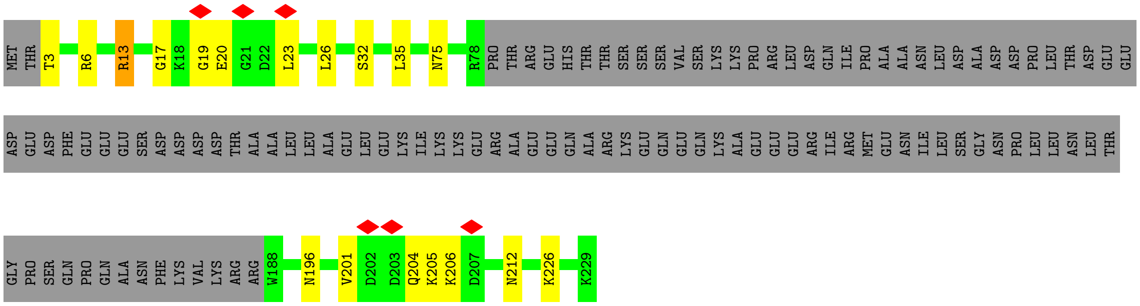
Chain O:



- Molecule 11: Spliceosome-associated protein CWC15 homolog

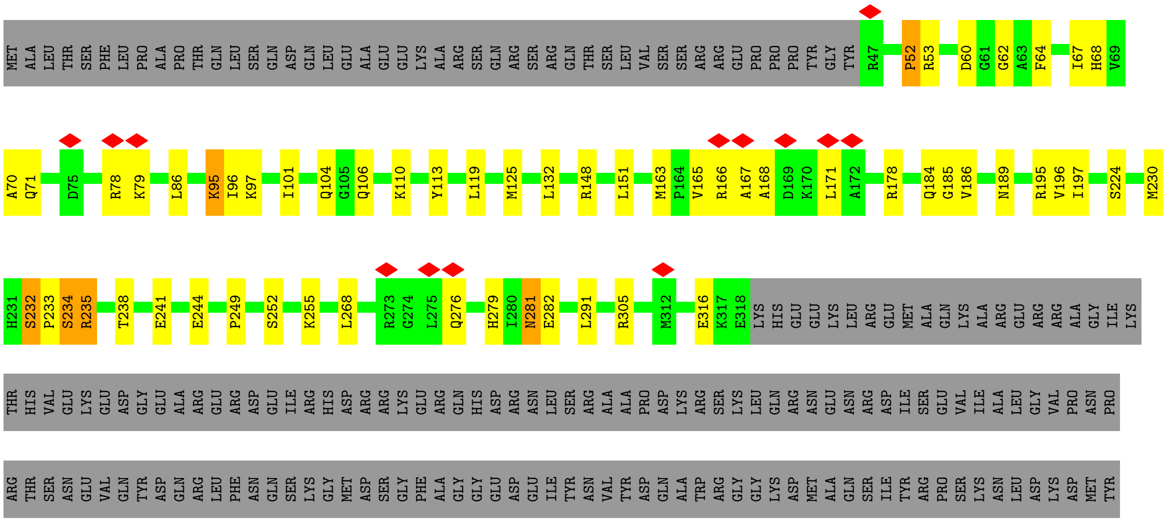
Chain P:

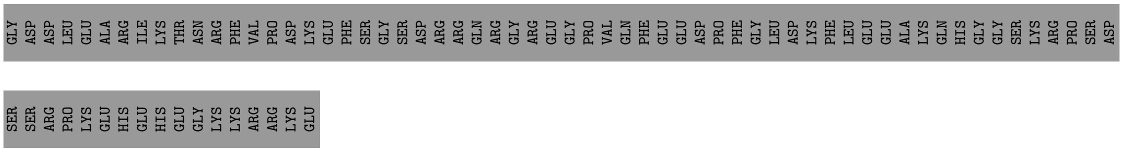




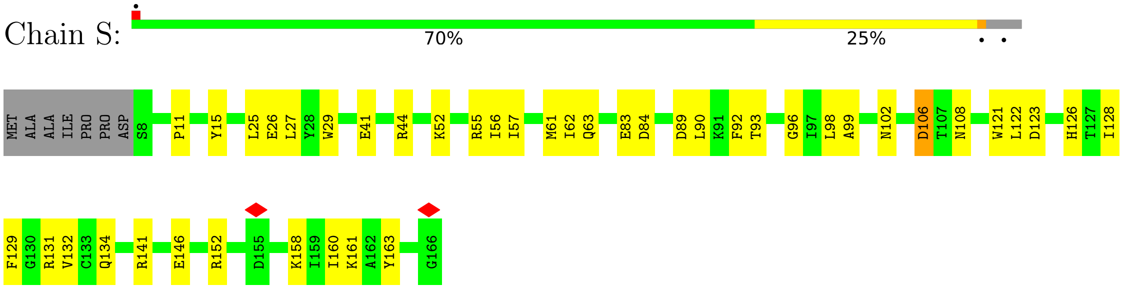
- Molecule 12: SNW domain-containing protein 1

Chain R:

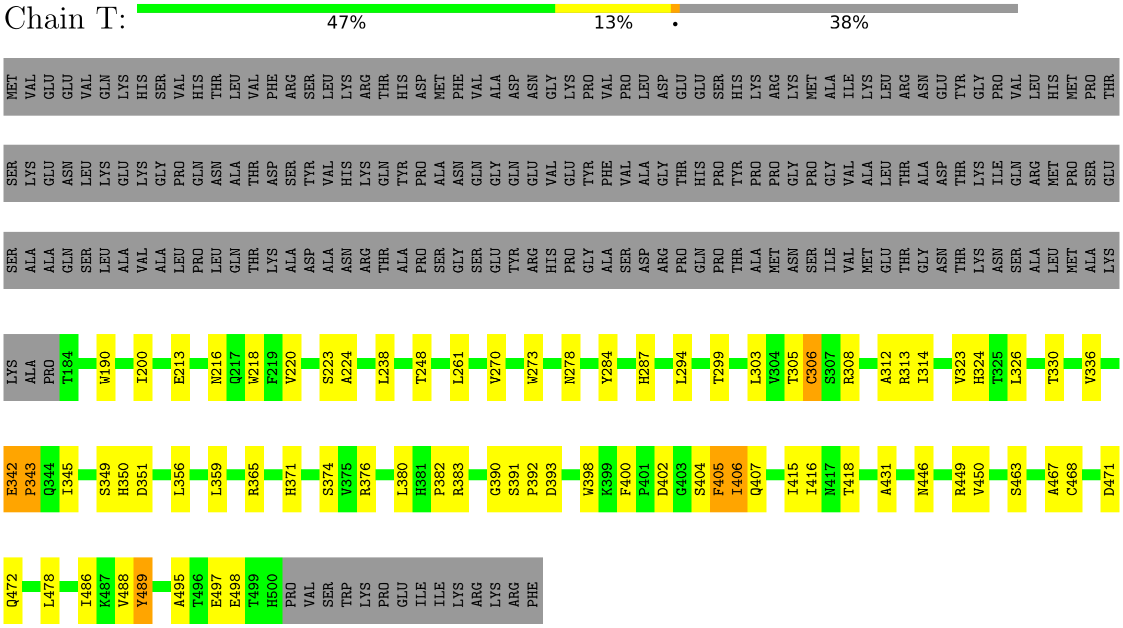




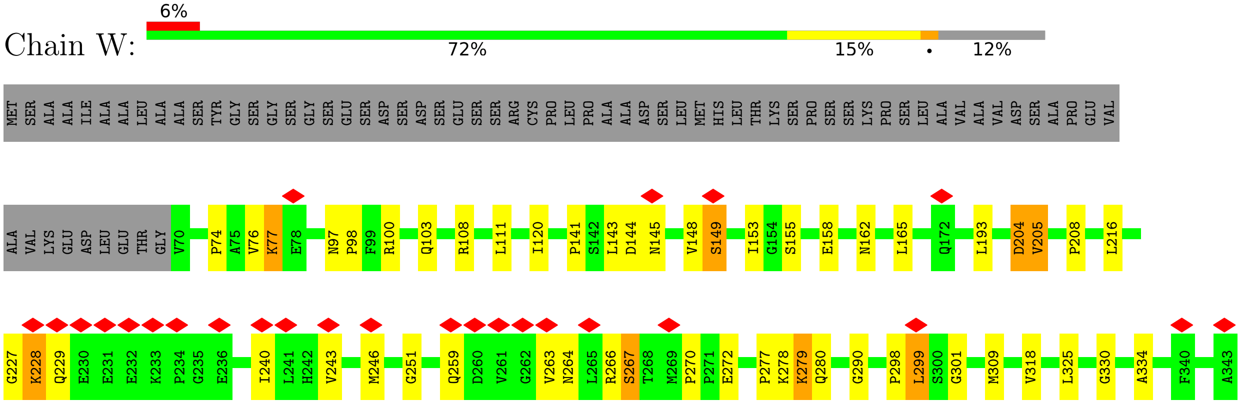
- Molecule 13: Peptidyl-prolyl cis-trans isomerase-like 1

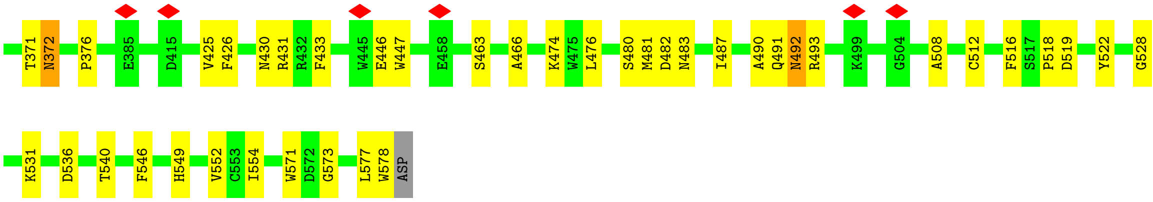


- Molecule 14: Pleiotropic regulator 1

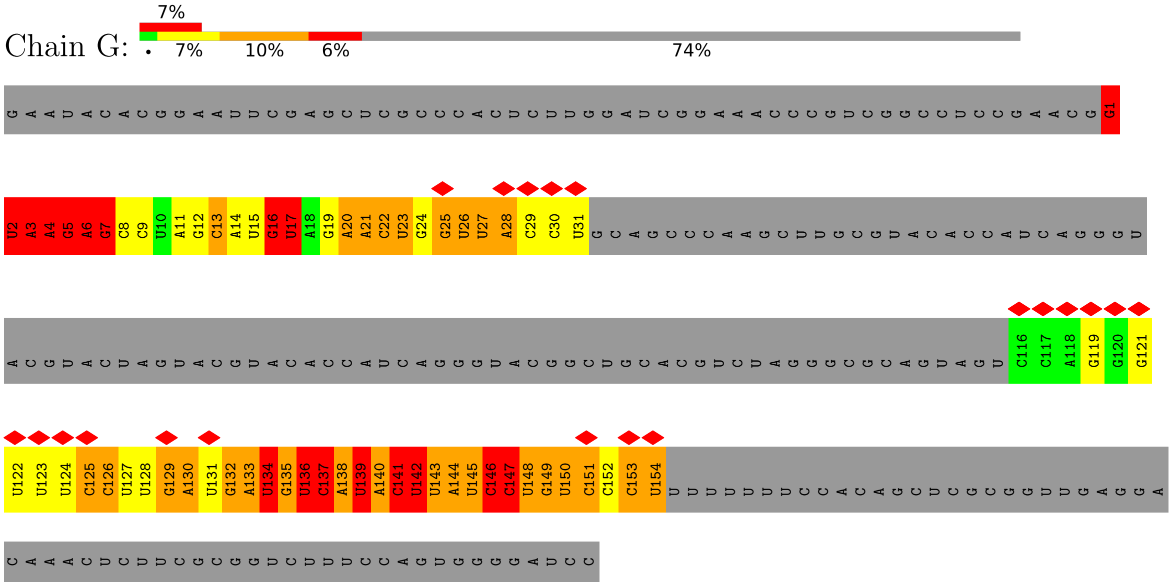


- Molecule 15: Pre-mRNA-processing factor 17

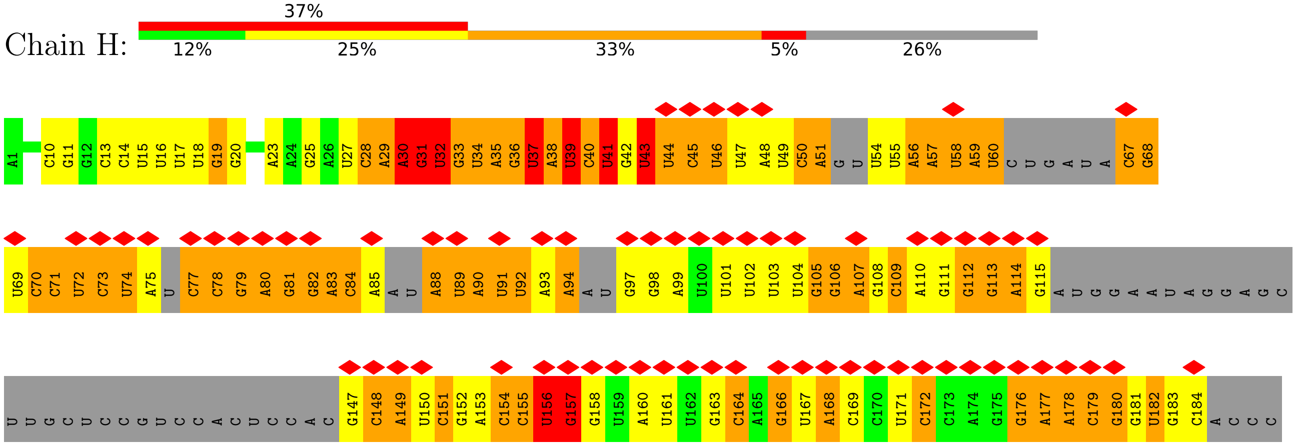




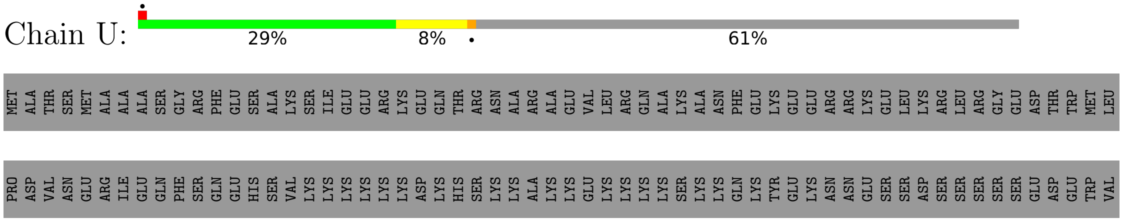
- Molecule 16: pre-mRNA

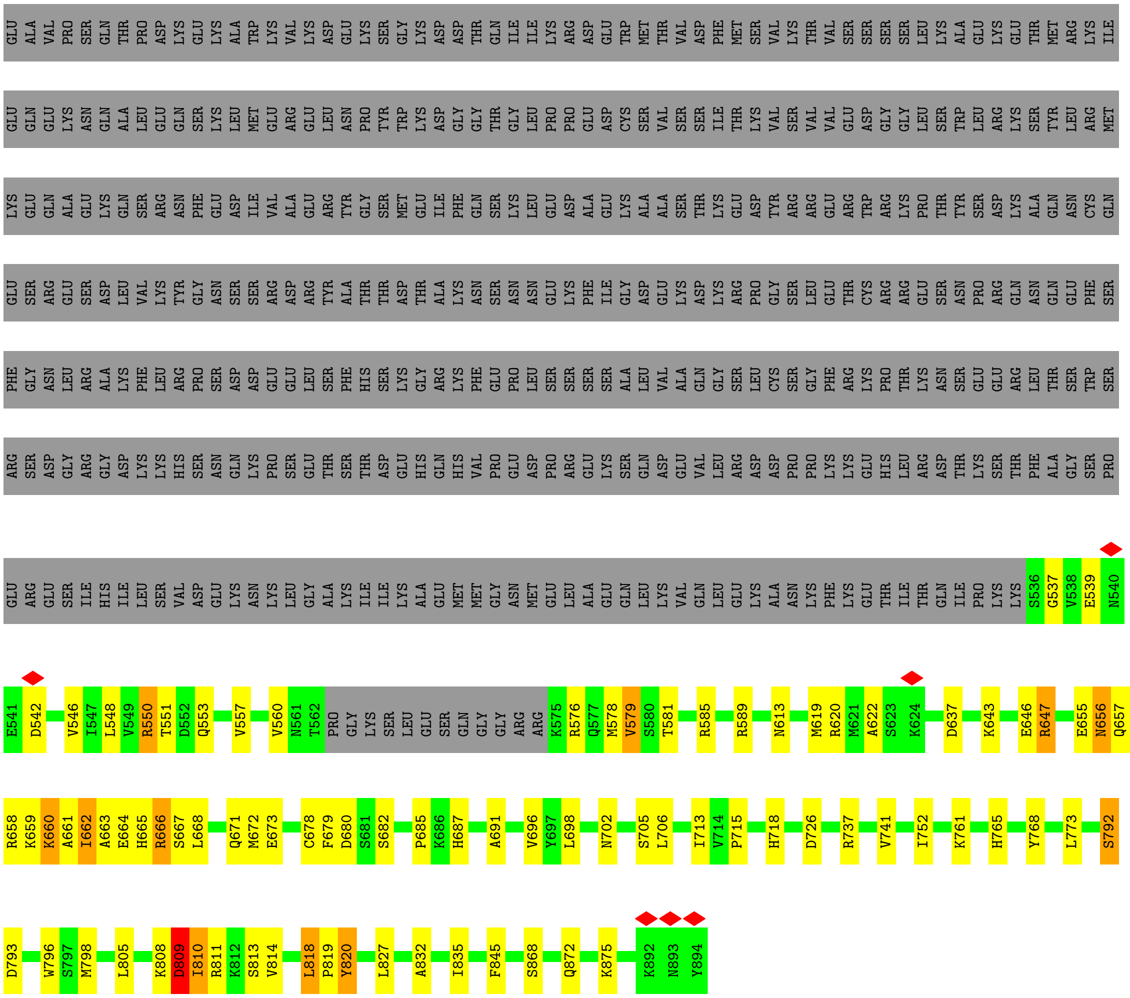


- Molecule 17: U2snRNA



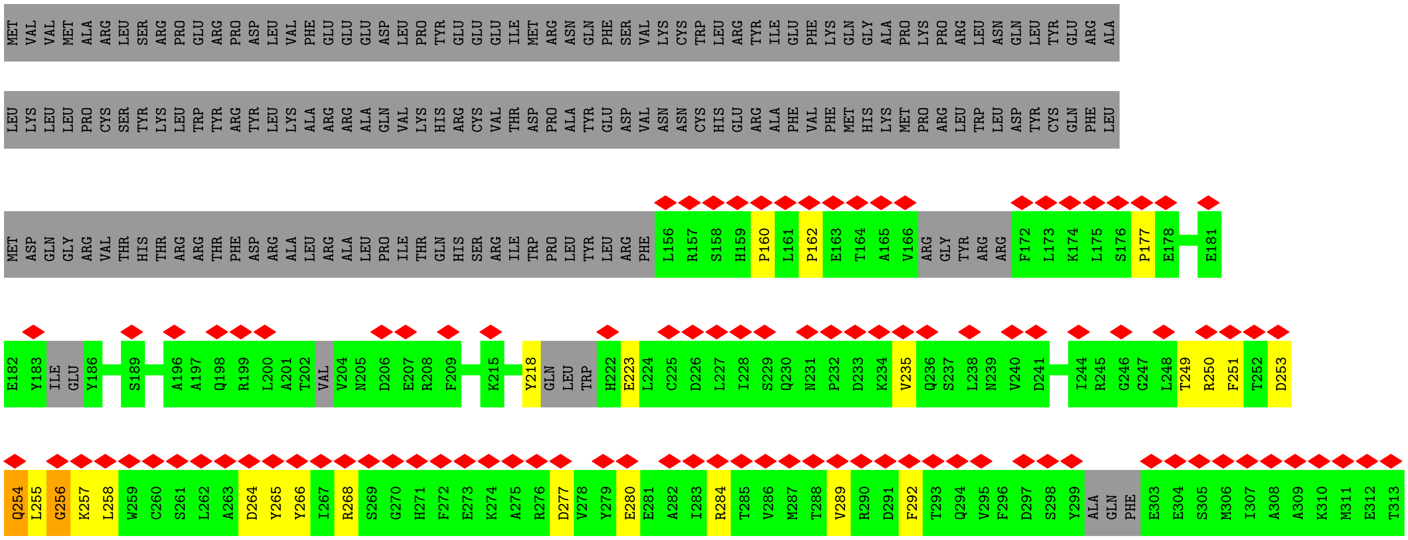
- Molecule 18: CWF19-like protein 2

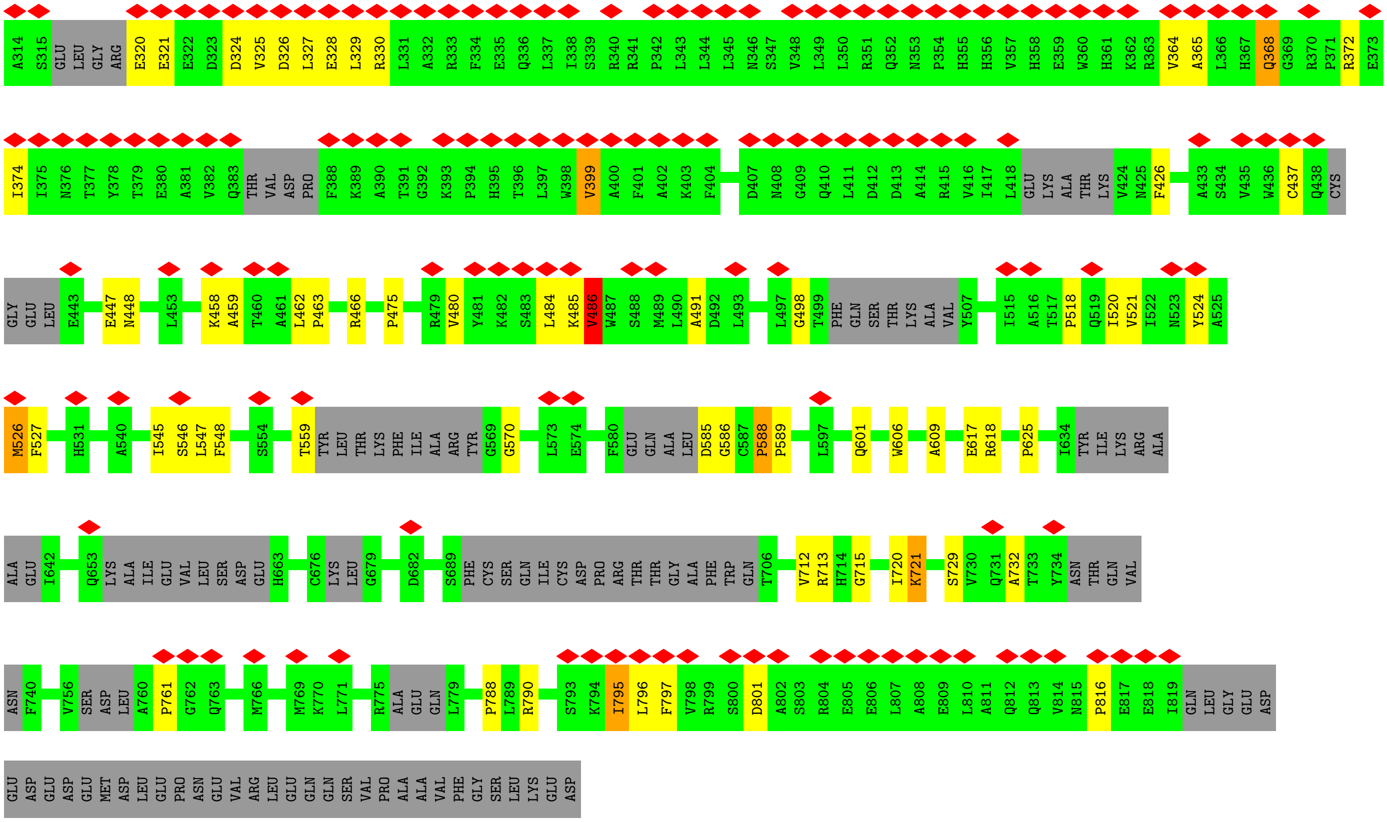




- Molecule 19: Pre-mRNA-splicing factor SYF1

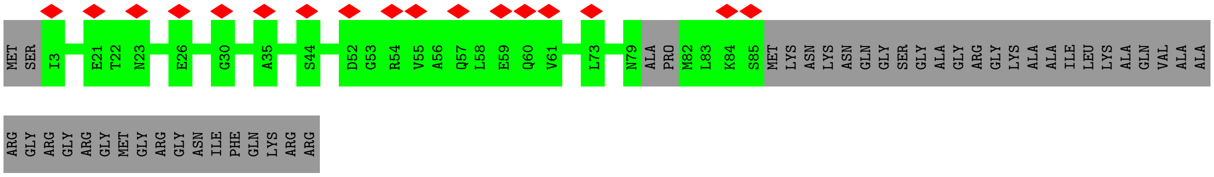
Chain I:





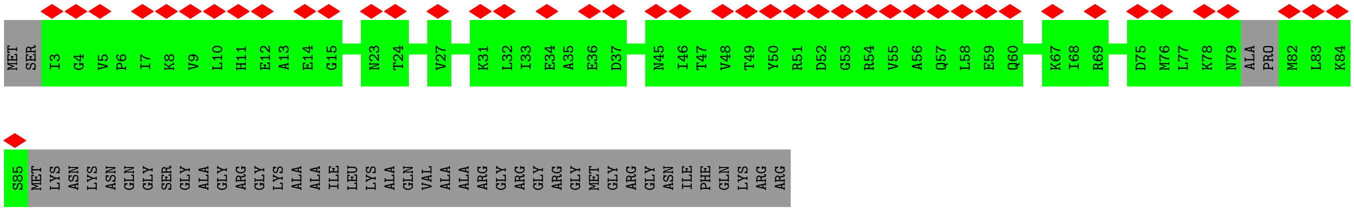
- Molecule 20: Small nuclear ribonucleoprotein Sm D3

Chain a:



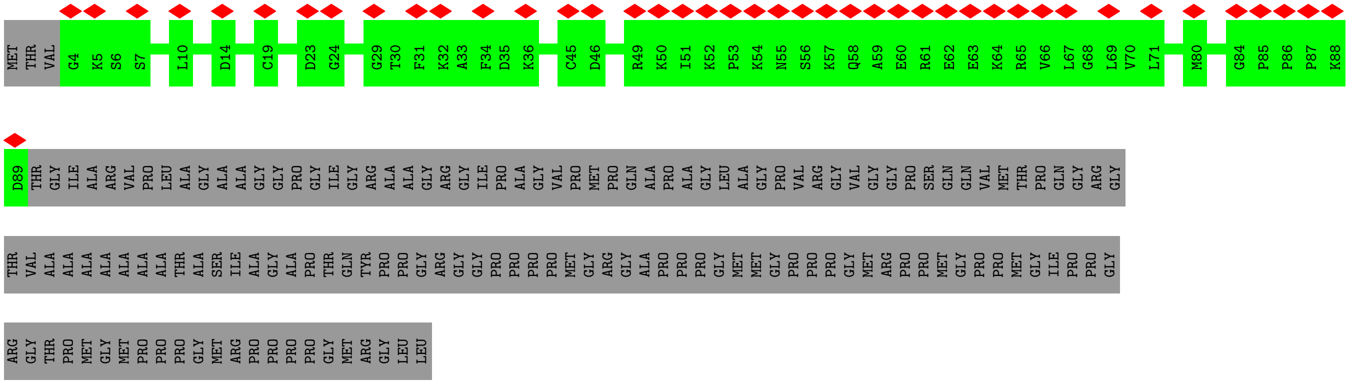
- Molecule 20: Small nuclear ribonucleoprotein Sm D3

Chain h:



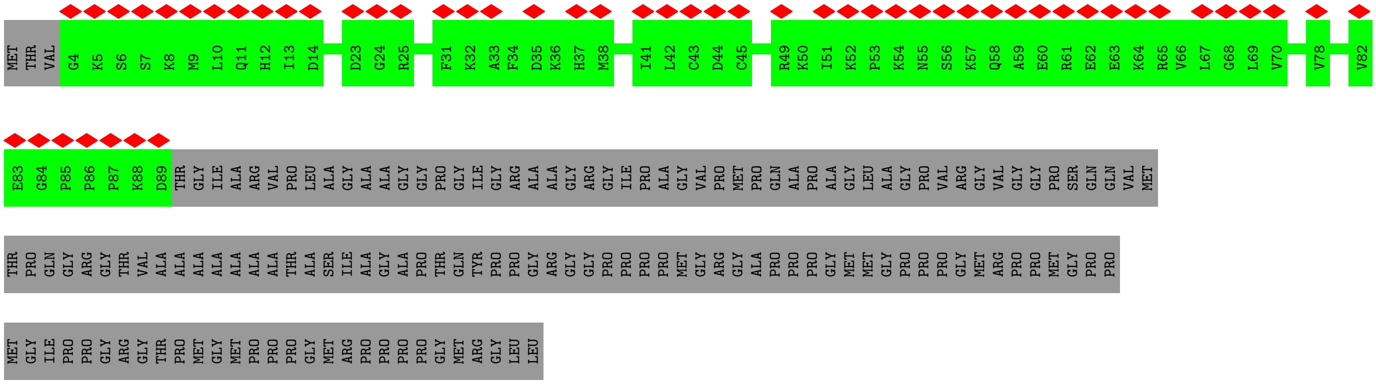
- Molecule 21: Small nuclear ribonucleoprotein-associated protein

Chain b:



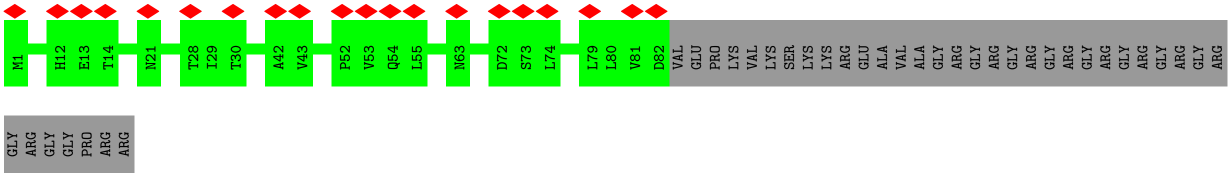
- Molecule 21: Small nuclear ribonucleoprotein-associated protein

Chain i:



- Molecule 22: Small nuclear ribonucleoprotein Sm D1

Chain c:



- Molecule 22: Small nuclear ribonucleoprotein Sm D1

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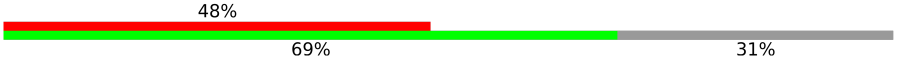
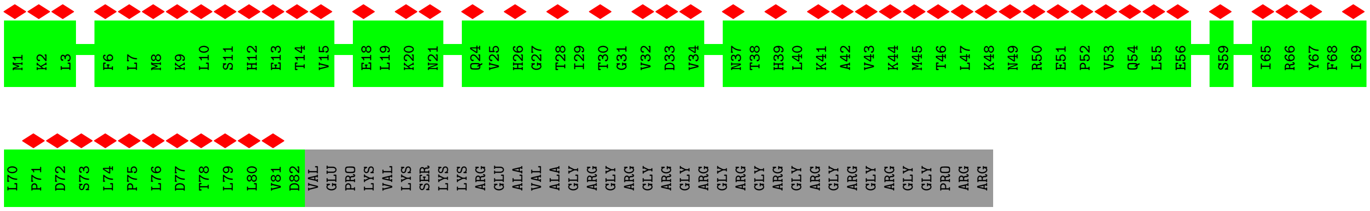
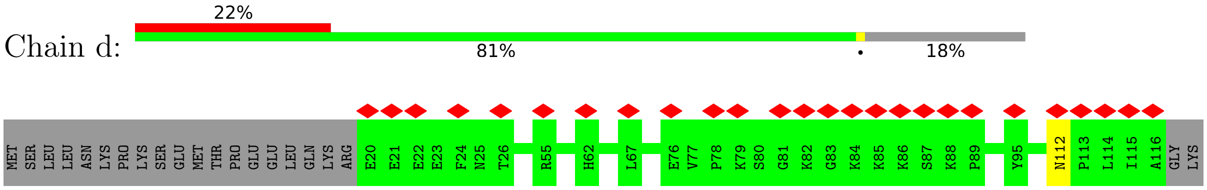




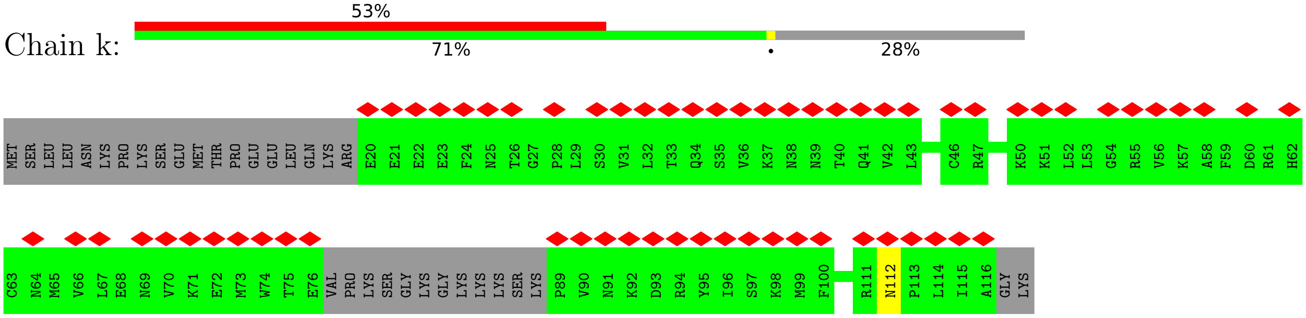
- Molecule 23: Small nuclear ribonucleoprotein Sm D2

Chain d:



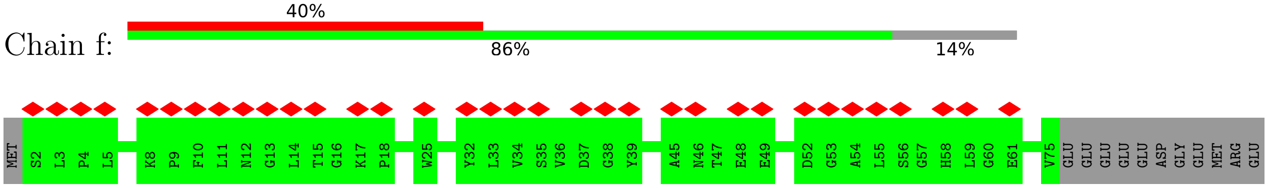
- Molecule 23: Small nuclear ribonucleoprotein Sm D2

Chain k:



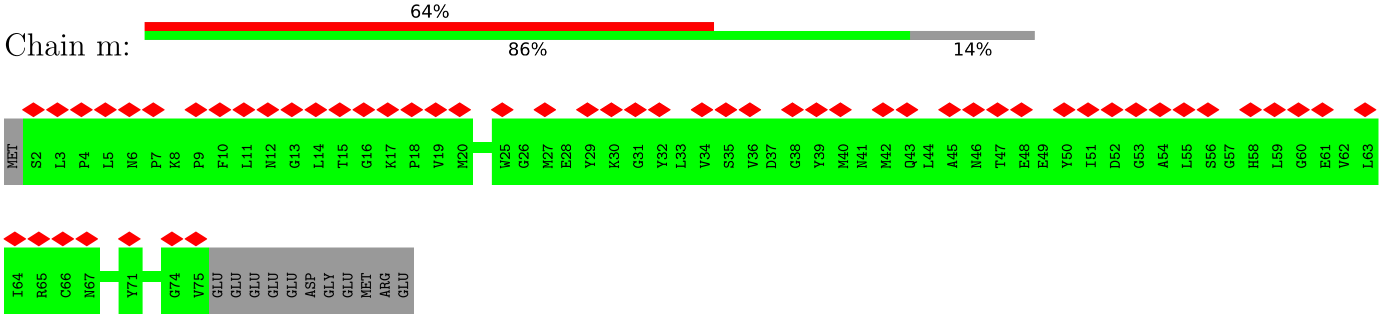
- Molecule 24: Small nuclear ribonucleoprotein F

Chain f:



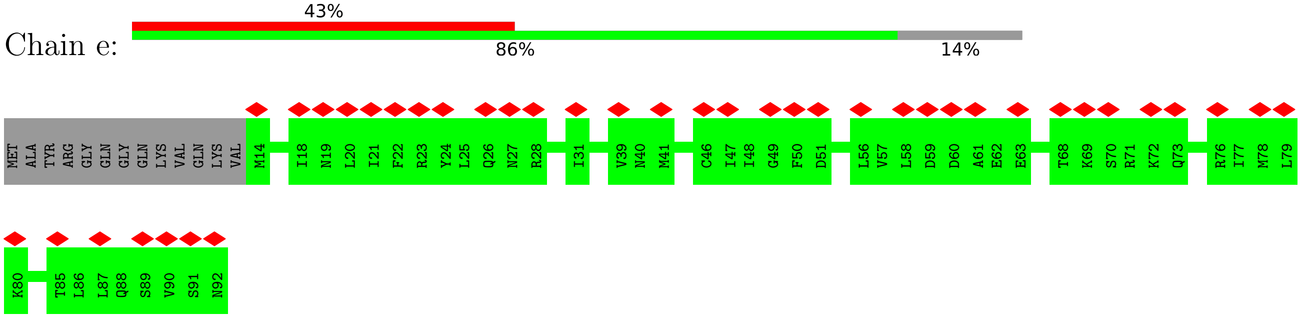
- Molecule 24: Small nuclear ribonucleoprotein F

Chain m:



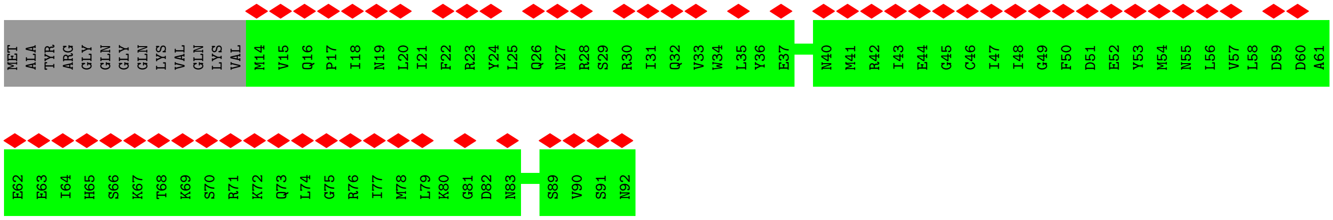
- Molecule 25: Small nuclear ribonucleoprotein E

Chain e:



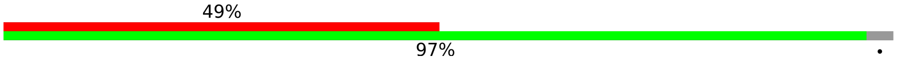
- Molecule 25: Small nuclear ribonucleoprotein E

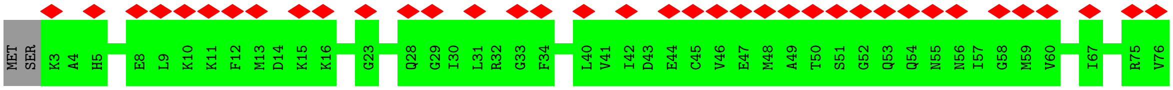
Chain l:



- Molecule 26: Small nuclear ribonucleoprotein G

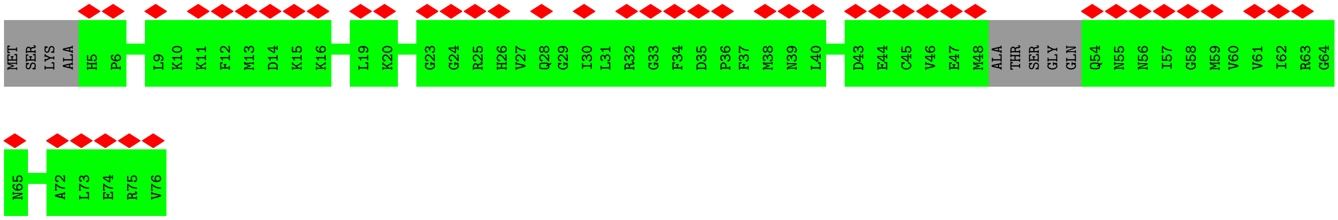
Chain g:





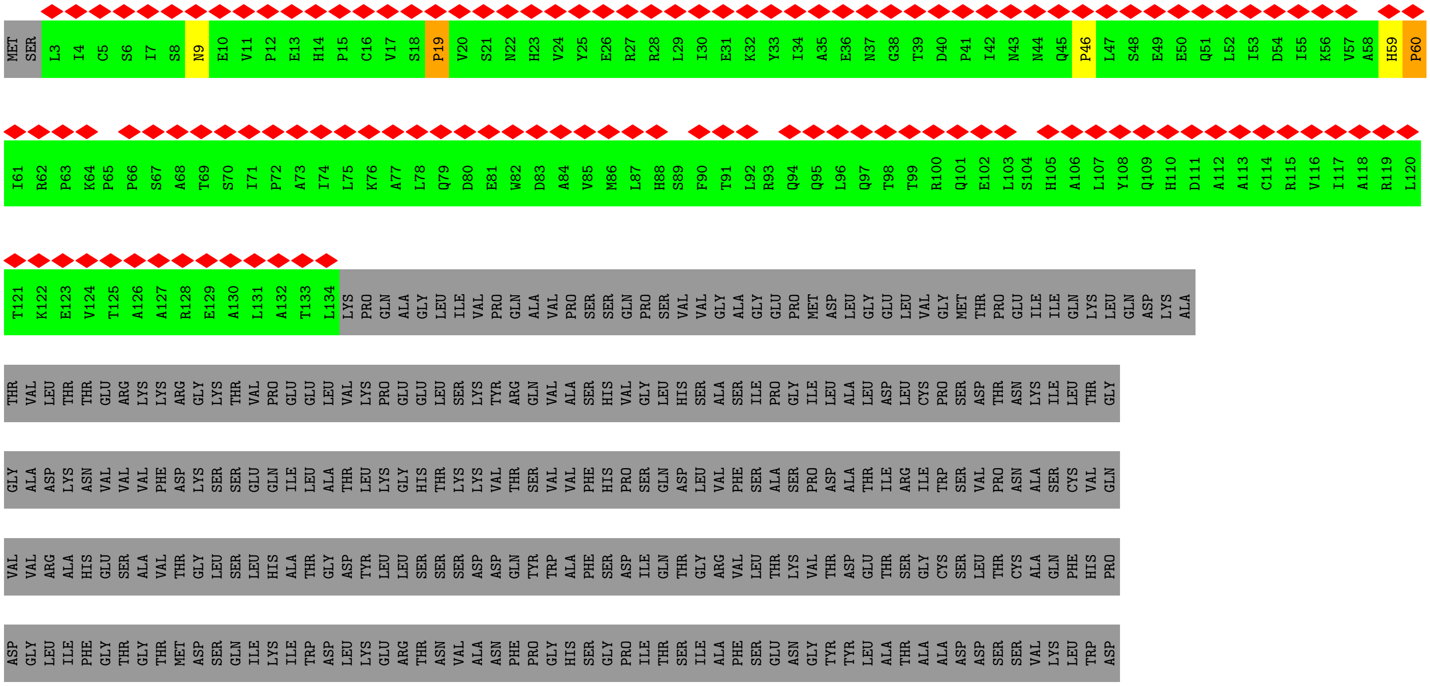
- Molecule 26: Small nuclear ribonucleoprotein G

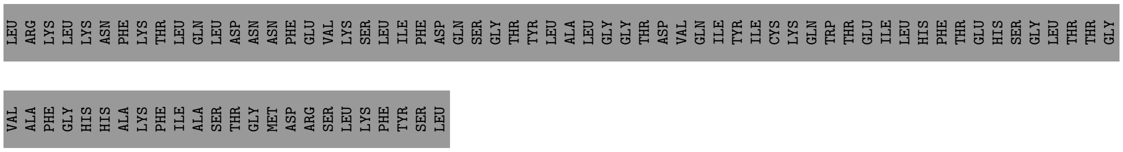
Chain n:



- Molecule 27: Pre-mRNA-processing factor 19

Chain q:





- Molecule 27: Pre-mRNA-processing factor 19

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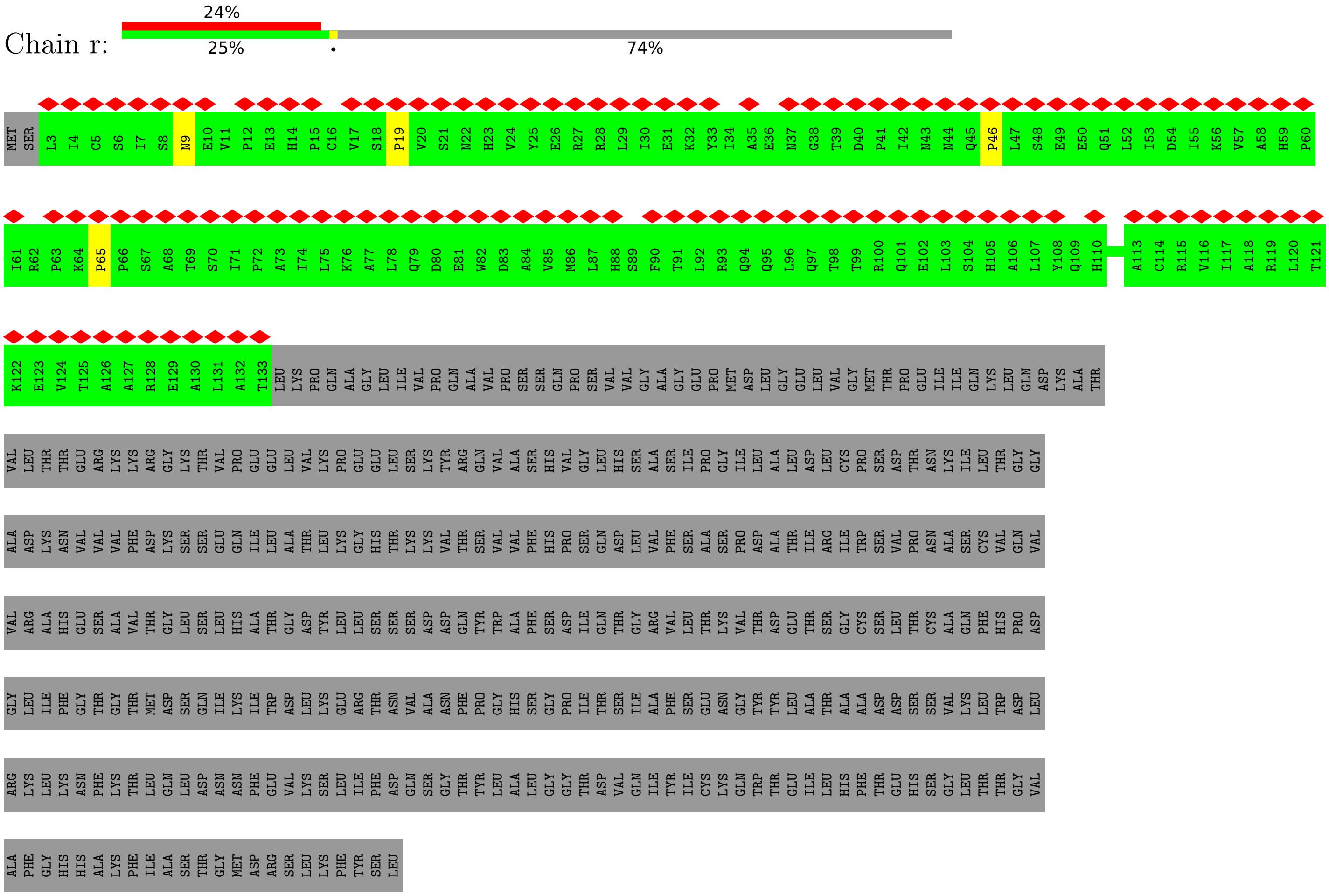
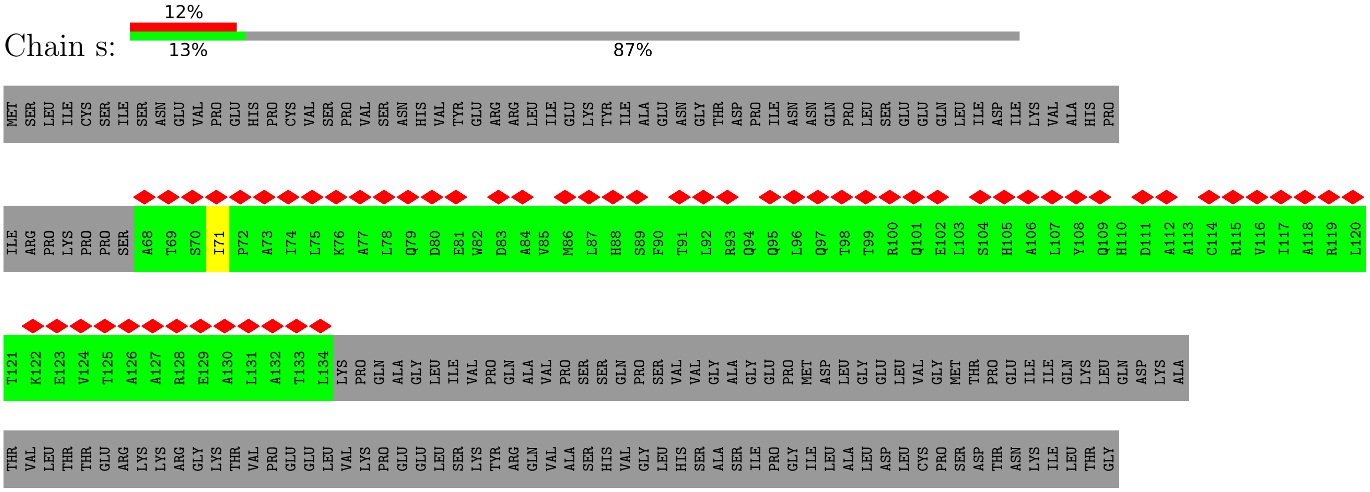
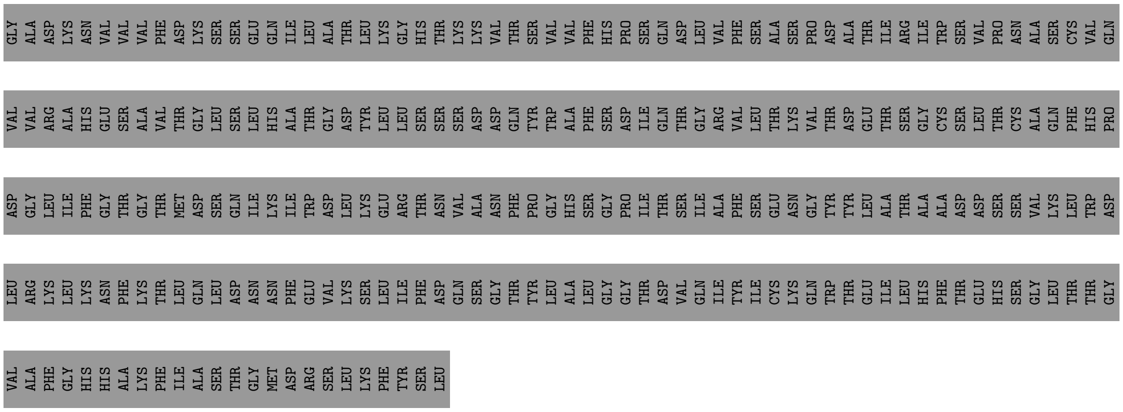


- Molecule 27: Pre-mRNA-processing factor 19

Chain s:





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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

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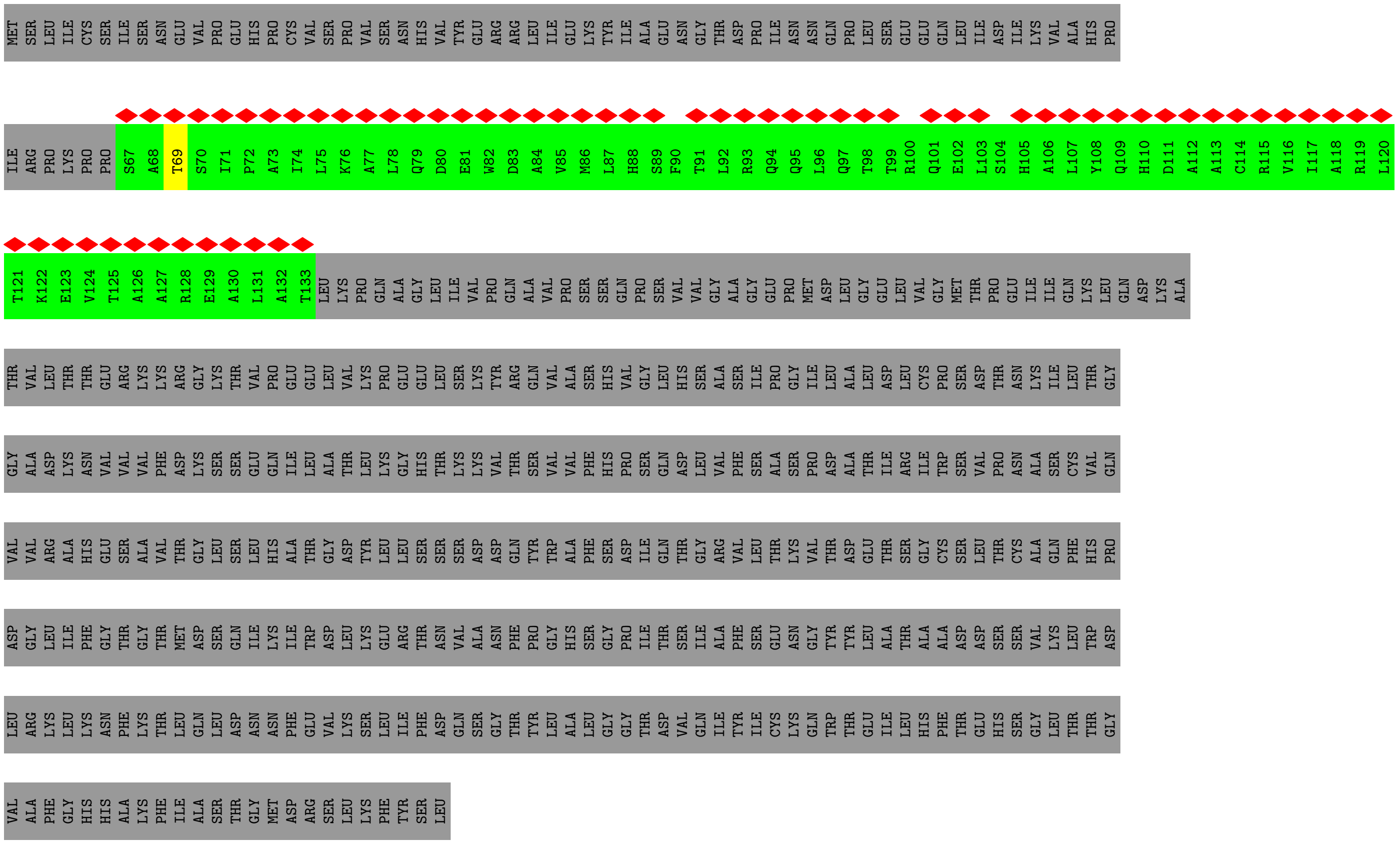
- Molecule 27: Pre-mRNA-processing factor 19

Chain t:



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T121 K122 E123 V124 T125 A126 A127 R128 E129 A130 L131 A132 T133 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

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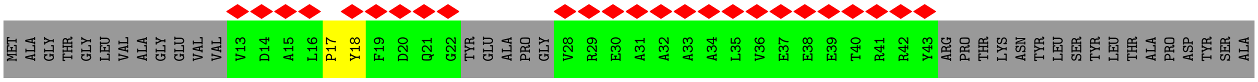
- Molecule 28: Pre-mRNA-splicing factor SPF27

Chain K:



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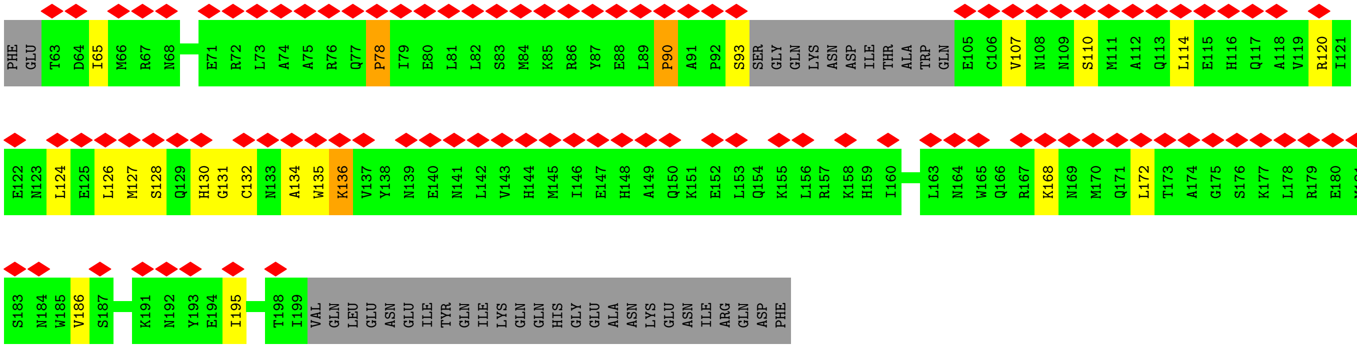
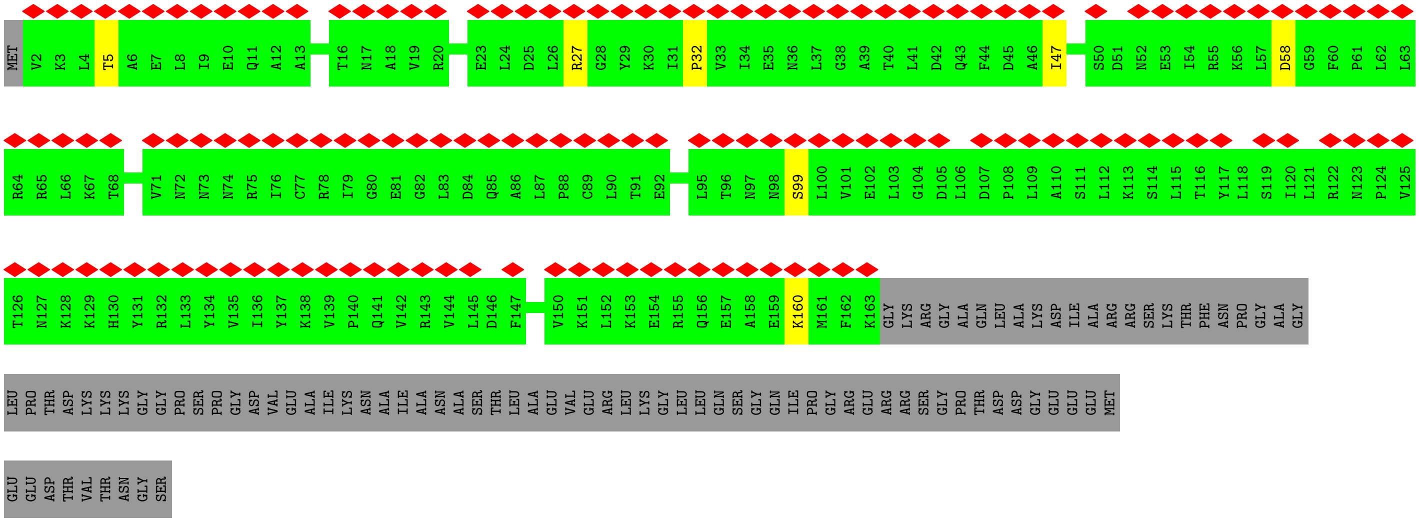


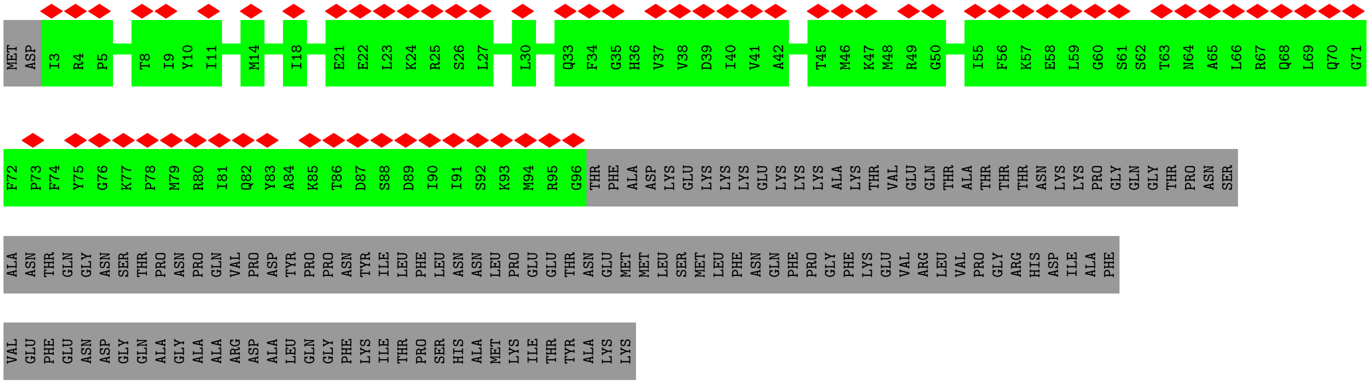
- Molecule 29: U2 small nuclear ribonucleoprotein A'

Chain o:



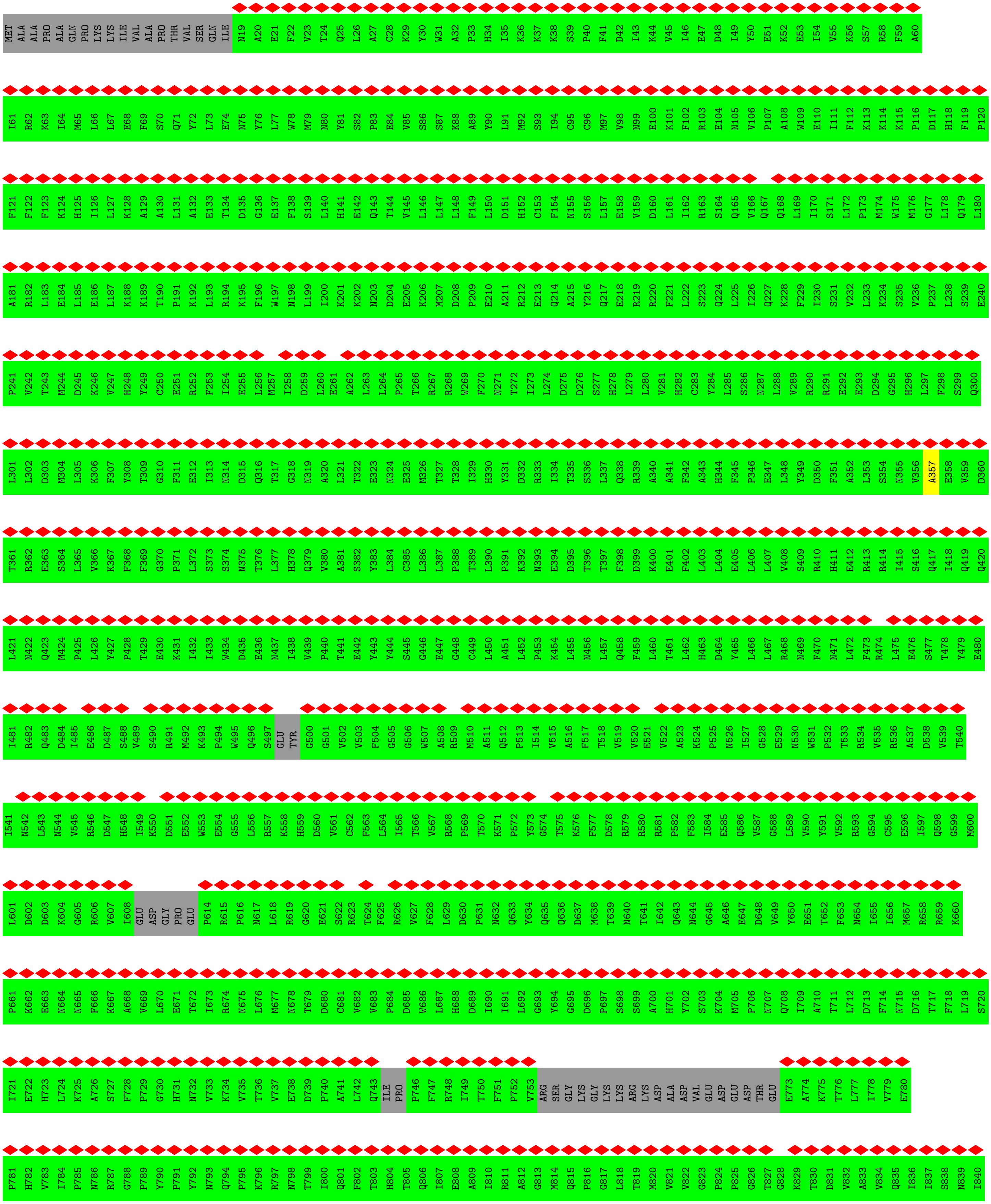
- Molecule 30: U2 small nuclear ribonucleoprotein B"

Chain p:



- Molecule 31: RNA helicase aquarius

Chain Q: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I61 R62 K63 I64 M65 L66 L67 E68 F69 S70 Q71 Y72 L73 E74 N75 Y76 L77 W78 M79 N80 Y81 S82 P83 E84 V85 S86 S87 K88 A89 Y90 L91 M92 S93 I94 C95 C96 M97 V98 N99 E100 K101 F102 R103 E104 N105 V106 P107 A108 W109 E110 I111 F112 K113 K114 K115 P116 D117 H118 F119 P120
F121 F122 F123 K124 H125 I126 L127 K128 A129 A130 L131 A132 E133 T134 D135 G136 E137 F138 S139 L140 H141 E142 Q143 T144 V145 L146 L147 F148 F149 L150 D151 H152 C153 F154 N155 S156 L157 E158 V159 D160 L161 I162 R163 S164 Q165 V166 Q167 Q168 L169 I170 S171 L172 P173 M174 W175 M176 G177 L178 Q179 L180
A181 R182 L183 E184 L185 E186 L187 K188 K189 T190 P191 K192 L193 R194 K195 F196 W197 N198 L199 I200 K201 K202 N203 D204 E205 K206 M207 D208 P209 E210 A211 R212 E213 Q214 A215 Y216 Q217 E218 R219 R220 F221 L222 S223 Q224 L225 I226 Q227 K228 F229 I230 S231 V232 L233 K234 S235 V236 P237 L238 S239 E240
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L601 D602 D603 K604 G605 R606 V607 I608 GLU ASP GLY PRO GLU P614 R615 P616 N617 L618 R619 G620 E621 S622 R623 T624 F625 R626 V627 F628 L629 D630 P631 N632 Q633 Y634 Q635 Q636 D637 M638 T639 N640 T641 I642 Q643 N644 G645 A646 E647 D648 V649 Y650 E651 T652 F653 N654 I655 I656 M657 R658 R659 K660
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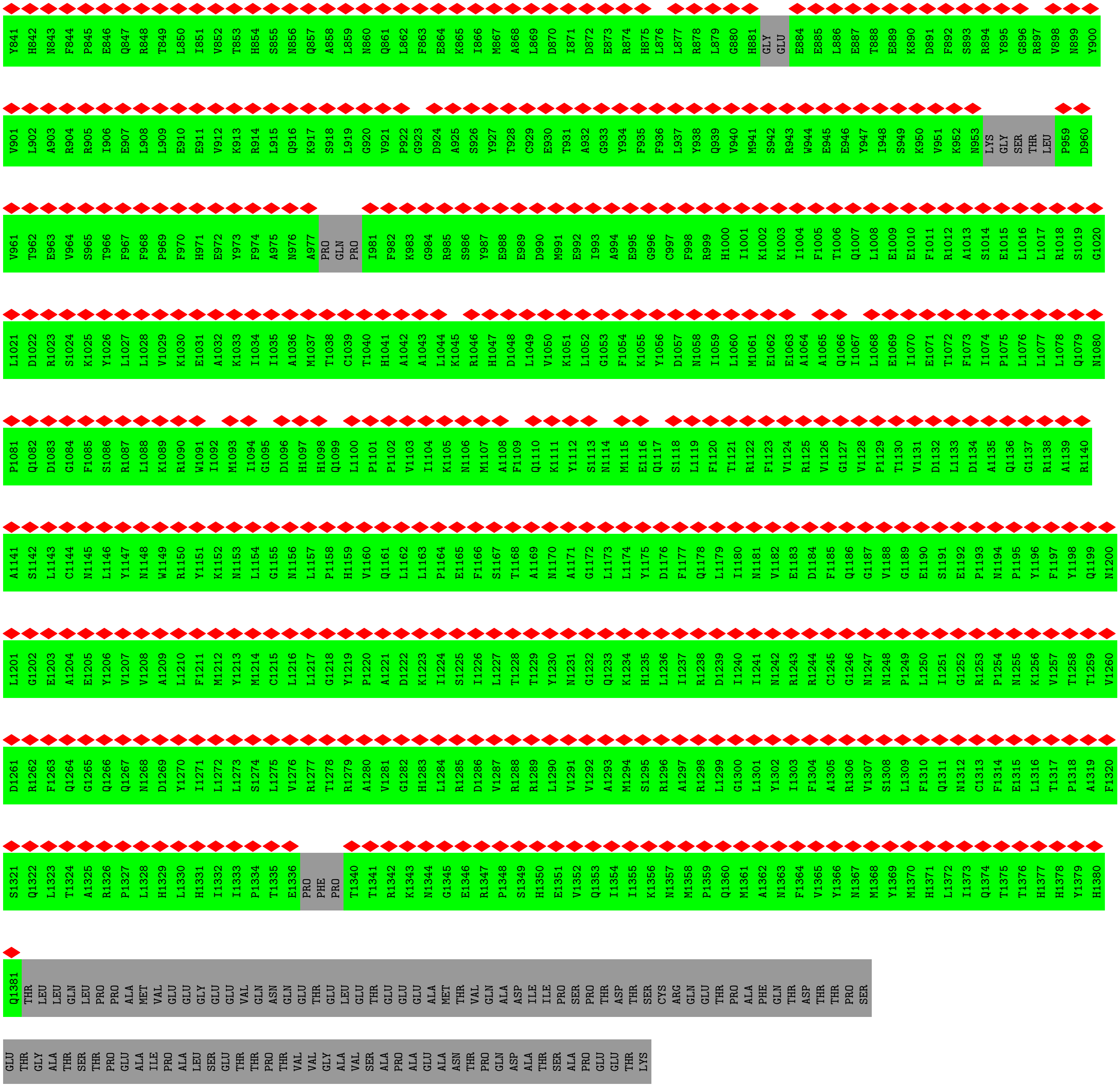
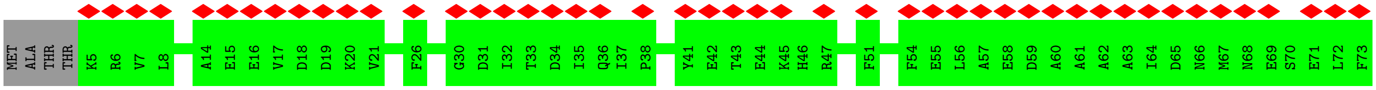
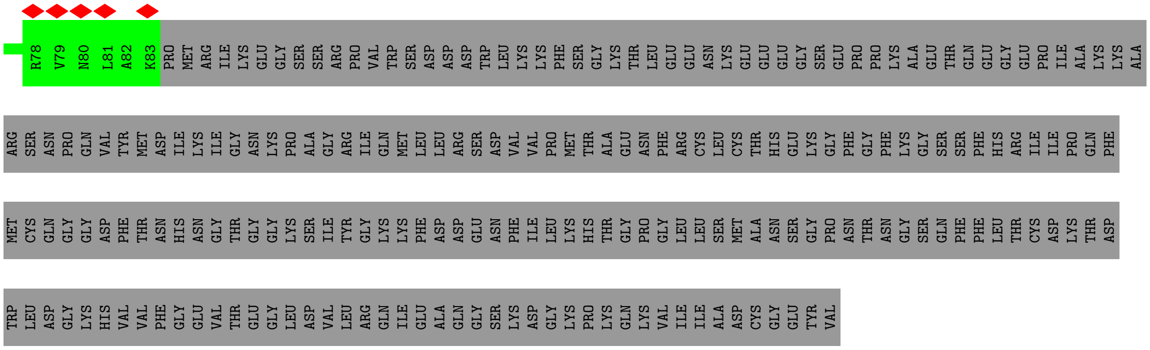


- Molecule 32: Peptidyl-prolyl cis-trans isomerase E

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V79
N80
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 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 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

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	390072	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.543	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z| >5$	RMSZ	$\#|Z| >5$
1	A	0.41	0/16926	0.64	9/22947 (0.0%)
2	B	0.54	1/2296 (0.0%)	1.09	15/3569 (0.4%)
3	C	0.33	0/7181	0.65	3/9758 (0.0%)
4	E	0.32	0/2420	0.64	1/3281 (0.0%)
5	F	0.64	0/2323	1.14	11/3619 (0.3%)
6	J	0.43	0/3802	0.59	6/5162 (0.1%)
7	L	0.35	0/3267	0.61	9/4418 (0.2%)
8	M	0.33	0/1119	0.59	1/1497 (0.1%)
9	N	0.99	6/1210 (0.5%)	0.74	0/1622
10	O	0.39	0/2390	0.62	3/3227 (0.1%)
11	P	0.36	0/1000	0.58	0/1330
12	R	0.38	0/2186	0.71	4/2937 (0.1%)
13	S	0.33	0/1268	0.61	2/1714 (0.1%)
14	T	0.55	1/2562 (0.0%)	0.74	0/3492
15	W	0.47	0/3038	0.72	3/4171 (0.1%)
16	G	0.74	5/1378 (0.4%)	1.46	31/2133 (1.5%)
17	H	0.81	20/3308 (0.6%)	1.37	64/5135 (1.2%)
18	U	0.37	0/2928	0.71	4/3928 (0.1%)
19	I	0.34	0/2803	0.58	11/3870 (0.3%)
20	a	0.47	0/397	0.62	0/549
20	h	0.47	0/396	0.61	0/547
21	b	0.51	0/423	0.72	0/587
21	i	0.50	0/423	0.73	0/587
22	c	0.57	0/405	0.73	0/563
22	j	0.57	0/405	0.73	0/563
23	d	0.69	0/479	0.85	0/666
23	k	0.70	0/420	0.85	0/583
24	f	0.75	0/360	0.81	0/497
24	m	0.75	0/360	0.81	0/497
25	e	0.65	0/390	0.80	0/542
25	l	0.64	0/390	0.80	0/542
26	g	0.54	0/362	0.71	0/501

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	n	0.53	0/327	0.72	0/451
27	q	0.35	0/658	0.58	3/919 (0.3%)
27	r	0.33	0/653	0.56	2/912 (0.2%)
27	s	0.26	0/334	0.37	0/466
27	t	0.31	0/334	0.38	0/466
28	K	0.39	1/753 (0.1%)	0.53	3/1046 (0.3%)
29	o	0.64	0/803	1.49	5/1119 (0.4%)
30	p	0.62	0/463	1.27	0/643
31	Q	0.21	0/6565	0.42	0/9143
32	y	0.25	0/389	0.62	0/540
All	All	0.46	34/79894 (0.0%)	0.76	190/110739 (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
1	A	0	16
3	C	0	6
4	E	0	1
5	F	0	1
6	J	0	1
9	N	0	1
12	R	0	8
14	T	0	5
15	W	0	3
16	G	0	5
17	H	0	1
18	U	0	6
23	d	0	1
23	k	0	1
All	All	0	56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	137	CYS	CB-SG	-11.04	1.63	1.82
9	N	119	CYS	CB-SG	-8.86	1.67	1.82
9	N	142	CYS	CB-SG	-8.41	1.68	1.82
9	N	101	CYS	CB-SG	-8.37	1.68	1.82
17	H	77	C	C1'-N1	7.34	1.59	1.48

The worst 5 of 190 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	147	C	O5'-P-OP1	-13.09	93.92	105.70
16	G	5	G	N3-C4-C5	-12.87	122.16	128.60
16	G	17	U	N1-C2-O2	9.52	129.47	122.80
16	G	2	U	N1-C1'-C2'	9.23	126.00	114.00
16	G	17	U	N3-C2-O2	-8.73	116.09	122.20

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1019	TYR	Peptide
1	A	107	PRO	Peptide
1	A	135	VAL	Peptide
1	A	320	TYR	Peptide
1	A	940	ILE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16477	0	16462	234	0
2	B	2060	0	1044	79	0
3	C	7022	0	7047	163	0
4	E	2366	0	2303	70	0
5	F	2075	0	1048	43	0
6	J	3758	0	2888	46	0
7	L	3237	0	2680	38	0
8	M	1098	0	1082	16	0
9	N	1184	0	1189	11	0
10	O	2340	0	2316	45	0
11	P	985	0	965	14	0
12	R	2165	0	2214	36	0
13	S	1236	0	1210	28	0
14	T	2496	0	2446	46	0
15	W	3008	0	1977	60	0
16	G	1246	0	631	212	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	H	2968	0	1504	256	0
18	U	2864	0	2814	80	0
19	I	2822	0	1319	64	0
20	a	399	0	173	0	0
20	h	398	0	172	0	0
21	b	424	0	179	0	0
21	i	424	0	179	0	0
22	c	406	0	170	0	0
22	j	406	0	170	0	0
23	d	480	0	200	0	0
23	k	422	0	175	0	0
24	f	361	0	158	0	0
24	m	361	0	158	0	0
25	e	391	0	163	0	0
25	l	391	0	163	0	0
26	g	363	0	160	0	0
26	n	329	0	138	0	0
27	q	659	0	296	0	0
27	r	654	0	294	0	0
27	s	335	0	168	0	0
27	t	335	0	168	0	0
28	K	757	0	338	18	0
29	o	804	0	350	0	0
30	p	464	0	205	0	0
31	Q	6562	0	2836	2	0
32	y	390	0	190	0	0
33	A	36	0	6	1	0
34	C	32	0	12	22	0
35	C	1	0	0	0	0
35	F	6	0	0	0	0
36	N	3	0	0	0	0
36	O	3	0	0	0	0
36	U	1	0	0	0	0
All	All	78004	0	60360	1359	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 11.

The worst 5 of 1359 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)
19:I:437:CYS:CB	19:I:447:GLU:CB	1.98	1.42
5:F:44:G:N2	16:G:3:A:C2	1.84	1.38
18:U:546:VAL:HG21	18:U:665:HIS:CE1	1.56	1.38
5:F:44:G:N2	16:G:3:A:H2	1.14	1.36
5:F:41:A:N6	16:G:6:A:H61	1.17	1.34

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1977/2335 (85%)	1793 (91%)	165 (8%)	19 (1%)	15	45
3	C	886/972 (91%)	788 (89%)	96 (11%)	2 (0%)	47	78
4	E	301/357 (84%)	280 (93%)	20 (7%)	1 (0%)	41	71
6	J	520/848 (61%)	473 (91%)	42 (8%)	5 (1%)	15	45
7	L	459/802 (57%)	423 (92%)	31 (7%)	5 (1%)	14	42
8	M	128/243 (53%)	116 (91%)	12 (9%)	0	100	100
9	N	141/144 (98%)	128 (91%)	12 (8%)	1 (1%)	22	54
10	O	288/420 (69%)	262 (91%)	25 (9%)	1 (0%)	41	71
11	P	114/229 (50%)	98 (86%)	15 (13%)	1 (1%)	17	48
12	R	268/536 (50%)	227 (85%)	38 (14%)	3 (1%)	14	42
13	S	157/166 (95%)	141 (90%)	16 (10%)	0	100	100
14	T	315/514 (61%)	292 (93%)	21 (7%)	2 (1%)	25	58
15	W	507/579 (88%)	433 (85%)	46 (9%)	28 (6%)	2	5
18	U	343/894 (38%)	277 (81%)	58 (17%)	8 (2%)	6	23
19	I	528/855 (62%)	491 (93%)	23 (4%)	14 (3%)	5	19
20	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	h	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
21	b	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
21	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
22	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
22	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
23	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
23	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
24	f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
24	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
25	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
25	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
26	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
26	n	63/76 (83%)	61 (97%)	2 (3%)	0	100	100
27	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	4	16
27	r	129/504 (26%)	119 (92%)	8 (6%)	2 (2%)	9	32
27	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	10	34
27	t	65/504 (13%)	64 (98%)	0	1 (2%)	10	34
28	K	144/225 (64%)	130 (90%)	8 (6%)	6 (4%)	3	10
29	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	12	37
30	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
31	Q	1308/1485 (88%)	1283 (98%)	25 (2%)	0	100	100
32	y	77/301 (26%)	75 (97%)	2 (3%)	0	100	100
All	All	10193/16097 (63%)	9369 (92%)	718 (7%)	106 (1%)	20	45

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1306	LYS
1	A	1367	ASN
1	A	1639	VAL
1	A	1653	ASP
1	A	1654	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1792/2108 (85%)	1767 (99%)	25 (1%)	67	89
3	C	787/866 (91%)	769 (98%)	18 (2%)	50	80
4	E	259/300 (86%)	254 (98%)	5 (2%)	57	84
6	J	242/751 (32%)	236 (98%)	6 (2%)	47	78
7	L	228/709 (32%)	225 (99%)	3 (1%)	69	90
8	M	117/209 (56%)	114 (97%)	3 (3%)	46	77
9	N	130/130 (100%)	129 (99%)	1 (1%)	81	94
10	O	259/361 (72%)	254 (98%)	5 (2%)	57	84
11	P	104/203 (51%)	101 (97%)	3 (3%)	42	76
12	R	227/457 (50%)	218 (96%)	9 (4%)	31	65
13	S	129/134 (96%)	127 (98%)	2 (2%)	62	86
14	T	273/441 (62%)	270 (99%)	3 (1%)	73	92
15	W	135/502 (27%)	133 (98%)	2 (2%)	65	87
18	U	313/806 (39%)	302 (96%)	11 (4%)	36	70
19	I	7/749 (1%)	2 (29%)	5 (71%)	0	0
All	All	5002/8726 (57%)	4901 (98%)	101 (2%)	57	82

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	M	134	GLN
12	R	165	VAL
19	I	526	MET
8	M	215	ASN
10	O	249	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
8	M	212	ASN
12	R	189	ASN
18	U	718	HIS
9	N	37	HIS
10	O	113	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	G	69/272 (25%)	55 (79%)	12 (17%)
17	H	133/188 (70%)	52 (39%)	8 (6%)
2	B	97/117 (82%)	44 (45%)	5 (5%)
5	F	96/107 (89%)	41 (42%)	6 (6%)
All	All	395/684 (57%)	192 (48%)	31 (7%)

5 of 192 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	8	G
2	B	9	G
2	B	10	U
2	B	11	U
2	B	20	G

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	G	16	G
17	H	46	U
16	G	133	A
17	H	50	C
17	H	30	A

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

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	$\#\|Z\| > 2$
12	SEP	R	224	12	8,9,10	0.85	0	8,12,14	2.02	1 (12%)
12	SEP	R	232	12	8,9,10	0.91	0	8,12,14	2.06	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
12	SEP	R	224	12	-	1/5/8/10	-
12	SEP	R	232	12	-	3/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	232	SEP	OG-CB-CA	5.17	113.17	108.14
12	R	224	SEP	OG-CB-CA	4.66	112.67	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	R	232	SEP	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	IHP	A	3000	-	36,36,36	0.70	0	54,60,60	0.97	0
34	GTP	C	1500	35	26,34,34	0.96	1 (3%)	32,54,54	1.46	4 (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
33	IHP	A	3000	-	-	8/30/54/54	0/1/1/1
34	GTP	C	1500	35	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	1500	GTP	C6-N1	-2.74	1.33	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	1500	GTP	PA-O3A-PB	-3.98	119.17	132.83
34	C	1500	GTP	PB-O3B-PG	-3.53	120.71	132.83
34	C	1500	GTP	C5-C6-N1	2.44	118.26	113.95
34	C	1500	GTP	C8-N7-C5	2.43	107.61	102.99

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	A	3000	IHP	C6-C1-O11-P1
33	A	3000	IHP	C4-O14-P4-O44
33	A	3000	IHP	C6-O16-P6-O26
34	C	1500	GTP	C5'-O5'-PA-O3A
33	A	3000	IHP	C2-C1-O11-P1

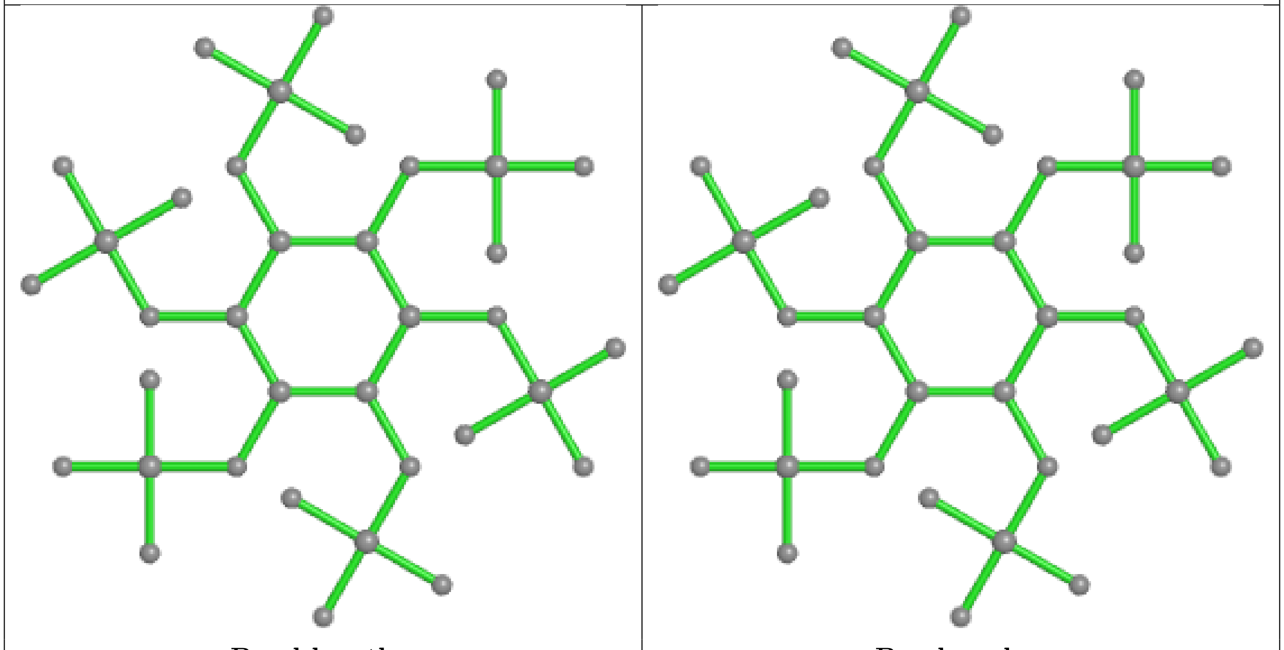
There are no ring outliers.

2 monomers are involved in 23 short contacts:

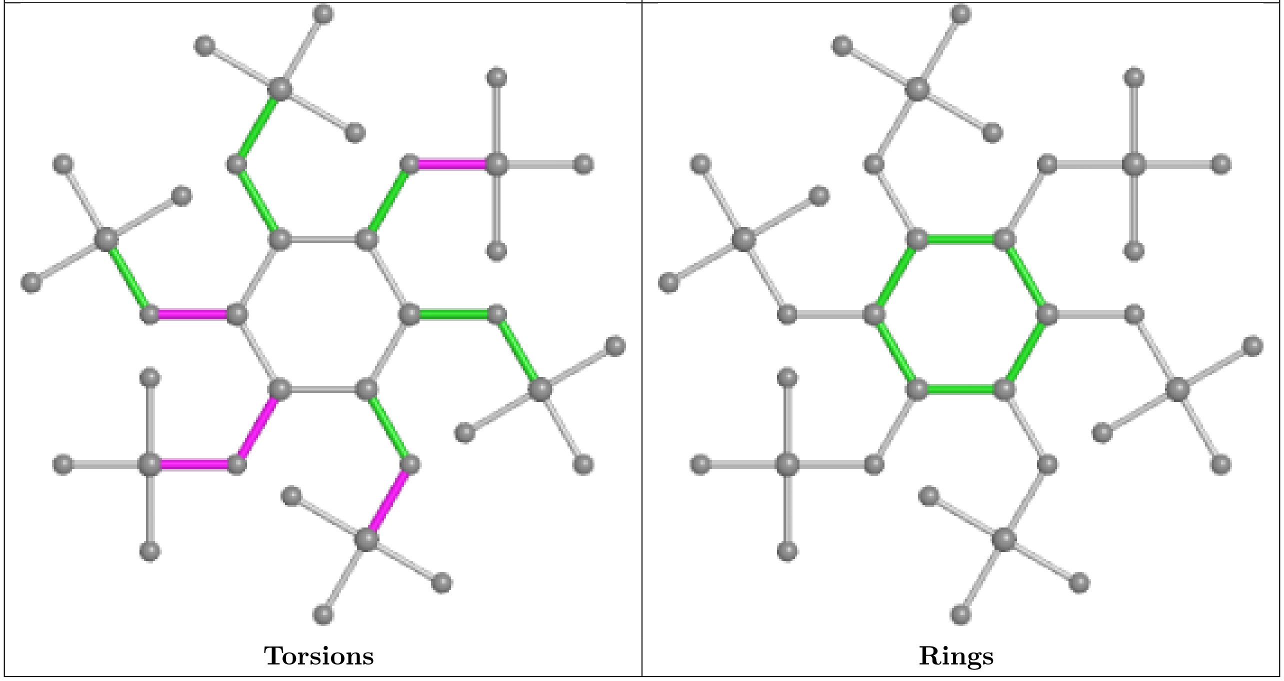
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	3000	IHP	1	0
34	C	1500	GTP	22	0

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

Ligand IHP A 3000

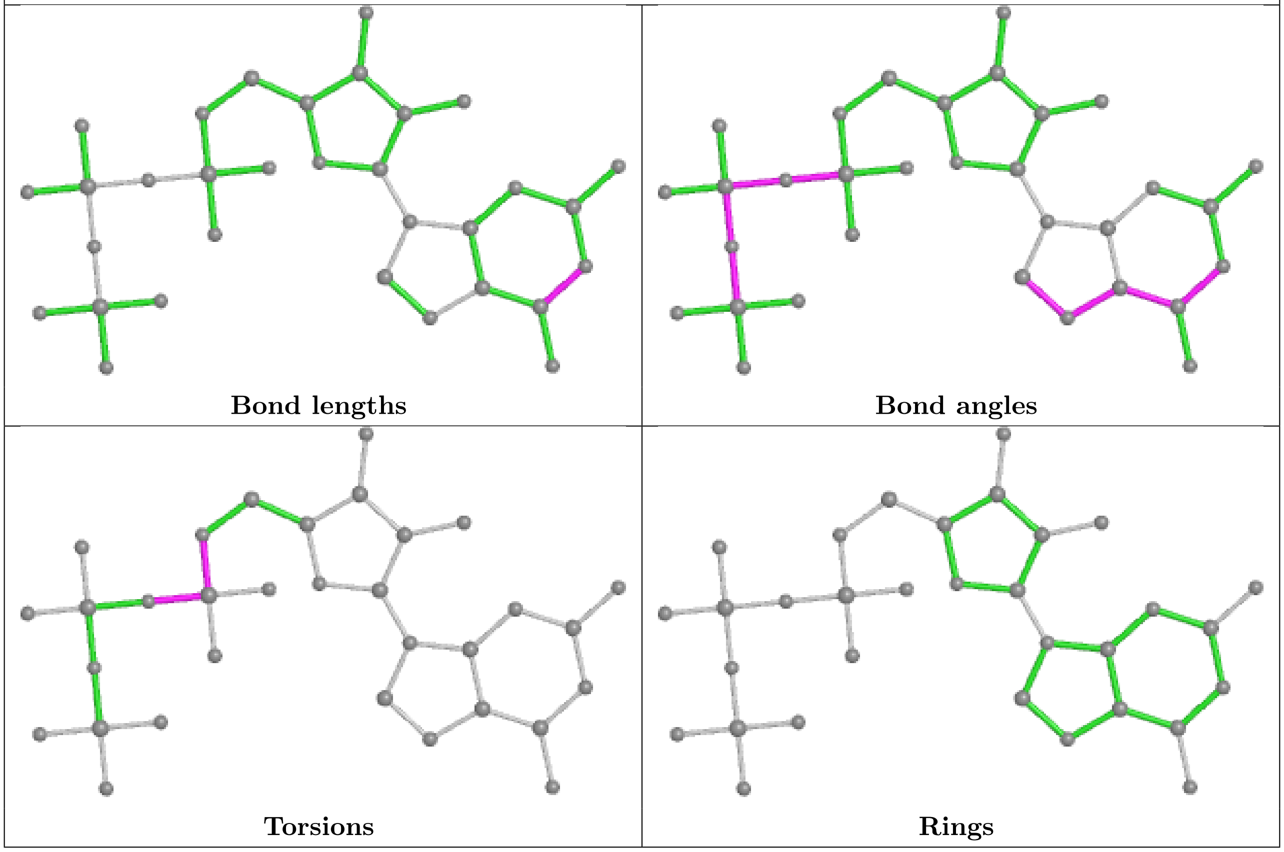


Bond lengths **Bond angles**



Torsions **Rings**

Ligand GTP C 1500



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

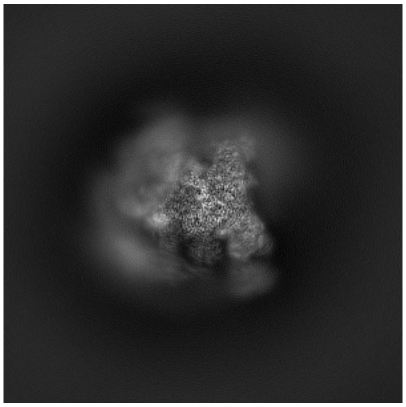
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-9646. These allow visual inspection of the internal detail of the map and identification of artifacts.

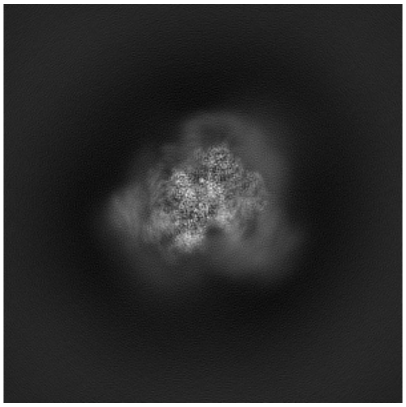
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

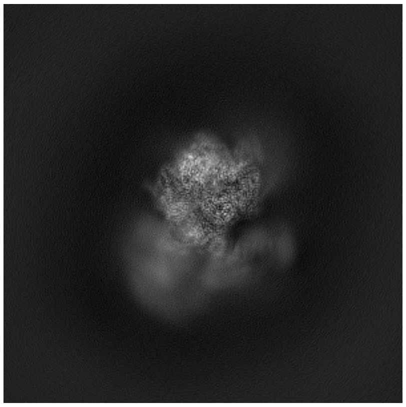
6.1.1 Primary map



X



Y

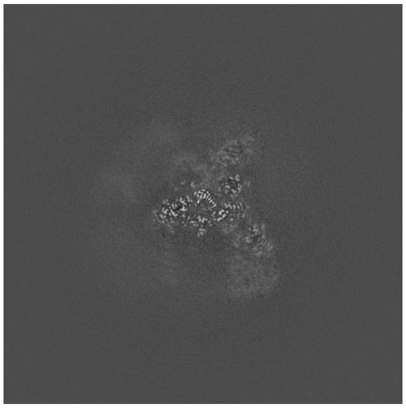


Z

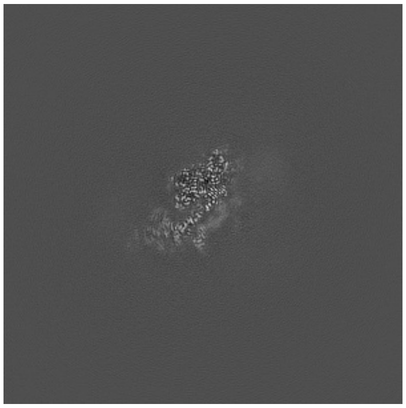
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

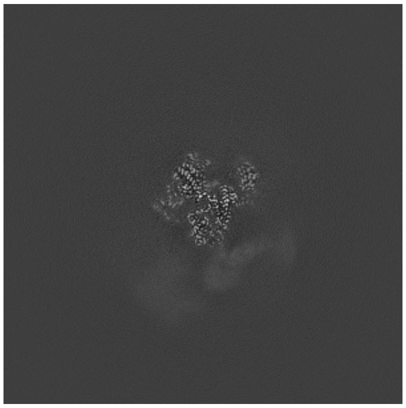
6.2.1 Primary map



X Index: 200



Y Index: 200

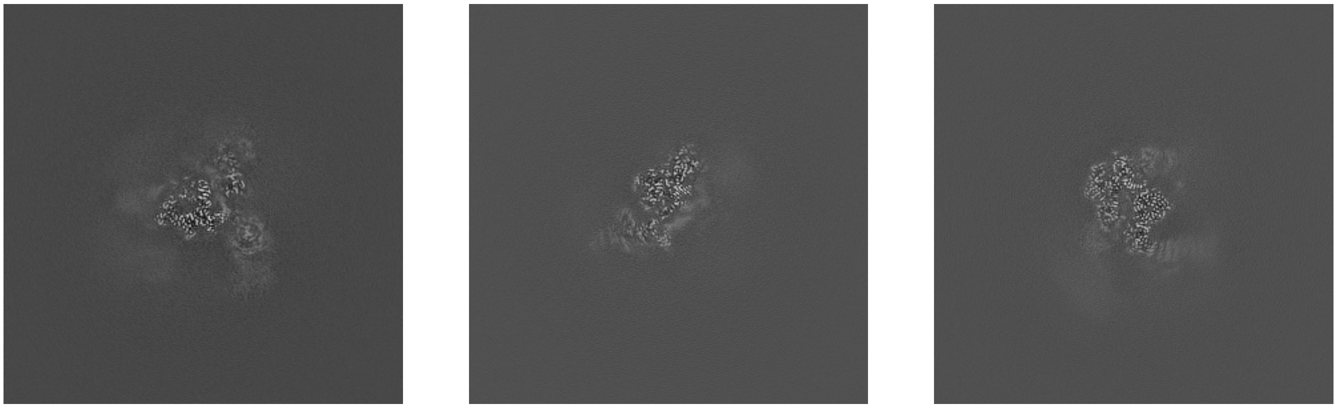


Z Index: 200

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

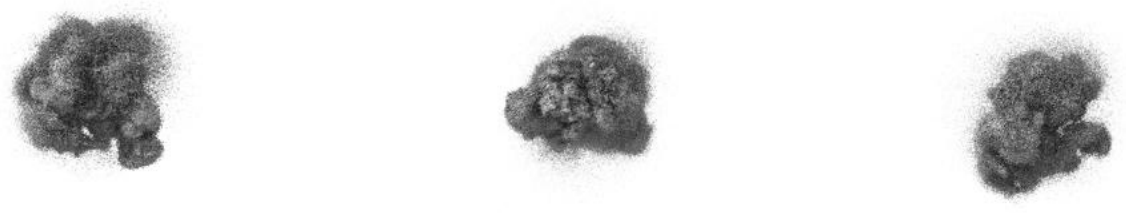


X Index: 210 Y Index: 201 Z Index: 185

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

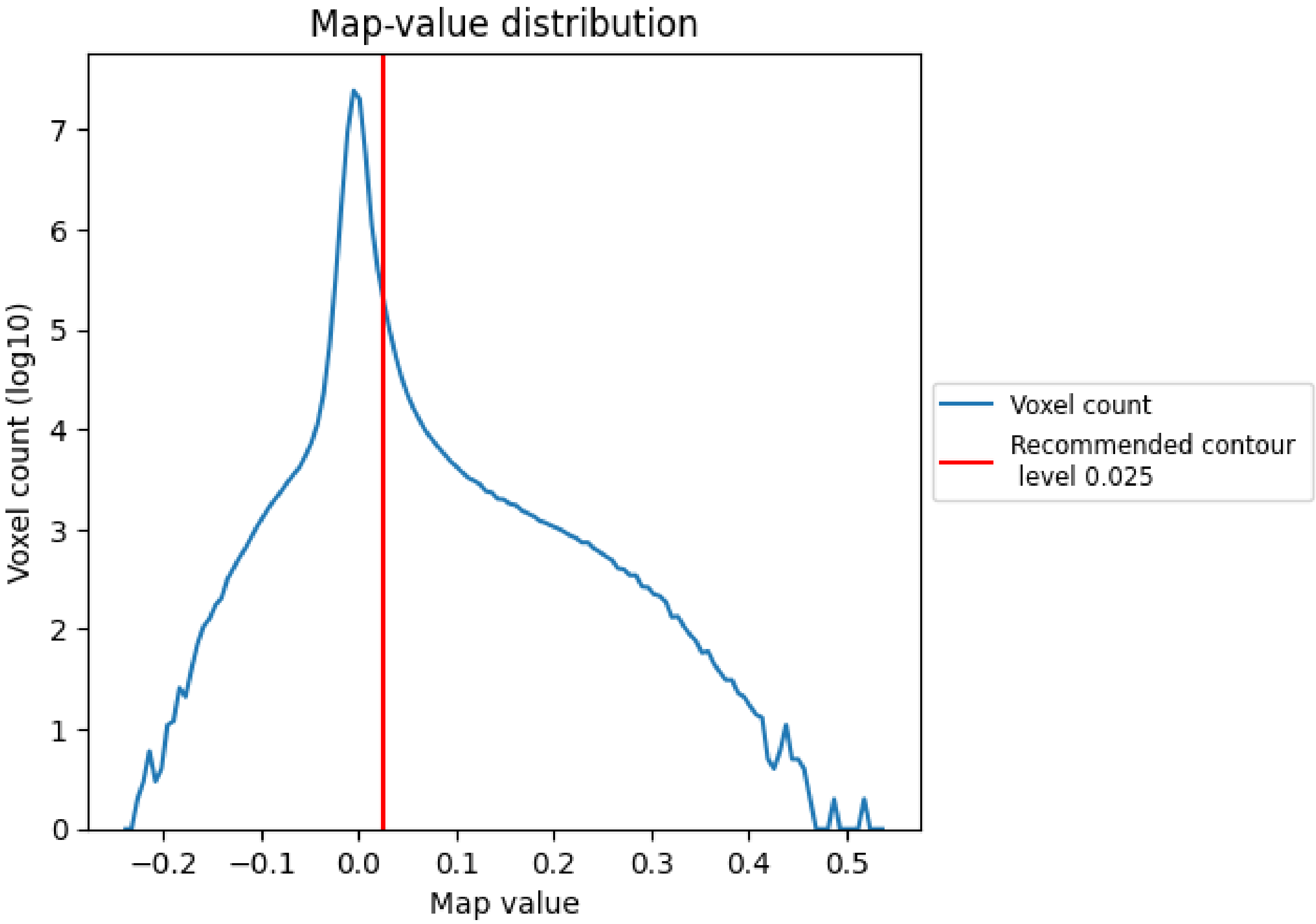
6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

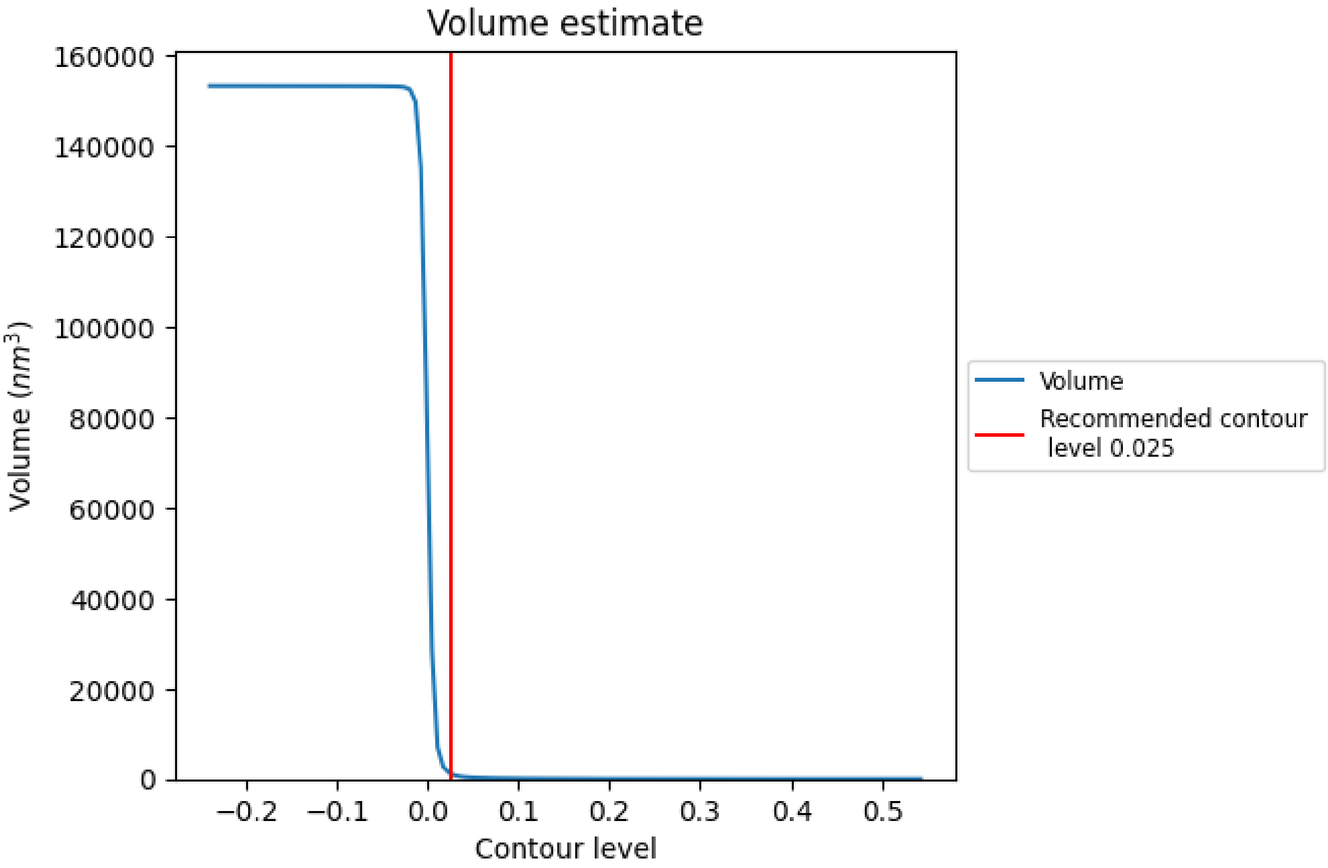
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

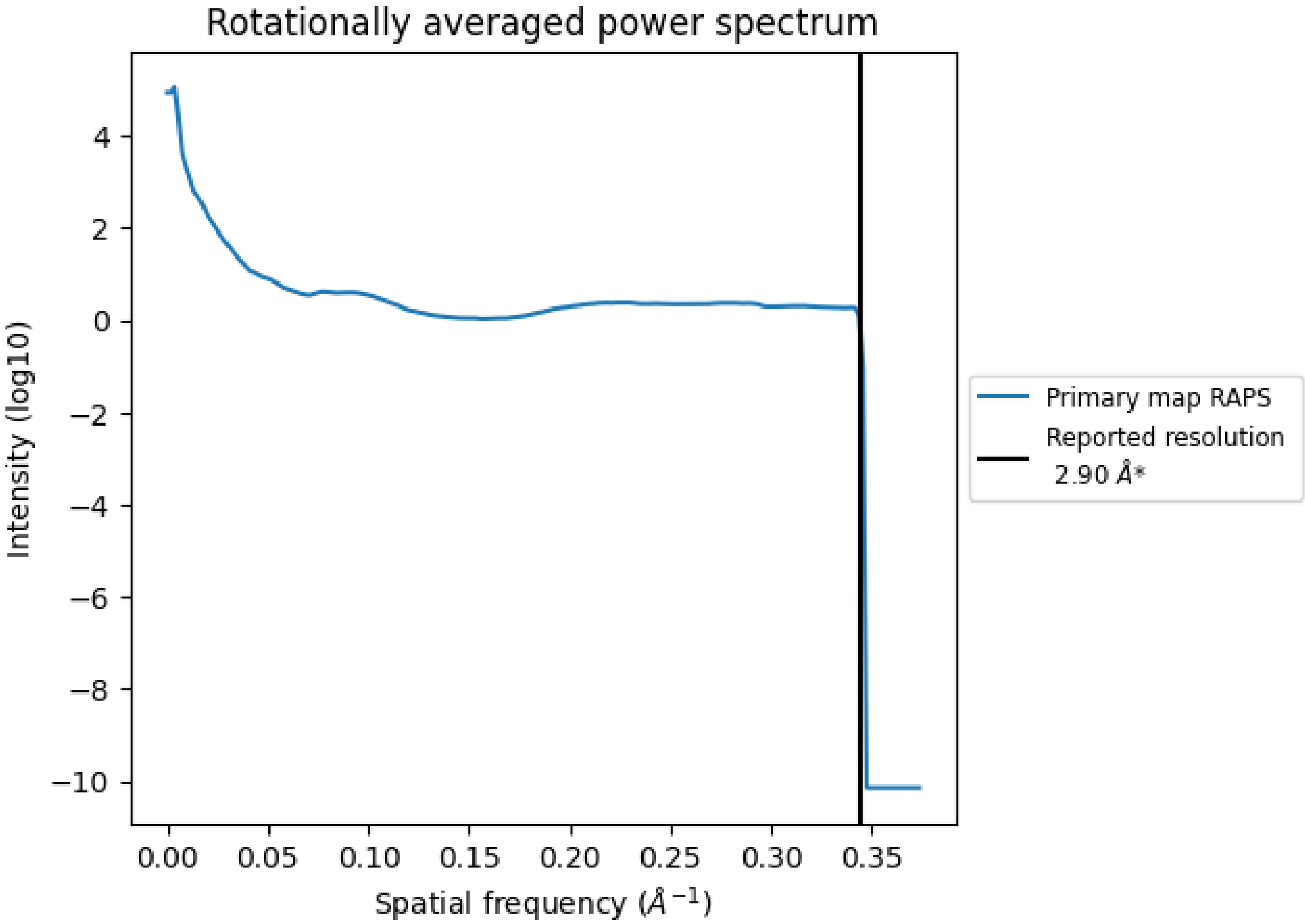
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1297 nm^3; this corresponds to an approximate mass of 1172 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

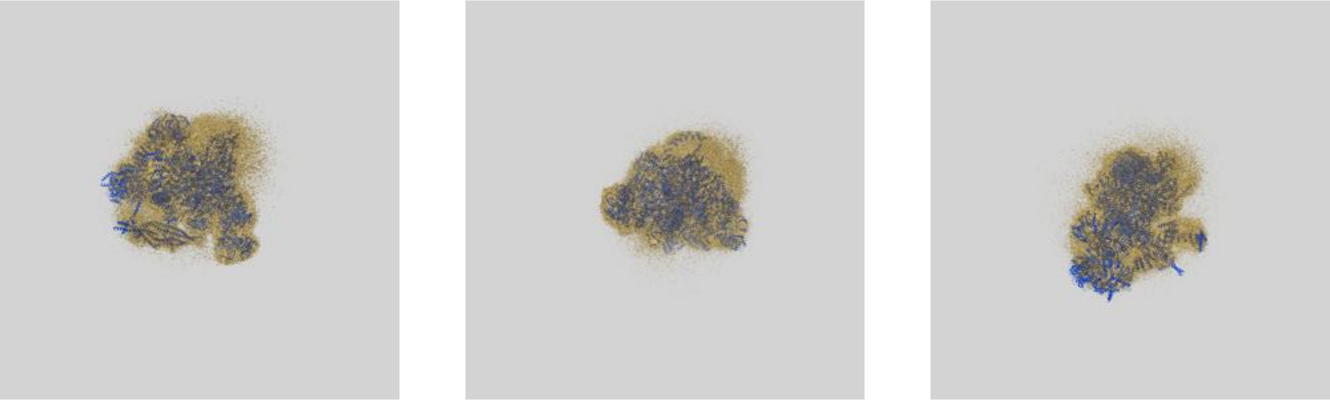
8 Fourier-Shell correlation

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-9646 and PDB model 6ID0. Per-residue inclusion information can be found in section 3 on page 12.

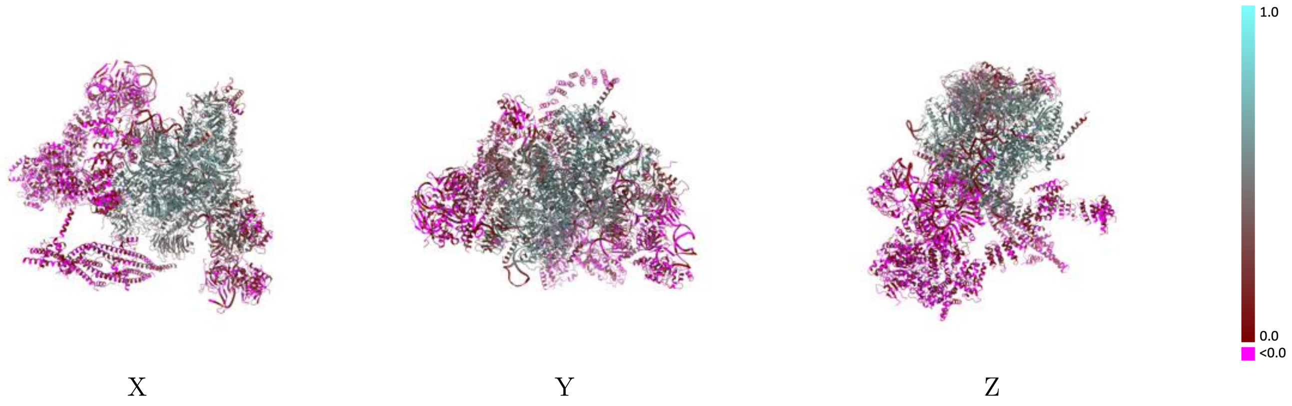
9.1 Map-model overlay ⓘ



X Y Z

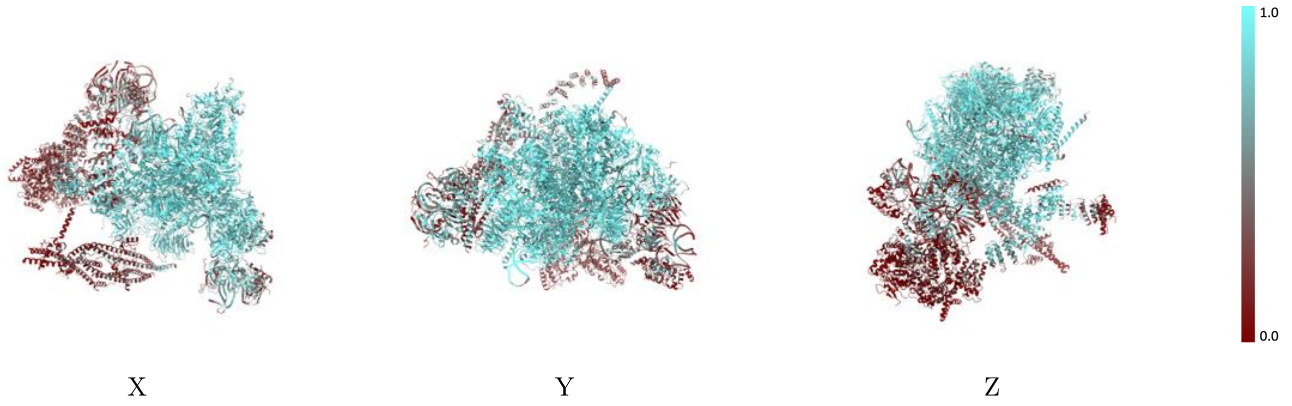
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



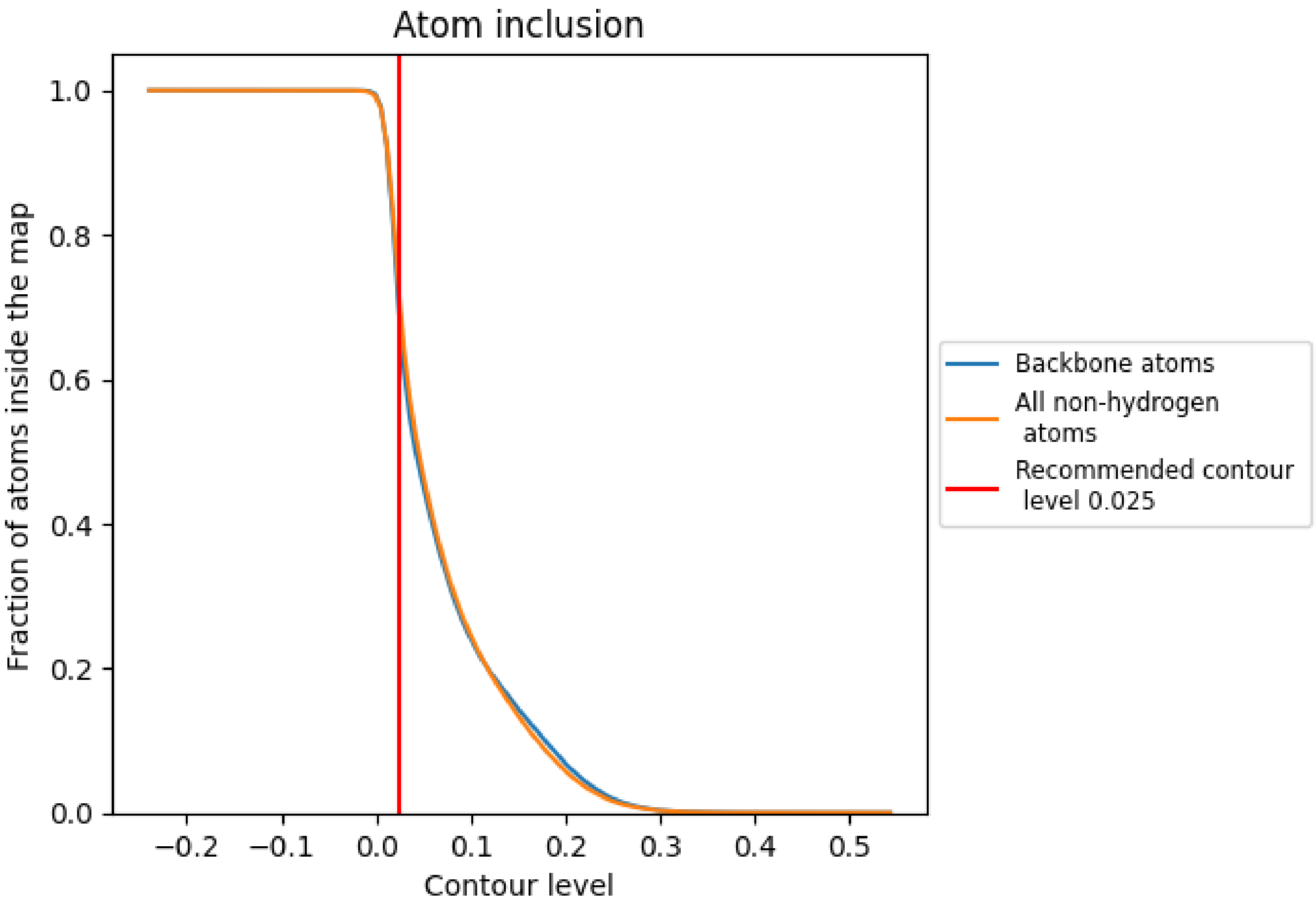
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 68% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7052	0.3140
A	0.9229	0.5020
B	0.8301	0.3370
C	0.8521	0.3270
E	0.8908	0.4110
F	0.9423	0.4650
G	0.6677	0.1420
H	0.5128	0.1100
I	0.5354	0.0560
J	0.7367	0.3250
K	0.2563	0.0580
L	0.6485	0.3380
M	0.8872	0.4960
N	0.9566	0.5500
O	0.8314	0.3930
P	0.8377	0.4610
Q	0.0687	-0.0050
R	0.8696	0.4660
S	0.9192	0.4670
T	0.9762	0.5980
U	0.8778	0.4540
W	0.8618	0.3360
a	0.6667	0.1900
b	0.4906	0.0340
c	0.6478	0.0540
d	0.6396	0.0330
e	0.4808	0.0550
f	0.4931	-0.0020
g	0.4848	0.0500
h	0.4698	0.0160
i	0.3656	0.0240
j	0.3522	-0.0110
k	0.3009	-0.0100
l	0.2532	-0.0090
m	0.3130	0.0350

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Chain	Atom inclusion	Q-score
n	🟫 0.3830	🟥 0.0330
o	🟫 0.1866	🟪 -0.0010
p	🟫 0.3728	🟥 0.0250
q	🟫 0.1153	🟥 0.0380
r	🟫 0.1850	🟥 0.0200
s	🟫 0.2328	🟥 0.0550
t	🟫 0.1403	🟥 0.0050
y	🟫 0.3923	🟥 0.0170