Full wwPDB EM Validation Report (i)

May 15, 2023 – 06:43 pm BST

PDB ID	:	5NRL
EMDB ID	:	EMD-3683
Title	:	Structure of a pre-catalytic spliceosome.
Authors	:	Plaschka, C.; Lin, P.-C.; Nagai, K.
Deposited on	:	2017-04-24
Resolution	:	7.20 Å(reported)

This is a Full wwPDB EM Validation 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:

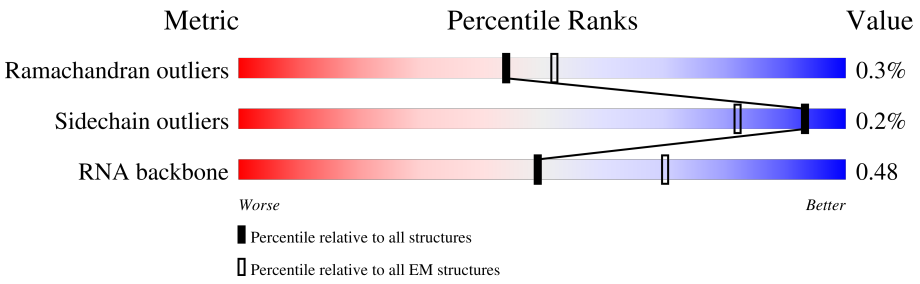
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 7.20 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	2	1175	9%; 5% 6% • 87%
2	3	89	31%; 87% 13%
3	4	160	•; 46% 24% • 29%
4	5	214	7%; 48% 31% 21%
5	6	112	•; 53% 32% 15%
6	7	115	26%; 57% 43%
7	8	109	20%; 59% 41%
8	A	2413	5%; 92% 8%

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Mol	Chain	Length	Quality of chain
9	B	2163	19% 78% 21%
10	C	1008	84% 16%
11	D	143	8% 99%
12	E	587	7% 21% 79%
13	F	494	5% 83% 16%
14	G	469	8% 79% 21%
15	H	465	92% 8%
16	I	95	21% 9% 69%
17	J	899	5% 88% 11%
18	K	126	8% 98%
19	L	194	56% 44%
20	M	242	7% 71% 28%
21	N	291	5% 29% 71%
22	O	971	21% 86% 14%
23	P	1361	26% 86% 13%
24	Q	435	21% 50% 49%
25	R	213	37% 81% 19%
26	S	107	16% 96%
27	T	530	77% 86% 13%
28	U	266	55% 73% 26%
29	V	280	45% 45% 55%
30	W	238	71% 62% 8% 29%
31	X	111	14% 27% 73%
32	Y	111	76% 74% 24%
33	Z	85	20% 96%

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Mol	Chain	Length	Quality of chain
34	a	95	23% 94% 5%
35	b	196	7% 36% 64%
35	k	196	16% 36% 64%
35	s	196	36% 36% 64%
36	d	101	12% 82% 18%
36	n	101	50% 79% 19%
36	v	101	81% 79% 19%
37	e	94	16% 82% 18%
37	p	94	31% 81% 18%
37	w	94	82% 81% 18%
38	f	86	20% 84% 16%
38	q	86	30% 85% 15%
38	x	86	85% 85% 15%
39	g	77	17% 92% 8%
39	r	77	66% 94%
39	y	77	97% 94%
40	h	146	7% 55% 45%
40	l	146	38% 66% 32%
40	t	146	49% 49% 51%
41	i	110	14% 84% 16%
41	m	110	35% 84% 16%
41	u	110	84% 84% 16%
42	j	187	18% 40% 60%
43	o	93	17% 81% 19%
44	z	86	34% 86% 14%

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 118701 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	155	3275	1464	552	1104	155	0	0

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	77	611	382	105	121	3	0	0

- Molecule 3 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	114	2423	1084	419	806	114	0	0

- Molecule 4 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	5	170	3615	1618	640	1188	169	0	0

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	6	95	2019	904	355	665	95	0	0

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	66	504	325	85	91	3	0	0

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	8	64	498	320	86	90	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A	2216	18122	11661	3103	3294	64	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	1699	13607	8720	2269	2564	54	1	0

- Molecule 10 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	850	6784	4392	1129	1237	26	0	0

- Molecule 11 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D	142	1164	736	202	215	11	0	0

- Molecule 12 is a protein called 66 kDa U4/U6.U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E	124	825	501	153	170	1	0	0

- Molecule 13 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	F	413	3238	2064	578	584	12	0	0

- Molecule 14 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	G	372	2835	1786	523	512	14	0	0

- Molecule 15 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	H	429	3396	2120	609	653	14	0	0

- Molecule 16 is a RNA chain called Yeast UBC4 gene for ubiquitin-conjugating enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	I	29	600	271	95	205	29	0	0

- Molecule 17 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	J	800	6485	4151	1106	1201	27	0	0

- Molecule 18 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	K	124	936	597	161	174	4	0	0

- Molecule 19 is a protein called 23 kDa U4/U6.U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	L	109	882	570	150	159	3	0	0

- Molecule 20 is a protein called Pre-mRNA-splicing factor 38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	M	174	1407	915	236	249	7	0	0

- Molecule 21 is a protein called Pre-mRNA-splicing factor SPP381.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	N	85	425	255	85	85	0	0

- Molecule 22 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	O	833	6612	4258	1121	1192	41	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	1186	9437	6034	1589	1763	51	0	0

- Molecule 24 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	220	1786	1157	307	313	9	0	0

- Molecule 25 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	173	1429	930	239	258	2	0	0

- Molecule 26 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	S	103	814	503	154	143	14	0	0

- Molecule 27 is a protein called Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	T	462	3915	2487	677	735	16	0	0

- Molecule 28 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	U	196	1488	933	258	291	6	0	0

- Molecule 29 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	V	127	1084	689	193	196	6	0	0

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	W	170	1383	866	253	257	7	0	0

- Molecule 31 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	X	30	150	90	30	30	0	0

- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Y	84	683	439	119	122	3	0	0

- Molecule 33 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Z	83	685	424	129	131	1	0	0

- Molecule 34 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	a	90	735	469	124	139	3	0	0

- Molecule 35 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	70	Total	C	N	O	S	0	0
			563	360	98	102	3		
35	k	70	Total	C	N	O	S	0	0
			563	360	98	102	3		
35	s	70	Total	C	N	O	S	0	0
			563	360	98	102	3		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	83	Total	C	N	O	S	0	0
			641	408	111	120	2		
36	n	82	Total	C	N	O	S	0	0
			632	402	109	119	2		
36	v	82	Total	C	N	O	S	0	0
			632	402	109	119	2		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	77	Total	C	N	O	S	0	0
			602	396	95	108	3		
37	p	77	Total	C	N	O	S	0	0
			602	396	95	108	3		
37	w	77	Total	C	N	O	S	0	0
			602	396	95	108	3		

- Molecule 38 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	72	Total	C	N	O	S	0	0
			578	371	101	105	1		
38	q	73	Total	C	N	O	S	0	0
			585	376	102	106	1		
38	x	73	Total	C	N	O	S	0	0
			585	376	102	106	1		

- Molecule 39 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	71	Total	C	N	O	S	0	0
			549	345	96	106	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	r	75	577	363	100	112	2	0	0
39	y	75	577	363	100	112	2	0	0

- Molecule 40 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	h	80	630	402	108	118	2	0	0
40	l	99	751	475	137	137	2	0	0
40	t	72	569	364	99	104	2	0	0

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	i	92	752	481	136	131	4	0	0
41	m	92	752	481	136	131	4	0	0
41	u	92	752	481	136	131	4	0	0

- Molecule 42 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	j	74	588	381	96	108	3	0	0

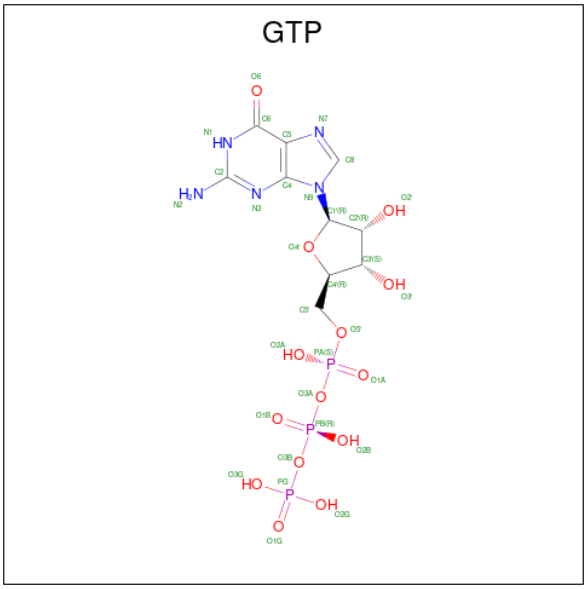
- Molecule 43 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	75	588	378	98	110	2	0	0

- Molecule 44 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	z	74	577	364	95	116	2	0	0

- Molecule 45 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	
45	C	1	32	10	5	14	3	0

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

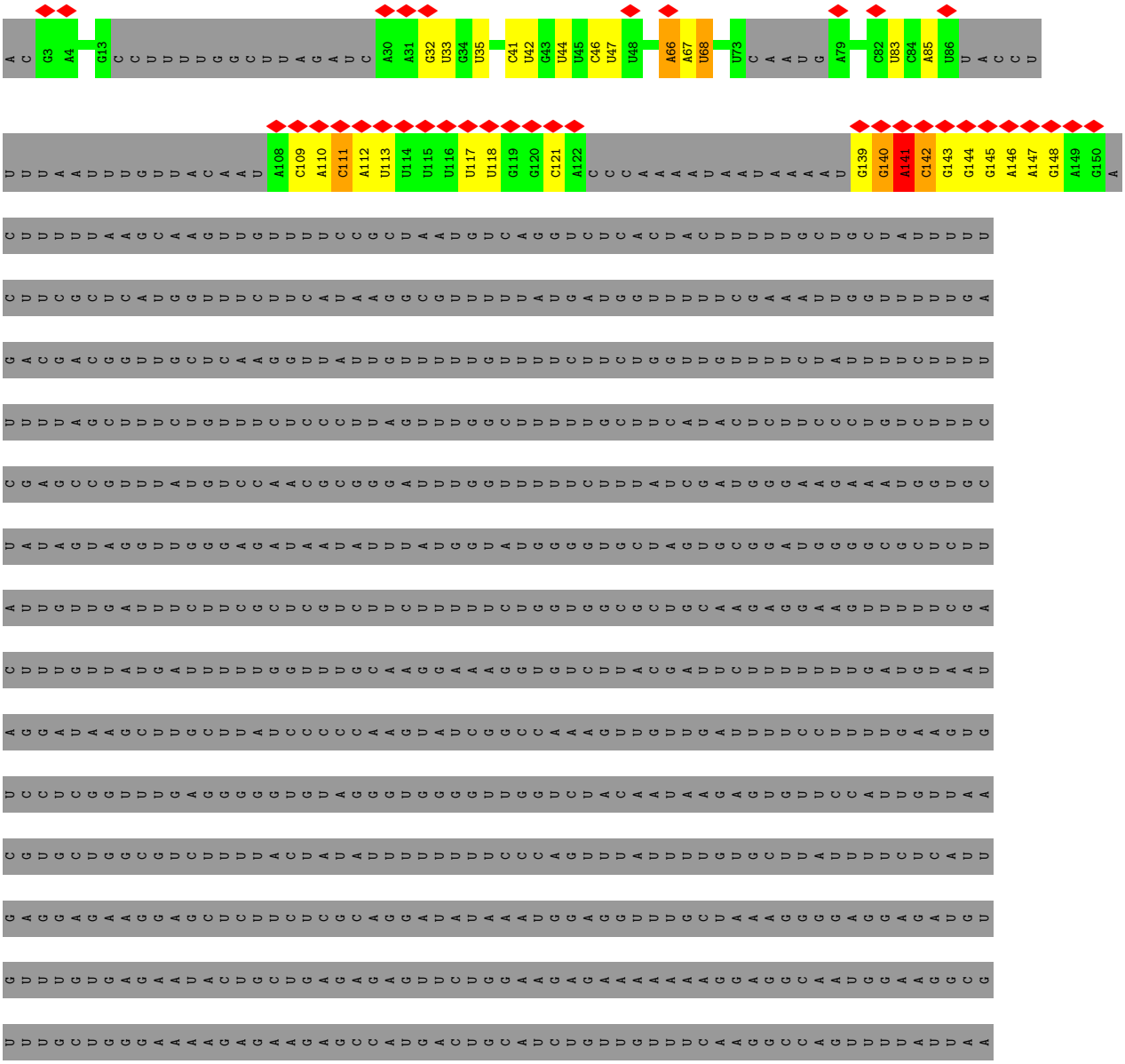
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
46	L	1	1	1	0
46	S	3	3	3	0
46	T	2	2	2	0
46	U	1	1	1	0

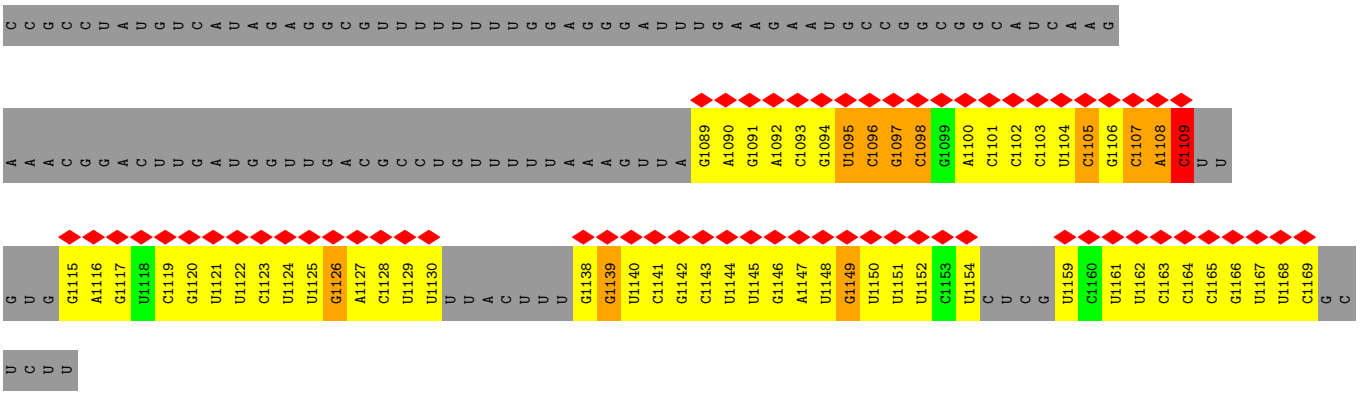
3 Residue-property plots (i)

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: U2 snRNA

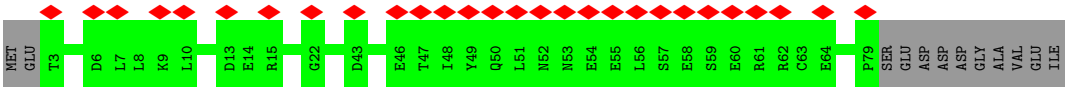
Chain 2:





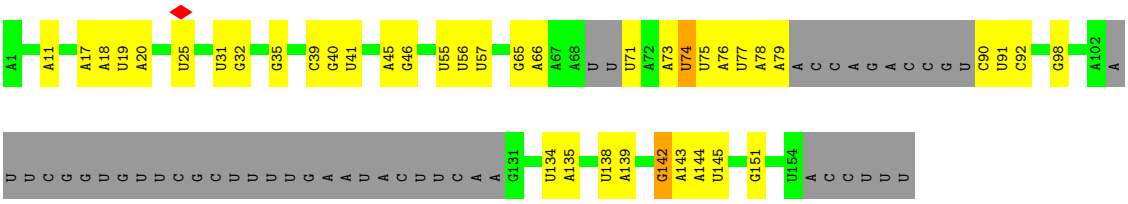
- Molecule 2: U6 snRNA-associated Sm-like protein LSm3

Chain 3:



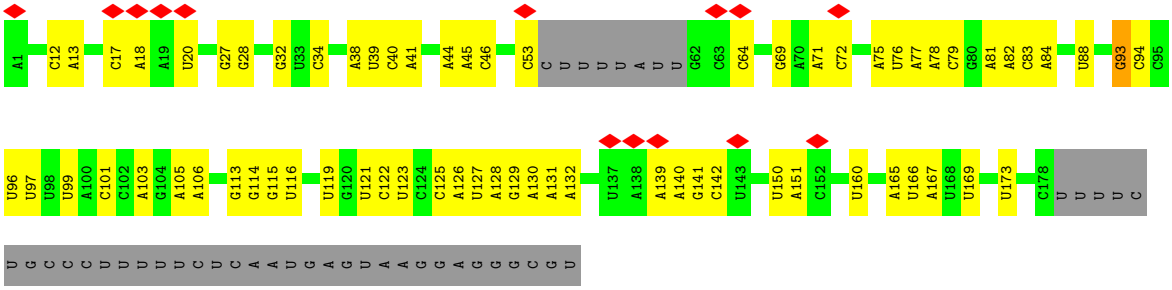
- Molecule 3: U4 snRNA

Chain 4:



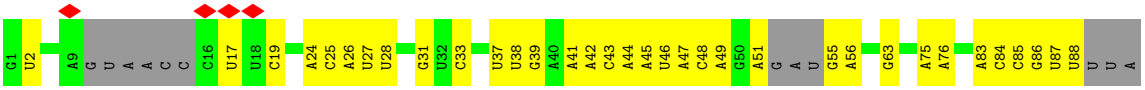
- Molecule 4: U5 snRNA

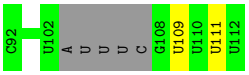
Chain 5:



- Molecule 5: U6 snRNA

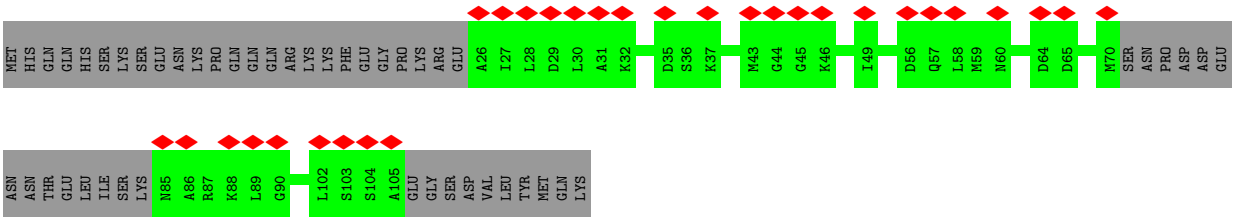
Chain 6:





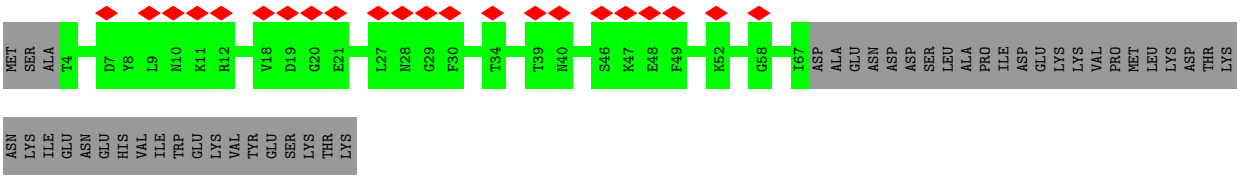
• Molecule 6: U6 snRNA-associated Sm-like protein LSm7

Chain 7:



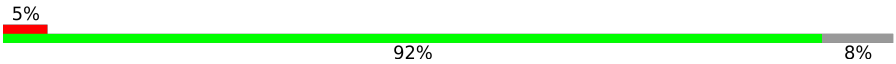
• Molecule 7: U6 snRNA-associated Sm-like protein LSm8

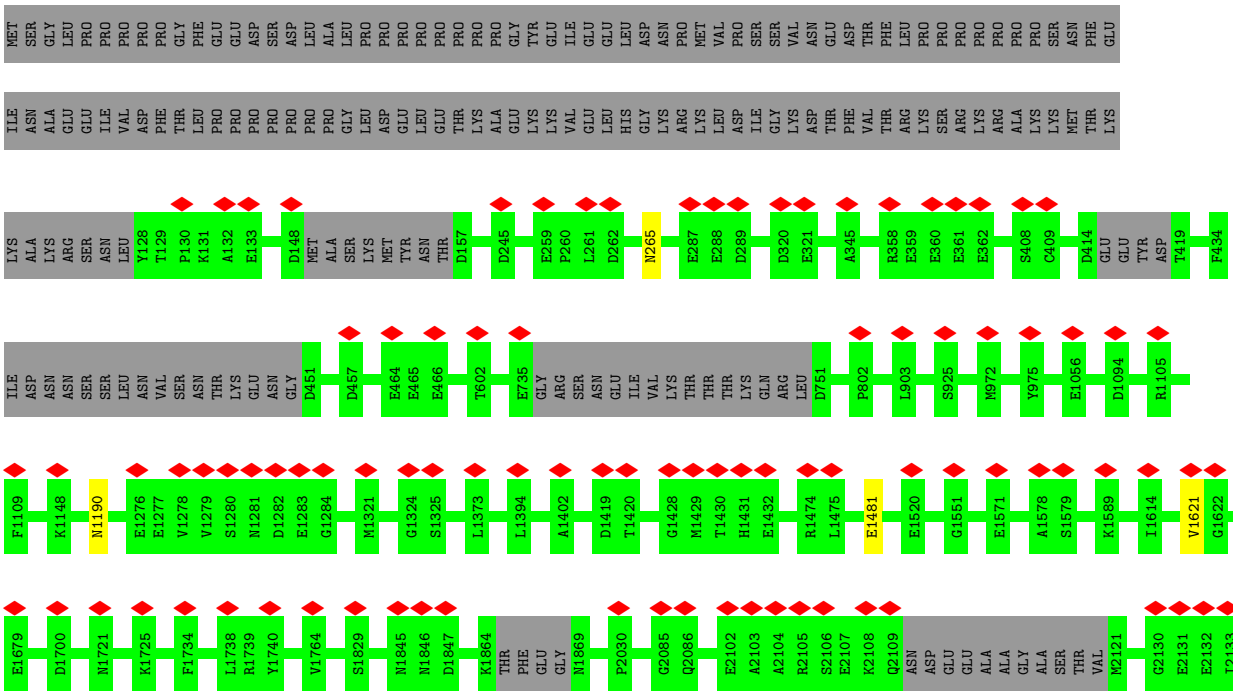
Chain 8:

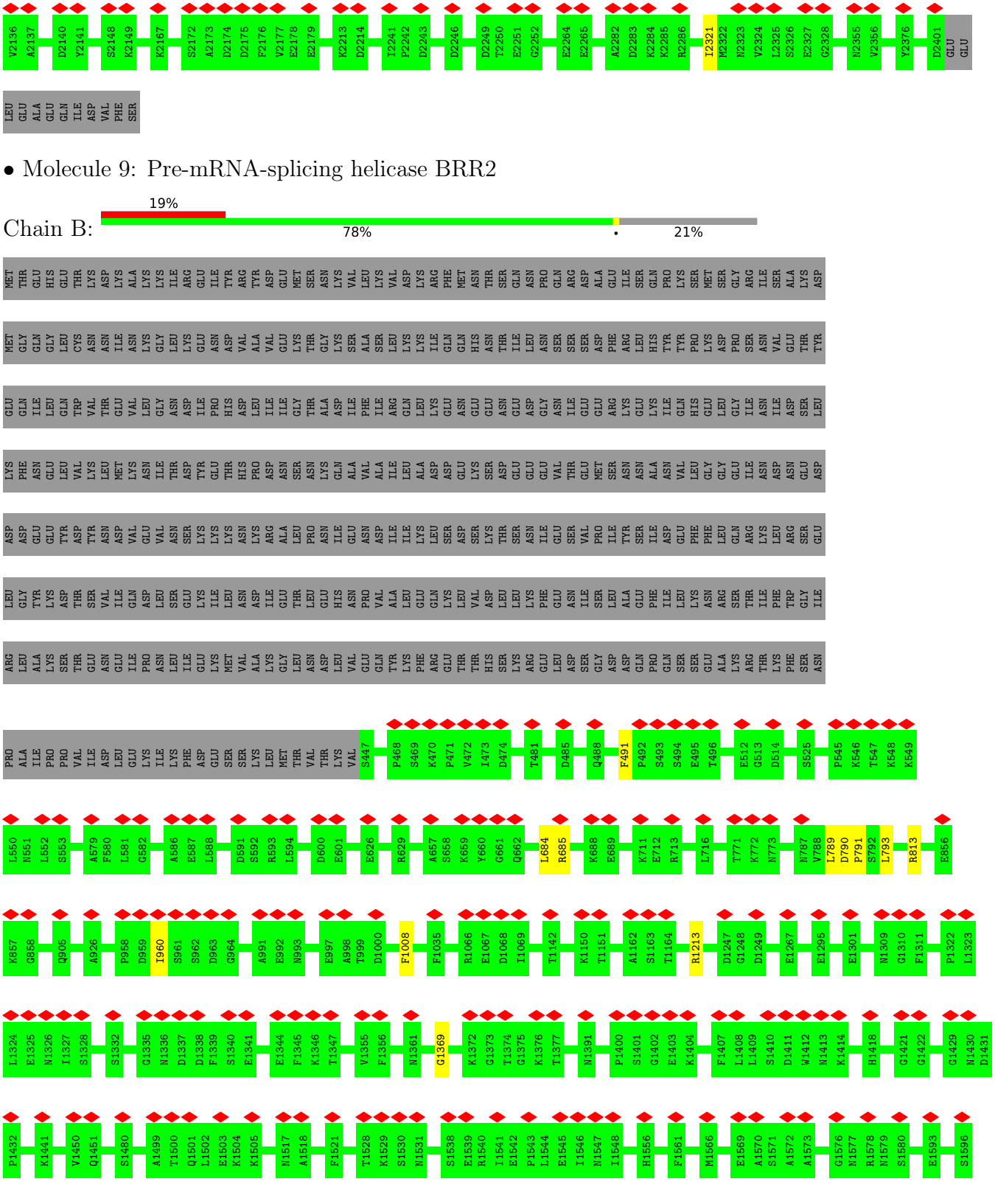


• Molecule 8: Pre-mRNA-splicing factor 8

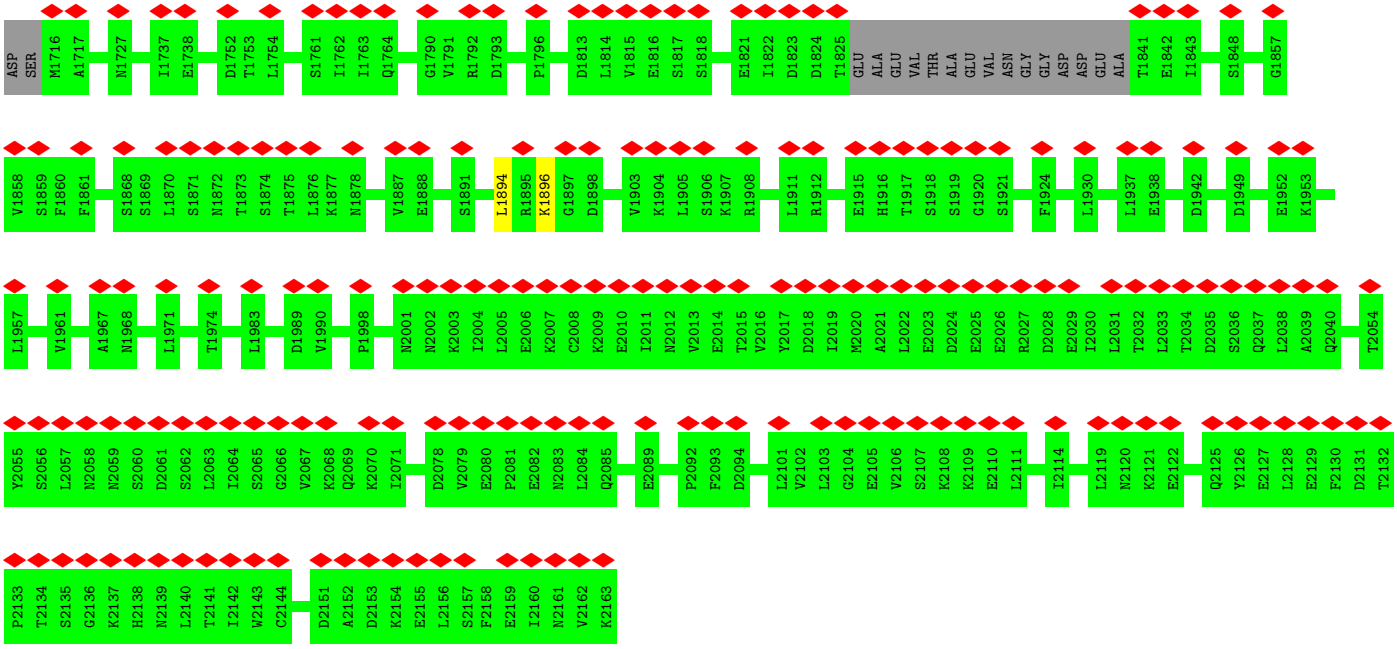
Chain A:





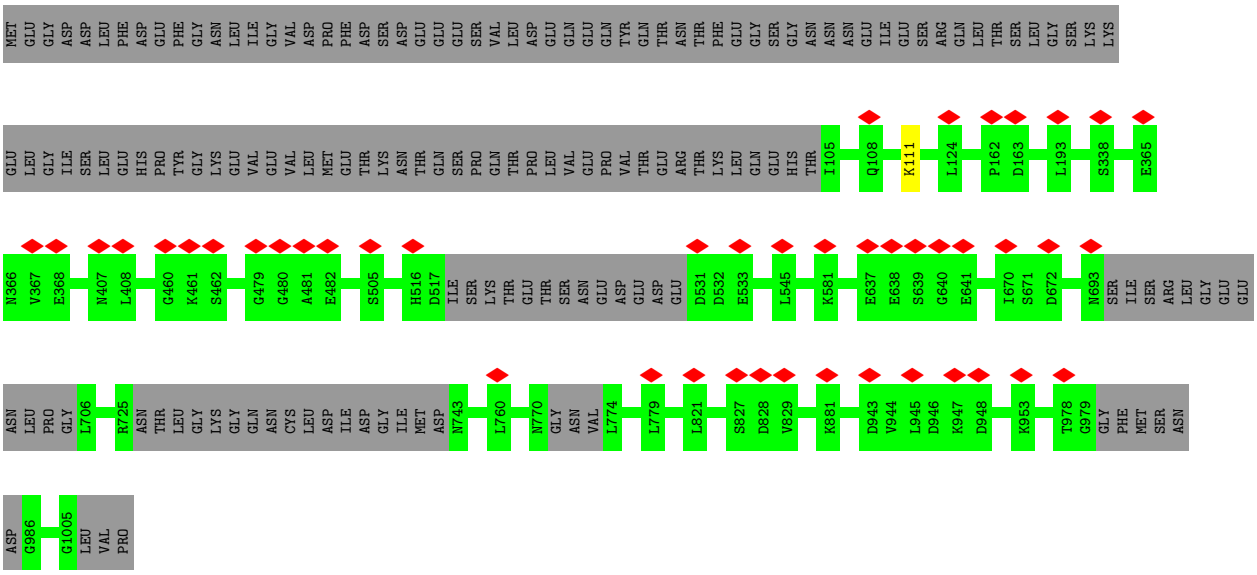


• Molecule 9: Pre-mRNA-splicing helicase BRR2



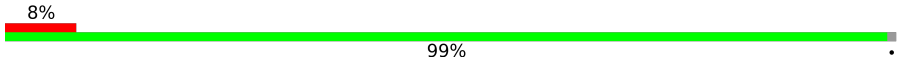
- Molecule 10: Pre-mRNA-splicing factor SNU114

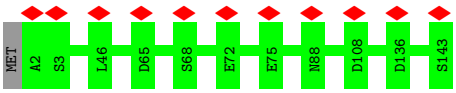
Chain C:



- Molecule 11: Spliceosomal protein DIB1

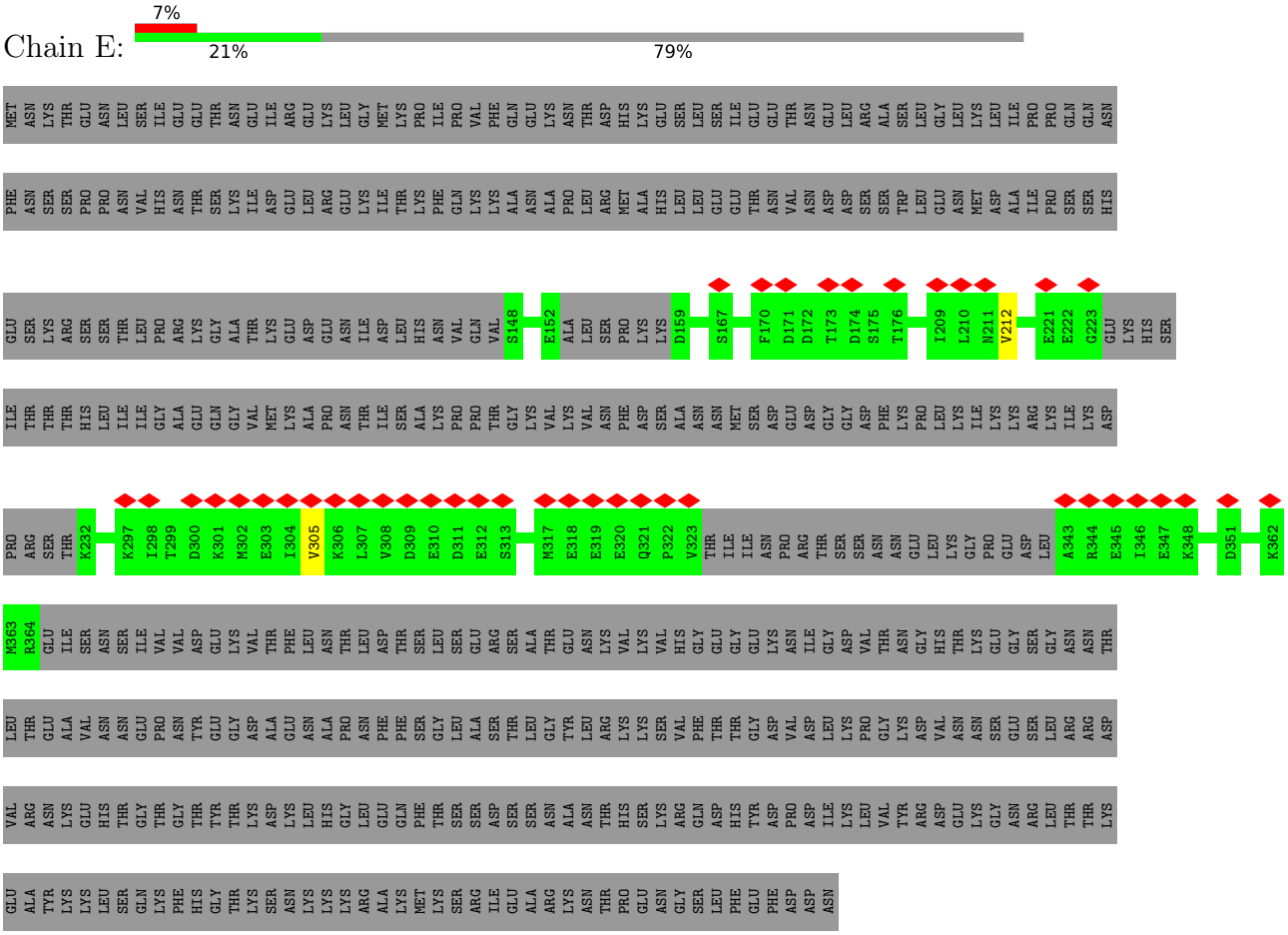
Chain D:





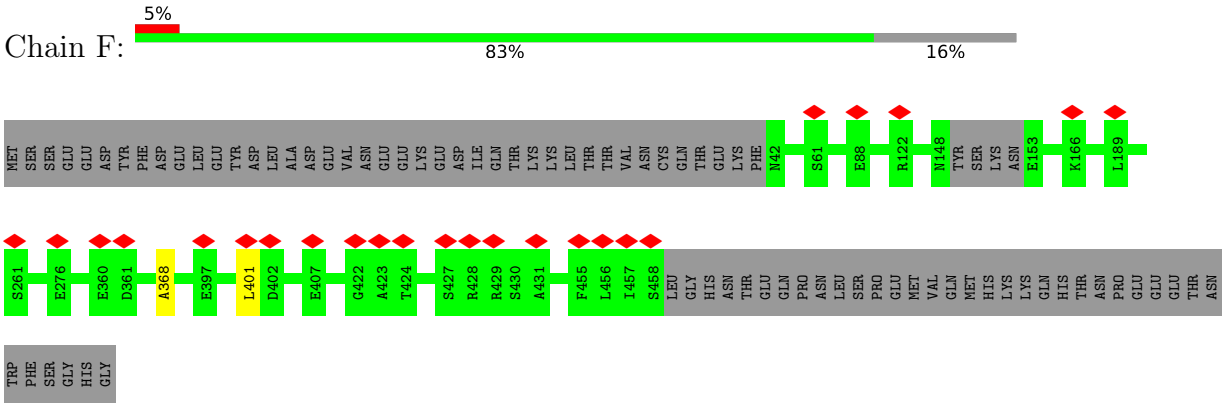
- Molecule 12: 66 kDa U4/U6.U5 small nuclear ribonucleoprotein component

Chain E:



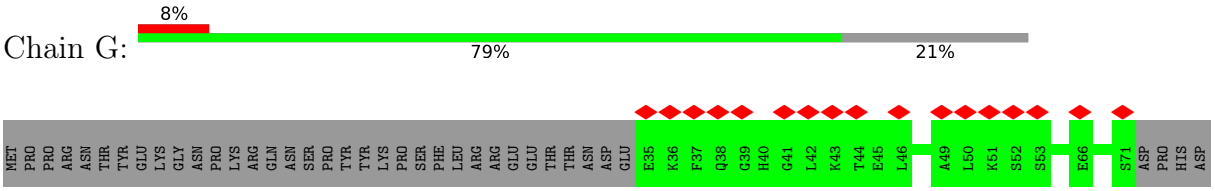
- Molecule 13: Pre-mRNA-processing factor 31

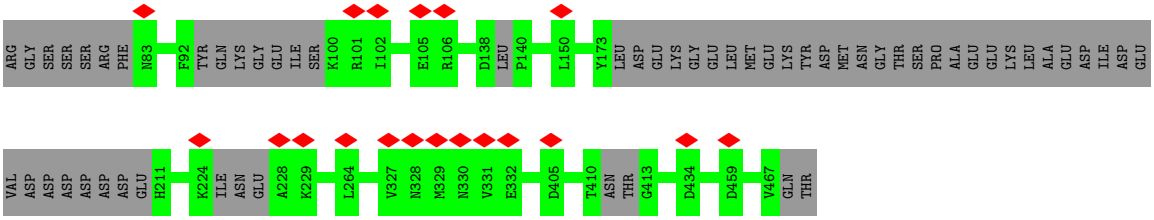
Chain F:



- Molecule 14: U4/U6 small nuclear ribonucleoprotein PRP3

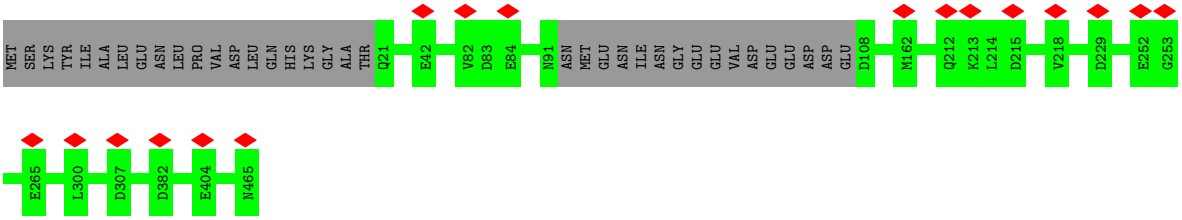
Chain G:





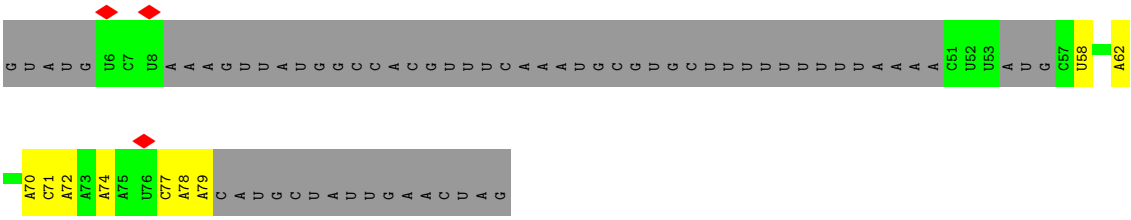
• Molecule 15: U4/U6 small nuclear ribonucleoprotein PRP4

Chain H:



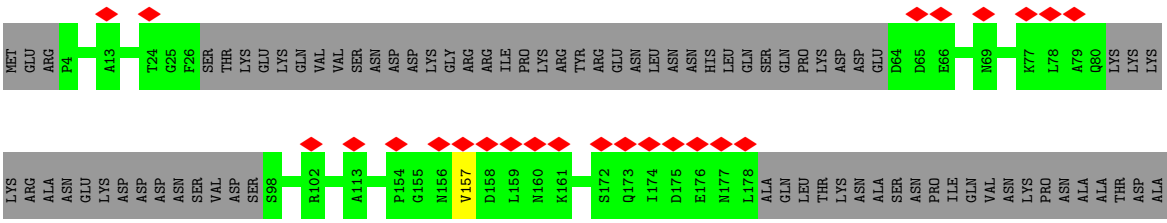
• Molecule 16: Yeast UBC4 gene for ubiquitin-conjugating enzyme

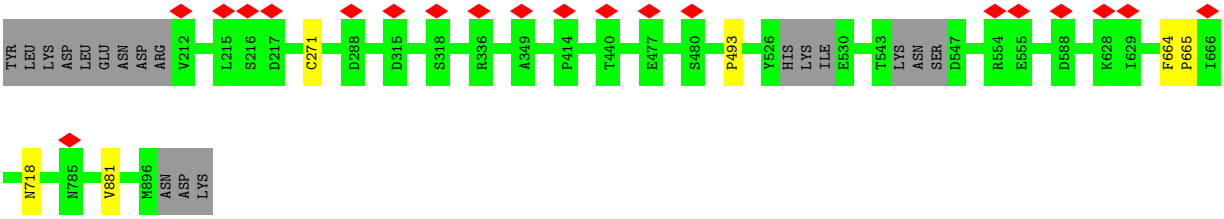
Chain I:



• Molecule 17: Pre-mRNA-splicing factor 6

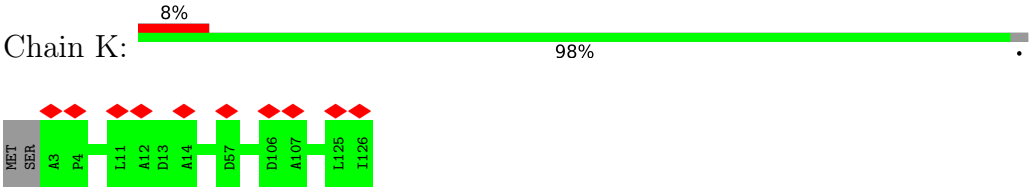
Chain J:





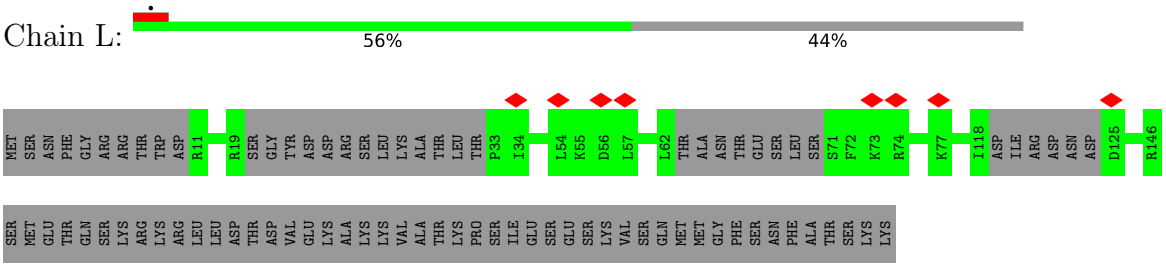
• Molecule 18: 13 kDa ribonucleoprotein-associated protein

Chain K:



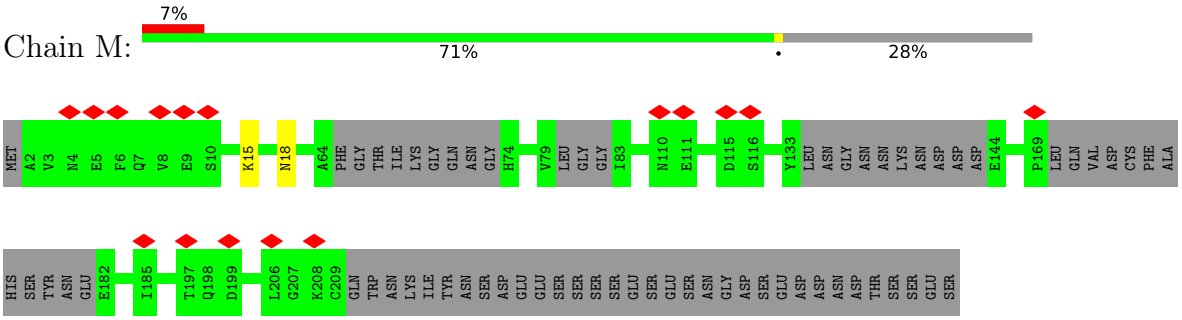
• Molecule 19: 23 kDa U4/U6.U5 small nuclear ribonucleoprotein component

Chain L:



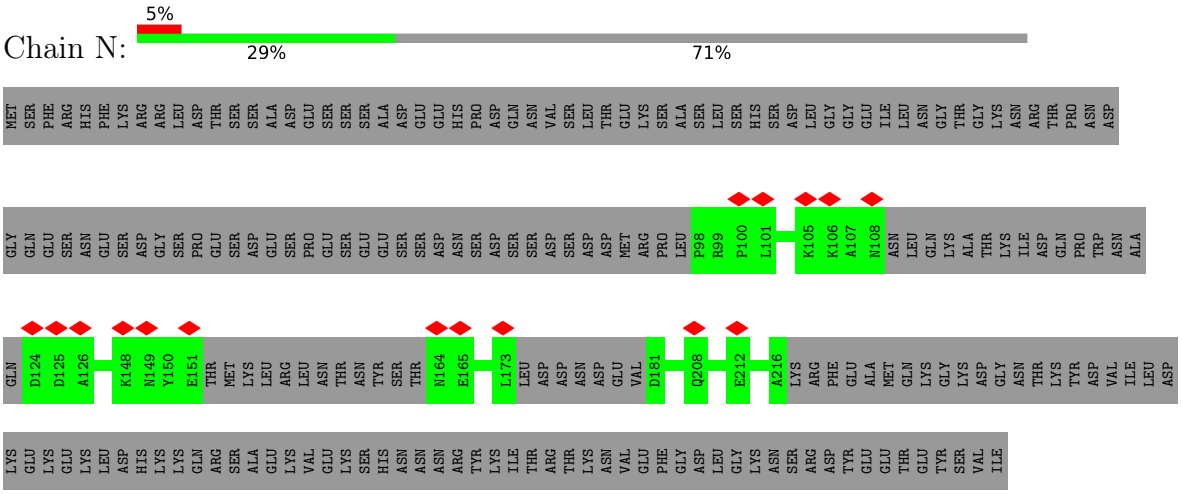
• Molecule 20: Pre-mRNA-splicing factor 38

Chain M:



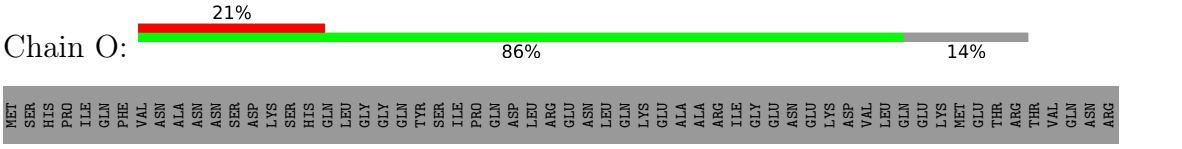
• Molecule 21: Pre-mRNA-splicing factor SPP381

Chain N:



• Molecule 22: U2 snRNP component HSH155

Chain O:



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

ASP SER ALA LEU VAL ASN VAL GLU GLY ILE HIS D132 L133 M134 F135 F136 K137 P138 S139 D140 H141 K142 Y143 F144 A145 D146 V147 I148 S149 LYS LYS PRO ILE ASP GLU LEU N157 K158 D159 E160 K161 K162 E163 R164 M168 L169 L170 K174 T178 A179 S180 R181 D190 K191 A192 V193

T194 F195 G196 L204 L209 D210 R211 S212 L213 E214 D215 L232 G233 D234 V246 D253 E254 S260 L275 K276 L279 R283 P284 D285 E289 D290 E291 Y292 A300 K306 N311 Q312 L313 L314 P315 C321 H322 S323 R324 K325 S326 I340 G341 I342 L343

L344 D361 M364 D365 D366 H367 Y388 V395 E398 K402 R405 S406 H407 R408 G409 P428 E429 T436 M439 R444 D447 S448 P449 D450 D451 A466 V467 E468 S469 I470 T471 P472 K473 R476 E477 E478 P481 E482 Q485 K486 V489 R490 R491

L494 D495 R496 K511 K512 D520 R527 D528 E529 A530 E531 L547 L548 A551 D552 L553 D554 E555 R556 R560 E571 Q572 T573 N574 S575 D576 P596 K612 T613 P614 L615 E636 F637 E638 M639 G652 E653 V654 Y655 M673 D676 K713 L714 A715 P716

L732 E733 K736 E755 N768 K771 V772 Q773 E774 K790 V791 Y826 N829 Y834 T838 N859 V860 A865 S869 H873 E874 D875 A876 F877 L880 T891 I896 I899 L900 E901 G902 L903 E904 A905 Q908 A909 L910 R936 D947

V955 E961 E965 E966 L967 D968 L969 V970 L971

- Molecule 23: Pre-mRNA-splicing factor RSE1

Chain P: 26% 86% 13%

MET TRP GLY GLY GLY LYS MET ALA VAL VAL SER LEU SER PRO HIS THR ALA LYS MET ARG LYS LEU PHE GLY GLN ALA SER THR THR MET ALA TYR ASP GLY LEU LYS ARG GLU ALA GLU ARG ARG THR ARG SER ASP HIS ASN ILE THR MET VAL A53 K54 D55 D56 E57 L58 Y59

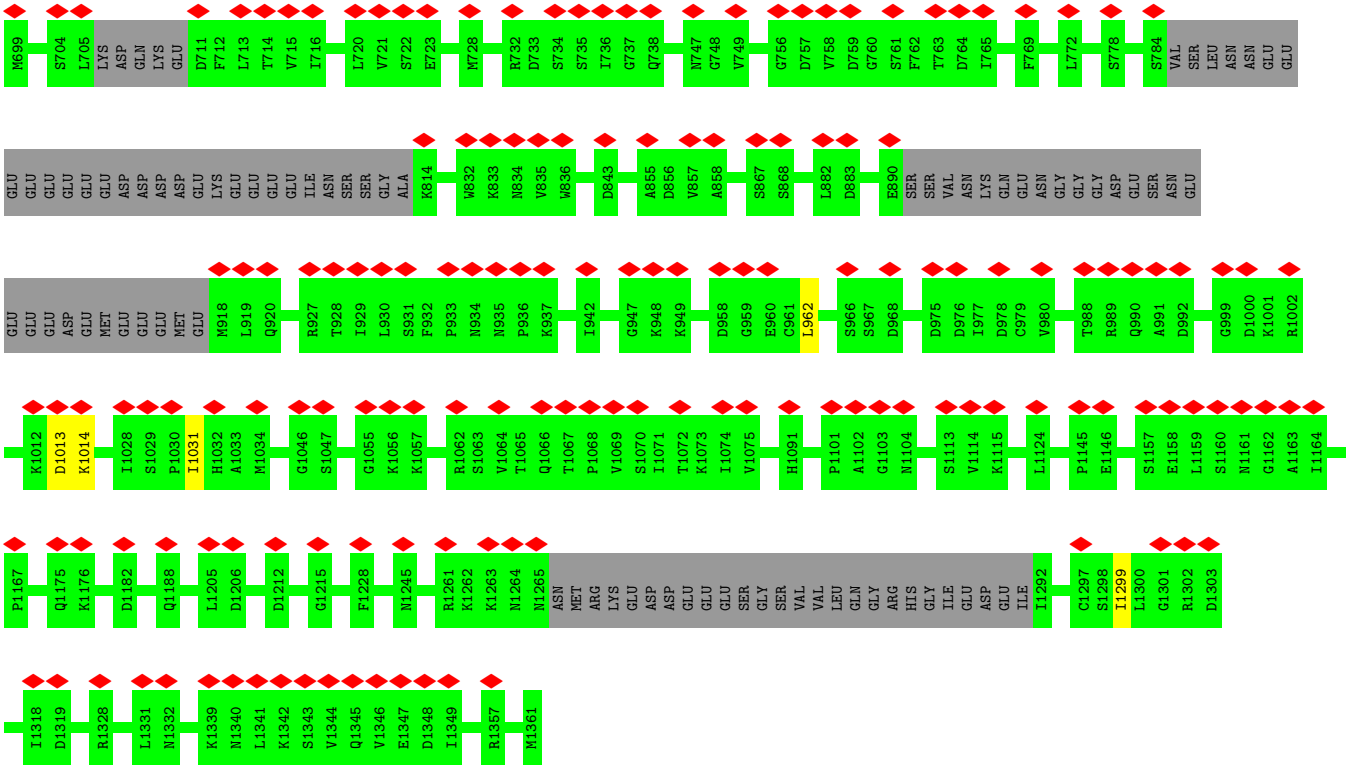
L63 T64 L65 K66 H73 I76 D81 L82 E83 A84 G85 S86 K87 R88 E89 A107 D108 G109 E110 L111 L120 M127 D131 L132 P133 HIS SER GLY SER ARG ALA LYS ALA SER ASN W144 A149 L150 I159 M164 H165 A166 G167 A168 L174 V175 L179 T180

R181 T182 S188 P189 I190 S191 P197 C201 I202 D217 Y218 A219 Q220 K221 L222 R223 S226 P227 L228 E229 I230 I231 H234 D239 V243 D244 V245 N246 F247 N248 N249 A260 A261 T262 S265 G276 L277 K282 K283 A284 D285 Y286 L296 S297 L298 N305

ILE THR THR SER LEU SER ASP ASN ASN TYR ASP ALA ASP TYR ASP THR LEU F323 N324 N341 G342 F343 L346 K347 S354 I355 T356 N357 S358 R359 H360 K361 N362 V363 T364 G368 K374 N375 V379 L380 L381 S394 P395 D396 T397 N398 D399 R400 I413 H417

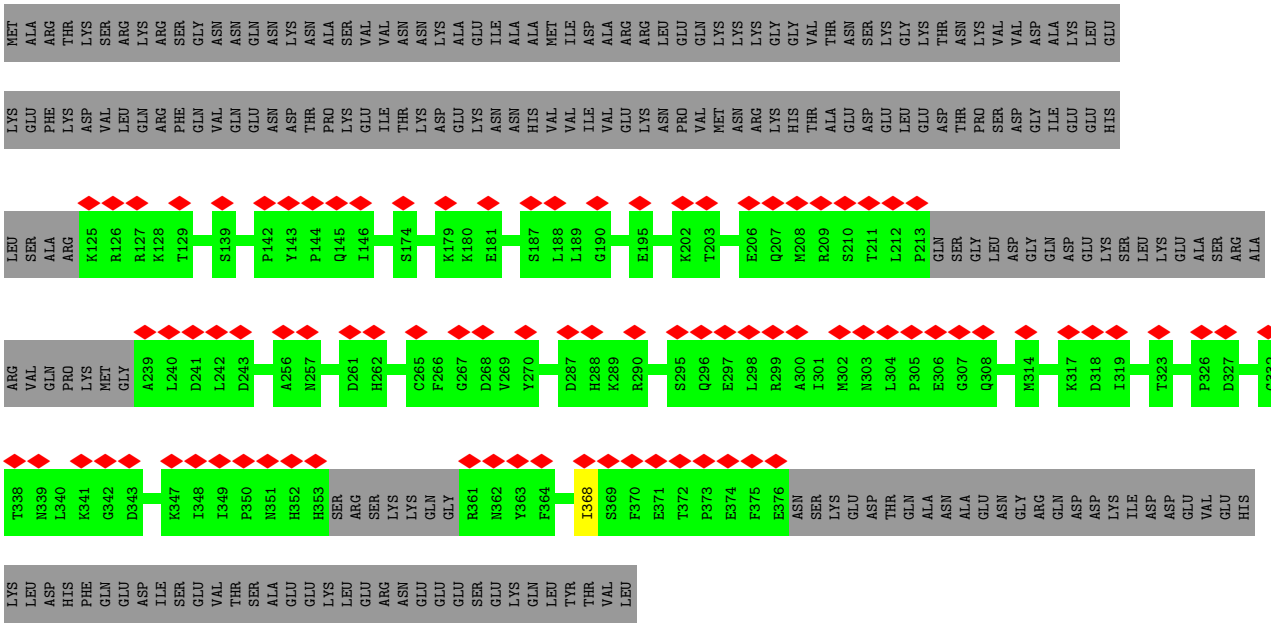
H420 K423 N424 E447 K448 N449 D450 F451 S452 N453 K458 D459 P460 N461 K462 S463 L464 V465 F466 E467 P468 S469 I470 K471 L472 Q473 L478 S479 L482 N483 P486 S487 I488 K489 I492 V493 S494 D495 T542 T543 G544 D545 P555 K556 L571 THR PRO ASP GLU ALA

THR ARG SER ALA F581 Q585 G595 S596 H597 T613 G614 K615 S616 R617 K621 V625 P626 P627 A628 G629 I630 R631 Y649 I656 D657 V658 S659 S660 D661 T667 T668 H669 P670 E671 L672 D673 T674 K678 D684 T685 Q686 H687 A688 D689 L690 D695 N696 E697 G698



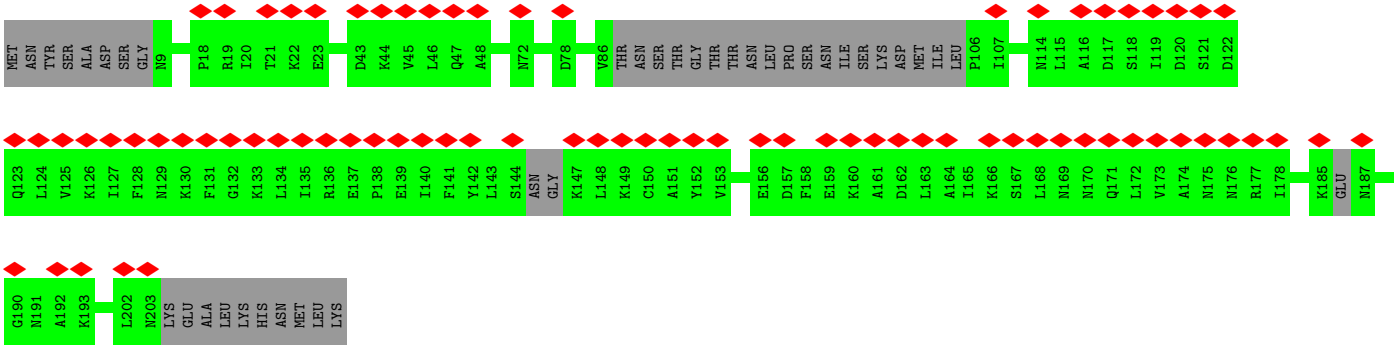
- Molecule 24: Cold sensitive U2 snRNA suppressor 1

Chain Q:



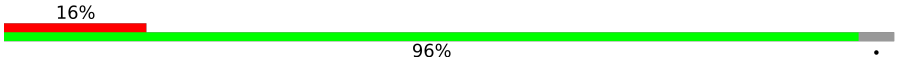
- Molecule 25: Protein HSH49

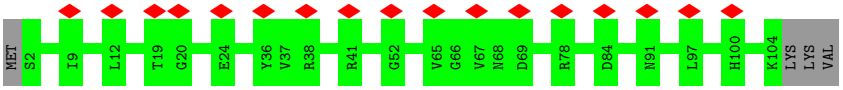
Chain R:



- Molecule 26: Pre-mRNA-splicing factor RDS3

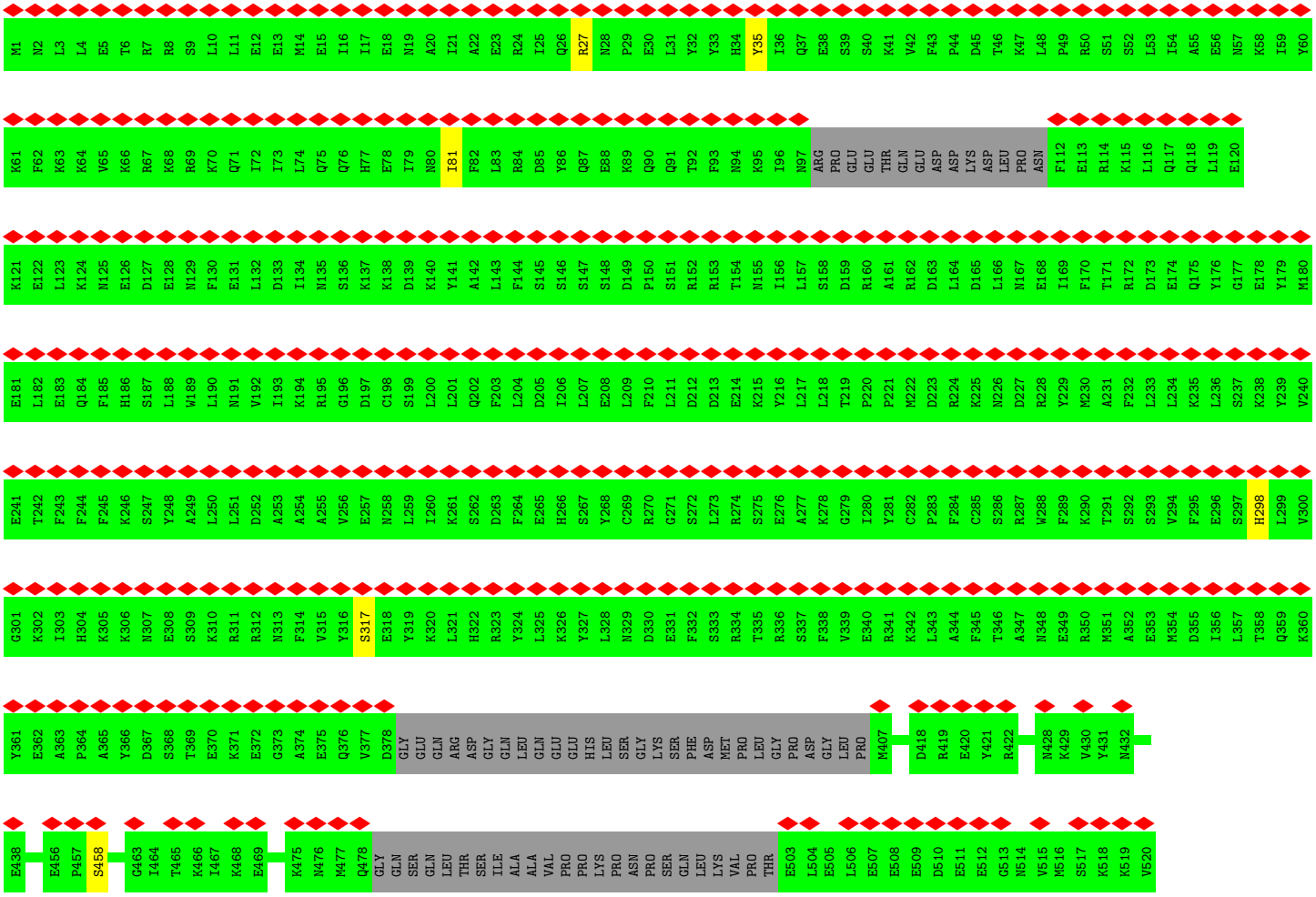
Chain S:





- Molecule 27: Pre-mRNA-splicing factor PRP9

Chain T:



Y521 D522 E523 L524 K525 K526 Q527 G528 LEU VAL

- Molecule 28: Pre-mRNA-splicing factor PRP11

Chain U: 55% 73% • 26%

MET ASN TYR LEU GLU GLY VAL GLY SER LYS LYS GLY GLY GLY GLY ILE ALA SER GLU SER GLN PHE ASN LEU GLN ARG ARG LYS GLU VAL GLU SER LEU L34 S35 K36 G37 E38 N39 Q45 D46 E47 LYS ASP ASP Q51 V52 R53 S54 G56 I95 G98 I101 E102 K103

S104 S105 LEU GLY ARG GLU GLY GLN THR THR HIS D115 F116 R117 Q118 Q119 Q120 K121 I122 I123 E124 A125 K126 Q127 S128 L129 K130 N131 N132 G133 T134 I135 P136 VAL CYS LYS ILE ALA THR VAL LYS ASN PRO LYS ASN G149 S150 V151 G152 L153 A154 I155 Q156 V157 N158 Y159 S160 S161 E162 V163

K164 E165 N166 S167 V168 D169 S170 D171 D172 K173 A174 K175 V176 P177 P178 L179 I180 R181 I182 V183 S184 G185 L186 E187 L188 S189 D190 T191 K192 Q193 K194 G195 K196 K197 F198 L199 V200 I201 A202 Y203 E204 P205 F206 E207 N208 I209 A210 I211 E212 L213 P214 P215 N216 E217 I218 L219 F220 S221 E222 N223

N224 D225 M226 D227 N228 N229 N230 D231 G232 V233 D234 E235 L236 N237 K238 K239 C240 T241 F242 W243 D244 A245 I246 S247 K248 L249 Y250 Y251 V252 Q253 PHE PHE PHE LYS GLN ALA GLU GLN GLU GLN ALA ASP VAL

- Molecule 29: Pre-mRNA-splicing factor PRP21

Chain V: 45% 45% • 55%

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

SER GLY GLU ASP ASN ASP ARG LYS SER GLU ARG GLU ILE ALA ARG PRO PRO ASP PHE LEU PHE SER GLN TYR ASP THR GLY ILE S89 R90 R91 D92 M93 E94 V95 I96 K97 L98 T99 A100 R101 Y102 Y103 A104 K105 D106 K107 S108 I109 V110 E111 Q112 M113 I114 S115 K116 D117 G118 E119 A120

R121 L122 N123 F124 M125 N126 S127 S128 H129 P130 L131 H132 K133 T134 F135 T136 D137 F138 V139 A140 Q141 Y142 K143 R144 V145 Y146 S147 F148 T149 G150 Q151 E152 I153 K154 K155 S156 K157 R158 T159 I160 L161 D162 N163 C164 F165 E166 R167 T168 Q169 Y170 W171 E172 F173 E174 K175 D176 K177 D178 R179 E180

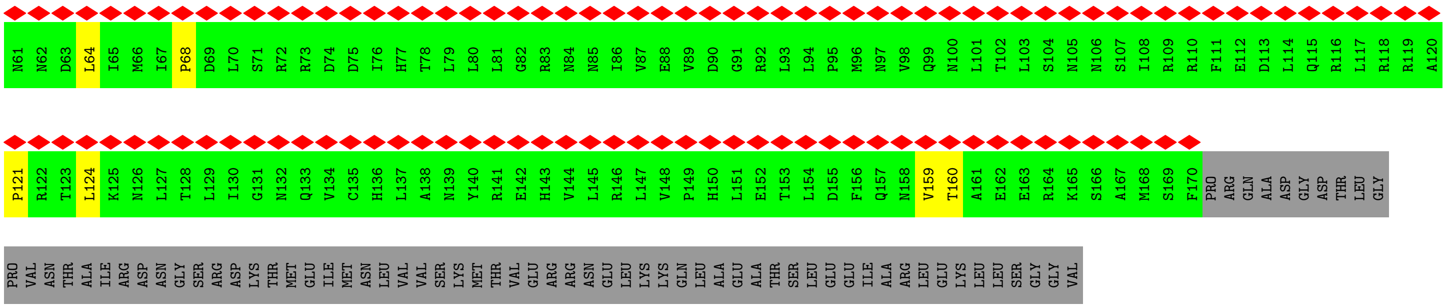
H181 D182 K183 L184 V185 E186 L187 C188 K189 I190 Q191 F192 A193 A194 I195 P196 W197 D198 K199 F200 T201 Q202 V203 A204 K205 F206 SER ILE PRO GLU ASP THR GLU ILE PHE GLU GLY SER LEU D220 L221 E222 Q223 M224 R225 L226 R227 R228 VAL GLN THR GLY ILE LYS LEU PHE ASP SER ILE LYS

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

- Molecule 30: U2 small nuclear ribonucleoprotein A'

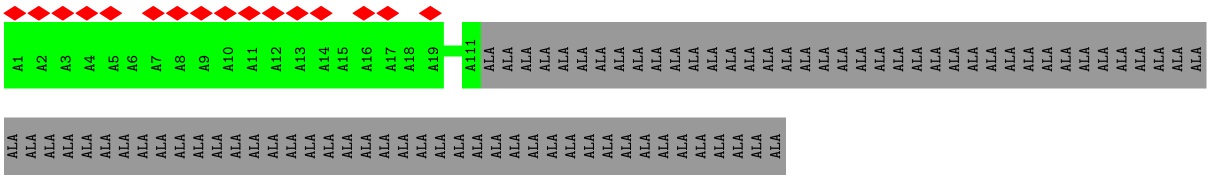
Chain W: 71% 62% 8% • 29%

M1 K2 F3 T4 P5 S6 I7 V8 I9 D10 A11 P12 Q13 Y14 Y15 V16 D17 H18 F19 N20 G21 K22 Y23 N24 V25 D26 K27 C28 V29 I30 L31 R32 D33 L34 Q35 L36 E37 T38 D39 S40 E41 S42 M43 P44 S45 S46 L47 K48 H49 L50 T51 K52 P53 T54 H55 I56 L57 D58 L59 T60



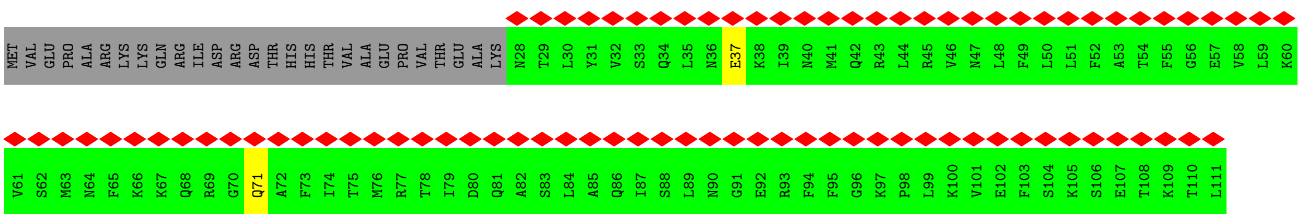
• Molecule 31: Unknown

Chain X:



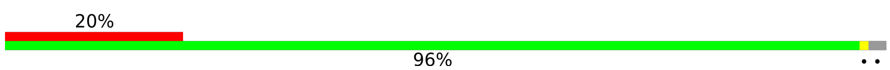
• Molecule 32: U2 small nuclear ribonucleoprotein B”

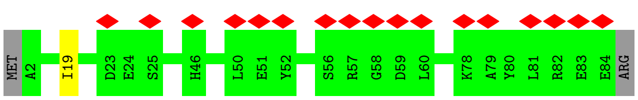
Chain Y:



• Molecule 33: RDS3 complex subunit 10

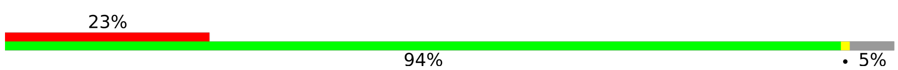
Chain Z:

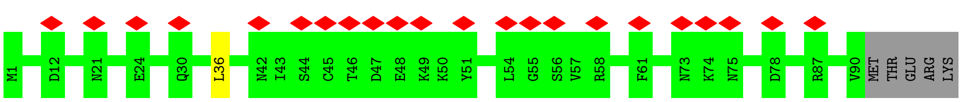




• Molecule 34: U6 snRNA-associated Sm-like protein LSm2

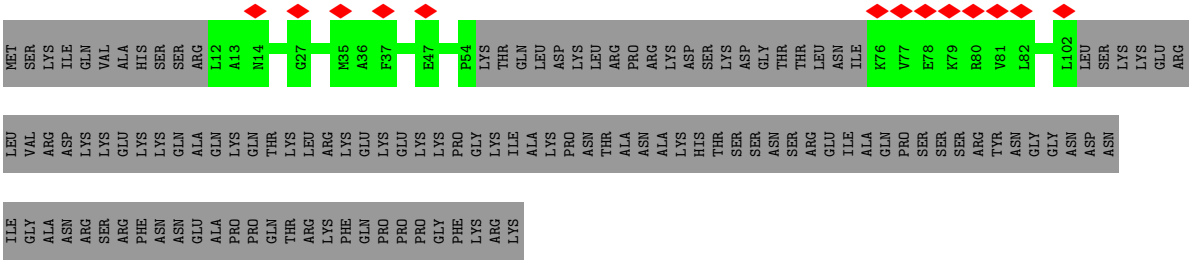
Chain a:





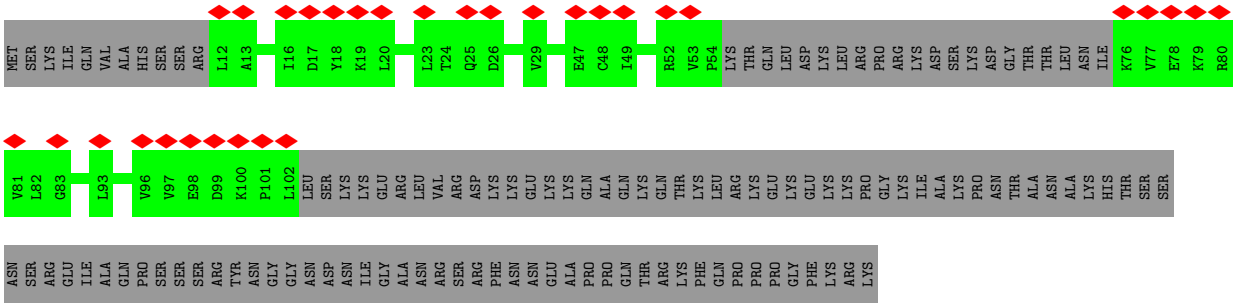
• Molecule 35: Small nuclear ribonucleoprotein-associated protein B

Chain b:



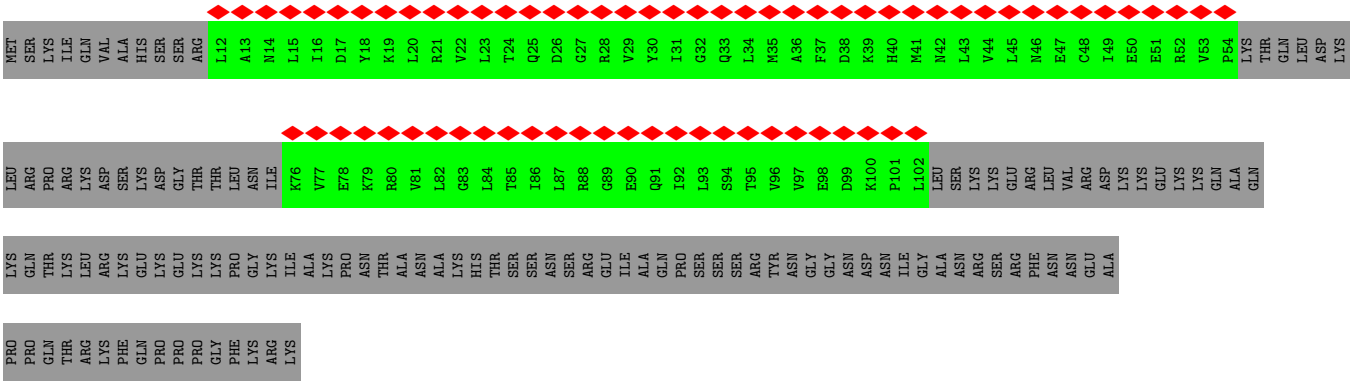
• Molecule 35: Small nuclear ribonucleoprotein-associated protein B

Chain k:



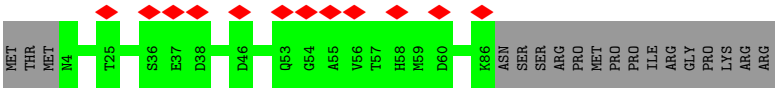
• Molecule 35: Small nuclear ribonucleoprotein-associated protein B

Chain s:



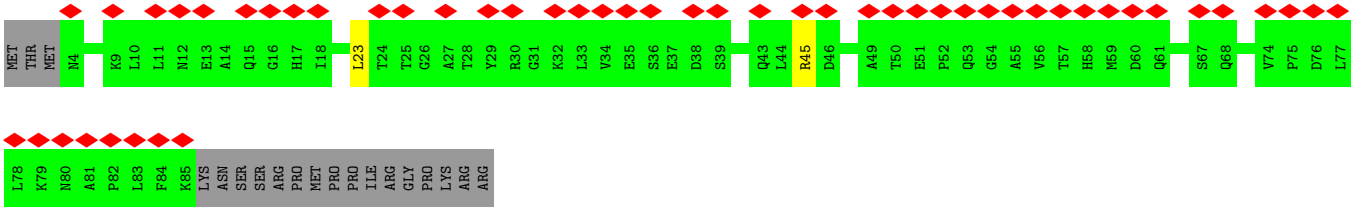
• Molecule 36: Small nuclear ribonucleoprotein Sm D3

Chain d:



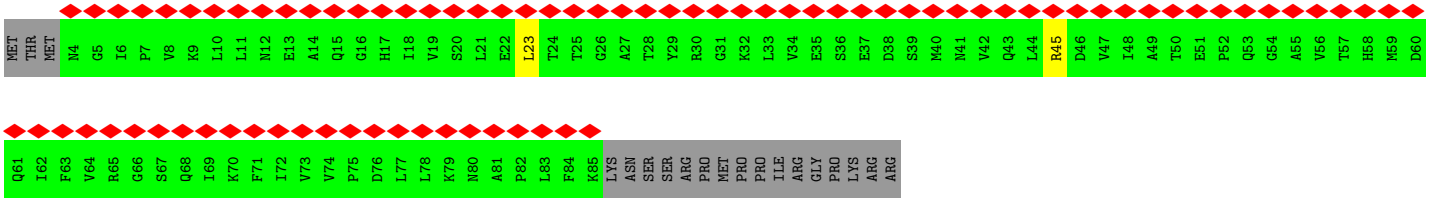
• Molecule 36: Small nuclear ribonucleoprotein Sm D3

Chain n:



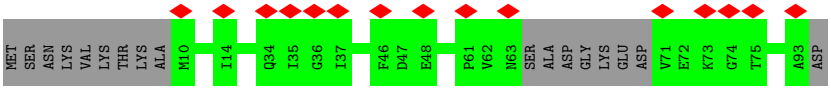
• Molecule 36: Small nuclear ribonucleoprotein Sm D3

Chain v:



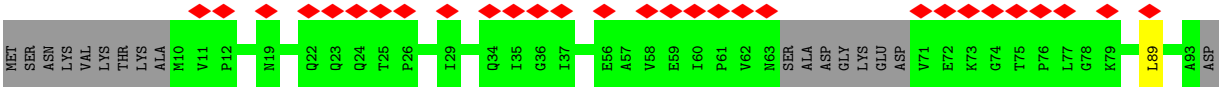
• Molecule 37: Small nuclear ribonucleoprotein E

Chain e:



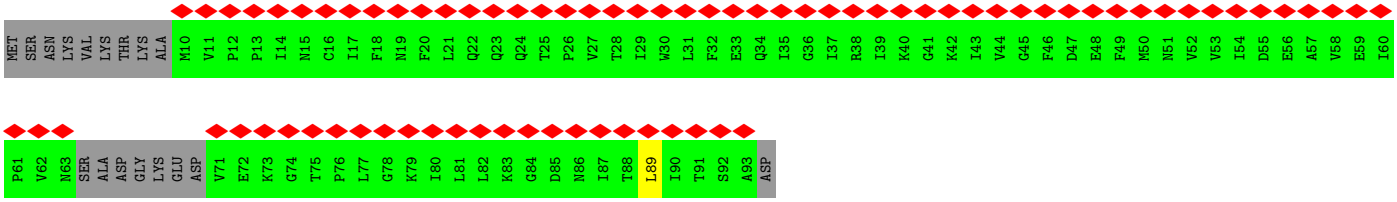
• Molecule 37: Small nuclear ribonucleoprotein E

Chain p:



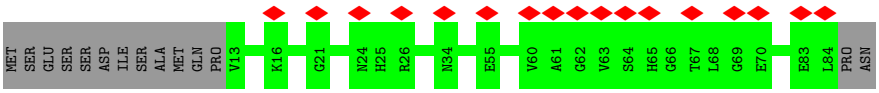
• Molecule 37: Small nuclear ribonucleoprotein E

Chain w:



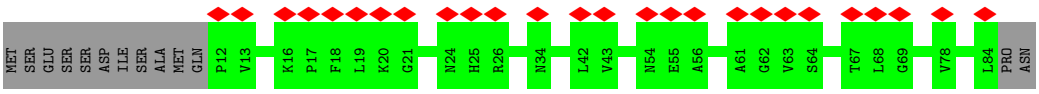
• Molecule 38: Small nuclear ribonucleoprotein F

Chain f:



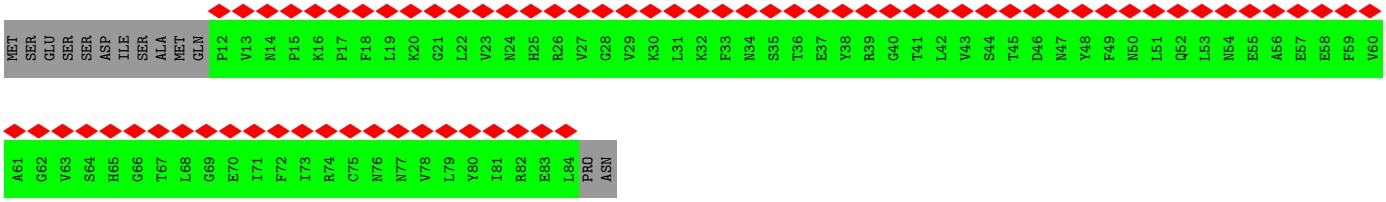
• Molecule 38: Small nuclear ribonucleoprotein F

Chain q:



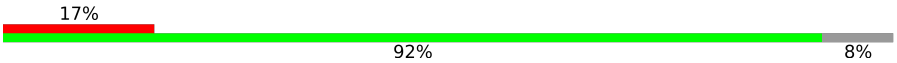
• Molecule 38: Small nuclear ribonucleoprotein F

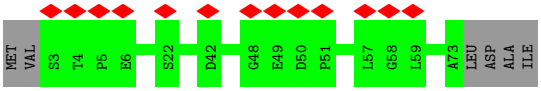
Chain x:



• Molecule 39: Small nuclear ribonucleoprotein G

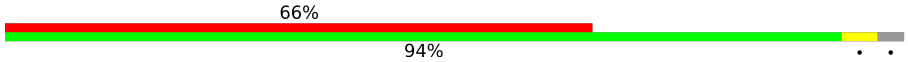
Chain g:

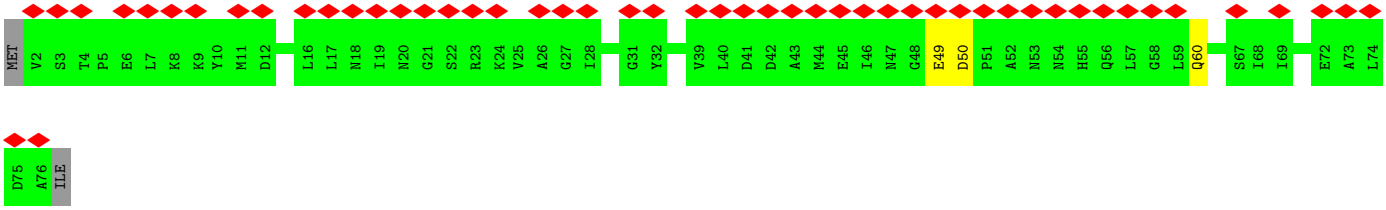




• Molecule 39: Small nuclear ribonucleoprotein G

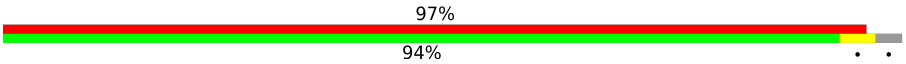
Chain r:

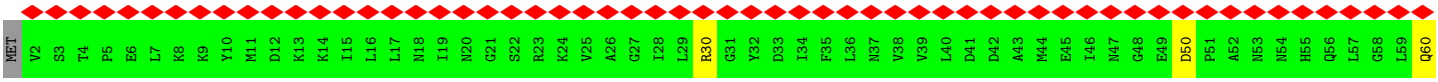


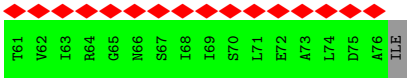


• Molecule 39: Small nuclear ribonucleoprotein G

Chain y:

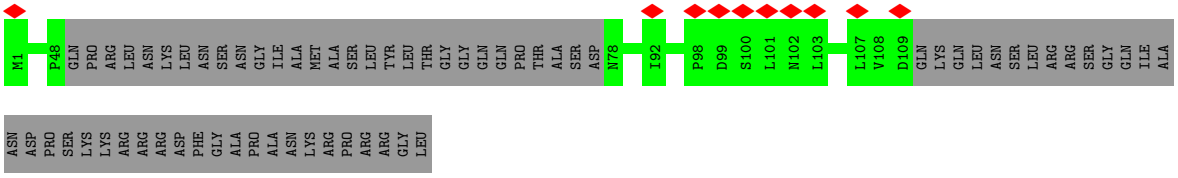






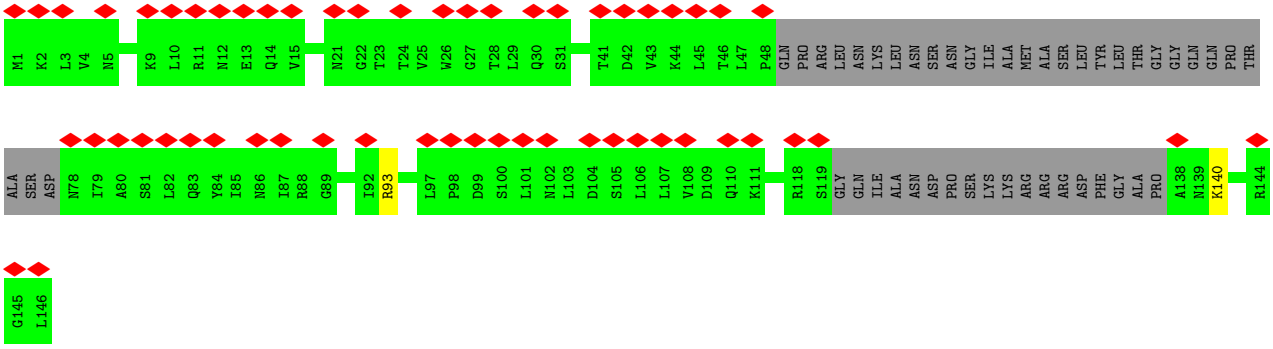
• Molecule 40: Small nuclear ribonucleoprotein Sm D1

Chain h:



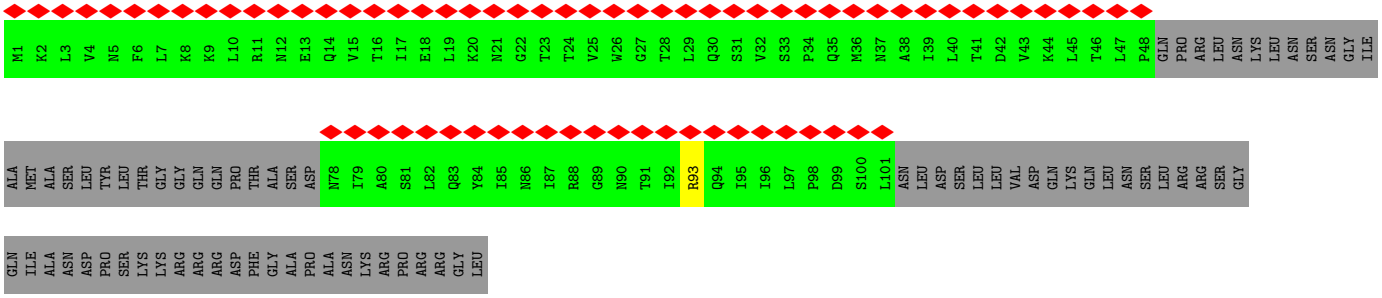
• Molecule 40: Small nuclear ribonucleoprotein Sm D1

Chain l:



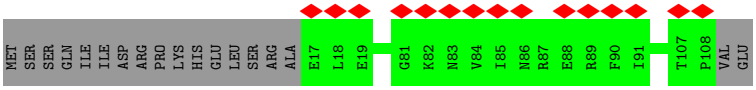
• Molecule 40: Small nuclear ribonucleoprotein Sm D1

Chain t:



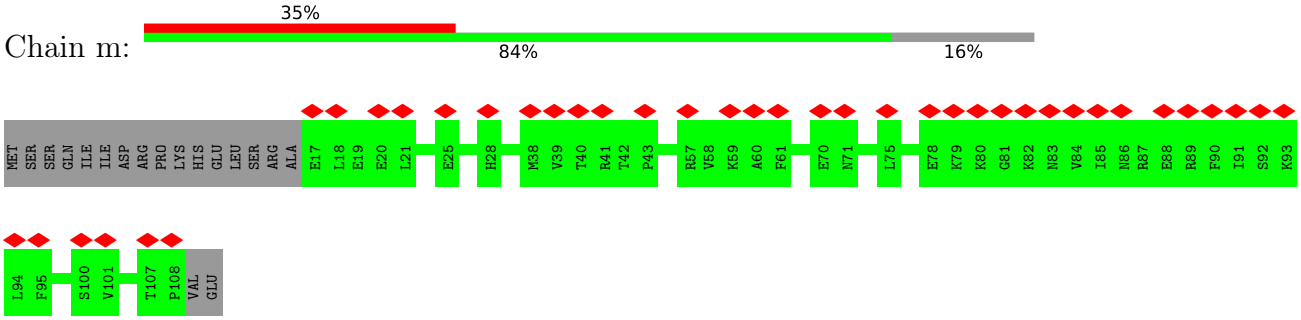
• Molecule 41: Small nuclear ribonucleoprotein Sm D2

Chain i:



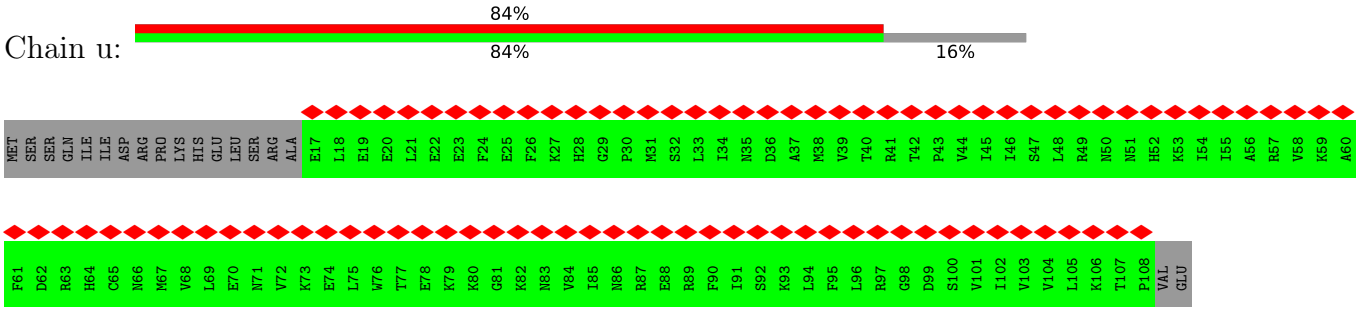
• Molecule 41: Small nuclear ribonucleoprotein Sm D2

Chain m:



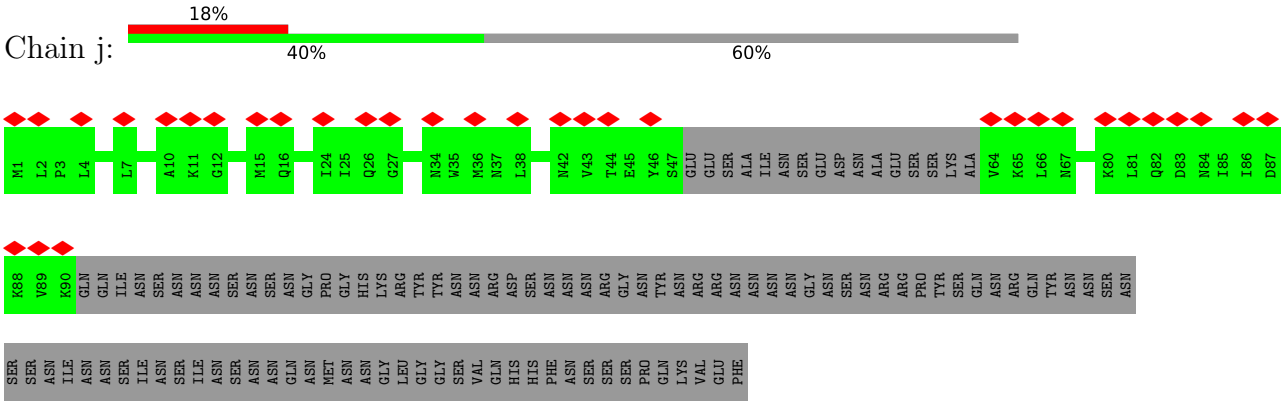
- Molecule 41: Small nuclear ribonucleoprotein Sm D2

Chain u:



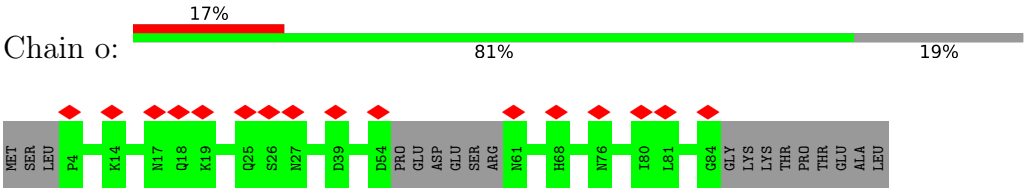
- Molecule 42: U6 snRNA-associated Sm-like protein LSm4

Chain j:



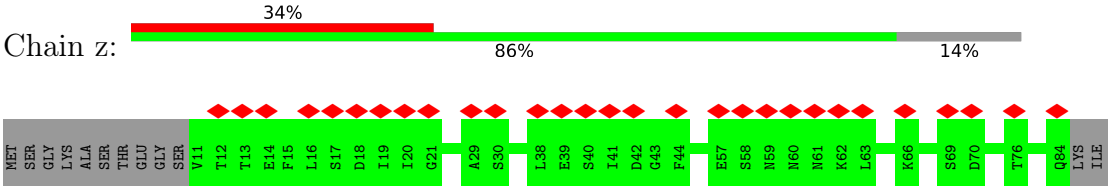
- Molecule 43: U6 snRNA-associated Sm-like protein LSm5

Chain o:



- Molecule 44: U6 snRNA-associated Sm-like protein LSm6

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9559	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 ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	350	Depositor
Maximum defocus (nm)	5300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.019	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0258	Depositor
Map size (Å)	686.39996, 686.39996, 686.39996	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	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, PSU, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	2	1.35	52/3579 (1.5%)	1.69	123/5551 (2.2%)
2	3	0.25	0/617	0.45	0/836
3	4	0.45	4/2705 (0.1%)	0.95	10/4204 (0.2%)
4	5	0.42	1/4039 (0.0%)	0.90	6/6284 (0.1%)
5	6	0.24	0/2253	0.83	3/3497 (0.1%)
6	7	0.24	0/505	0.44	0/675
7	8	0.24	0/501	0.45	0/673
8	A	0.29	0/18580	0.46	1/25189 (0.0%)
9	B	0.40	1/13905 (0.0%)	0.62	6/18852 (0.0%)
10	C	0.32	0/6928	0.47	0/9377
11	D	0.28	0/1185	0.46	0/1596
12	E	0.24	0/822	0.40	0/1109
13	F	0.27	0/3292	0.45	1/4432 (0.0%)
14	G	0.29	0/2885	0.45	0/3882
15	H	0.27	0/3455	0.49	0/4663
16	I	0.28	0/665	0.82	0/1024
17	J	0.26	0/6613	0.43	0/8942
18	K	0.26	0/949	0.45	0/1292
19	L	0.25	0/899	0.44	0/1204
20	M	0.24	0/1430	0.44	0/1927
21	N	0.22	0/421	0.29	0/583
22	O	0.28	0/6745	0.45	0/9157
23	P	0.30	1/9623 (0.0%)	0.53	1/13041 (0.0%)
24	Q	0.27	0/1835	0.46	0/2480
25	R	0.26	0/1453	0.42	0/1954
26	S	0.29	0/827	0.46	0/1105
27	T	0.27	0/3992	0.41	0/5346
28	U	0.25	0/1511	0.41	1/2038 (0.0%)
29	V	0.24	0/1105	0.36	0/1475
30	W	0.42	0/1406	0.69	4/1905 (0.2%)
31	X	0.25	0/148	0.39	0/204
32	Y	0.30	0/692	0.54	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Z	0.28	0/694	0.47	0/929
34	a	0.26	0/745	0.51	1/1005 (0.1%)
35	b	0.29	0/567	0.47	0/762
35	k	0.41	0/567	0.61	0/762
35	s	0.40	0/567	0.63	0/762
36	d	0.30	0/650	0.50	0/879
36	n	0.41	0/641	0.65	2/868 (0.2%)
36	v	0.43	0/641	0.65	2/868 (0.2%)
37	e	0.26	0/612	0.44	0/830
37	p	0.39	0/612	0.59	1/830 (0.1%)
37	w	0.40	0/612	0.61	1/830 (0.1%)
38	f	0.27	0/589	0.46	0/796
38	q	0.39	0/597	0.62	0/807
38	x	0.42	0/597	0.63	0/807
39	g	0.25	0/554	0.53	0/746
39	r	0.32	0/582	0.63	0/785
39	y	0.26	0/582	0.49	0/785
40	h	0.25	0/635	0.48	0/861
40	l	0.38	0/756	0.70	1/1023 (0.1%)
40	t	0.41	0/574	0.68	1/777 (0.1%)
41	i	0.25	0/764	0.44	0/1026
41	m	0.38	0/764	0.57	0/1026
41	u	0.40	0/764	0.57	0/1026
42	j	0.25	0/594	0.42	0/802
43	o	0.24	0/595	0.41	0/806
44	z	0.24	0/584	0.43	0/787
All	All	0.39	59/122004 (0.0%)	0.62	165/167605 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	2
8	A	0	2
9	B	0	4
17	J	0	2
20	M	0	2
23	P	0	2
27	T	0	1
30	W	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	r	0	1
All	All	0	17

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1149	G	O3'-P	24.35	1.90	1.61
1	2	143	G	O3'-P	18.92	1.83	1.61
4	5	105	A	O3'-P	18.04	1.82	1.61
1	2	1161	U	O3'-P	-15.56	1.42	1.61
1	2	143	G	C3'-O3'	15.28	1.63	1.42
1	2	1092	A	O3'-P	-14.79	1.43	1.61
1	2	1090	A	O3'-P	14.49	1.78	1.61
1	2	144	G	O3'-P	-14.29	1.44	1.61
1	2	1116	A	O3'-P	-11.58	1.47	1.61
1	2	1166	G	O3'-P	9.99	1.73	1.61
1	2	1149	G	C3'-O3'	9.99	1.56	1.42
1	2	1163	C	O5'-C5'	9.13	1.59	1.44
1	2	1116	A	C3'-O3'	-8.93	1.29	1.42
1	2	1127	A	O3'-P	-8.69	1.50	1.61
1	2	1167	U	O3'-P	8.63	1.71	1.61
1	2	1164	C	O3'-P	-8.23	1.51	1.61
1	2	1090	A	C3'-O3'	7.79	1.53	1.42
3	4	142	G	N7-C5	-7.73	1.34	1.39
1	2	1162	U	P-O5'	7.53	1.67	1.59
1	2	1163	C	P-O5'	7.49	1.67	1.59
1	2	1117	G	P-O5'	7.31	1.67	1.59
1	2	144	G	P-O5'	7.10	1.66	1.59
1	2	1096	C	O3'-P	6.96	1.69	1.61
1	2	1154	U	C1'-N1	6.95	1.59	1.48
1	2	1128	C	C5'-C4'	-6.95	1.43	1.51
1	2	1140	U	C1'-N1	6.88	1.59	1.48
1	2	1165	C	O3'-P	6.55	1.69	1.61
1	2	1095	U	O3'-P	6.54	1.69	1.61
1	2	145	G	P-O5'	-6.44	1.53	1.59
1	2	1169	C	C1'-N1	6.44	1.58	1.48
1	2	1150	U	O5'-C5'	6.37	1.54	1.44
1	2	1090	A	C4'-O4'	6.36	1.53	1.45
1	2	1117	G	C5'-C4'	6.25	1.58	1.51
1	2	1168	U	C5'-C4'	-6.22	1.43	1.51
1	2	1162	U	O3'-P	6.22	1.68	1.61
1	2	1165	C	O5'-C5'	6.05	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	73	A	C1'-N9	-6.04	1.38	1.46
23	P	188	SER	C-N	-6.03	1.22	1.34
1	2	1162	U	O5'-C5'	6.01	1.54	1.44
3	4	142	G	C2-N2	-6.01	1.28	1.34
1	2	1162	U	C2-N3	5.96	1.42	1.37
1	2	1151	U	O5'-C5'	-5.88	1.33	1.42
1	2	1163	C	O3'-P	5.81	1.68	1.61
1	2	68	U	C1'-N1	5.78	1.57	1.48
1	2	1161	U	C3'-O3'	-5.73	1.34	1.42
3	4	74	U	C1'-N1	5.72	1.57	1.48
1	2	1097	G	O3'-P	5.70	1.68	1.61
1	2	1162	U	C3'-C2'	-5.60	1.46	1.52
1	2	118	U	C1'-N1	5.59	1.57	1.48
1	2	144	G	C3'-O3'	-5.50	1.34	1.42
1	2	143	G	P-O5'	-5.46	1.54	1.59
1	2	121	C	C1'-N1	5.44	1.56	1.48
1	2	111	C	C1'-N1	5.38	1.56	1.48
1	2	109	C	C1'-N1	5.29	1.56	1.48
1	2	147	A	O3'-P	-5.24	1.54	1.61
1	2	1166	G	C5'-C4'	5.23	1.57	1.51
1	2	1090	A	O5'-C5'	5.16	1.52	1.44
1	2	85	A	C1'-N9	-5.09	1.39	1.46
9	B	1695	TYR	CE1-CZ	-5.02	1.32	1.38

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	144	G	C4'-C3'-O3'	-16.52	74.71	109.40
1	2	1093	C	P-O5'-C5'	14.80	144.59	120.90
1	2	1162	U	C5'-C4'-O4'	14.80	126.86	109.10
1	2	1147	A	C5'-C4'-C3'	-14.15	93.35	116.00
1	2	1092	A	C2'-C3'-O3'	14.11	140.53	109.50
1	2	143	G	C4'-C3'-O3'	13.61	140.22	113.00
1	2	1098	C	N1-C1'-C2'	-13.39	96.59	114.00
1	2	1151	U	C4'-C3'-O3'	-12.56	83.02	109.40
1	2	144	G	C2'-C3'-O3'	12.27	136.49	109.50
9	B	1213	ARG	NE-CZ-NH2	-12.11	114.25	120.30
1	2	143	G	P-O3'-C3'	11.89	133.97	119.70
1	2	1149	G	P-O3'-C3'	11.89	133.97	119.70
1	2	144	G	C5'-C4'-O4'	-11.80	94.94	109.10
1	2	1151	U	P-O5'-C5'	11.68	139.59	120.90
1	2	1117	G	C5'-C4'-O4'	11.40	122.78	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	145	G	C5'-C4'-C3'	-11.24	98.02	116.00
1	2	1109	C	C2-N1-C1'	11.21	131.14	118.80
1	2	1109	C	C6-N1-C1'	-11.15	107.42	120.80
1	2	1150	U	C5'-C4'-C3'	11.08	133.72	116.00
1	2	1117	G	C5'-C4'-C3'	-10.88	98.59	116.00
1	2	1163	C	C5'-C4'-O4'	10.55	121.76	109.10
1	2	141	A	N9-C1'-C2'	-10.47	100.38	114.00
1	2	144	G	C5'-C4'-C3'	10.44	132.71	116.00
1	2	1126	G	N9-C1'-C2'	-10.02	100.97	114.00
1	2	143	G	C5'-C4'-C3'	-9.89	100.17	116.00
1	2	1091	G	C5'-C4'-C3'	9.88	131.81	116.00
3	4	142	G	N1-C6-O6	-9.83	114.00	119.90
4	5	88	U	P-O3'-C3'	9.73	131.38	119.70
1	2	1139	G	N9-C1'-C2'	-9.71	101.31	112.00
1	2	1163	C	C5'-C4'-C3'	-9.72	100.45	116.00
1	2	1147	A	P-O5'-C5'	9.59	136.25	120.90
1	2	1090	A	P-O3'-C3'	9.52	131.12	119.70
1	2	1162	U	C5'-C4'-C3'	-9.20	101.28	116.00
1	2	1168	U	C4'-C3'-O3'	-8.97	90.56	109.40
1	2	1150	U	C4'-C3'-O3'	-8.96	90.59	109.40
1	2	142	C	N1-C1'-C2'	-8.85	102.27	112.00
3	4	142	G	C5-C6-O6	8.78	133.87	128.60
1	2	1152	U	P-O5'-C5'	8.70	134.82	120.90
1	2	1151	U	O4'-C1'-N1	8.64	115.11	108.20
1	2	1090	A	C4'-C3'-O3'	8.63	130.26	113.00
1	2	1148	U	C4'-C3'-O3'	-8.54	91.46	109.40
1	2	1092	A	P-O5'-C5'	8.52	134.54	120.90
1	2	145	G	P-O5'-C5'	8.31	134.20	120.90
1	2	1165	C	C5'-C4'-C3'	-8.27	102.77	116.00
1	2	1109	C	C4'-C3'-O3'	8.25	129.50	113.00
1	2	148	G	C5'-C4'-C3'	-8.24	102.81	116.00
3	4	142	G	N1-C2-N3	8.21	128.82	123.90
1	2	1150	U	C2'-C3'-O3'	8.14	127.41	109.50
1	2	1151	U	C5'-C4'-O4'	8.13	118.86	109.10
1	2	1090	A	C5'-C4'-O4'	8.09	118.81	109.10
1	2	1109	C	O4'-C1'-N1	8.05	114.64	108.20
1	2	144	G	O3'-P-O5'	-8.02	88.75	104.00
1	2	1149	G	O3'-P-O5'	8.01	119.22	104.00
1	2	1150	U	P-O5'-C5'	7.98	133.67	120.90
1	2	1168	U	P-O5'-C5'	-7.93	108.21	120.90
1	2	1167	U	C2'-C3'-O3'	7.88	126.84	109.50
1	2	1092	A	C4'-C3'-O3'	-7.83	92.96	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1165	C	C5'-C4'-O4'	7.79	118.44	109.10
1	2	1147	A	C4'-C3'-O3'	7.77	128.53	113.00
3	4	71	U	C2-N1-C1'	7.76	127.01	117.70
1	2	1107	C	N1-C1'-C2'	-7.75	103.47	112.00
1	2	1161	U	C5'-C4'-C3'	-7.74	103.61	116.00
1	2	1093	C	C5'-C4'-C3'	-7.71	103.66	116.00
1	2	1169	C	P-O5'-C5'	-7.65	108.66	120.90
1	2	1097	G	C3'-C2'-O2'	7.61	135.37	113.30
1	2	1165	C	C4'-C3'-O3'	7.53	128.06	113.00
5	6	24	A	OP2-P-O3'	-7.34	89.04	105.20
3	4	71	U	N1-C2-O2	7.32	127.92	122.80
1	2	1168	U	C2'-C3'-O3'	7.29	125.53	109.50
1	2	1128	C	C5'-C4'-O4'	7.28	117.84	109.10
5	6	24	A	P-O3'-C3'	7.26	128.41	119.70
1	2	1089	G	C4'-C3'-O3'	7.26	127.51	113.00
1	2	1115	G	O5'-P-OP1	-7.22	99.20	105.70
1	2	1149	G	C4'-C3'-O3'	7.22	127.45	113.00
1	2	1159	U	O5'-P-OP1	-7.22	99.20	105.70
30	W	50	LEU	CA-CB-CG	7.17	131.78	115.30
1	2	139	G	O5'-P-OP1	-7.16	99.26	105.70
1	2	139	G	O5'-P-OP2	-7.15	99.27	105.70
1	2	1089	G	O5'-P-OP2	-7.12	99.29	105.70
1	2	1159	U	O5'-P-OP2	-7.12	99.30	105.70
1	2	1089	G	O5'-P-OP1	-7.11	99.30	105.70
1	2	1115	G	C4'-C3'-O3'	7.04	127.08	113.00
1	2	1115	G	O5'-P-OP2	-7.04	99.37	105.70
8	A	265	ASN	C-N-CA	-6.72	104.89	121.70
1	2	1090	A	C5'-C4'-C3'	-6.71	105.26	116.00
4	5	105	A	P-O3'-C3'	-6.71	111.64	119.70
1	2	1096	C	C1'-C2'-O2'	-6.68	90.55	110.60
40	l	93	ARG	CG-CD-NE	-6.64	97.86	111.80
1	2	1129	U	C5'-C4'-O4'	6.61	117.03	109.10
1	2	148	G	C5'-C4'-O4'	6.56	116.98	109.10
36	n	45	ARG	NE-CZ-NH1	-6.56	117.02	120.30
3	4	142	G	C6-N1-C2	-6.55	121.17	125.10
40	t	93	ARG	CG-CD-NE	-6.49	98.17	111.80
1	2	140	G	N9-C1'-C2'	-6.47	104.88	112.00
34	a	36	LEU	CA-CB-CG	6.45	130.14	115.30
1	2	1166	G	O5'-C5'-C4'	6.37	123.81	111.70
1	2	145	G	O4'-C1'-N9	6.31	113.25	108.20
1	2	1166	G	C5'-C4'-C3'	6.31	126.09	116.00
5	6	24	A	OP1-P-O3'	6.30	119.07	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	4	71	U	N3-C2-O2	-6.27	117.81	122.20
1	2	1092	A	N9-C1'-C2'	6.25	122.12	114.00
1	2	145	G	O5'-C5'-C4'	-6.23	99.87	111.70
36	v	45	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	2	1152	U	C5'-C4'-C3'	-6.14	106.17	116.00
1	2	1096	C	C4'-C3'-O3'	6.12	125.24	113.00
4	5	93	G	C5-C6-O6	6.10	132.26	128.60
37	w	89	LEU	CA-CB-CG	6.09	129.31	115.30
9	B	1213	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	2	1167	U	P-O3'-C3'	-6.05	112.44	119.70
1	2	143	G	O4'-C1'-N9	6.04	113.03	108.20
1	2	1151	U	O3'-P-O5'	-5.99	92.61	104.00
1	2	143	G	O3'-P-O5'	5.98	115.37	104.00
1	2	144	G	P-O3'-C3'	-5.96	112.55	119.70
1	2	1167	U	C5'-C4'-O4'	-5.90	102.02	109.10
1	2	1091	G	O5'-C5'-C4'	5.89	122.90	111.70
1	2	1108	A	C3'-C2'-C1'	5.89	106.21	101.50
1	2	1162	U	C4'-C3'-O3'	5.89	124.78	113.00
1	2	1150	U	N1-C1'-C2'	5.83	121.57	114.00
30	W	36	LEU	CA-CB-CG	5.83	128.70	115.30
28	U	136	PRO	N-CA-CB	5.77	110.22	103.30
1	2	1115	G	P-O3'-C3'	5.76	126.61	119.70
1	2	1148	U	C5'-C4'-O4'	5.75	116.01	109.10
1	2	1162	U	C2'-C3'-O3'	-5.75	96.86	109.50
3	4	142	G	C8-N9-C4	-5.72	104.11	106.40
1	2	141	A	C4'-C3'-O3'	5.69	124.38	113.00
37	p	89	LEU	CA-CB-CG	5.63	128.25	115.30
30	W	57	LEU	CA-CB-CG	5.63	128.24	115.30
4	5	93	G	N1-C6-O6	-5.61	116.53	119.90
1	2	1167	U	C5'-C4'-C3'	5.59	124.94	116.00
4	5	88	U	OP1-P-O3'	5.56	117.44	105.20
1	2	1097	G	C2'-C3'-O3'	-5.55	97.30	109.50
3	4	71	U	C6-N1-C1'	-5.54	113.44	121.20
1	2	1162	U	P-O3'-C3'	5.53	126.33	119.70
1	2	145	G	C3'-C2'-O2'	-5.49	97.37	113.30
1	2	1091	G	C4'-C3'-O3'	-5.49	97.88	109.40
1	2	145	G	C5'-C4'-O4'	5.48	115.68	109.10
9	B	789	LEU	CA-CB-CG	5.48	127.90	115.30
1	2	1105	C	C4'-C3'-O3'	-5.45	97.95	109.40
4	5	88	U	OP2-P-O3'	-5.45	93.21	105.20
1	2	1162	U	C4'-C3'-C2'	5.43	108.03	102.60
1	2	1151	U	N1-C1'-C2'	5.43	121.05	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1168	U	C4'-C3'-C2'	-5.41	97.19	102.60
36	n	23	LEU	CA-CB-CG	5.40	127.72	115.30
36	v	23	LEU	CA-CB-CG	5.39	127.70	115.30
1	2	1089	G	P-O3'-C3'	5.34	126.11	119.70
1	2	1168	U	O3'-P-O5'	-5.33	93.86	104.00
1	2	144	G	C1'-C2'-O2'	-5.32	94.63	110.60
1	2	1150	U	P-O3'-C3'	-5.28	113.37	119.70
3	4	90	C	C2-N3-C4	5.25	122.52	119.90
9	B	813	ARG	CG-CD-NE	5.20	122.72	111.80
1	2	1152	U	O4'-C4'-C3'	5.18	110.25	106.10
1	2	66	A	C4'-C3'-O3'	5.17	123.35	113.00
1	2	1163	C	C4'-C3'-O3'	5.15	123.30	113.00
1	2	1148	U	P-O5'-C5'	5.12	129.10	120.90
1	2	145	G	C4'-C3'-O3'	5.12	123.24	113.00
9	B	793	LEU	CA-CB-CG	5.12	127.07	115.30
23	P	962	LEU	CA-CB-CG	5.11	127.04	115.30
9	B	1894	LEU	CA-CB-CG	5.10	127.03	115.30
30	W	34	LEU	CB-CG-CD2	-5.08	102.36	111.00
13	F	401	LEU	CA-CB-CG	5.08	126.99	115.30
1	2	1169	C	O5'-C5'-C4'	-5.06	102.08	111.70
1	2	1147	A	O5'-C5'-C4'	5.04	121.28	111.70
1	2	146	A	C5'-C4'-C3'	-5.03	107.96	116.00
1	2	1161	U	C5'-C4'-O4'	5.02	115.13	109.10
1	2	145	G	P-O3'-C3'	5.02	125.72	119.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	1109	C	Sidechain
1	2	141	A	Sidechain
8	A	1190	ASN	Peptide
8	A	1481	GLU	Peptide
9	B	1369	GLY	Peptide
9	B	684	LEU	Peptide
9	B	685	ARG	Peptide
9	B	790	ASP	Peptide
17	J	271	CYS	Peptide
17	J	664	PHE	Peptide
20	M	15	LYS	Peptide
20	M	18	ASN	Peptide
23	P	1013	ASP	Peptide

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Mol	Chain	Res	Type	Group
23	P	1014	LYS	Peptide
27	T	458	SER	Peptide
30	W	16	VAL	Peptide
39	r	50	ASP	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
2	3	75/89 (84%)	74 (99%)	1 (1%)	0	100	100
6	7	62/115 (54%)	62 (100%)	0	0	100	100
7	8	62/109 (57%)	61 (98%)	1 (2%)	0	100	100
8	A	2202/2413 (91%)	2095 (95%)	105 (5%)	2 (0%)	51	86
9	B	1694/2163 (78%)	1631 (96%)	60 (4%)	3 (0%)	47	81
10	C	838/1008 (83%)	785 (94%)	52 (6%)	1 (0%)	51	86
11	D	140/143 (98%)	126 (90%)	14 (10%)	0	100	100
12	E	114/587 (19%)	103 (90%)	9 (8%)	2 (2%)	8	40
13	F	409/494 (83%)	387 (95%)	21 (5%)	1 (0%)	47	81
14	G	358/469 (76%)	335 (94%)	23 (6%)	0	100	100
15	H	425/465 (91%)	398 (94%)	27 (6%)	0	100	100
17	J	788/899 (88%)	722 (92%)	61 (8%)	5 (1%)	25	66
18	K	122/126 (97%)	121 (99%)	1 (1%)	0	100	100
19	L	101/194 (52%)	94 (93%)	7 (7%)	0	100	100
20	M	164/242 (68%)	141 (86%)	23 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	N	77/291 (26%)	76 (99%)	1 (1%)	0	100	100
22	O	829/971 (85%)	789 (95%)	40 (5%)	0	100	100
23	P	1170/1361 (86%)	1059 (90%)	104 (9%)	7 (1%)	25	66
24	Q	214/435 (49%)	202 (94%)	11 (5%)	1 (0%)	29	69
25	R	165/213 (78%)	162 (98%)	3 (2%)	0	100	100
26	S	101/107 (94%)	88 (87%)	13 (13%)	0	100	100
27	T	454/530 (86%)	416 (92%)	38 (8%)	0	100	100
28	U	188/266 (71%)	159 (85%)	28 (15%)	1 (0%)	29	69
29	V	123/280 (44%)	112 (91%)	11 (9%)	0	100	100
30	W	168/238 (71%)	129 (77%)	28 (17%)	11 (6%)	1	16
31	X	26/111 (23%)	26 (100%)	0	0	100	100
32	Y	82/111 (74%)	76 (93%)	5 (6%)	1 (1%)	13	50
33	Z	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	50
34	a	88/95 (93%)	81 (92%)	7 (8%)	0	100	100
35	b	66/196 (34%)	61 (92%)	5 (8%)	0	100	100
35	k	66/196 (34%)	62 (94%)	4 (6%)	0	100	100
35	s	66/196 (34%)	62 (94%)	4 (6%)	0	100	100
36	d	81/101 (80%)	79 (98%)	2 (2%)	0	100	100
36	n	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
36	v	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
37	e	73/94 (78%)	71 (97%)	2 (3%)	0	100	100
37	p	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
37	w	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
38	f	70/86 (81%)	67 (96%)	3 (4%)	0	100	100
38	q	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
38	x	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
39	g	69/77 (90%)	63 (91%)	6 (9%)	0	100	100
39	r	73/77 (95%)	66 (90%)	5 (7%)	2 (3%)	5	31
39	y	73/77 (95%)	64 (88%)	6 (8%)	3 (4%)	3	22
40	h	76/146 (52%)	75 (99%)	1 (1%)	0	100	100
40	l	93/146 (64%)	89 (96%)	3 (3%)	1 (1%)	14	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	t	68/146 (47%)	67 (98%)	1 (2%)	0	100	100
41	i	90/110 (82%)	90 (100%)	0	0	100	100
41	m	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
41	u	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
42	j	70/187 (37%)	67 (96%)	3 (4%)	0	100	100
43	o	71/93 (76%)	66 (93%)	5 (7%)	0	100	100
44	z	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
All	All	13125/17406 (75%)	12318 (94%)	765 (6%)	42 (0%)	44	77

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	J	881	VAL
23	P	1299	ILE
24	Q	368	ILE
30	W	34	LEU
30	W	52	LYS
39	y	50	ASP
13	F	368	ALA
23	P	363	VAL
23	P	413	ILE
30	W	17	ASP
30	W	18	HIS
30	W	51	THR
30	W	68	PRO
30	W	121	PRO
30	W	124	LEU
32	Y	71	GLN
40	l	140	LYS
9	B	791	PRO
9	B	1896	LYS
10	C	111	LYS
30	W	29	VAL
39	r	60	GLN
8	A	2321	ILE
9	B	960	ILE
12	E	212	VAL
17	J	157	VAL
17	J	665	PRO
23	P	107	ALA

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Mol	Chain	Res	Type
30	W	12	PRO
33	Z	19	ILE
17	J	493	PRO
28	U	232	GLY
39	r	49	GLU
39	y	30	ARG
39	y	60	GLN
23	P	364	THR
23	P	486	PRO
30	W	159	VAL
17	J	718	ASN
8	A	1621	VAL
12	E	305	VAL
23	P	1031	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3	71/81 (88%)	71 (100%)	0	100	100
6	7	56/103 (54%)	56 (100%)	0	100	100
7	8	56/99 (57%)	56 (100%)	0	100	100
8	A	1982/2182 (91%)	1982 (100%)	0	100	100
9	B	1525/1955 (78%)	1523 (100%)	2 (0%)	93	97
10	C	761/910 (84%)	761 (100%)	0	100	100
11	D	131/132 (99%)	131 (100%)	0	100	100
12	E	60/534 (11%)	60 (100%)	0	100	100
13	F	354/445 (80%)	354 (100%)	0	100	100
14	G	267/436 (61%)	267 (100%)	0	100	100
15	H	377/410 (92%)	377 (100%)	0	100	100
17	J	708/813 (87%)	708 (100%)	0	100	100
18	K	102/104 (98%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	L	92/179 (51%)	92 (100%)	0	100	100
20	M	154/224 (69%)	154 (100%)	0	100	100
22	O	739/867 (85%)	738 (100%)	1 (0%)	93	97
23	P	1093/1244 (88%)	1093 (100%)	0	100	100
24	Q	192/391 (49%)	192 (100%)	0	100	100
25	R	154/189 (82%)	154 (100%)	0	100	100
26	S	93/97 (96%)	93 (100%)	0	100	100
27	T	429/492 (87%)	424 (99%)	5 (1%)	71	83
28	U	158/236 (67%)	157 (99%)	1 (1%)	86	92
29	V	118/259 (46%)	116 (98%)	2 (2%)	60	78
30	W	161/219 (74%)	151 (94%)	10 (6%)	18	43
32	Y	76/100 (76%)	75 (99%)	1 (1%)	69	81
33	Z	75/77 (97%)	75 (100%)	0	100	100
34	a	85/91 (93%)	85 (100%)	0	100	100
35	b	64/176 (36%)	64 (100%)	0	100	100
35	k	64/176 (36%)	64 (100%)	0	100	100
35	s	64/176 (36%)	64 (100%)	0	100	100
36	d	72/89 (81%)	72 (100%)	0	100	100
36	n	71/89 (80%)	71 (100%)	0	100	100
36	v	71/89 (80%)	71 (100%)	0	100	100
37	e	69/83 (83%)	69 (100%)	0	100	100
37	p	69/83 (83%)	69 (100%)	0	100	100
37	w	69/83 (83%)	69 (100%)	0	100	100
38	f	64/77 (83%)	64 (100%)	0	100	100
38	q	65/77 (84%)	65 (100%)	0	100	100
38	x	65/77 (84%)	65 (100%)	0	100	100
39	g	61/66 (92%)	61 (100%)	0	100	100
39	r	64/66 (97%)	64 (100%)	0	100	100
39	y	64/66 (97%)	64 (100%)	0	100	100
40	h	75/129 (58%)	75 (100%)	0	100	100
40	l	81/129 (63%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	t	67/129 (52%)	67 (100%)	0	100	100
41	i	85/103 (82%)	85 (100%)	0	100	100
41	m	85/103 (82%)	85 (100%)	0	100	100
41	u	85/103 (82%)	85 (100%)	0	100	100
42	j	64/172 (37%)	64 (100%)	0	100	100
43	o	66/84 (79%)	66 (100%)	0	100	100
44	z	66/75 (88%)	66 (100%)	0	100	100
All	All	11739/15369 (76%)	11717 (100%)	22 (0%)	93	96

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	B	491	PHE
9	B	1008	PHE
22	O	321	CYS
27	T	27	ARG
27	T	35	TYR
27	T	81	ILE
27	T	298	HIS
27	T	317	SER
28	U	246	ILE
29	V	129	HIS
29	V	158	ARG
30	W	4	THR
30	W	8	VAL
30	W	30	ILE
30	W	31	LEU
30	W	34	LEU
30	W	36	LEU
30	W	41	GLU
30	W	50	LEU
30	W	64	LEU
30	W	160	THR
32	Y	37	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (193) such sidechains are listed below:

Mol	Chain	Res	Type
2	3	31	GLN

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Mol	Chain	Res	Type
7	8	28	ASN
8	A	185	GLN
8	A	344	ASN
8	A	404	ASN
8	A	487	ASN
8	A	508	GLN
8	A	559	GLN
8	A	570	GLN
8	A	592	HIS
8	A	658	ASN
8	A	760	ASN
8	A	784	GLN
8	A	796	ASN
8	A	848	ASN
8	A	907	ASN
8	A	952	ASN
8	A	974	ASN
8	A	976	GLN
8	A	997	GLN
8	A	1030	GLN
8	A	1087	ASN
8	A	1128	GLN
8	A	1173	HIS
8	A	1218	GLN
8	A	1471	GLN
8	A	1522	ASN
8	A	1531	HIS
8	A	1532	HIS
8	A	1647	GLN
8	A	1667	GLN
8	A	1677	GLN
8	A	1883	ASN
8	A	1895	HIS
8	A	1947	HIS
8	A	2047	GLN
8	A	2144	GLN
8	A	2306	ASN
8	A	2338	GLN
9	B	516	ASN
9	B	568	GLN
9	B	621	ASN
9	B	676	ASN

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Mol	Chain	Res	Type
9	B	706	GLN
9	B	739	GLN
9	B	768	HIS
9	B	804	HIS
9	B	894	ASN
9	B	904	GLN
9	B	921	ASN
9	B	1103	GLN
9	B	1148	GLN
9	B	1281	GLN
9	B	1349	ASN
9	B	1418	HIS
9	B	1443	HIS
9	B	1611	ASN
9	B	1726	HIS
9	B	1931	GLN
9	B	1968	ASN
9	B	1996	GLN
9	B	2069	GLN
9	B	2139	ASN
10	C	183	GLN
10	C	220	ASN
10	C	251	GLN
10	C	290	HIS
10	C	309	ASN
10	C	423	HIS
10	C	471	HIS
10	C	511	GLN
10	C	554	HIS
10	C	693	ASN
10	C	869	HIS
11	D	101	ASN
11	D	104	ASN
11	D	138	ASN
13	F	113	HIS
13	F	136	GLN
13	F	171	GLN
13	F	244	HIS
13	F	270	HIS
13	F	418	GLN
13	F	443	HIS
14	G	145	HIS

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Mol	Chain	Res	Type
14	G	276	ASN
15	H	38	GLN
15	H	160	GLN
15	H	200	GLN
15	H	203	ASN
15	H	306	HIS
15	H	392	HIS
15	H	394	ASN
15	H	420	ASN
17	J	99	ASN
17	J	140	GLN
17	J	303	ASN
17	J	367	GLN
17	J	379	GLN
17	J	657	ASN
17	J	673	GLN
17	J	733	ASN
17	J	785	ASN
17	J	803	ASN
17	J	884	GLN
18	K	25	GLN
18	K	38	ASN
19	L	104	HIS
20	M	19	ASN
20	M	43	ASN
20	M	112	ASN
22	O	376	HIS
22	O	539	HIS
22	O	695	ASN
22	O	769	ASN
22	O	853	HIS
22	O	882	ASN
22	O	887	ASN
22	O	894	HIS
22	O	908	GLN
23	P	209	GLN
23	P	248	ASN
23	P	375	ASN
23	P	382	GLN
23	P	385	HIS
23	P	436	ASN
23	P	481	GLN

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Mol	Chain	Res	Type
23	P	504	HIS
23	P	546	ASN
23	P	590	HIS
23	P	609	HIS
23	P	738	GLN
23	P	920	GLN
23	P	944	ASN
23	P	945	HIS
23	P	950	GLN
23	P	1023	HIS
23	P	1117	HIS
23	P	1154	HIS
23	P	1203	HIS
23	P	1359	ASN
24	Q	145	GLN
24	Q	204	ASN
24	Q	288	HIS
25	R	31	GLN
25	R	47	GLN
25	R	50	GLN
25	R	170	ASN
27	T	34	HIS
27	T	91	GLN
27	T	167	ASN
27	T	202	GLN
27	T	415	HIS
27	T	440	HIS
30	W	55	HIS
30	W	85	ASN
30	W	99	GLN
30	W	133	GLN
30	W	157	GLN
30	W	158	ASN
32	Y	47	ASN
32	Y	90	ASN
33	Z	7	GLN
33	Z	37	ASN
33	Z	41	ASN
34	a	83	GLN
38	f	25	HIS
38	f	65	HIS
38	f	77	ASN

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Mol	Chain	Res	Type
39	g	53	ASN
39	g	54	ASN
39	g	56	GLN
39	g	60	GLN
41	i	28	HIS
42	j	14	GLN
42	j	16	GLN
35	k	33	GLN
40	l	30	GLN
41	m	52	HIS
36	n	4	ASN
43	o	77	ASN
38	q	76	ASN
38	q	77	ASN
39	r	20	ASN
39	r	54	ASN
35	s	33	GLN
40	t	30	GLN
41	u	51	ASN
41	u	52	HIS
36	v	4	ASN
38	x	77	ASN
39	y	20	ASN
39	y	54	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	147/1175 (12%)	47 (31%)	25 (17%)
16	I	26/95 (27%)	8 (30%)	2 (7%)
3	4	110/160 (68%)	33 (30%)	6 (5%)
4	5	166/214 (77%)	61 (36%)	8 (4%)
5	6	91/112 (81%)	33 (36%)	8 (8%)
All	All	540/1756 (30%)	182 (33%)	49 (9%)

All (182) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	33	U
1	2	41	C
1	2	46	C

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Mol	Chain	Res	Type
1	2	47	U
1	2	66	A
1	2	67	A
1	2	68	U
1	2	83	U
1	2	111	C
1	2	112	A
1	2	113	U
1	2	117	U
1	2	140	G
1	2	141	A
1	2	142	C
1	2	1094	G
1	2	1095	U
1	2	1096	C
1	2	1097	G
1	2	1098	C
1	2	1100	A
1	2	1101	C
1	2	1102	C
1	2	1103	C
1	2	1104	U
1	2	1105	C
1	2	1106	G
1	2	1107	C
1	2	1108	A
1	2	1109	C
1	2	1119	C
1	2	1120	G
1	2	1121	U
1	2	1122	U
1	2	1123	C
1	2	1124	U
1	2	1125	U
1	2	1126	G
1	2	1130	U
1	2	1139	G
1	2	1141	C
1	2	1142	G
1	2	1143	C
1	2	1144	U
1	2	1145	U

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Mol	Chain	Res	Type
1	2	1146	G
1	2	1149	G
3	4	11	A
3	4	18	A
3	4	19	U
3	4	20	A
3	4	25	U
3	4	31	U
3	4	32	G
3	4	35	G
3	4	40	G
3	4	41	U
3	4	45	A
3	4	46	G
3	4	55	U
3	4	56	U
3	4	57	U
3	4	65	G
3	4	66	A
3	4	74	U
3	4	75	U
3	4	76	A
3	4	77	U
3	4	78	A
3	4	79	A
3	4	92	C
3	4	98	G
3	4	134	U
3	4	135	A
3	4	138	U
3	4	139	A
3	4	143	A
3	4	144	A
3	4	145	U
3	4	151	G
4	5	12	C
4	5	13	A
4	5	18	A
4	5	20	U
4	5	27	G
4	5	28	G
4	5	32	G

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Mol	Chain	Res	Type
4	5	34	C
4	5	38	A
4	5	39	U
4	5	41	A
4	5	44	A
4	5	45	A
4	5	46	C
4	5	53	C
4	5	64	C
4	5	69	G
4	5	71	A
4	5	72	C
4	5	75	A
4	5	76	U
4	5	77	A
4	5	78	A
4	5	79	C
4	5	81	A
4	5	82	A
4	5	83	C
4	5	84	A
4	5	93	G
4	5	94	C
4	5	96	U
4	5	97	U
4	5	99	U
4	5	101	C
4	5	103	A
4	5	106	A
4	5	113	G
4	5	115	G
4	5	116	U
4	5	119	U
4	5	121	U
4	5	122	C
4	5	123	U
4	5	125	C
4	5	126	A
4	5	127	U
4	5	128	A
4	5	129	G
4	5	131	A

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Mol	Chain	Res	Type
4	5	132	A
4	5	139	A
4	5	140	A
4	5	141	G
4	5	142	C
4	5	151	A
4	5	160	U
4	5	165	A
4	5	166	U
4	5	167	A
4	5	169	U
4	5	173	U
5	6	2	U
5	6	17	U
5	6	19	C
5	6	25	C
5	6	26	A
5	6	27	U
5	6	28	U
5	6	31	G
5	6	33	C
5	6	37	U
5	6	38	U
5	6	39	G
5	6	41	A
5	6	42	A
5	6	44	A
5	6	45	A
5	6	46	U
5	6	47	A
5	6	48	C
5	6	49	A
5	6	51	A
5	6	56	A
5	6	63	G
5	6	75	A
5	6	76	A
5	6	83	A
5	6	84	C
5	6	85	C
5	6	86	G
5	6	87	U

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Mol	Chain	Res	Type
5	6	88	U
5	6	109	U
5	6	111	U
16	I	58	U
16	I	62	A
16	I	70	A
16	I	71	C
16	I	72	A
16	I	74	A
16	I	78	A
16	I	79	A

All (49) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	32	G
1	2	46	C
1	2	66	A
1	2	67	A
1	2	110	A
1	2	1095	U
1	2	1096	C
1	2	1097	G
1	2	1100	A
1	2	1101	C
1	2	1102	C
1	2	1105	C
1	2	1107	C
1	2	1119	C
1	2	1120	G
1	2	1121	U
1	2	1122	U
1	2	1123	C
1	2	1124	U
1	2	1125	U
1	2	1138	G
1	2	1141	C
1	2	1142	G
1	2	1144	U
1	2	1145	U
3	4	17	A
3	4	19	U

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Mol	Chain	Res	Type
3	4	39	C
3	4	91	U
3	4	134	U
3	4	142	G
4	5	17	C
4	5	40	C
4	5	82	A
4	5	83	C
4	5	114	G
4	5	128	A
4	5	130	A
4	5	150	U
5	6	26	A
5	6	27	U
5	6	38	U
5	6	43	C
5	6	45	A
5	6	55	G
5	6	83	A
5	6	84	C
16	I	77	C
16	I	78	A

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

3 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	$\#\|Z\| > 2$
1	PSU	2	35	1,16	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
1	PSU	2	44	1,16	18,21,22	1.03	1 (5%)	22,30,33	1.65	4 (18%)
1	PSU	2	42	1,16	18,21,22	1.08	1 (5%)	22,30,33	1.73	4 (18%)

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
1	PSU	2	35	1,16	-	0/7/25/26	0/2/2/2
1	PSU	2	44	1,16	-	0/7/25/26	0/2/2/2
1	PSU	2	42	1,16	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	42	PSU	C6-C5	3.46	1.39	1.35
1	2	35	PSU	C6-C5	3.35	1.39	1.35
1	2	44	PSU	C6-C5	3.22	1.39	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	42	PSU	C4-N3-C2	-4.57	119.75	126.34
1	2	35	PSU	C4-N3-C2	-4.49	119.87	126.34
1	2	42	PSU	N1-C2-N3	4.43	120.14	115.13
1	2	35	PSU	N1-C2-N3	4.37	120.08	115.13
1	2	44	PSU	N1-C2-N3	4.28	119.98	115.13
1	2	44	PSU	C4-N3-C2	-4.07	120.47	126.34
1	2	44	PSU	C6-N1-C2	-2.72	119.90	122.68
1	2	44	PSU	O2-C2-N1	-2.44	120.11	122.79
1	2	35	PSU	O2-C2-N1	-2.38	120.17	122.79
1	2	42	PSU	O2-C2-N1	-2.23	120.34	122.79
1	2	35	PSU	C6-N1-C2	-2.22	120.42	122.68
1	2	42	PSU	C6-N1-C2	-2.13	120.50	122.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
45	GTP	C	1101	-	26,34,34	1.19	2 (7%)	32,54,54	1.66	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	C	1101	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1101	GTP	C5-C6	-4.24	1.38	1.47
45	C	1101	GTP	C2-N3	2.11	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C	1101	GTP	PB-O3B-PG	-4.88	116.09	132.83
45	C	1101	GTP	PA-O3A-PB	-3.57	120.59	132.83
45	C	1101	GTP	C5-C6-N1	3.39	119.93	113.95
45	C	1101	GTP	C2-N1-C6	-2.98	119.61	125.10
45	C	1101	GTP	C8-N7-C5	2.94	108.60	102.99
45	C	1101	GTP	C3'-C2'-C1'	2.89	105.33	100.98
45	C	1101	GTP	O6-C6-C5	-2.16	120.16	124.37

There are no chirality outliers.

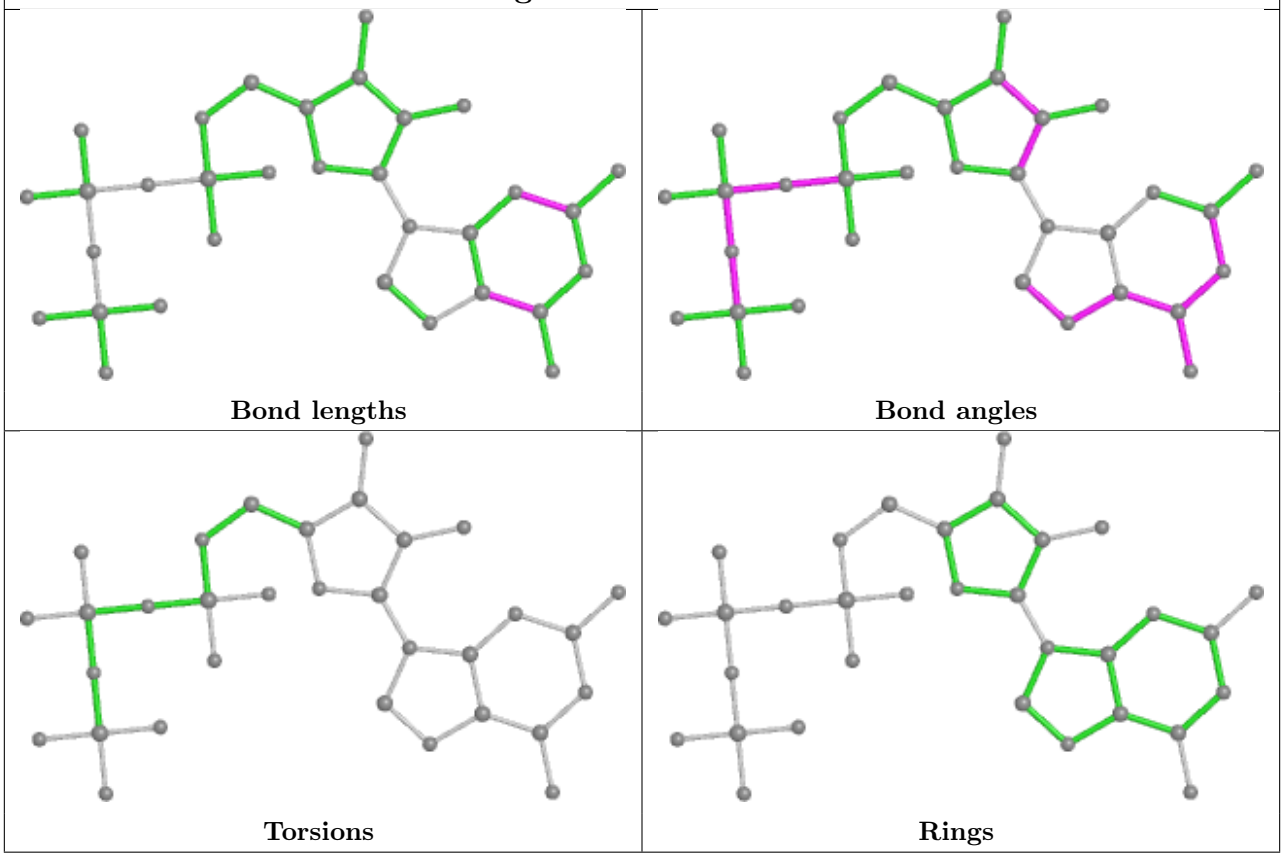
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand GTP C 1101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	5	3
1	2	3
12	E	1
31	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	236:SER	C	297:LYS	N	126.30
1	X	19:ALA	C	101:ALA	N	56.70
1	5	72:C	O3'	73:U	P	3.93
1	5	42:A	O3'	43:G	P	3.10
1	2	1149:G	O3'	1150:U	P	1.90
1	2	143:G	O3'	144:G	P	1.83
1	5	105:A	O3'	106:A	P	1.82
1	2	1090:A	O3'	1091:G	P	1.78

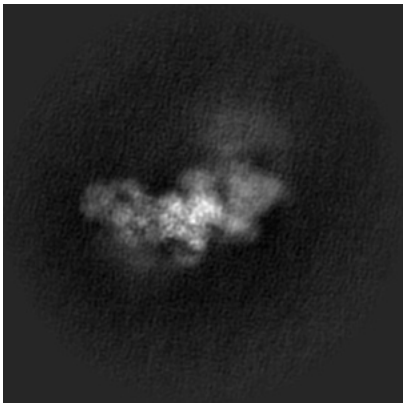
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3683. These allow visual inspection of the internal detail of the map and identification of artifacts.

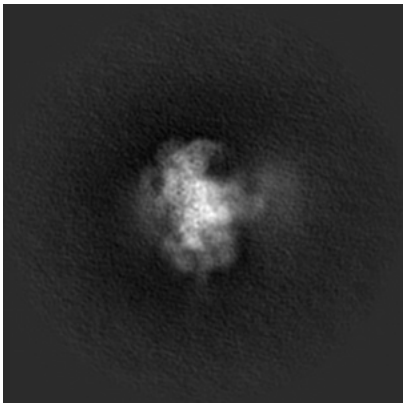
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

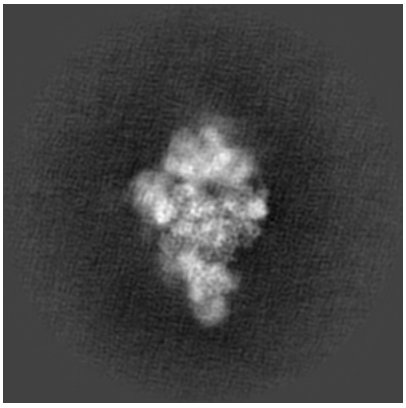
6.1.1 Primary map



X



Y

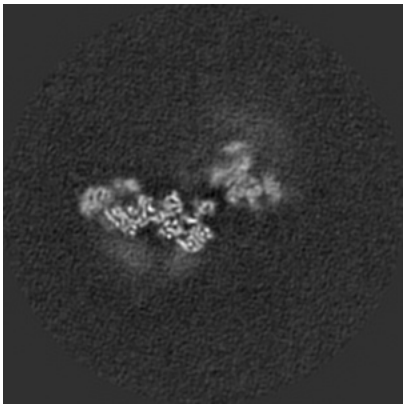


Z

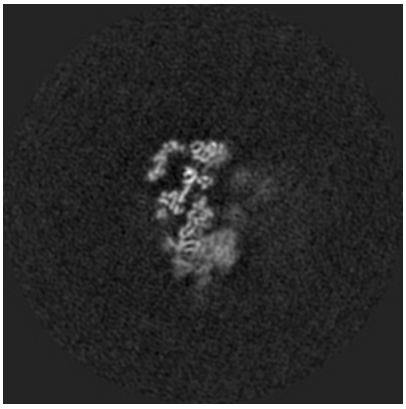
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

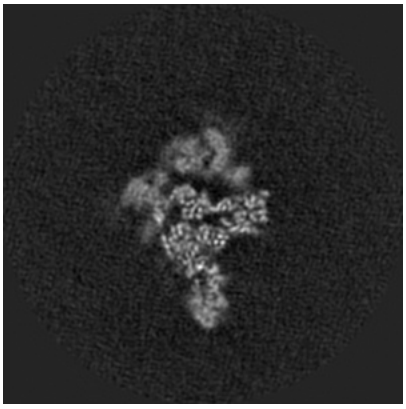
6.2.1 Primary map



X Index: 240



Y Index: 240

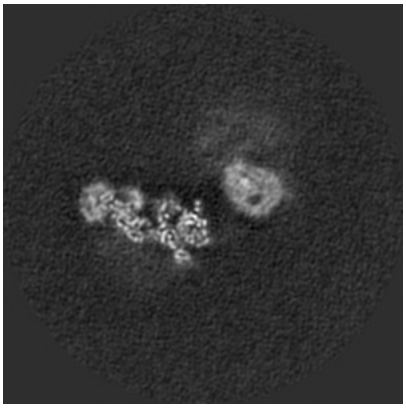


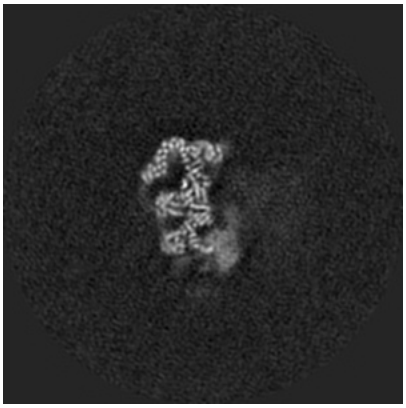
Z Index: 240

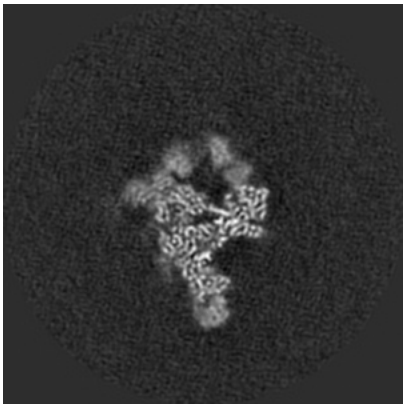
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 253

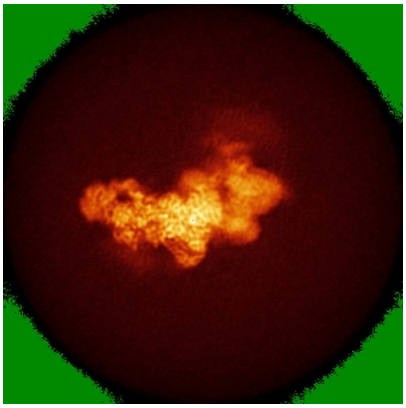

Y Index: 232

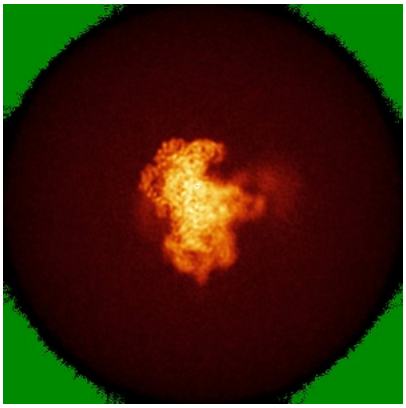

Z Index: 232

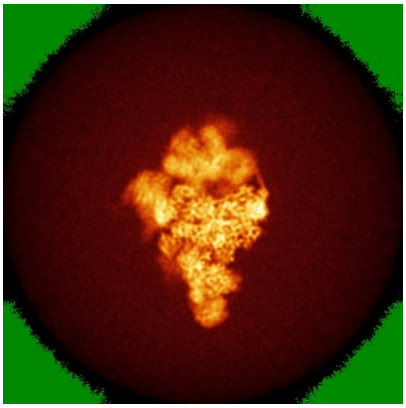
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0258. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

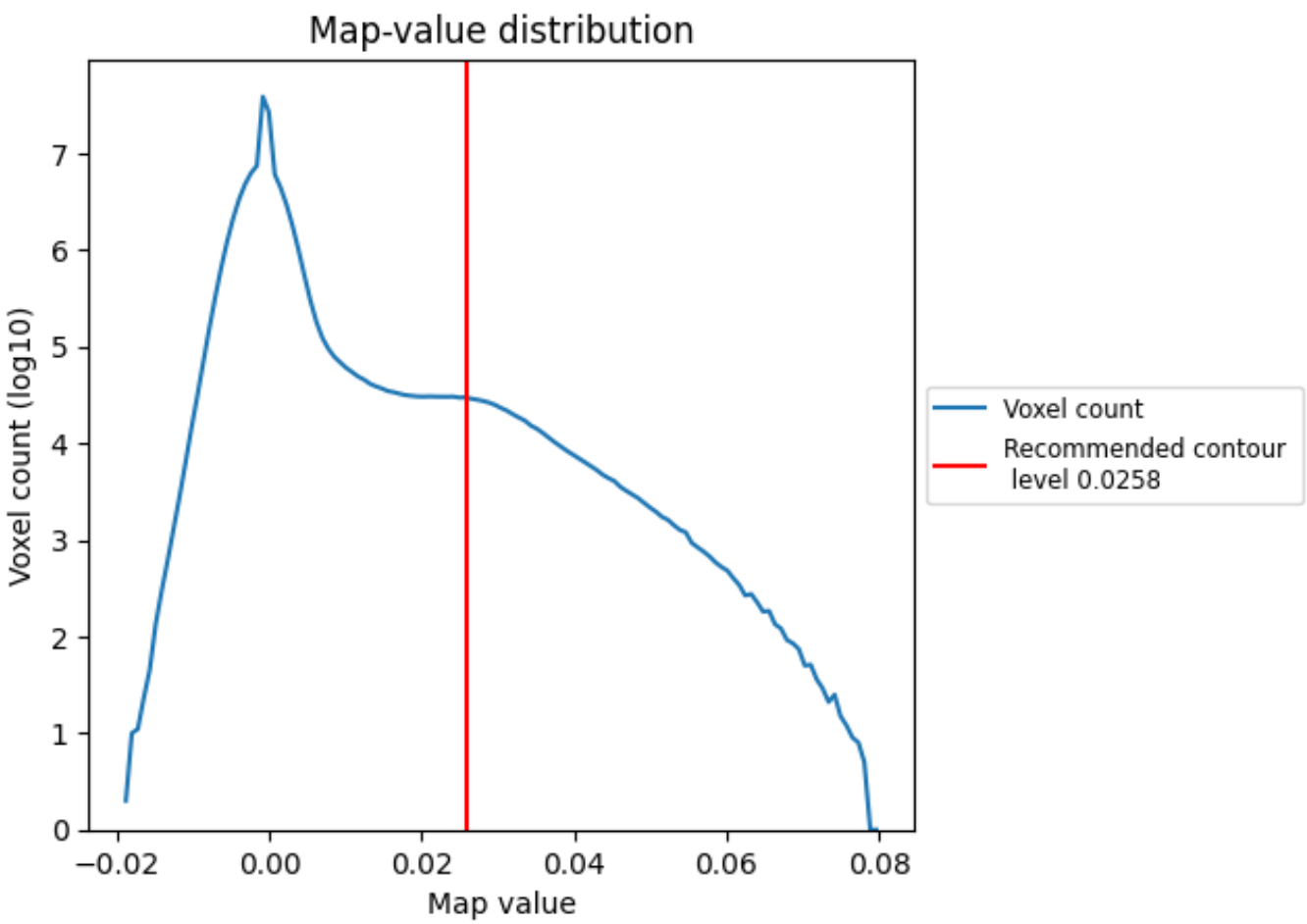
6.6 Mask visualisation (i)

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

7 Map analysis (i)

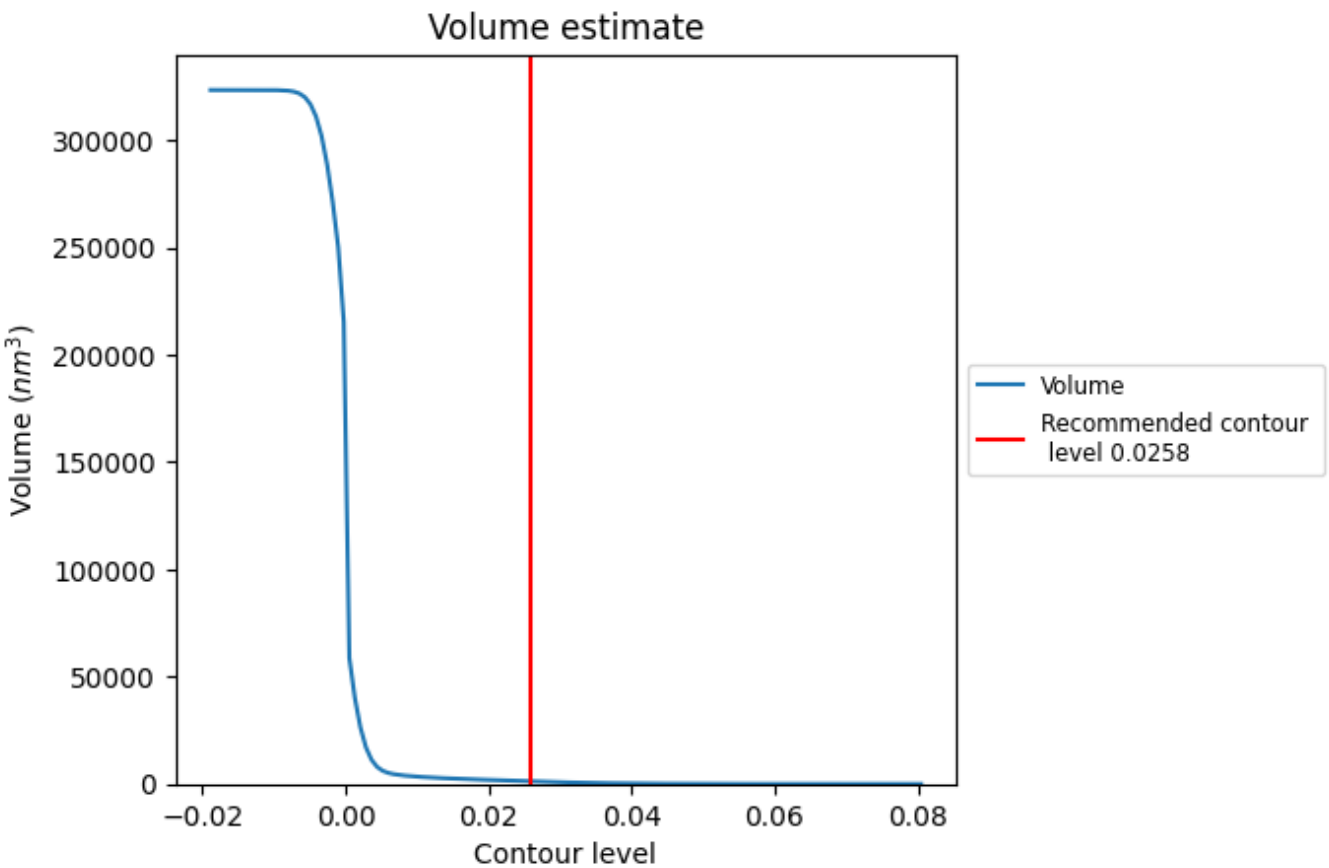
This section contains the results of statistical analysis of the map.

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.

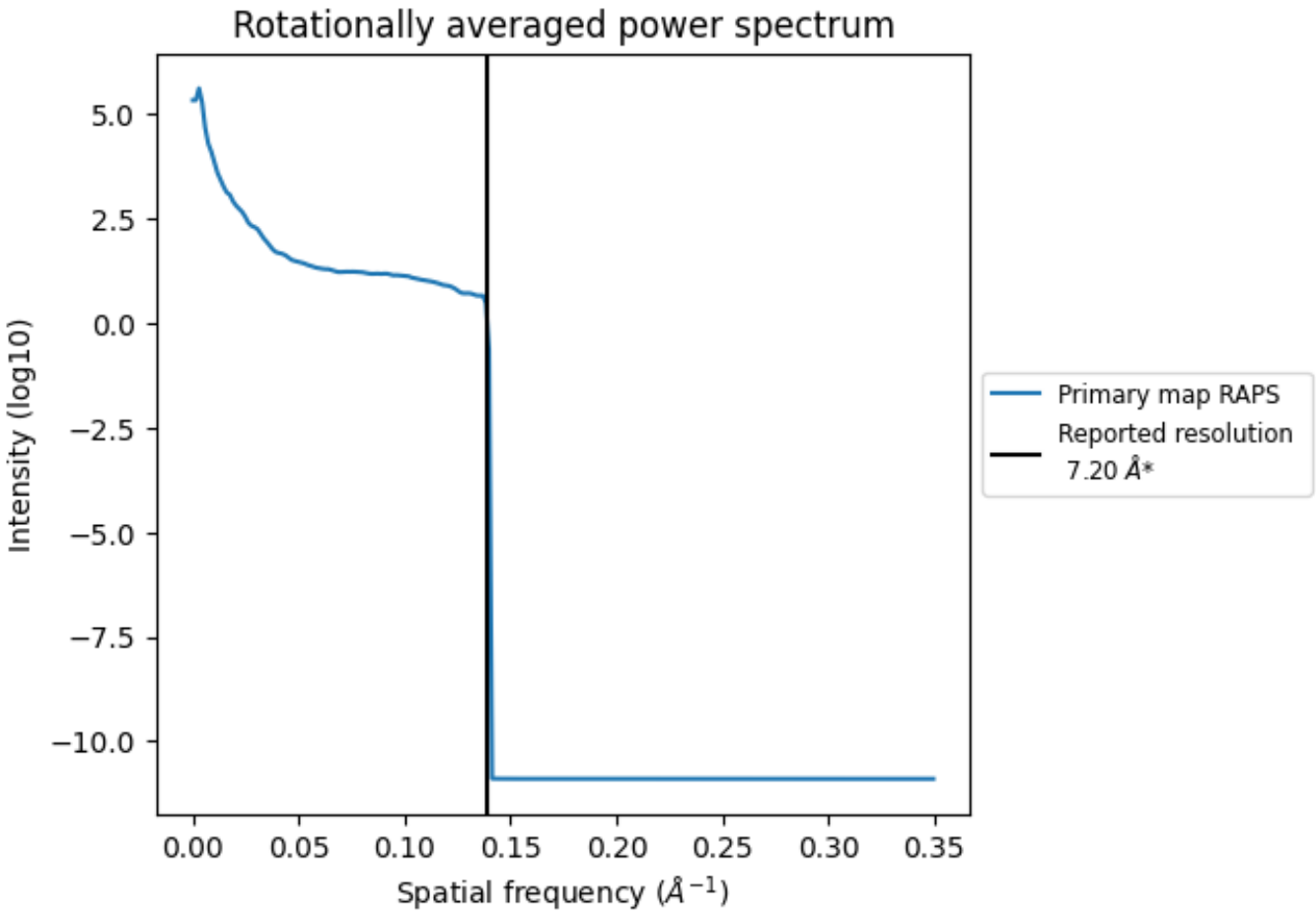
7.2 Volume estimate (i)



The volume at the recommended contour level is 1240 nm^3; this corresponds to an approximate mass of 1120 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 0.139 Å^{-1}

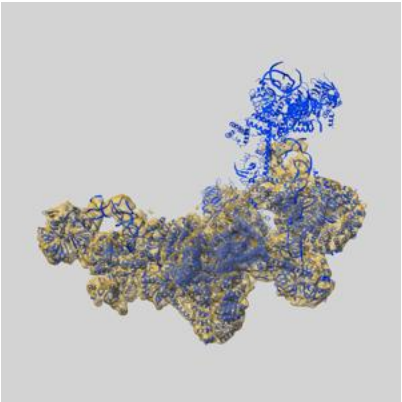
8 Fourier-Shell correlation (i)

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

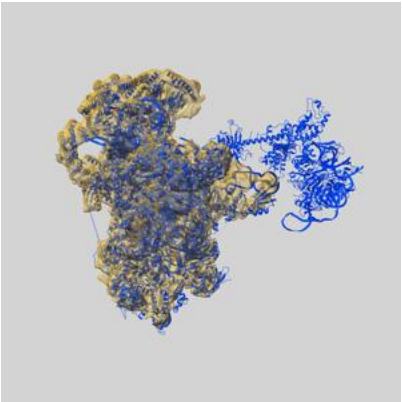
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3683 and PDB model 5NRL. Per-residue inclusion information can be found in section 3 on page 13.

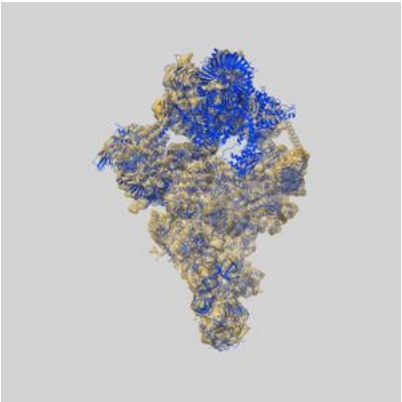
9.1 Map-model overlay (i)



X



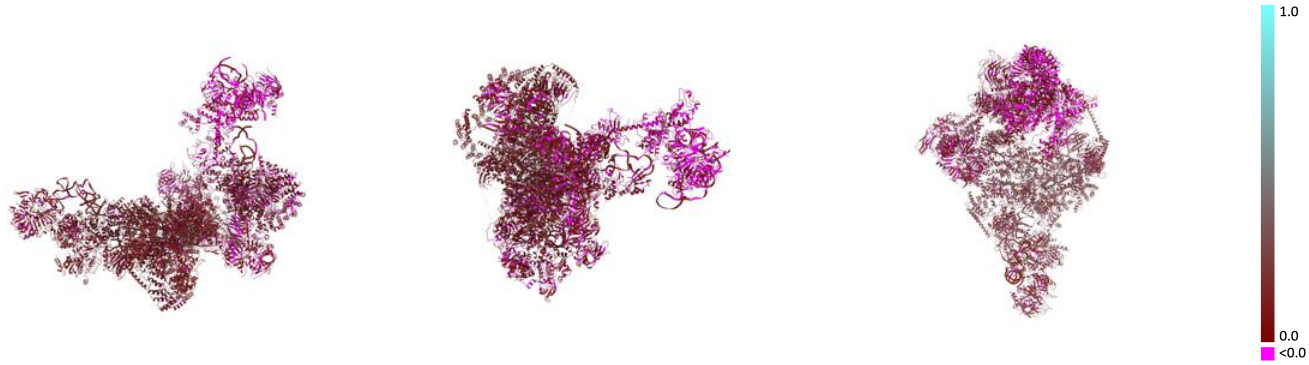
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0258 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.

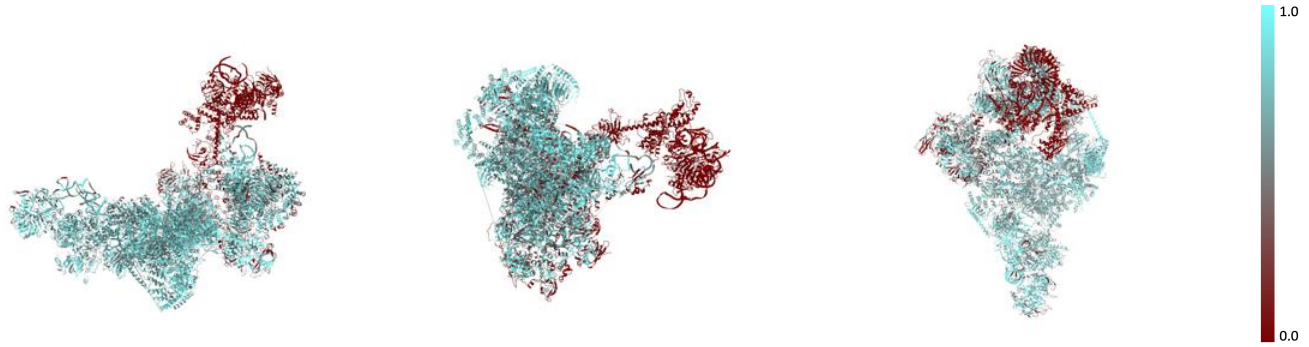
9.2 Q-score mapped to coordinate model (i)



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.

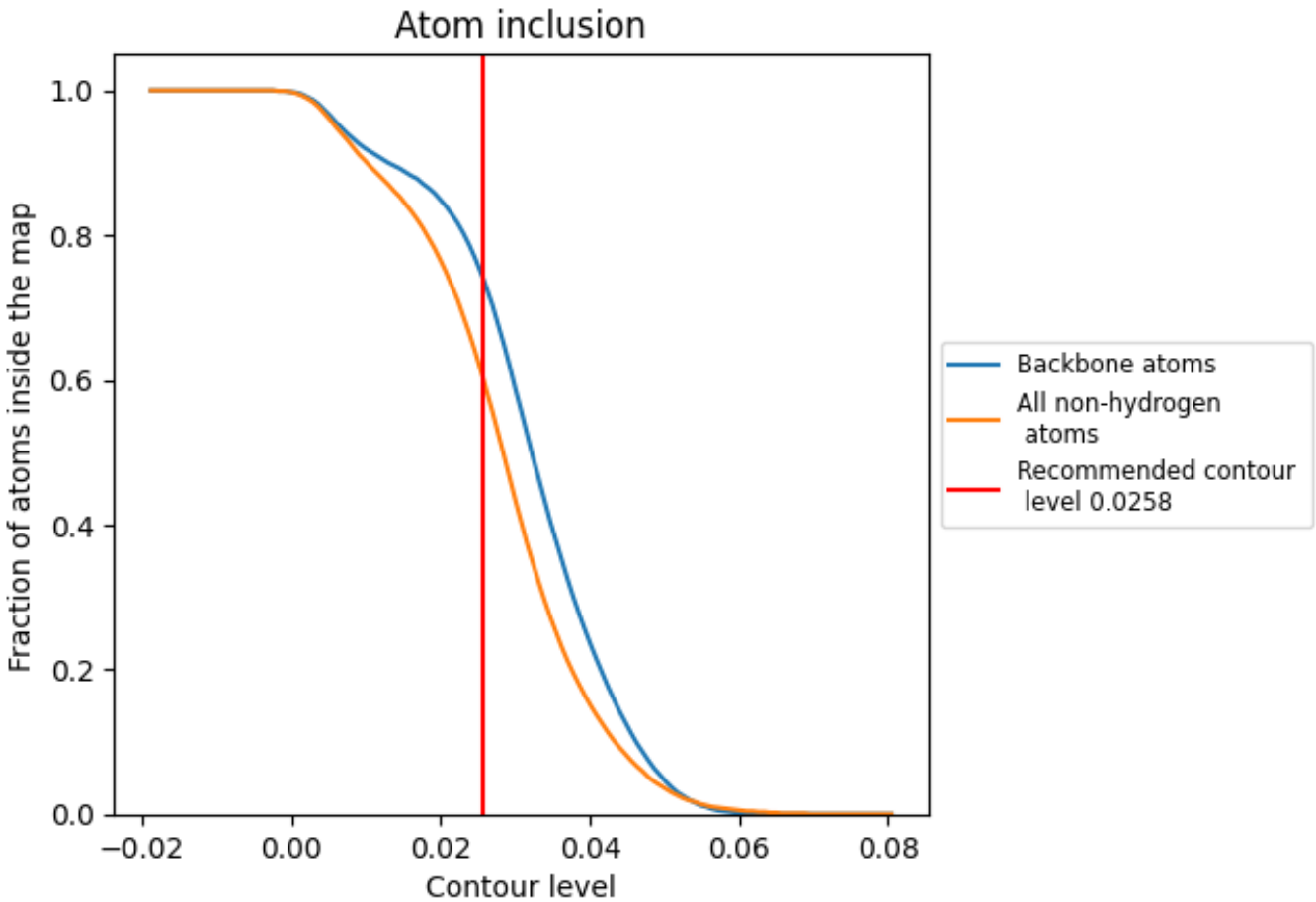
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0258).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 60% 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 (0.0258) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5990	0.1170
2	0.2760	0.0470
3	0.5440	0.0880
4	0.9080	0.1920
5	0.8050	0.1610
6	0.8490	0.1950
7	0.5250	0.0490
8	0.5600	0.0820
A	0.7100	0.1500
B	0.6040	0.1240
C	0.7390	0.1500
D	0.6650	0.1440
E	0.5550	0.1590
F	0.7210	0.1670
G	0.7410	0.1600
H	0.7760	0.1380
I	0.7900	0.1290
J	0.7460	0.1600
K	0.6930	0.1580
L	0.7210	0.1510
M	0.7060	0.1400
N	0.7880	0.2460
O	0.6550	0.1020
P	0.6160	0.0950
Q	0.5210	0.1160
R	0.4630	0.0960
S	0.7310	0.0980
T	0.1060	0.0240
U	0.2500	0.0420
V	0.0000	0.0440
W	0.0000	-0.0000
X	0.5070	0.2310
Y	0.0000	0.0080
Z	0.6490	0.1080
a	0.6180	0.0880

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Chain	Atom inclusion	Q-score
b	0.6820	0.1200
d	0.6500	0.1270
e	0.6880	0.1190
f	0.6930	0.1170
g	0.6540	0.1230
h	0.7060	0.1050
i	0.7160	0.1360
j	0.5100	0.0780
k	0.4970	0.0340
l	0.3620	0.0730
m	0.4950	0.0640
n	0.3060	0.0440
o	0.6960	0.0800
p	0.5580	0.0620
q	0.5850	0.0790
r	0.3290	0.0510
s	0.0000	0.0010
t	0.0000	0.0150
u	0.0000	-0.0050
v	0.0000	-0.0080
w	0.0000	0.0040
x	0.0000	-0.0260
y	0.0000	-0.0010
z	0.5740	0.0700