Full wwPDB EM Validation Report (i)

Nov 14, 2022 – 12:50 PM JST

PDB ID	:	6J6G
EMDB ID	:	EMD-0686
Title	:	Cryo-EM structure of the yeast B*-a2 complex at an average resolution of 3.2 angstrom
Authors	:	Wan, R.; Bai, R.; Yan, C.; Lei, J.; Shi, Y.
Deposited on	:	2019-01-15
Resolution	:	3.20 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:

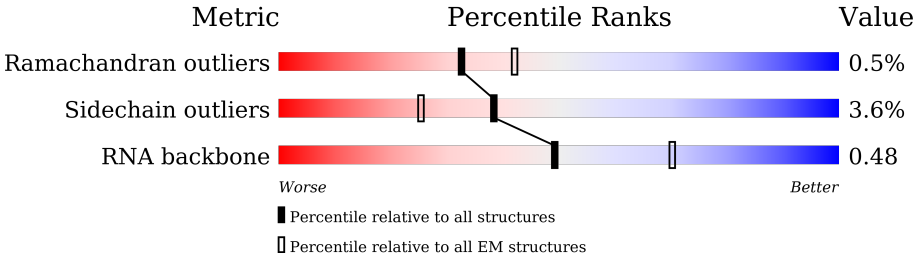
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	A	2413	• 78% • 21%
2	C	1008	90% • 9%
3	J	135	20% 80%
4	O	451	78% • 21%
5	P	379	5% 54% 46%
6	Q	364	78% • 20%
7	R	339	75% • 23%
8	S	175	• 39% • 60%

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Mol	Chain	Length	Quality of chain
9	T	157	99%
10	Z	577	13% 76% 23%
11	c	590	36% 71% 26%
12	d	687	7% 80% 18%
13	I	215	47% 53%
14	n	455	55% 62% 34%
15	H	235	21% 9% 70%
16	B	679	5% 91%
17	D	214	57% 26% 16%
18	E	112	61% 31% 8%
19	L	1175	12% 5% 82%
20	v	859	10% 82% 16%
21	a	111	26% 75% 24%
22	b	238	21% 68% 29%
23	t	175	77% 81% 8% 11%
24	i	94	76% 21%
24	u	94	43% 78% 21%
25	m	146	5% 75% 6% 18%
25	z	146	10% 74% 26%
26	j	77	86% 12%
26	x	77	74% 95%
27	h	86	79% 21%
27	w	86	27% 79% 21%
28	e	110	29% 85% 7% 8%
28	g	110	85% 6% 8%

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Mol	Chain	Length	Quality of chain
29	k	196	44% 6% 49%
29	s	196	10% 46% 53%
30	l	101	61% 21% 18%
30	y	101	41% 80% 20%
31	o	503	18% 24% 75%
31	p	503	19% 25% 75%
31	q	503	24% 25% 74%
31	r	503	18% 24% 75%

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 79042 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-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1913	15793	10154	2714	2868	57	0	0

- Molecule 2 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	920	7348	4733	1223	1362	30	0	0

- Molecule 3 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	J	27	190	112	38	40	0	0

- Molecule 4 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	O	357	2810	1777	493	530	10	0	0

- Molecule 5 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	P	205	1608	1003	294	304	7	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Q	292	2301	1461	399	426	15	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	R	261	2089	1320	369	388	12	0	0

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	S	70	567	355	113	98	1	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	T	157	1291	808	240	232	11	0	0

- Molecule 10 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Z	447	3651	2343	602	688	18	0	0

- Molecule 11 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	c	436	2978	1843	552	575	8	0	0

- Molecule 12 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	d	566	3881	2433	707	732	9	0	0

- Molecule 13 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	102	822	504	152	165	1	0	0

- Molecule 14 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
14	n	299	1894	1175	340	372	1	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	H	70	617	390	115	111	1	0	0

- Molecule 16 is a RNA chain called ACT1 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	B	60	1266	567	213	426	60	0	0

- Molecule 17 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	D	179	3795	1699	660	1258	178	0	0

- Molecule 18 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	E	103	2192	982	391	716	103	0	0

- Molecule 19 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	L	208	4382	1962	732	1480	208	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	v	722	4625	2893	825	895	12	0	0

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	a	84	416	248	84	84	0	0

- Molecule 22 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	b	169	841	503	169	169	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	t	156	926	585	160	180	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	u	74	526	346	87	90	3	0	0
24	i	74	541	358	90	90	3	0	0

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	m	119	917	575	163	176	3	0	0
25	z	108	824	521	142	158	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	j	75	552	350	98	103	1	0	0
26	x	75	552	350	98	103	1	0	0

- Molecule 27 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	h	68	518	337	96	84	1	0	0
27	w	68	518	337	96	84	1	0	0

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	g	101	785	504	149	128	4	0	0
28	e	101	785	504	149	128	4	0	0

- Molecule 29 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	k	100	809	514	150	142	3	0	0
29	s	93	749	476	138	132	3	0	0

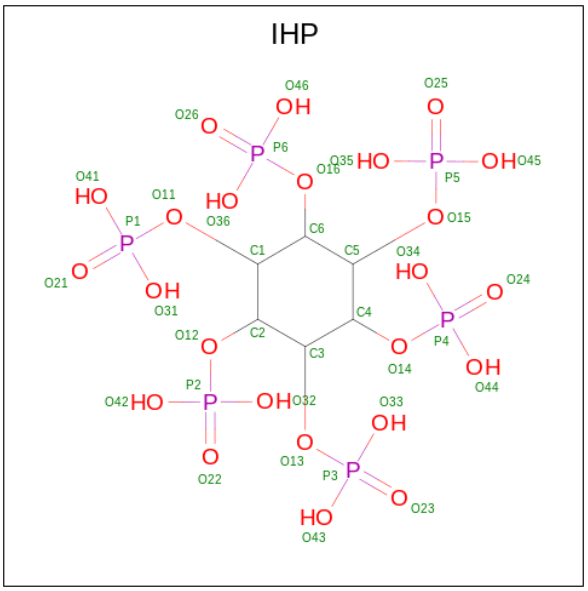
- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	l	83	641	408	111	120	2	0	0
30	y	81	616	394	107	113	2	0	0

- Molecule 31 is a protein called Pre-mRNA-processing factor 19.

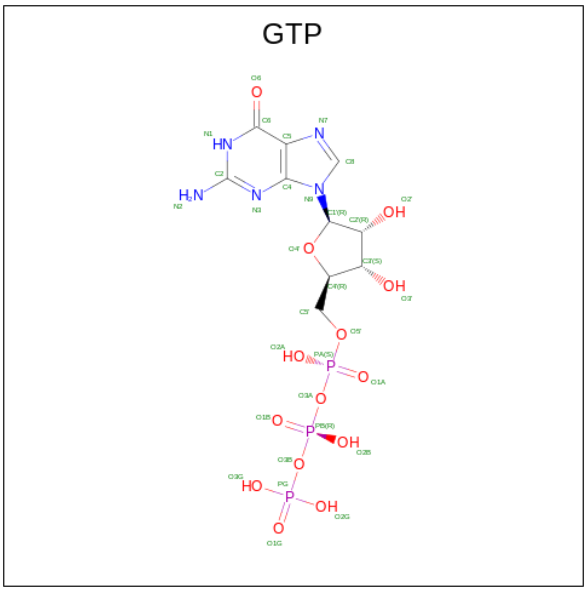
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	r	125	823	521	133	167	2	0	0
31	p	128	843	532	136	173	2	0	0
31	q	129	850	537	137	174	2	0	0
31	o	126	830	525	134	169	2	0	0

- Molecule 32 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 33 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	
33	C	1	32	10	5	14	3	0

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
34	C	1	1	1	0
			Total	Mg	
34	E	5	5	5	0

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

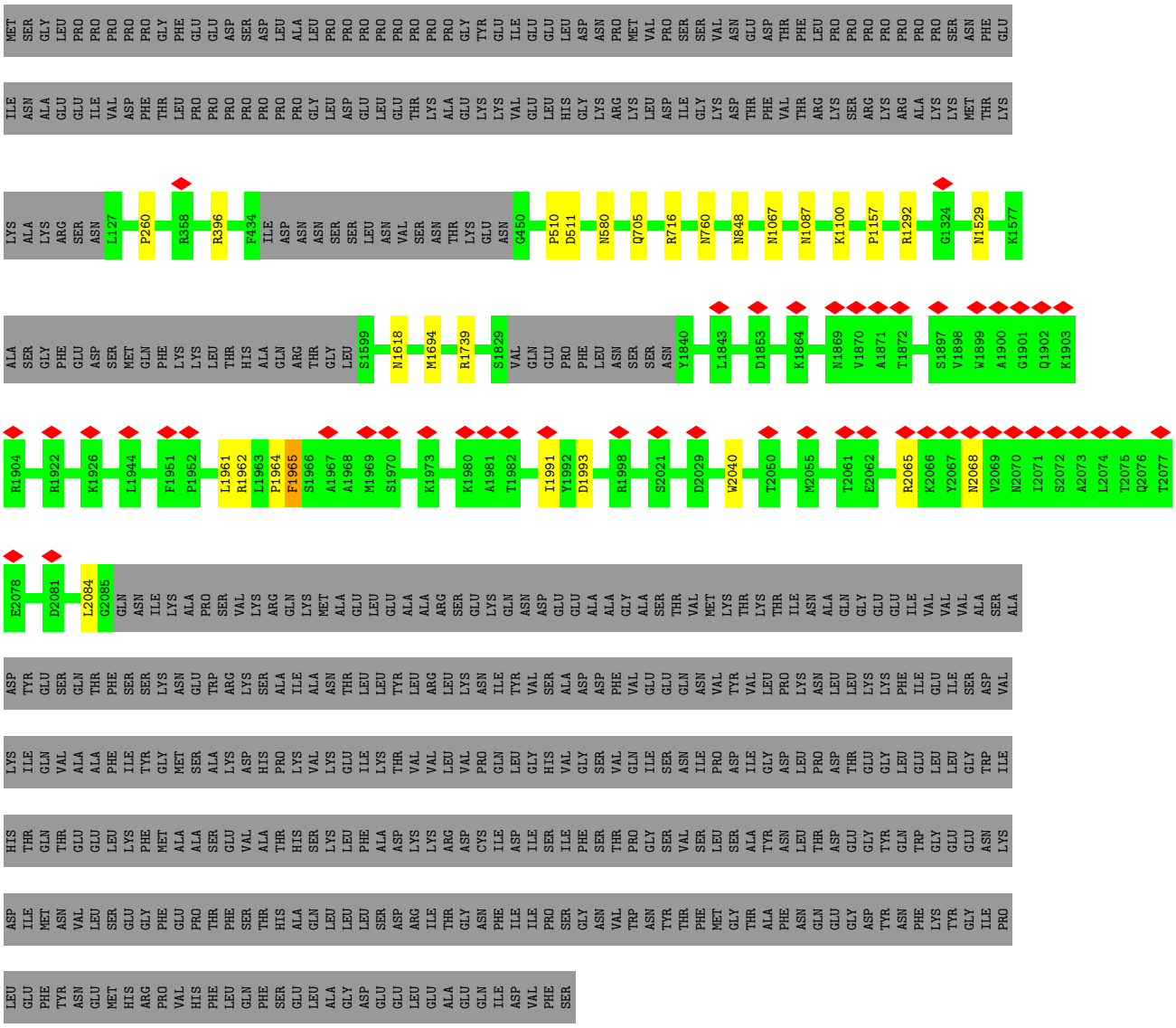
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
35	Q	2	2	2	0
			Total	Zn	
35	R	1	1	1	0
			Total	Zn	
35	T	3	3	3	0

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.

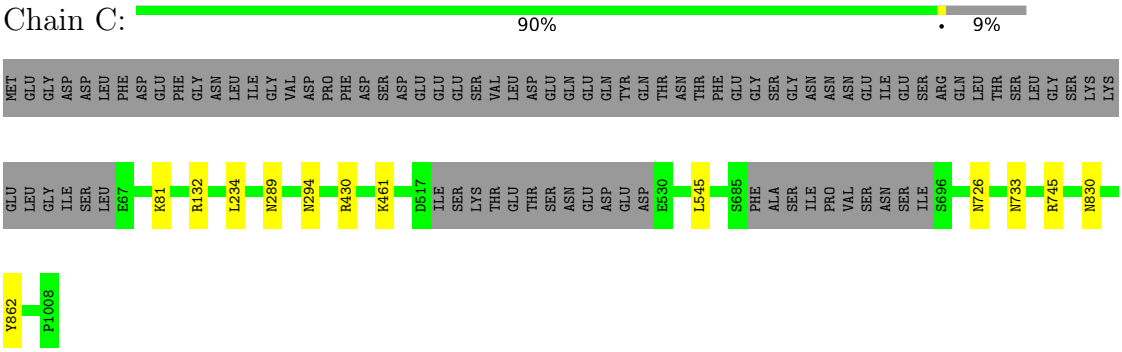
- Molecule 1: Pre-mRNA-splicing factor 8

Chain A: 78% 21%



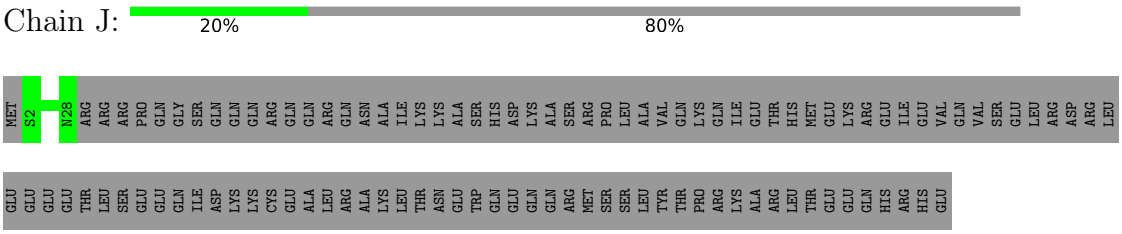
- Molecule 2: Pre-mRNA-splicing factor SNU114

Chain C:



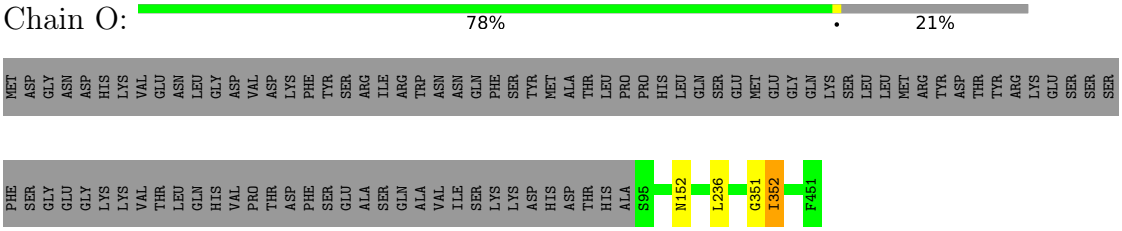
- Molecule 3: Pre-mRNA-splicing factor CWC21

Chain J:



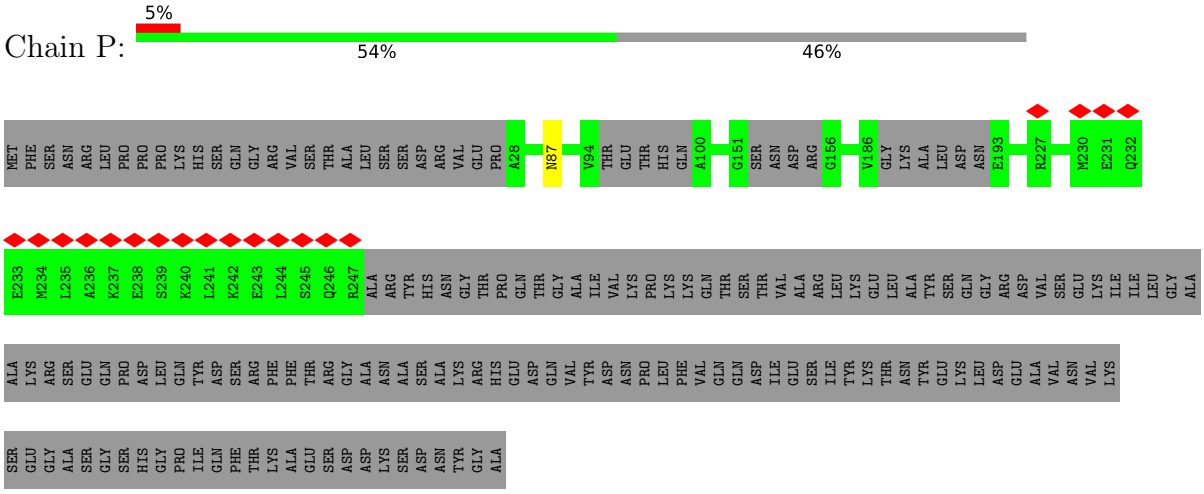
- Molecule 4: Pre-mRNA-splicing factor PRP46

Chain O:



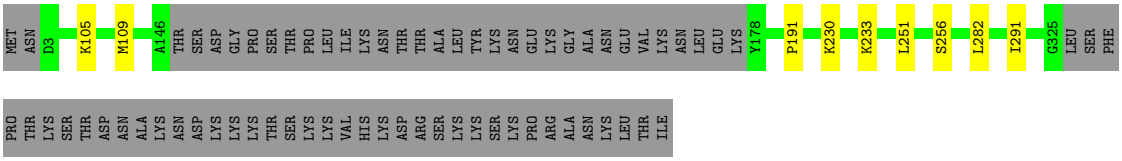
- Molecule 5: Pre-mRNA-processing protein 45

Chain P:



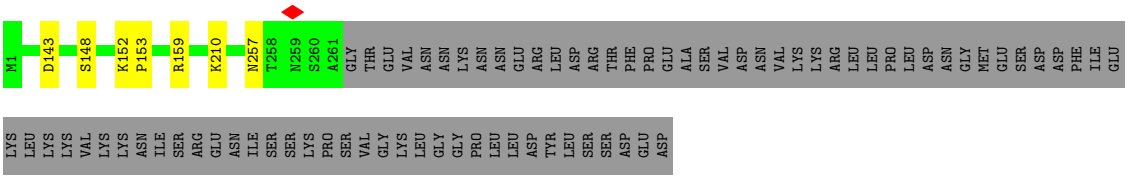
- Molecule 6: Pre-mRNA-splicing factor SLT11

Chain Q:



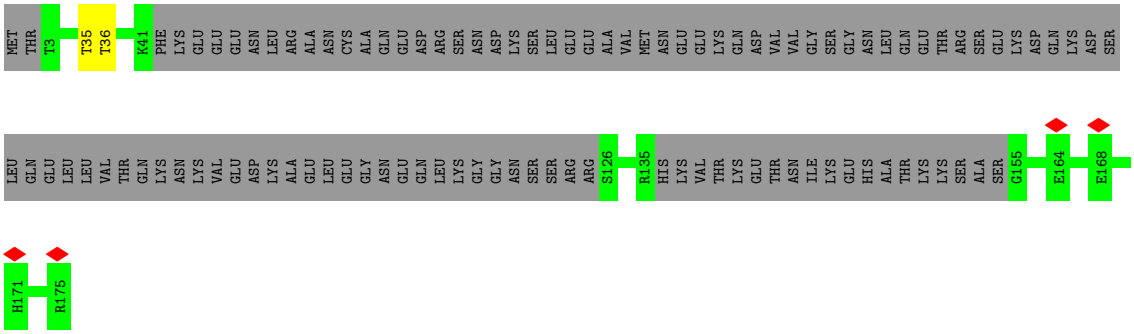
• Molecule 7: Pre-mRNA-splicing factor CWC2

Chain R:



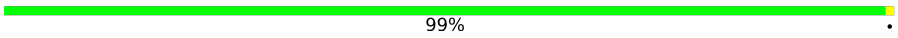
• Molecule 8: Pre-mRNA-splicing factor CWC15

Chain S:



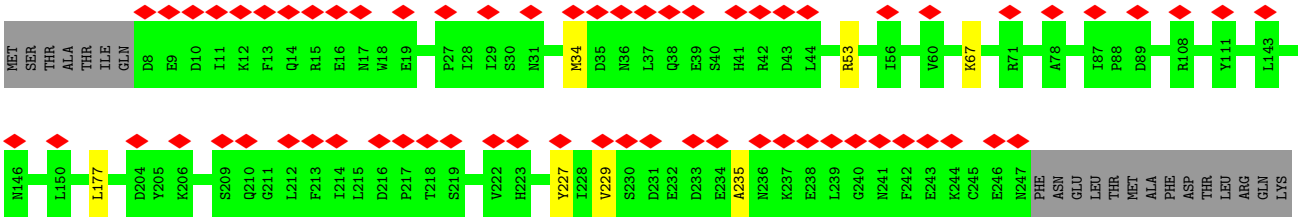
• Molecule 9: Pre-mRNA-splicing factor BUD31

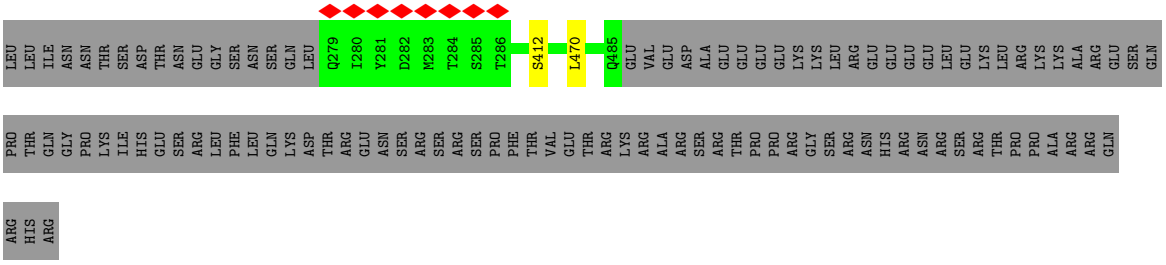
Chain T:



• Molecule 10: Pre-mRNA-splicing factor CWC22

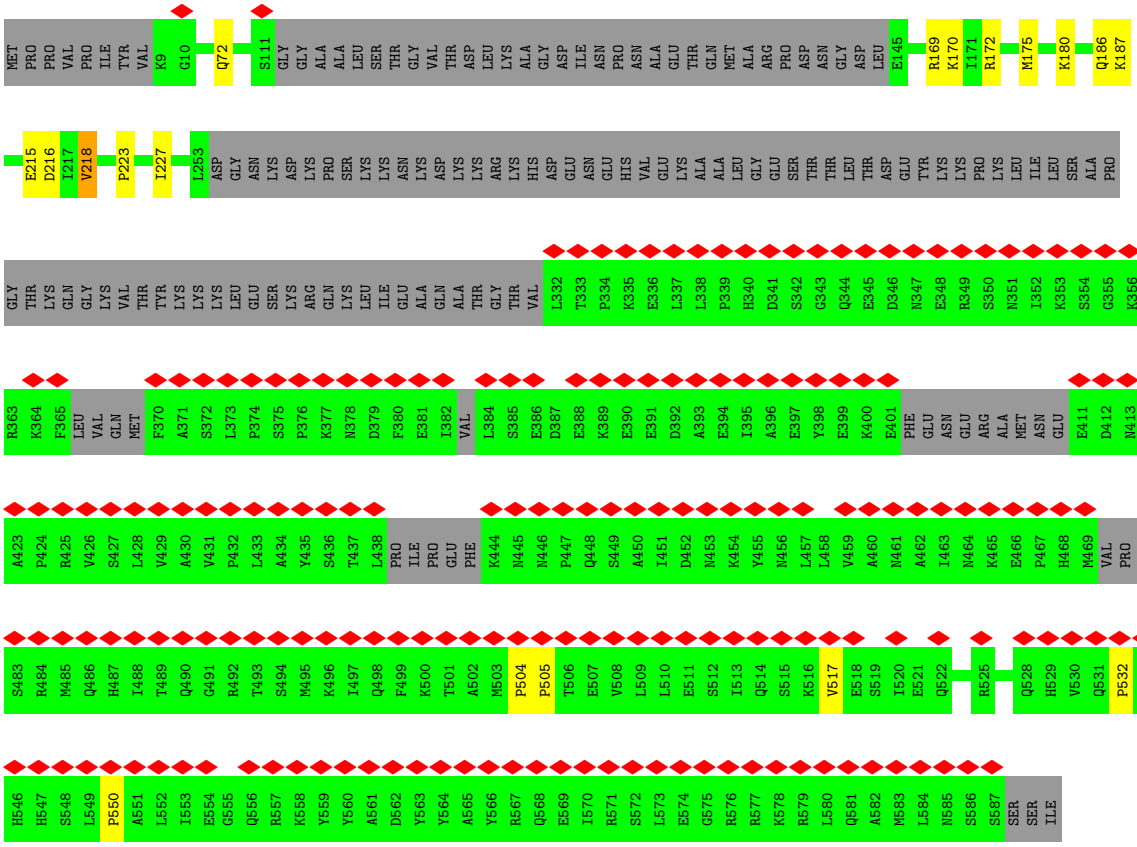
Chain Z:





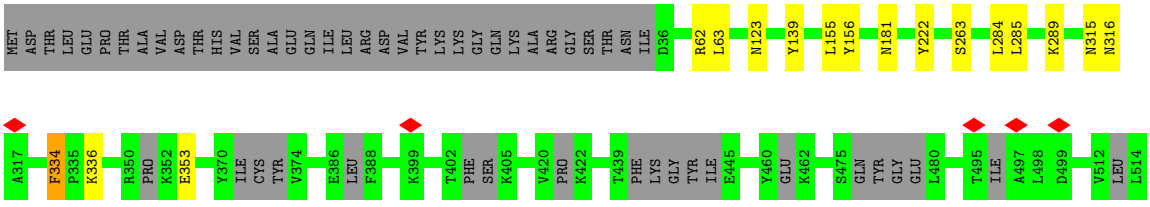
- Molecule 11: Pre-mRNA-splicing factor CEF1

Chain c:



- Molecule 12: Pre-mRNA-splicing factor CLF1

Chain d:



E523 E526 PHE GLU LYS ALA R531 K532 L533 Y534 Y537 W548 ILE GLU PHE ALA MET Y554 Q571 SER GLU ASN V575 D576 E577 D578 I579 E580 F581 E582 I583 T584 D585 E586 N587 K588 L589 E590 A591 R592 K593 VAL F595 E596 E597 A598 I599 V600 K603 L612 S613 I614 L615

E616 A617 LEU LYS D620 Y621 E622 E623 T624 Y625 G626 T627 E628 L629 D630 Q631 E632 T633 V634 K635 K636 ARG PHE PRO LYS VAL ILE LYS LYS VAL ARG LEU GLN ASN GLY VAL GLU GLU GLU PHE VAL ASP TYR ILE PHE PRO ASP ASP ILE ASP ASP ASP LYS PRO LYS PRO SER LYS PHE LEU

GLU LEU ALA LYS LYS TRP LYS GLN GLU GLN ALA LEU

- Molecule 13: Pre-mRNA-splicing factor SYF2

Chain I: 47% 53%

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

SER PRO GLU LYS GLU LYS ALA PHE HIS TYR THR VAL GLN GLU TYR ASP ALA TRP GLU ARG ARG HIS PRO GLN GLY LYS THR GLY GLN SER GLN R92 D123 SER SER ALA ASP GLU GLU ASP ASN LYS ASN VAL PRO LYS LYS GLY ARG ILE GLY K142 V192 R209 E210 S211 LYS

GLY SER GLU

- Molecule 14: Pre-mRNA-processing factor 17

Chain n: 55% 62% • 34%

MET GLY LEU VAL ASP GLY TYR ASP THR SER SER ASP SER ASP LEU ASN PHE ASP GLU GLY LYS SER VAL HIS GLU LYS LYS ASN GLY ASN LEU HIS GLU ASP THR SER TYR GLU PRO SER SER ASN ASN ILE HIS LYS ARG LYS SER HIS F51 S73 SER SER ASP ASP GLU THR SER

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

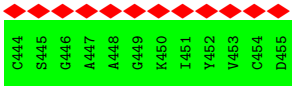
GLU GLU ARG ILE SER PHE ARG CYS TYR LEU P151 K152 K153 V154 I155 R156 N157 Y158 P159 G160 H161 P162 E163 G164 T165 T166 A167 L168 K169 F170 L171 P172 K173 T174 G175 H176 L177 I178 L179 S180 G181 G182 N183 D184 H185 T186 I187 K188 I189 W190 D191 F192 TYR HIS ASP TYR E197 C198 L199 R200

D201 F202 Q203 G204 H205 N206 K207 P208 I209 K210 A211 L212 R213 F214 T215 E216 D217 C218 Q219 S220 F221 L222 S223 S224 S225 F226 D227 R228 S229 V230 K231 I232 W233 D234 T235 E236 T237 G238 K239 V240 K241 T242 R243 L244 H245 L246 N247 S248 T249 P250 A251 D252 V253 E254 S255 R256 P257 T258 N259 P260

H261 E262 F263 I264 V265 G266 L267 S268 N269 I272 L273 H274 Y275 D276 D277 ARG VAL SER GLU ASN GLN GLY LEU V286 Q287 T288 Y289 D290 H291 H292 L293 S294 S295 I296 L297 A298 L299 K300 Y301 F302 P303 D304 G305 S306 K307 F308 I309 S312 E313 D314 K315 T316 V317 R318 I319 W320 E321 N322

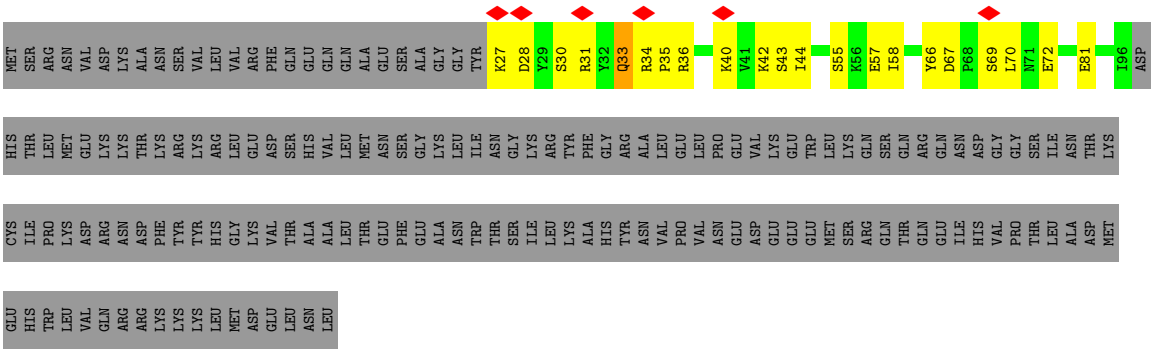
Q323 I324 N325 V326 P327 I328 K329 Q330 I331 S332 D333 T334 A335 GLN HIS S338 M339 P340 F341 L342 N343 V344 H345 P346 SER GLN N349 Y350 F351 C352 A353 Q354 S355 M356 D357 N358 R359 I360 Y361 S362 F363 S364 LEU LYS PRO K368 R371 H372 P373 K374 K375 I376 PHE LYS GLY H380 S381 S382 A383

G384 Y385 G386 I387 S388 L389 A390 F391 S392 G393 D394 G395 R396 Y397 I398 C399 S400 G401 D402 S403 K404 S405 R406 L407 F408 T409 W410 D411 W412 N413 T414 S415 R416 L417 L418 ASN ASN ILE LYS T423 P424 G425 N426 K427 P428 I429 T430 Q431 V432 D433 W434 H435 P436 GLN GLU THR S440 K441 V442 T443



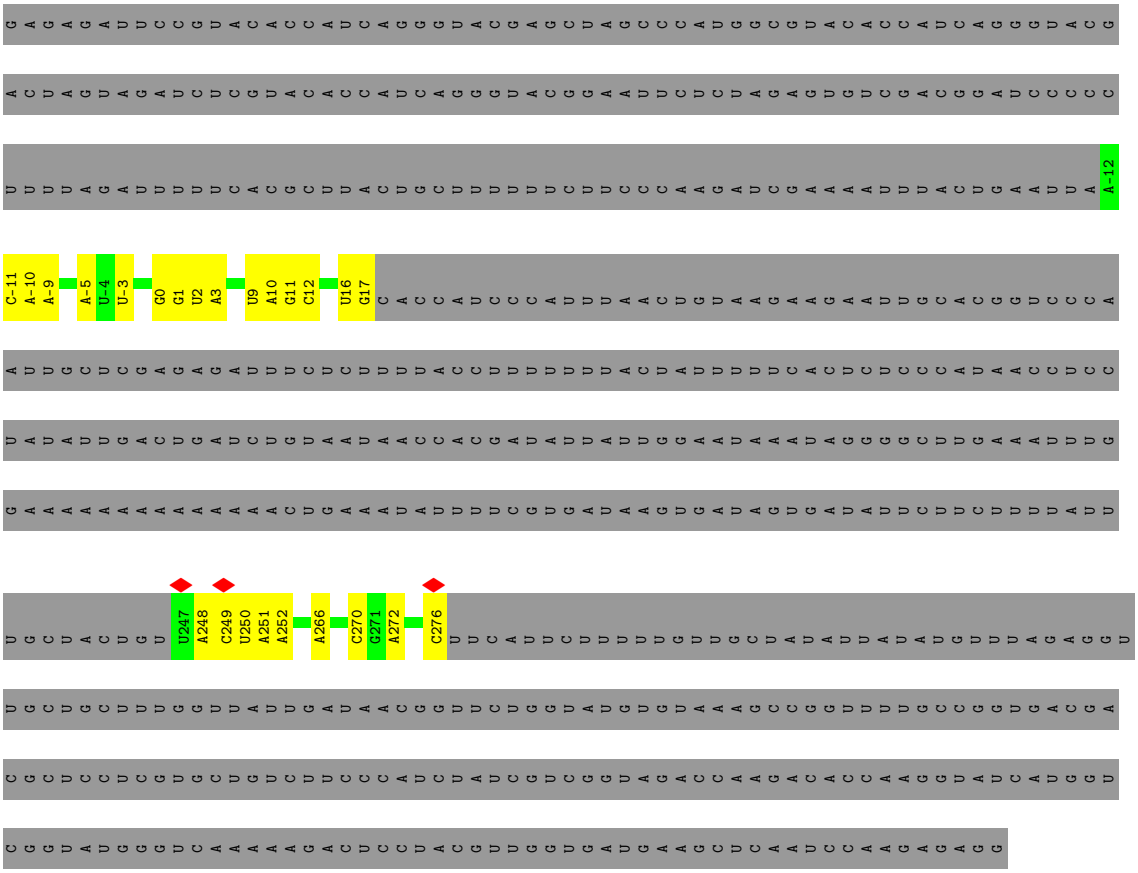
• Molecule 15: Pre-mRNA-splicing factor ISY1

Chain H:



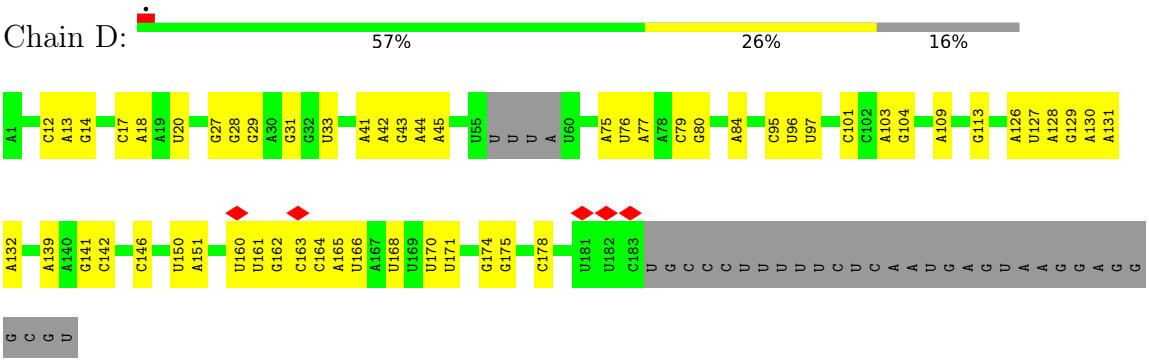
• Molecule 16: ACT1 pre-mRNA

Chain B:



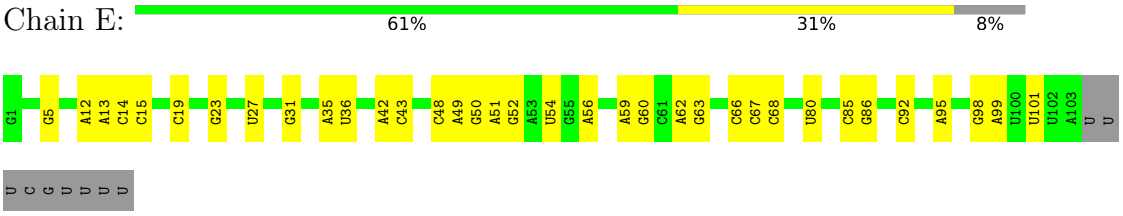
• Molecule 17: U5 snRNA

Chain D:



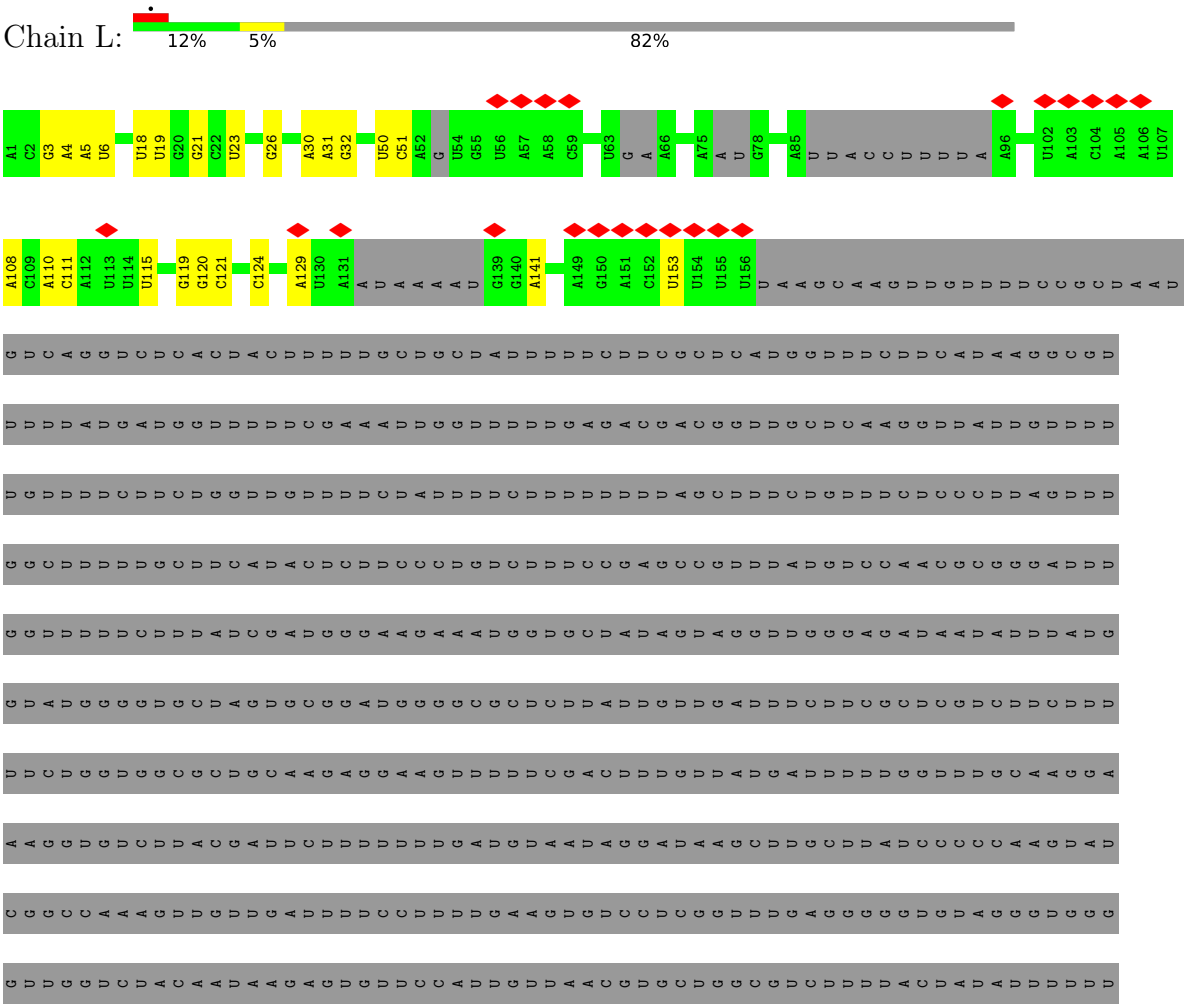
- Molecule 18: U6 snRNA

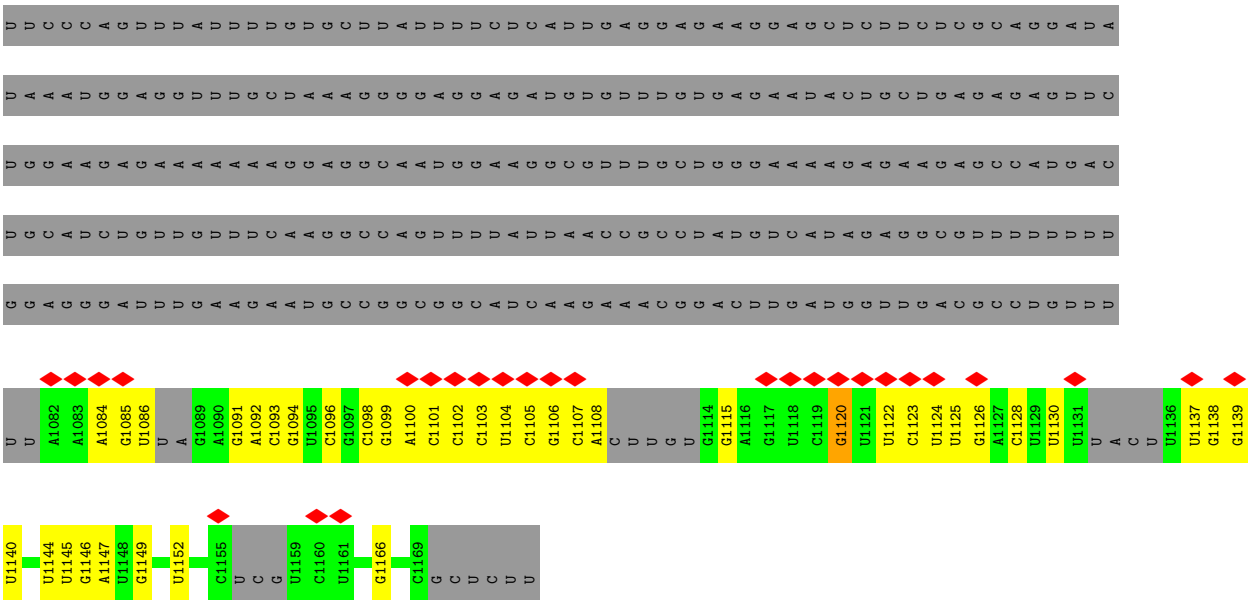
Chain E:



- Molecule 19: U2 snRNA

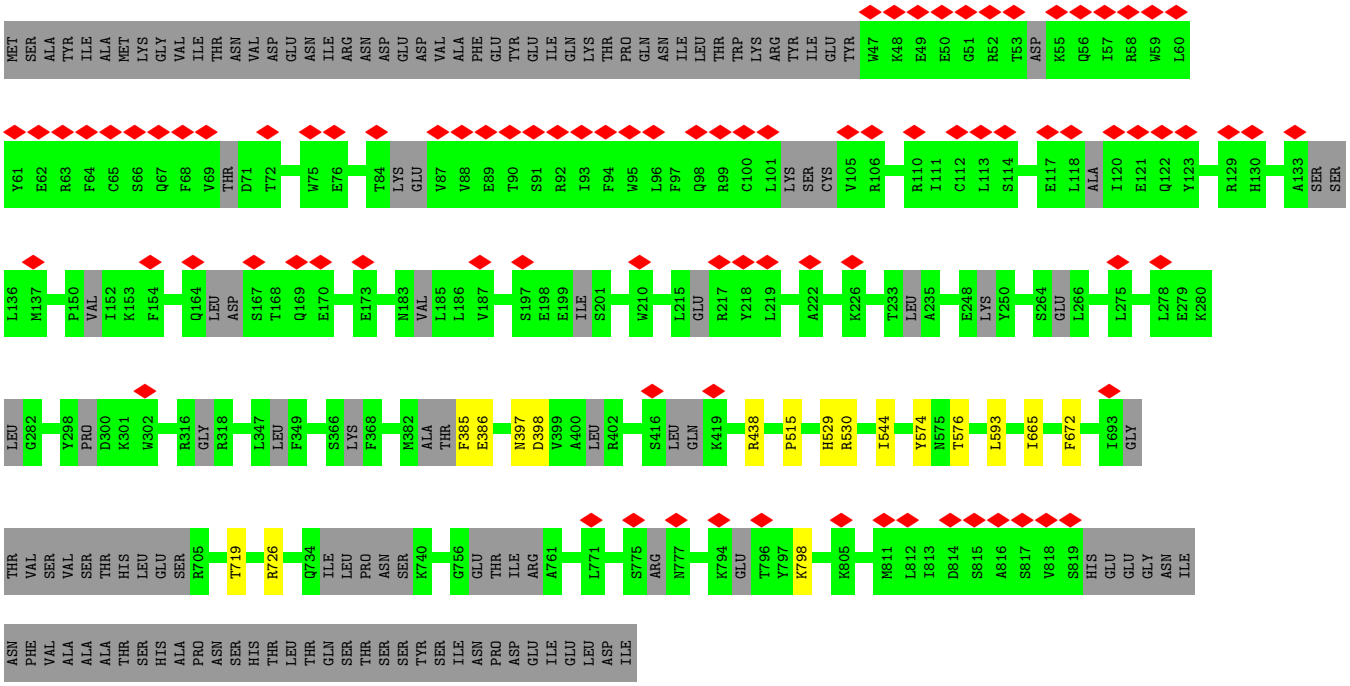
Chain L:





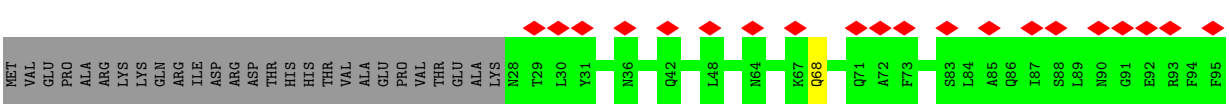
• Molecule 20: Pre-mRNA-splicing factor SYF1

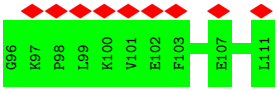
Chain v:



• Molecule 21: U2 small nuclear ribonucleoprotein B”

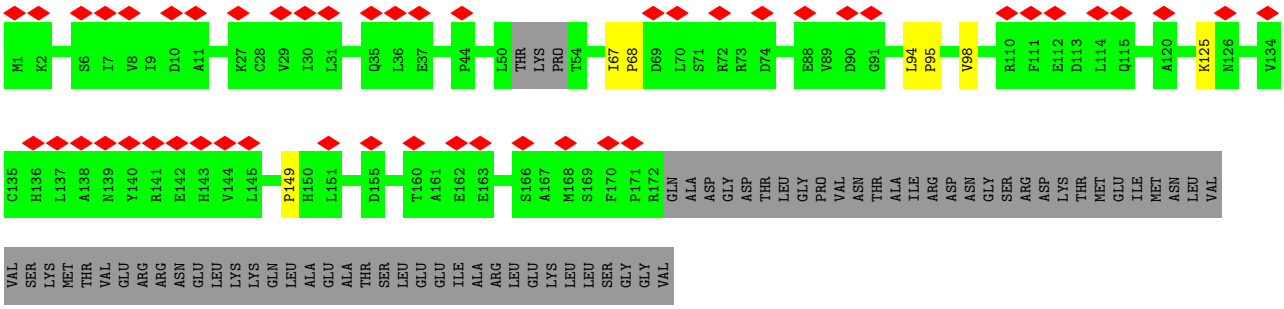
Chain a:





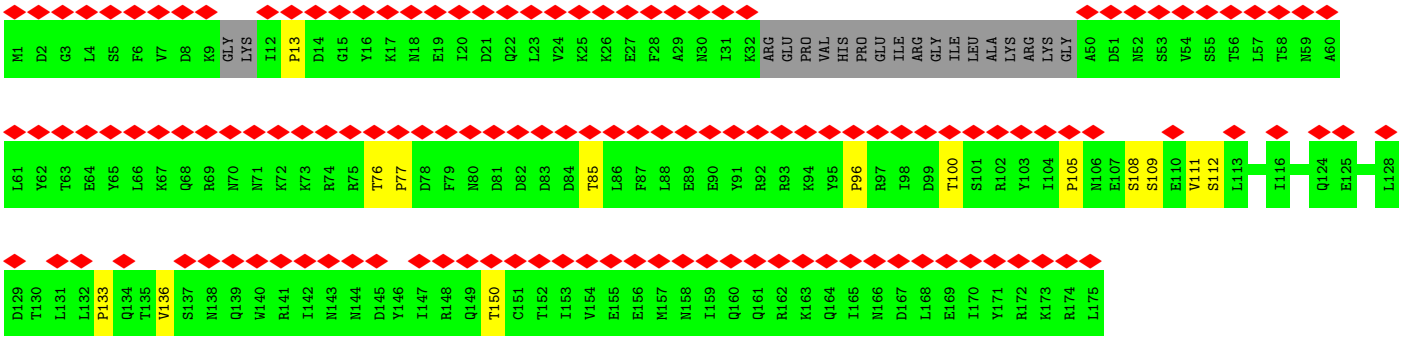
• Molecule 22: U2 small nuclear ribonucleoprotein A'

Chain b:



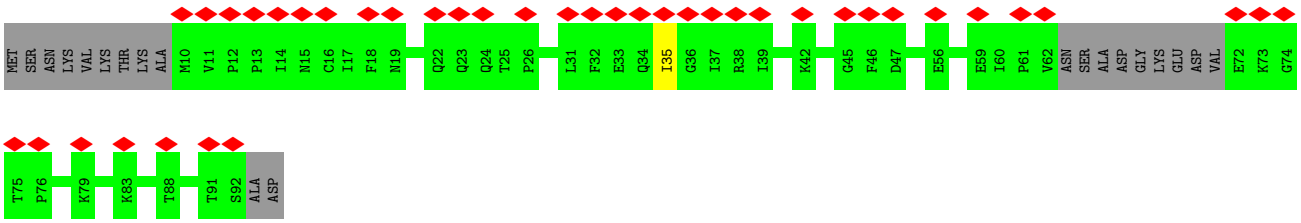
• Molecule 23: Pre-mRNA-splicing factor SNT309

Chain t:



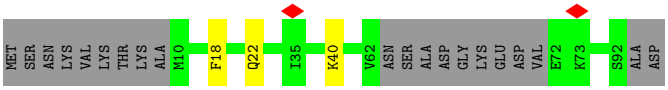
• Molecule 24: Small nuclear ribonucleoprotein E

Chain u:



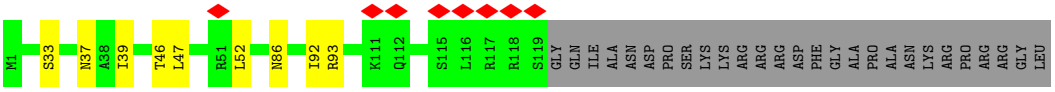
• Molecule 24: Small nuclear ribonucleoprotein E

Chain i:



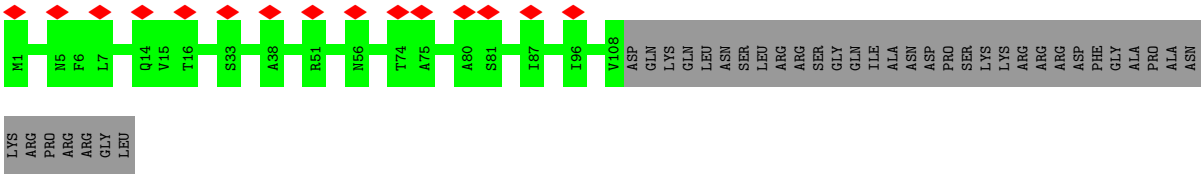
• Molecule 25: Small nuclear ribonucleoprotein Sm D1

Chain m:



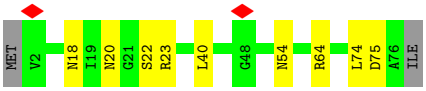
• Molecule 25: Small nuclear ribonucleoprotein Sm D1

Chain z:



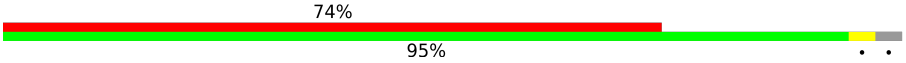
• Molecule 26: Small nuclear ribonucleoprotein G

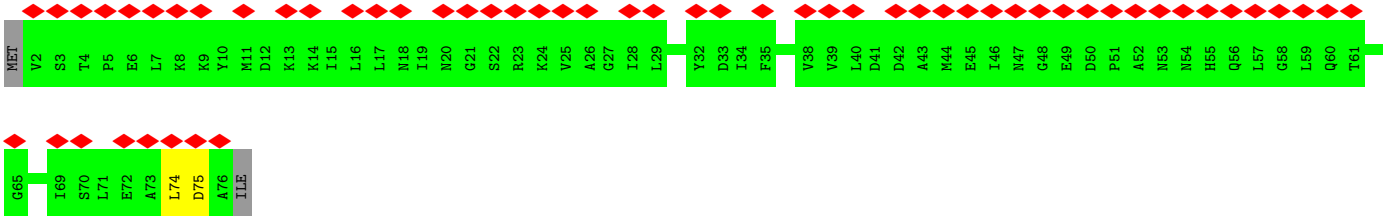
Chain j:



• Molecule 26: Small nuclear ribonucleoprotein G

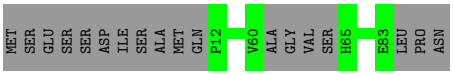
Chain x:





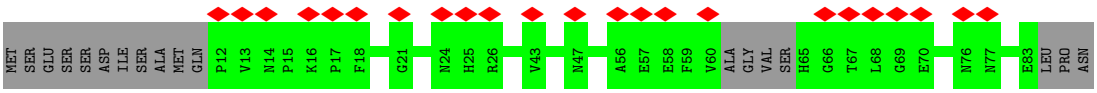
• Molecule 27: Small nuclear ribonucleoprotein F

Chain h:



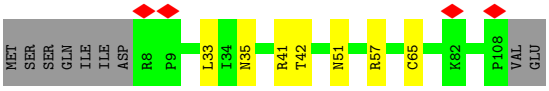
• Molecule 27: Small nuclear ribonucleoprotein F

Chain w:



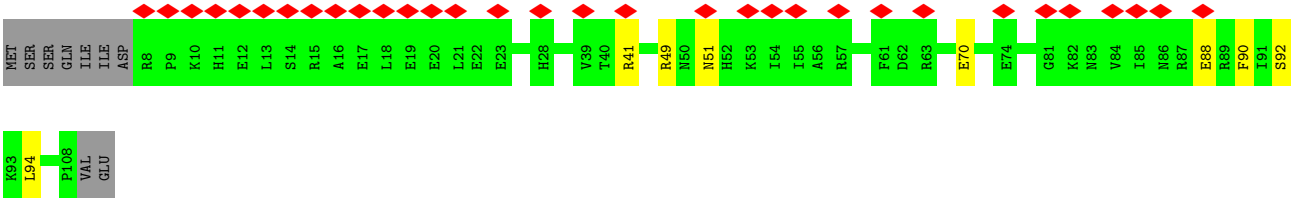
• Molecule 28: Small nuclear ribonucleoprotein Sm D2

Chain g:



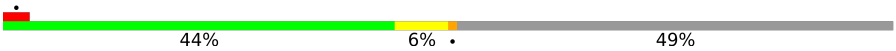
• Molecule 28: Small nuclear ribonucleoprotein Sm D2

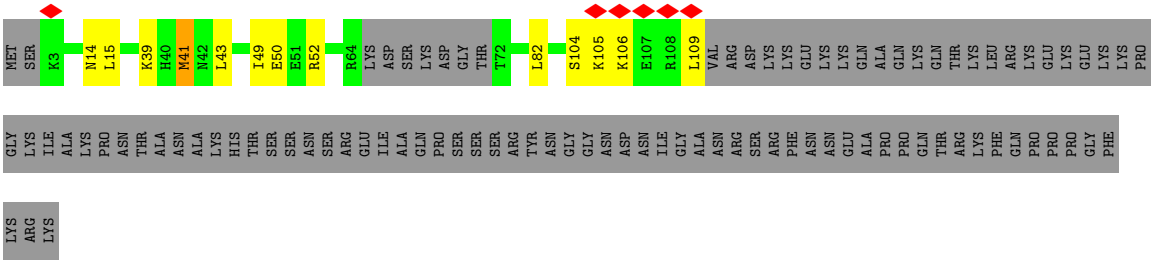
Chain e:



• Molecule 29: Small nuclear ribonucleoprotein-associated protein B

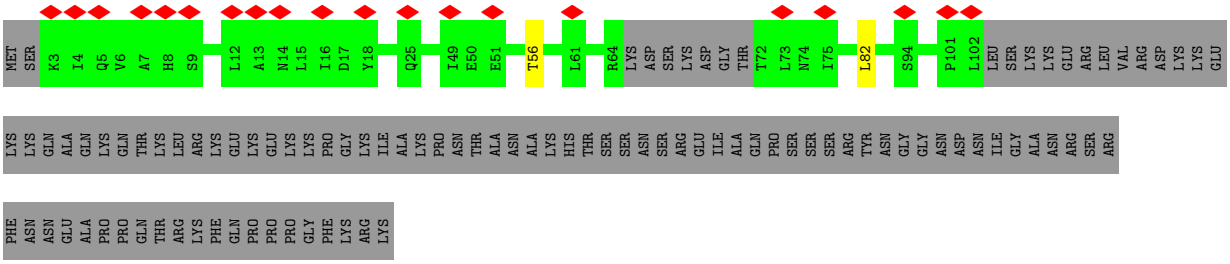
Chain k:





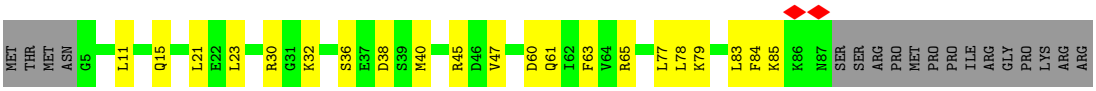
• Molecule 29: Small nuclear ribonucleoprotein-associated protein B

Chain s:



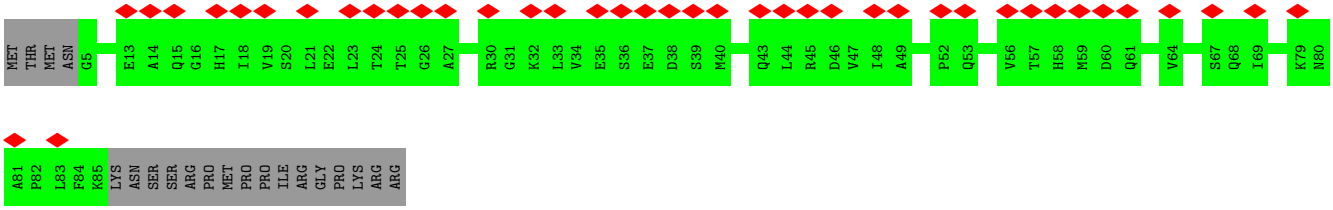
• Molecule 30: Small nuclear ribonucleoprotein Sm D3

Chain l:



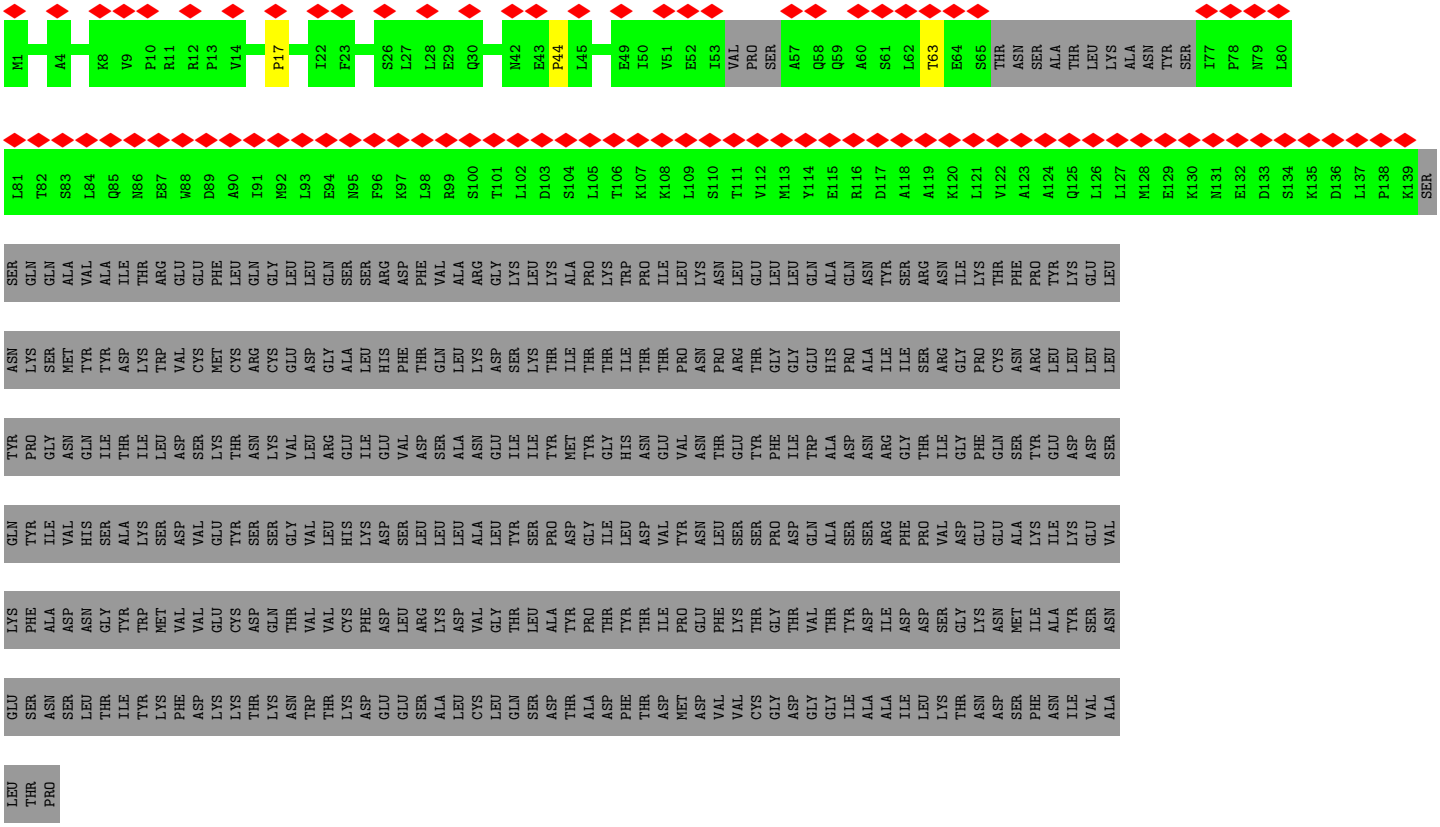
• Molecule 30: Small nuclear ribonucleoprotein Sm D3

Chain y:



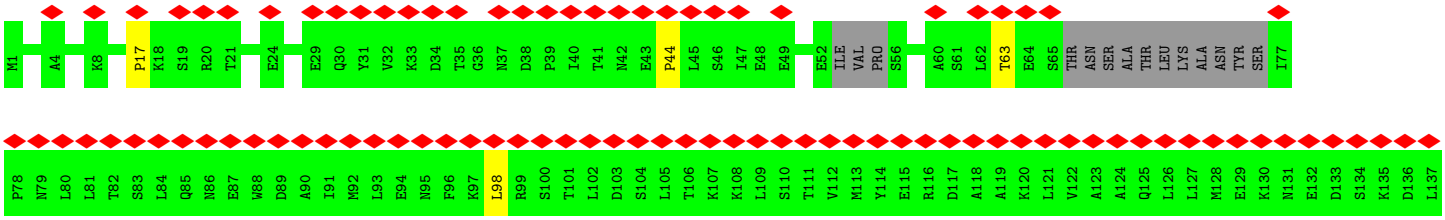
• Molecule 31: Pre-mRNA-processing factor 19

Chain r:



• Molecule 31: Pre-mRNA-processing factor 19

Chain p:



P138 K139 S140 S141 Q142 GLN ALA VAL ALA ILE THR ARG GLU GLU PHE LEU GLN GLY LEU LEU GLN SER SER ARG ASP PHE VAL ALA ARG GLY LYS LEU LYS ALA PRO LYS TRP PRO ILE LEU LYS ASN LEU GLU LEU LEU GLN ALA GLN ASN TYR SER ARG ASN ILE LYS THR PHE PRO TYR

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

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

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

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

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

ILE VAL ALA LEU THR PRO

- Molecule 31: Pre-mRNA-processing factor 19

Chain q: 24% 25% 74%

M1 L2 C3 A4 I5 S6 G7 K8 V9 P10 R11 R12 P13 V14 L15 S16 P17 K18 S19 R20 T21 I22 F23 E24 K25 S26 L27 L28 E29 Q30 Y31 V32 K33 D34 T35 G36 N37 D38 P39 I40 T41 N42 E43 P44 L45 S46 I47 E48 E49 I50 V51 E52 I53 V54 P55 Q58 Q59 A60 S61

LEU THR GLU SER THR ASN SER ALA THR LEU LYS ALA ASN TYR S76 I77 P78 N79 L80 L81 T82 S83 L84 Q85 N86 E87 W88 D89 A90 I91 M92 L93 E94 N95 F96 K97 L98 R99 S100 T101 L102 D103 S104 L105 T106 K107 K108 L109 S110 T111 V112 M113 Y114 E115 R116 D117 A118 A119 K120 L121

V122 A123 A124 Q125 L126 L127 M128 E129 K130 N131 E132 D133 S134 K135 D136 L137 P138 K139 S140 S141 Q142 Q143 ALA VAL ALA ILE THR ARG GLU GLU PHE LEU GLN GLY LEU LEU GLN SER SER ARG ASP PHE VAL ALA ARG GLY LYS LEU LYS ALA PRO LYS TRP PRO ILE LEU LYS ASN LEU GLU

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

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

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

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

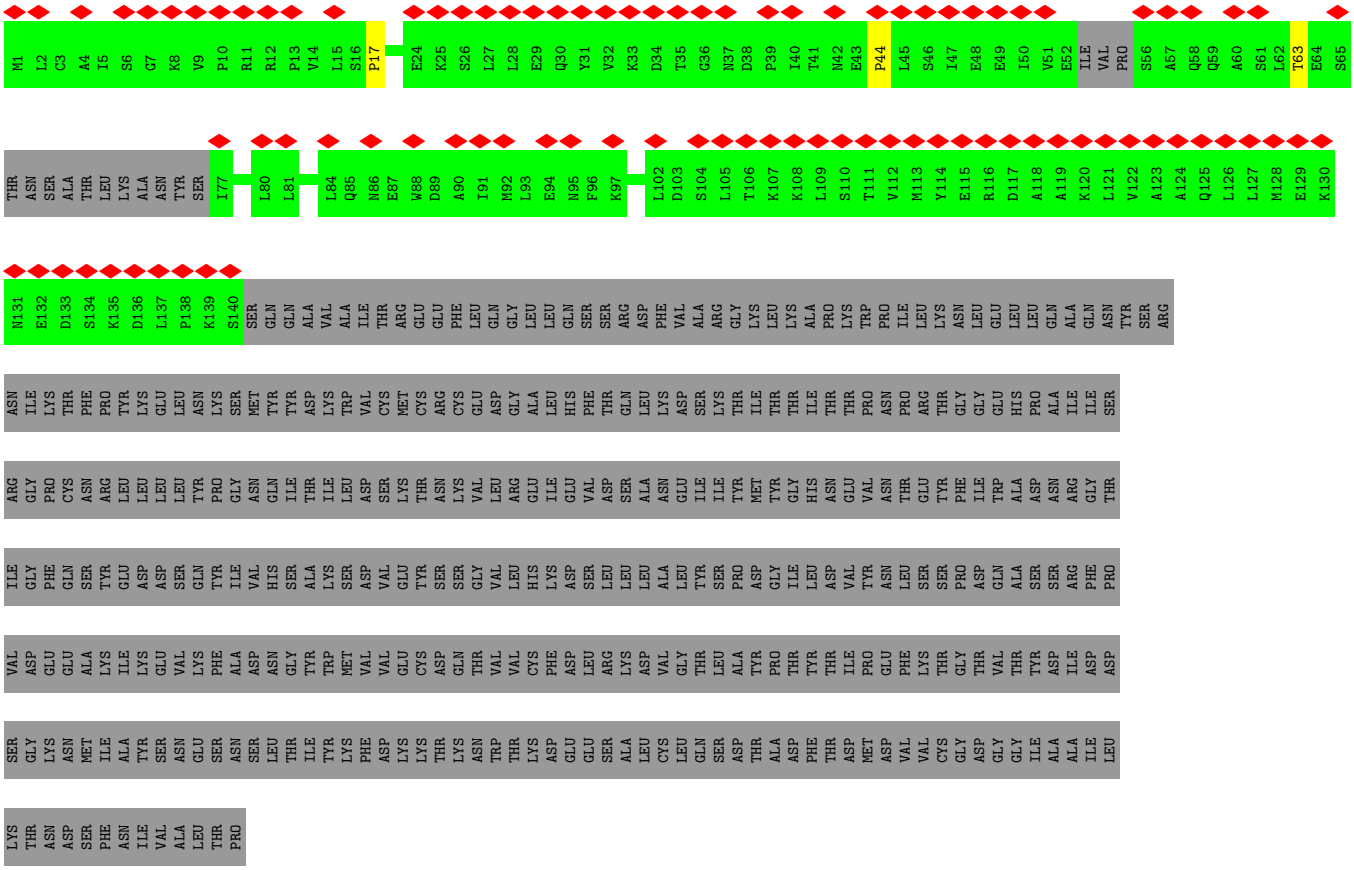
GLY THR VAL THR TYR ASP ILE ASP ASP SER GLY LYS ASN MET ILE ALA TYR SER ASN GLU SER ASN SER LEU THR ILE TYR LYS PHE ASP LYS LYS THR LYS ASN TRP THR LYS ASP GLU GLU SER ALA LEU CYS LEU GLN SER ASP THR ALA ASP PHE THR ASP MET ASP VAL VAL CYS

GLY ASP GLY GLY ILE ALA ALA ILE LEU LYS THR ASN ASP SER PHE ASN ILE VAL ALA LEU THR PRO

- Molecule 31: Pre-mRNA-processing factor 19

Chain o:

18%
24%
75%


M1 L2 C3 A4 I5 S6 G7 K8 V9 P10 R11 R12 P13 V14 L15 S16 P17 E24 K25 S26 L27 L28 E29 Q30 Y31 V32 K33 D34 T35 G36 N37 D38 P39 I40 T41 N42 E43 P44 L45 S46 I47 E48 E49 I50 V51 E52 ILE VAL PRO S56 A57 Q58 Q59 A60 S61 L62 T63 E64 S65
THR ASN SER ALA THR LEU LYS ALA ASN TYR SER I77 L80 L81 L84 Q85 N86 E87 W88 D89 A90 I91 M92 L93 E94 N95 F96 K97 L102 D103 S104 L105 T106 K107 K108 L109 S110 T111 V112 M113 Y114 E115 R116 D117 A118 A119 K120 L121 V122 A123 A124 Q125 L126 L127 M128 E129 K130
N131 E132 D133 S134 K135 D136 L137 P138 K139 S140 SER GLN GLN ALA VAL ALA ILE THR ARG GLU GLU PHE LEU GLN GLY LEU LEU GLN SER SER ARG ASP PHE VAL ALA ARG GLY LYS LEU LYS ALA PRO LYS TRP PRO ILE LEU LYS ASN LEU GLU LEU LYS ALA GLN ASN TYR SER ARG
ASN ILE LYS THR PHE PRO TYR LYS GLU LEU ASN LYS SER MET TYR TYR ASP LYS TRP VAL CYS MET CYS ARG CYS GLU ASP GLY ALA LEU HIS PHE THR GLN LEU LYS ASP SER LYS THR ILE THR THR ILE THR THR PRO ASN PRO ARG THR GLY GLY GLU HIS PRO ALA ILE ILE SER
ARG GLY PRO CYS ASN ARG LEU LEU LEU LEU TYR PRO GLY ASN GLN ILE THR ILE LEU ASP SER LYS THR ASN LYS VAL LEU ARG GLU ILE GLU VAL ASP SER ALA ASN GLU ILE ILE TYR MET TYR GLY HIS ASN GLU VAL ASN THR GLU TYR PHE ILE TRP ALA ASP ASN ARG GLY THR
ILE GLY PHE GLN SER TYR GLU ASP ASP SER GLN TYR ILE VAL HIS SER ALA LYS SER ASP VAL GLU TYR SER SER GLY VAL LEU HIS LYS ASP SER LEU LEU LEU ALA LEU TYR SER PRO ASP GLY ILE LEU ASP VAL TYR ASN LEU SER SER PRO ASP GLN ALA SER SER ARG PHE PRO
VAL ASP GLU GLU ALA LYS ILE LYS GLU VAL LYS PHE ALA ASP ASN GLY TYR TRP MET VAL VAL GLU CYS ASP GLN THR VAL VAL CYS PHE ASP LEU ARG LYS ASP VAL GLY THR LEU ALA TYR PRO THR TYR THR ILE PRO GLU PHE LYS THR GLY THR VAL THR TYR ASP ILE ASP ASP
SER GLY LYS ASN MET ILE ALA TYR SER ASN GLU SER ASN SER LEU THR ILE TYR LYS PHE ASP LYS LYS THR LYS ASN TRP THR LYS ASP GLU GLU SER ALA LEU CYS LEU GLN SER ASP THR ALA ASP PHE THR ASP MET ASP VAL VAL CYS GLY ASP GLY GLY ILE ALA ALA ILE LEU
LYS THR ASN ASP SER PHE ASN ILE VAL ALA LEU THR PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	555036	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 ($e^-/Å^2$)	49.3	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	0.343	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	532.0, 532.0, 532.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.37	0/16198	0.56	0/21958
2	C	0.36	0/7503	0.57	0/10159
3	J	0.30	0/191	0.51	0/254
4	O	0.39	0/2872	0.60	0/3902
5	P	0.30	0/1629	0.53	0/2194
6	Q	0.36	0/2339	0.61	0/3154
7	R	0.37	0/2135	0.56	0/2871
8	S	0.27	0/581	0.49	0/776
9	T	0.35	0/1315	0.54	0/1759
10	Z	0.33	0/3712	0.53	0/5004
11	c	0.31	0/2996	0.47	0/4033
12	d	0.33	0/3931	0.48	0/5356
13	I	0.25	0/826	0.42	0/1097
14	n	0.27	0/1894	0.55	0/2529
15	H	0.61	0/631	0.60	0/846
16	B	0.32	0/1411	0.82	0/2191
17	D	0.42	0/4239	0.88	0/6598
18	E	0.51	0/2452	0.89	0/3817
19	L	0.28	1/4877 (0.0%)	0.75	0/7562
20	v	0.42	0/4662	0.51	0/6358
21	a	0.42	0/415	0.56	0/577
22	b	0.68	0/839	0.70	0/1169
23	t	0.29	0/924	0.42	0/1244
24	i	0.29	0/551	0.50	0/750
24	u	0.29	0/535	0.48	0/730
25	m	0.35	0/926	0.55	0/1257
25	z	0.30	0/833	0.53	0/1134
26	j	0.45	0/557	0.54	0/756
26	x	0.34	0/557	0.51	0/756
27	h	0.28	0/529	0.50	0/715
27	w	0.28	0/529	0.50	0/715
28	e	0.38	0/799	0.52	0/1078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
28	g	0.40	0/799	0.55	0/1078
29	k	0.41	0/815	0.60	0/1092
29	s	0.35	0/755	0.59	0/1014
30	l	0.49	0/650	0.57	0/879
30	y	0.31	0/625	0.50	0/847
31	o	0.28	0/835	0.50	0/1126
31	p	0.25	0/848	0.51	0/1143
31	q	0.30	0/856	0.52	0/1155
31	r	0.29	0/828	0.54	0/1117
All	All	0.37	1/81399 (0.0%)	0.61	0/112750

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	1120	G	O3'-P	-5.54	1.54	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	
1	A	1905/2413 (79%)	1815 (95%)	84 (4%)	6 (0%)	41	74
2	C	914/1008 (91%)	881 (96%)	33 (4%)	0	100	100
3	J	25/135 (18%)	23 (92%)	2 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	355/451 (79%)	318 (90%)	35 (10%)	2 (1%)	25	64
5	P	197/379 (52%)	190 (96%)	7 (4%)	0	100	100
6	Q	288/364 (79%)	264 (92%)	22 (8%)	2 (1%)	22	61
7	R	259/339 (76%)	246 (95%)	11 (4%)	2 (1%)	19	58
8	S	64/175 (37%)	63 (98%)	1 (2%)	0	100	100
9	T	155/157 (99%)	150 (97%)	5 (3%)	0	100	100
10	Z	443/577 (77%)	425 (96%)	16 (4%)	2 (0%)	29	67
11	c	418/590 (71%)	396 (95%)	20 (5%)	2 (0%)	29	67
12	d	534/687 (78%)	513 (96%)	16 (3%)	5 (1%)	17	56
13	I	98/215 (46%)	96 (98%)	2 (2%)	0	100	100
14	n	279/455 (61%)	265 (95%)	12 (4%)	2 (1%)	22	61
15	H	68/235 (29%)	64 (94%)	2 (3%)	2 (3%)	4	28
20	v	666/859 (78%)	642 (96%)	22 (3%)	2 (0%)	41	74
21	a	82/111 (74%)	78 (95%)	3 (4%)	1 (1%)	13	49
22	b	165/238 (69%)	138 (84%)	20 (12%)	7 (4%)	3	20
23	t	150/175 (86%)	145 (97%)	4 (3%)	1 (1%)	22	61
24	i	70/94 (74%)	67 (96%)	3 (4%)	0	100	100
24	u	70/94 (74%)	67 (96%)	3 (4%)	0	100	100
25	m	117/146 (80%)	111 (95%)	6 (5%)	0	100	100
25	z	106/146 (73%)	100 (94%)	6 (6%)	0	100	100
26	j	73/77 (95%)	67 (92%)	5 (7%)	1 (1%)	11	46
26	x	73/77 (95%)	65 (89%)	7 (10%)	1 (1%)	11	46
27	h	64/86 (74%)	60 (94%)	4 (6%)	0	100	100
27	w	64/86 (74%)	61 (95%)	3 (5%)	0	100	100
28	e	99/110 (90%)	95 (96%)	3 (3%)	1 (1%)	15	54
28	g	99/110 (90%)	93 (94%)	4 (4%)	2 (2%)	7	38
29	k	96/196 (49%)	90 (94%)	5 (5%)	1 (1%)	15	54
29	s	89/196 (45%)	83 (93%)	6 (7%)	0	100	100
30	l	81/101 (80%)	79 (98%)	0	2 (2%)	5	32
30	y	79/101 (78%)	75 (95%)	4 (5%)	0	100	100
31	o	120/503 (24%)	115 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	p	122/503 (24%)	118 (97%)	4 (3%)	0	100	100
31	q	125/503 (25%)	116 (93%)	9 (7%)	0	100	100
31	r	119/503 (24%)	112 (94%)	7 (6%)	0	100	100
All	All	8731/13195 (66%)	8286 (95%)	401 (5%)	44 (0%)	32	67

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	PRO
1	A	1965	PHE
7	R	152	LYS
7	R	153	PRO
12	d	181	ASN
12	d	353	GLU
14	n	387	ILE
21	a	68	GLN
22	b	68	PRO
22	b	95	PRO
22	b	125	LYS
22	b	149	PRO
26	j	75	ASP
1	A	1964	PRO
4	O	351	GLY
4	O	352	ILE
11	c	218	VAL
15	H	33	GLN
20	v	798	LYS
22	b	98	VAL
23	t	112	SER
28	g	51	ASN
28	g	65	CYS
29	k	41	MET
28	e	51	ASN
30	l	78	LEU
1	A	510	PRO
1	A	511	ASP
10	Z	235	ALA
12	d	63	LEU
12	d	336	LYS
14	n	427	LYS
20	v	515	PRO

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Mol	Chain	Res	Type
22	b	67	ILE
22	b	94	LEU
30	l	40	MET
26	x	75	ASP
1	A	1157	PRO
6	Q	256	SER
10	Z	229	VAL
6	Q	191	PRO
11	c	418	PRO
12	d	334	PHE
15	H	35	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1737/2182 (80%)	1714 (99%)	23 (1%)	69	87
2	C	830/910 (91%)	817 (98%)	13 (2%)	62	84
3	J	21/121 (17%)	21 (100%)	0	100	100
4	O	312/397 (79%)	309 (99%)	3 (1%)	76	90
5	P	175/328 (53%)	174 (99%)	1 (1%)	86	94
6	Q	265/332 (80%)	258 (97%)	7 (3%)	46	76
7	R	224/296 (76%)	219 (98%)	5 (2%)	52	79
8	S	57/151 (38%)	55 (96%)	2 (4%)	36	69
9	T	141/141 (100%)	140 (99%)	1 (1%)	84	94
10	Z	417/538 (78%)	410 (98%)	7 (2%)	60	83
11	c	214/525 (41%)	196 (92%)	18 (8%)	11	39
12	d	274/633 (43%)	261 (95%)	13 (5%)	26	62
13	I	92/193 (48%)	91 (99%)	1 (1%)	73	88
14	n	121/412 (29%)	108 (89%)	13 (11%)	6	27
15	H	68/216 (32%)	48 (71%)	20 (29%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	v	294/786 (37%)	279 (95%)	15 (5%)	24	60
23	t	39/165 (24%)	26 (67%)	13 (33%)	0	0
24	i	55/83 (66%)	52 (94%)	3 (6%)	21	57
24	u	52/83 (63%)	51 (98%)	1 (2%)	57	81
25	m	106/129 (82%)	97 (92%)	9 (8%)	10	38
25	z	95/129 (74%)	95 (100%)	0	100	100
26	j	56/66 (85%)	48 (86%)	8 (14%)	3	15
26	x	56/66 (85%)	55 (98%)	1 (2%)	59	82
27	h	51/77 (66%)	51 (100%)	0	100	100
27	w	51/77 (66%)	51 (100%)	0	100	100
28	e	82/103 (80%)	75 (92%)	7 (8%)	10	38
28	g	82/103 (80%)	77 (94%)	5 (6%)	18	54
29	k	92/176 (52%)	79 (86%)	13 (14%)	3	16
29	s	85/176 (48%)	83 (98%)	2 (2%)	49	77
30	l	72/89 (81%)	53 (74%)	19 (26%)	0	2
30	y	68/89 (76%)	68 (100%)	0	100	100
31	o	60/451 (13%)	57 (95%)	3 (5%)	24	60
31	p	62/451 (14%)	58 (94%)	4 (6%)	17	51
31	q	62/451 (14%)	59 (95%)	3 (5%)	25	61
31	r	60/451 (13%)	57 (95%)	3 (5%)	24	60
All	All	6528/11576 (56%)	6292 (96%)	236 (4%)	38	69

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	396	ARG
1	A	580	ASN
1	A	705	GLN
1	A	716	ARG
1	A	760	ASN
1	A	848	ASN
1	A	1067	ASN
1	A	1087	ASN
1	A	1100	LYS
1	A	1292	ARG

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Mol	Chain	Res	Type
1	A	1529	ASN
1	A	1618	ASN
1	A	1694	MET
1	A	1739	ARG
1	A	1961	LEU
1	A	1962	ARG
1	A	1965	PHE
1	A	1991	ILE
1	A	1993	ASP
1	A	2040	TRP
1	A	2065	ARG
1	A	2068	ASN
1	A	2084	LEU
2	C	81	LYS
2	C	132	ARG
2	C	234	LEU
2	C	289	ASN
2	C	294	ASN
2	C	430	ARG
2	C	461	LYS
2	C	545	LEU
2	C	726	ASN
2	C	733	ASN
2	C	745	ARG
2	C	830	ASN
2	C	862	TYR
4	O	152	ASN
4	O	236	LEU
4	O	352	ILE
5	P	87	ASN
6	Q	105	LYS
6	Q	109	MET
6	Q	230	LYS
6	Q	233	LYS
6	Q	251	LEU
6	Q	282	LEU
6	Q	291	ILE
7	R	143	ASP
7	R	148	SER
7	R	159	ARG
7	R	210	LYS
7	R	257	ASN

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Mol	Chain	Res	Type
8	S	35	THR
8	S	36	THR
9	T	153	CYS
10	Z	34	MET
10	Z	53	ARG
10	Z	67	LYS
10	Z	177	LEU
10	Z	227	TYR
10	Z	412	SER
10	Z	470	LEU
11	c	72	GLN
11	c	169	ARG
11	c	170	LYS
11	c	172	ARG
11	c	175	MET
11	c	180	LYS
11	c	186	GLN
11	c	187	LYS
11	c	215	GLU
11	c	216	ASP
11	c	218	VAL
11	c	223	PRO
11	c	227	ILE
11	c	504	PRO
11	c	505	PRO
11	c	517	VAL
11	c	532	PRO
11	c	550	PRO
12	d	62	ARG
12	d	123	ASN
12	d	139	TYR
12	d	155	LEU
12	d	156	TYR
12	d	222	TYR
12	d	263	SER
12	d	284	LEU
12	d	285	LEU
12	d	289	LYS
12	d	315	ASN
12	d	316	ASN
12	d	334	PHE
13	I	209	ARG

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Mol	Chain	Res	Type
14	n	159	PRO
14	n	162	PRO
14	n	165	THR
14	n	208	PRO
14	n	257	PRO
14	n	260	PRO
14	n	327	PRO
14	n	340	PRO
14	n	373	PRO
14	n	424	PRO
14	n	428	PRO
14	n	430	THR
14	n	436	PRO
15	H	27	LYS
15	H	28	ASP
15	H	30	SER
15	H	31	ARG
15	H	33	GLN
15	H	34	ARG
15	H	36	ARG
15	H	40	LYS
15	H	42	LYS
15	H	43	SER
15	H	44	ILE
15	H	55	SER
15	H	57	GLU
15	H	58	ILE
15	H	66	TYR
15	H	67	ASP
15	H	69	SER
15	H	70	LEU
15	H	72	GLU
15	H	81	GLU
20	v	385	PHE
20	v	386	GLU
20	v	397	ASN
20	v	398	ASP
20	v	438	ARG
20	v	529	HIS
20	v	530	ARG
20	v	544	ILE
20	v	574	TYR

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Mol	Chain	Res	Type
20	v	576	THR
20	v	593	LEU
20	v	665	ILE
20	v	672	PHE
20	v	719	THR
20	v	726	ARG
23	t	13	PRO
23	t	76	THR
23	t	77	PRO
23	t	85	THR
23	t	96	PRO
23	t	100	THR
23	t	105	PRO
23	t	108	SER
23	t	109	SER
23	t	111	VAL
23	t	133	PRO
23	t	136	VAL
23	t	150	THR
24	u	35	ILE
25	m	33	SER
25	m	37	ASN
25	m	39	ILE
25	m	46	THR
25	m	47	LEU
25	m	52	LEU
25	m	86	ASN
25	m	92	ILE
25	m	93	ARG
26	j	18	ASN
26	j	20	ASN
26	j	22	SER
26	j	23	ARG
26	j	40	LEU
26	j	54	ASN
26	j	64	ARG
26	j	74	LEU
28	g	33	LEU
28	g	35	ASN
28	g	41	ARG
28	g	42	THR
28	g	57	ARG

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Mol	Chain	Res	Type
29	k	14	ASN
29	k	15	LEU
29	k	39	LYS
29	k	41	MET
29	k	43	LEU
29	k	49	ILE
29	k	50	GLU
29	k	52	ARG
29	k	82	LEU
29	k	104	SER
29	k	105	LYS
29	k	106	LYS
29	k	109	LEU
28	e	41	ARG
28	e	49	ARG
28	e	70	GLU
28	e	88	GLU
28	e	90	PHE
28	e	92	SER
28	e	94	LEU
29	s	56	THR
29	s	82	LEU
30	l	11	LEU
30	l	15	GLN
30	l	21	LEU
30	l	23	LEU
30	l	30	ARG
30	l	32	LYS
30	l	36	SER
30	l	38	ASP
30	l	45	ARG
30	l	47	VAL
30	l	60	ASP
30	l	61	GLN
30	l	63	PHE
30	l	65	ARG
30	l	77	LEU
30	l	79	LYS
30	l	83	LEU
30	l	84	PHE
30	l	85	LYS
24	i	18	PHE

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Mol	Chain	Res	Type
24	i	22	GLN
24	i	40	LYS
26	x	74	LEU
31	r	17	PRO
31	r	44	PRO
31	r	63	THR
31	p	17	PRO
31	p	44	PRO
31	p	63	THR
31	p	98	LEU
31	q	17	PRO
31	q	44	PRO
31	q	55	PRO
31	o	17	PRO
31	o	44	PRO
31	o	63	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	310	ASN
1	A	541	ASN
1	A	580	ASN
1	A	658	ASN
1	A	713	ASN
1	A	864	GLN
1	A	1034	ASN
1	A	1067	ASN
1	A	1128	GLN
1	A	1368	GLN
1	A	1449	ASN
1	A	1529	ASN
1	A	1538	ASN
1	A	1540	ASN
1	A	1618	ASN
1	A	1687	HIS
1	A	1707	HIS
1	A	1863	HIS
1	A	1947	HIS
1	A	1990	ASN
1	A	2068	ASN

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Mol	Chain	Res	Type
2	C	84	GLN
2	C	101	GLN
2	C	183	GLN
2	C	218	HIS
2	C	220	ASN
2	C	251	GLN
2	C	289	ASN
2	C	310	ASN
2	C	431	GLN
2	C	608	GLN
2	C	647	ASN
2	C	726	ASN
2	C	733	ASN
2	C	869	HIS
3	J	19	HIS
4	O	99	ASN
4	O	317	HIS
5	P	87	ASN
5	P	140	ASN
6	Q	243	ASN
7	R	54	GLN
7	R	58	HIS
7	R	91	HIS
7	R	155	GLN
7	R	257	ASN
8	S	8	GLN
8	S	173	HIS
9	T	58	GLN
10	Z	54	ASN
10	Z	84	ASN
10	Z	107	ASN
10	Z	116	ASN
10	Z	131	HIS
10	Z	182	GLN
10	Z	202	GLN
10	Z	310	HIS
10	Z	354	HIS
10	Z	368	ASN
11	c	31	HIS
11	c	161	ASN
11	c	214	ASN
12	d	79	HIS

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Mol	Chain	Res	Type
12	d	123	ASN
12	d	147	ASN
12	d	315	ASN
12	d	316	ASN
13	I	115	GLN
15	H	93	GLN
20	v	397	ASN
20	v	643	HIS
24	u	86	ASN
25	m	12	ASN
25	m	14	GLN
25	m	21	ASN
25	m	30	GLN
25	m	83	GLN
25	m	86	ASN
25	m	94	GLN
26	j	18	ASN
26	j	20	ASN
26	j	54	ASN
28	g	50	ASN
28	g	52	HIS
28	g	86	ASN
29	k	14	ASN
28	e	64	HIS
28	e	66	ASN
28	e	71	ASN
28	e	86	ASN
30	l	15	GLN
30	l	41	ASN
30	l	43	GLN
30	l	68	GLN
27	w	50	ASN
26	x	20	ASN
25	z	12	ASN
25	z	14	GLN
25	z	21	ASN
25	z	30	GLN

5.3.3 RNA (i)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	B	58/679 (8%)	24 (41%)	2 (3%)
17	D	177/214 (82%)	54 (30%)	7 (3%)
18	E	102/112 (91%)	35 (34%)	1 (0%)
19	L	197/1175 (16%)	63 (31%)	7 (3%)
All	All	534/2180 (24%)	176 (32%)	17 (3%)

All (176) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	B	-11	C
16	B	-10	A
16	B	-9	A
16	B	-5	A
16	B	-3	U
16	B	0	G
16	B	1	G
16	B	2	U
16	B	3	A
16	B	9	U
16	B	10	A
16	B	11	G
16	B	12	C
16	B	16	U
16	B	17	G
16	B	248	A
16	B	249	C
16	B	250	U
16	B	251	A
16	B	252	A
16	B	266	A
16	B	270	C
16	B	272	A
16	B	276	C
17	D	12	C
17	D	13	A
17	D	14	G
17	D	18	A
17	D	20	U
17	D	27	G
17	D	28	G
17	D	29	G

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Mol	Chain	Res	Type
17	D	31	G
17	D	33	U
17	D	41	A
17	D	42	A
17	D	43	G
17	D	44	A
17	D	45	A
17	D	75	A
17	D	76	U
17	D	77	A
17	D	79	C
17	D	80	G
17	D	84	A
17	D	95	C
17	D	96	U
17	D	97	U
17	D	101	C
17	D	103	A
17	D	104	G
17	D	109	A
17	D	113	G
17	D	126	A
17	D	127	U
17	D	128	A
17	D	129	G
17	D	130	A
17	D	131	A
17	D	132	A
17	D	139	A
17	D	141	G
17	D	142	C
17	D	146	C
17	D	151	A
17	D	160	U
17	D	161	U
17	D	162	G
17	D	163	C
17	D	164	C
17	D	165	A
17	D	166	U
17	D	168	U
17	D	170	U

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Mol	Chain	Res	Type
17	D	171	U
17	D	174	G
17	D	175	G
17	D	178	C
18	E	5	G
18	E	12	A
18	E	13	A
18	E	14	C
18	E	15	C
18	E	19	C
18	E	23	G
18	E	27	U
18	E	31	G
18	E	35	A
18	E	36	U
18	E	42	A
18	E	43	C
18	E	48	C
18	E	49	A
18	E	50	G
18	E	51	A
18	E	52	G
18	E	54	U
18	E	56	A
18	E	59	A
18	E	60	G
18	E	62	A
18	E	63	G
18	E	66	C
18	E	67	C
18	E	68	C
18	E	80	U
18	E	85	C
18	E	86	G
18	E	92	C
18	E	95	A
18	E	98	G
18	E	99	A
18	E	101	U
19	L	3	G
19	L	4	A
19	L	5	A

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Mol	Chain	Res	Type
19	L	6	U
19	L	18	U
19	L	19	U
19	L	21	G
19	L	23	U
19	L	26	G
19	L	30	A
19	L	31	A
19	L	32	G
19	L	50	U
19	L	51	C
19	L	108	A
19	L	110	A
19	L	111	C
19	L	115	U
19	L	119	G
19	L	120	G
19	L	121	C
19	L	124	C
19	L	129	A
19	L	141	A
19	L	153	U
19	L	1084	A
19	L	1085	G
19	L	1086	U
19	L	1091	G
19	L	1093	C
19	L	1094	G
19	L	1096	C
19	L	1098	C
19	L	1099	G
19	L	1100	A
19	L	1101	C
19	L	1102	C
19	L	1103	C
19	L	1104	U
19	L	1105	C
19	L	1106	G
19	L	1107	C
19	L	1108	A
19	L	1115	G
19	L	1120	G

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Mol	Chain	Res	Type
19	L	1122	U
19	L	1123	C
19	L	1124	U
19	L	1125	U
19	L	1126	G
19	L	1128	C
19	L	1130	U
19	L	1137	U
19	L	1138	G
19	L	1139	G
19	L	1140	U
19	L	1144	U
19	L	1145	U
19	L	1146	G
19	L	1147	A
19	L	1149	G
19	L	1152	U
19	L	1166	G

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	B	9	U
16	B	248	A
17	D	17	C
17	D	27	G
17	D	28	G
17	D	95	C
17	D	130	A
17	D	150	U
17	D	163	C
18	E	49	A
19	L	120	G
19	L	1085	G
19	L	1092	A
19	L	1093	C
19	L	1106	G
19	L	1107	C
19	L	1146	G

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
14	SEP	n	73	14	8,9,10	1.52	1 (12%)	8,12,14	1.54	2 (25%)

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
14	SEP	n	73	14	-	3/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	73	SEP	P-O1P	3.29	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	73	SEP	P-OG-CB	-3.21	109.46	118.30
14	n	73	SEP	OG-CB-CA	2.26	110.34	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	n	73	SEP	CB-OG-P-O1P
14	n	73	SEP	CB-OG-P-O2P
14	n	73	SEP	CB-OG-P-O3P

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 14 ligands modelled in this entry, 12 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	$\#\|Z\| > 2$
32	IHP	A	3000	-	36,36,36	0.74	0	54,60,60	0.53	0
33	GTP	C	1500	34	26,34,34	1.25	1 (3%)	32,54,54	1.65	6 (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
32	IHP	A	3000	-	-	11/30/54/54	0/1/1/1
33	GTP	C	1500	34	-	1/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	1500	GTP	C5-C6	-4.38	1.38	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	1500	GTP	PB-O3B-PG	-4.45	117.56	132.83
33	C	1500	GTP	C5-C6-N1	3.34	119.85	113.95
33	C	1500	GTP	C3'-C2'-C1'	3.00	105.49	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	1500	GTP	C8-N7-C5	2.95	108.61	102.99
33	C	1500	GTP	C2-N1-C6	-2.90	119.76	125.10
33	C	1500	GTP	O6-C6-C5	-2.24	120.00	124.37

There are no chirality outliers.

All (12) torsion outliers are listed below:

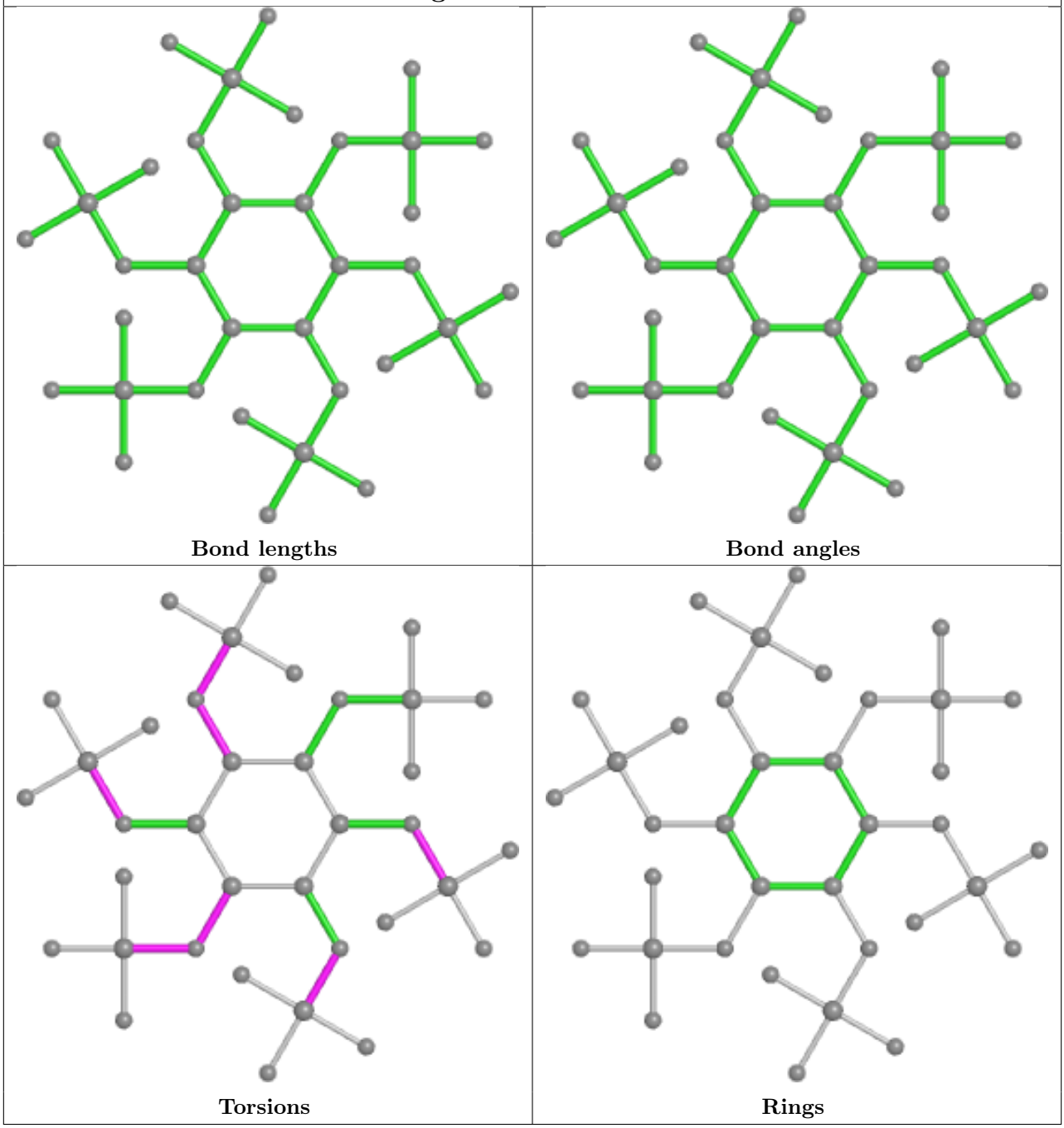
Mol	Chain	Res	Type	Atoms
32	A	3000	IHP	C2-C1-O11-P1
32	A	3000	IHP	C6-C1-O11-P1
32	A	3000	IHP	C1-O11-P1-O31
32	A	3000	IHP	C5-O15-P5-O25
32	A	3000	IHP	C6-O16-P6-O26
32	A	3000	IHP	C2-O12-P2-O22
32	A	3000	IHP	C3-O13-P3-O23
32	A	3000	IHP	C2-C3-O13-P3
32	A	3000	IHP	C4-C3-O13-P3
32	A	3000	IHP	C2-O12-P2-O32
33	C	1500	GTP	PB-O3A-PA-O2A
32	A	3000	IHP	C5-O15-P5-O45

There are no ring outliers.

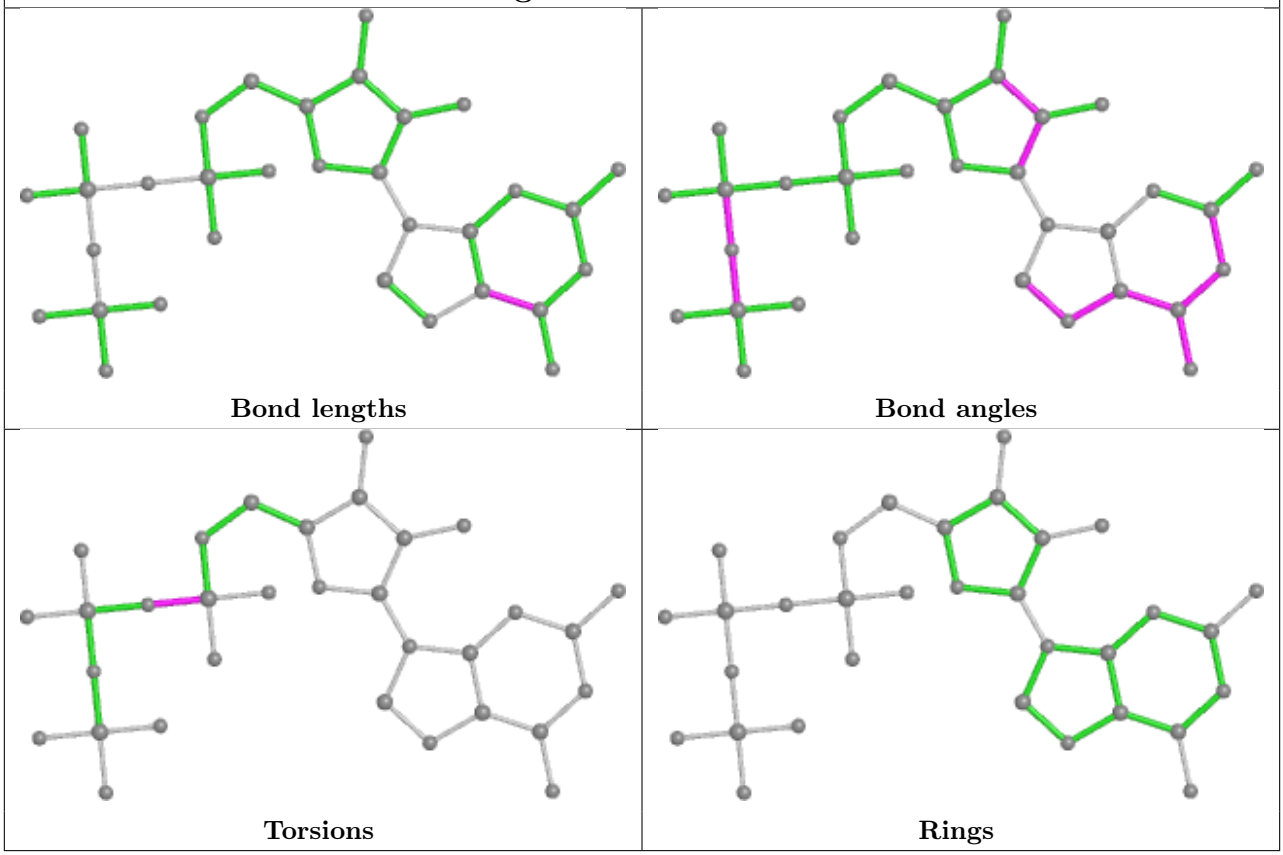
No monomer is involved in short contacts.

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

Ligand IHP A 3000



Ligand GTP C 1500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

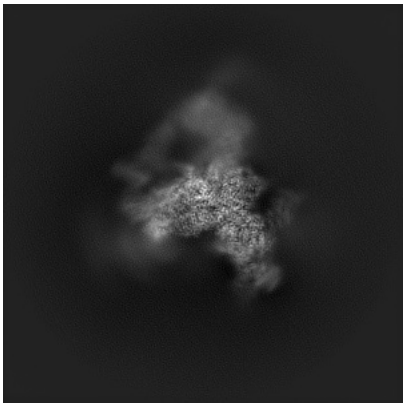
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0686. These allow visual inspection of the internal detail of the map and identification of artifacts.

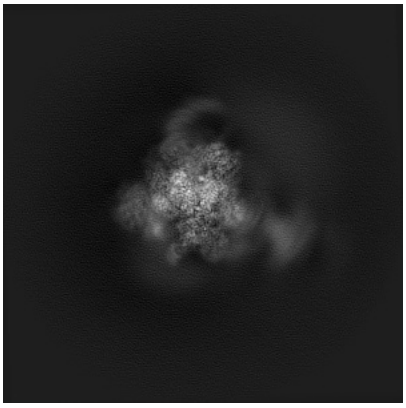
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

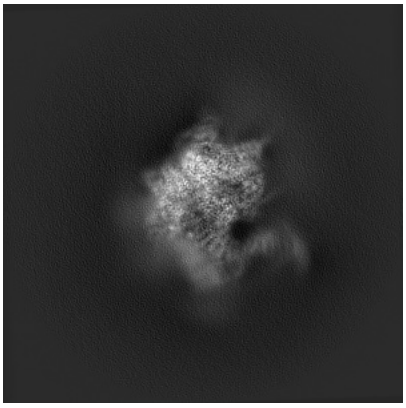
6.1.1 Primary map



X



Y

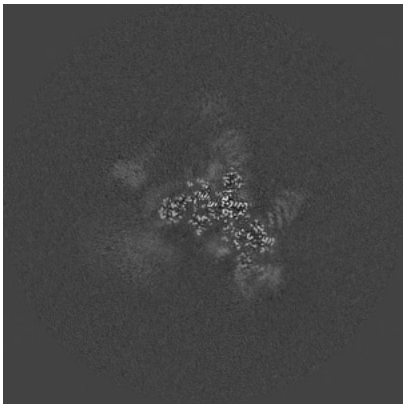


Z

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

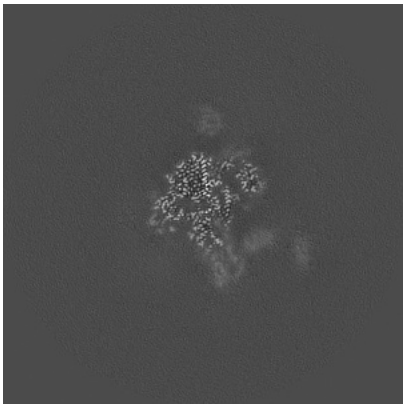
6.2 Central slices (i)

6.2.1 Primary map



X Index: 200

Y Index: 200

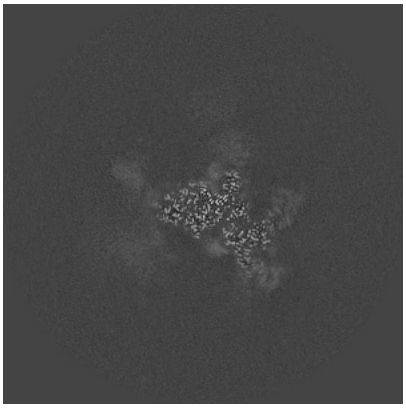


Z Index: 200

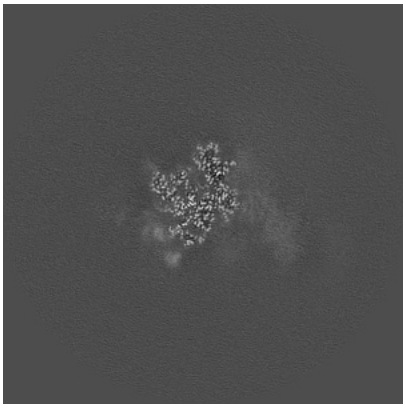
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

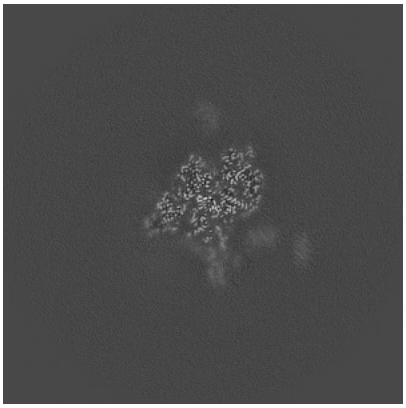
6.3.1 Primary map



X Index: 204



Y Index: 228



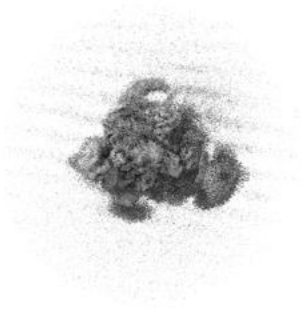
Z Index: 206

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

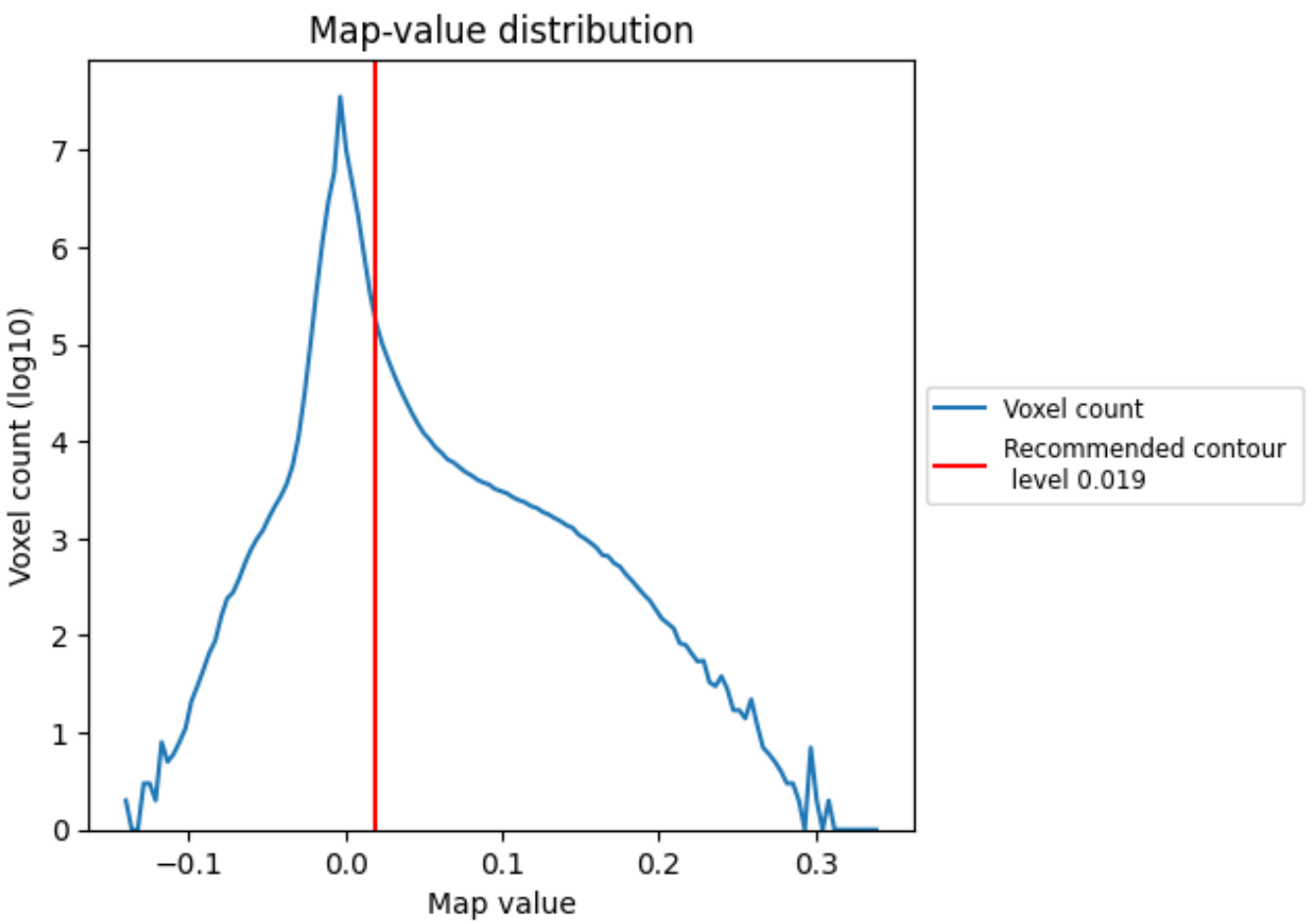
6.5 Mask visualisation (i)

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

7 Map analysis (i)

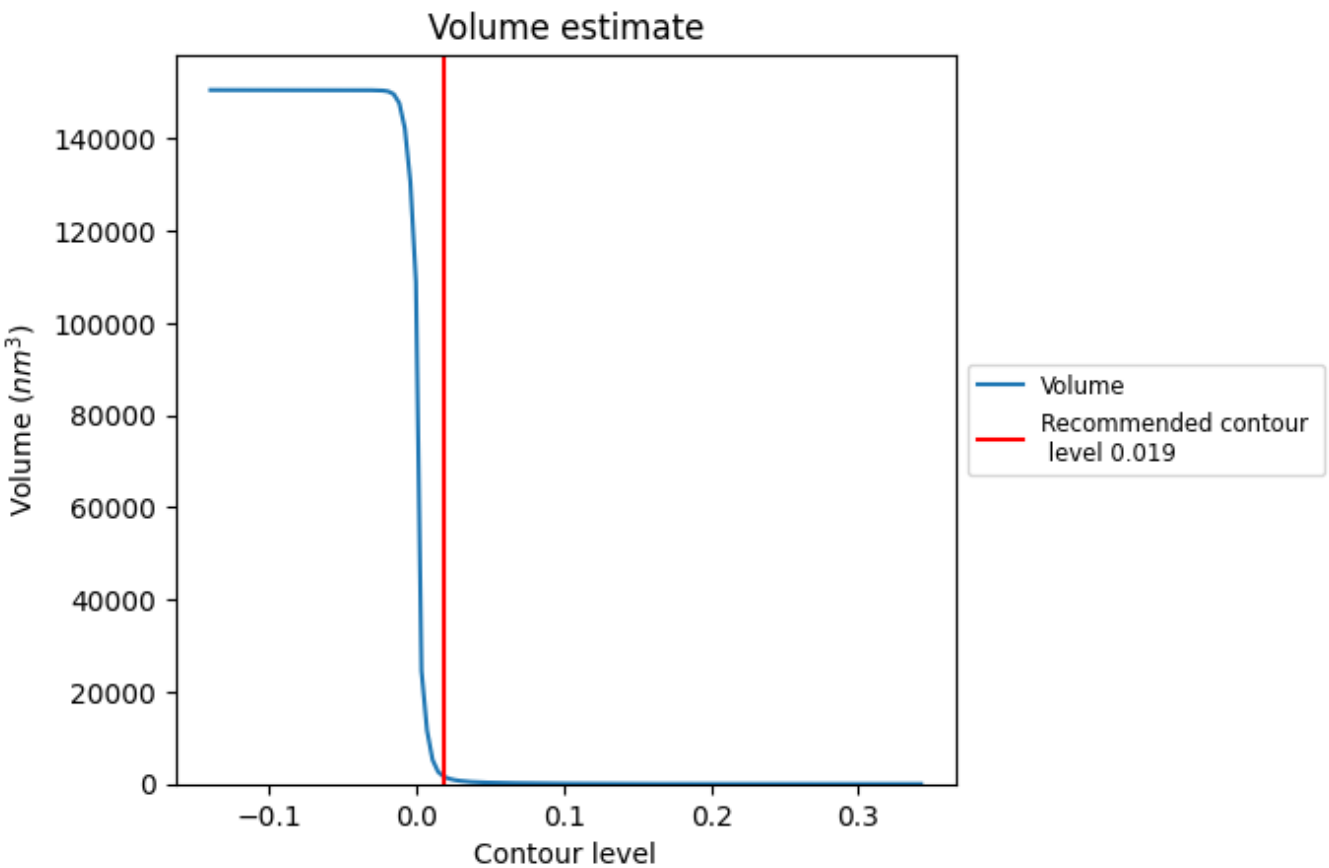
This section contains the results of statistical analysis of the map.

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.

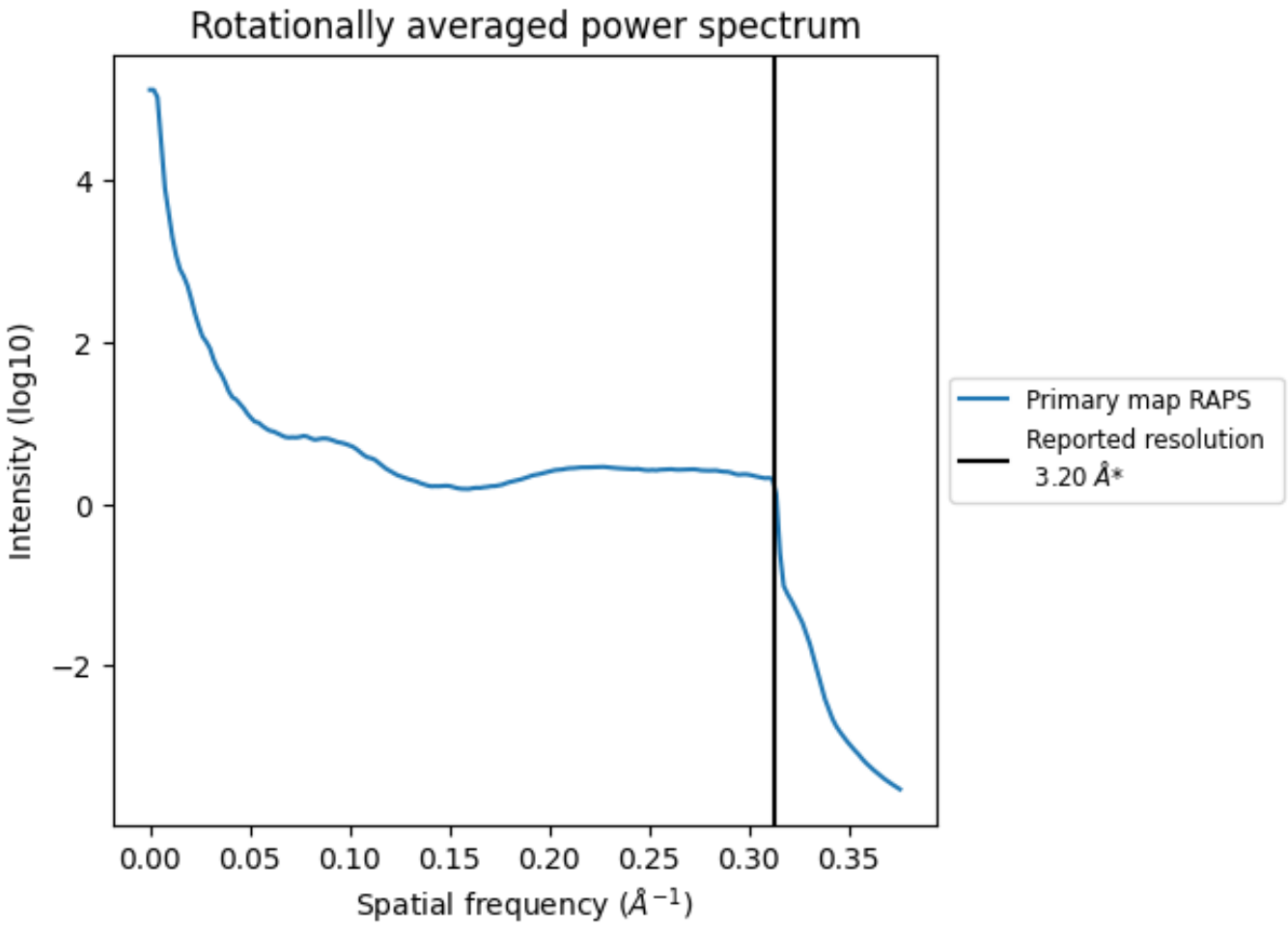
7.2 Volume estimate (i)



The volume at the recommended contour level is 1533 nm^3; this corresponds to an approximate mass of 1385 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 0.312 Å^{-1}

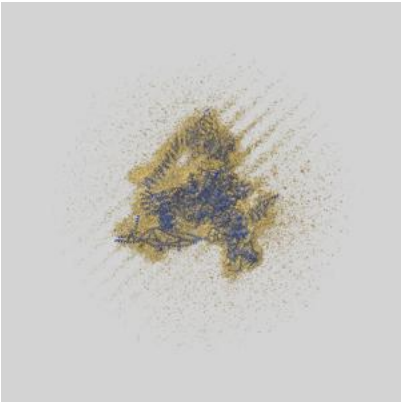
8 Fourier-Shell correlation (i)

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

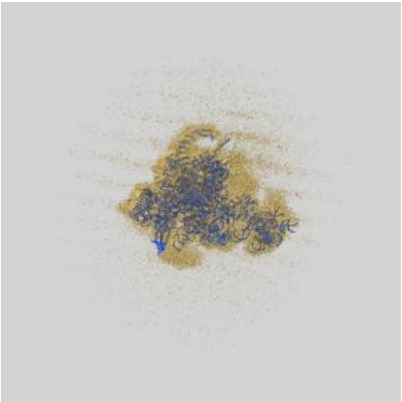
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0686 and PDB model 6J6G. Per-residue inclusion information can be found in section 3 on page 12.

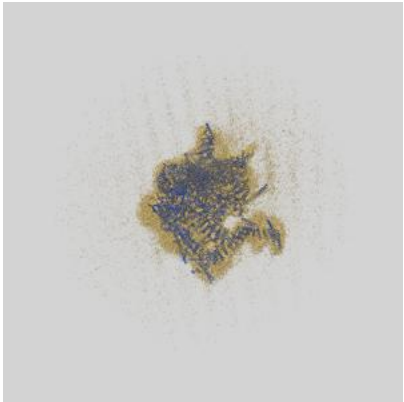
9.1 Map-model overlay (i)



X



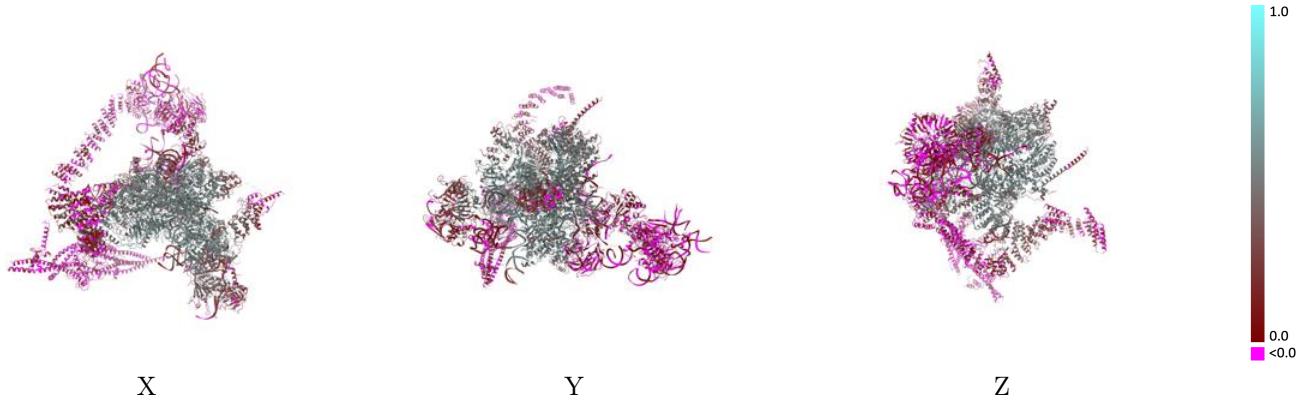
Y



Z

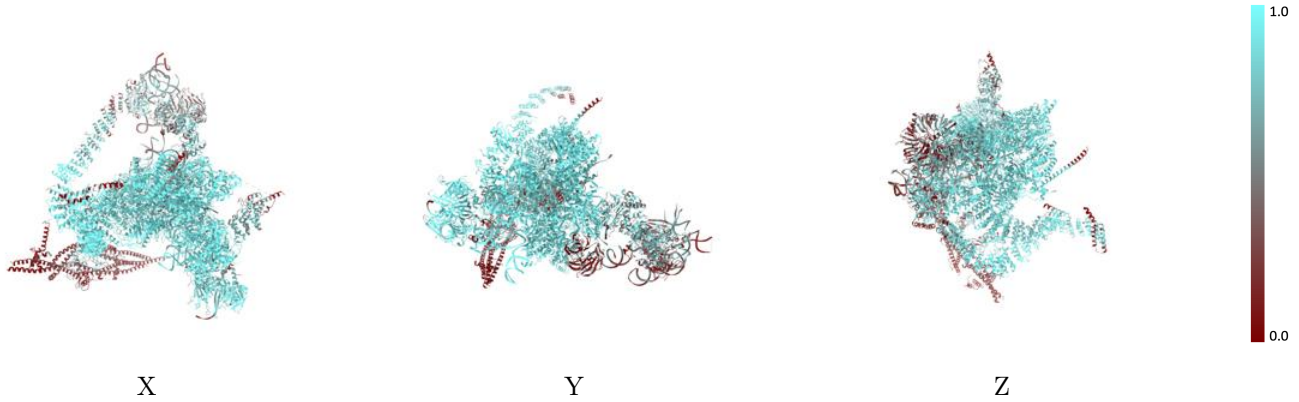
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



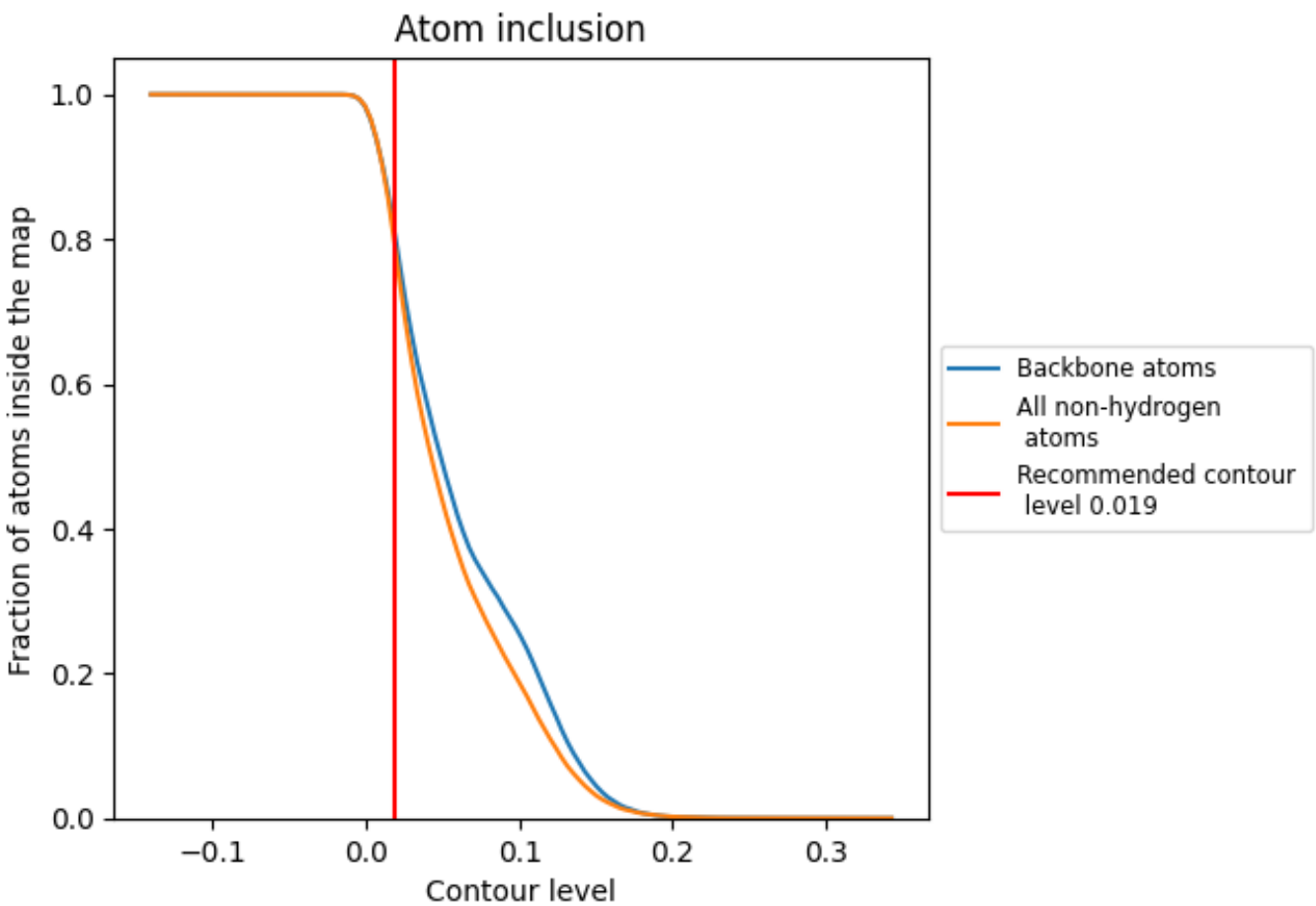
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7911	0.3170
A	0.9167	0.4650
B	0.8389	0.2280
C	0.9562	0.4980
D	0.9515	0.3350
E	0.9936	0.4850
H	0.7876	0.1160
I	0.9169	0.4460
J	0.9465	0.5140
L	0.6162	0.0890
O	0.9677	0.5330
P	0.8607	0.4420
Q	0.9269	0.4400
R	0.9483	0.4880
S	0.8522	0.4900
T	0.9603	0.5230
Z	0.7222	0.3010
a	0.5938	0.0290
b	0.6397	0.0370
c	0.5732	0.2700
d	0.8872	0.3180
e	0.5612	0.0280
g	0.8346	0.1540
h	0.9132	0.1340
i	0.9164	0.2180
j	0.8824	0.2820
k	0.8226	0.2940
l	0.8959	0.4280
m	0.8031	0.2240
n	0.2195	0.0850
o	0.2676	0.0010
p	0.2217	0.0180
q	0.1170	0.0040
r	0.2405	-0.0030
s	0.6115	-0.0010

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Chain	Atom inclusion	Q-score
t	0.1330	-0.0220
u	0.3867	0.0270
v	0.8388	0.1440
w	0.5562	0.0120
x	0.2757	0.0440
y	0.4072	-0.0060
z	0.6344	0.0060