Full wwPDB EM Validation Report (i)

Nov 14, 2022 – 03:20 PM JST

PDB ID	:	6J6N
EMDB ID	:	EMD-0691
Title	:	Cryo-EM structure of the yeast B*-b1 complex at an average resolution of 3.86 angstrom
Authors	:	Wan, R.; Bai, R.; Yan, C.; Lei, J.; Shi, Y.
Deposited on	:	2019-01-15
Resolution	:	3.86 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:

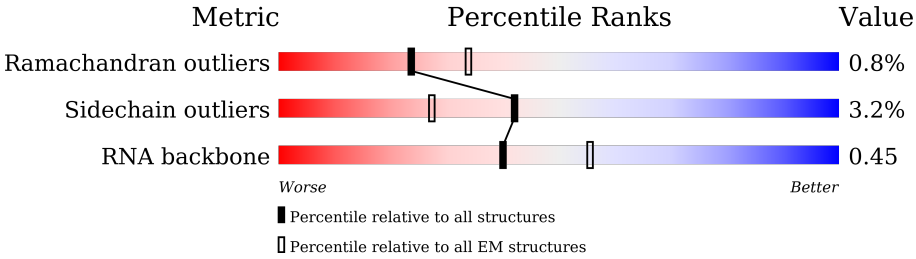
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.86 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	6% 77% • 21%
2	C	1008	• 90% • 9%
3	J	135	20% 80%
4	O	451	76% • 21%
5	P	379	6% 51% • • 46%
6	Q	364	• 78% • 20%
7	R	339	• 76% • 23%
8	S	175	• 39% • 60%

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Mol	Chain	Length	Quality of chain
9	T	157	97%
10	Z	577	31%, 77%, 23%
11	c	590	39%, 73%, 26%
12	d	687	15%, 82%, 18%
13	I	215	5%, 47%, 53%
14	n	455	58%, 62%, 34%
15	H	235	16%, 30%, 70%
16	B	246	6%, 9%, 14%, 77%
17	D	214	56%, 28%, 16%
18	E	112	54%, 38%, 8%
19	L	1175	8%, 11%, 6%, 83%
20	v	859	22%, 82%, 16%
21	a	111	35%, 75%, 24%
22	b	238	32%, 68%, 29%
23	t	175	88%, 81%, 8%, 11%
24	i	94	76%, 21%
24	u	94	59%, 78%, 21%
25	m	146	12%, 75%, 6%, 18%
25	z	146	42%, 74%, 26%
26	j	77	13%, 86%, 12%
26	x	77	78%, 95%
27	h	86	79%, 21%
27	w	86	48%, 79%, 21%
28	e	110	62%, 84%, 8%, 8%
28	g	110	15%, 85%, 6%, 8%

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Mol	Chain	Length	Quality of chain
29	k	196	5% 44% 6% 49%
29	s	196	20% 46% 53%
30	l	101	61% 21% 18%
30	y	101	53% 80% 20%
31	o	503	22% 24% 75%
31	p	503	22% 25% 75%
31	q	503	25% 25% 74%
31	r	503	23% 24% 75%

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 78937 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	71	629	399	116	113	1	0	0

- Molecule 16 is a RNA chain called UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	B	57	1206	542	209	398	57	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	205	4325	1936	728	1456	205	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

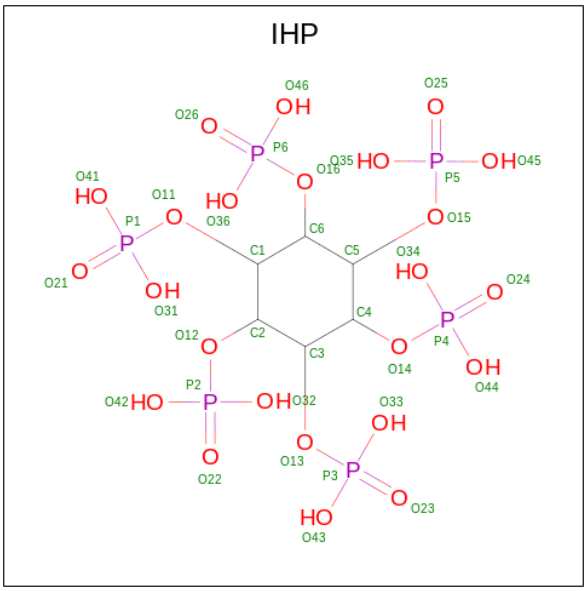
- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D3.

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.

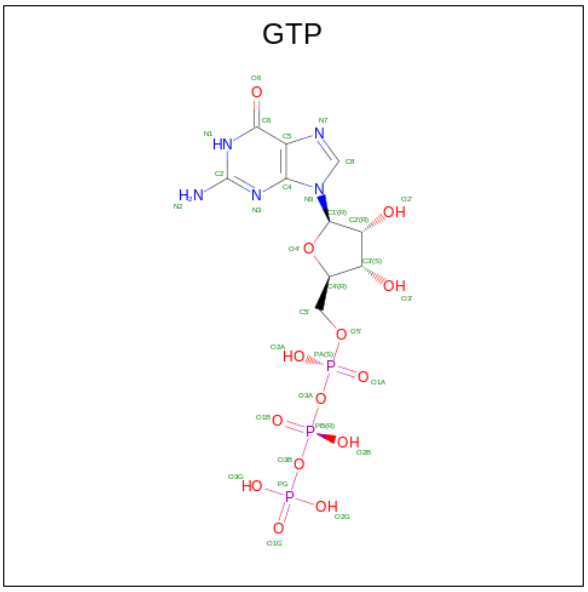
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	r	125	823	521	133	167	2	0	0
31	p	128	843	532	136	173	2	0	0
31	q	129	850	537	137	174	2	0	0
31	o	126	830	525	134	169	2	0	0

- 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).

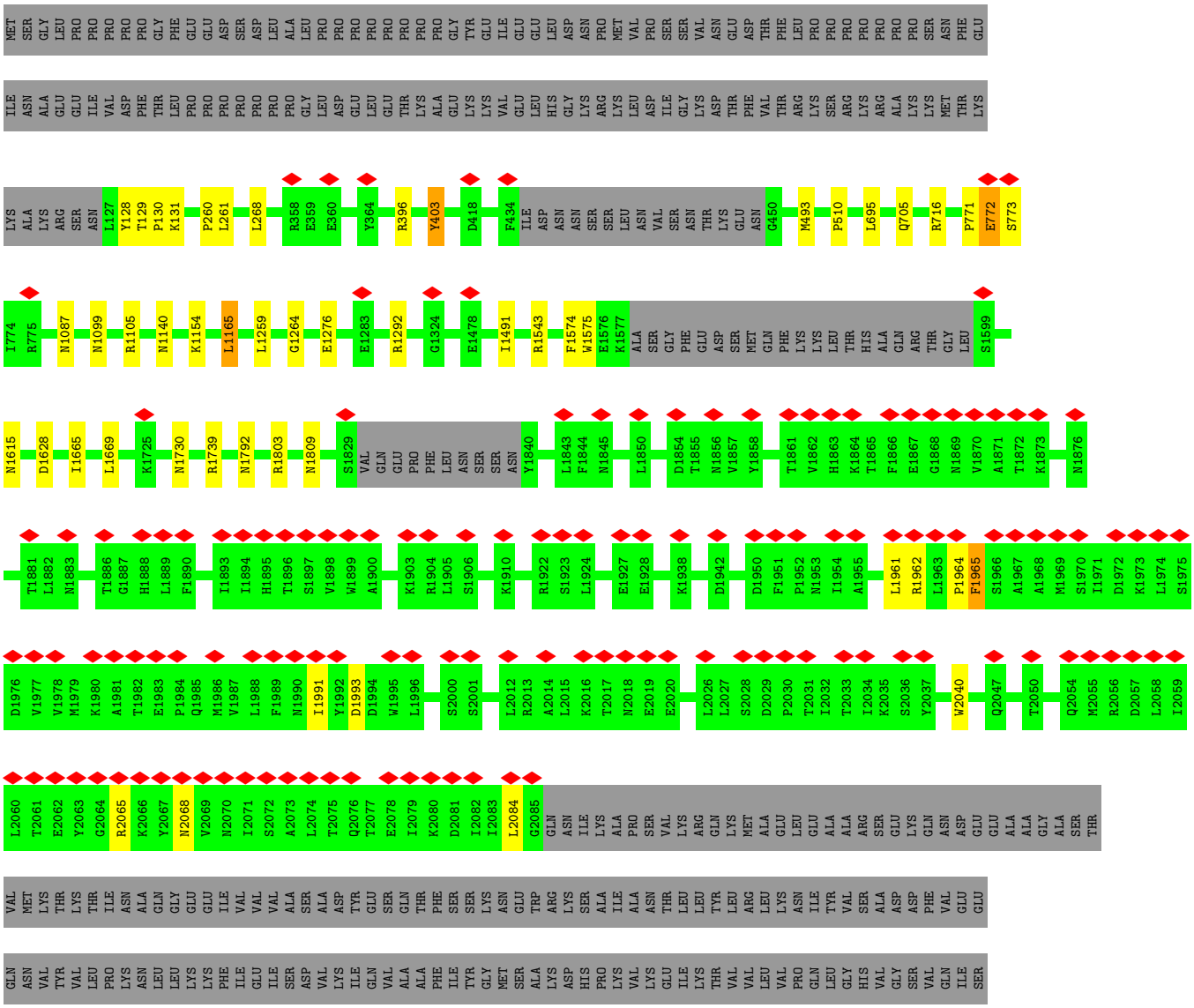
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
35	Q	2	2	2	0
			Total	Zn	
35	R	1	1	1	0
			Total	Zn	
35	T	3	3	3	0

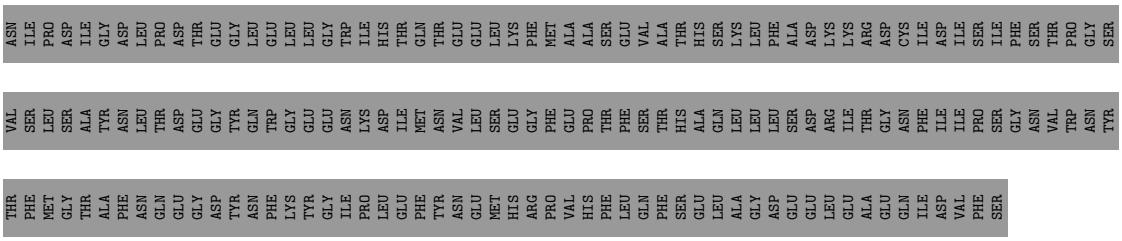
3 Residue-property plots (i)

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

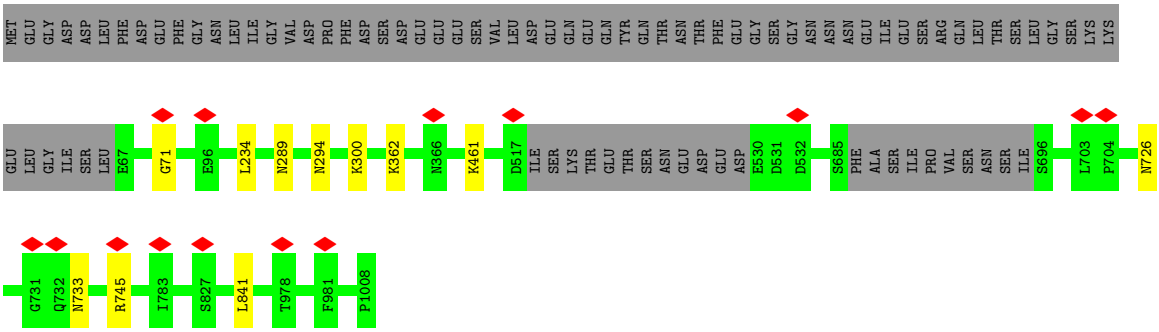
Chain A:





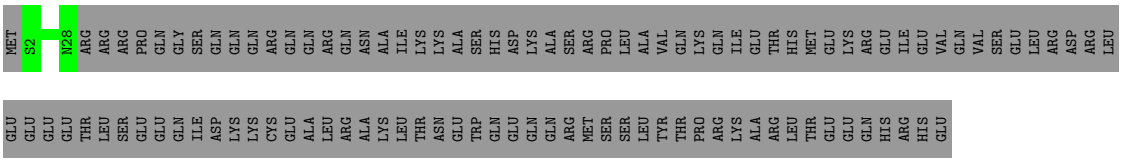
• Molecule 2: Pre-mRNA-splicing factor SNU114

Chain C:



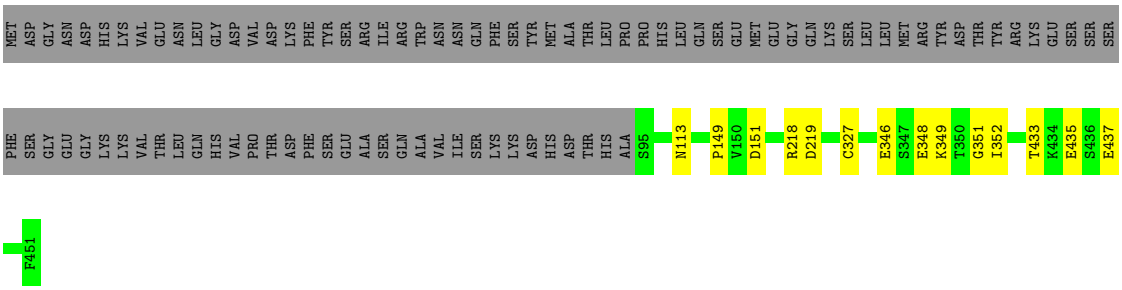
• Molecule 3: Pre-mRNA-splicing factor CWC21

Chain J:



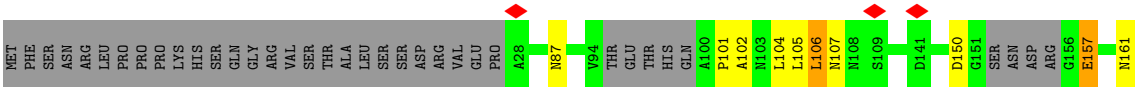
• Molecule 4: Pre-mRNA-splicing factor PRP46

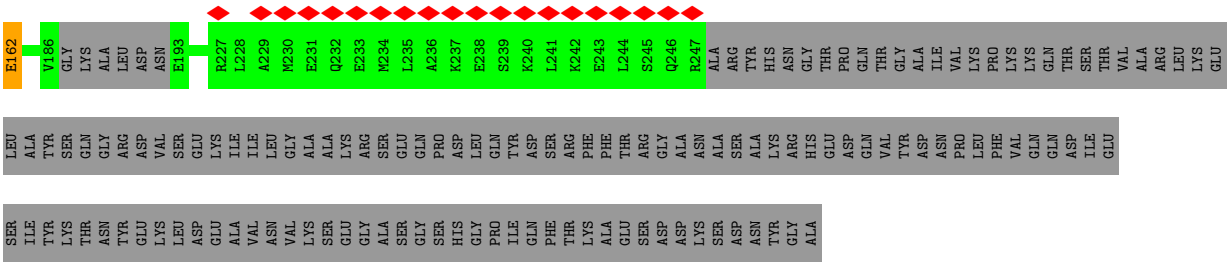
Chain O:



• Molecule 5: Pre-mRNA-processing protein 45

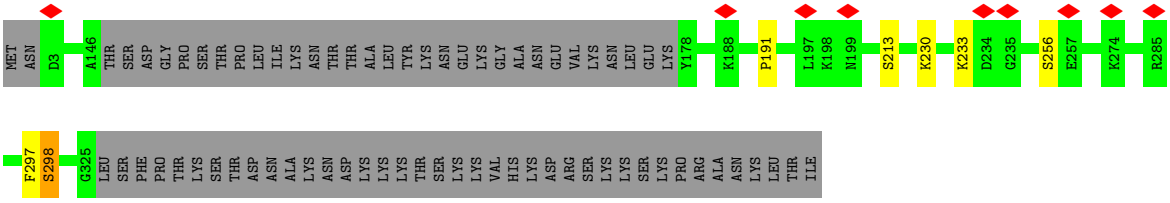
Chain P:





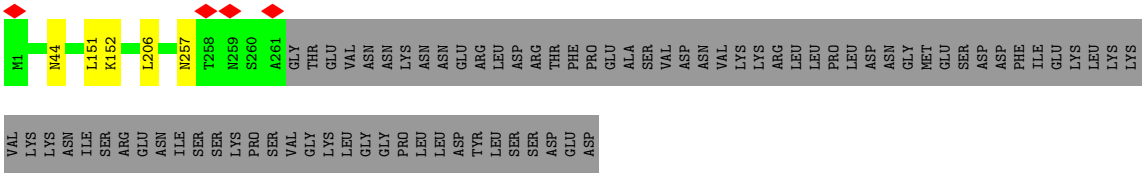
- Molecule 6: Pre-mRNA-splicing factor SLT11

Chain Q:



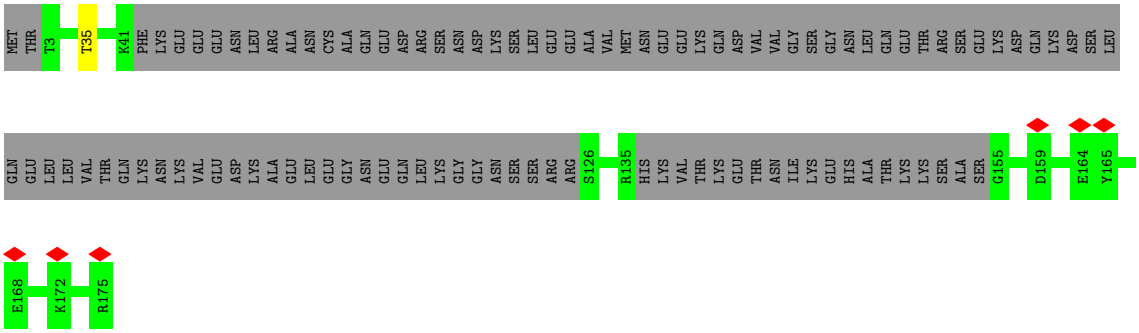
- Molecule 7: Pre-mRNA-splicing factor CWC2

Chain R:



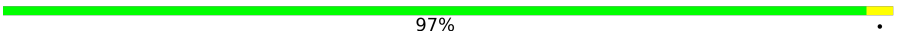
- Molecule 8: Pre-mRNA-splicing factor CWC15

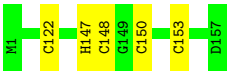
Chain S:



- Molecule 9: Pre-mRNA-splicing factor BUD31

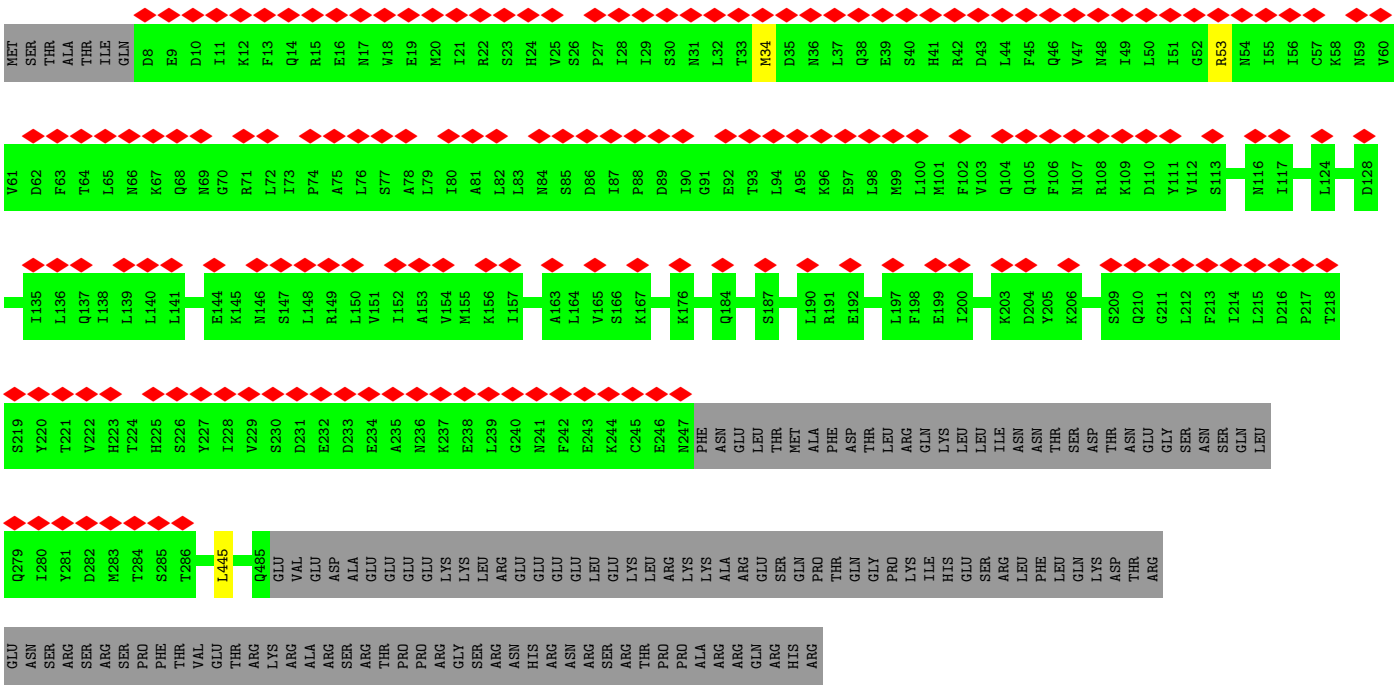
Chain T:





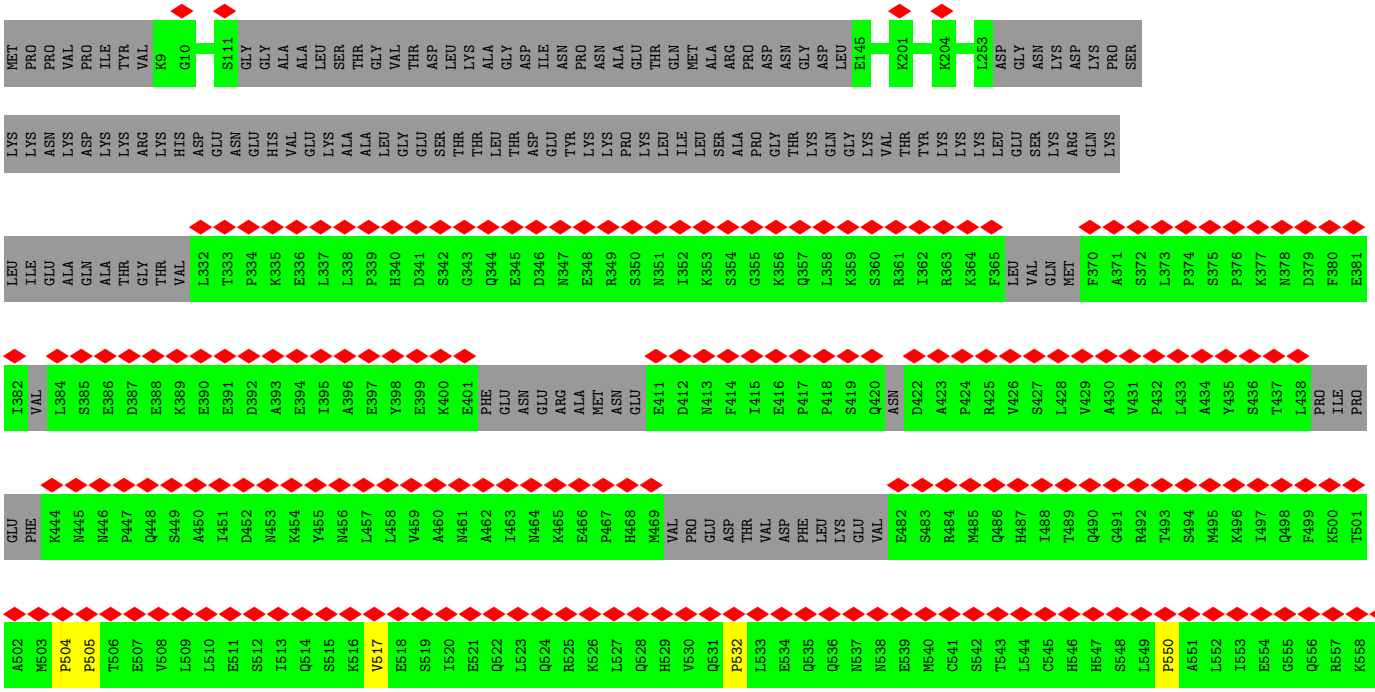
• Molecule 10: Pre-mRNA-splicing factor CWC22

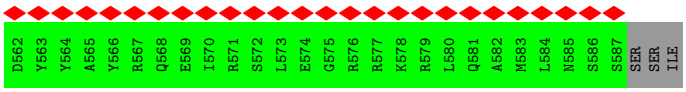
Chain Z:



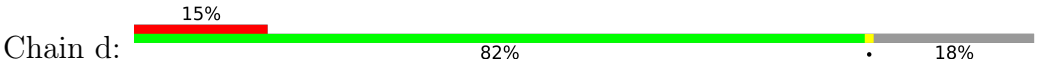
• Molecule 11: Pre-mRNA-splicing factor CEF1

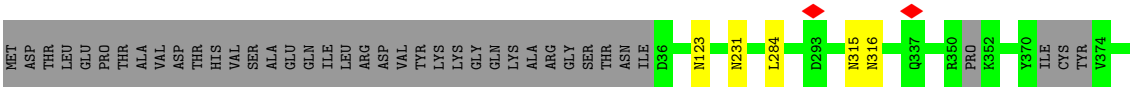
Chain c:

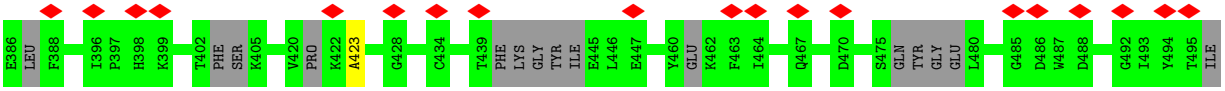


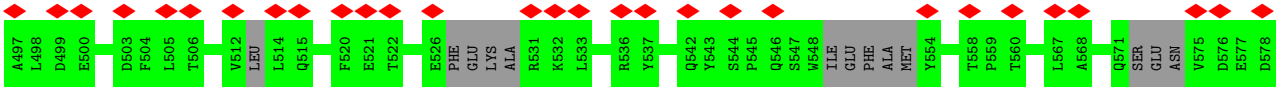


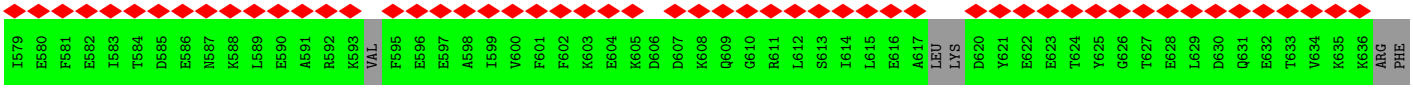
• Molecule 12: Pre-mRNA-splicing factor CLF1



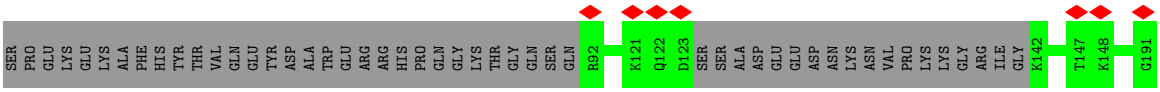


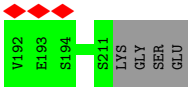




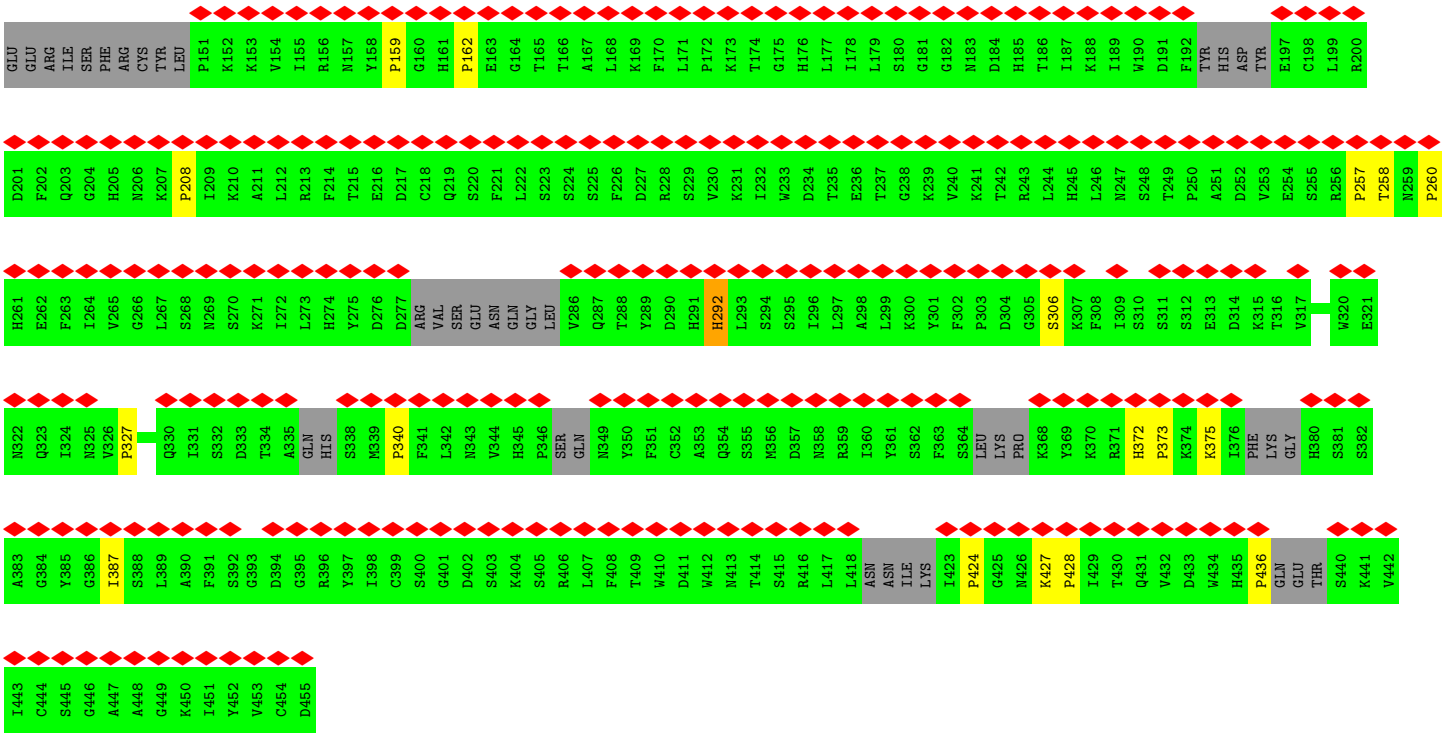


• Molecule 13: Pre-mRNA-splicing factor SYF2



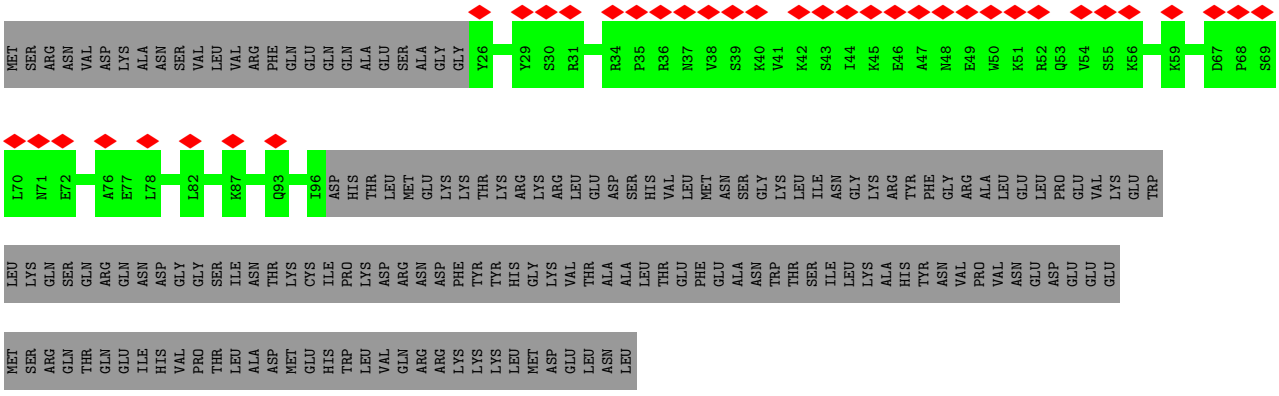


• Molecule 14: Pre-mRNA-processing factor 17



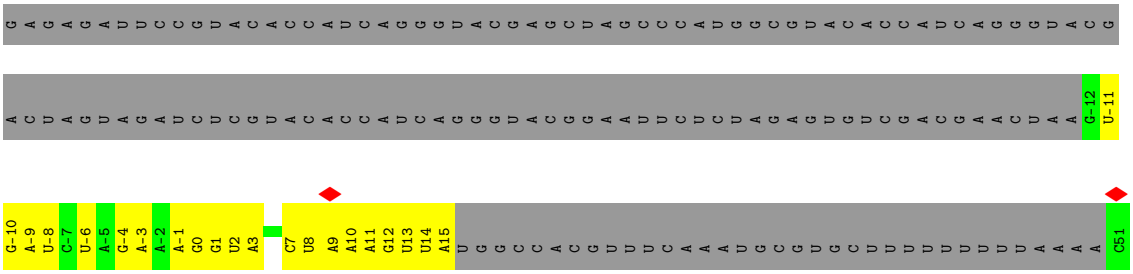
- Molecule 15: Pre-mRNA-splicing factor ISY1

Chain H:



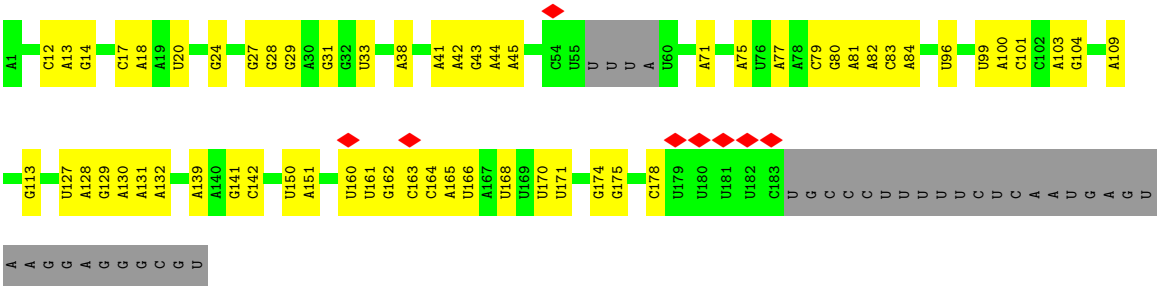
- Molecule 16: UBC4 pre-mRNA

Chain B:



• Molecule 17: U5 snRNA

Chain D:

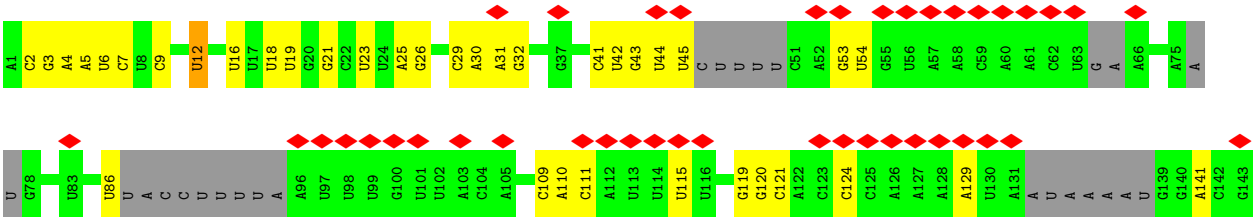


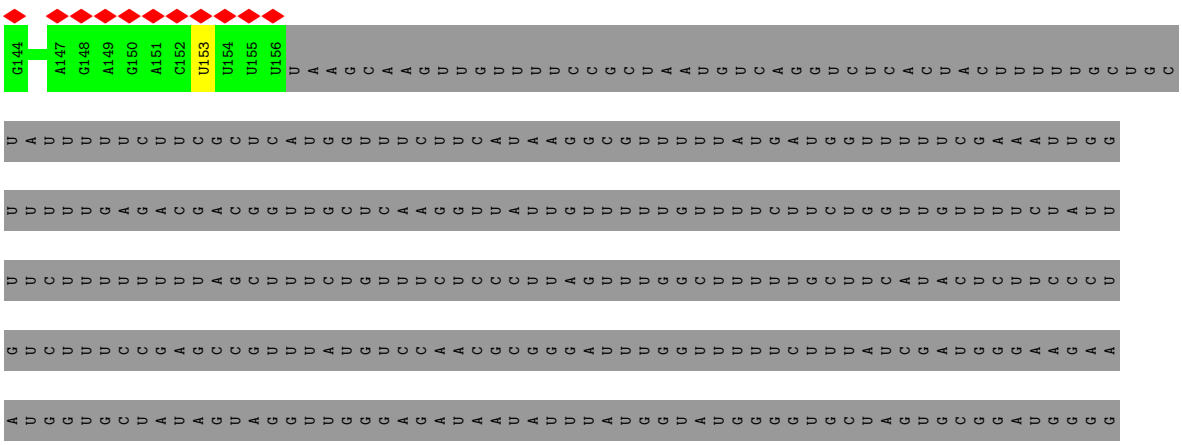
• Molecule 18: U6 snRNA

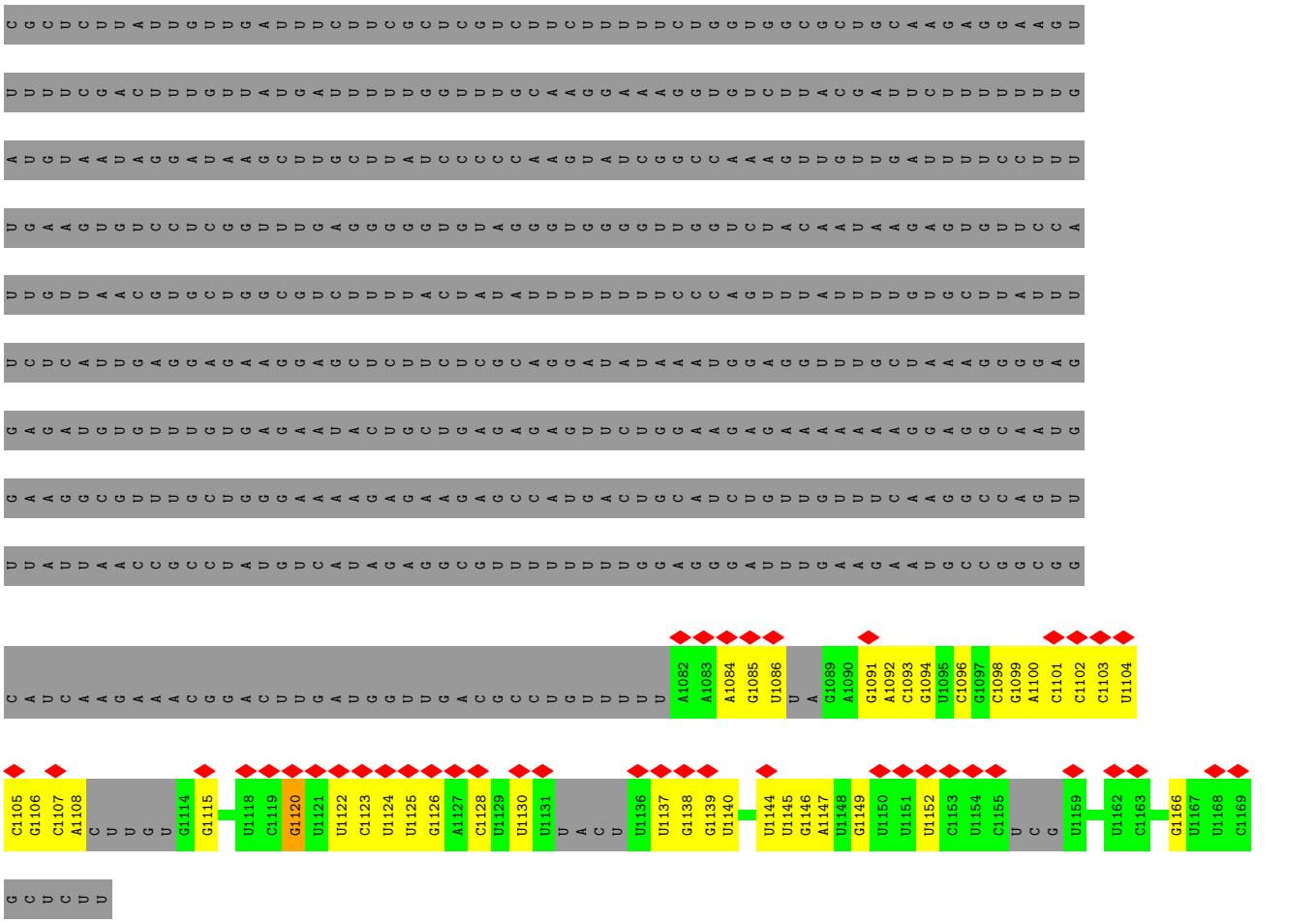
Chain E:

• Molecule 19: U2 snRNA

Chain L:

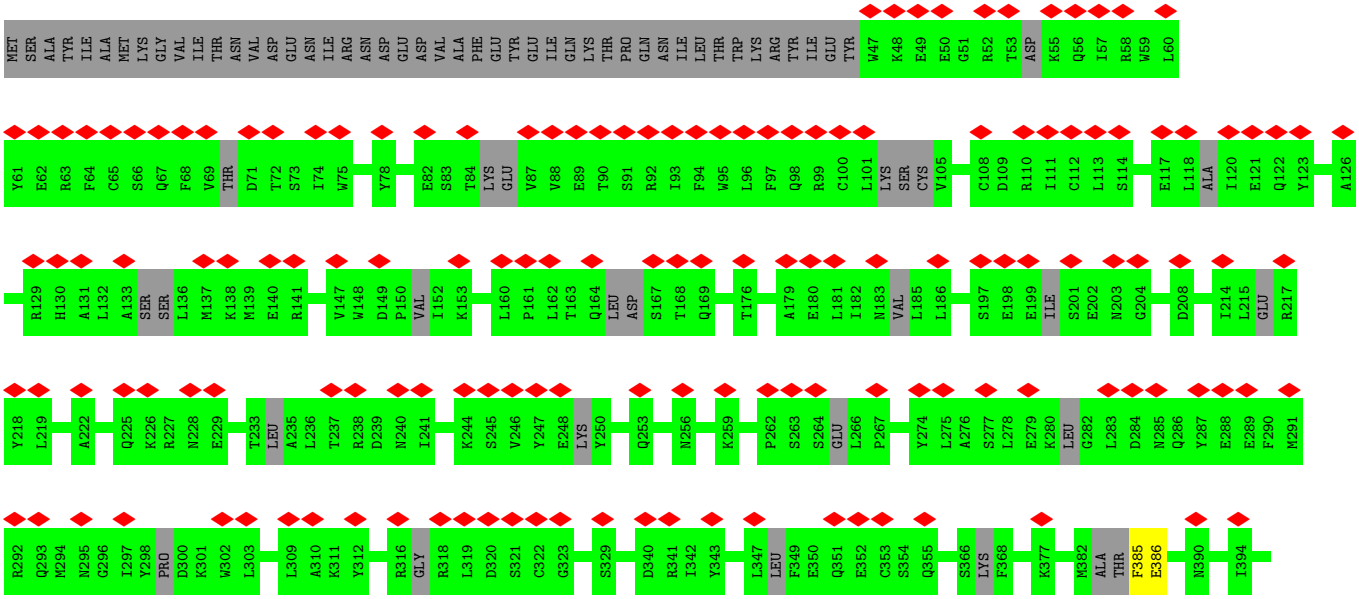


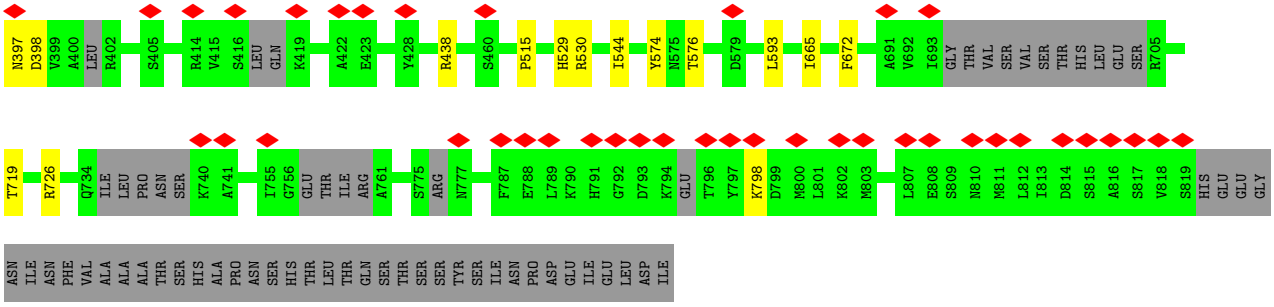




• Molecule 20: Pre-mRNA-splicing factor SYF1

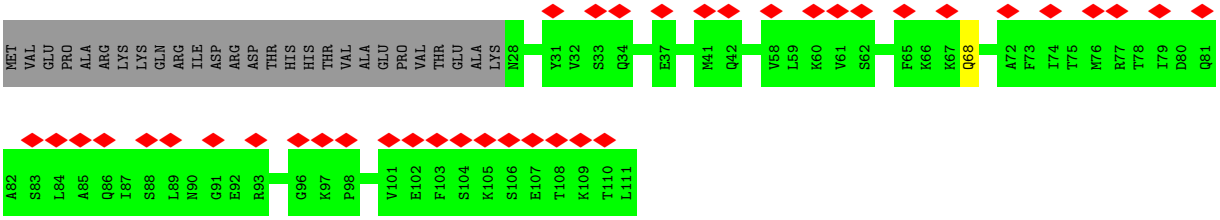
Chain v: 22% 82% • 16%





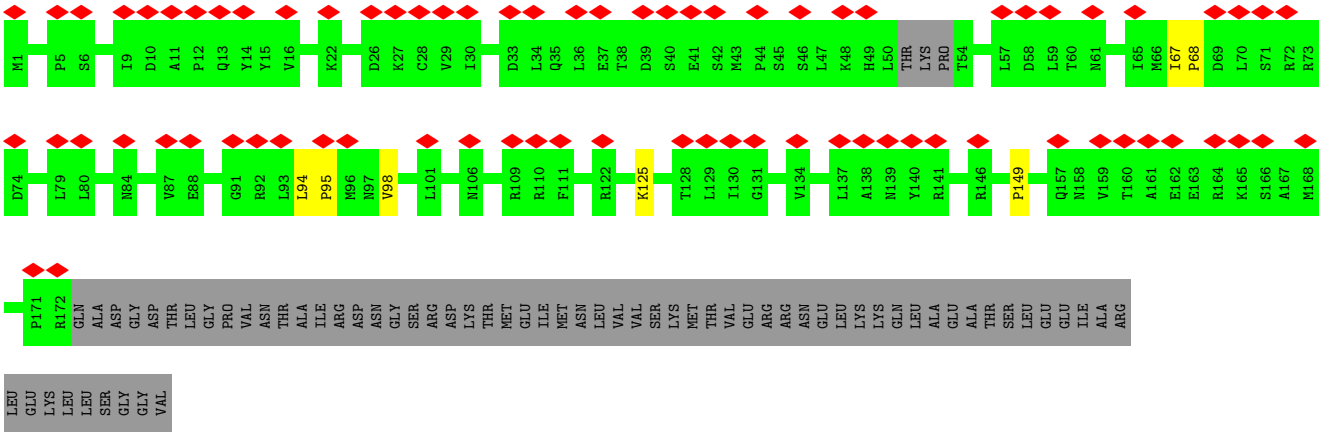
- Molecule 21: U2 small nuclear ribonucleoprotein B”

Chain a:



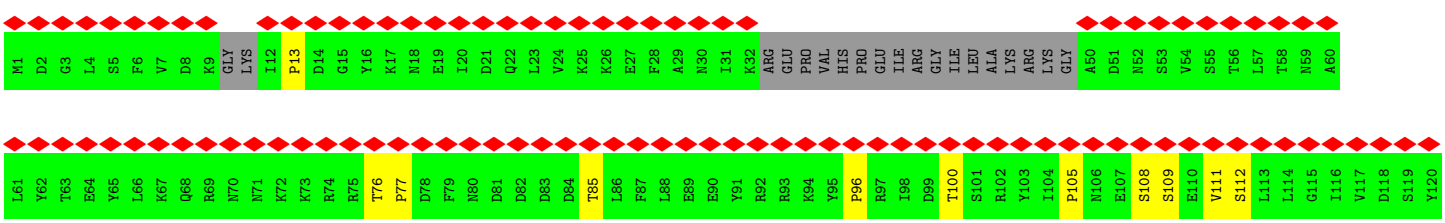
- Molecule 22: U2 small nuclear ribonucleoprotein A’

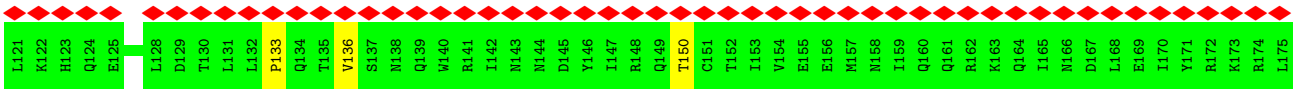
Chain b:



- Molecule 23: Pre-mRNA-splicing factor SNT309

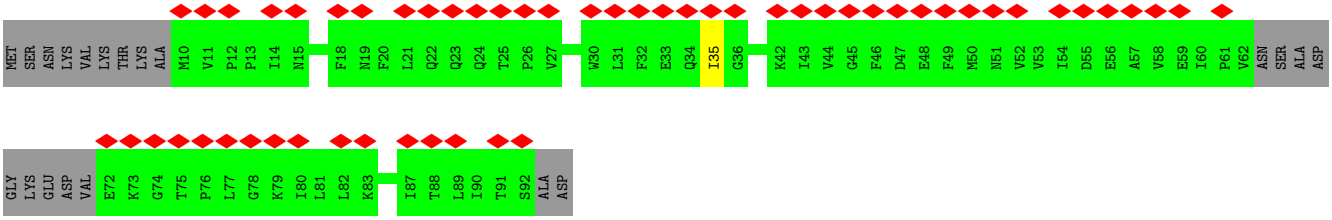
Chain t:





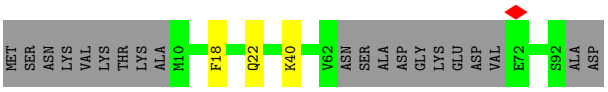
• Molecule 24: Small nuclear ribonucleoprotein E

Chain u:



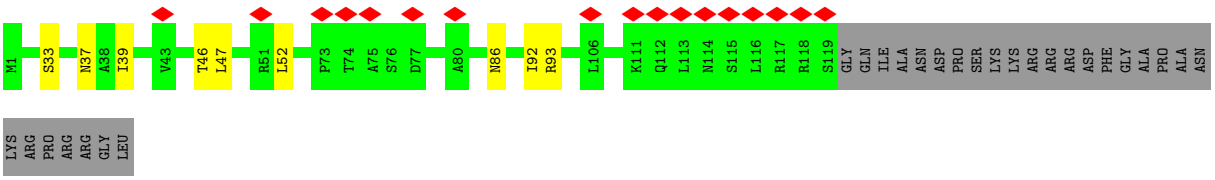
• Molecule 24: Small nuclear ribonucleoprotein E

Chain i:



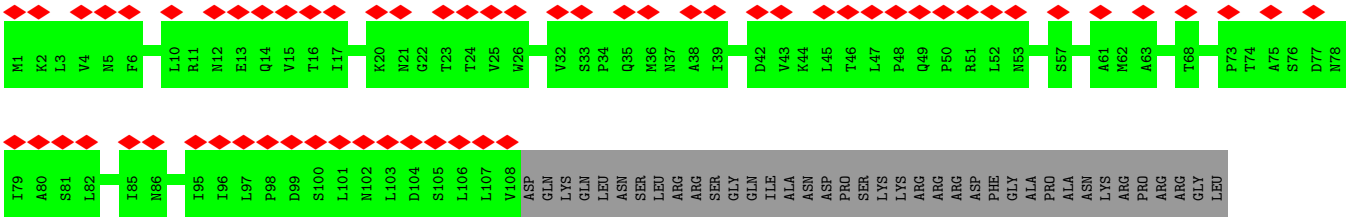
• Molecule 25: Small nuclear ribonucleoprotein Sm D1

Chain m:



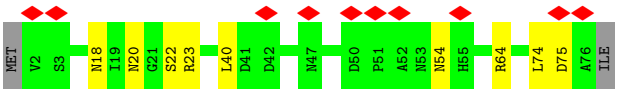
• Molecule 25: Small nuclear ribonucleoprotein Sm D1

Chain z:



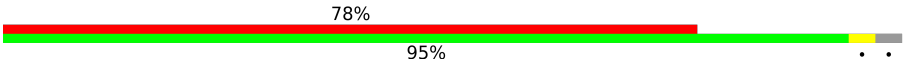
• Molecule 26: Small nuclear ribonucleoprotein G

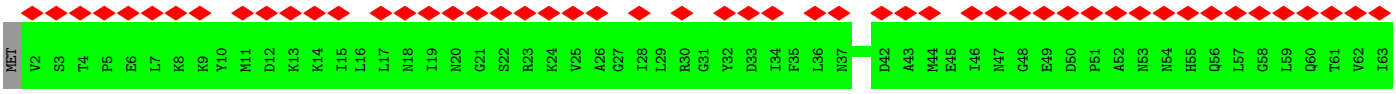
Chain j:

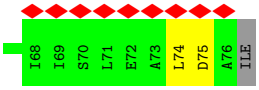


• Molecule 26: Small nuclear ribonucleoprotein G

Chain x:

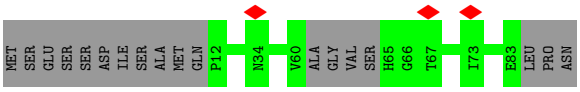






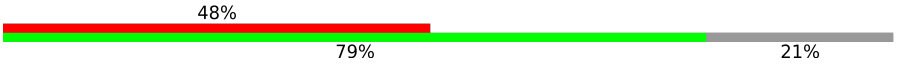
• Molecule 27: Small nuclear ribonucleoprotein F

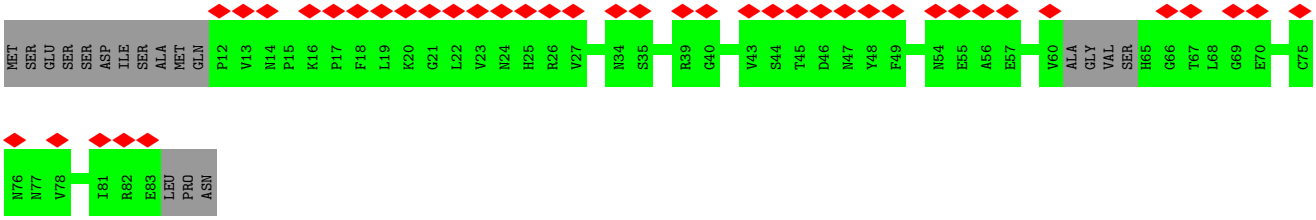
Chain h:



• Molecule 27: Small nuclear ribonucleoprotein F

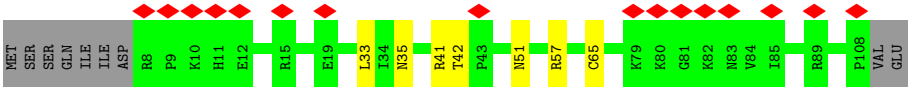
Chain w:





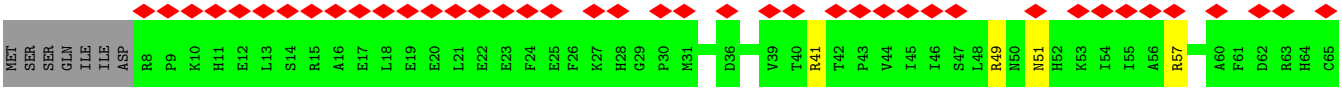
• Molecule 28: Small nuclear ribonucleoprotein Sm D2

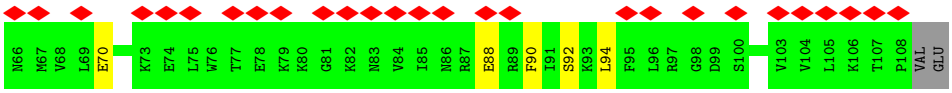
Chain g:



• Molecule 28: Small nuclear ribonucleoprotein Sm D2

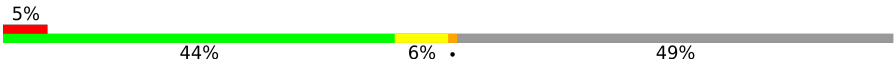
Chain e:

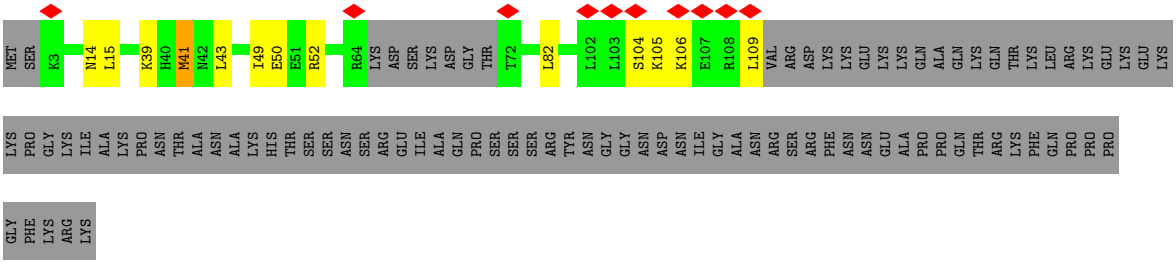




• Molecule 29: Small nuclear ribonucleoprotein-associated protein B

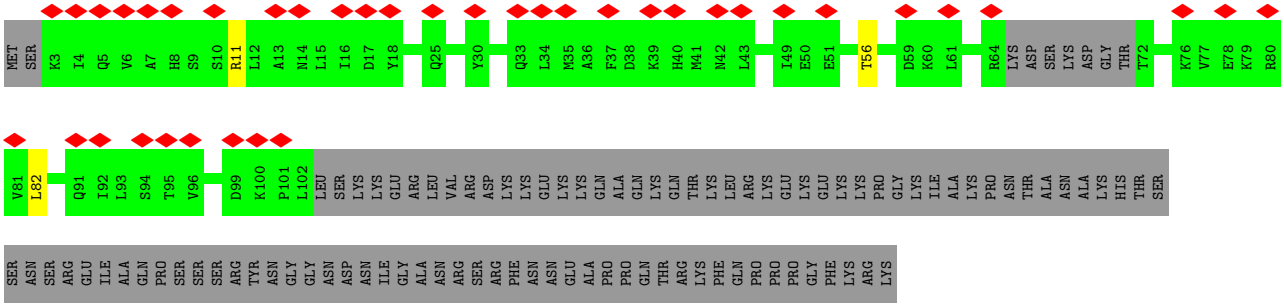
Chain k:





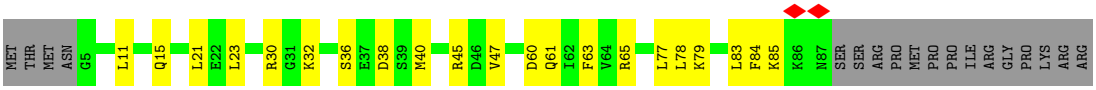
• Molecule 29: Small nuclear ribonucleoprotein-associated protein B

Chain s:



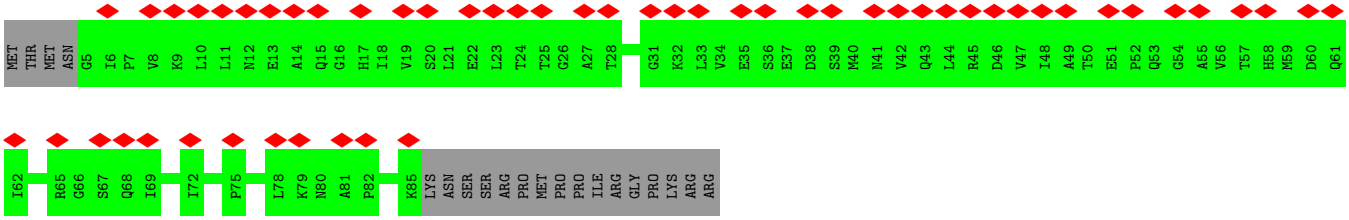
• Molecule 30: Small nuclear ribonucleoprotein Sm D3

Chain l:



• Molecule 30: Small nuclear ribonucleoprotein Sm D3

Chain y:



• Molecule 31: Pre-mRNA-processing factor 19

Chain r: 23% 24% 75%

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 D34 T35 G36 N37 D38 T41 N42 E43 P44 L45 S46 E49 I50 V51 E52 I53 VAL PRO SER A57 Q58 Q59 A60 S61 L62 T63

E64 S65 THR ASN SER ALA THR LEU LYS ALA ASN TYR SER 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 SER 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 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 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 p: 22% 25% 75%

M1 L2 C3 A4 I5 S6 G7 K8 R11 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 E49 I50 V51 E52 ILE VAL PRO S56 A60 S61 L62 T63 E64 S65 THR

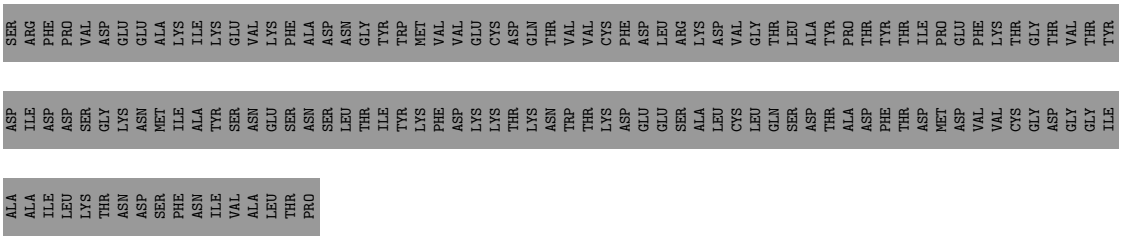
ASN SER ALA THR LEU LYS ALA ASN TYR SER I77 P78 N79 L80 L81 T82 S83 L84 Q85 N86 E87 W88 D89 A90 I91 M92 L93 E94 N95 F96 K97 L98 R99 S100 T101 L102 D103 S104 L105 T106 K107 K108 L109 S110 T111 V112 M113 Y114 E115 R116 D117 A118 A119 K120 L121 V122 A123 A124 Q125 L126

L127 M128 E129 K130 N131 E132 D133 S134 K135 D136 L137 P138 K139 S140 S141 Q142 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 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 ASP SER LYS THR ILE THR THR ILE THR THR PRO ASN PRO ARG THR GLY GLY ALA

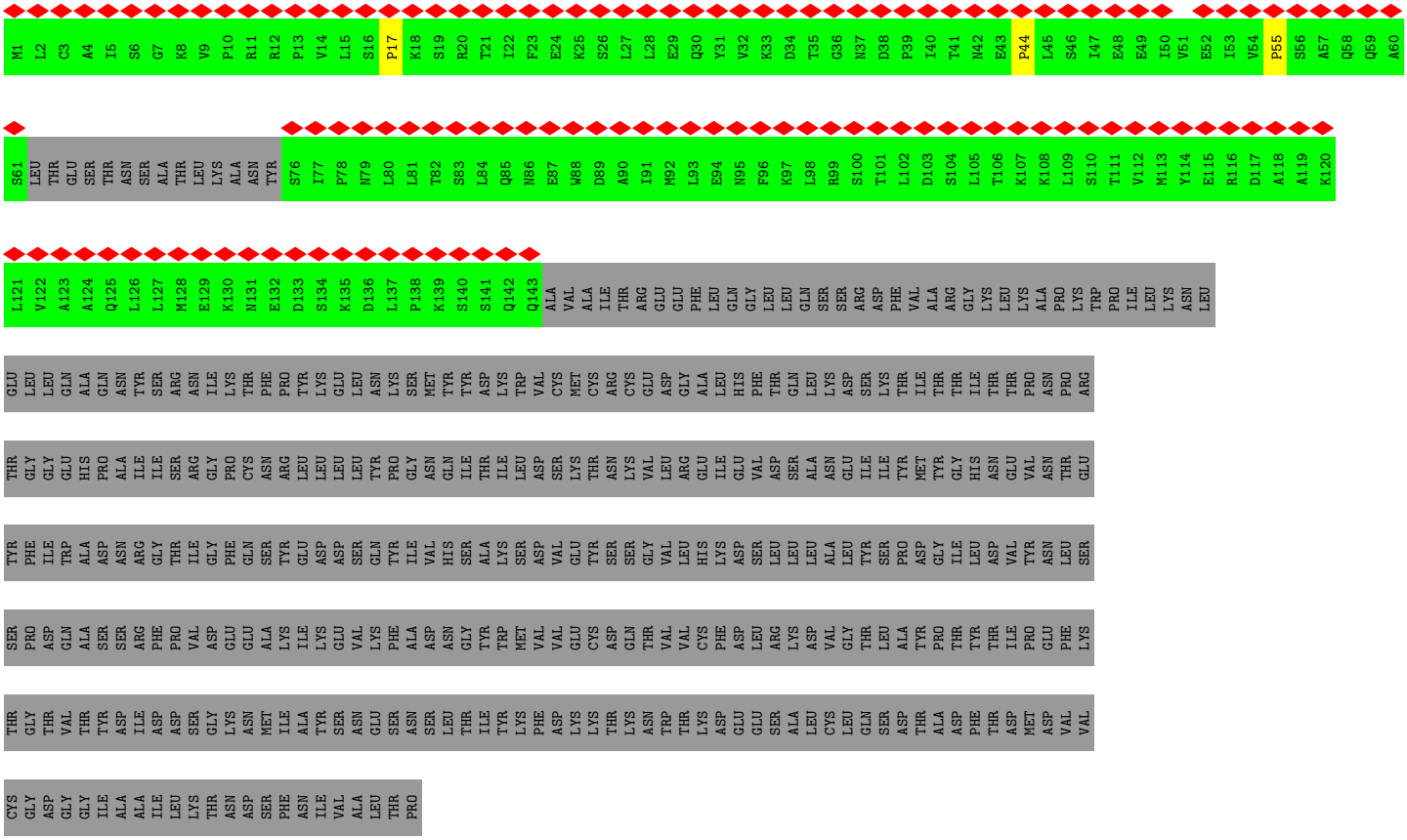
ALA ILE ILE SER ARG GLY PRO CYS ASN ARG LEU LEU LEU LEU TYR PRO GLY ASN GLN ILE THR ILE LEU ASP SER LYS THR ASN LYS VAL LEU ARG GLU ILE GLU VAL ASP SER ALA ASN GLU ILE ILE TYR MET TYR GLY HIS ASN GLU VAL ASN THR GLU TYR PHE ILE TRP ALA ASP

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



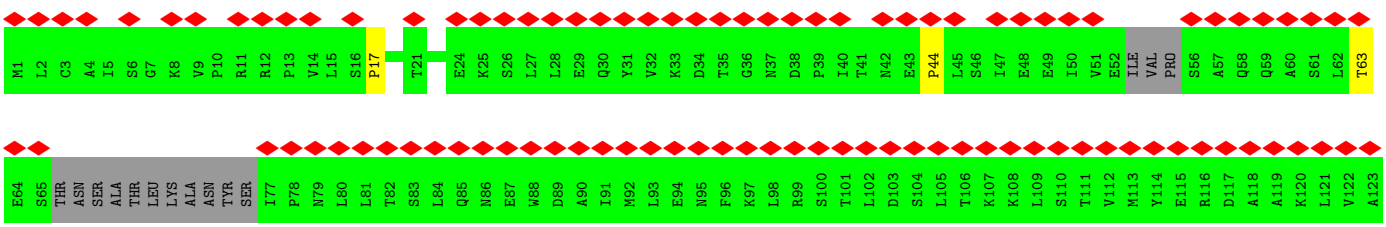
• Molecule 31: Pre-mRNA-processing factor 19

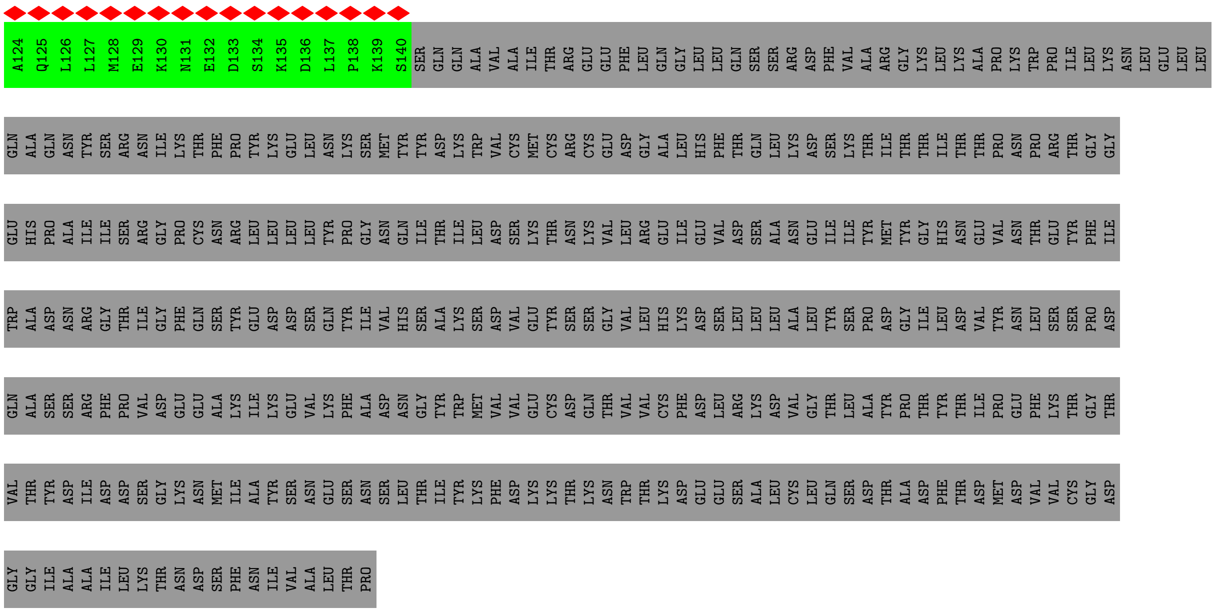
Chain q:



• Molecule 31: Pre-mRNA-processing factor 19

Chain o:




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 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 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	395458	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	0.209	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.028	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: IHP, MG, ZN, SEP, GTP

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	0.45	0/16198	0.61	0/21958
2	C	0.44	0/7503	0.62	0/10159
3	J	0.40	0/191	0.67	0/254
4	O	0.52	0/2872	0.65	0/3902
5	P	0.38	0/1629	0.55	0/2194
6	Q	0.38	0/2339	0.62	0/3154
7	R	0.41	0/2135	0.58	0/2871
8	S	0.33	0/581	0.56	0/776
9	T	0.49	0/1315	0.59	0/1759
10	Z	0.35	0/3712	0.56	0/5004
11	c	0.32	0/2996	0.48	0/4033
12	d	0.36	0/3931	0.50	0/5356
13	I	0.36	0/826	0.51	0/1097
14	n	0.34	0/1894	0.58	0/2529
15	H	0.37	0/644	0.70	0/864
16	B	0.49	0/1347	0.92	0/2091
17	D	0.56	0/4239	0.96	0/6598
18	E	0.80	1/2452 (0.0%)	0.95	0/3817
19	L	0.37	2/4815 (0.0%)	0.79	0/7467
20	v	0.42	0/4662	0.51	0/6358
21	a	0.42	0/415	0.57	0/577
22	b	0.69	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	0.54	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	0.36	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	0.43	3/81286 (0.0%)	0.64	0/112573

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	12	U	O3'-P	7.07	1.69	1.61
19	L	1120	G	O3'-P	-5.48	1.54	1.61
18	E	81	G	O3'-P	-5.11	1.55	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%)	1793 (94%)	95 (5%)	17 (1%)	17 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	914/1008 (91%)	872 (95%)	41 (4%)	1 (0%)	51	83
3	J	25/135 (18%)	23 (92%)	2 (8%)	0	100	100
4	O	355/451 (79%)	316 (89%)	33 (9%)	6 (2%)	9	42
5	P	197/379 (52%)	183 (93%)	6 (3%)	8 (4%)	3	26
6	Q	288/364 (79%)	263 (91%)	20 (7%)	5 (2%)	9	42
7	R	259/339 (76%)	247 (95%)	10 (4%)	2 (1%)	19	56
8	S	64/175 (37%)	60 (94%)	4 (6%)	0	100	100
9	T	155/157 (99%)	146 (94%)	6 (4%)	3 (2%)	8	40
10	Z	443/577 (77%)	422 (95%)	21 (5%)	0	100	100
11	c	418/590 (71%)	398 (95%)	20 (5%)	0	100	100
12	d	534/687 (78%)	520 (97%)	13 (2%)	1 (0%)	47	78
13	I	98/215 (46%)	94 (96%)	4 (4%)	0	100	100
14	n	279/455 (61%)	249 (89%)	25 (9%)	5 (2%)	8	41
15	H	69/235 (29%)	61 (88%)	8 (12%)	0	100	100
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	48
22	b	165/238 (69%)	138 (84%)	20 (12%)	7 (4%)	3	26
23	t	150/175 (86%)	145 (97%)	4 (3%)	1 (1%)	22	59
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	45
26	x	73/77 (95%)	65 (89%)	7 (10%)	1 (1%)	11	45
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	51
28	g	99/110 (90%)	93 (94%)	4 (4%)	2 (2%)	7	39
29	k	96/196 (49%)	90 (94%)	5 (5%)	1 (1%)	15	51
29	s	89/196 (45%)	83 (93%)	6 (7%)	0	100	100
30	l	81/101 (80%)	79 (98%)	0	2 (2%)	5	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	y	79/101 (78%)	75 (95%)	4 (5%)	0	100	100
31	o	120/503 (24%)	115 (96%)	5 (4%)	0	100	100
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	8732/13195 (66%)	8224 (94%)	441 (5%)	67 (1%)	24	56

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	A	260	PRO
1	A	403	TYR
1	A	773	SER
1	A	1575	TRP
1	A	1965	PHE
4	O	151	ASP
5	P	106	LEU
9	T	148	CYS
9	T	150	CYS
12	d	423	ALA
14	n	292	HIS
14	n	372	HIS
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	510	PRO
1	A	771	PRO
1	A	1491	ILE
1	A	1964	PRO
2	C	71	GLY
4	O	219	ASP
4	O	351	GLY
5	P	102	ALA
5	P	105	LEU
5	P	157	GLU
5	P	162	GLU

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Mol	Chain	Res	Type
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	128	TYR
4	O	218	ARG
5	P	150	ASP
6	Q	256	SER
6	Q	297	PHE
6	Q	298	SER
7	R	151	LEU
9	T	122	CYS
14	n	375	LYS
20	v	515	PRO
22	b	67	ILE
22	b	94	LEU
1	A	772	GLU
1	A	1165	LEU
1	A	1264	GLY
4	O	352	ILE
5	P	101	PRO
30	l	40	MET
26	x	75	ASP
1	A	268	LEU
1	A	1276	GLU
5	P	161	ASN
6	Q	213	SER
7	R	206	LEU
14	n	387	ILE
14	n	427	LYS
1	A	130	PRO
4	O	149	PRO
6	Q	191	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%)	1700 (98%)	37 (2%)	53	73
2	C	830/910 (91%)	820 (99%)	10 (1%)	71	83
3	J	21/121 (17%)	21 (100%)	0	100	100
4	O	312/397 (79%)	304 (97%)	8 (3%)	46	68
5	P	175/328 (53%)	169 (97%)	6 (3%)	37	62
6	Q	265/332 (80%)	262 (99%)	3 (1%)	73	84
7	R	224/296 (76%)	221 (99%)	3 (1%)	69	81
8	S	57/151 (38%)	56 (98%)	1 (2%)	59	77
9	T	141/141 (100%)	139 (99%)	2 (1%)	67	81
10	Z	417/538 (78%)	414 (99%)	3 (1%)	84	90
11	c	214/525 (41%)	209 (98%)	5 (2%)	50	70
12	d	274/633 (43%)	269 (98%)	5 (2%)	59	77
13	I	92/193 (48%)	92 (100%)	0	100	100
14	n	122/412 (30%)	108 (88%)	14 (12%)	5	26
15	H	69/216 (32%)	69 (100%)	0	100	100
20	v	294/786 (37%)	279 (95%)	15 (5%)	24	53
23	t	39/165 (24%)	26 (67%)	13 (33%)	0	2
24	i	55/83 (66%)	52 (94%)	3 (6%)	21	51
24	u	52/83 (63%)	51 (98%)	1 (2%)	57	75
25	m	106/129 (82%)	97 (92%)	9 (8%)	10	39
25	z	95/129 (74%)	95 (100%)	0	100	100
26	j	56/66 (85%)	48 (86%)	8 (14%)	3	20
26	x	56/66 (85%)	55 (98%)	1 (2%)	59	77
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%)	74 (90%)	8 (10%)	8	31
28	g	82/103 (80%)	77 (94%)	5 (6%)	18	48
29	k	92/176 (52%)	79 (86%)	13 (14%)	3	21
29	s	85/176 (48%)	82 (96%)	3 (4%)	36	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	l	72/89 (81%)	53 (74%)	19 (26%)	0	4
30	y	68/89 (76%)	68 (100%)	0	100	100
31	o	60/451 (13%)	57 (95%)	3 (5%)	24	53
31	p	62/451 (14%)	58 (94%)	4 (6%)	17	46
31	q	62/451 (14%)	59 (95%)	3 (5%)	25	54
31	r	60/451 (13%)	57 (95%)	3 (5%)	24	53
All	All	6530/11576 (56%)	6322 (97%)	208 (3%)	42	63

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	261	LEU
1	A	396	ARG
1	A	403	TYR
1	A	493	MET
1	A	695	LEU
1	A	705	GLN
1	A	716	ARG
1	A	772	GLU
1	A	1087	ASN
1	A	1099	ASN
1	A	1105	ARG
1	A	1140	ASN
1	A	1154	LYS
1	A	1165	LEU
1	A	1259	LEU
1	A	1292	ARG
1	A	1543	ARG
1	A	1574	PHE
1	A	1615	ASN
1	A	1628	ASP
1	A	1665	ILE
1	A	1669	LEU
1	A	1730	ASN
1	A	1739	ARG
1	A	1792	ASN
1	A	1803	ARG
1	A	1809	ASN
1	A	1961	LEU

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Mol	Chain	Res	Type
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	234	LEU
2	C	289	ASN
2	C	294	ASN
2	C	300	LYS
2	C	362	LYS
2	C	461	LYS
2	C	726	ASN
2	C	733	ASN
2	C	745	ARG
2	C	841	LEU
4	O	113	ASN
4	O	327	CYS
4	O	346	GLU
4	O	348	GLU
4	O	349	LYS
4	O	433	THR
4	O	435	GLU
4	O	437	GLU
5	P	87	ASN
5	P	104	LEU
5	P	106	LEU
5	P	107	ASN
5	P	157	GLU
5	P	162	GLU
6	Q	230	LYS
6	Q	233	LYS
6	Q	298	SER
7	R	44	ASN
7	R	152	LYS
7	R	257	ASN
8	S	35	THR
9	T	147	HIS
9	T	153	CYS
10	Z	34	MET

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Mol	Chain	Res	Type
10	Z	53	ARG
10	Z	445	LEU
11	c	504	PRO
11	c	505	PRO
11	c	517	VAL
11	c	532	PRO
11	c	550	PRO
12	d	123	ASN
12	d	231	ASN
12	d	284	LEU
12	d	315	ASN
12	d	316	ASN
14	n	159	PRO
14	n	162	PRO
14	n	208	PRO
14	n	257	PRO
14	n	258	THR
14	n	260	PRO
14	n	292	HIS
14	n	306	SER
14	n	327	PRO
14	n	340	PRO
14	n	373	PRO
14	n	424	PRO
14	n	428	PRO
14	n	436	PRO
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	57	ARG
28	e	70	GLU
28	e	88	GLU
28	e	90	PHE
28	e	92	SER
28	e	94	LEU
29	s	11	ARG
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
24	i	22	GLN
24	i	40	LYS
26	x	74	LEU
31	r	17	PRO
31	r	44	PRO

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Mol	Chain	Res	Type
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 (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	405	ASN
1	A	541	ASN
1	A	658	ASN
1	A	796	ASN
1	A	861	GLN
1	A	864	GLN
1	A	1034	ASN
1	A	1087	ASN
1	A	1099	ASN
1	A	1140	ASN
1	A	1156	HIS
1	A	1197	ASN
1	A	1221	ASN
1	A	1368	GLN
1	A	1431	HIS
1	A	1449	ASN
1	A	1455	GLN
1	A	1532	HIS
1	A	1540	ASN
1	A	1652	HIS
1	A	1687	HIS
1	A	1730	ASN
1	A	1792	ASN
1	A	1809	ASN
1	A	1863	HIS
1	A	1947	HIS

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Mol	Chain	Res	Type
1	A	1990	ASN
1	A	2068	ASN
2	C	103	HIS
2	C	180	ASN
2	C	183	GLN
2	C	220	ASN
2	C	255	GLN
2	C	289	ASN
2	C	294	ASN
2	C	647	ASN
2	C	683	ASN
2	C	726	ASN
2	C	733	ASN
4	O	99	ASN
4	O	306	HIS
5	P	87	ASN
5	P	107	ASN
5	P	111	HIS
5	P	161	ASN
6	Q	106	ASN
6	Q	141	ASN
6	Q	243	ASN
6	Q	317	ASN
7	R	39	GLN
7	R	44	ASN
7	R	91	HIS
8	S	34	HIS
8	S	173	HIS
9	T	56	HIS
9	T	57	HIS
9	T	112	ASN
9	T	144	GLN
10	Z	84	ASN
10	Z	223	HIS
10	Z	310	HIS
10	Z	354	HIS
10	Z	441	ASN
11	c	214	ASN
12	d	123	ASN
12	d	315	ASN
12	d	316	ASN
15	H	48	ASN

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Mol	Chain	Res	Type
20	v	397	ASN
20	v	529	HIS
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	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)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	B	55/246 (22%)	33 (60%)	5 (9%)
17	D	177/214 (82%)	56 (31%)	8 (4%)
18	E	102/112 (91%)	43 (42%)	5 (4%)
19	L	194/1175 (16%)	75 (38%)	13 (6%)
All	All	528/1747 (30%)	207 (39%)	31 (5%)

All (207) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	B	-11	U
16	B	-10	G
16	B	-9	A
16	B	-8	U
16	B	-6	U
16	B	-4	G
16	B	-3	A
16	B	-1	A
16	B	0	G
16	B	1	G
16	B	2	U
16	B	3	A
16	B	7	C
16	B	8	U
16	B	9	A
16	B	10	A
16	B	11	A
16	B	12	G
16	B	13	U
16	B	14	U
16	B	15	A
16	B	52	U
16	B	53	U
16	B	54	A
16	B	55	U
16	B	56	G
16	B	57	C
16	B	58	U
16	B	70	A
16	B	71	C
16	B	74	A
16	B	75	A
16	B	78	A
17	D	12	C
17	D	13	A
17	D	14	G
17	D	18	A
17	D	20	U
17	D	24	G
17	D	27	G
17	D	28	G
17	D	29	G
17	D	31	G

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Mol	Chain	Res	Type
17	D	33	U
17	D	38	A
17	D	41	A
17	D	42	A
17	D	43	G
17	D	44	A
17	D	45	A
17	D	71	A
17	D	75	A
17	D	77	A
17	D	79	C
17	D	80	G
17	D	81	A
17	D	82	A
17	D	84	A
17	D	96	U
17	D	99	U
17	D	100	A
17	D	101	C
17	D	103	A
17	D	104	G
17	D	109	A
17	D	113	G
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	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	16	C
18	E	23	G
18	E	31	G
18	E	36	U
18	E	39	G
18	E	40	A
18	E	42	A
18	E	51	A
18	E	52	G
18	E	54	U
18	E	55	G
18	E	56	A
18	E	58	C
18	E	59	A
18	E	60	G
18	E	62	A
18	E	63	G
18	E	64	U
18	E	65	U
18	E	66	C
18	E	67	C
18	E	68	C
18	E	73	A
18	E	74	U
18	E	79	A
18	E	80	U
18	E	81	G
18	E	85	C
18	E	86	G
18	E	87	U
18	E	88	U
18	E	90	U
18	E	91	A

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Mol	Chain	Res	Type
18	E	92	C
18	E	98	G
18	E	100	U
18	E	101	U
18	E	102	U
19	L	2	C
19	L	3	G
19	L	4	A
19	L	5	A
19	L	6	U
19	L	7	C
19	L	9	C
19	L	12	U
19	L	16	U
19	L	18	U
19	L	19	U
19	L	21	G
19	L	23	U
19	L	25	A
19	L	26	G
19	L	29	C
19	L	30	A
19	L	31	A
19	L	32	G
19	L	41	C
19	L	43	G
19	L	44	U
19	L	45	U
19	L	53	G
19	L	54	U
19	L	86	U
19	L	109	C
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

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Mol	Chain	Res	Type
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
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 (31) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type

Mol	Chain	Res	Type
16	B	2	U
16	B	7	C
16	B	9	A
16	B	57	C
16	B	69	A
17	D	17	C
17	D	27	G
17	D	28	G
17	D	83	C
17	D	99	U
17	D	127	U
17	D	150	U
17	D	163	C
18	E	14	C
18	E	55	G
18	E	64	U
18	E	85	C
18	E	100	U
19	L	3	G
19	L	5	A
19	L	31	A
19	L	42	U
19	L	53	G
19	L	109	C
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	1.51	1 (12%)	8,12,14	0.99	0

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

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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	$\#\|Z\| > 2$
33	GTP	C	1500	34	26,34,34	0.95	2 (7%)	32,54,54	0.68	0
32	IHP	A	3000	-	36,36,36	0.76	0	54,60,60	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	GTP	C	1500	34	-	9/18/38/38	0/3/3/3
32	IHP	A	3000	-	-	6/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	1500	GTP	C5-C6	-2.56	1.42	1.47
33	C	1500	GTP	C8-N7	-2.10	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	3000	IHP	C2-C3-O13-P3
32	A	3000	IHP	C5-O15-P5-O25
33	C	1500	GTP	C5'-O5'-PA-O3A
33	C	1500	GTP	C5'-O5'-PA-O1A
33	C	1500	GTP	C3'-C4'-C5'-O5'
33	C	1500	GTP	O4'-C4'-C5'-O5'
32	A	3000	IHP	C4-C3-O13-P3
32	A	3000	IHP	C4-O14-P4-O24
33	C	1500	GTP	PB-O3B-PG-O2G
33	C	1500	GTP	PB-O3B-PG-O3G

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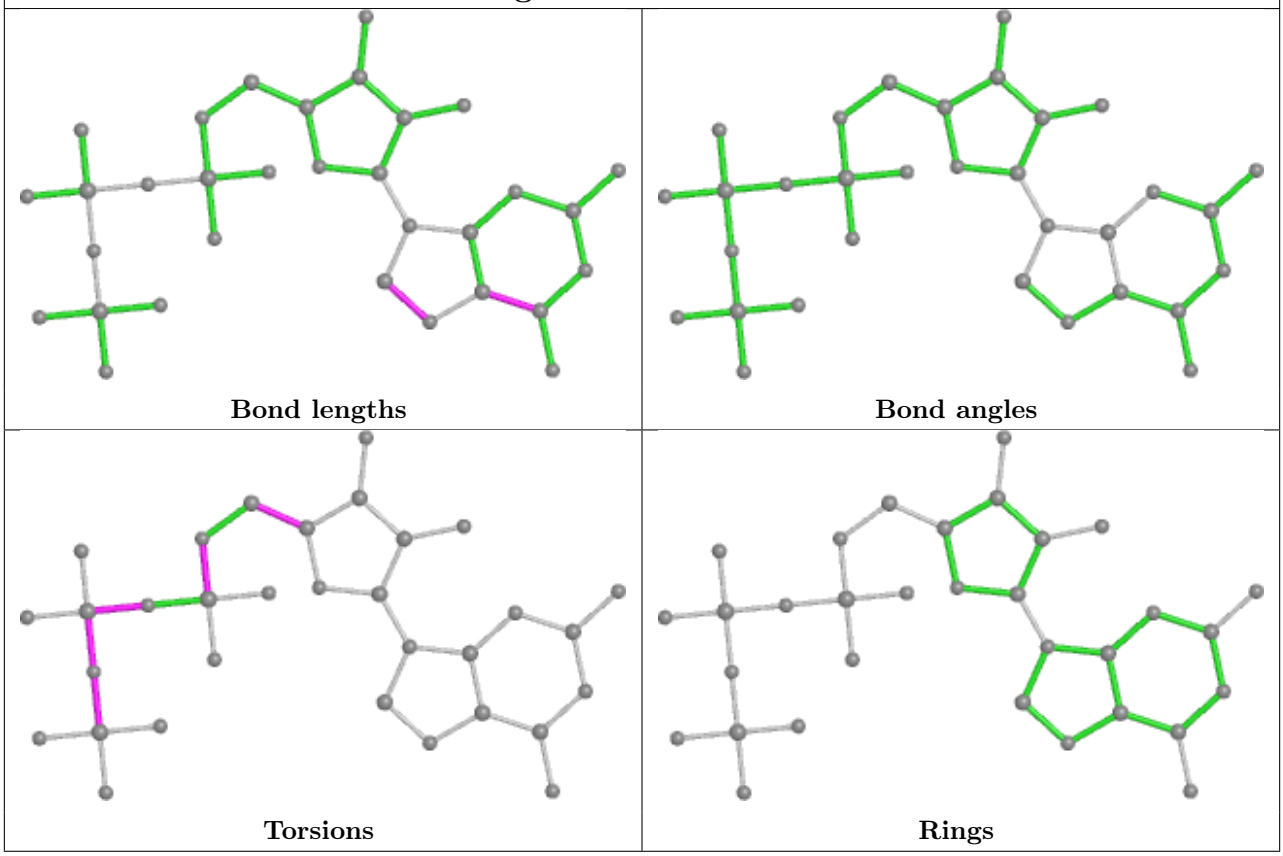
Mol	Chain	Res	Type	Atoms
32	A	3000	IHP	C3-O13-P3-O43
32	A	3000	IHP	C5-O15-P5-O35
33	C	1500	GTP	C5'-O5'-PA-O2A
33	C	1500	GTP	PG-O3B-PB-O1B
33	C	1500	GTP	PA-O3A-PB-O2B

There are no ring outliers.

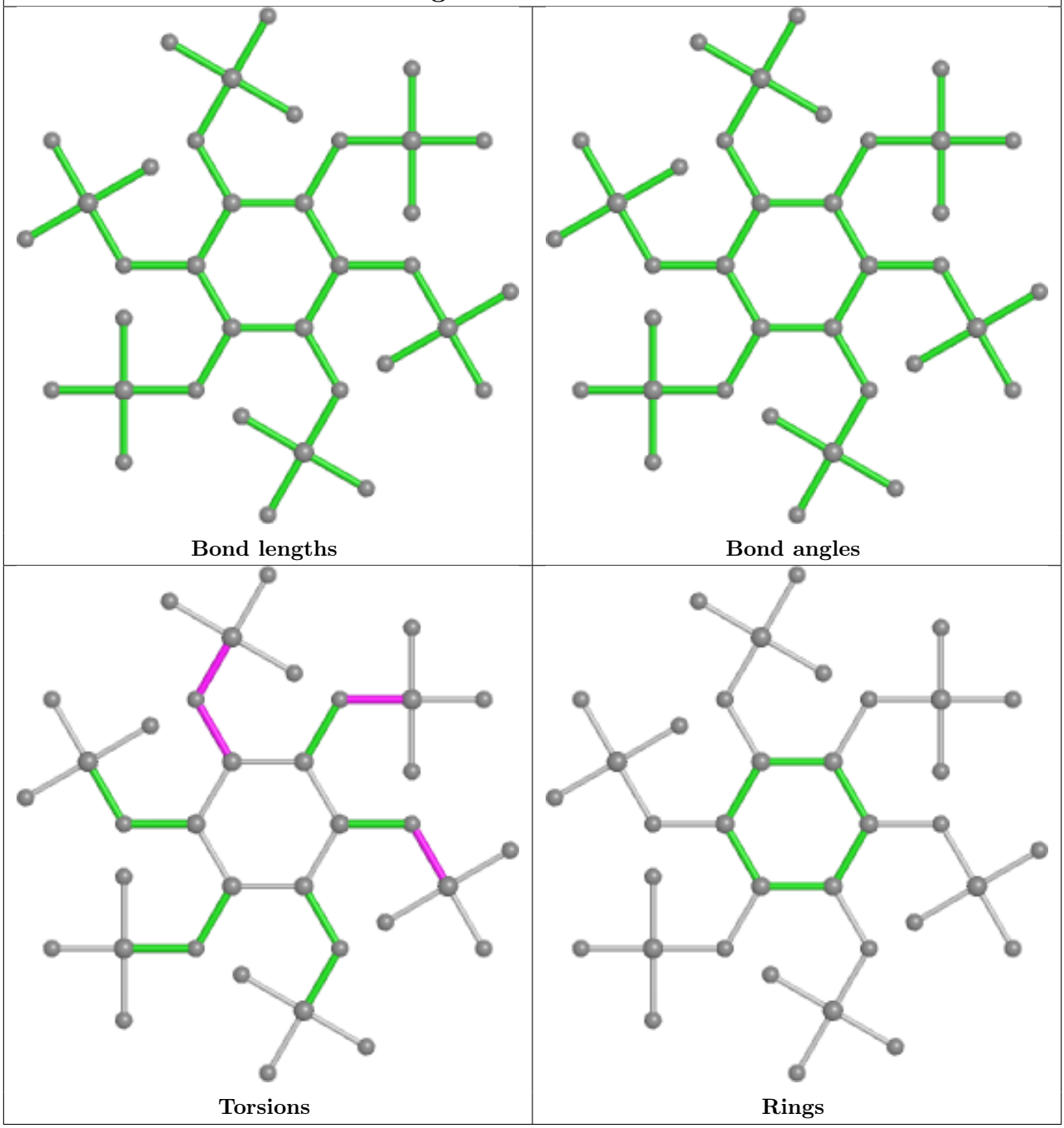
No monomer is involved in short contacts.

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 1500



Ligand IHP A 3000



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.

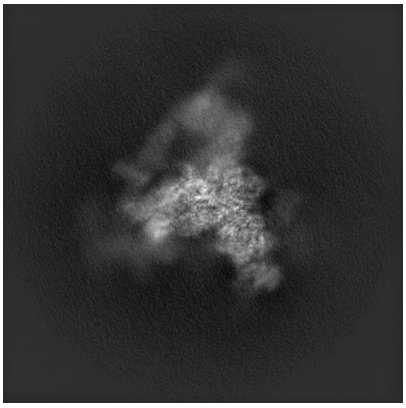
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0691. These allow visual inspection of the internal detail of the map and identification of artifacts.

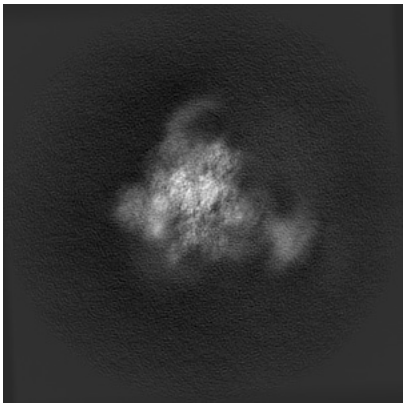
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

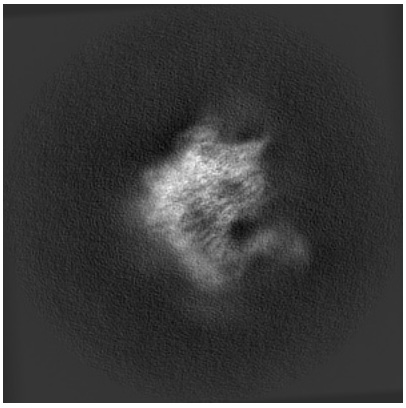
6.1.1 Primary map



X



Y

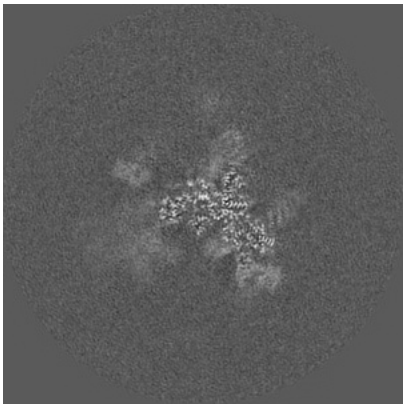


Z

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

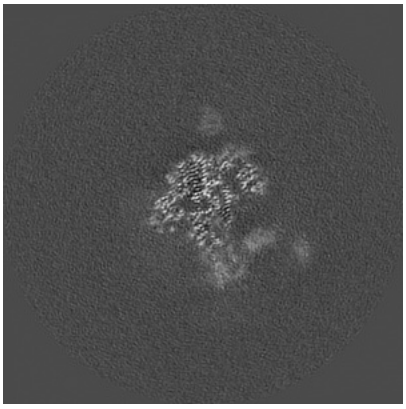
6.2 Central slices (i)

6.2.1 Primary map



X Index: 200

Y Index: 200

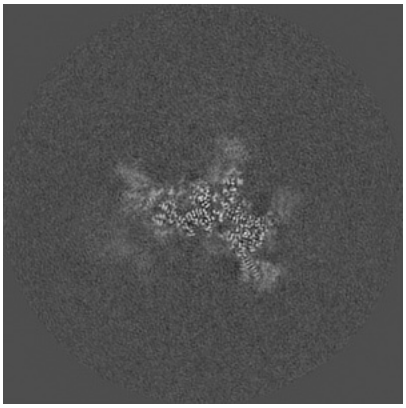


Z Index: 200

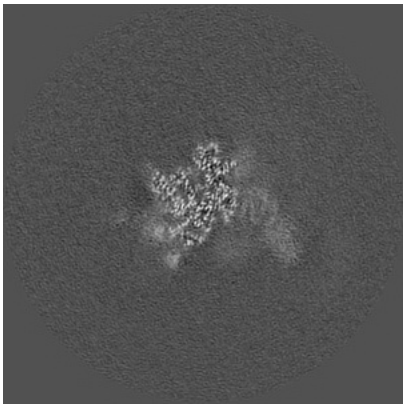
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

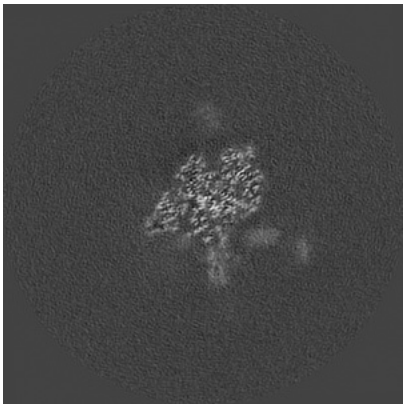
6.3.1 Primary map



X Index: 210



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

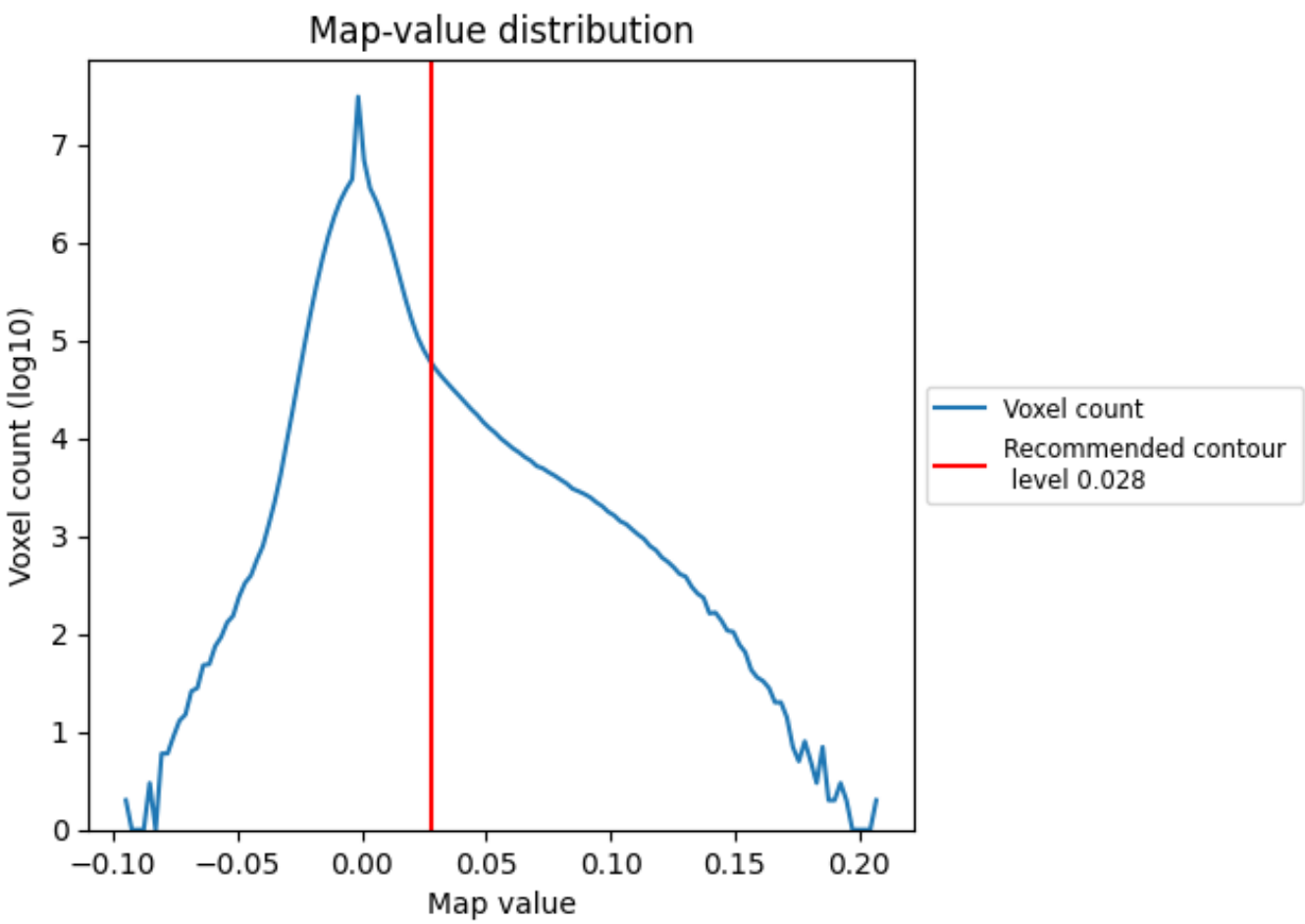
6.5 Mask visualisation (i)

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

7 Map analysis (i)

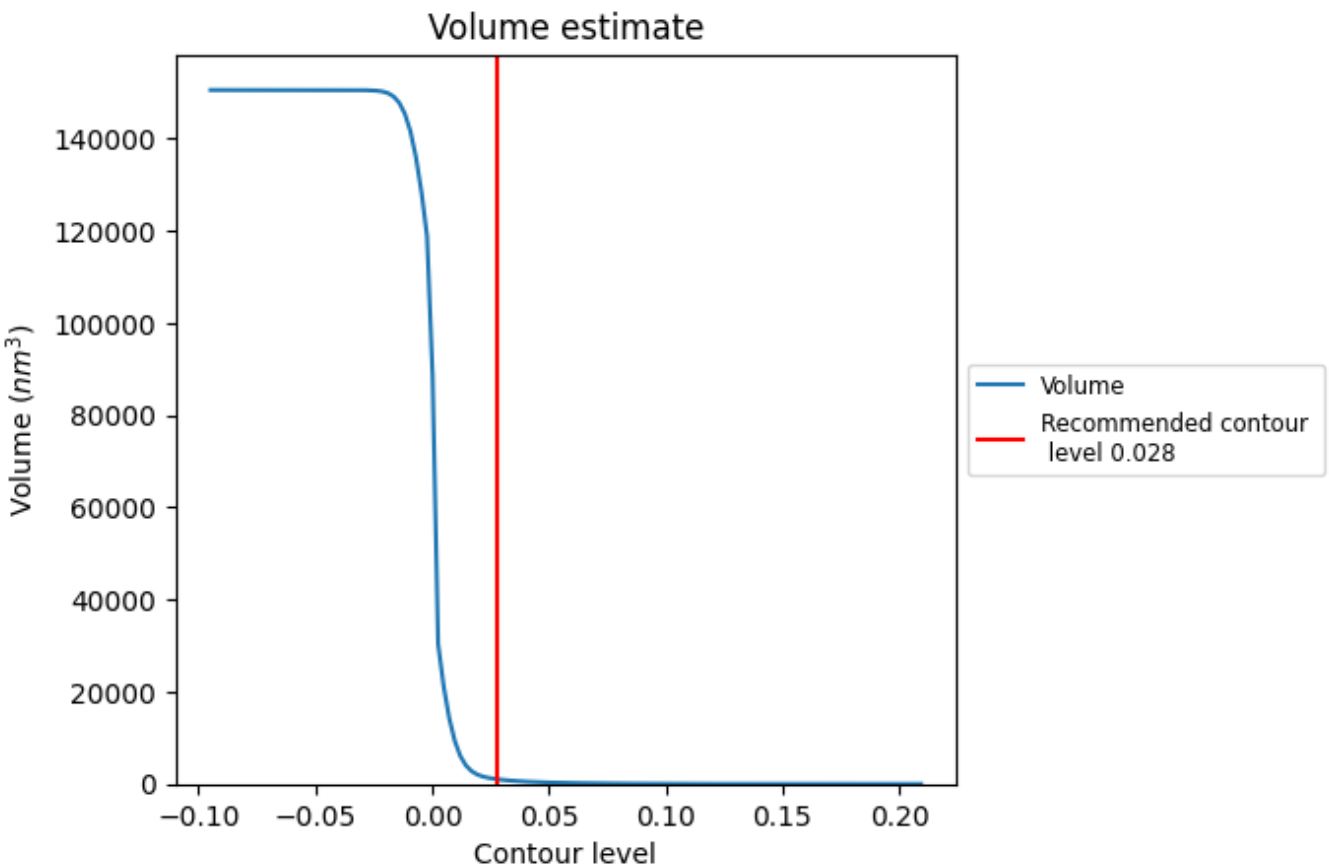
This section contains the results of statistical analysis of the map.

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.

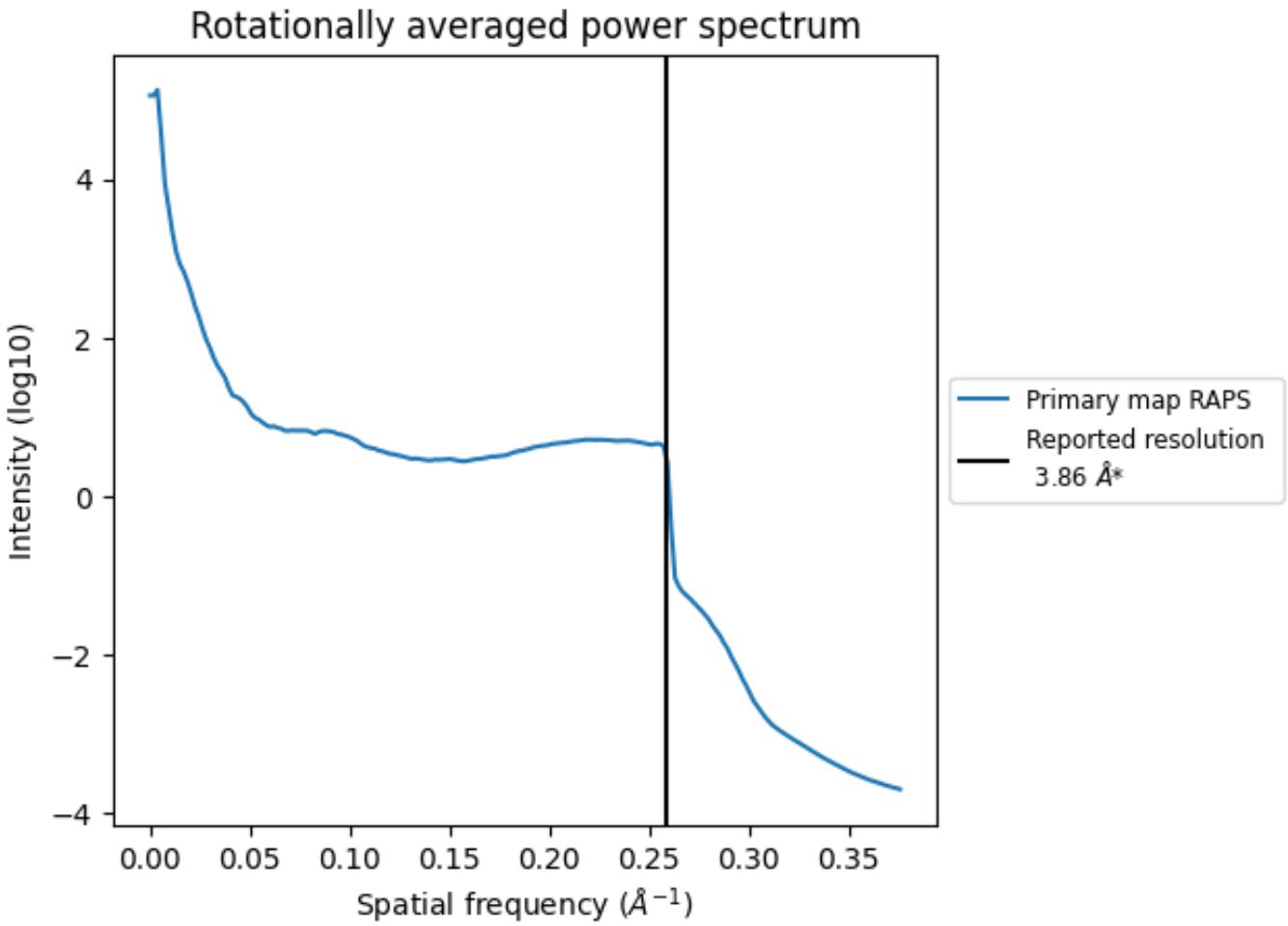
7.2 Volume estimate (i)



The volume at the recommended contour level is 1021 nm^3; this corresponds to an approximate mass of 922 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 0.259 Å^{-1}

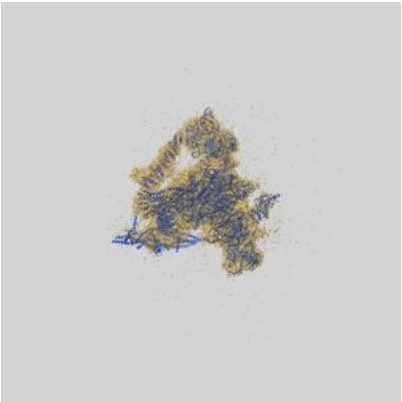
8 Fourier-Shell correlation (i)

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

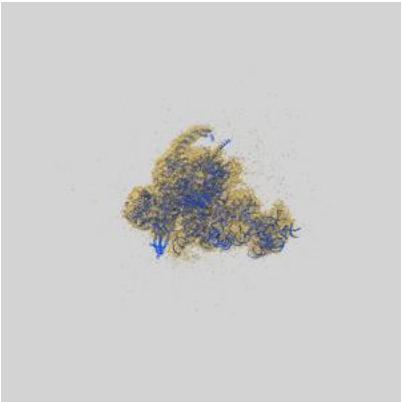
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0691 and PDB model 6J6N. Per-residue inclusion information can be found in section 3 on page 12.

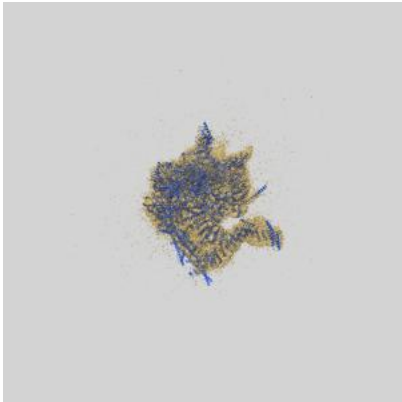
9.1 Map-model overlay (i)



X



Y



Z

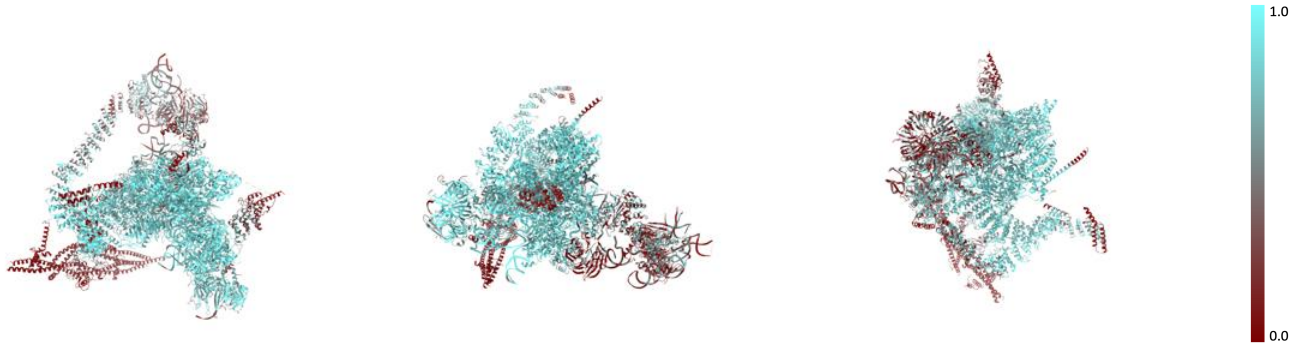
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

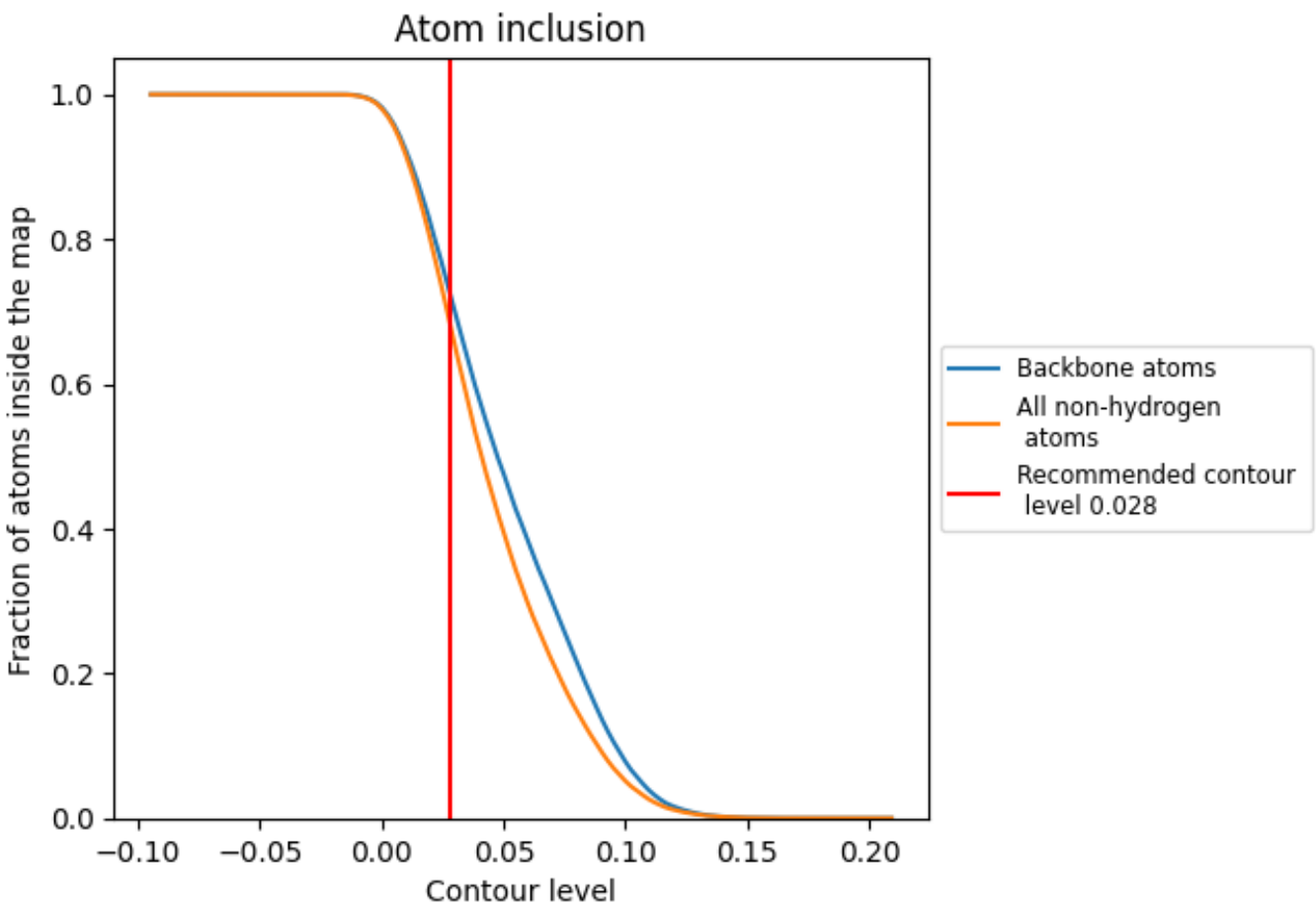
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 68% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6827	0.2480
A	0.8210	0.3620
B	0.6891	0.2110
C	0.8762	0.3900
D	0.9033	0.2580
E	0.9599	0.3630
H	0.4023	0.0970
I	0.7531	0.2890
J	0.8717	0.3970
L	0.4985	0.0780
O	0.8802	0.4260
P	0.7562	0.3360
Q	0.8185	0.3290
R	0.8721	0.3760
S	0.7628	0.3950
T	0.9030	0.4020
Z	0.5325	0.2310
a	0.5072	0.0430
b	0.5125	0.0450
c	0.4814	0.2030
d	0.7700	0.2460
e	0.3073	0.0600
g	0.7018	0.1280
h	0.8600	0.1290
i	0.8346	0.1430
j	0.7426	0.2110
k	0.7338	0.2230
l	0.8202	0.3080
m	0.6637	0.1580
n	0.1444	0.0390
o	0.1017	-0.0100
p	0.1204	0.0050
q	0.0154	-0.0080
r	0.0916	-0.0100
s	0.4596	0.0150

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Chain	Atom inclusion	Q-score
t	0.0324	0.0250
u	0.3048	0.0290
v	0.6845	0.1200
w	0.3609	0.0580
x	0.2390	0.0380
y	0.3235	0.0380
z	0.3877	0.0460