



wwPDB EM Validation Summary Report ⓘ

Mar 22, 2026 – 03:29 PM UTC

PDB ID : 6AHD / pdb_00006ahd
EMDB ID : EMD-9624
Title : The Cryo-EM Structure of Human Pre-catalytic Spliceosome (B complex) at 3.8 angstrom resolution
Authors : Zhan, X.; Yan, C.; Zhang, X.; Shi, Y.
Deposited on : 2018-08-17
Resolution : 3.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

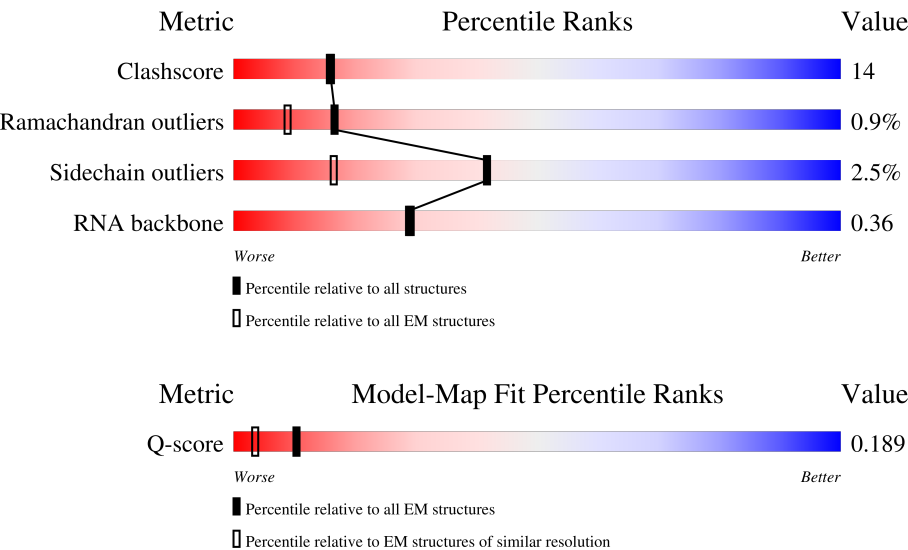
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2335	77%17%5% 47%38%38%19%6% 34%31%45%22%
2	I	144	
3	B	117	

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Mol	Chain	Length	Quality of chain
4	F	107	
5	G	274	
6	O	142	
7	C	972	
8	N	941	
9	M	128	
10	L	499	
11	9	800	
12	J	683	
13	U	231	
13	a	231	
13	i	231	
14	V	119	
14	b	119	
14	j	119	
15	P	118	
15	c	118	
15	k	118	
16	Q	86	
16	d	86	
16	l	86	
17	R	92	
17	e	92	
17	m	92	
18	S	76	

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Mol	Chain	Length	Quality of chain
18	f	76	
18	n	76	
19	T	126	
19	g	126	
19	h	126	
20	E	357	
21	X	376	
22	W	177	
23	A0	73	
24	0	439	
25	Z	312	
26	8	199	
27	Y	513	
28	H	188	
29	o	255	
30	p	225	
31	u	793	
32	v	464	
33	w	501	
34	q	95	
35	r	102	
36	s	139	
37	t	91	
38	x	80	
39	y	103	

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Mol	Chain	Length	Quality of chain
40	z	96	
41	K	522	
42	1	1304	
43	3	1217	
44	5	125	
45	6	110	
46	7	86	
47	2	895	
48	4	424	
49	D	2136	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	IHP	A	3000	-	-	X	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 85302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2209	Total	C	N	O	S	0	0
			17290	10998	3094	3128	70		

- Molecule 2 is a RNA chain called U4snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	136	Total	C	N	O	P	0	0
			2881	1288	498	959	136		

- Molecule 3 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	115	Total	C	N	O	P	0	0
			2420	1084	403	818	115		

- Molecule 4 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	94	Total	C	N	O	P	0	0
			1995	891	362	648	94		

- Molecule 5 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	77	Total	C	N	O	P	0	0
			1612	722	261	552	77		

- Molecule 6 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	141	Total	C	N	O	S	0	0
			1152	739	194	209	10		

- Molecule 7 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	818	Total	C	N	O	S	0	0
			6440	4117	1086	1205	32		

- Molecule 8 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	781	Total	C	N	O	S	0	0
			4518	2759	876	878	5		

- Molecule 9 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	124	Total	C	N	O	S	0	0
			962	608	171	178	5		

- Molecule 10 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	376	Total	C	N	O	S	0	0
			2874	1788	524	550	12		

- Molecule 11 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	9	165	Total	C	N	O	S	0	0
			1087	669	205	212	1		

- Molecule 12 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	227	Total	C	N	O	S	0	0
			1273	724	283	263	3		

- Molecule 13 is a protein called SmB.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	a	86	Total	C	N	O	0	0
			344	172	86	86		
13	i	86	Total	C	N	O	0	0
			344	172	86	86		

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Mol	Chain	Residues	Atoms				AltConf	Trace
13	U	64	Total	C	N	O	0	0
			256	128	64	64		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	b	82	Total	C	N	O	0	0
			328	164	82	82		
14	j	82	Total	C	N	O	0	0
			328	164	82	82		
14	V	82	Total	C	N	O	0	0
			334	170	82	82		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	c	97	Total	C	N	O	0	0
			388	194	97	97		
15	k	85	Total	C	N	O	0	0
			340	170	85	85		
15	P	74	Total	C	N	O	0	0
			300	152	74	74		

- Molecule 16 is a protein called SmE.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	d	74	Total	C	N	O	0	0
			296	148	74	74		
16	l	74	Total	C	N	O	0	0
			296	148	74	74		
16	Q	71	Total	C	N	O	0	0
			292	150	71	71		

- Molecule 17 is a protein called SmF.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	e	79	Total	C	N	O	0	0
			316	158	79	79		
17	m	79	Total	C	N	O	0	0
			316	158	79	79		
17	R	78	Total	C	N	O	0	0
			314	158	78	78		

- Molecule 18 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	f	74	Total	C	N	O	0	0
			296	148	74	74		
18	n	68	Total	C	N	O	0	0
			272	136	68	68		
18	S	73	Total	C	N	O	0	0
			298	152	73	73		

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	g	81	Total	C	N	O	0	0
			324	162	81	81		
19	h	80	Total	C	N	O	0	0
			320	160	80	80		
19	T	71	Total	C	N	O	0	0
			288	146	71	71		

- Molecule 20 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	E	299	Total	C	N	O	0	0
			1196	598	299	299		

- Molecule 21 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	X	75	Total	C	N	O	0	0
			378	228	75	75		

- Molecule 22 is a protein called Peptidyl-prolyl cis-trans isomerase H.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	169	Total	C	N	O	0	0
			844	506	169	169		

- Molecule 23 is a protein called Ubiquitin-like protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A0	73	Total	C	N	O	S	0	0
			581	375	93	109	4		

- Molecule 24 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	0	45	Total	C	N	O	0	0
			225	135	45	45		

- Molecule 25 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	176	Total	C	N	O	0	0
			883	531	176	176		

- Molecule 26 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	8	56	Total	C	N	O	0	0
			277	165	56	56		

- Molecule 27 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Y	453	Total	C	N	O	0	0
			2258	1352	453	453		

- Molecule 28 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	109	Total	C	N	O	P	0	0
			2311	1032	396	774	109		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	o	162	Total	C	N	O	0	0
			648	324	162	162		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
30	p	94	Total	C	N	O	0	0
			376	188	94	94		

- Molecule 31 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	u	124	Total	C	N	O	0	0
			496	248	124	124		

- Molecule 32 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	v	94	Total	C	N	O	0	0
			376	188	94	94		

- Molecule 33 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	w	423	Total	C	N	O	0	0
			1693	847	423	423		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
34	q	90	Total	C	N	O	0	0
			360	180	90	90		

- Molecule 35 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	r	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 36 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	s	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 37 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	t	72	Total	C	N	O	0	0
			288	144	72	72		

- Molecule 38 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	x	70	Total	C	N	O	0	0
			280	140	70	70		

- Molecule 39 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	y	65	Total	C	N	O	0	0
			260	130	65	65		

- Molecule 40 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	z	61	Total	C	N	O	0	0
			244	122	61	61		

- Molecule 41 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	K	414	Total	C	N	O	S	0	0
			1821	969	423	428	1		

- Molecule 42 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	1	1048	Total	C	N	O	0	0
			4192	2096	1048	1048		

- Molecule 43 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	3	1168	Total	C	N	O	0	0
			4672	2336	1168	1168		

- Molecule 44 is a protein called SF3b14a, Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	5	108	Total	C	N	O	0	0
			432	216	108	108		

- Molecule 45 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	6	89	Total	C	N	O	0	0
			356	178	89	89		

- Molecule 46 is a protein called SF3b5, Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	7	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 47 is a protein called SF3b145, Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	2	182	Total	C	N	O	0	0
			728	364	182	182		

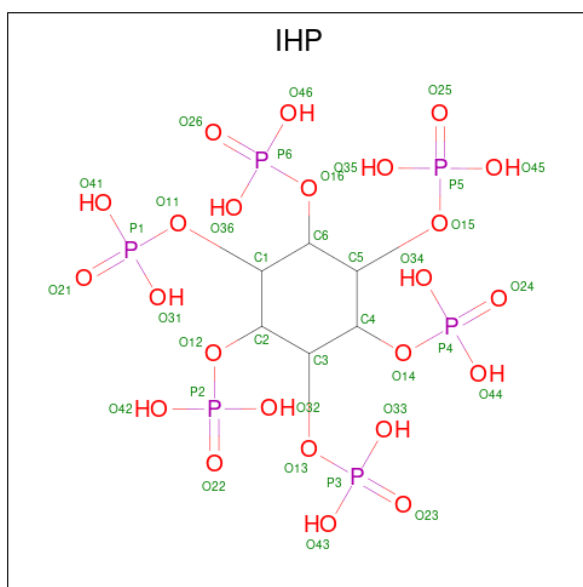
- Molecule 48 is a protein called SF3b49, Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	4	78	Total	C	N	O	0	0
			312	156	78	78		

- Molecule 49 is a protein called Brr2, U5 small nuclear ribonucleoprotein 200 kDa helicase.

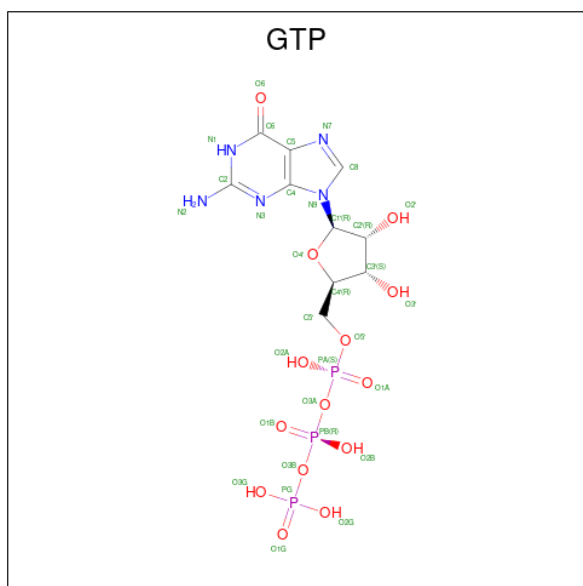
Mol	Chain	Residues	Atoms				AltConf	Trace
49	D	1699	Total	C	N	O	0	0
			6796	3398	1699	1699		

- Molecule 50 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 51 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

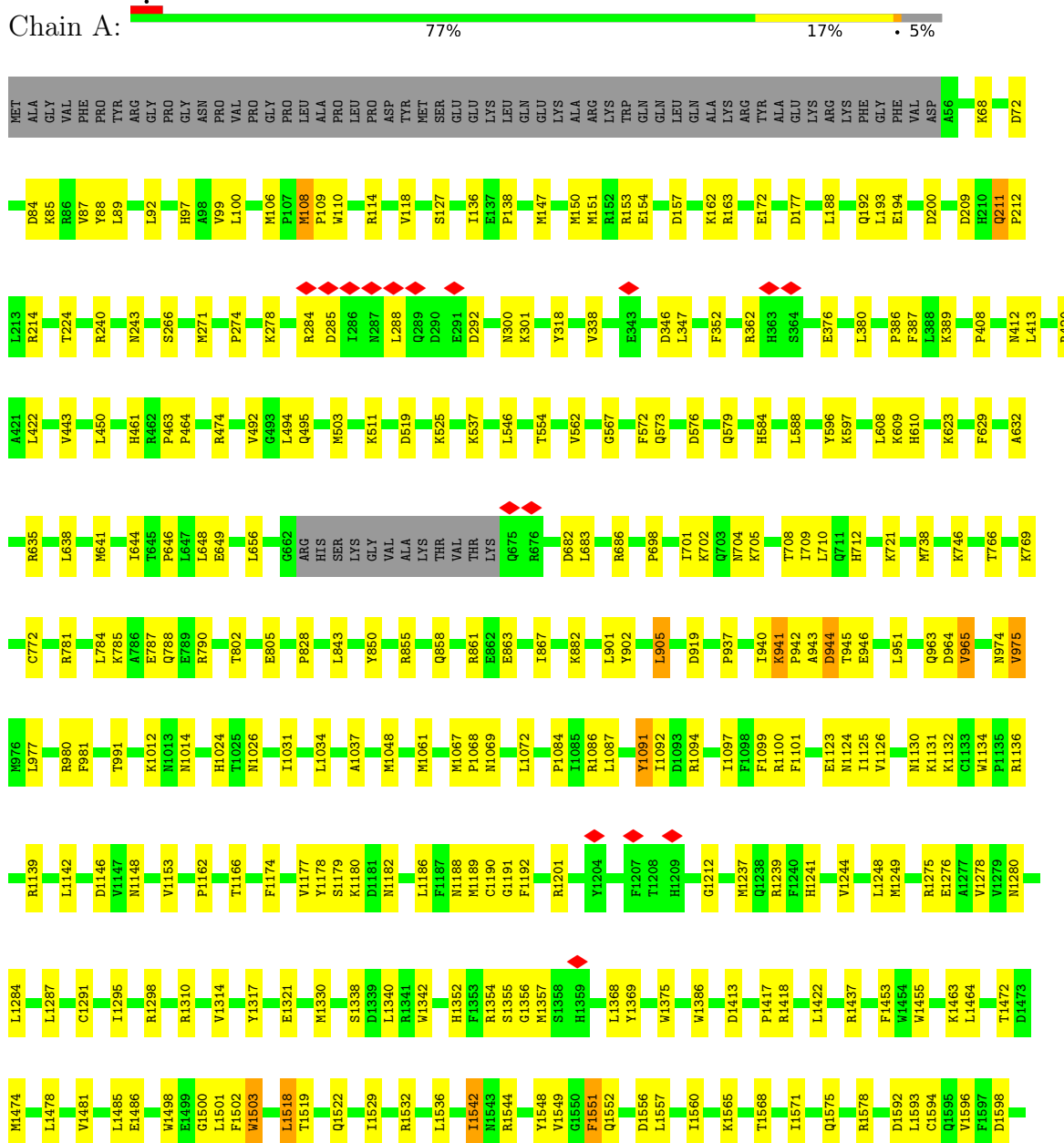
- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

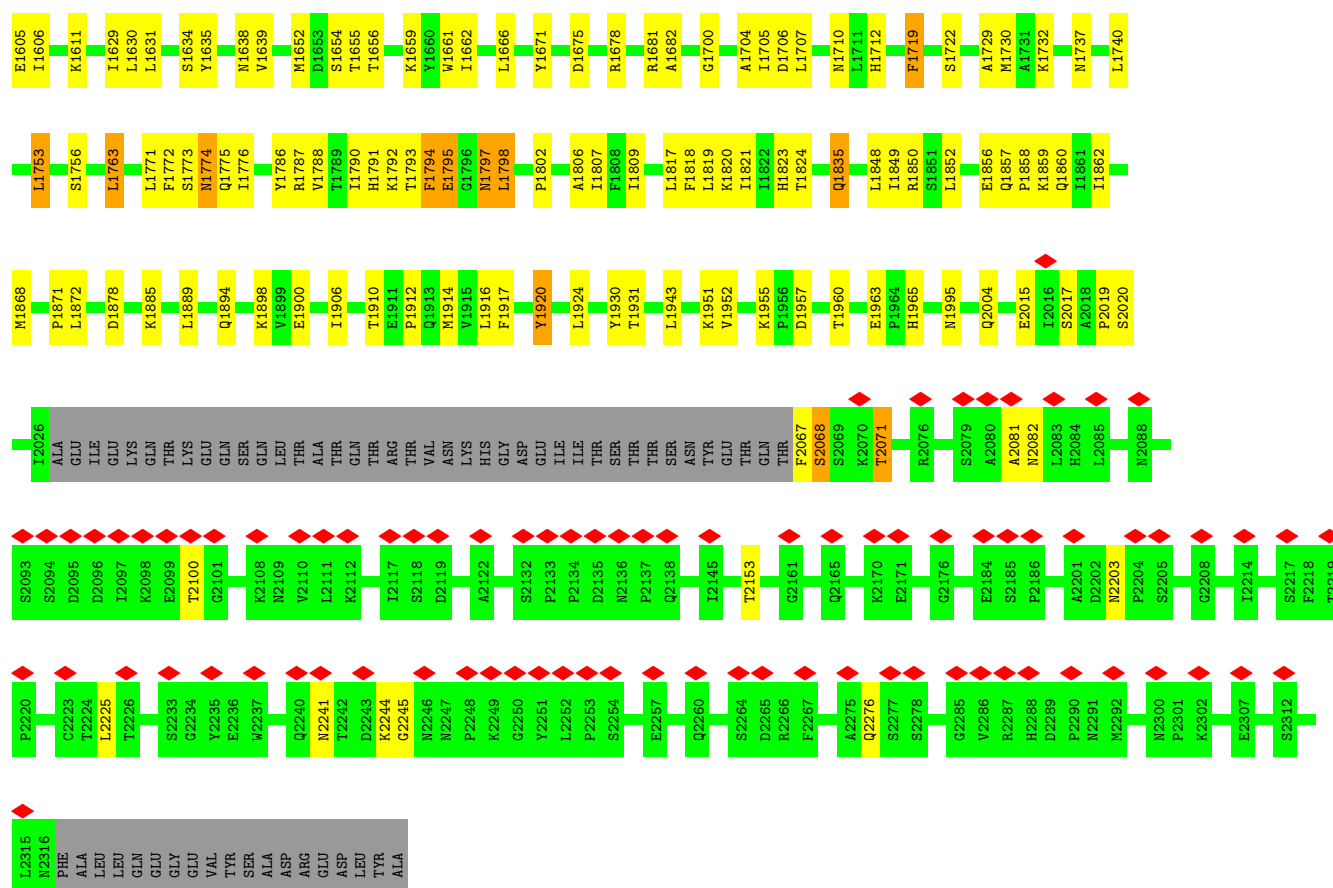
Mol	Chain	Residues	Atoms		AltConf
52	C	1	Total	Mg	0
			1	1	

3 Residue-property plots

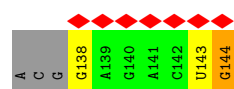
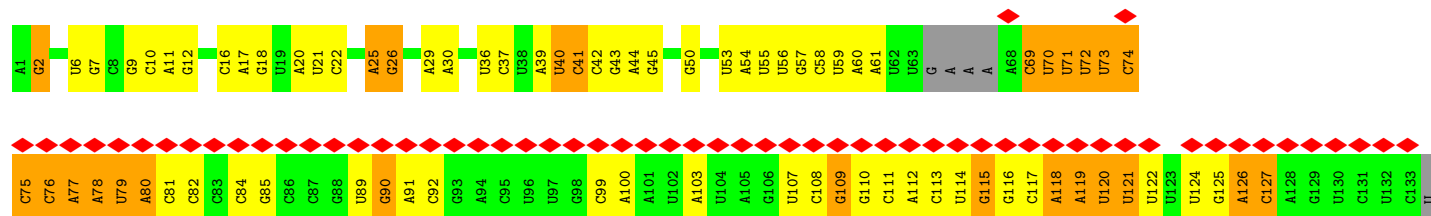
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

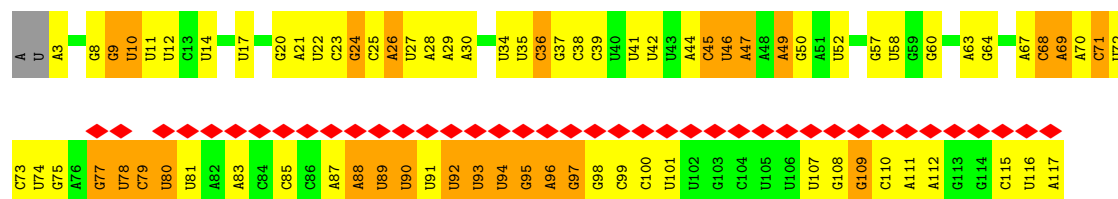


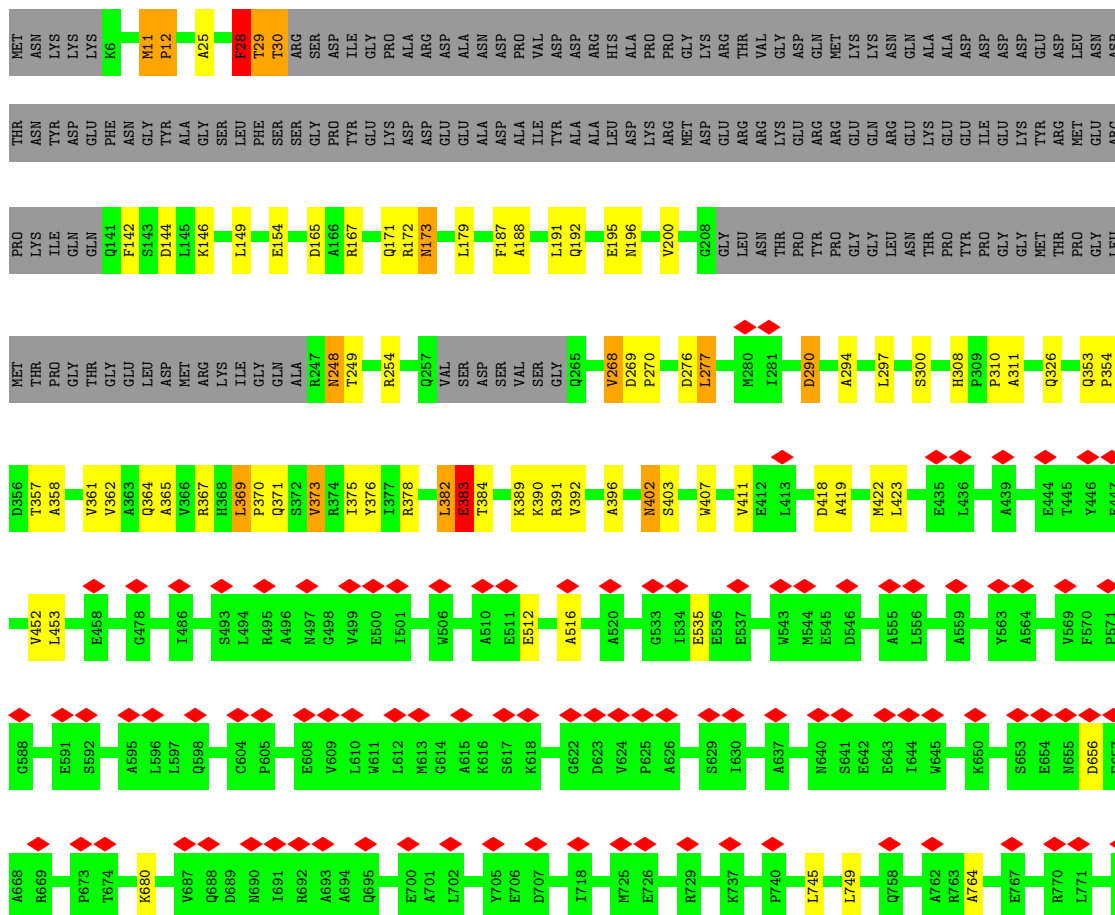


• Molecule 2: U4snRNA

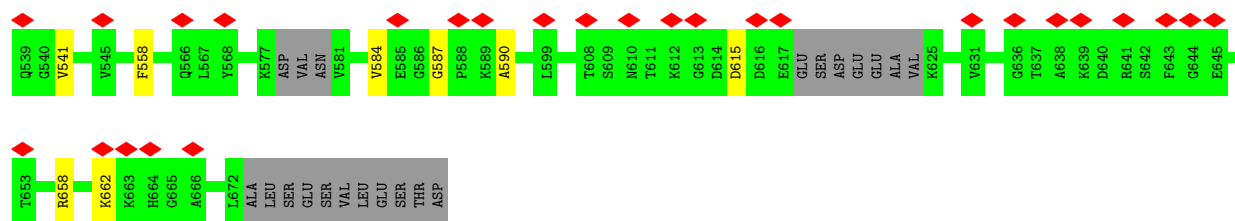


• Molecule 3: U5snRNA

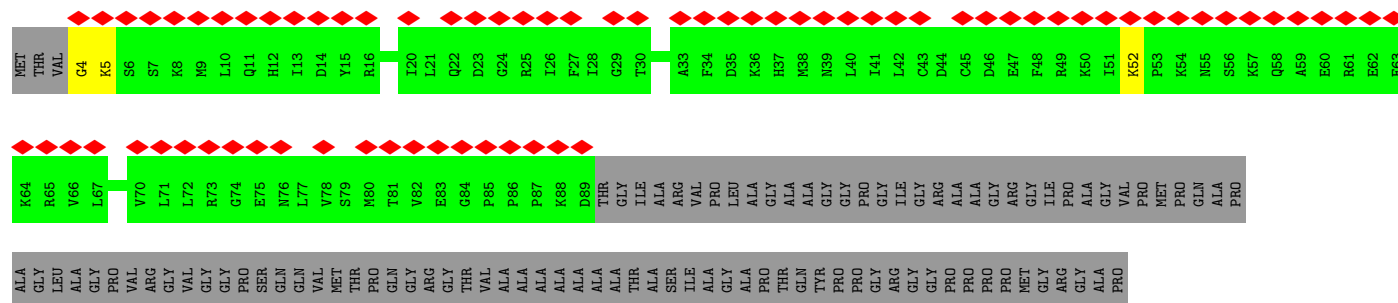




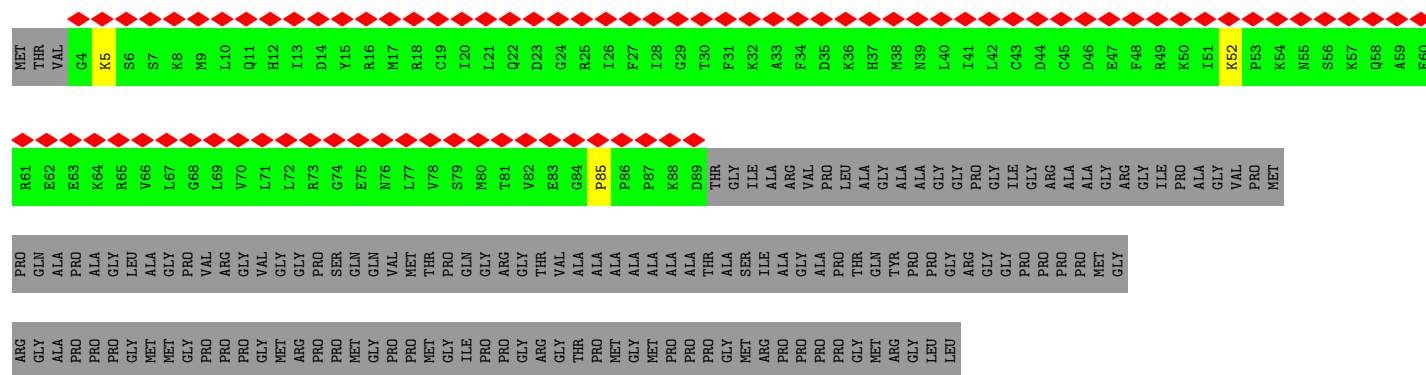




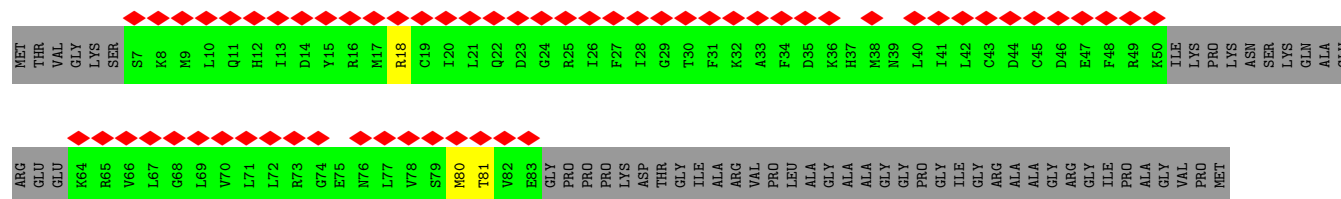
● Molecule 13: SmB



● Molecule 13: SmB

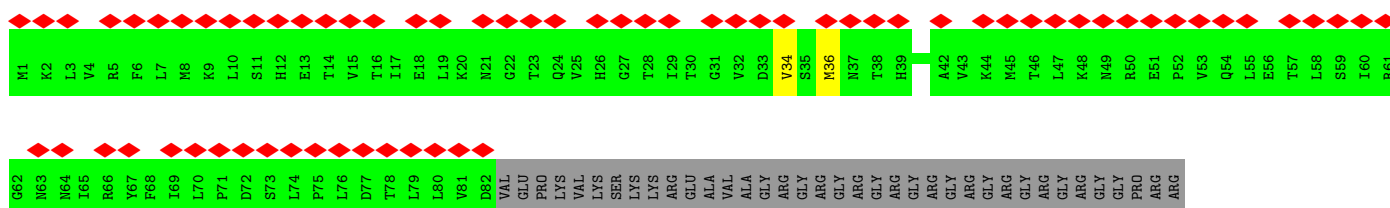


● Molecule 13: SmB

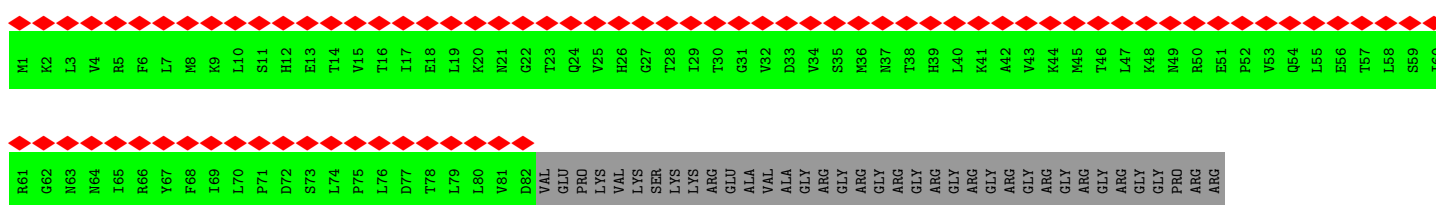


[illegible]

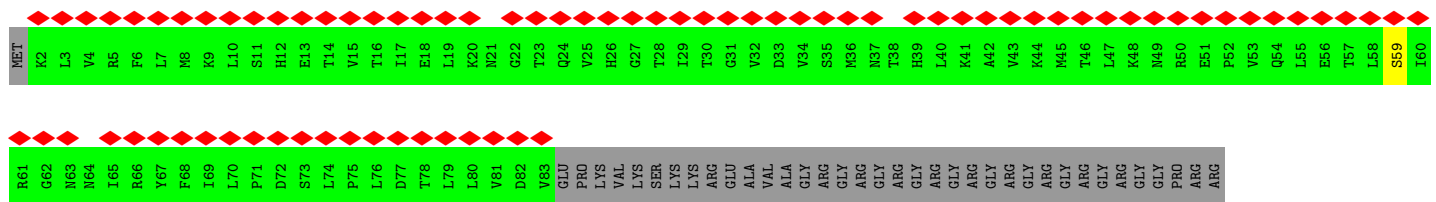
Chain b: 58% 67% 31%



Chain j: 69% 31%



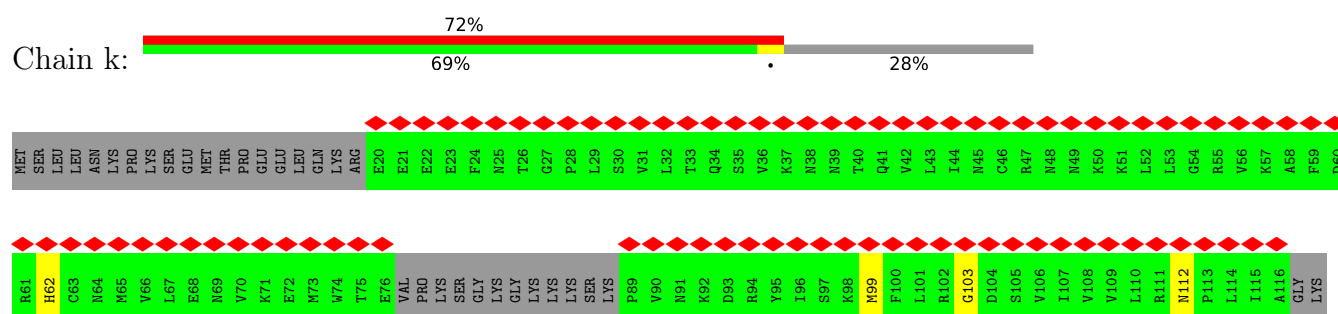
Chain V:



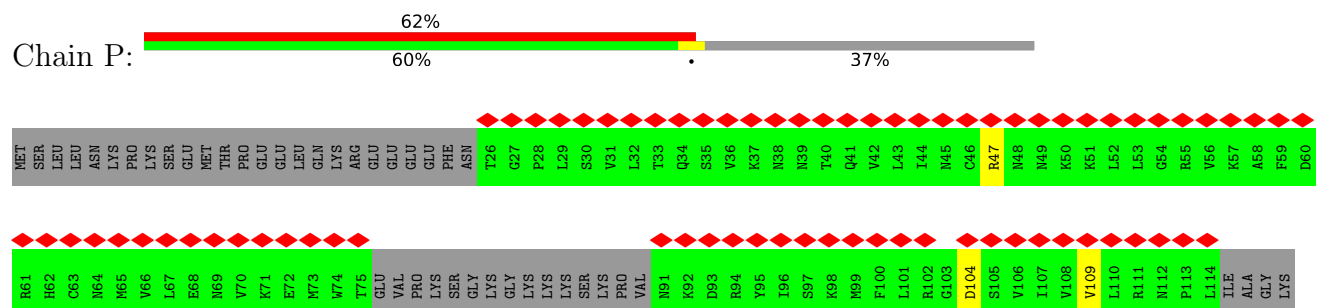
Chain c: 81% 79% 18%



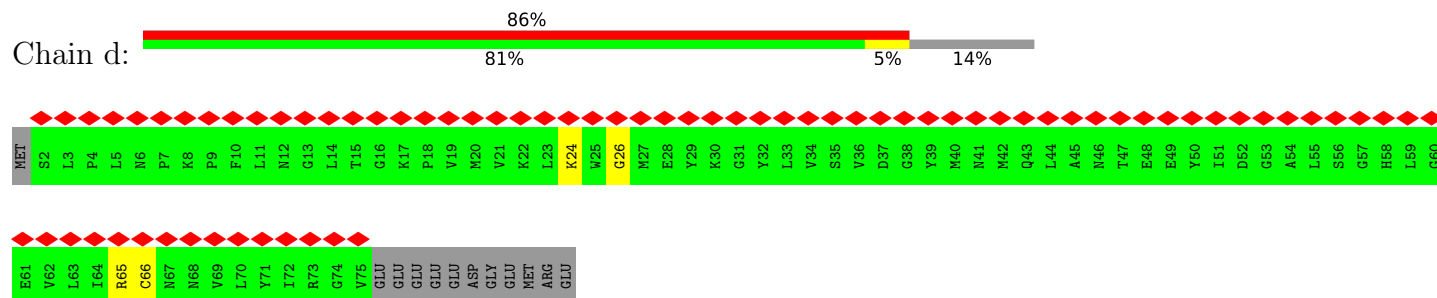
WORLD WIDE
PDB
PROTEIN DATA BANK



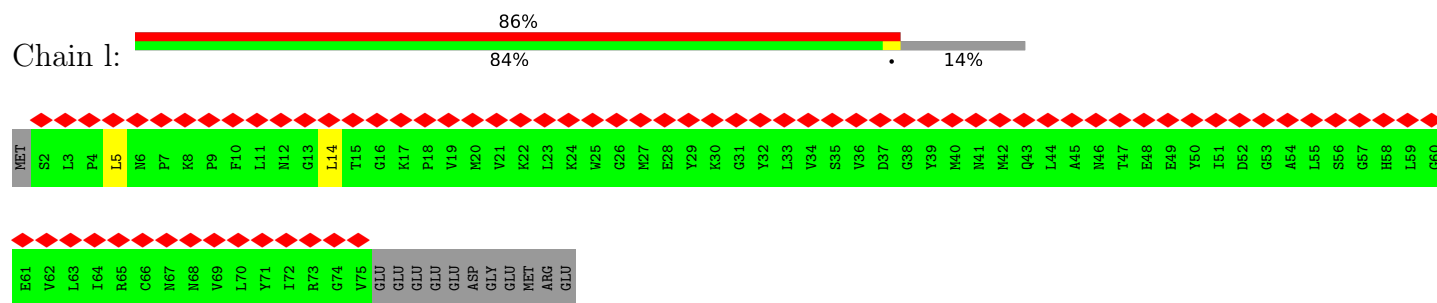
- Molecule 15: Small nuclear ribonucleoprotein Sm D2



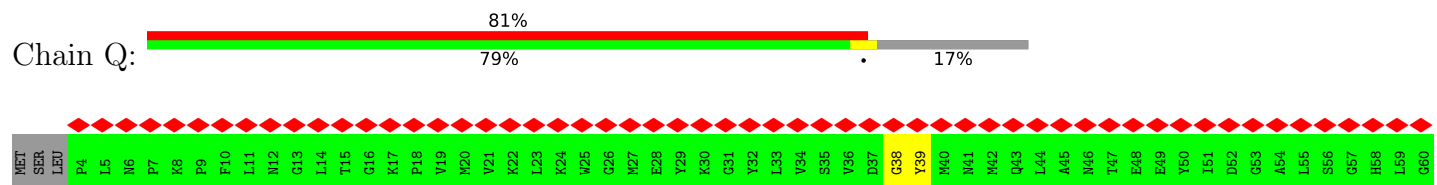
- Molecule 16: SmE



- Molecule 16: SmE

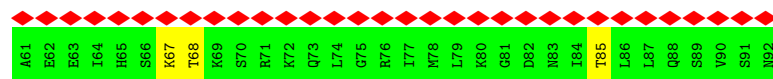
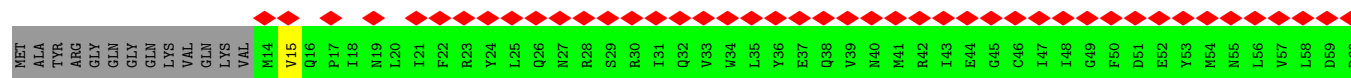
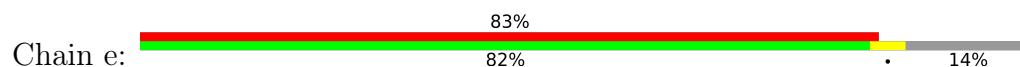


- Molecule 16: SmE

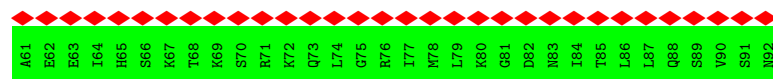
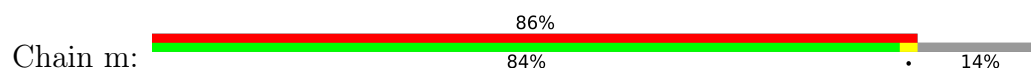




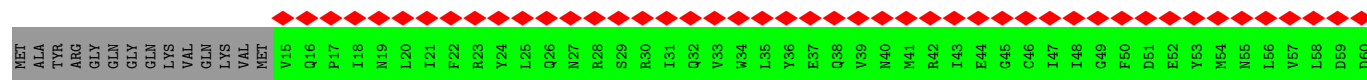
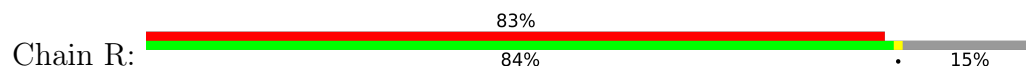
• Molecule 17: SmF



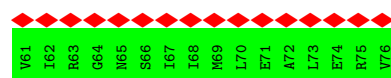
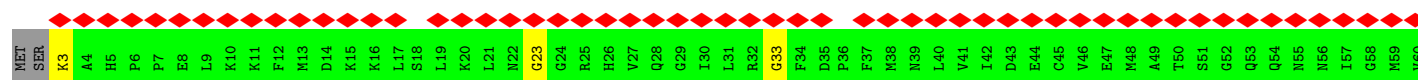
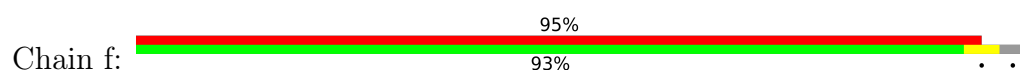
• Molecule 17: SmF



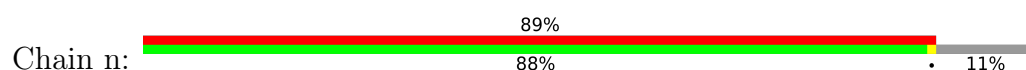
• Molecule 17: SmF

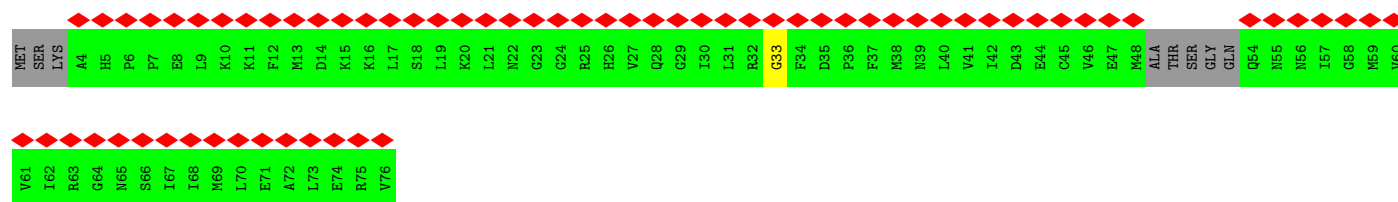


• Molecule 18: Small nuclear ribonucleoprotein G

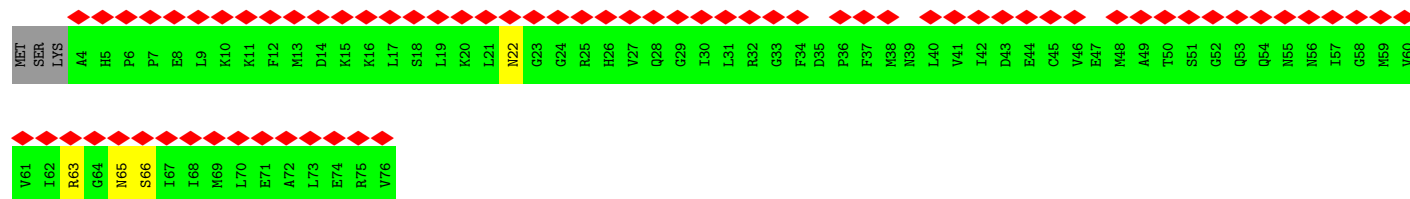
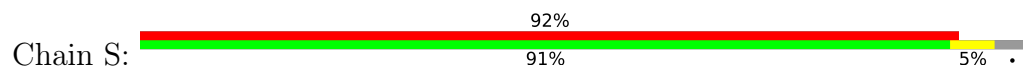


• Molecule 18: Small nuclear ribonucleoprotein G

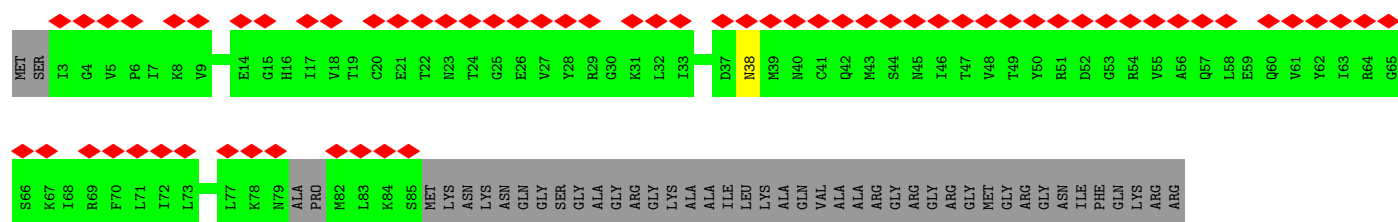




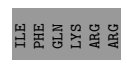
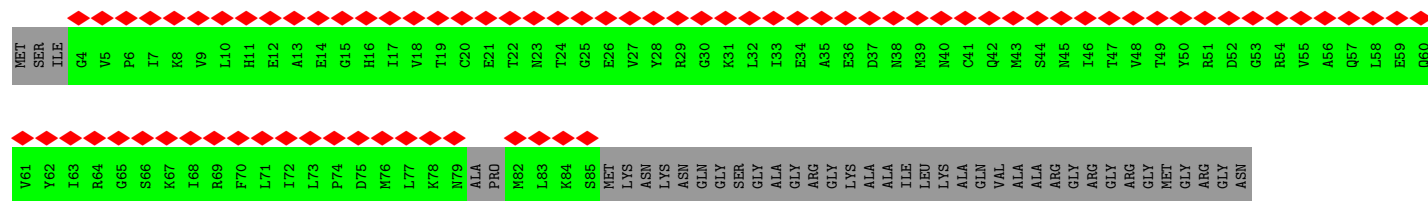
• Molecule 18: Small nuclear ribonucleoprotein G



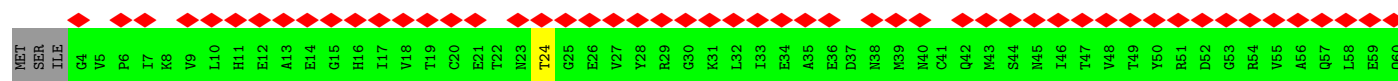
• Molecule 19: Small nuclear ribonucleoprotein Sm D3

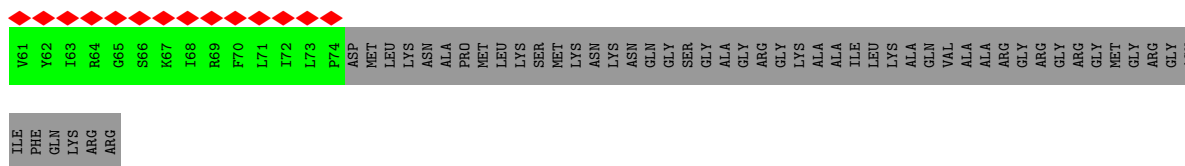


• Molecule 19: Small nuclear ribonucleoprotein Sm D3

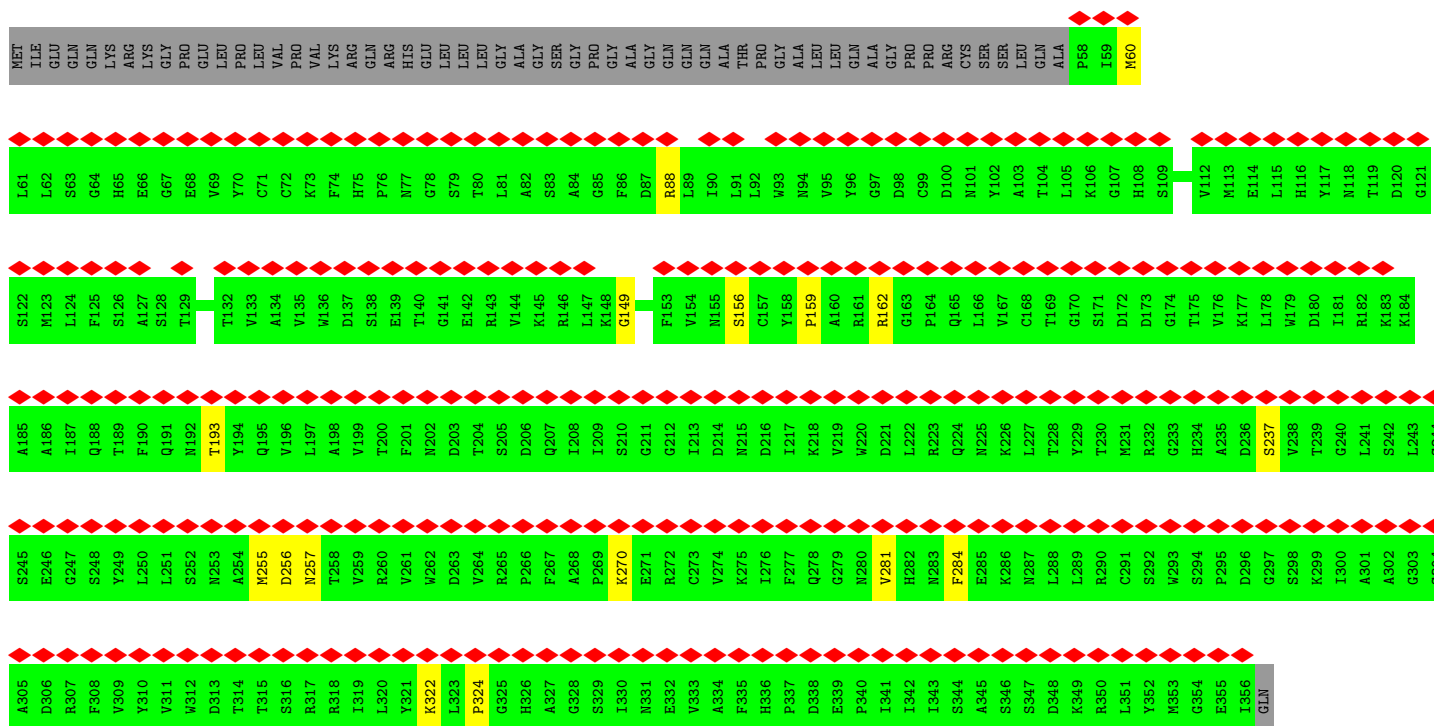
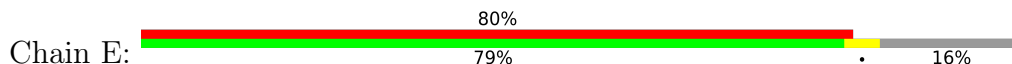


• Molecule 19: Small nuclear ribonucleoprotein Sm D3

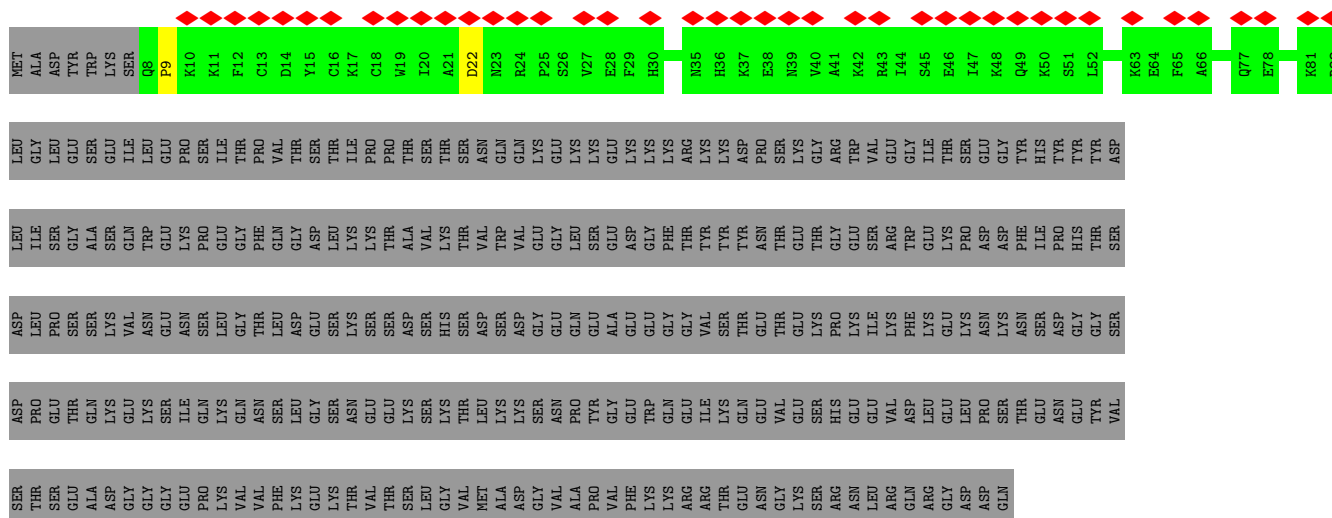




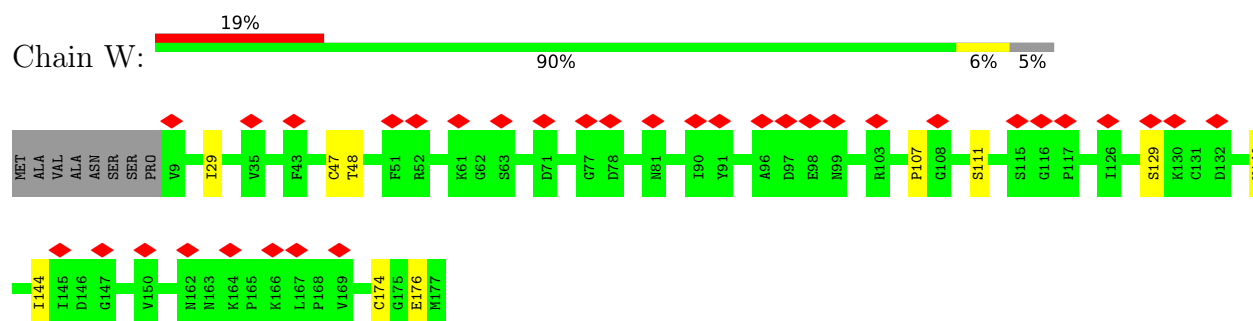
- Molecule 20: U5 small nuclear ribonucleoprotein 40 kDa protein



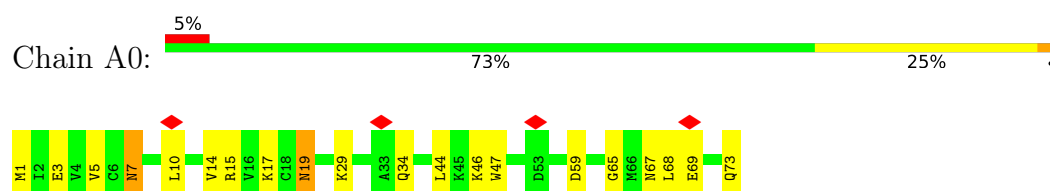
- Molecule 21: WW domain-binding protein 4



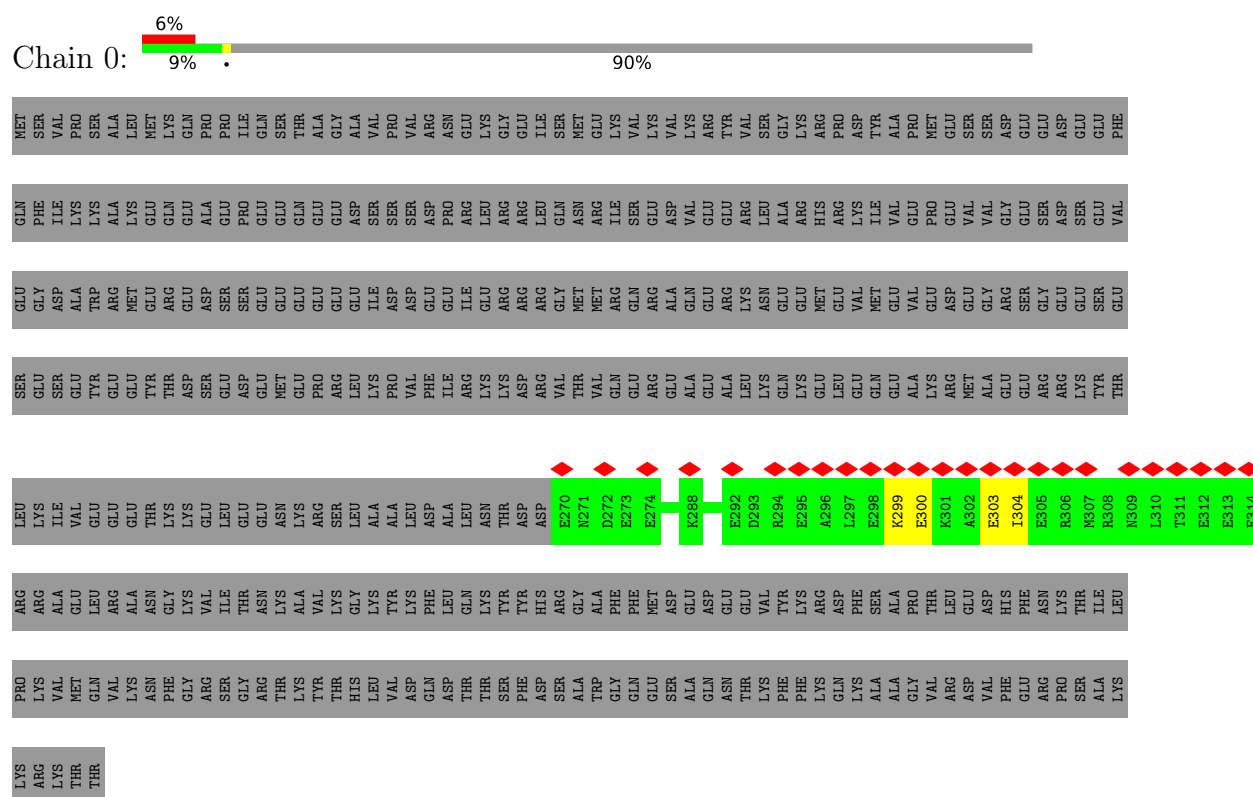
- Molecule 22: Peptidyl-prolyl cis-trans isomerase H



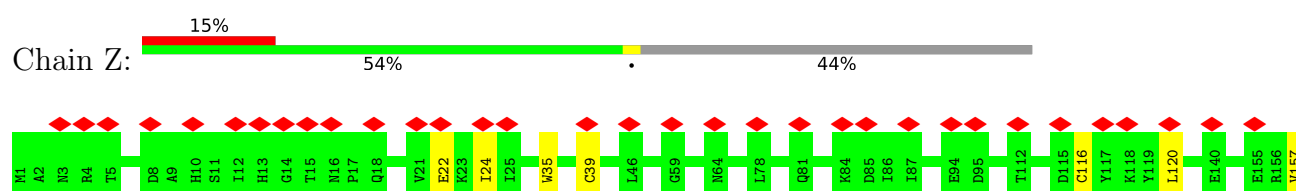
- Molecule 23: Ubiquitin-like protein 5



- Molecule 24: Microfibrillar-associated protein 1

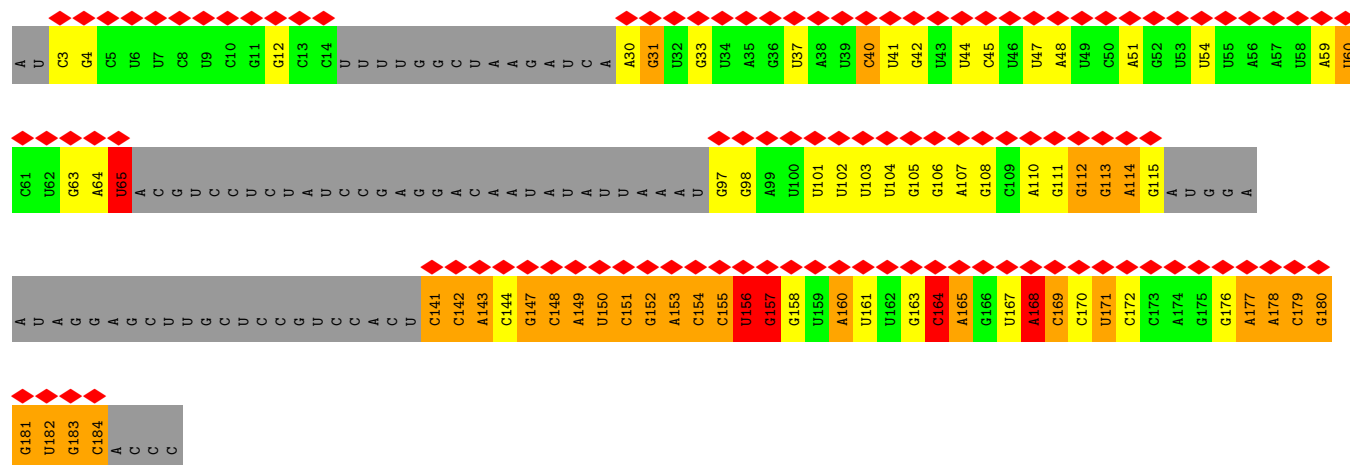


- Molecule 25: Pre-mRNA-splicing factor 38A

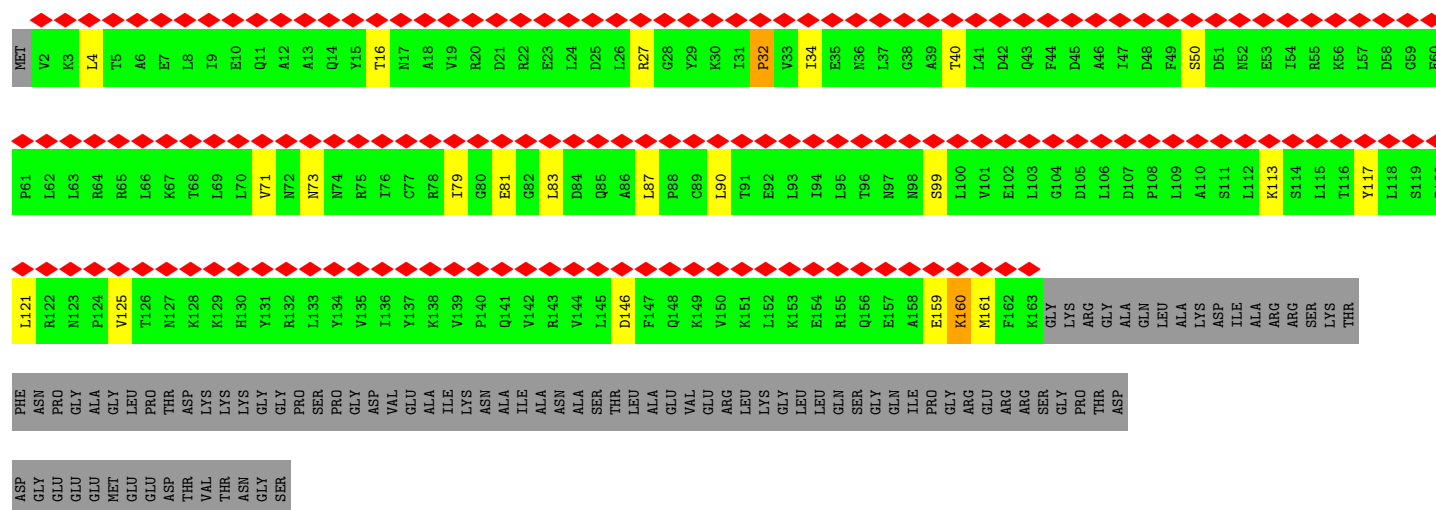




• Molecule 28: U2snRNA



• Molecule 29: U2 small nuclear ribonucleoprotein A'



• Molecule 30: U2 small nuclear ribonucleoprotein B''



ILE	LEU	GLY	VAL	LEU	VAL	PHI	THR	LEU	PRO	LEU	THR	ASP	GLN	VAL	SER	VAL	ILE	VAL	VAL	LYS	LYS	LYS	ILE	HIS	GLU	THR	GLY	MET	PRO	ALA	LYS	LYS	GLN	LYS	LEU	LYS	ASP	SER	ASN	ALA	ALA	LEU	TYR	TYR	ASN	MET	ASN	GLY	VAL	ALA	VAL	LYS
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- Molecule 32: Splicing factor 3A subunit 2



THR	LEU	HIS	LEU	ASP	MET	THR	LEU	HIS	LEU	ASP	MET
HIS	LEU	HIS	LEU	ASP	MET	HIS	LEU	HIS	LEU	ASP	MET
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLU	GLY	GLY	GLY	GLY	GLY	GLU	GLY	GLY	GLY	GLY	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
K118	K118	K118	K118	K118	K118	K118	K118	K118	K118	K118	K118
V119	V119	V119	V119	V119	V119	V119	V119	V119	V119	V119	V119

K121	Q122	R123	D124	S125	E126	M127	GLY	GLN	GLN	SER	LEU	LEU	PHE	GLN	GLN	ASP	Y138	P139	E140	I141	A142	E143	G144	I145	M146	P147	R148	H149	R150	F151	M152	M153	A154	Y155	E156	Q157	R158	I159	E160	P161	P162	D163	R164	R165	W166	Q167	Y168	L169	L170	M171	A172	A173	E174	Y175	E177	T178	I179	M180
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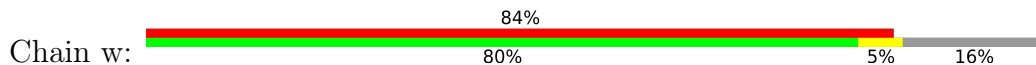
F181	K182	V183	P184	S185	R186	E187	I188	D189	K190	A191	E192	G193	K194	PHE	TRP	T197	H198	W199	N200	R201	E202	T203	K204	Q205	F206	T207	L208	Q209	F210	H211	F212	K213	M214	E215	K216	T217	F218	A219	P220	P221	S222	L223	PRO	ALA	GLY	PRO	PRO	GLY	GLY	VAL	LYS	ARG	PRO	PRO	PRO	PRO	LEU	MET	ASN
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LEU	PRO	PRO	ARG	PRO	PRO	LEU	LEU	GLU	SER	LEU	PRO	PRO	PRO	PRO	PRO	GLY	GLY	LEU	PRO	PRO	THR	PRO	PRO	ALA	SER	SER	GLY	PRO	PRO	GLY	PRO	PRO	PRO	GLN	LEU	PRO	PRO	PRO	ALA	GLY	GLY	VAL	HIS	PRO	PRO	ALA	ALA	VAL	VAL	HIS	PRO	PRO	ALA	ALA	SER	GLY
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[illegible][illegible]

VAL	HIS	PRO	GLN	PRO	PRO	GLY	VAL	HIS	PRO	SER	ASN	PRO	GLY	VAL	HIS	PRO	PRO	THR	PRO	MET	PRO	PRO	MET	LEU	ARG	PRO	PRO	LEU	PRO	SER	GLU	GLY	GLY	ASN	ILE	PRO	PRO	PRO	PRO	THR	ASN
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- Molecule 33: Splicing factor 3A subunit 3

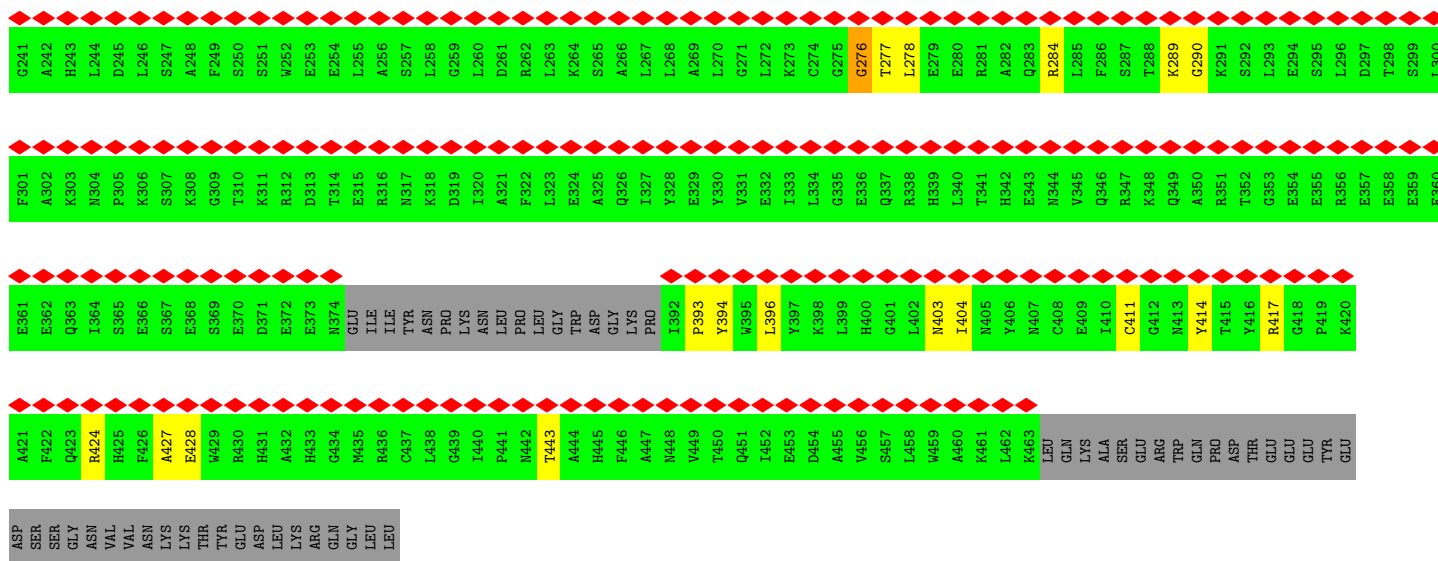


M1	E2	T3	I4	L5	E6	Q7	Q8	R9	R10	Y11	H12	E13	E14	K15	E16	R17	L18	M19	D20	V21	M22	A23	K24	E25	M26	L27	T28	K29	K30	S31	T32	L33	R34	D35	Q36	L37	N38	S39	D40	H41	R42	T43	R44	A45	M46	Q47	D48	R49	Y50	M51	E52	V53	S54	E55	N56	L57	R58	D59	E60
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Y61	D62	D63	K64	D65	G66	L67	R68	K69	E70	E71	L72	W73	A74	L75	S76	G77	F78	H79	N80	F81	A82	S83	F84	Y85	N86	R87	L88	K89	Q90	I91	K92	E93	F94	H95	R96	K97	H98	PRO	ASN	GLU	ILE	CYS	VAL	PRO	MET	SER	VAL	GLU	F110	E111	E112	L113	L114	K115	A116	R117	E118	N119	P120
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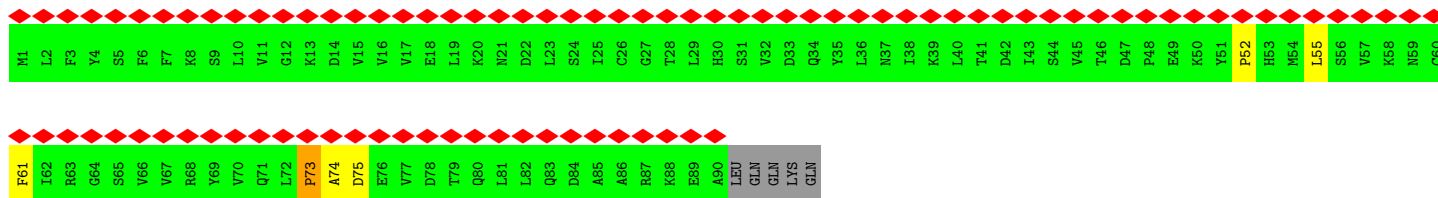
S121	E122	E123	A124	Q125	N126	L127	V128	E129	F130	T131	D132	E133	E134	G135	V136	G137	R138	V139	L140	D141	L142	H143	ASP	CYS	TYR	LEU	LYS	V149	I150	N151	L152	K153	A154	S155	E156	L158	D159	V160	I161	T162	V163	L164	S165	I166	F167	Q169	L170	F171	D172	I173	P174	K175	E176	R177	K178	N179	A180
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E181	Y182	R183	R184	Y185	L186	E187	M188	L189	L190	E191	Y192	Q193	Q194	D195	Y196	T197	D198	L199	V200	K201	P202	L203	Q204	D205	Q206	E207	N208	L209	F210	GLY	LYS	ILE	GLN	ALA	GLU	PHE	E218	K219	K220	W221	E222	N223	Q224	T225	F226	P227	Q228	W229	P230	K231	F232	T233	Q234	S235	A236	L237	T238	H239	A240
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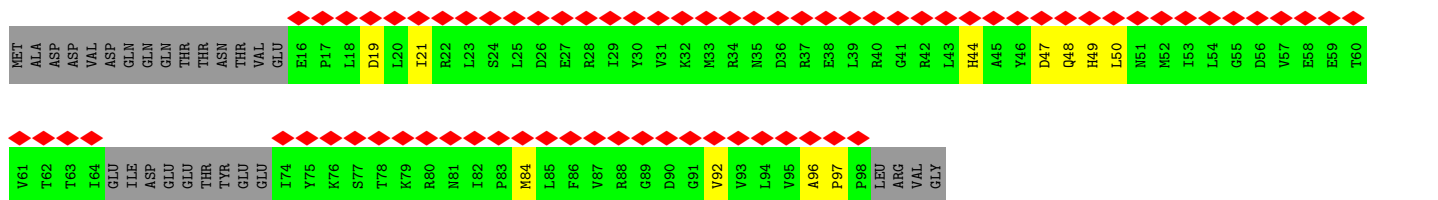
• Molecule 34: U6 snRNA-associated Sm-like protein LSm2

Chain q: 95% 88% 5% • 5%



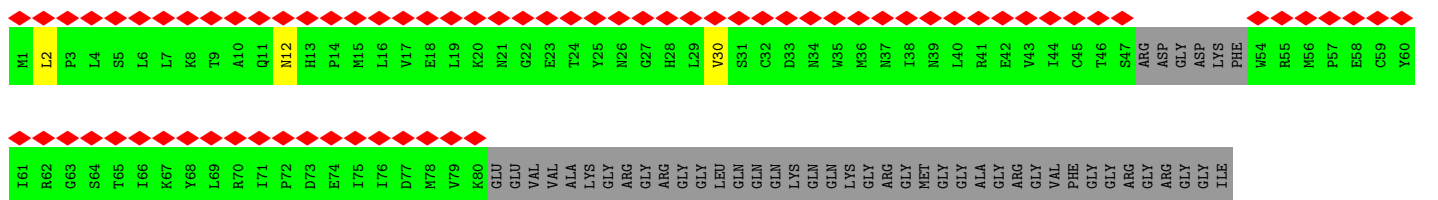
• Molecule 35: U6 snRNA-associated Sm-like protein LSm3

Chain r: 73% 62% 11% 27%



• Molecule 36: U6 snRNA-associated Sm-like protein LSm4

Chain s: 53% 51% 47%



PRO GLY THR GLY ARG GLN PRO GLU LYS LYS PRO GLY ARG GLN ALA ALA LYS LYS

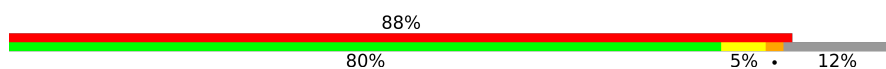
- Molecule 37: U6 snRNA-associated Sm-like protein LSm5

Chain t: 

MET ALA ALA ASN THR THR ASN PRO S10 Q11 L12 L13 P14 L15 E16 L17 V18 D19 K20 C21 T22 G23 S24 R25 T26 H27 T28 V29 K30 K31 K32 D33 K34 E35 I36 V37 Q38 T39 L40 L41 Q42 F43 D44 D45 F46 V47 M48 M49 V50 L51 E52 D53 V54 T55 E56 F57 E58 I59 THR

PRO GLU R64 R65 I66 T67 K68 L69 D70 Q71 I72 L73 L74 N75 G76 N77 N78 I79 T80 M81 L82 V83 P84 G85 GLY GLY P80 GLU VAL

- Molecule 38: U6 snRNA-associated Sm-like protein LSm6

Chain x: 

MET SER LEU ARG GLN T7 P8 S9 D10 F11 L12 K13 Q14 I15 I16 G17 R18 P19 V20 V21 V22 K23 L24 N25 S26 G27 V28 D29 D30 R31 G32 V33 L34 A35 C36 L37 D38 G39 Y40 M41 N42 I43 A44 L45 E46 Q47 T48 E49 E50 Y51 V52 N53 G54 Q55 L56 K57 N58 K59 Y60

G61 D62 A63 F64 I65 R66 G67 N68 N69 V70 L71 Y72 I73 S74 T75 Q76 LYS ARG ARG MET

- Molecule 39: U6 snRNA-associated Sm-like protein LSm7

Chain y: 

MET ALA ASP GLU LYS LYS LYS LYS S11 I12 L13 D14 L15 S16 K17 Y18 I19 D20 K21 T22 T23 R24 V25 K26 F27 Q28 G29 G30 R31 E32 A33 S34 G35 I36 L37 G38 K38 G39 F40 D41 P42 L43 L44 N45 N46 V47 L48 D49 G50 T51 I52 E53 Y54 W55 ARG ASP PRO ASP

GLN THR LEU THR ASP T68 R69 Q70 L71 G72 L73 V74 V75 C76 R77 G78 T79 S80 V81 V82 L83 I84 C85 P86 Q87 ASP GLY MET GLU ALA ILE PRO ASN PHE ILE GLN GLN ASP ALA

- Molecule 40: U6 snRNA-associated Sm-like protein LSm8

Chain z: 

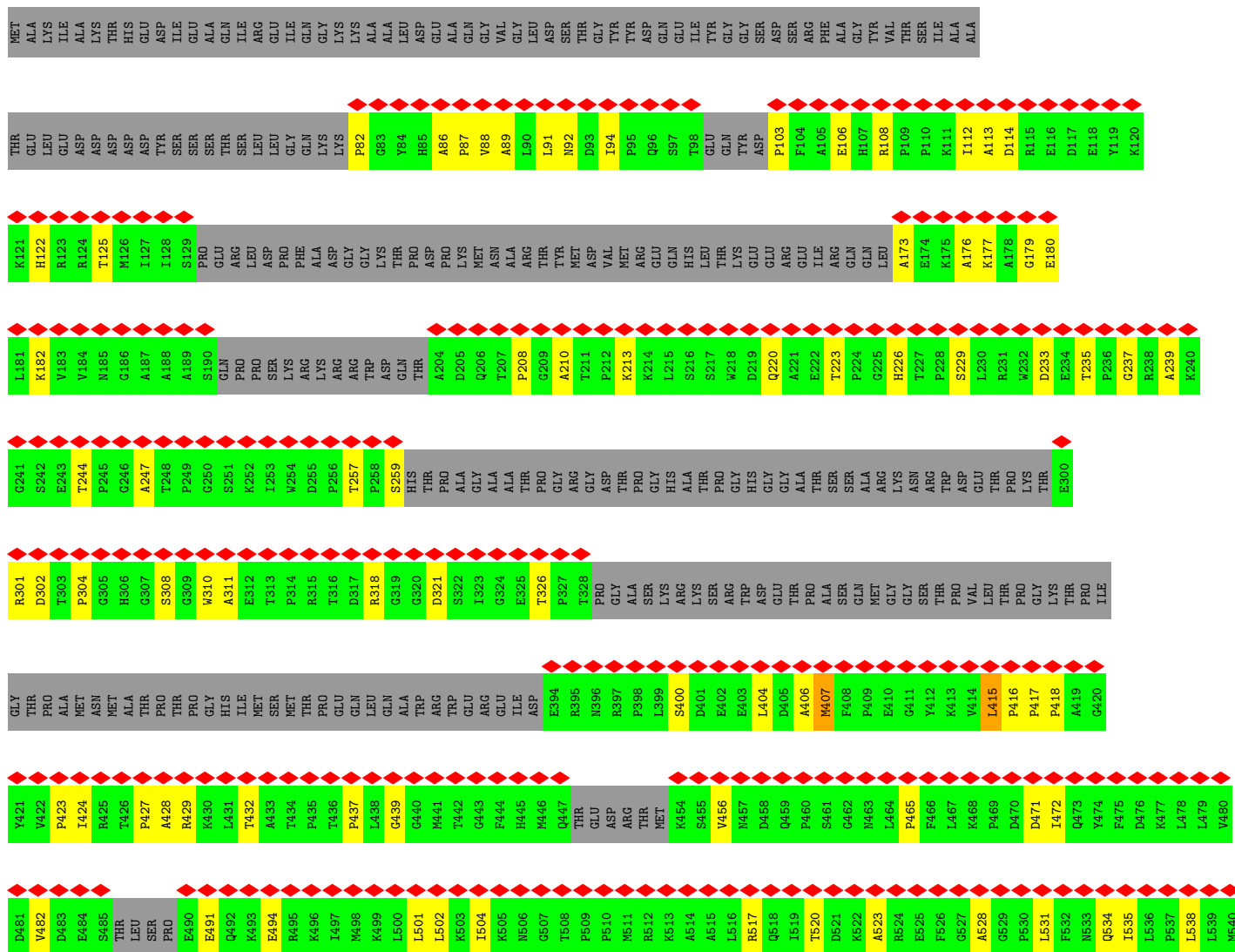
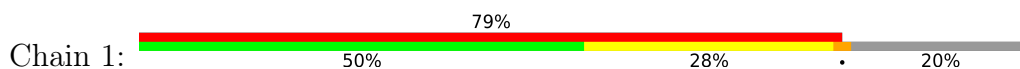
MET THR SER A4 L5 E6 N7 Y8 I9 N10 N11 T12 V13 A14 V15 I16 T17 S18 D19 G20 R21 M22 I23 V24 G25 T26 Q27 L27 K28 G29 F30 D31 Q32 T33 I34 N35 L36 I37 L38 D39 E40 S41 H42 E43 ARG VAL PHE SER SER SER GLN GLY VAL E53 Q54 V55 V56 L57 G58 L59 Y60

I61 V62 R63 G64 D65 N66 V67 A68 V69 I70 G71 E72 I73 ASP GLU THR ASP SER ALA LEU ASP LEU GLY ASN ILE ARG ALA GLU PRO LEU ASN SER VAL ALA HIS

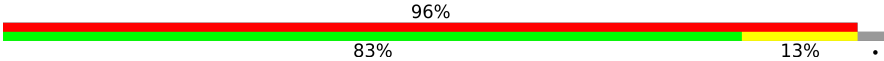
- Molecule 41: U4/U6 small nuclear ribonucleoprotein Prp4

Chain K: 

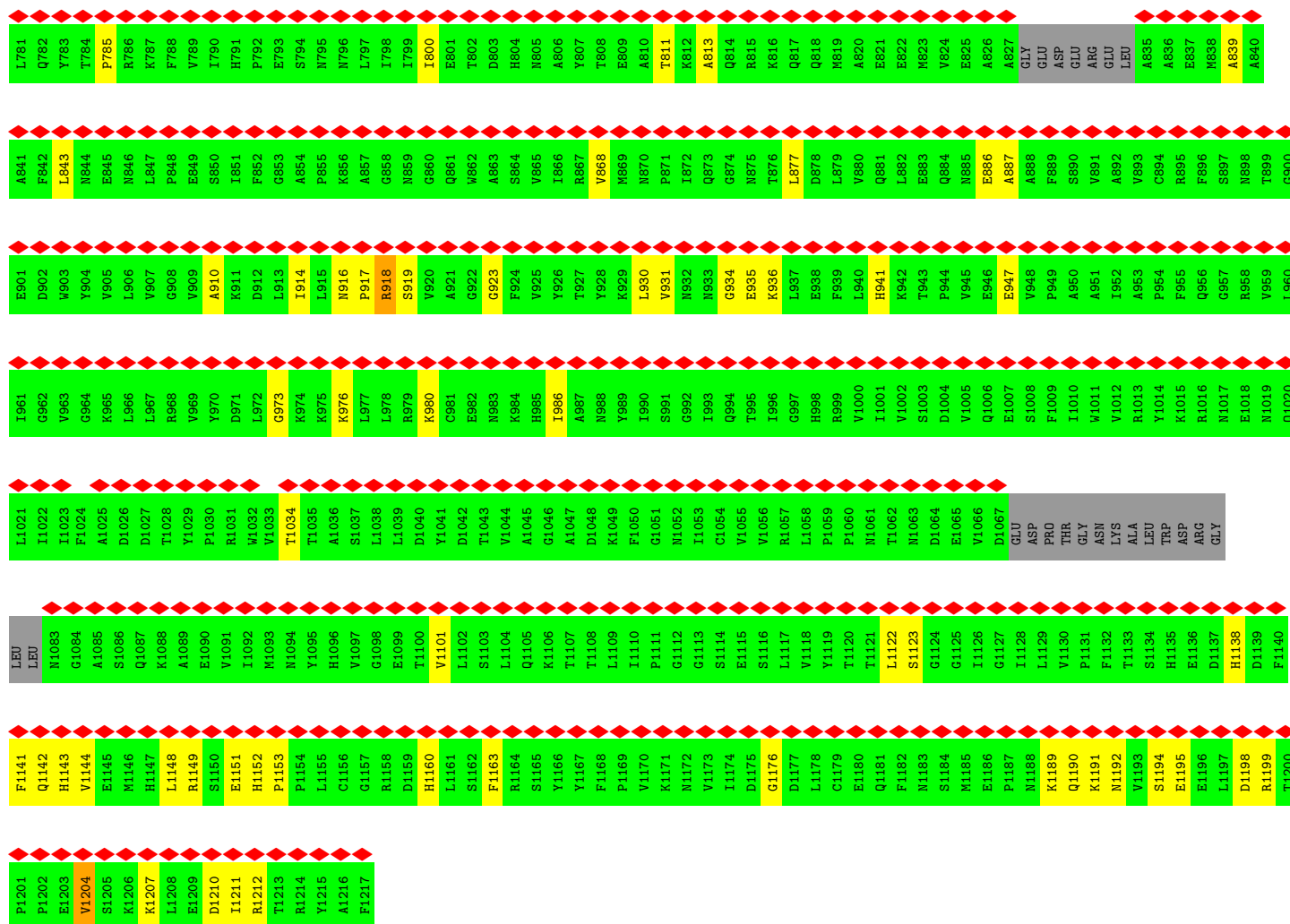
- Molecule 42: Splicing factor 3B subunit 1



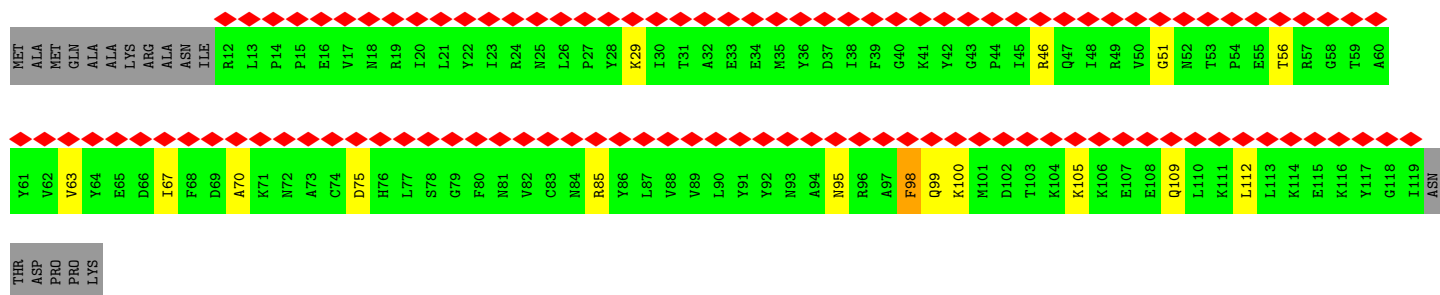
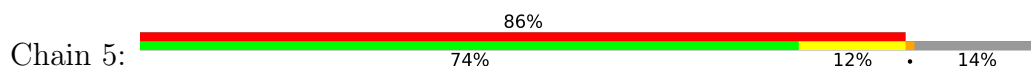
- Molecule 43: Splicing factor 3B subunit 3

Chain 3: 

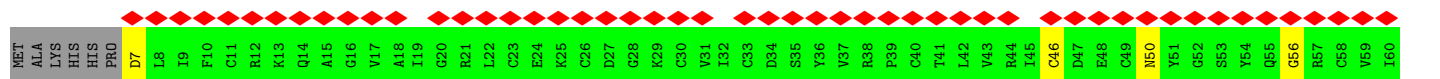
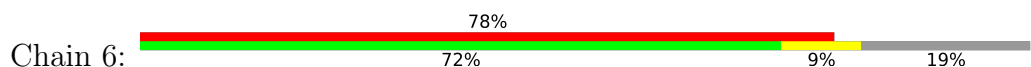
M1	F2	L3	Y4	N5	L6	T7	L8	Q9	R10	A11	T12	G13	I14	S15	F16	A17	I18	H19	G20	N21	F22	S23	G24	T25	K26	Q27	Q28	E29	I30	V31	V32	S33	R34	G35	K36	I37	L38	E39	L40	L41	R42	P43	D44	P45	N46	T47	G48	K49	V50	H51	T52	L53	L54	T55	V56	E57	V58	F59	G60	
V61	I62	R63	S64	L65	M66	A67	F68	R69	L70	T71	G72	T73	G74	K75	D76	Y77	I78	V79	V80	G81	S82	D83	S84	G85	R86	I87	V88	I89	L90	E91	Y92	Q93	P94	S95	K96	N97	L98	F99	E100	K101	I102	H103	Q104	E105	L106	F107	G108	K109	S110	G111	C112	R113	R114	T115	V116	P117	G118	Q119	F120	
L121	A122	V123	D124	K125	K126	G127	R128	A129	V130	M131	I132	S133	A134	I135	A136	K137	Q138	K139	L140	V141	Y142	I143	L144	N145	R146	D147	A148	A149	L150	R151	L152	T153	I154	S155	S156	L157	L158	E159	A160	H161	K162	A163	N164	T165	L166	V167	Y168	H169	V170	V171	G172	V173	D174	R175	G176	F177	E178	N179	P180	
M181	F182	A183	C184	L185	E186	M187	D188	Y189	E190	E191	A192	D193	N194	D195	P196	T197	G198	E199	A200	A201	A202	M203	T204	N205	Q206	T207	L208	T209	F210	Y211	E212	L213	D214	L215	G216	L217	N218	H219	V220	V221	R222	K223	V224	S225	E226	P227	L228	E229	H231	G232	M233	F234	L235	T236	T237	V238	P239	G240		
G241	S242	D243	G244	P245	S246	G247	V248	L249	C251	S252	E253	N254	Y255	T256	T257	Y258	K259	N260	F261	G262	D263	Q264	P265	D266	L267	R268	C269	P270	I271	P272	R273	R274	R275	N276	D277	L278	D279	D280	P281	E282	R283	G284	N285	L286	F287	V288	C289	S290	A291	T292	H293	G294	T295	K296	S297	N298	F299	F300		
F301	L302	A303	Q304	T305	E306	Q307	G308	D309	I310	F311	K312	I313	T314	L315	E316	T317	D318	E319	D320	N321	V322	T323	E324	I325	R326	L327	K328	Y329	F330	D331	T332	V333	P334	V335	A336	A337	A338	K339	C340	V341	L342	K343	T344	G345	N346	L347	F348	V349	S351	E352	F353	G354	N355	H356	Y357	L358	Y359	Q360		
I361	A362	H363	L364	G365	D366	D367	D368	E369	E370	P371	E372	F373	S374	S375	A376	R377	PRO	LEU	GLU	GLY	ASP	T384	F385	F386	F387	Q388	P389	R390	P391	L392	K393	N394	L395	V396	L397	V398	D399	E400	L401	D402	S403	L404	S405	P406	L407	L408	F409	C410	Q411	L412	A413	D414	L415	A416	N417	E418	D419	T420		
P421	Q422	L423	V424	V425	G426	C427	G428	R429	G430	P431	R432	S433	S434	L435	R436	V437	L438	R439	HIS	G441	L442	E443	V444	S445	E446	N447	A448	V449	S450	L451	L452	P453	G454	N455	P456	N457	A458	V459	W460	T461	V462	R463	R464	H465	L466	E467	D468	E469	F470	D471	A472	Y473	L474	L475	V476	S477	F478	V479	N480	
A481	T482	L483	V484	L485	S486	L487	G488	E489	T490	V491	E492	E493	V494	T495	D496	S497	G498	F499	L500	G501	T502	T503	P504	T505	S507	S507	C508	S509	L510	L511	G512	D513	D514	A515	L516	V517	Q518	V519	Y520	P521	D522	G523	L524	R525	H526	I527	R528	A529	D530	K531	L532	L533	A534	E535	V536	K537	T538	P539	G540	
K541	K542	T543	I544	V545	K546	C547	A548	V549	N550	Q551	R552	Q553	V554	V555	T556	A557	T558	G559	G560	G561	E562	L563	V564	Y565	F566	E567	M568	D569	P570	S571	G572	Q573	L574	N575	E576	F577	T578	E579	R580	K581	C641	I642	V643	E644	M645	D586	V587	V588	C589	M590	S591	L592	A593	N594	V595	P596	F597	G598	E599	Q600
R601	S602	R603	F604	L605	A606	V607	G608	L609	V610	D611	N612	T613	V614	R615	T616	I617	S618	L619	D620	P621	S622	D623	C624	L625	Q626	P627	L628	S629	M630	Q631	A632	L633	P634	A635	Q636	P637	E638	S639	L640	C641	I642	V643	E644	M645	D586	V587	V588	C589	M590	S591	L592	A593	N594	V595	P596	F597	G598	E599	Q600	
GLY	F662	L663	Y664	L665	N666	I667	G668	L669	Q670	N671	G672	V673	L674	L675	R676	T677	V678	L679	D680	P681	V682	T683	G684	D685	L686	S687	D688	T689	R690	T691	ARG	TYR	G695	S696	R697	P698	V699	K700	L701	F702	T703	V704	R705	M706	Q707	G708	Q709	E710	A711	V712	L713	A714	F715	S716	S717	R718	S719	W720		
L721	S722	Y723	S724	Y725	N726	S727	R728	L729	H730	L731	T732	F733	L734	S735	Y736	E737	T738	L739	E740	F741	A742	S743	G744	F745	A746	S747	E748	Q749	C750	F751	E752	G753	I754	V755	A756	I757	S758	T759	N760	T761	L762	R763	I764	L765	A766	L767	E768	K769	L770	G771	ALA	V773	F774	N775	Q776	V777	A778	F779	P780	

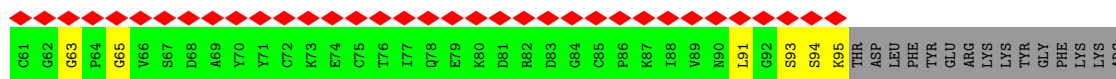


• Molecule 44: SF3b14a, Splicing factor 3B subunit 6

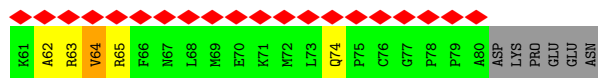
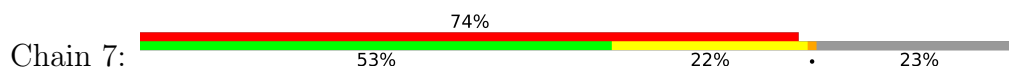


• Molecule 45: PHD finger-like domain-containing protein 5A

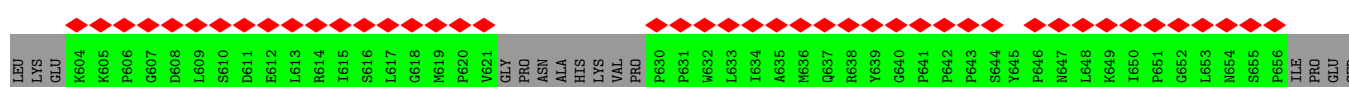
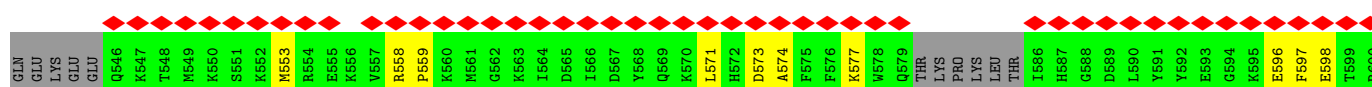
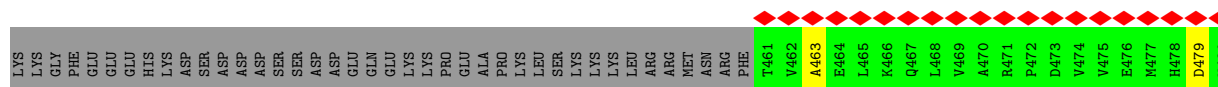
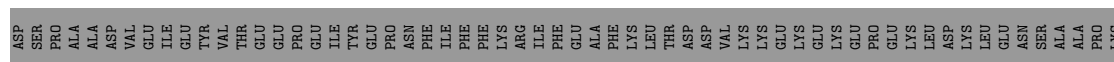
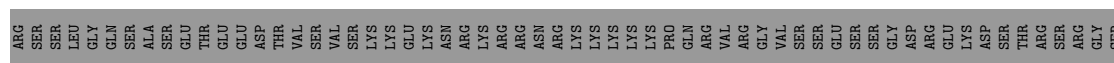
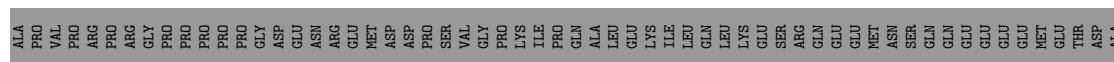
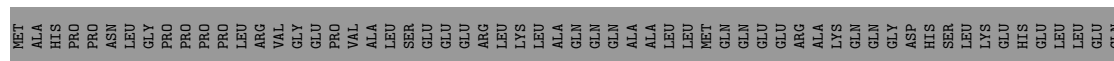
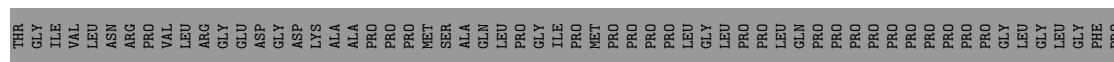
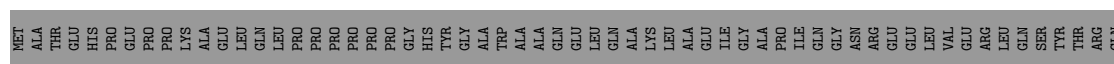




• Molecule 46: SF3b5, Splicing factor 3B subunit 5



• Molecule 47: SF3b145, Splicing factor 3B subunit 2



L1289	L1290	L1291	K1294	Y1295	P1297	P1298	P1299	E1231	E1300	L1301	L1302	D1303	L1304	Q1305	P1306	L1307	P1308	V1309	S1310	A1311	L1312	L1313	M1314	S1315	F1317	E1318	S1319	L1320	Y1321	Q1322	P1323	K1324	F1325	P1326	F1327	F1328	P1329	P1330	L1331	T1332	T1333	Q1334	F1335	N1336	N1337	T1338	Y1339	Y1340	M1341	S1342	D1343	F1347	G1349	A1350		
V1222	I1223	V1225	E1226	D1227	V1228	S1230	E1231	V1232	I1233	L1234	H1235	H1236	E1237	Y1238	F1239	L1240	K1241	A1243	K1244	Y1245	Q1247	D1248	E1249	H1250	L1251	I1252	T1253	V1256	P1257	V1258	F1259	E1260	P1261	L1262	P1263	P1264	P1265	Y1266	V1271	R1274	W1275	L1276	S1277	C1278	E1279	L1282	S1285	F1286	R1287	H1288						
K1145	K1146	N1147	P1149	F1150	E1151	L1153	Y1154	L1155	L1156	N1157	H1158	N1159	E1160	E1163	L1164	I1165	R1166	Q1171	K1172	T1173	K1176	H1179	K1183	L1184	E1185	L1186	L1190	Q1191	P1192	I1193	T1194	L1195	S1196	T1197	T1205	P1206	D1207	F1208	Q1209	W1210	D1211	E1212	K1213	Y1214	H1215	G1216	S1217	A1220	F1221							
I1052	E1053	F1066	I1067	S1068	L1072	E1073	L1077	A1078	D1080	M1081	V1082	Y1083	V1084	Q1085	T1086	S1087	A1088	G1089	R1093	A1094	I1095	F1096	E1097	L1098	V1099	L1100	N1101	R1102	G1103	W1104	A1105	Q1106	L1107	T1108	D1109	K1110	L1114	C1127	R1130	Q1131	F1132	R1133	K1134	L1135	V1140	K1141	K1142	I1143	E1144							
D973	K974	K975	T976	Q977	N978	F979	Q980	N981	A988	Y991	Y992	I993	T994	N995	D996	Y1001	N1002	Q1003	L1004	L1005	K1006	P1007	T1008	L1009	S1010	I1011	E1012	E1013	L1014	F1015	R1016	V1017	F1018	S1019	D942	L1020	S1021	G945	D946	P947	L948	N949	D950	Q951	L954	V957	H958	T959	A960	A961	L962	D965	Y972			
L869	A757	L762	E767	Q768	C769	K770	K775	D776	L777	N657	A662	D668	P669	A670	K671	G672	L673	F674	Y675	N678	T688	Y689	V690	T693	E694	K695	K696	K718	M719	H726	K729	A735	D740	M741	C742	L743	E744	K745	D746	L747	L748	G749	L750	F751	E754											
L559	A560	Y562	G563	I564	T565	V566	A567	E568	L569	T570	G571	H573	Q574	L575	C576	K577	E578	E579	I580	S581	T583	Q584	I585	T586	Y587	E591	K592	W593	G600	G601	E602	R603	T604	Y605	T606	Q607	D608	V609	R610	K611	I612	L613	L614	D615	D623	V627	L628	E629	A630	L631	V632	A633				
R490	A491	A492	L493	E494	T495	D496	Q497	N498	L499	L500	P504	A507	G508	K509	T510	N511	V512	A513	L514	M515	C516	M517	L518	E519	I521	G522	K523	H524	I525	N526	M527	D528	G529	T530	I531	N532	V533	D534	D535	F536	F475	K537	I538	I539	M544	R545	S546	E550	M551	V552	G553	S554	F555	G556		
HIS	PHE	MET	ALA	ASN	LYS	R427	C428	Q429	L430	P431	D432	R436	R439	K440	G441	E444	A449	L450	P454	F455	G456	S457	E458	E459	Q460	L461	L462	P463	I464	E465	K466	L467	P468	K469	Y470	A471	Q472	A473	G474	F475	E476	G477	F478	T480	L481	M482	R483	I484	Q485	S486	K487	L488	Y489			
GLU	CYS	GLU	ASN	GLN	LEU	LEU	VAL	LEU	VAL	THR	GLU	THR	GLU	THR	ASP	PHE	ILE	LYS	VAL	ARG	ASP	VAL	ARG	GLN	HIS	ARG	MET	TRP	MET	ILE	LEU	GLN	TYR	ARG	GLN	THR	LEU	SER	LEU	ALA	ASP	ALA	GLN	GLY	SER	ALA	GLY	GLU	ALA	VAL	ALA	GLU	LEU	LYS	GLY	LEU
SER	ALA	ASN	VAL	ALA	SER	GLY	GLU	LEU	ASP	PHE	SER	ASP	THR	LYS	LYS	ASP	ILE	HIS	PRO	ASP	ASP	VAL	ARG	ILE	ASP	PHE	THR	MET	TRP	ASP	ALA	GLN	ILE	GLY	GLU	ALA	VAL	SER	GLN	LYS	GLY	LEU	VAL	GLU	LEU	ILE	ASP	LEU	LYS	THR	ALA	SER	ASP	ASP	ARG	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.338, 1.338, 1.338	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, 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	0/17735	0.78	16/23951 (0.1%)
2	I	0.30	0/3214	0.48	0/4998
3	B	0.31	0/2698	0.47	0/4195
4	F	0.29	0/2230	0.49	1/3468 (0.0%)
5	G	0.60	8/1793 (0.4%)	0.71	4/2783 (0.1%)
6	O	0.42	0/1180	0.74	0/1594
7	C	0.33	0/6584	0.73	6/8942 (0.1%)
8	N	0.63	0/4568	0.88	18/6320 (0.3%)
9	M	0.33	0/974	0.66	2/1316 (0.2%)
10	L	0.33	0/2912	0.72	2/3924 (0.1%)
11	9	1.09	1/1091 (0.1%)	1.19	5/1478 (0.3%)
12	J	0.72	1/1278 (0.1%)	0.95	4/1657 (0.2%)
13	U	0.13	0/254	0.39	0/314
13	a	0.86	0/343	1.20	3/427 (0.7%)
13	i	0.86	0/343	1.20	3/427 (0.7%)
14	V	0.14	0/333	0.46	0/416
14	b	0.89	0/327	1.11	0/407
14	j	0.89	0/327	1.10	0/407
15	P	0.15	0/298	0.49	0/370
15	c	1.14	0/387	1.21	1/482 (0.2%)
15	k	1.18	0/338	1.20	1/419 (0.2%)
16	Q	0.21	0/291	0.47	0/363
16	d	1.23	0/295	1.26	0/367
16	l	1.24	1/295 (0.3%)	1.26	0/367
17	R	0.16	0/313	0.46	0/390
17	e	1.03	0/315	1.27	1/392 (0.3%)
17	m	1.02	0/315	1.26	0/392
18	S	0.23	0/297	0.59	0/371
18	f	0.86	0/295	1.05	0/367
18	n	0.86	0/270	1.05	0/334
19	T	0.13	0/287	0.35	0/358
19	g	0.80	0/322	1.01	0/399

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	h	0.81	0/318	1.01	0/394
20	E	1.08	0/1195	1.22	5/1492 (0.3%)
21	X	0.15	0/379	0.44	0/530
22	W	0.18	0/853	0.47	0/1188
23	A0	0.32	0/591	0.83	0/799
24	0	0.08	0/224	0.35	0/312
25	Z	0.16	0/888	0.52	0/1241
26	8	0.15	0/276	0.55	0/383
27	Y	0.16	0/2265	0.48	1/3156 (0.0%)
28	H	0.71	12/2576 (0.5%)	1.11	27/4003 (0.7%)
29	o	0.99	0/647	2.34	33/807 (4.1%)
30	p	0.97	0/375	1.97	7/467 (1.5%)
31	u	0.36	0/493	0.97	2/611 (0.3%)
32	v	0.37	0/373	1.77	4/461 (0.9%)
33	w	0.38	0/1688	0.92	3/2102 (0.1%)
34	q	0.69	0/359	1.28	0/447
35	r	0.75	0/294	1.37	3/364 (0.8%)
36	s	0.58	0/294	1.32	3/364 (0.8%)
37	t	0.71	0/286	1.28	2/354 (0.6%)
38	x	0.71	0/279	1.40	2/347 (0.6%)
39	y	0.60	0/258	1.14	0/319
40	z	0.68	0/242	1.21	1/299 (0.3%)
41	K	0.30	0/1818	0.93	8/2308 (0.3%)
42	1	1.72	38/4184 (0.9%)	1.43	25/5216 (0.5%)
43	3	1.39	25/4664 (0.5%)	1.20	9/5816 (0.2%)
44	5	1.26	2/431 (0.5%)	1.27	1/537 (0.2%)
45	6	1.15	0/355	1.12	0/442
46	7	1.59	1/263 (0.4%)	1.23	0/327
47	2	1.17	0/722	1.25	3/892 (0.3%)
48	4	1.02	0/311	0.99	0/387
49	D	0.53	0/6795	1.27	41/8492 (0.5%)
All	All	0.73	89/87198 (0.1%)	0.95	247/117252 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
7	C	0	6
8	N	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	c	0	1
15	k	0	1
23	A0	0	2
33	w	0	1
42	1	0	11
43	3	0	11
44	5	0	1
46	7	0	1
47	2	0	3
49	D	0	1
All	All	0	59

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	407	MET	N-CA	22.52	1.71	1.46
42	1	406	ALA	C-N	15.04	1.52	1.33
42	1	1243	PRO	N-CA	-9.50	1.35	1.47
42	1	944	SER	N-CA	-8.38	1.34	1.46
43	3	84	SER	CA-C	-7.84	1.42	1.53

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	v	146	MET	CA-C-N	21.08	146.19	119.84
32	v	146	MET	C-N-CA	21.08	146.19	119.84
49	D	946	ASP	CA-C-N	19.95	140.60	118.85
49	D	946	ASP	C-N-CA	19.95	140.60	118.85
42	1	406	ALA	CA-C-N	17.65	147.36	120.89

There are no chirality outliers.

5 of 59 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	MET	Peptide
1	A	211	GLN	Peptide
1	A	408	PRO	Peptide
1	A	463	PRO	Peptide
1	A	802	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17290	0	16495	395	0
2	I	2881	0	1461	125	0
3	B	2420	0	1226	130	0
4	F	1995	0	1006	63	0
5	G	1612	0	821	195	0
6	O	1152	0	1123	21	0
7	C	6440	0	6465	135	0
8	N	4518	0	3121	99	0
9	M	962	0	1012	12	0
10	L	2874	0	2856	50	0
11	9	1087	0	921	256	0
12	J	1273	0	903	33	0
13	U	256	0	70	2	0
13	a	344	0	93	3	0
13	i	344	0	93	4	0
14	V	334	0	92	1	0
14	b	328	0	89	5	0
14	j	328	0	89	0	0
15	P	300	0	80	5	0
15	c	388	0	102	6	0
15	k	340	0	87	1	0
16	Q	292	0	93	7	0
16	d	296	0	87	10	0
16	l	296	0	87	1	0
17	R	314	0	86	3	0
17	e	316	0	85	4	0
17	m	316	0	85	2	0
18	S	298	0	89	5	0
18	f	296	0	84	9	0
18	n	272	0	75	1	0
19	T	288	0	84	1	0
19	g	324	0	89	4	0
19	h	320	0	88	0	0
20	E	1196	0	337	2	0
21	X	378	0	190	1	0
22	W	844	0	426	16	0
23	A0	581	0	567	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	0	225	0	98	2	0
25	Z	883	0	414	6	0
26	8	277	0	114	2	0
27	Y	2258	0	1064	38	0
28	H	2311	0	1170	149	0
29	o	648	0	167	1	0
30	p	376	0	102	0	0
31	u	496	0	118	2	0
32	v	376	0	85	0	0
33	w	1693	0	454	22	0
34	q	360	0	95	2	0
35	r	296	0	76	5	0
36	s	296	0	77	0	0
37	t	288	0	78	0	0
38	x	280	0	81	8	0
39	y	260	0	75	0	0
40	z	244	0	71	3	0
41	K	1821	0	759	50	0
42	1	4192	0	1110	233	0
43	3	4672	0	1260	71	0
44	5	432	0	114	6	0
45	6	356	0	105	7	0
46	7	264	0	70	11	0
47	2	728	0	183	9	0
48	4	312	0	87	3	0
49	D	6796	0	1778	111	0
50	A	36	0	6	9	0
51	C	32	0	12	0	0
52	C	1	0	0	0	0
All	All	85302	0	50580	1943	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 1943 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1790:ILE:HD13	11:9:266:PHE:CE2	1.27	1.66
11:9:352:GLU:HG3	11:9:357:ALA:CB	1.28	1.59
1:A:1790:ILE:HD13	11:9:266:PHE:CD2	1.40	1.54
42:1:407:MET:N	42:1:407:MET:CA	1.71	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1790:ILE:CD1	11:9:266:PHE:CE2	1.92	1.46

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2203/2335 (94%)	2043 (93%)	150 (7%)	10 (0%)	24	57
6	O	139/142 (98%)	125 (90%)	13 (9%)	1 (1%)	18	51
7	C	814/972 (84%)	756 (93%)	54 (7%)	4 (0%)	24	57
8	N	773/941 (82%)	685 (89%)	78 (10%)	10 (1%)	9	38
9	M	122/128 (95%)	118 (97%)	4 (3%)	0	100	100
10	L	372/499 (74%)	351 (94%)	21 (6%)	0	100	100
11	9	155/800 (19%)	141 (91%)	13 (8%)	1 (1%)	21	54
12	J	221/683 (32%)	207 (94%)	12 (5%)	2 (1%)	14	45
13	U	60/231 (26%)	57 (95%)	3 (5%)	0	100	100
13	a	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
13	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
14	V	80/119 (67%)	76 (95%)	4 (5%)	0	100	100
14	b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
14	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
15	P	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
15	c	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
15	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
16	Q	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
16	d	72/86 (84%)	69 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	l	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
17	R	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
17	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
17	m	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
18	S	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
18	f	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
18	n	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
19	T	69/126 (55%)	69 (100%)	0	0	100	100
19	g	77/126 (61%)	75 (97%)	2 (3%)	0	100	100
19	h	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
20	E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	3	25
21	X	73/376 (19%)	70 (96%)	3 (4%)	0	100	100
22	W	167/177 (94%)	158 (95%)	9 (5%)	0	100	100
23	A0	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
24	0	43/439 (10%)	42 (98%)	1 (2%)	0	100	100
25	Z	174/312 (56%)	158 (91%)	15 (9%)	1 (1%)	21	54
26	8	54/199 (27%)	47 (87%)	7 (13%)	0	100	100
27	Y	445/513 (87%)	432 (97%)	12 (3%)	1 (0%)	43	73
29	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	38
30	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
31	u	118/793 (15%)	106 (90%)	6 (5%)	6 (5%)	1	17
32	v	88/464 (19%)	63 (72%)	16 (18%)	9 (10%)	0	7
33	w	413/501 (82%)	367 (89%)	41 (10%)	5 (1%)	10	40
34	q	88/95 (93%)	77 (88%)	7 (8%)	4 (4%)	2	18
35	r	70/102 (69%)	64 (91%)	3 (4%)	3 (4%)	2	19
36	s	70/139 (50%)	63 (90%)	6 (9%)	1 (1%)	9	37
37	t	68/91 (75%)	63 (93%)	4 (6%)	1 (2%)	8	36
38	x	68/80 (85%)	64 (94%)	2 (3%)	2 (3%)	3	25
39	y	61/103 (59%)	56 (92%)	5 (8%)	0	100	100
40	z	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	6	33
41	K	406/522 (78%)	343 (84%)	62 (15%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	1	1032/1304 (79%)	844 (82%)	166 (16%)	22 (2%)	5	31
43	3	1152/1217 (95%)	1053 (91%)	89 (8%)	10 (1%)	14	45
44	5	106/125 (85%)	84 (79%)	19 (18%)	3 (3%)	4	26
45	6	87/110 (79%)	76 (87%)	10 (12%)	1 (1%)	11	41
46	7	64/86 (74%)	55 (86%)	7 (11%)	2 (3%)	3	25
47	2	170/895 (19%)	151 (89%)	15 (9%)	4 (2%)	4	29
48	4	76/424 (18%)	75 (99%)	1 (1%)	0	100	100
49	D	1697/2136 (79%)	1604 (94%)	82 (5%)	11 (1%)	21	54
All	All	13852/21253 (65%)	12701 (92%)	1024 (7%)	127 (1%)	16	45

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	474	LEU
8	N	842	HIS
12	J	541	VAL
20	E	193	THR
27	Y	383	CYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1775/2108 (84%)	1752 (99%)	23 (1%)	61	71
6	O	126/130 (97%)	125 (99%)	1 (1%)	73	76
7	C	719/866 (83%)	713 (99%)	6 (1%)	73	76
8	N	196/792 (25%)	186 (95%)	10 (5%)	21	46
9	M	108/111 (97%)	108 (100%)	0	100	100
10	L	299/424 (70%)	293 (98%)	6 (2%)	48	65
11	9	81/681 (12%)	54 (67%)	27 (33%)	0	1
12	J	72/599 (12%)	69 (96%)	3 (4%)	26	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	X	2/333 (1%)	2 (100%)	0	100	100
22	W	10/148 (7%)	10 (100%)	0	100	100
23	A0	60/66 (91%)	59 (98%)	1 (2%)	53	67
25	Z	6/293 (2%)	6 (100%)	0	100	100
27	Y	11/450 (2%)	11 (100%)	0	100	100
41	K	29/442 (7%)	17 (59%)	12 (41%)	0	0
All	All	3494/7443 (47%)	3405 (98%)	89 (2%)	42	61

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	9	267	ARG
11	9	353	GLN
11	9	270	GLU
11	9	303	ASN
12	J	527	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
10	L	276	HIS
10	L	398	HIS
12	J	491	GLN
1	A	1487	HIS
1	A	1460	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	133/144 (92%)	54 (40%)	5 (3%)
28	H	105/188 (55%)	22 (20%)	3 (2%)
3	B	114/117 (97%)	43 (37%)	6 (5%)
4	F	90/107 (84%)	32 (35%)	5 (5%)
5	G	76/274 (27%)	45 (59%)	15 (19%)
All	All	518/830 (62%)	196 (37%)	34 (6%)

5 of 196 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	2	G
2	I	9	G
2	I	11	A
2	I	12	G
2	I	18	G

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	G	153	C
5	G	155	U
28	H	164	C
4	F	35	A
4	F	28	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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	$\# Z > 2$
50	IHP	A	3000	-	36,36,36	0.82	0	60,60,60	1.26	3 (5%)
51	GTP	C	1500	52	33,34,34	1.07	3 (9%)	50,54,54	1.67	11 (22%)

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
50	IHP	A	3000	-	-	5/30/54/54	0/1/1/1
51	GTP	C	1500	52	-	5/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	C	1500	GTP	C5-N7	-2.47	1.34	1.39
51	C	1500	GTP	C2-N3	2.37	1.38	1.33
51	C	1500	GTP	O4'-C4'	-2.01	1.40	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	C	1500	GTP	C5-C4-N3	-5.34	119.90	128.39
51	C	1500	GTP	N9-C4-N3	4.70	135.34	125.95
50	A	3000	IHP	C6-C5-C4	3.79	118.73	110.43
51	C	1500	GTP	C2-N3-C4	3.41	118.17	112.30
50	A	3000	IHP	P5-O15-C5	-2.80	115.95	123.43

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	C	1500	GTP	C3'-C4'-C5'-O5'
51	C	1500	GTP	C4'-C5'-O5'-PA
51	C	1500	GTP	O4'-C4'-C5'-O5'
50	A	3000	IHP	C3-O13-P3-O23
51	C	1500	GTP	C5'-O5'-PA-O3A

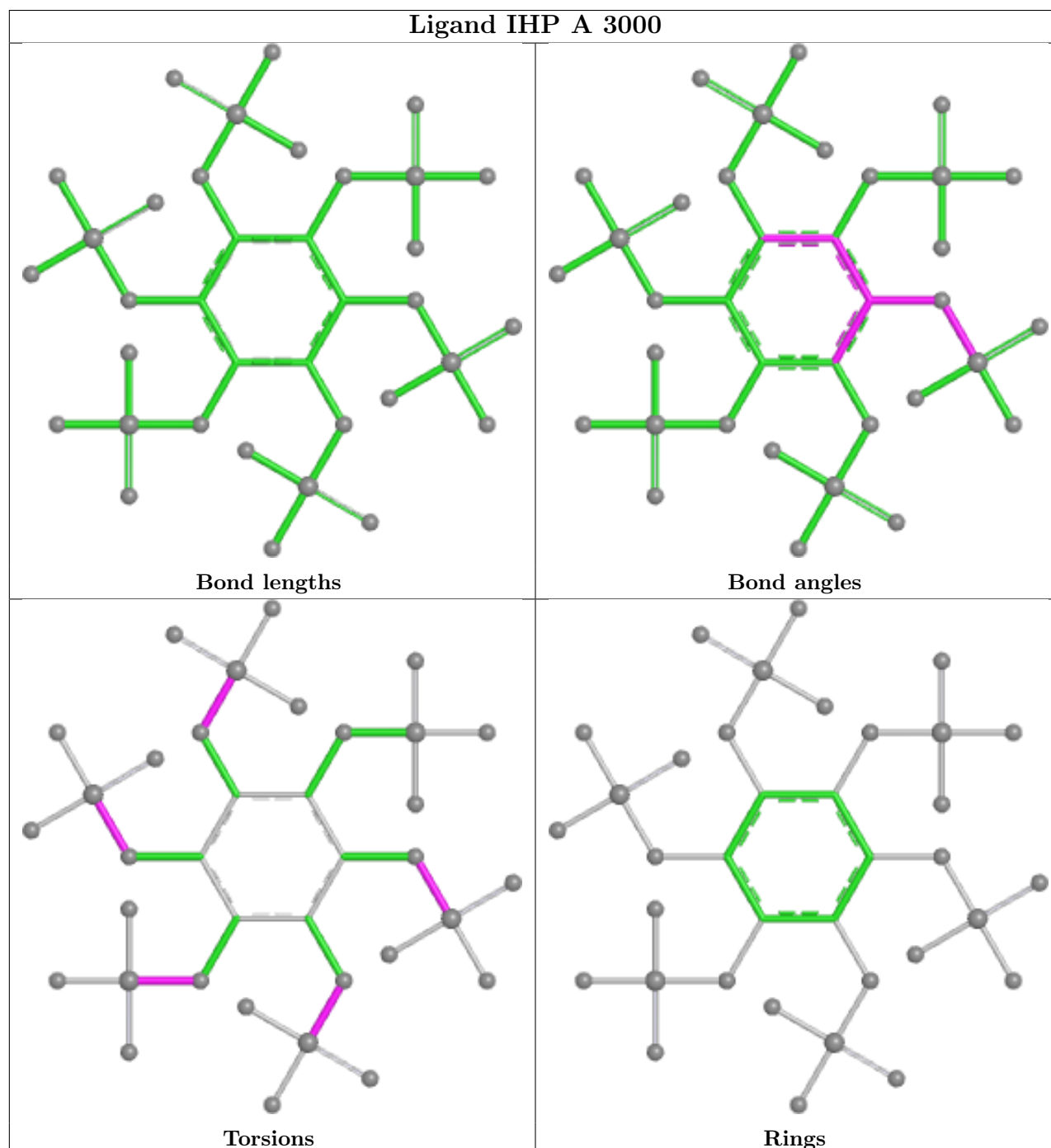
There are no ring outliers.

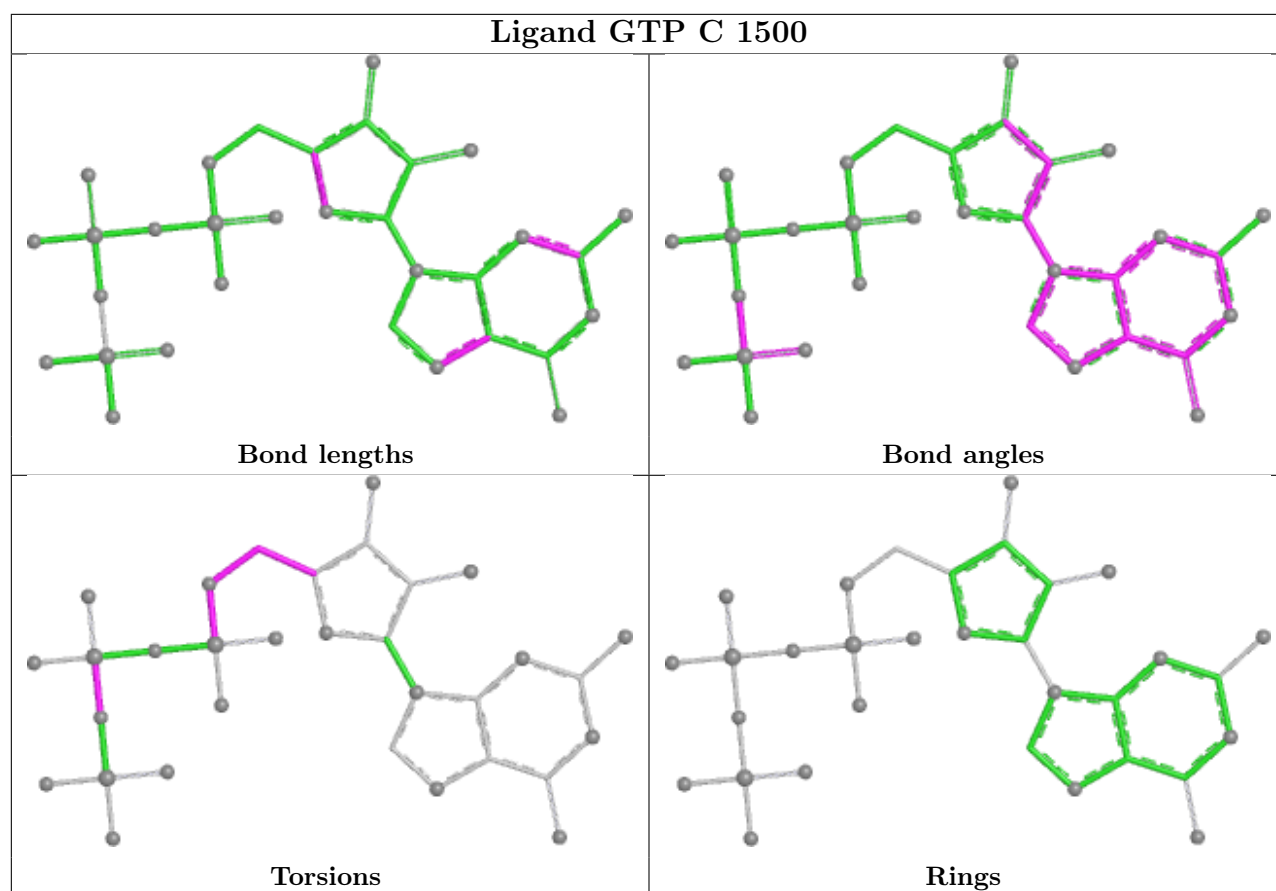
1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	A	3000	IHP	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 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.





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.

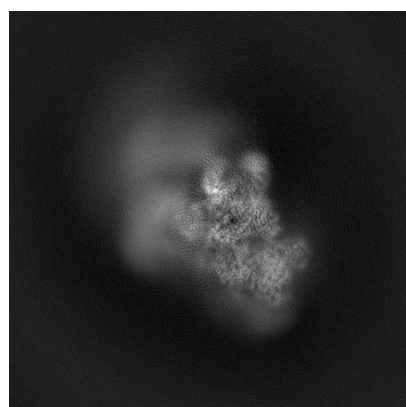
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9624. These allow visual inspection of the internal detail of the map and identification of artifacts.

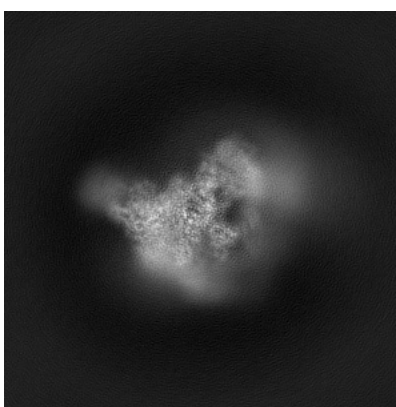
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

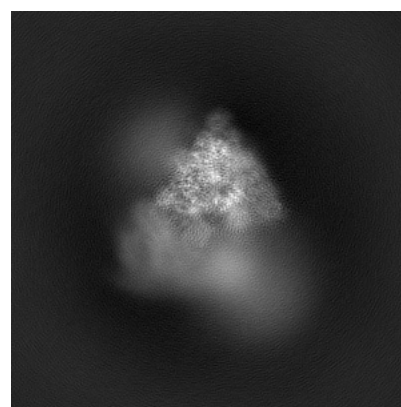
6.1.1 Primary map



X



Y

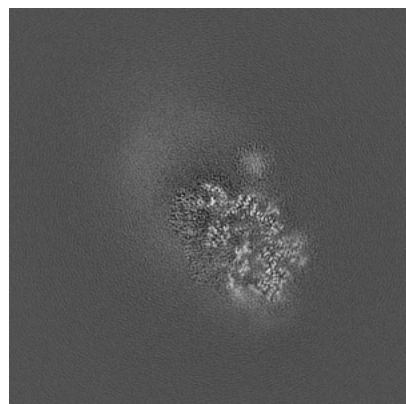


Z

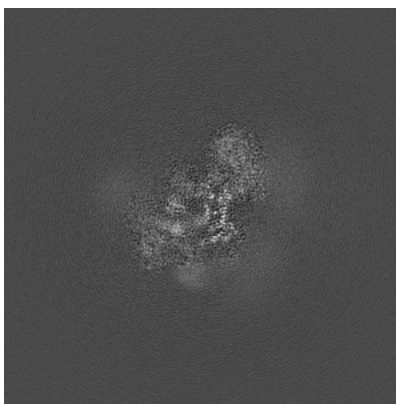
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

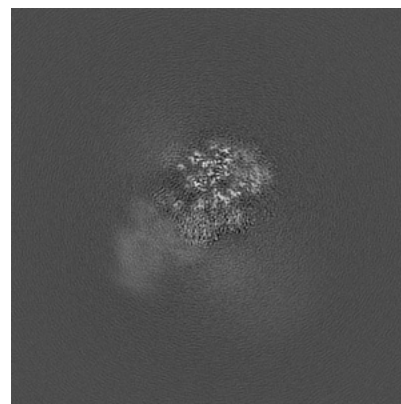
6.2.1 Primary map



X Index: 200



Y Index: 200

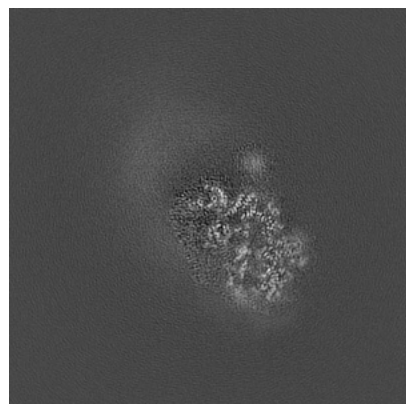


Z Index: 200

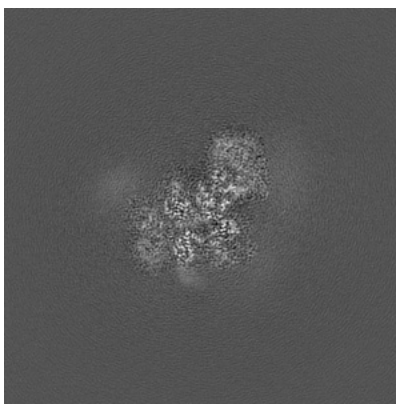
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

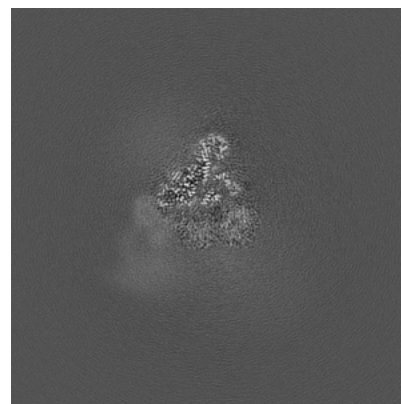
6.3.1 Primary map



X Index: 201



Y Index: 207

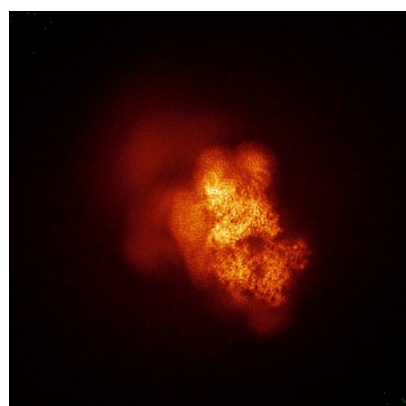


Z Index: 181

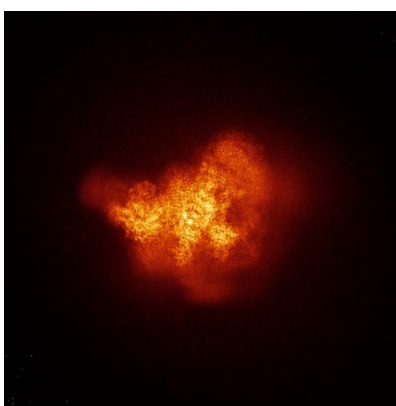
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

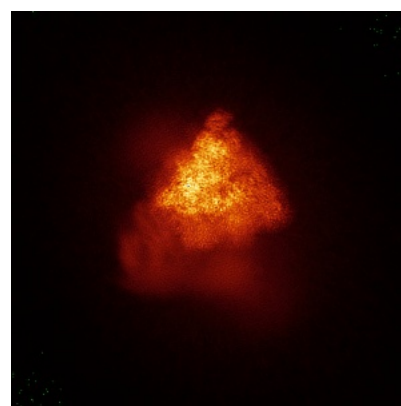
6.4.1 Primary map



X



Y

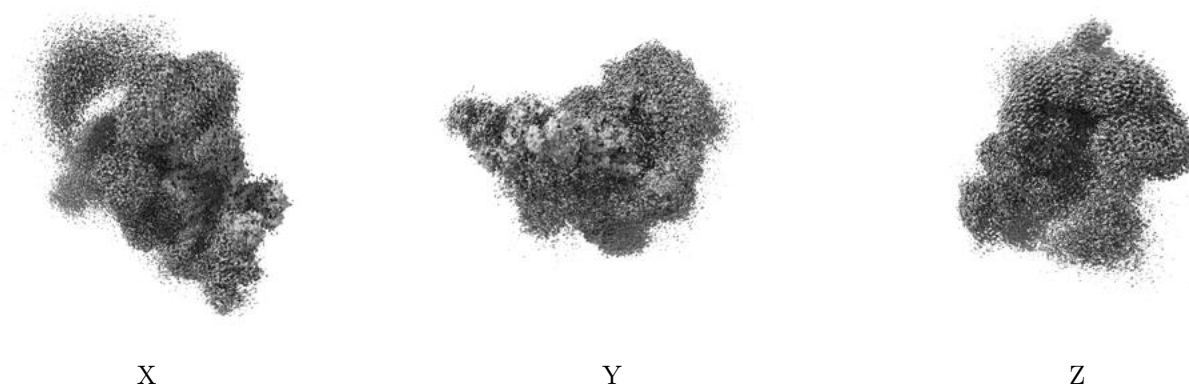


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

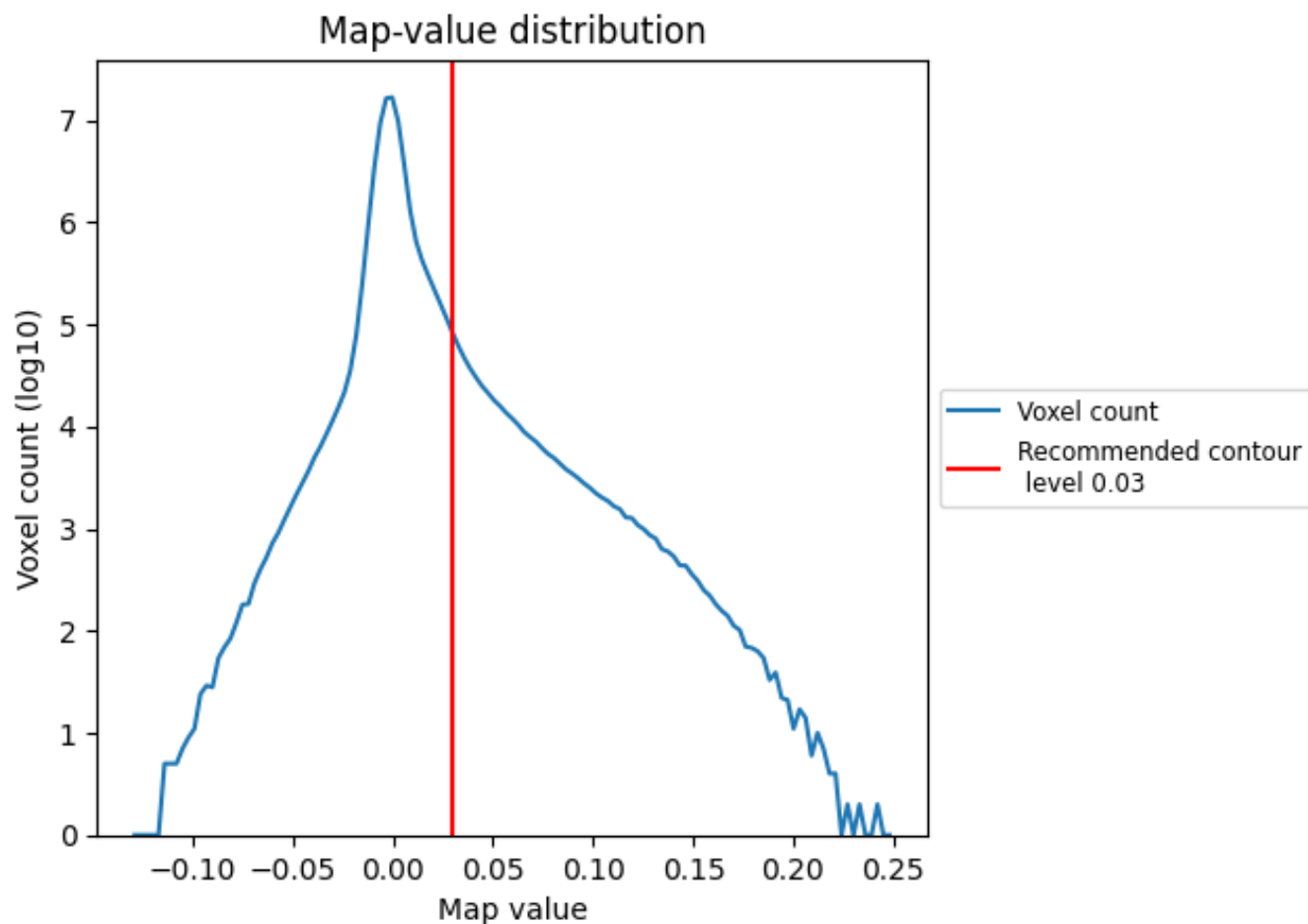
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

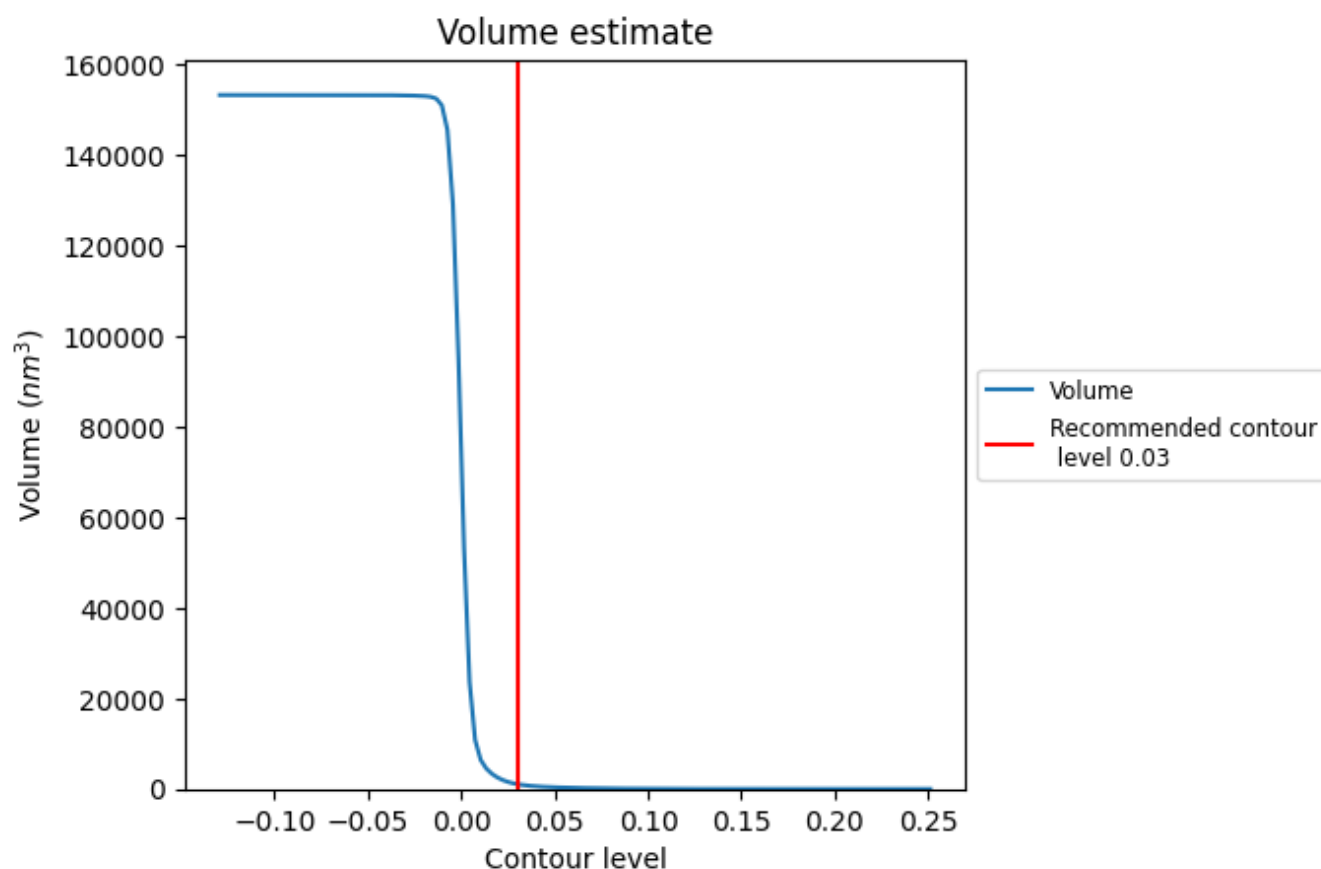
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

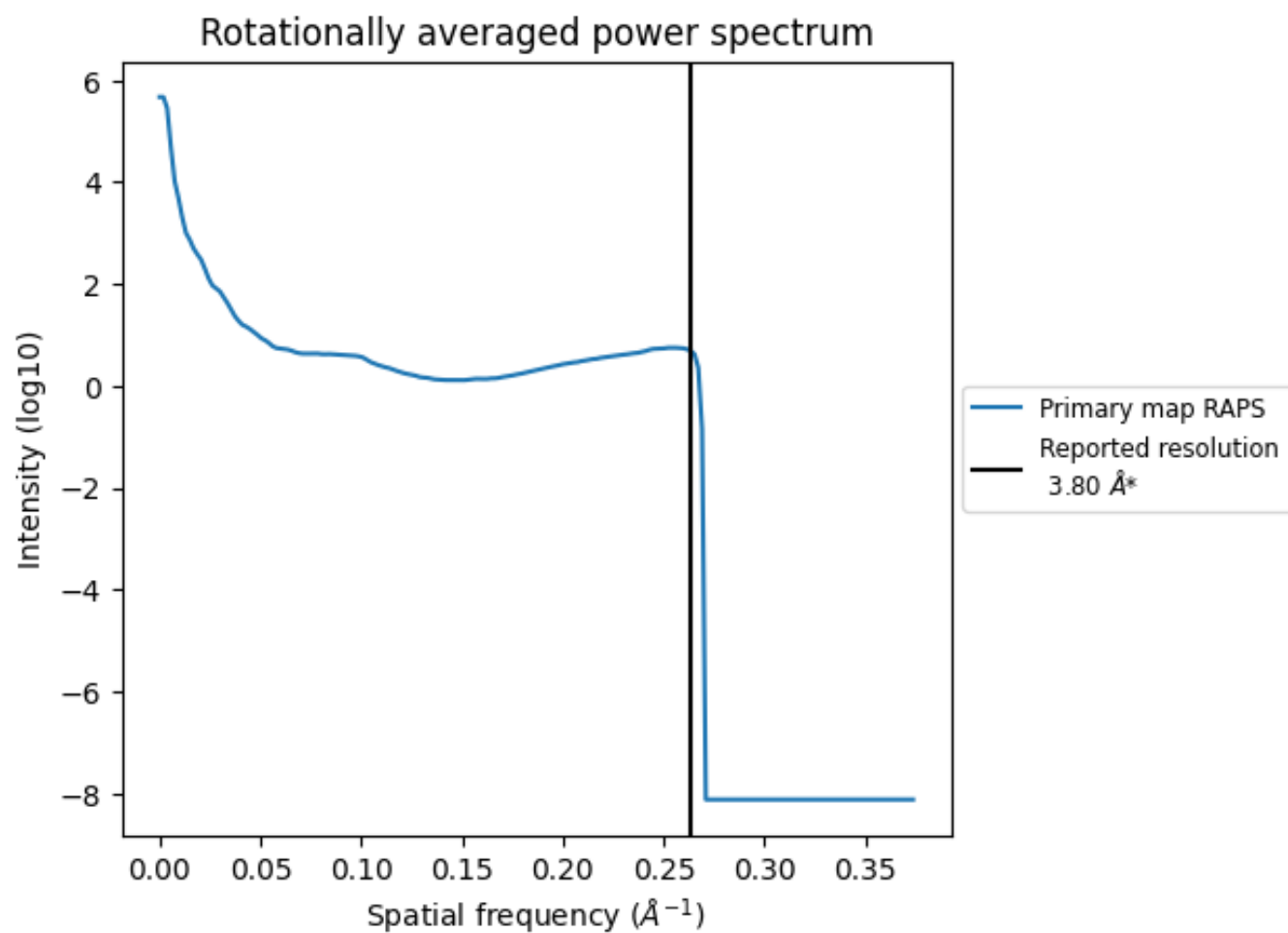
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1073 nm³; this corresponds to an approximate mass of 969 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

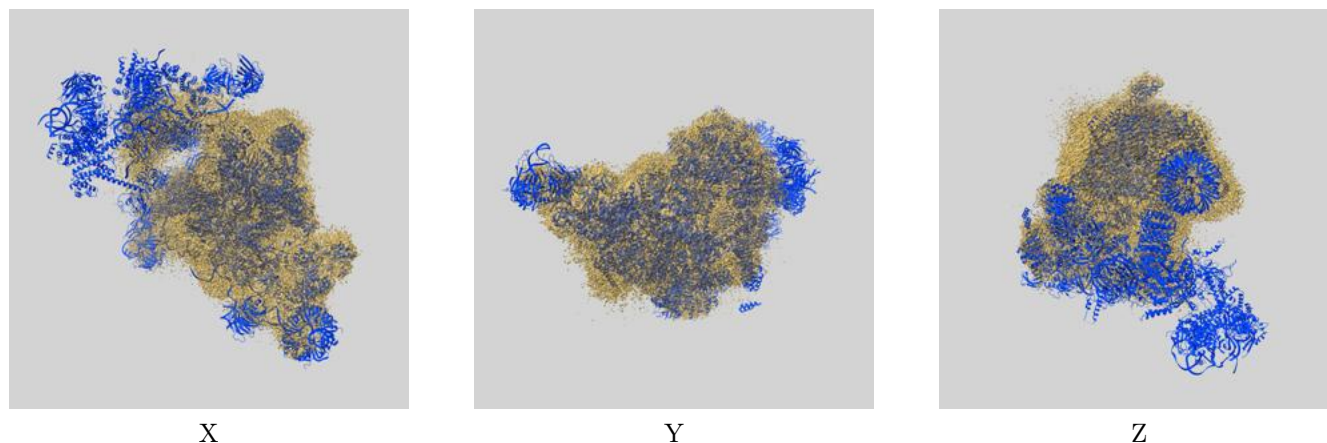
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

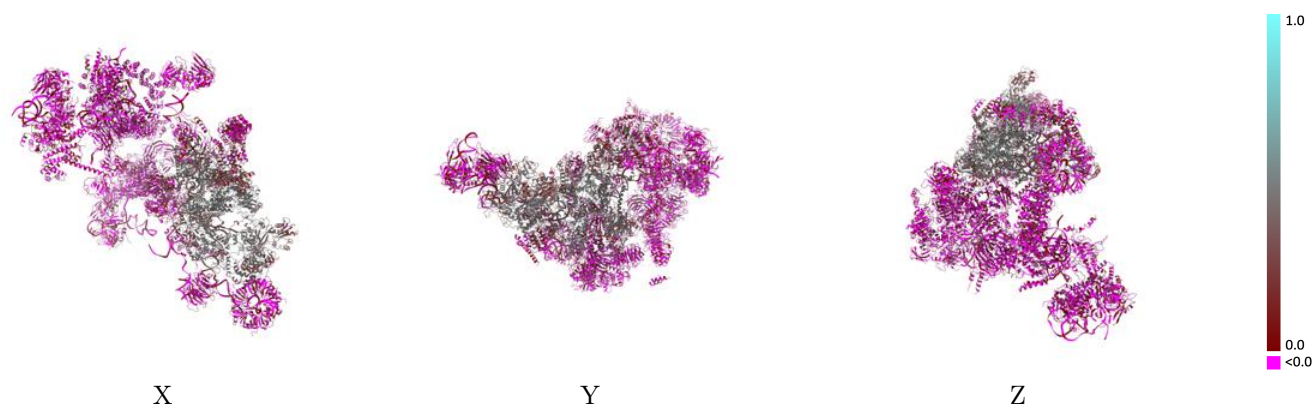
This section contains information regarding the fit between EMDB map EMD-9624 and PDB model 6AHD. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



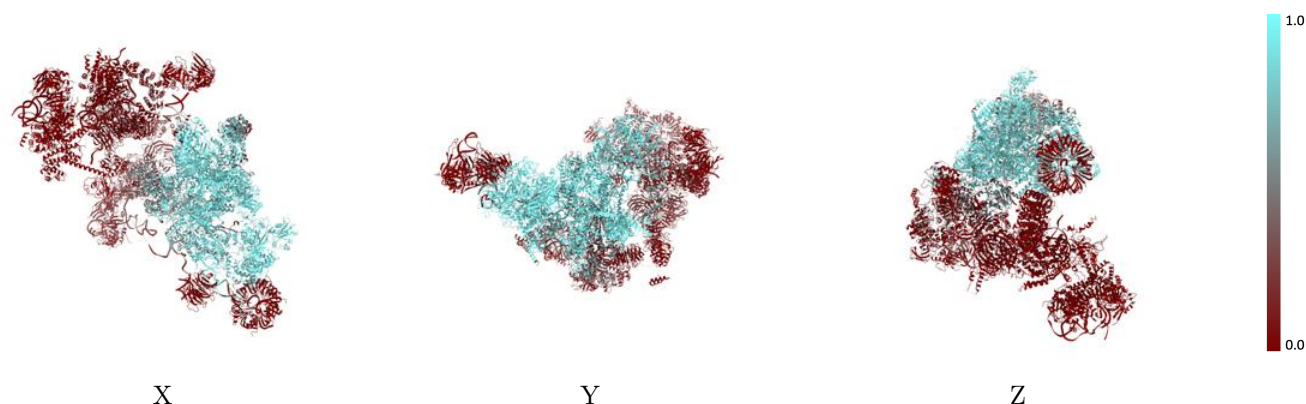
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



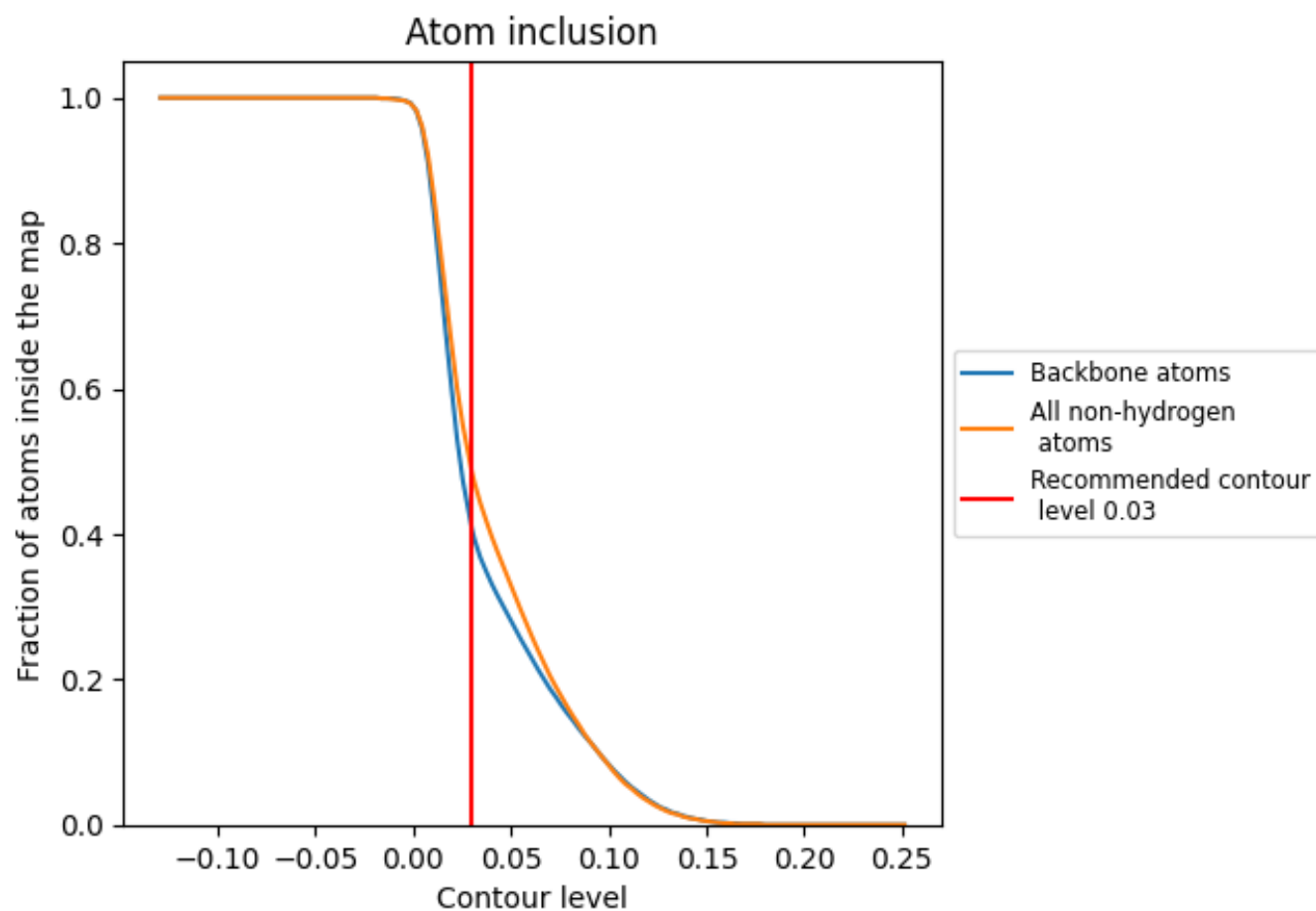
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 41% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4850	 0.1890
0	 0.4620	 0.0350
1	 0.0200	 -0.0020
2	 0.0510	 0.0150
3	 0.0100	 -0.0120
4	 0.0450	 0.0080
5	 0.0000	 -0.0120
6	 0.0450	 0.0060
7	 0.0490	 -0.0460
8	 0.6250	 0.1170
9	 0.8110	 0.3010
A	 0.8920	 0.4270
A0	 0.7330	 0.3980
B	 0.6270	 0.2100
C	 0.9040	 0.3920
D	 0.2710	 0.0170
E	 0.0430	 0.0270
F	 0.4840	 0.1360
G	 0.3250	 0.0910
H	 0.0290	 0.0170
I	 0.5260	 0.1780
J	 0.7910	 0.2650
K	 0.8960	 0.2760
L	 0.8380	 0.3490
M	 0.8950	 0.4130
N	 0.7580	 0.2080
O	 0.9210	 0.4500
P	 0.0270	 -0.0080
Q	 0.0170	 -0.0430
R	 0.0380	 0.0530
S	 0.0570	 0.0580
T	 0.0520	 0.0070
U	 0.0510	 0.0040
V	 0.0360	 0.0450
W	 0.6680	 0.0810



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Chain	Atom inclusion	Q-score
X	 0.4710	 0.0330
Y	 0.0260	 0.0100
Z	 0.6690	 0.1560
a	 0.1280	 -0.0110
b	 0.1250	 0.0190
c	 0.0410	 0.0080
d	 0.0100	 -0.0090
e	 0.0220	 0.0010
f	 0.0340	 -0.0570
g	 0.1850	 0.0140
h	 0.0000	 -0.0180
i	 0.0000	 0.0150
j	 0.0000	 -0.0030
k	 0.0000	 -0.0090
l	 0.0000	 -0.0360
m	 0.0000	 0.0330
n	 0.0000	 -0.0400
o	 0.0000	 0.0220
p	 0.0000	 -0.0370
q	 0.0000	 0.0190
r	 0.0000	 0.0090
s	 0.0000	 -0.0050
t	 0.0000	 0.0350
u	 0.0000	 0.0260
v	 0.0000	 0.0080
w	 0.0010	 0.0110
x	 0.0070	 0.0140
y	 0.0000	 -0.0360
z	 0.0000	 -0.0230