



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:50 PM UTC

PDB ID : 6AH0 / pdb_00006ah0
EMDB ID : EMD-9621
Title : The Cryo-EM Structure of the Precursor of Human Pre-catalytic Spliceosome (pre-B complex)
Authors : Zhan, X.; Yan, C.; Zhang, X.; Shi, Y.
Deposited on : 2018-08-15
Resolution : 5.70 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

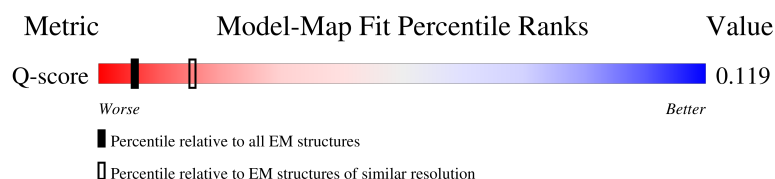
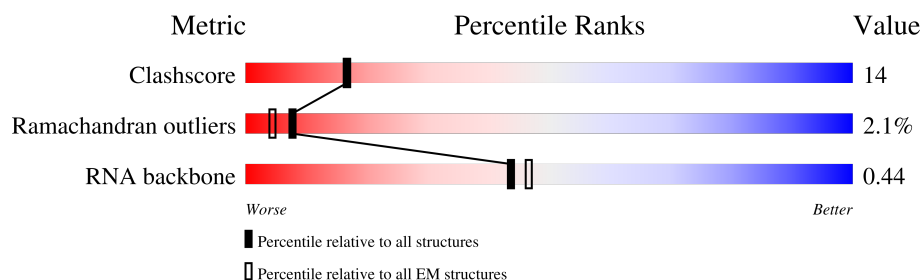
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	503 (5.20 - 6.20)

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	B	117	
2	D	2136	
3	E	357	
4	P	118	

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Mol	Chain	Length	Quality of chain
4	a	118	
4	k	118	
5	Q	86	
5	b	86	
5	m	86	
6	R	92	
6	c	92	
6	l	92	
7	S	76	
7	d	76	
7	n	76	
8	T	126	
8	e	126	
8	h	126	
9	U	231	
9	f	231	
9	i	231	
10	V	119	
10	g	119	
10	j	119	
11	F	107	
12	q	95	
13	r	102	
14	s	139	
15	t	91	

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Mol	Chain	Length	Quality of chain
16	x	80	
17	y	103	
18	z	96	
19	G	274	
20	H	188	
21	o	255	
22	p	225	
23	u	793	
24	v	464	
25	w	501	
26	1	1304	
27	2	895	
28	3	1217	
29	4	424	
30	5	125	
31	6	110	
32	7	86	
33	J	683	
34	K	522	
35	N	941	
36	L	499	
37	M	128	
38	O	142	
39	W	565	
40	I	144	

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Mol	Chain	Length	Quality of chain
41	X	820	50% 50%
42	A	2335	81% 13% 5%
43	C	972	74% 9% 16%

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 63369 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	115	Total	C	N	O	P	0	0
			2419	1084	402	818	115		

- Molecule 2 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	1874	Total	C	N	O	0	0
			7496	3748	1874	1874		

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

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

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	78	Total	C	N	O	0	0
			318	162	78	78		
4	k	85	Total	C	N	O	0	0
			340	170	85	85		
4	P	74	Total	C	N	O	0	0
			300	152	74	74		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	b	73	Total	C	N	O	0	0
			300	154	73	73		
5	m	74	Total	C	N	O	0	0
			296	148	74	74		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	Q	71	Total	C	N	O	0	0
			292	150	71	71		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	c	78	Total	C	N	O	0	0
			314	158	78	78		
6	l	79	Total	C	N	O	0	0
			316	158	79	79		
6	R	78	Total	C	N	O	0	0
			314	158	78	78		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	d	69	Total	C	N	O	0	0
			282	144	69	69		
7	n	68	Total	C	N	O	0	0
			272	136	68	68		
7	S	73	Total	C	N	O	0	0
			298	152	73	73		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	e	78	Total	C	N	O	0	0
			318	162	78	78		
8	h	80	Total	C	N	O	0	0
			320	160	80	80		
8	T	71	Total	C	N	O	0	0
			288	146	71	71		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	f	64	Total	C	N	O	0	0
			260	132	64	64		
9	i	73	Total	C	N	O	0	0
			292	146	73	73		
9	U	64	Total	C	N	O	0	0
			256	128	64	64		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	g	93	Total	C	N	O	0	0
			380	194	93	93		
10	j	82	Total	C	N	O	0	0
			328	164	82	82		
10	V	82	Total	C	N	O	0	0
			334	170	82	82		

- Molecule 11 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	69	Total	C	N	O	P	0	0
			1470	656	259	486	69		

- Molecule 12 is a protein called U6 snRNA-associated Sm-like protein LSm2.

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

- Molecule 13 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	r	75	Total	C	N	O	0	0
			300	150	75	75		

- Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm4.

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

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	t	75	Total	C	N	O	0	0
			300	150	75	75		

- Molecule 16 is a protein called U6 snRNA-associated Sm-like protein LSm6.

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

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm7.

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

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm8.

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

- Molecule 19 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	42	Total	C	N	O	P	0	0
			862	387	122	311	42		

- Molecule 20 is a RNA chain called U2snRNA.

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

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein A'.

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

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

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

- Molecule 23 is a protein called Splicing factor 3A subunit 1.

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

- Molecule 24 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	v	99	Total	C	N	O	0	0
			396	198	99	99		

- Molecule 25 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	w	443	Total	C	N	O	0	0
			1773	887	443	443		

- Molecule 26 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	1	1030	Total	C	N	O	0	0
			4120	2060	1030	1030		

- Molecule 27 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	2	186	Total	C	N	O	0	0
			744	372	186	186		

- Molecule 28 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	3	1174	Total	C	N	O	0	0
			4696	2348	1174	1174		

- Molecule 29 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	4	78	Total	C	N	O	0	0
			312	156	78	78		

- Molecule 30 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	5	108	Total	C	N	O	0	0
			432	216	108	108		

- Molecule 31 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	6	89	Total	C	N	O	0	0
			356	178	89	89		

- Molecule 32 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	7	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 33 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	J	167	Total	C	N	O	0	0
			668	334	167	167		

- Molecule 34 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	K	343	Total	C	N	O	0	0
			1371	686	343	342		

- Molecule 35 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	N	579	Total	C	N	O	0	0
			2316	1158	579	579		

- Molecule 36 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	L	226	Total	C	N	O	0	0
			904	452	226	226		

- Molecule 37 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	M	125	Total	C	N	O	0	0
			500	250	125	125		

- Molecule 38 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	O	139	Total	C	N	O	0	0
			556	278	139	139		

- Molecule 39 is a protein called U4/U6.U5 tri-snRNP-associated protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	W	463	Total	C	N	O	0	0
			1852	926	463	463		

- Molecule 40 is a RNA chain called U4snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	I	117	Total	C	N	O	P	0	0
			2491	1112	439	823	117		

- Molecule 41 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	X	414	Total	C	N	O	0	0
			1661	833	414	414		

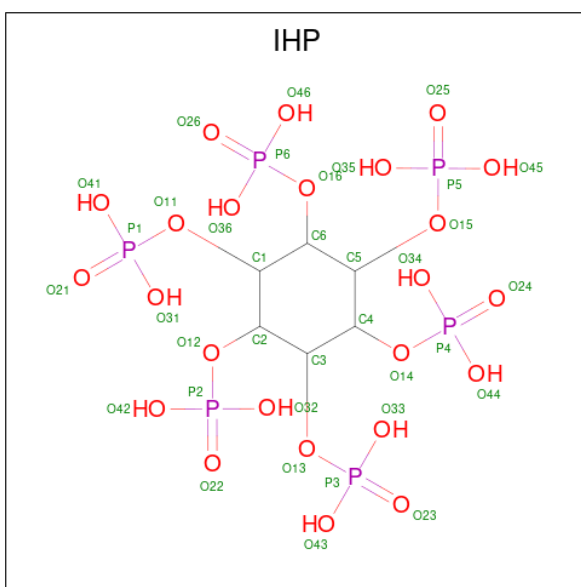
- Molecule 42 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	A	2221	Total	C	N	O	0	0
			8884	4442	2221	2221		

- Molecule 43 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

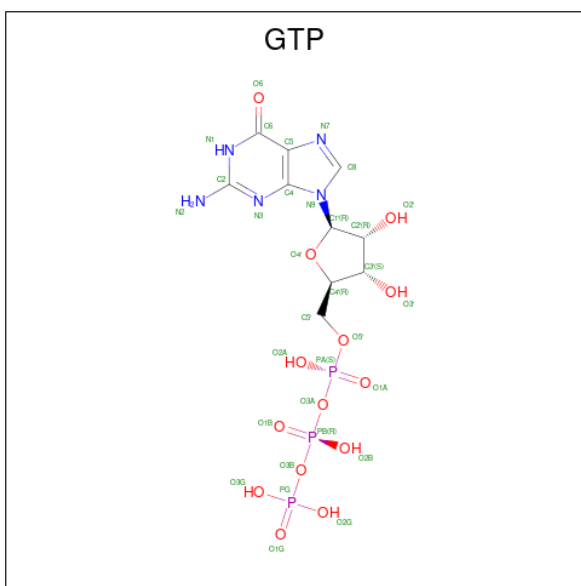
Mol	Chain	Residues	Atoms				AltConf	Trace
43	C	818	Total	C	N	O	0	0
			3272	1636	818	818		

- Molecule 44 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



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

- Molecule 45 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

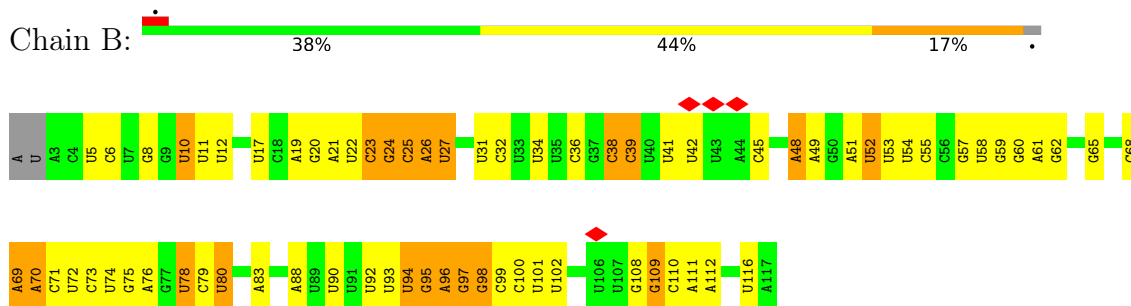
- Molecule 46 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

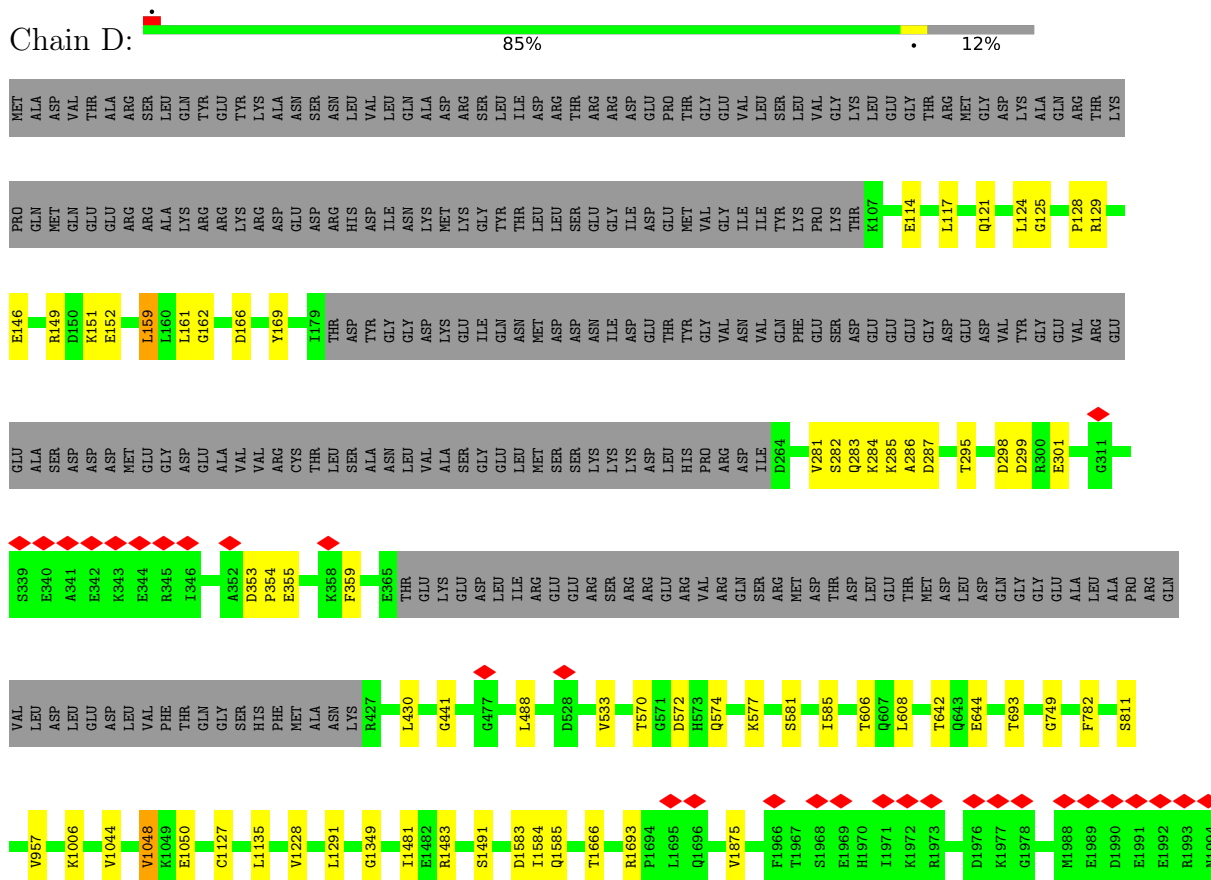
3 Residue-property plots

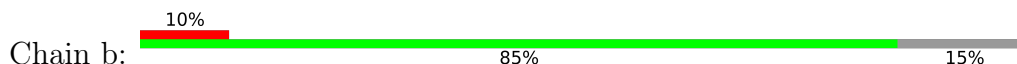
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

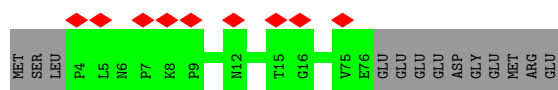
• Molecule 1: U5snRNA



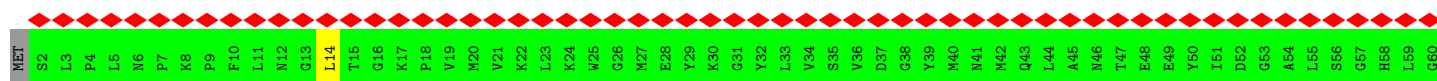
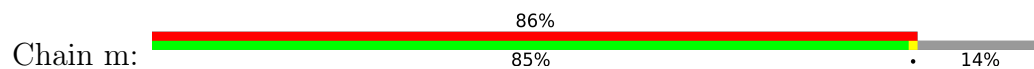
• Molecule 2: U5 small nuclear ribonucleoprotein 200 kDa helicase



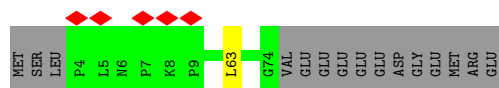
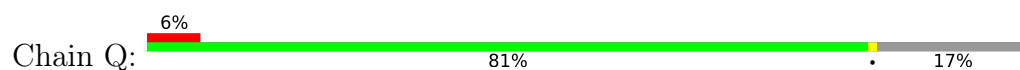




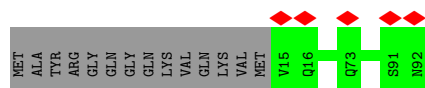
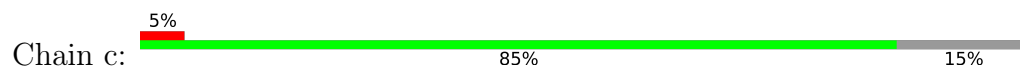
- Molecule 5: Small nuclear ribonucleoprotein F



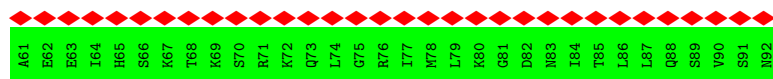
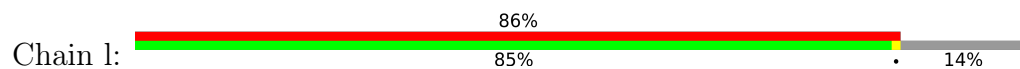
- Molecule 5: Small nuclear ribonucleoprotein F



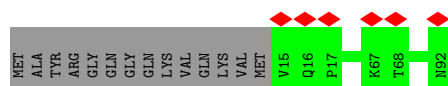
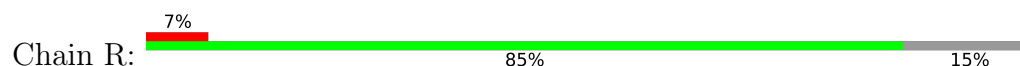
- Molecule 6: Small nuclear ribonucleoprotein E



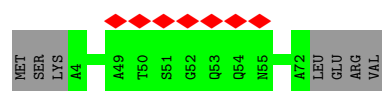
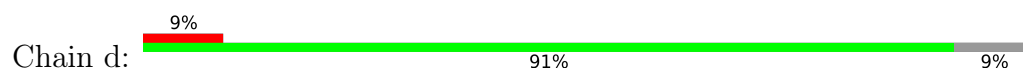
- Molecule 6: Small nuclear ribonucleoprotein E



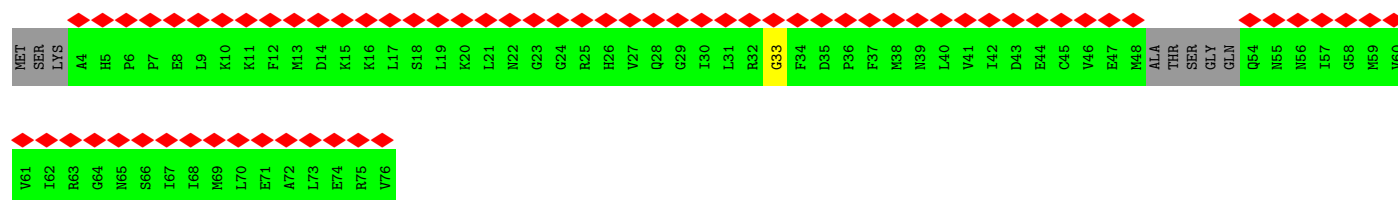
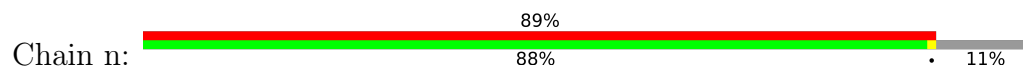
- Molecule 6: Small nuclear ribonucleoprotein E



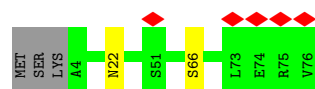
- Molecule 7: Small nuclear ribonucleoprotein G



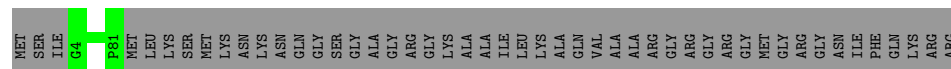
- Molecule 7: Small nuclear ribonucleoprotein G



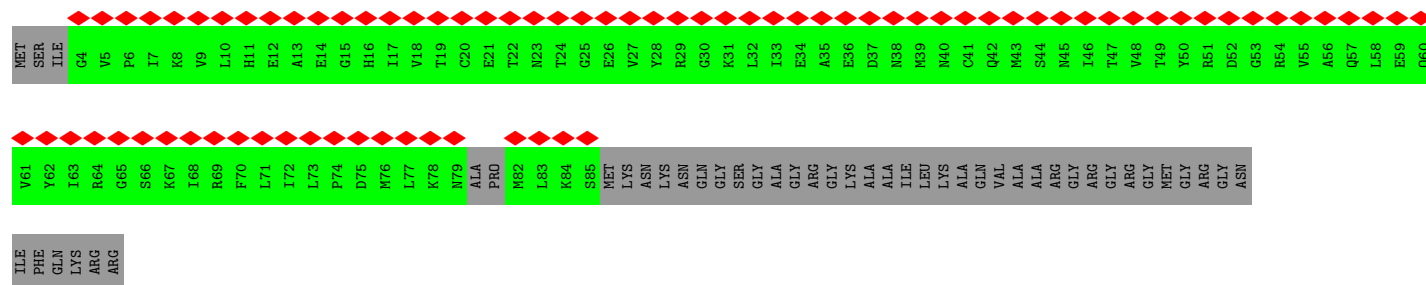
- Molecule 7: Small nuclear ribonucleoprotein G



- Molecule 8: Small nuclear ribonucleoprotein Sm D3



- Molecule 8: Small nuclear ribonucleoprotein Sm D3



- Molecule 8: Small nuclear ribonucleoprotein Sm D3





- | | | |
|-----|----|-----|
| MET | K2 | S36 | MET | R37 | V83 | V87 | K91 | E92 | F93 | A94 | V96 | ALA | GLY | ARG | GLY | GLY | ARG | ARG | GLY | GLY | ARG | ARG | GLY | GLY | ARG | ARG | GLY | GLY | PRO | ARG | ARG |
|-----|----|-----|

- | |
|-----|
| M1 | K2 | L3 | L4 | V5 | F6 | L7 | M8 | K9 | L10 | S11 | H12 | E13 | T14 | V15 | T16 | I17 | E18 | L19 | K20 | N21 | G22 | T23 | Q24 | V25 | M26 | G27 | T28 | L29 | T30 | G31 | V32 | A33 | V34 | S35 | M36 | N37 | T38 | H39 | L40 | K41 | A42 | G43 | K44 | M45 | T46 | L47 | K48 | N49 | R50 | E51 | P52 | V53 | Q54 | L55 | E56 | T57 | L58 | S59 | T60 |
| R61 | G62 | N63 | M64 | I65 | R66 | V67 | F68 | I69 | L70 | P71 | D72 | S73 | L74 | P75 | L76 | D77 | T78 | L79 | L80 | V81 | D82 | V83 | GLU | PRO | L85 | VAL | L86 | SER | L88 | L89 | GLU | ALA | VAL | ALA | GLY | ARG | GLY | ARG | GLY | ARG | GLY | GLY | GLY | ARG | GLY | GLY | PRO | PRO | ARG | ARG | | | | | | | | | |

- MET** K2 K20 N21 S59 N63 N64 165 D77 T78 V83 GLU PRO LYS VAL LYS SER LYS LYS ARG ALA VAL ALA GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG

-

A

A

U85

U86

U87

U88

U89

G90

A91

A92

G93

C94

G95

U96

U

C

C

A

U

A102

U103

U104

U105

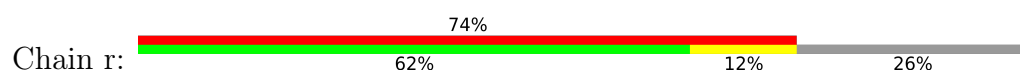
U106

U107

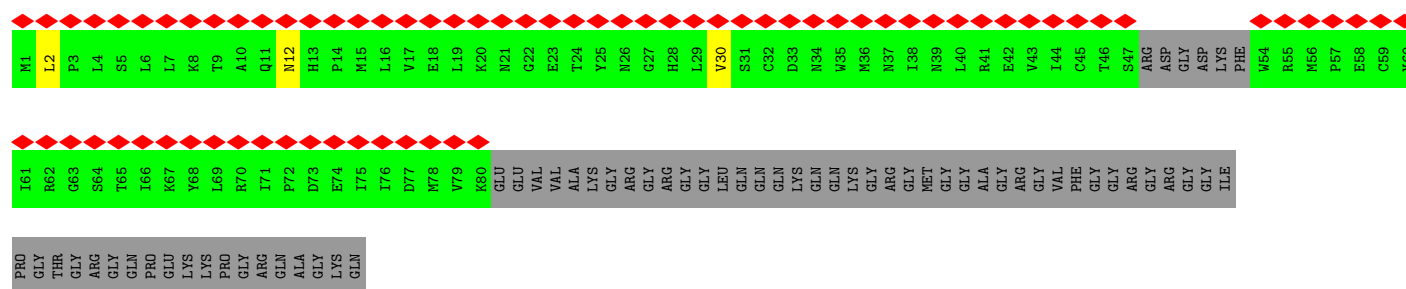
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|----|----|----|----|----|----|----|----|----|-----|
| M1 | L2 | F3 | Y4 | S5 | F6 | F7 | K8 | S9 | L10 | V11 | G12 | K13 | D14 | V15 | V16 | V17 | E18 | L19 | K20 | N21 | D22 | L23 | S24 | C26 | G27 | T28 | L29 | H30 | S31 | V32 | D33 | Q34 | Y35 | L36 | N37 | L38 | K39 | L40 | L41 | D42 | L43 | S44 | V45 | T46 | D47 | P48 | E49 | K50 | K51 | Y52 | P53 | H54 | L55 | S56 | V57 | K58 | N59 | L60 |
|----|----|----|----|----|----|----|----|----|-----|

F61	I62	R63	G64	S65	V66	V67	R68	Y69	V70	Q71	L72	P73	A74	D75	E76	V77	D78	T79	Q80	L81	L82	Q83	D84	A85	A86	R87	K88	E89	A90	LEU	GLN	GLN	GLN	LYS	LYS	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

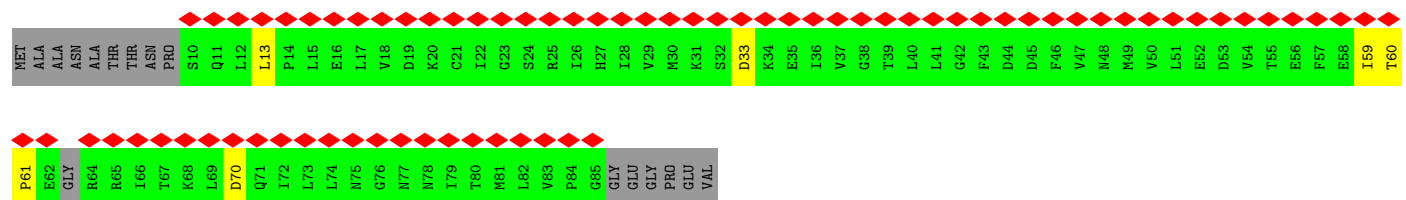
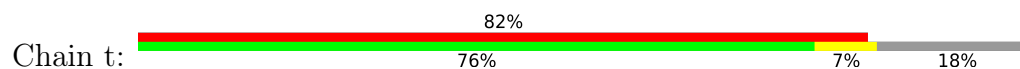
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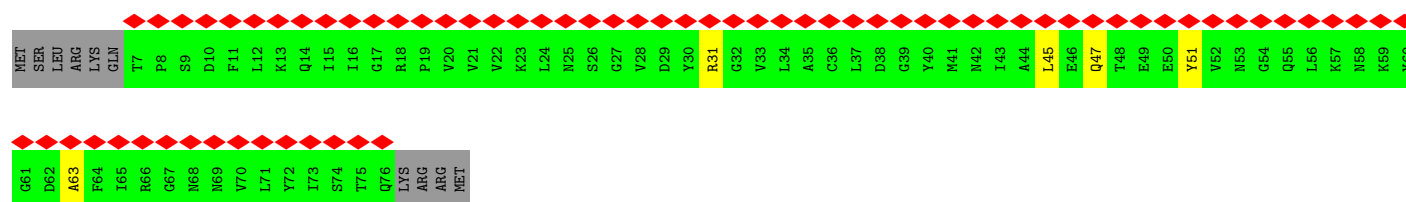
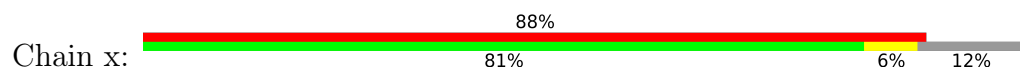
• Molecule 14: U6 snRNA-associated Sm-like protein LSm4



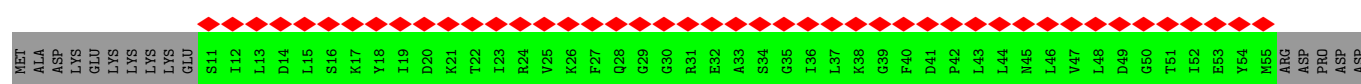
• Molecule 15: U6 snRNA-associated Sm-like protein LSm5



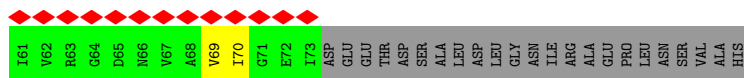
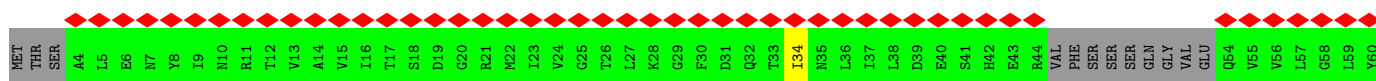
• Molecule 16: U6 snRNA-associated Sm-like protein LSm6



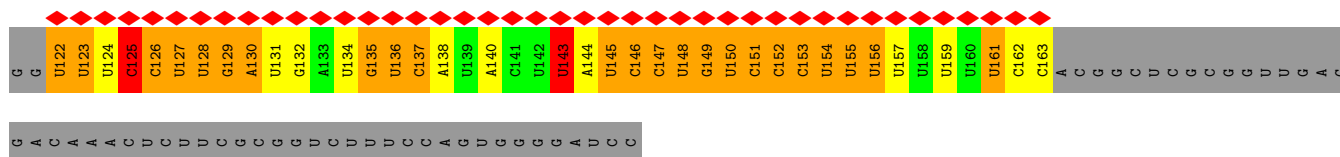
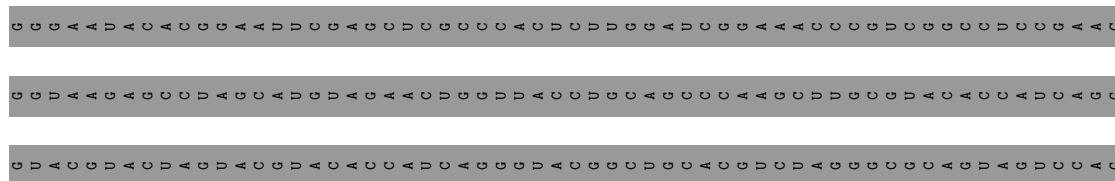
• Molecule 17: U6 snRNA-associated Sm-like protein LSm7



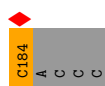
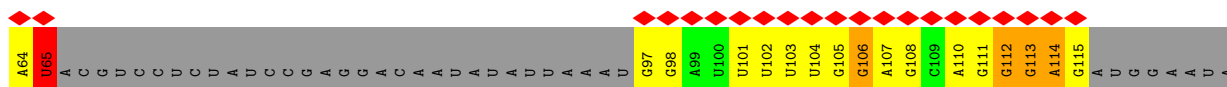
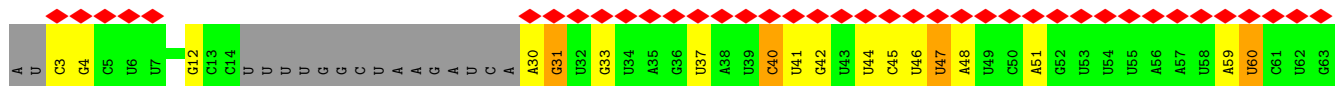
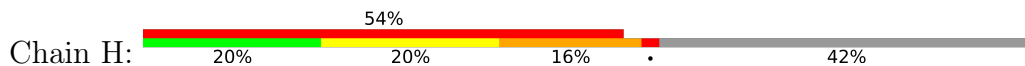
- Molecule 18: U6 snRNA-associated Sm-like protein LSm8



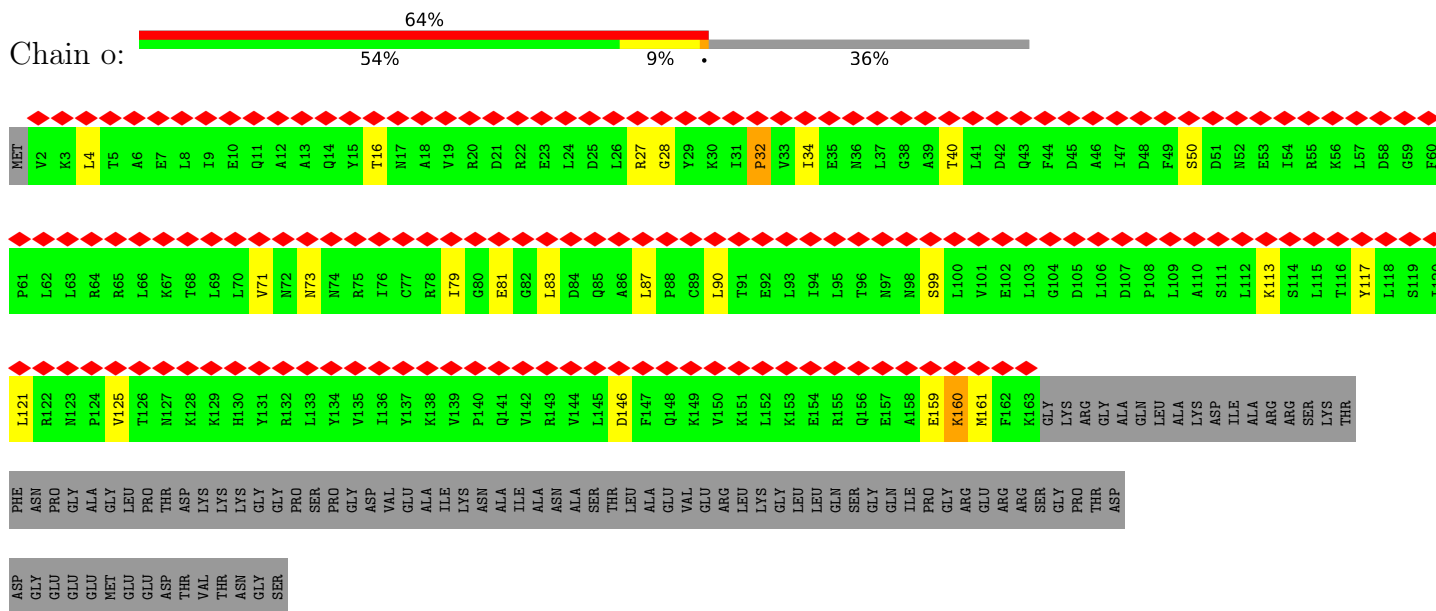
- Molecule 19: pre-mRNA



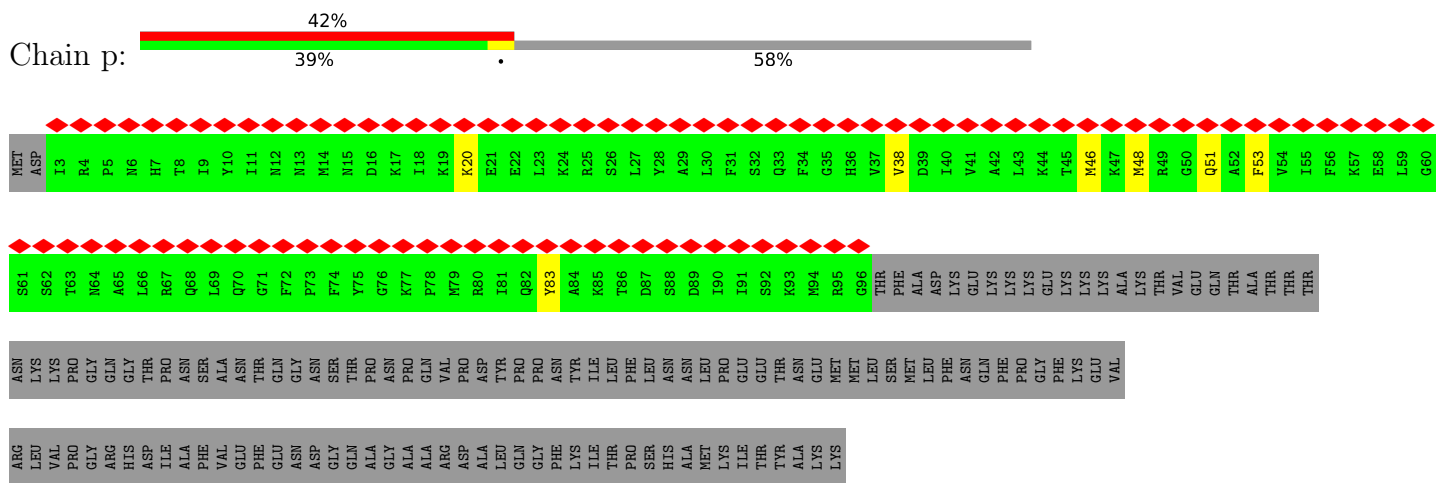
- Molecule 20: U2snRNA



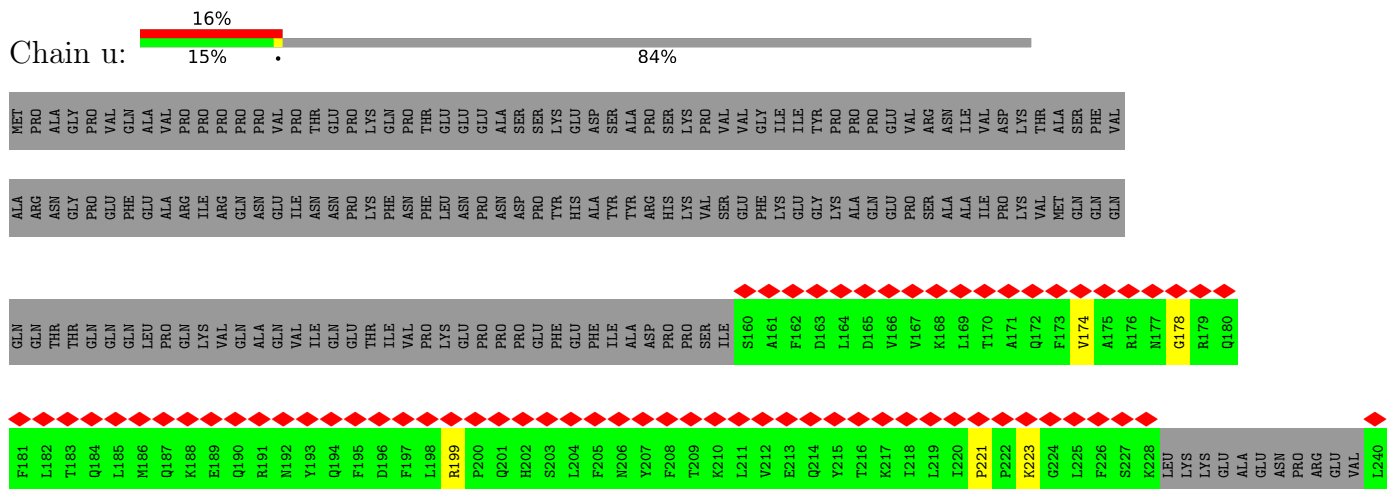
- Molecule 21: U2 small nuclear ribonucleoprotein A'

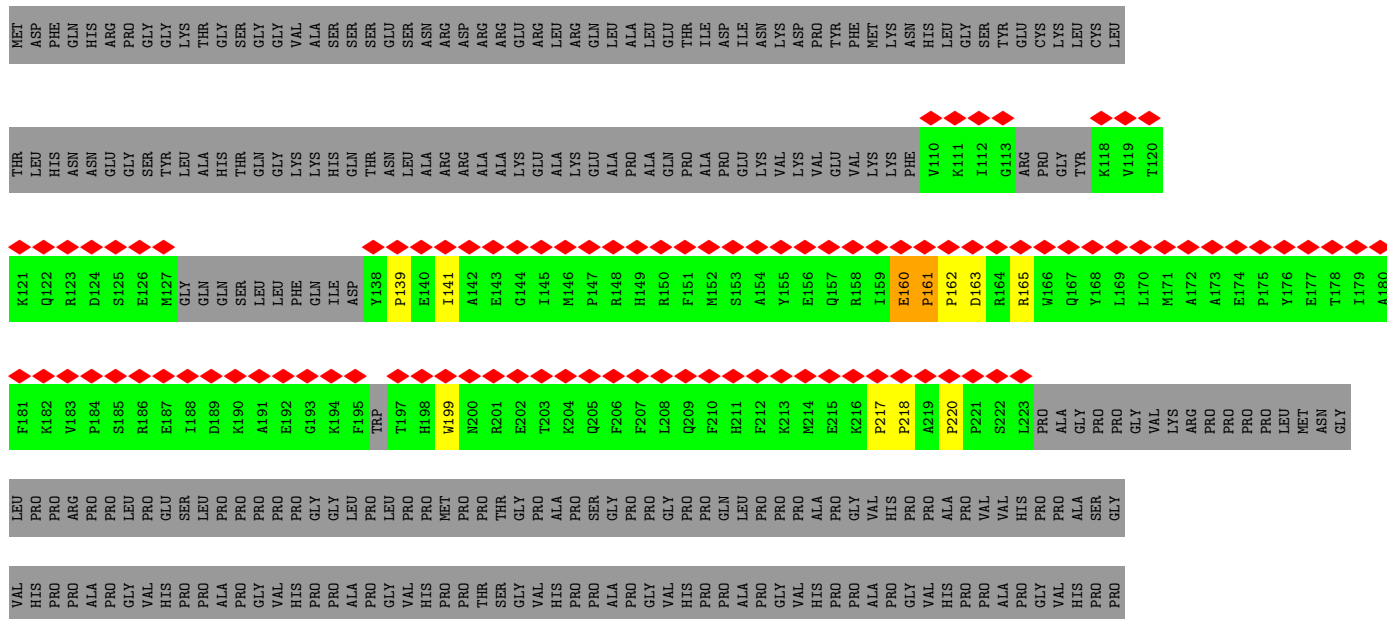


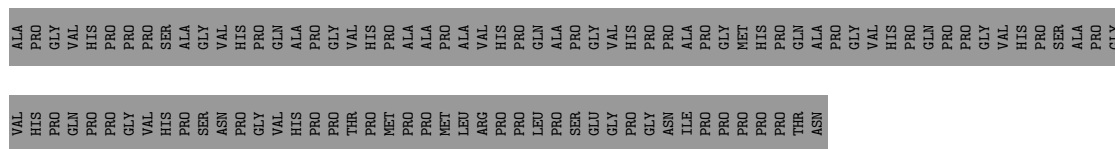
- Molecule 22: U2 small nuclear ribonucleoprotein B''



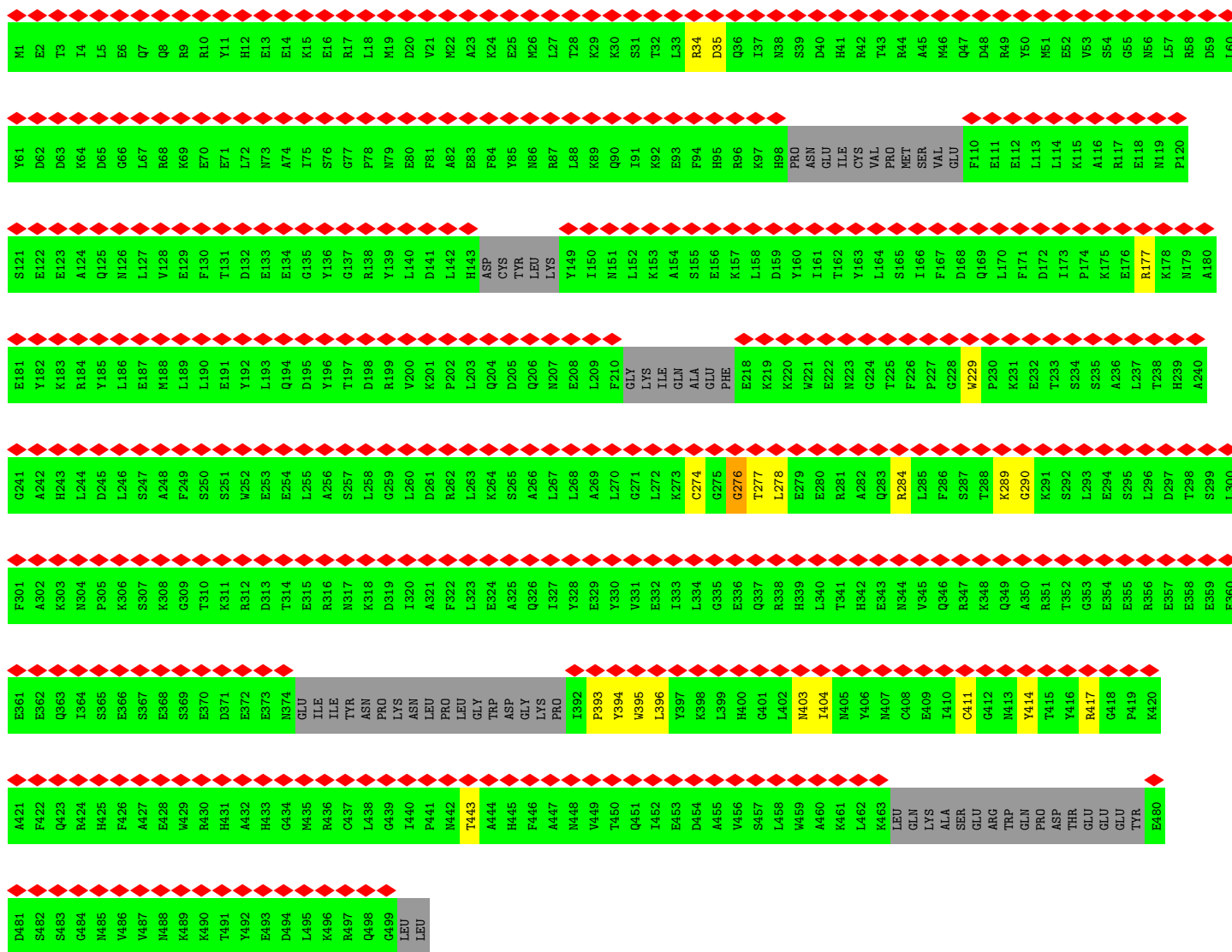
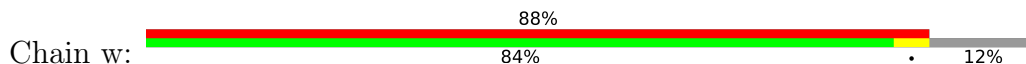
- Molecule 23: Splicing factor 3A subunit 1



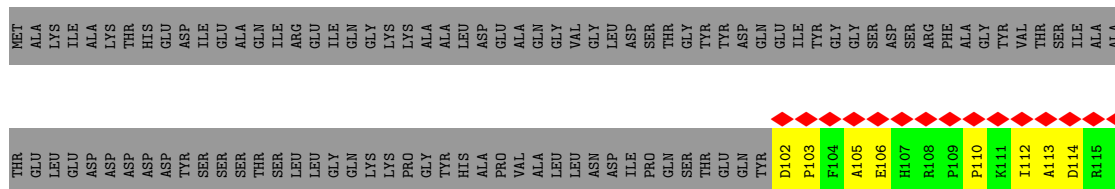
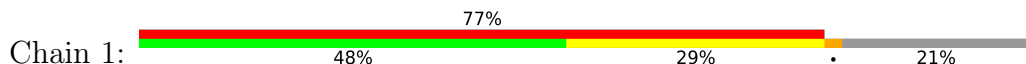




- Molecule 25: Splicing factor 3A subunit 3



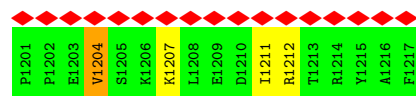
- Molecule 26: Splicing factor 3B subunit 1



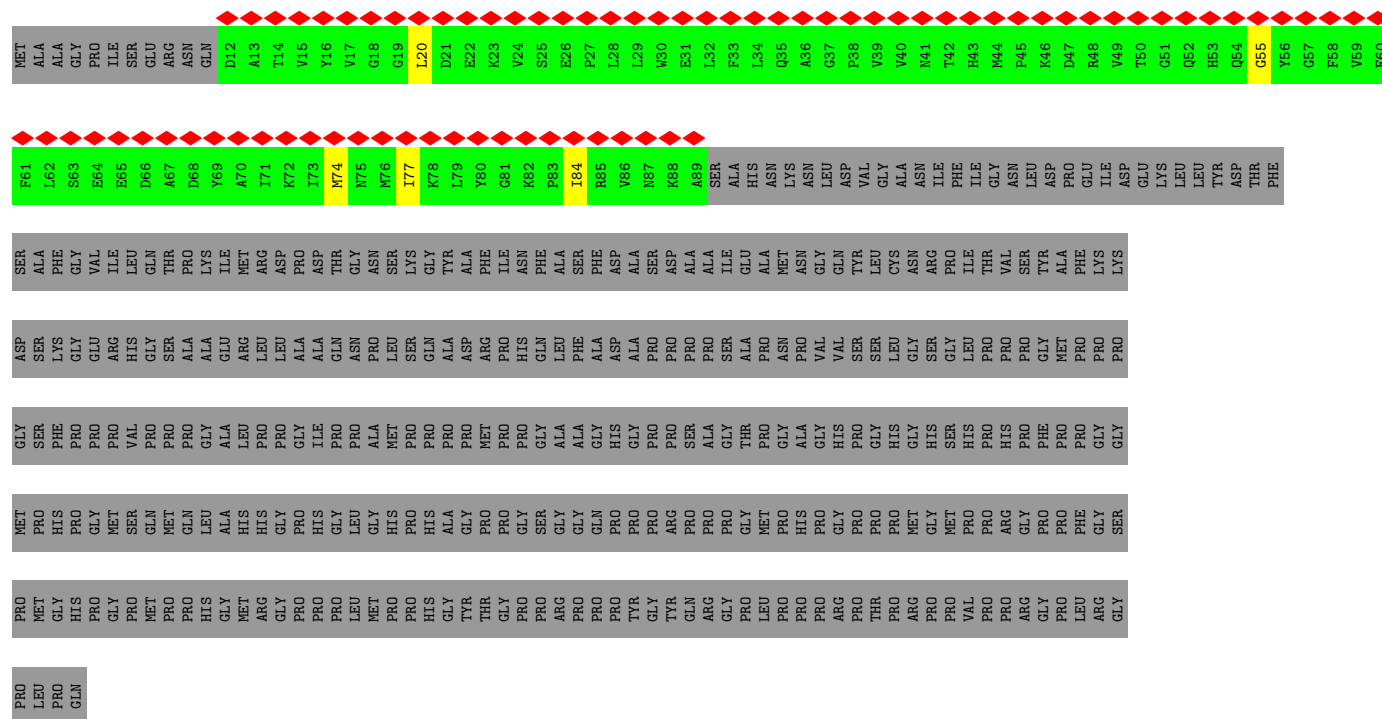
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E902	I842	E782	E722	A602	P542	V482	V422	THR	D302	S242	K182	H122
Q903	R843	E783	S723	A603	T543	D483	P423	PRO	T303	E243	V183	R123
T904	V844	M784	S724	A604	L544	E484	I424	ALA	P304	T244	V184	R124
T905	G845	K785	D725	G605	E545	S485	R425	ASN	G305	P245	N185	M125
E906	A846	K786	S726	L606	D546	THR	T426	MET	H306	G246	G186	M126
D907	A847	I787	S727	A607	Q547	LEU	P427	ALA	G307	A247	A187	I127
S908	E848	V788	L728	T608	E548	PRO	A428	THR	S308	T248	A188	I128
V909	I849	L789	K729	M609	R549	PRO	R429	PRO	G309	P249	A189	S129
M910	T850	K790	P730	M610	H550	GLY	K430	GLY	W310	G250	S190	PRO
L911	S851	V791	L731	S611	L551	HIS	L431	HIS	A311	S251	GLN	ARG
N912	R852	V792	W732	T612	L552	ILE	T432	ILE	E312	K252	PRO	GLU
G913	I853	K793	K733	M613	V553	SER	A433	SER	T313	I253	PRO	LEU
F914	V854	Q794	G734	R614	K554	THR	T434	THR	P314	W254	PRO	ASP
G915	D855	C795	I735	P615	V555	THR	P435	THR	R315	D255	ARG	PHE
T916	D856	C796	R736	D616	I556	PRO	T436	PRO	T316	P256	ARG	ALA
V917	L857	G797	Q737	L617	D557	GLN	P437	GLN	D317	T257	GLY	ASP
V918	K858	T798	H738	D618	R558	LEU	L438	LEU	R318	P258	TRP	GLY
N919	D859	D799	R739	M619	I559	GLN	G439	GLN	G319	S259	ASP	LYS
A920	E860	G800	G740	M620	L560	ALA	G440	ALA	G320	THR	THR	THR
L921	A861	V801	K741	D621	V561	TRP	M441	TRP	D321	ALA	ALA	PRO
K922	E862	E802	G742	E622	K562	ARG	T442	ARG	S322	D205	D205	PRO
K923	K863	L803	L743	P623	L563	GLU	G443	GLU	I323	Q206	Q206	LYS
R924	Y864	N804	A744	V624	D564	ARG	F444	ARG	G324	T207	T207	ASN
V925	R865	T805	A745	R625	D565	ILE	H445	ILE	E325	P208	P208	ALA
K926	K866	I806	F746	D626	I566	ASP	M446	ASP	T326	G209	G209	ARG
P927	M867	K807	L747	N626	V567	THR	Q447	THR	P327	GLY	A210	THR
V928	V868	T808	K748	T628	R568	GLU	GLU	GLU	T328	ARG	T211	TYR
L929	M869	E809	A749	A629	P569	ASP	ASP	ASP	P329	GLY	P212	MET
P930	E870	I810	I750	R630	V570	ARG	ARG	ARG	GLY	ASP	K213	VAL
Q931	T871	L811	G751	A631	V571	THR	THR	THR	ALA	PRO	P213	MET
I932	I872	P812	Y752	F632	H572	LYS	K454	LYS	LYS	GLY	K214	ARG
C933	E873	F813	L753	A633	K573	ALA	S455	ALA	LYS	ARG	L215	GLU
Q934	K874	F814	I754	V634	I574	LEU	V456	LEU	LYS	ALA	S216	GLN
T935	I875	F815	P755	V635	L575	LEU	M457	LEU	THR	GLY	W218	THR
V936	K876	K816	L756	A636	V576	GLY	D458	GLY	ASP	GLY	Q220	LYS
L937	G877	H817	K757	S637	V577	THR	Q459	THR	ALA	GLY	A221	GLU
V938	N878	F818	D758	A638	I578	PRO	P460	PRO	THR	ALA	E222	ARG
R939	L879	W819	A759	L639	E579	ALA	S461	ALA	ALA	THR	T223	ILE
L940	C880	Q820	E760	G640	P580	GLN	G462	GLN	SER	SER	P224	GLN
N941	A881	H821	Y761	I641	L581	ASN	A407	ASN	GLN	ALA	H226	LEU
K943	D883	M823	N763	S643	I582	GLY	L464	GLY	GLY	ARG	T227	A173
S944	I884	A824	I764	L644	D584	GLY	P465	GLY	GLY	ASN	P228	E174
A945	D885	L825	S765	L645	E585	THR	F466	THR	THR	THR	S229	K175
K946	H886	D826	A766	P646	D586	VAL	L467	VAL	PRO	ASP	L230	K177
V947	K887	R827	R767	F647	Y587	LEU	P469	LEU	GLU	GLU	R231	A176
R948	N888	H828	E768	L648	V588	THR	D470	THR	PRO	THR	W232	A178
Q949	E889	W829	V769	K649	A589	PRO	D471	PRO	LYS	GLY	D233	G179
N950	E890	Y830	W770	A650	R590	LYS	I472	LYS	THR	THR	E234	E180
A951	Q891	R831	L771	V651	V591	ILE	Q473	ILE	PRO	THR	T235	
A952	L892	Q832	I772	C652	E592	ILE	Y474	ILE	PRO	THR	G236	
D953	I893	L833	L773	K653	G593	THR	F475	THR	THR	THR	P237	
L954	V894	K834	I774	S654	R594	THR	D476	THR	THR	THR	G237	
I955	C895	D835	R775	K655	E595	THR	K477	THR	THR	THR	R238	
S956	I896	T836	E776	K656	I596	THR	L478	THR	THR	THR	A239	
R957	L897	T837	F777	S657	I597	THR	L479	THR	THR	THR	K240	
T958	V898	V838	Q778	V658	S598	THR	V480	THR	THR	THR		
A959	R899	E839	S779	Q659	N599	THR		THR	THR	THR		
V960	F900	L840	P780	A660	L600	THR		THR	THR	THR		



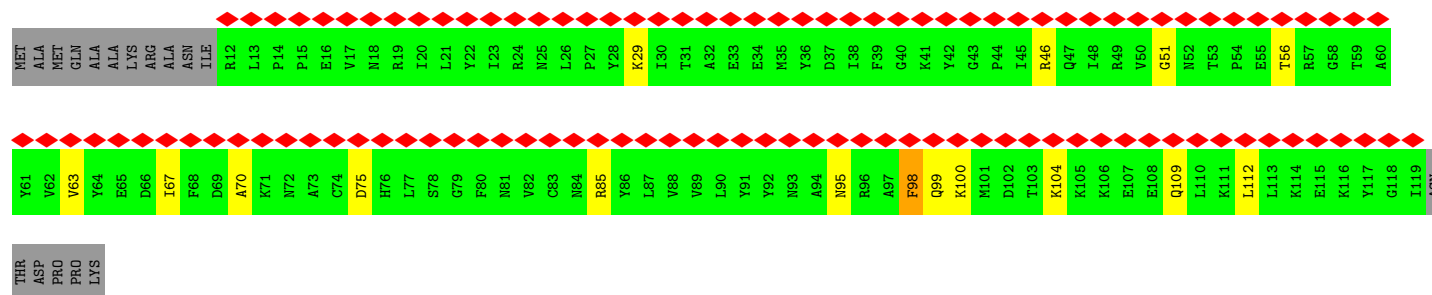
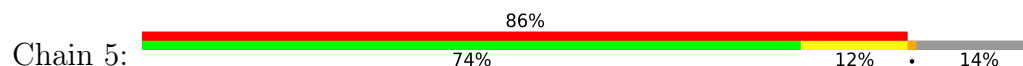




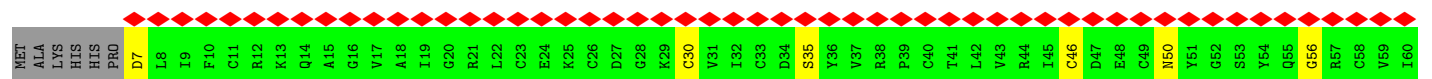
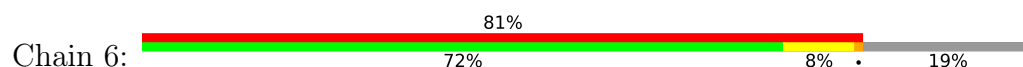
• Molecule 29: Splicing factor 3B subunit 4

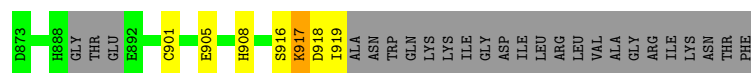


• Molecule 30: Splicing factor 3B subunit 6

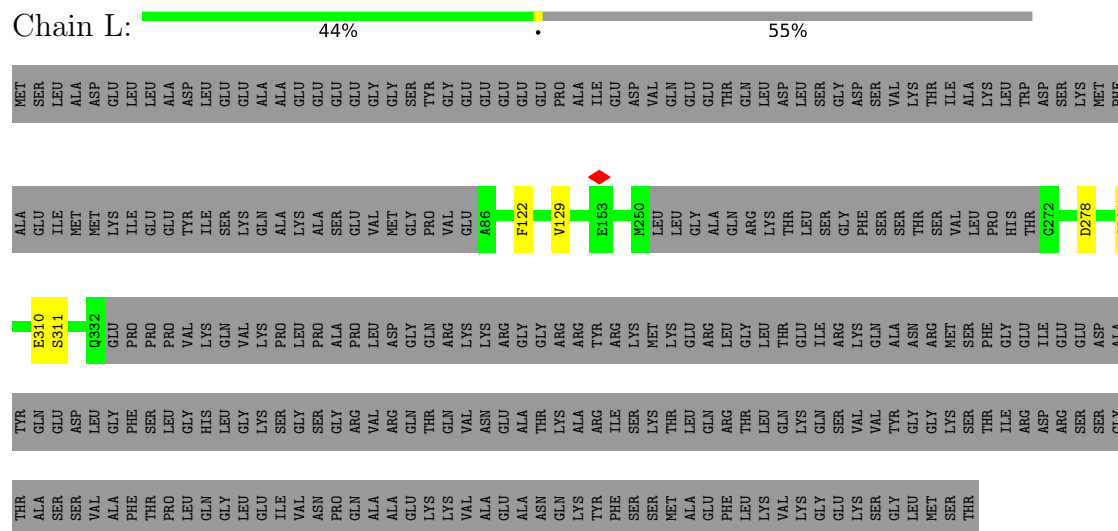


• Molecule 31: PHD finger-like domain-containing protein 5A

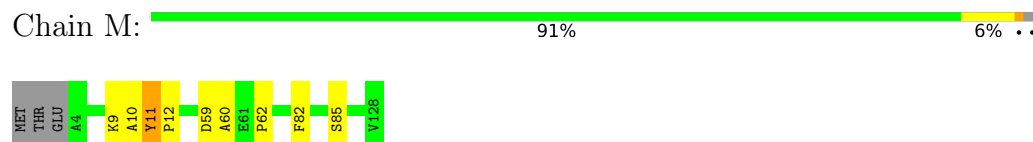




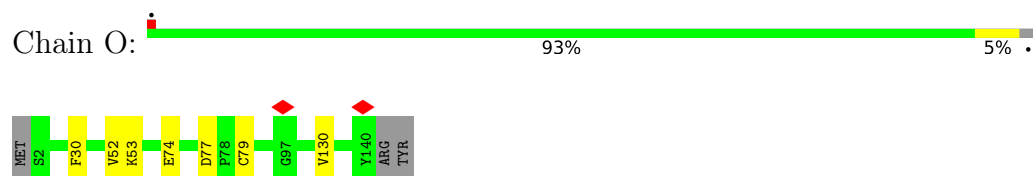
- Molecule 36: U4/U6 small nuclear ribonucleoprotein Prp31



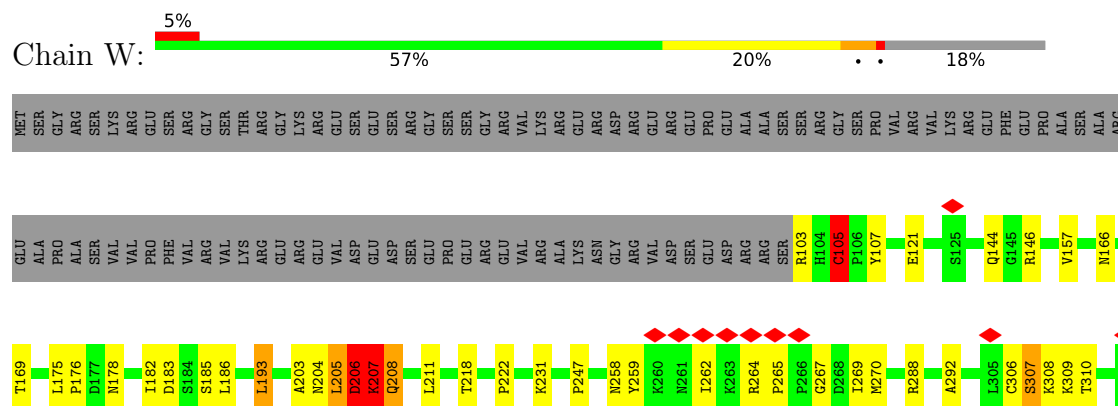
- Molecule 37: NHP2-like protein 1

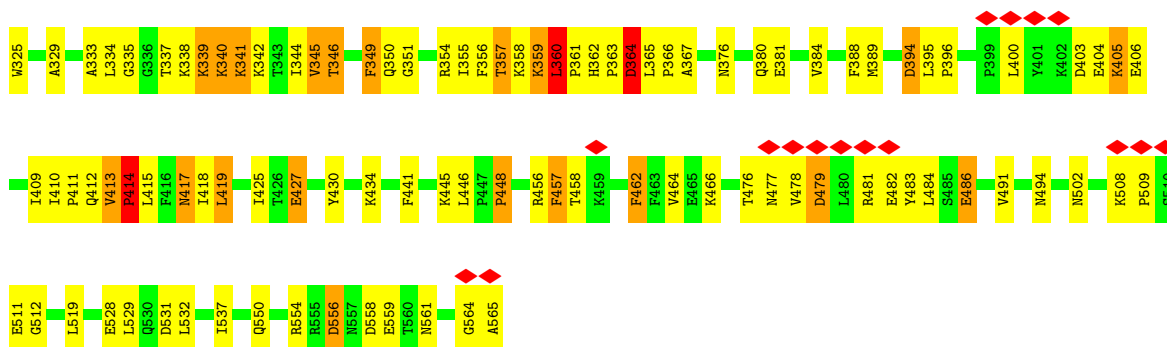


- Molecule 38: Thioredoxin-like protein 4A

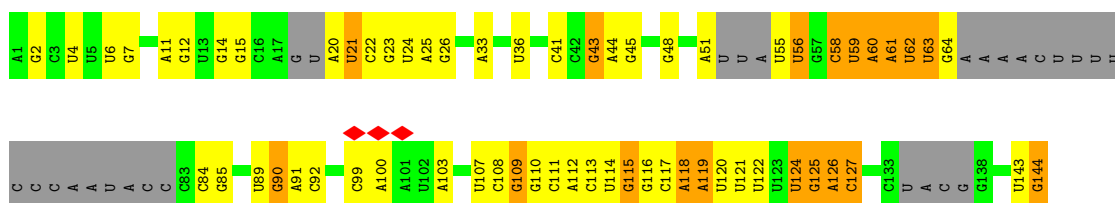


- Molecule 39: U4/U6.U5 tri-snRNP-associated protein 2

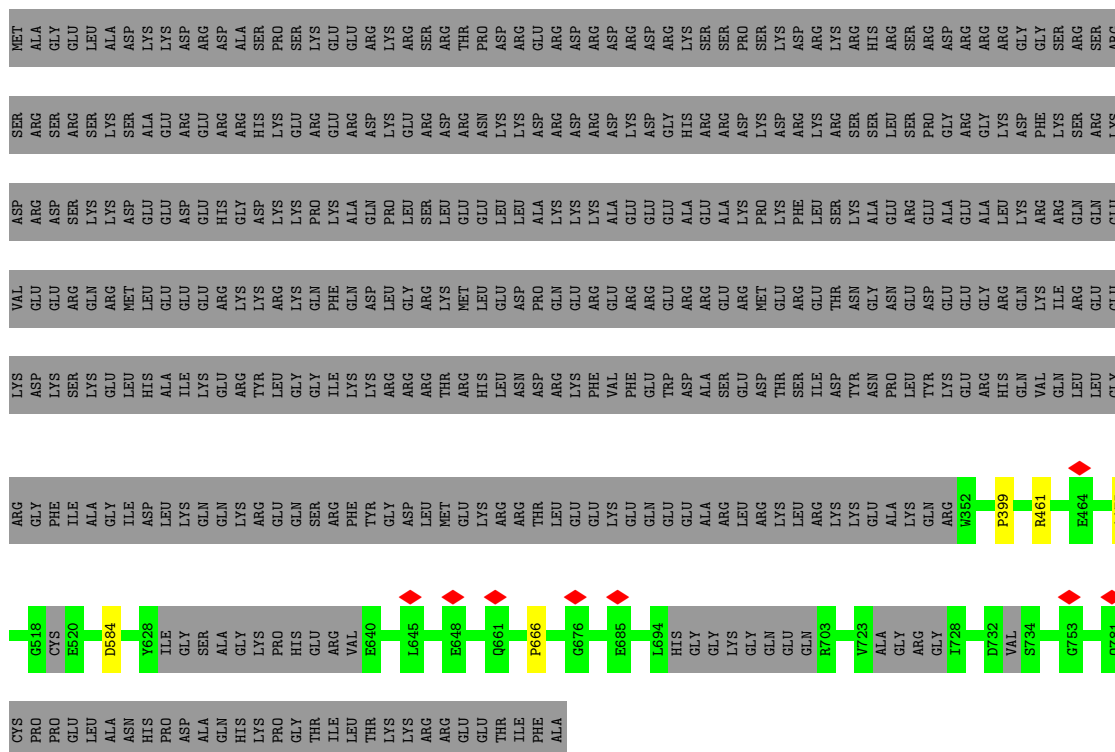




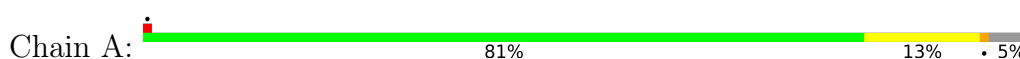
- Molecule 40: U4snRNA

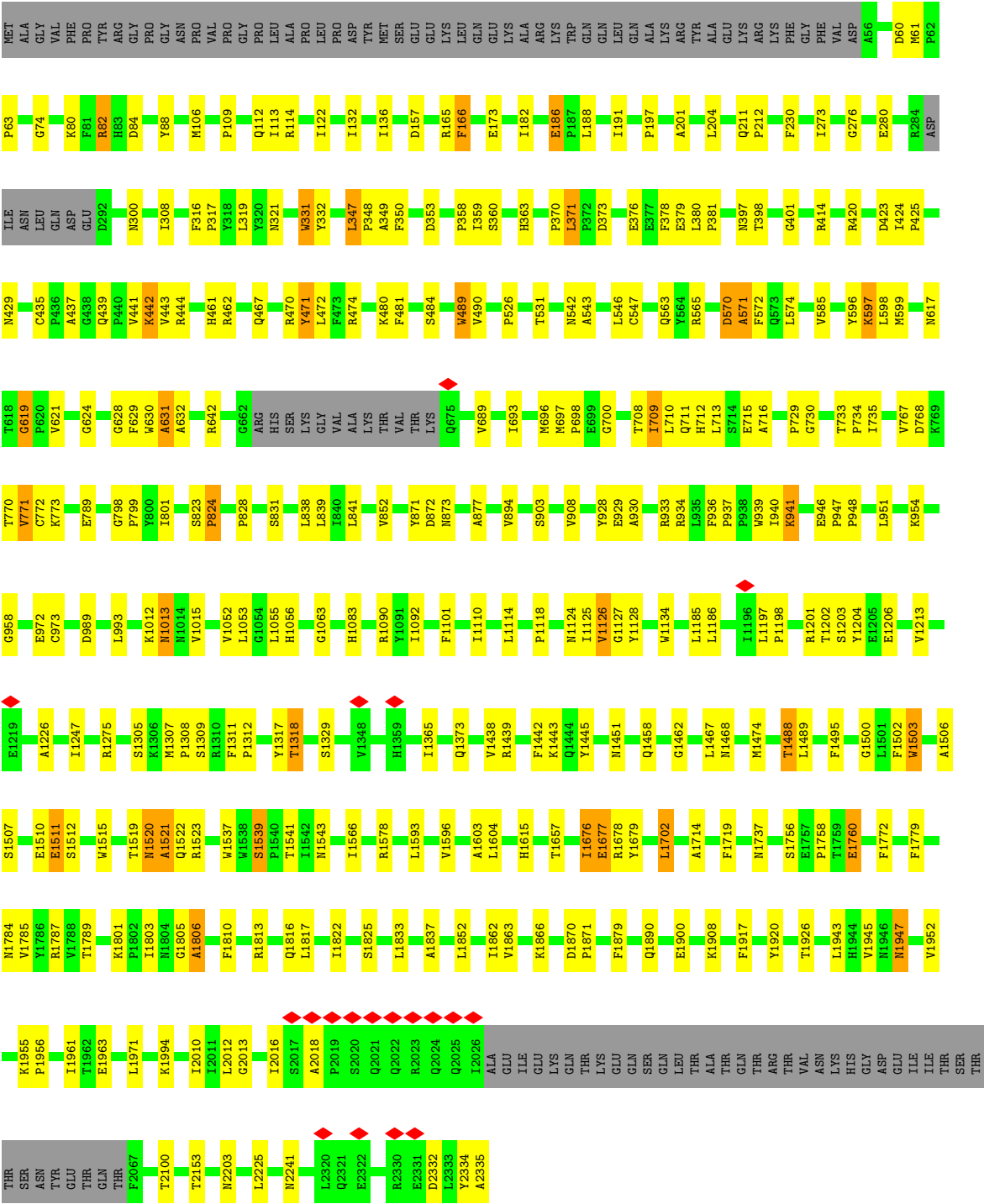


- Molecule 41: Probable ATP-dependent RNA helicase DDX23

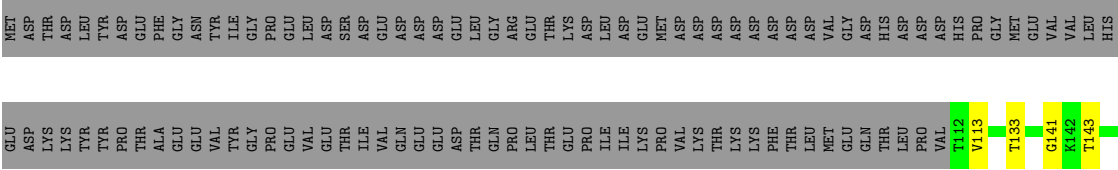


- Molecule 42: Pre-mRNA-processing-splicing factor 8





• Molecule 43: 116 kDa U5 small nuclear ribonucleoprotein component



E156	I157	R158	LYS	ARG	TYR	ASP	GLN	ASP	ASP	CYS	THR	ASP	ILE	LEU	PHE	T173	R177	V225	V226	M236	L237	I257	L263	K268	S310	Q313	D333	Y336	K341	R342	L343	W344	R354	K355	A360	P361	Q366	R367	V385	G386	D387	V388
F427	T428	Q436	H437	I438	P439	S440	G444	A445	K448	I449	T452	V457	D458	G462	P470	G471	G472	P473	L474	M475	V496	I497	S498	G499	L516	E519	A535	R536	G547	D556	I559	E572	E573	F577	R578	P615	I651	D652	I653	D657		
T661	E664	T665	V666	V667	N680	K681	K682	N683	K684	G736	L750	K756	A757	E776	G777	P778	D781	E782	R785	V795	V796	A797	Q798	E799	A823	T824	P825	R826	L827	A838	H856	L868	I906	V907	F908	G909	R919	E922	F923	Q924	A930	
K936	I943	SER	GLU	ASP	VAL	SER	ILE	SER	LYS	PHE	PHE	ASP	ASP	PRO	MET	LEU	LEU	GLU	LEU	ALA	LYS	GLN	ASP	VAL	VAL	LEU	ASN	TYR	PRO	MET												

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186162	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	0.116	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	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 ⓘ

5.1 Standard geometry ⓘ

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	B	0.12	0/2697	0.23	0/4193
2	D	0.55	0/7493	1.20	34/9361 (0.4%)
3	E	1.08	0/1195	1.22	5/1492 (0.3%)
4	P	0.15	0/298	0.49	0/370
4	a	0.13	0/316	0.46	0/392
4	k	1.18	0/338	1.20	1/419 (0.2%)
5	Q	0.20	0/291	0.47	0/363
5	b	0.20	0/299	0.45	0/373
5	m	1.24	1/295 (0.3%)	1.26	0/367
6	R	0.16	0/313	0.46	0/390
6	c	0.15	0/313	0.45	0/390
6	l	1.02	0/315	1.26	0/392
7	S	0.22	0/297	0.59	0/371
7	d	0.21	0/281	0.58	0/351
7	n	0.86	0/270	1.05	0/334
8	T	0.13	0/287	0.35	0/358
8	e	0.13	0/317	0.61	0/396
8	h	0.81	0/318	1.01	0/394
9	U	0.12	0/254	0.39	0/314
9	f	0.13	0/258	0.41	0/320
9	i	0.77	0/290	1.10	1/359 (0.3%)
10	V	0.14	0/333	0.46	0/416
10	g	0.13	0/378	0.44	0/471
10	j	0.89	0/327	1.11	0/407
11	F	0.25	1/1639 (0.1%)	0.38	2/2545 (0.1%)
12	q	0.69	0/359	1.28	0/447
13	r	0.74	0/298	1.87	5/369 (1.4%)
14	s	0.58	0/294	1.32	3/364 (0.8%)
15	t	0.69	0/298	1.27	2/369 (0.5%)
16	x	0.68	0/279	1.29	0/347
17	y	0.59	0/258	1.14	0/319
18	z	0.69	0/242	1.22	1/299 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	G	0.60	4/954 (0.4%)	0.80	2/1477 (0.1%)
20	H	0.68	12/2576 (0.5%)	1.00	18/4003 (0.4%)
21	o	0.98	0/647	2.34	34/807 (4.2%)
22	p	0.97	0/375	1.97	7/467 (1.5%)
23	u	0.36	0/493	0.97	2/611 (0.3%)
24	v	0.40	0/392	1.38	6/483 (1.2%)
25	w	0.37	0/1767	0.90	4/2199 (0.2%)
26	1	1.71	38/4112 (0.9%)	1.37	21/5126 (0.4%)
27	2	1.15	0/738	1.22	3/912 (0.3%)
28	3	1.39	26/4689 (0.6%)	1.19	7/5849 (0.1%)
29	4	1.07	0/311	1.15	1/387 (0.3%)
30	5	1.23	2/431 (0.5%)	1.27	1/537 (0.2%)
31	6	1.17	0/355	1.13	0/442
32	7	1.59	1/263 (0.4%)	1.23	0/327
33	J	1.13	2/664 (0.3%)	1.25	5/823 (0.6%)
34	K	1.20	3/1367 (0.2%)	1.40	18/1702 (1.1%)
35	N	0.89	2/2297 (0.1%)	1.51	18/2838 (0.6%)
36	L	0.63	0/902	1.13	4/1124 (0.4%)
37	M	0.67	0/499	1.25	5/622 (0.8%)
38	O	1.23	1/555 (0.2%)	1.24	1/692 (0.1%)
39	W	0.88	1/1851 (0.1%)	1.96	56/2312 (2.4%)
40	I	0.23	1/2779 (0.0%)	0.37	0/4319
41	X	0.74	0/1655	1.28	6/2062 (0.3%)
42	A	1.03	12/8880 (0.1%)	1.58	156/11093 (1.4%)
43	C	1.05	2/3270 (0.1%)	1.50	44/4084 (1.1%)
All	All	0.93	109/64262 (0.2%)	1.23	473/83350 (0.6%)

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
2	D	0	1
4	k	0	1
16	x	0	1
25	w	0	1
26	1	0	15
27	2	0	2
28	3	0	13
30	5	0	1
31	6	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	7	0	1
34	K	0	1
35	N	0	6
39	W	0	62
43	C	0	1
All	All	0	108

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	A	597	LYS	C-N	17.92	1.58	1.33
26	1	719	TYR	C-O	-13.59	1.11	1.24
42	A	877	ALA	C-N	12.10	1.50	1.33
26	1	718	PRO	CA-C	-11.67	1.41	1.52
26	1	1243	PRO	N-CA	-9.51	1.35	1.47

The worst 5 of 473 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	N	369	LEU	CA-C-N	-25.14	88.41	119.84
35	N	369	LEU	C-N-CA	-25.14	88.41	119.84
13	r	82	ILE	CA-C-N	17.59	141.83	119.84
13	r	82	ILE	C-N-CA	17.59	141.83	119.84
42	A	1451	ASN	CA-C-N	16.74	140.77	119.84

There are no chirality outliers.

5 of 108 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	110	PRO	Peptide
2	D	430	LEU	Peptide
4	k	112	ASN	Peptide
25	w	443	THR	Peptide
16	x	51	TYR	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	B	2419	0	1224	61	0
2	D	7496	0	1961	22	0
3	E	1196	0	337	2	0
4	P	300	0	80	10	0
4	a	318	0	86	0	0
4	k	340	0	87	0	0
5	Q	292	0	93	1	0
5	b	300	0	95	0	0
5	m	296	0	87	0	0
6	R	314	0	86	0	0
6	c	314	0	86	0	0
6	l	316	0	85	1	0
7	S	298	0	89	1	0
7	d	282	0	85	0	0
7	n	272	0	75	1	0
8	T	288	0	84	0	0
8	e	318	0	92	0	0
8	h	320	0	88	0	0
9	U	256	0	70	3	0
9	f	260	0	74	2	0
9	i	292	0	80	0	0
10	V	334	0	92	16	0
10	g	380	0	103	0	0
10	j	328	0	89	0	0
11	F	1470	0	745	49	0
12	q	360	0	95	3	0
13	r	300	0	77	6	0
14	s	296	0	77	0	0
15	t	300	0	80	1	0
16	x	280	0	81	3	0
17	y	260	0	75	0	0
18	z	244	0	71	1	0
19	G	862	0	441	140	0
20	H	2311	0	1170	154	0
21	o	648	0	167	1	0
22	p	376	0	102	0	0
23	u	496	0	118	1	0
24	v	396	0	91	0	0
25	w	1773	0	477	27	0
26	1	4120	0	1091	239	0
27	2	744	0	189	6	0
28	3	4696	0	1266	69	0
29	4	312	0	87	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	5	432	0	114	7	0
31	6	356	0	105	5	0
32	7	264	0	70	11	0
33	J	668	0	179	8	0
34	K	1371	0	384	17	0
35	N	2316	0	581	46	0
36	L	904	0	235	2	0
37	M	500	0	128	4	0
38	O	556	0	147	2	0
39	W	1852	0	477	34	0
40	I	2491	0	1262	118	0
41	X	1661	0	440	0	0
42	A	8884	0	2284	159	0
43	C	3272	0	874	51	0
44	A	36	0	6	0	0
45	C	32	0	12	4	0
46	C	1	0	0	0	0
All	All	63369	0	19126	1151	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 1151 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:145:U:C2'	19:G:146:C:H5''	1.54	1.37
33:J:536:ASP:CA	33:J:587:GLY:CA	2.11	1.28
43:C:470:PRO:CA	43:C:499:GLY:HA2	1.64	1.27
40:I:63:U:H2'	40:I:64:G:C8	1.69	1.26
33:J:536:ASP:CA	33:J:587:GLY:HA3	1.64	1.25

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	
2	D	1868/2136 (88%)	1770 (95%)	93 (5%)	5 (0%)	36	72
3	E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	3	22
4	P	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
4	a	74/118 (63%)	71 (96%)	3 (4%)	0	100	100
4	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
5	Q	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
5	b	71/86 (83%)	70 (99%)	1 (1%)	0	100	100
5	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
6	R	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
6	c	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
6	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
7	S	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
7	d	67/76 (88%)	63 (94%)	4 (6%)	0	100	100
7	n	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
8	T	69/126 (55%)	69 (100%)	0	0	100	100
8	e	76/126 (60%)	73 (96%)	3 (4%)	0	100	100
8	h	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
9	U	60/231 (26%)	57 (95%)	3 (5%)	0	100	100
9	f	60/231 (26%)	57 (95%)	3 (5%)	0	100	100
9	i	69/231 (30%)	68 (99%)	1 (1%)	0	100	100
10	V	80/119 (67%)	76 (95%)	4 (5%)	0	100	100
10	g	89/119 (75%)	84 (94%)	5 (6%)	0	100	100
10	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
12	q	88/95 (93%)	77 (88%)	7 (8%)	4 (4%)	2	16
13	r	71/102 (70%)	66 (93%)	3 (4%)	2 (3%)	4	24
14	s	70/139 (50%)	64 (91%)	5 (7%)	1 (1%)	9	39
15	t	71/91 (78%)	64 (90%)	4 (6%)	3 (4%)	2	17
16	x	68/80 (85%)	66 (97%)	2 (3%)	0	100	100
17	y	61/103 (59%)	56 (92%)	5 (8%)	0	100	100
18	z	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	41
22	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
23	u	118/793 (15%)	106 (90%)	6 (5%)	6 (5%)	1	14
24	v	91/464 (20%)	66 (72%)	16 (18%)	9 (10%)	0	7
25	w	431/501 (86%)	385 (89%)	41 (10%)	5 (1%)	10	43
26	1	1014/1304 (78%)	821 (81%)	171 (17%)	22 (2%)	5	28
27	2	174/895 (19%)	155 (89%)	14 (8%)	5 (3%)	3	23
28	3	1160/1217 (95%)	1062 (92%)	90 (8%)	8 (1%)	18	55
29	4	76/424 (18%)	74 (97%)	2 (3%)	0	100	100
30	5	106/125 (85%)	83 (78%)	20 (19%)	3 (3%)	4	24
31	6	87/110 (79%)	76 (87%)	11 (13%)	0	100	100
32	7	64/86 (74%)	55 (86%)	8 (12%)	1 (2%)	7	37
33	J	159/683 (23%)	148 (93%)	7 (4%)	4 (2%)	4	25
34	K	335/522 (64%)	295 (88%)	26 (8%)	14 (4%)	2	17
35	N	541/941 (58%)	475 (88%)	41 (8%)	25 (5%)	2	16
36	L	222/499 (44%)	214 (96%)	8 (4%)	0	100	100
37	M	123/128 (96%)	117 (95%)	6 (5%)	0	100	100
38	O	137/142 (96%)	126 (92%)	9 (7%)	2 (2%)	8	39
39	W	461/565 (82%)	327 (71%)	77 (17%)	57 (12%)	0	4
41	X	402/820 (49%)	393 (98%)	8 (2%)	1 (0%)	43	77
42	A	2213/2335 (95%)	2046 (92%)	100 (4%)	67 (3%)	3	22
43	C	814/972 (84%)	751 (92%)	40 (5%)	23 (3%)	4	24
All	All	13158/19749 (67%)	11964 (91%)	915 (7%)	279 (2%)	8	29

5 of 279 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	354	PRO
2	D	957	VAL
2	D	1584	ILE
3	E	193	THR
12	q	55	LEU

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	114/117 (97%)	38 (33%)	2 (1%)
11	F	65/107 (60%)	10 (15%)	2 (3%)
19	G	41/274 (14%)	28 (68%)	9 (21%)
20	H	105/188 (55%)	25 (23%)	2 (1%)
40	I	112/144 (77%)	31 (27%)	4 (3%)
All	All	437/830 (52%)	132 (30%)	19 (4%)

5 of 132 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	8	G
1	B	10	U
1	B	20	G
1	B	21	A
1	B	22	U

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	H	168	A
40	I	99	C
40	I	114	U
40	I	58	C
19	G	150	U

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

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
45	GTP	C	1500	46	33,34,34	1.54	5 (15%)	50,54,54	1.66	6 (12%)
44	IHP	A	3000	-	36,36,36	0.82	0	60,60,60	1.26	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	C	1500	46	-	3/22/38/38	0/3/3/3
44	IHP	A	3000	-	-	5/30/54/54	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1500	GTP	PA-O3A	4.30	1.64	1.59
45	C	1500	GTP	C6-N1	-3.44	1.32	1.38
45	C	1500	GTP	C5-C4	2.70	1.46	1.38
45	C	1500	GTP	C4-N9	-2.28	1.32	1.38
45	C	1500	GTP	C5-N7	-2.24	1.34	1.39

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C	1500	GTP	C5-C4-N3	-5.94	118.94	128.39
45	C	1500	GTP	C2-N3-C4	4.78	120.53	112.30
45	C	1500	GTP	N9-C4-N3	3.82	133.58	125.95
44	A	3000	IHP	C6-C5-C4	3.79	118.73	110.43
45	C	1500	GTP	C6-C5-N7	3.28	136.26	130.29

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

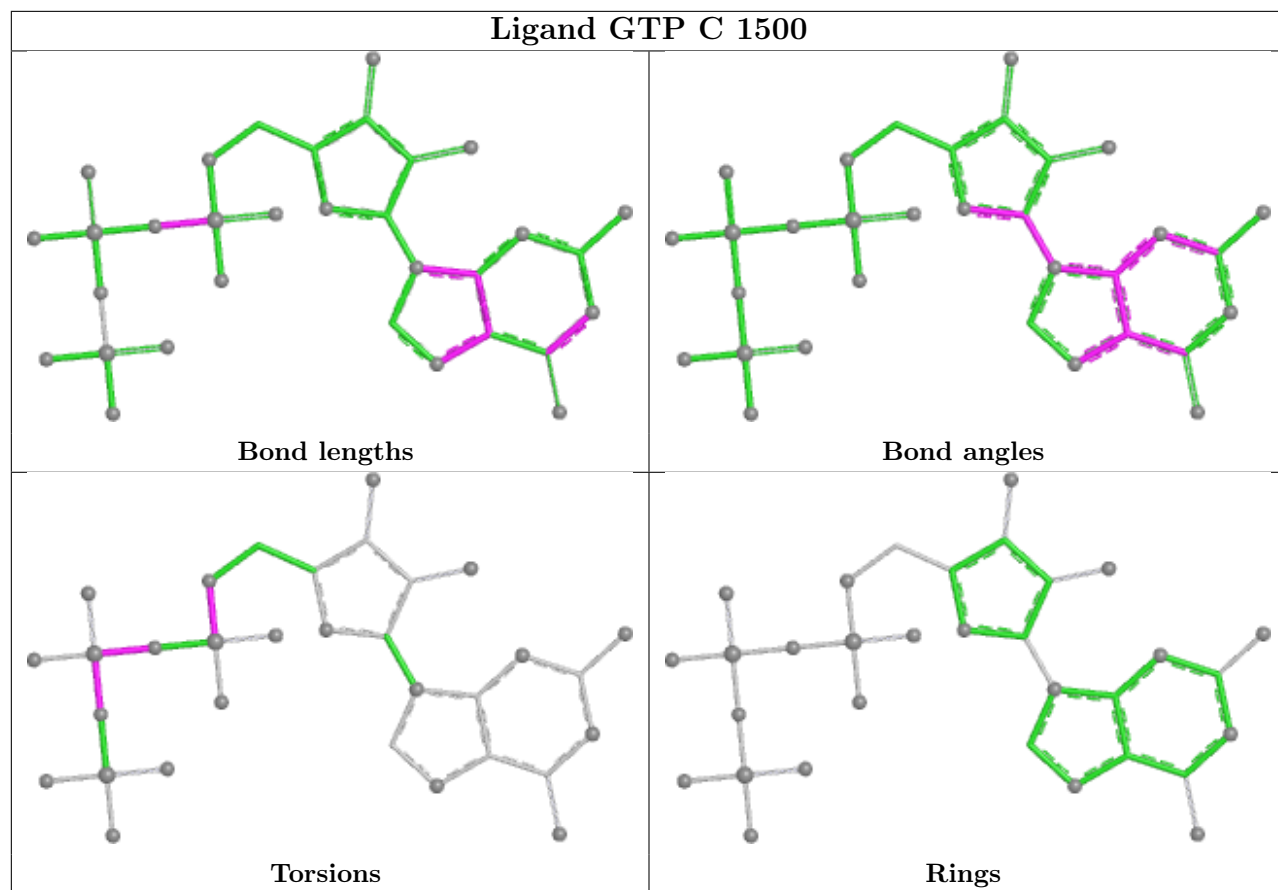
Mol	Chain	Res	Type	Atoms
45	C	1500	GTP	C5'-O5'-PA-O3A
44	A	3000	IHP	C3-O13-P3-O23
44	A	3000	IHP	C2-O12-P2-O42
44	A	3000	IHP	C5-O15-P5-O25
45	C	1500	GTP	PG-O3B-PB-O2B

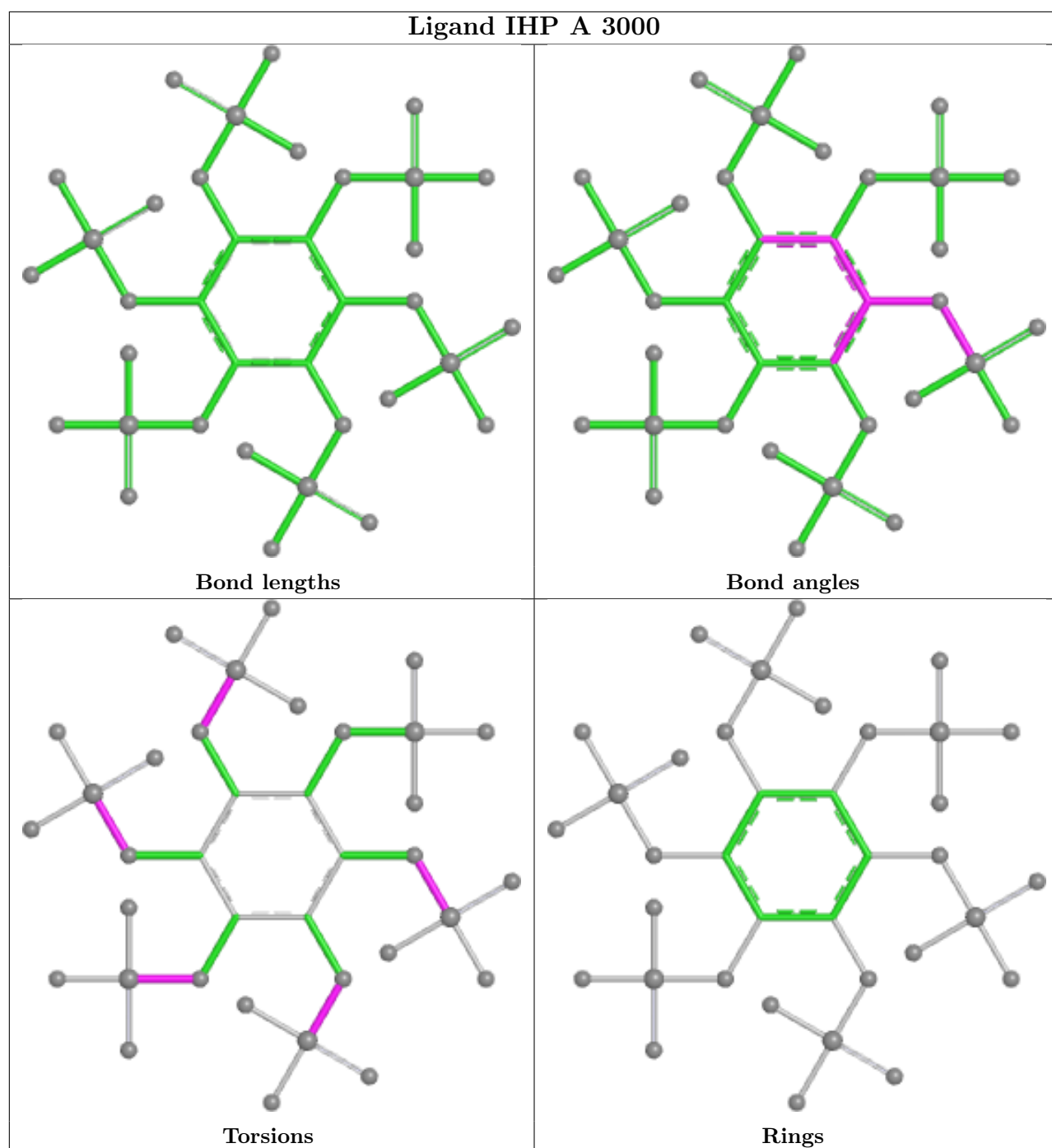
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	C	1500	GTP	4	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.

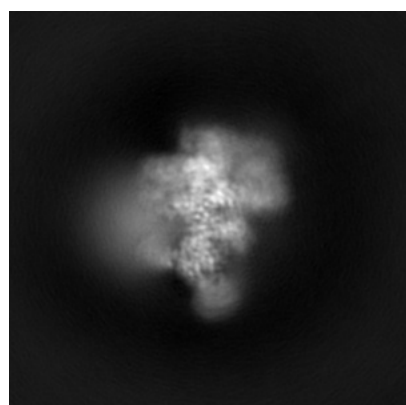
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9621. These allow visual inspection of the internal detail of the map and identification of artifacts.

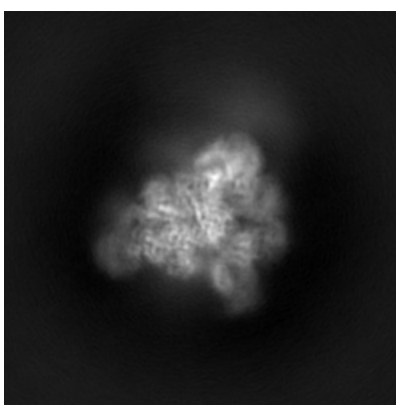
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

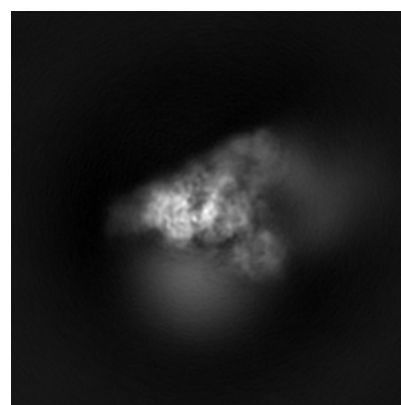
6.1.1 Primary map



X



Y

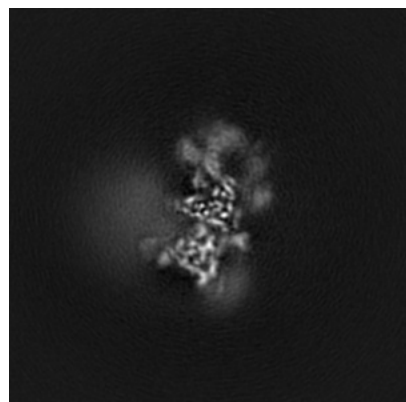


Z

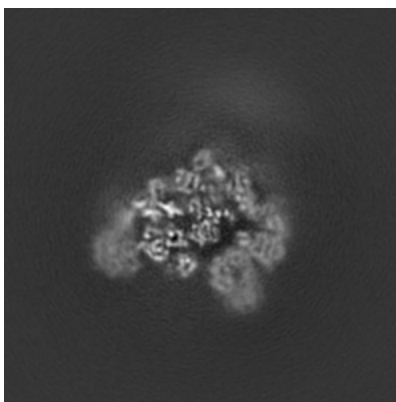
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

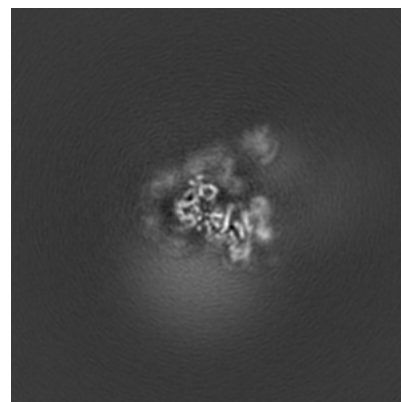
6.2.1 Primary map



X Index: 200



Y Index: 200

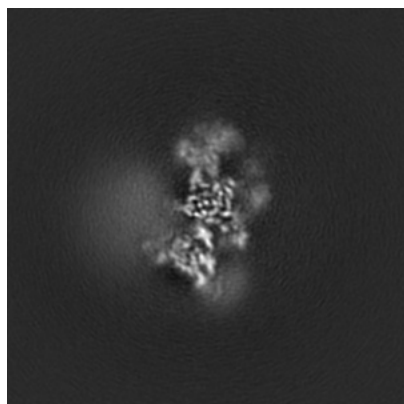


Z Index: 200

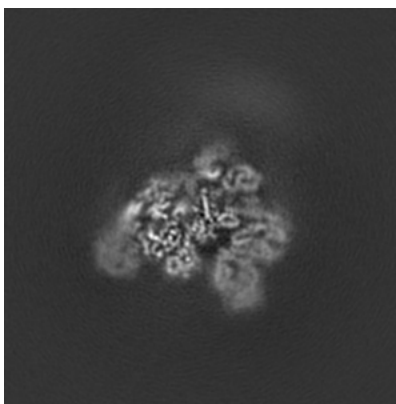
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

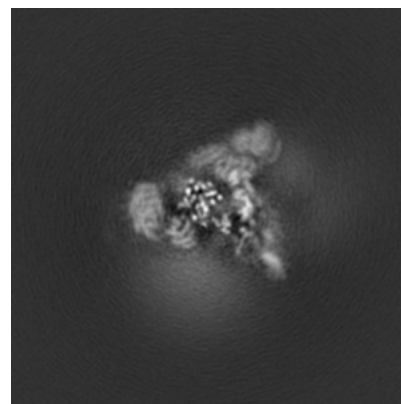
6.3.1 Primary map



X Index: 197



Y Index: 193

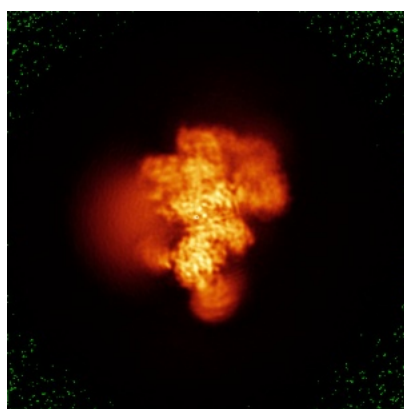


Z Index: 213

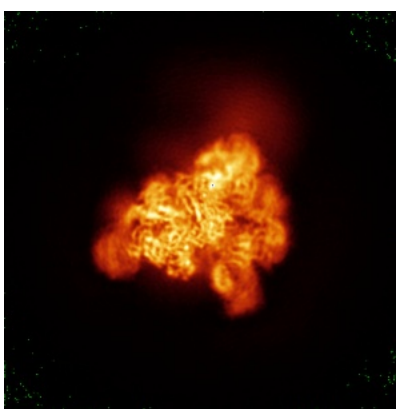
The images above show the largest variance slices of the map in three orthogonal directions.

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

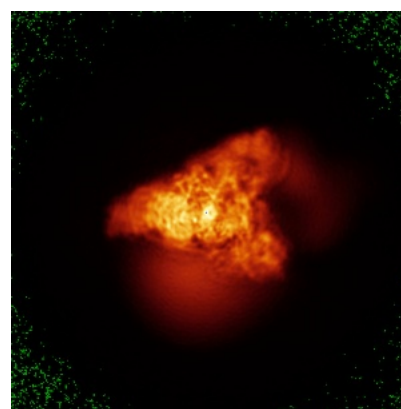
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

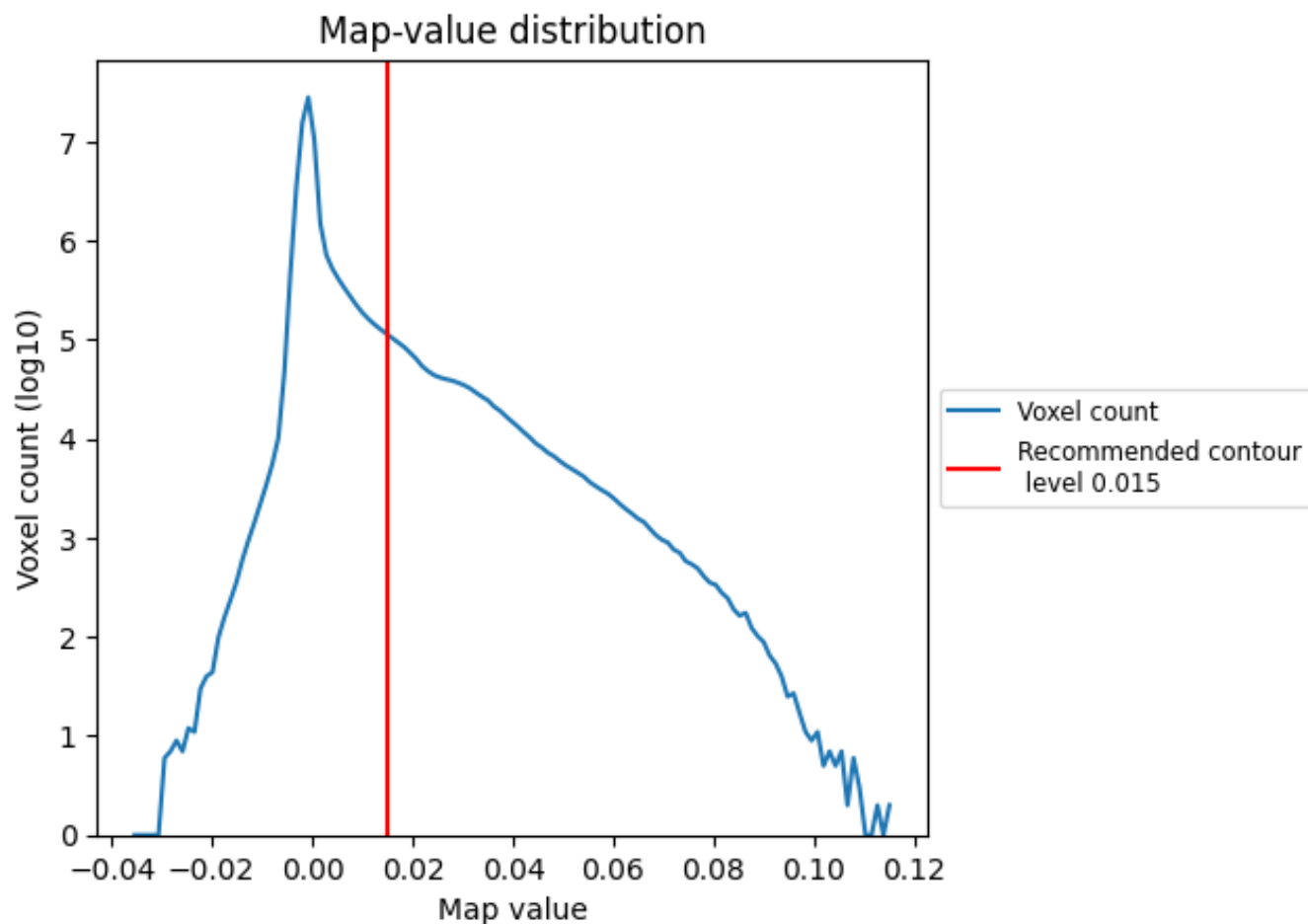
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

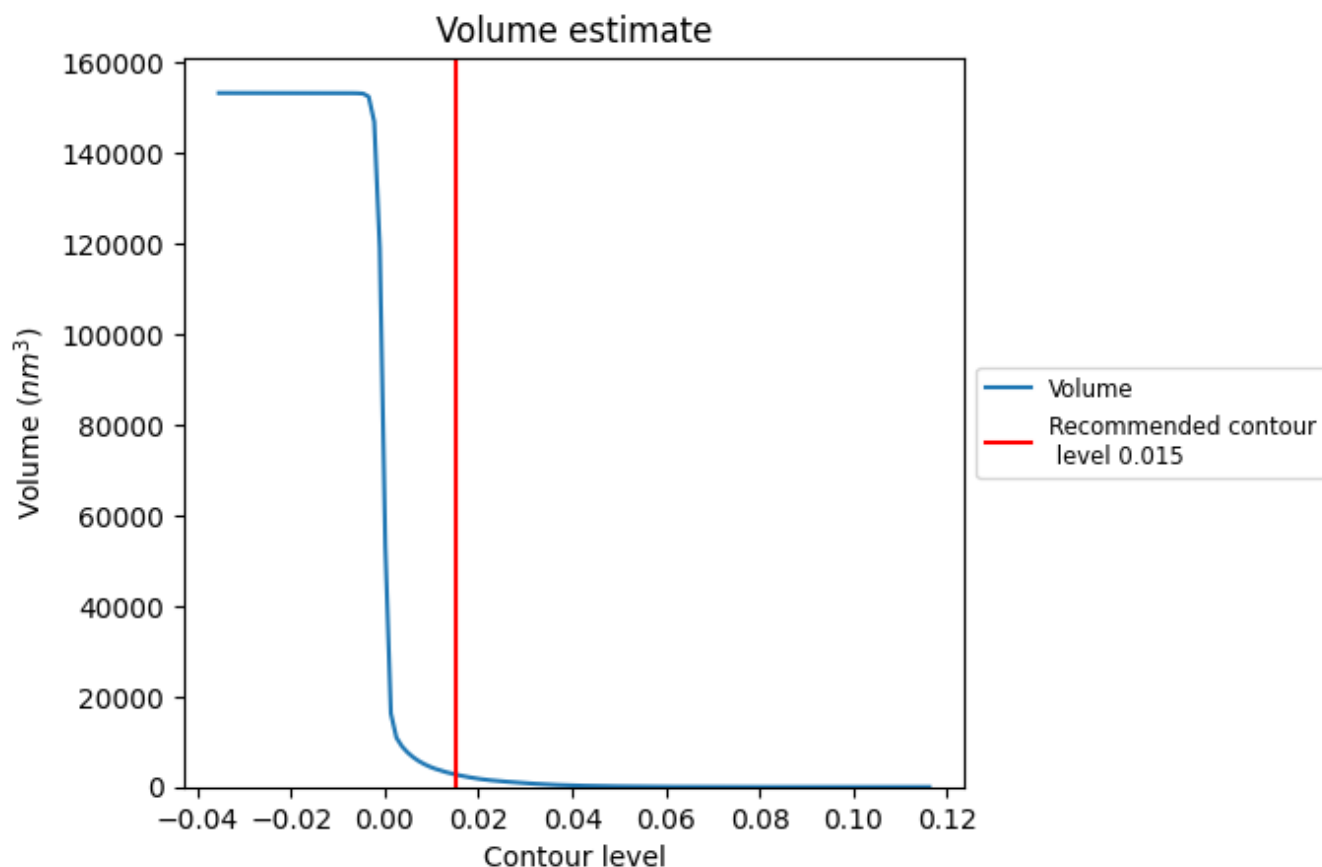
This section contains the results of statistical analysis of the map.

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.

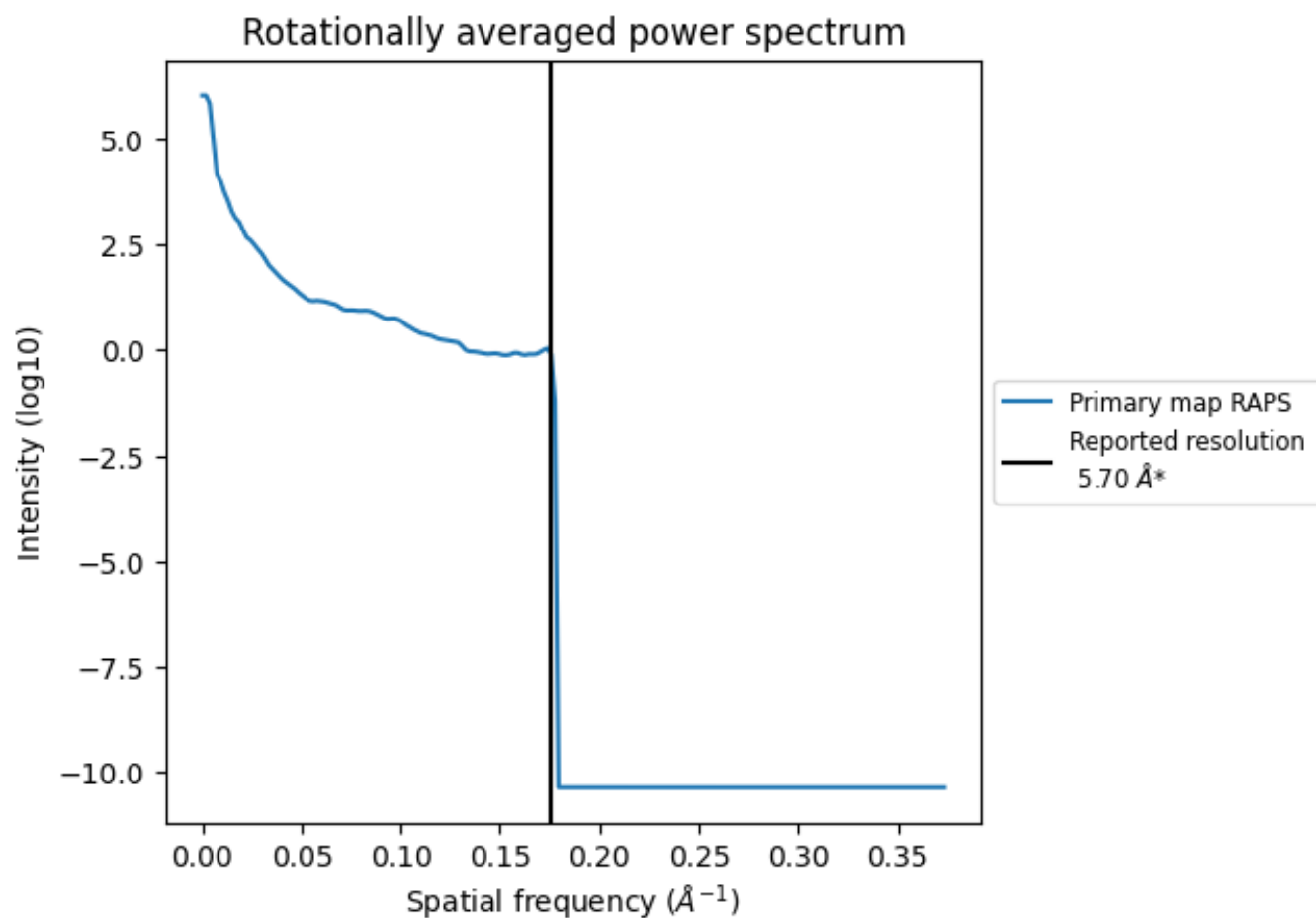
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2784 nm³; this corresponds to an approximate mass of 2515 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 0.175 $\text{\AA}^{-1}$

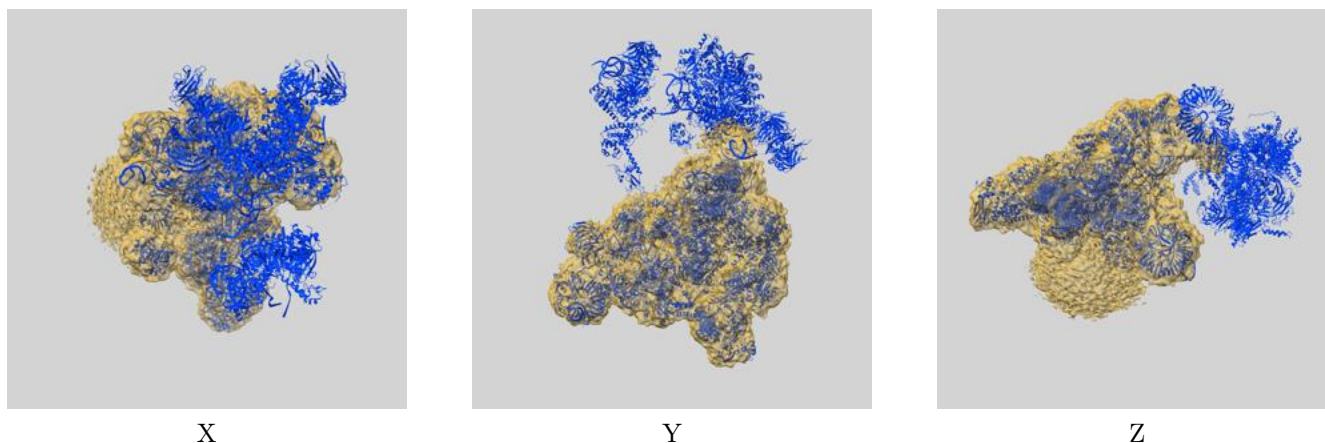
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

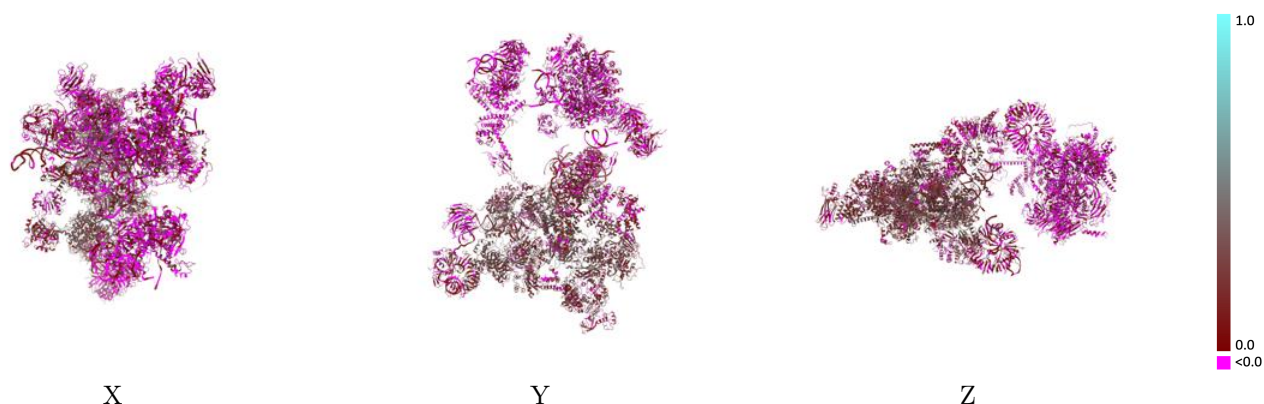
This section contains information regarding the fit between EMDB map EMD-9621 and PDB model 6AH0. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



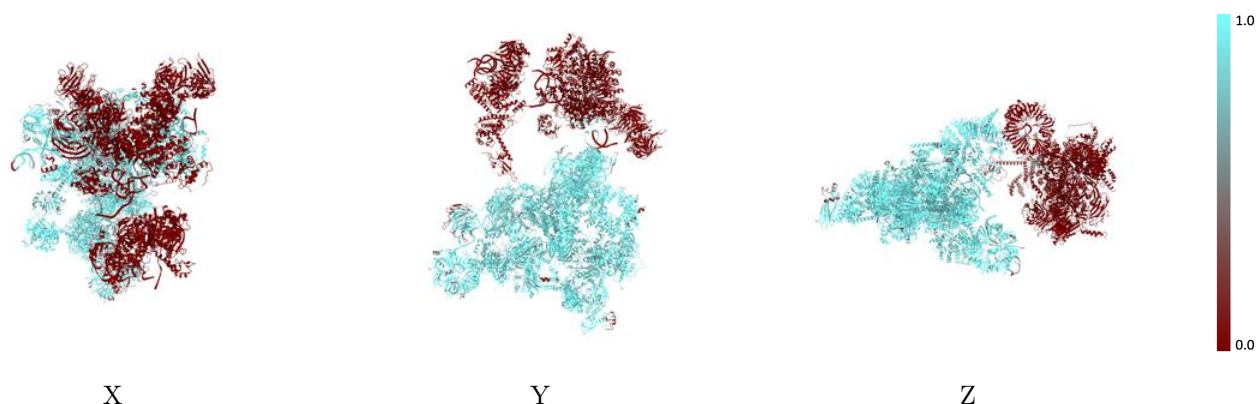
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



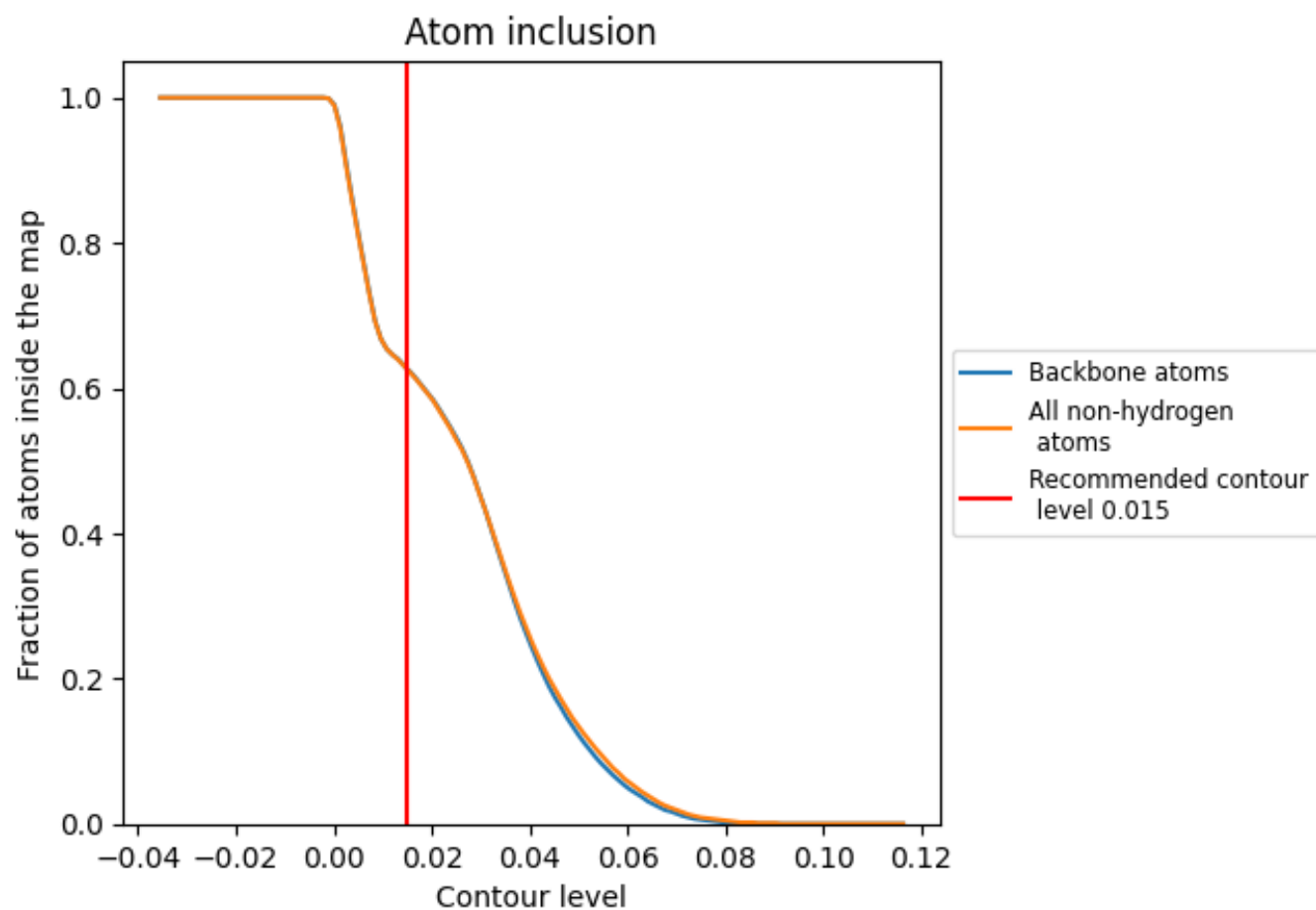
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 63% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6260	 0.1190
1	 0.0190	 0.0020
2	 0.0360	 0.0050
3	 0.0000	 -0.0030
4	 0.0000	 -0.0090
5	 0.0000	 -0.0110
6	 0.0000	 -0.0050
7	 0.0000	 0.0920
A	 0.9900	 0.2830
B	 0.9360	 0.1220
C	 1.0000	 0.2810
D	 0.9740	 0.1980
E	 0.7270	 -0.0190
F	 0.7860	 0.1010
G	 0.0000	 0.0150
H	 0.0530	 -0.0000
I	 0.9330	 0.1200
J	 0.9580	 0.0740
K	 0.9940	 0.0920
L	 0.9870	 0.1530
M	 0.9900	 0.2130
N	 0.9580	 0.1260
O	 0.9750	 0.2170
P	 0.9570	 0.1190
Q	 0.9210	 0.0870
R	 0.8920	 0.0800
S	 0.9230	 0.1050
T	 0.9060	 0.0760
U	 0.9100	 0.0820
V	 0.9550	 0.1500
W	 0.9250	 0.1840
X	 0.9610	 0.1200
a	 0.9650	 0.1010
b	 0.8400	 0.0480
c	 0.9040	 0.0990



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Chain	Atom inclusion	Q-score
d	 0.8760	 0.1480
e	 1.0000	 0.2090
f	 1.0000	 0.1490
g	 0.9290	 0.1560
h	 0.0000	 0.0120
i	 0.0000	 -0.0140
j	 0.0000	 -0.0180
k	 0.0000	 0.0390
l	 0.0000	 0.0120
m	 0.0000	 0.0380
n	 0.0000	 0.0170
o	 0.0000	 -0.0050
p	 0.0000	 0.0060
q	 0.0000	 0.0370
r	 0.0000	 0.0420
s	 0.0000	 -0.0520
t	 0.0000	 -0.0050
u	 0.0000	 0.0100
v	 0.0000	 0.0170
w	 0.0000	 -0.0140
x	 0.0000	 0.0050
y	 0.0000	 0.0190
z	 0.0000	 -0.0140