wwPDB EM Validation Summary Report (i)

Mar 27, 2026 – 08:41 PM UTC

PDB ID	:	8QO9 / pdb_00008qo9
EMDB ID	:	EMD-18529
Title	:	Cryo-EM structure of a human spliceosomal B complex protomer
Authors	:	Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Urlaub, H.; Stark, H.; Luehrmann, R.
Deposited on	:	2023-09-28
Resolution	:	5.29 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

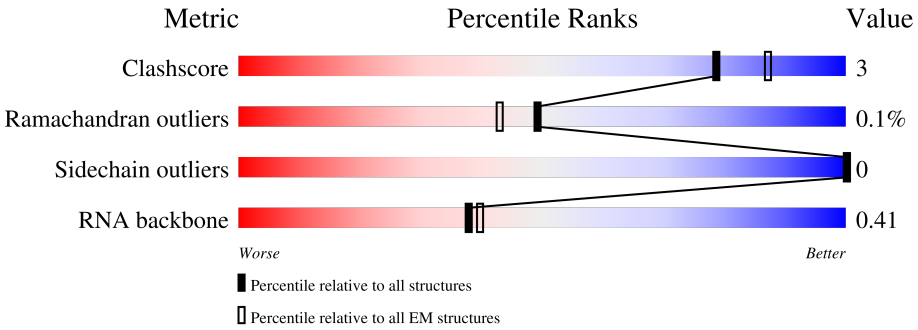
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

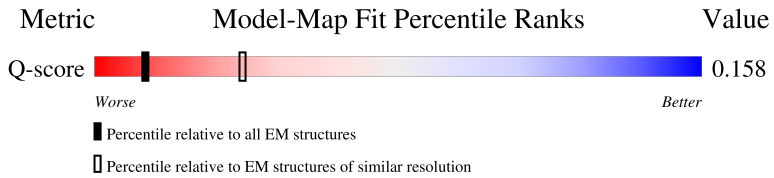
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.29 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	587 (4.79 - 5.75)

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

Mol	Chain	Length	Quality of chain
1	B4	424	18% 82%
2	8	464	14% 21% 78%
2	G	464	9% 91%

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Mol	Chain	Length	Quality of chain
3	9	501	45% 62% 38%
3	H	501	14% 86%
4	B2	895	23% 77%
5	B5	86	78% 20%
6	2	188	8% 23% 24% 5% 48%
7	B3	1217	7% 94%
8	BP	110	86% 5% 9%
9	B1	1304	66% 33%
10	B6	125	70% 28%
11	62	95	94% 5%
12	63	102	5% 73% 27%
13	64	139	18% 53% 47%
14	65	91	25% 77% 21%
15	66	80	9% 85% 12%
16	67	103	35% 61% 37%
17	68	96	63% 36%
18	2b	240	33% 66%
18	4b	240	31% 66%
18	5b	240	35% 64%
19	21	119	67% 33%
19	41	119	66% 32%
19	51	119	68% 31%
20	22	118	39% 75% 5% 19%
20	42	118	73% 5% 22%
20	52	118	82% 18%

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Mol	Chain	Length	Quality of chain
21	2f	86	62% 81% 16%
21	4f	86	78% 6% 16%
21	5f	86	86% 14%
22	2e	92	59% 82% 7% 12%
22	4e	92	79% 17%
22	5e	92	86% 14%
23	2g	76	22% 92%
23	4g	76	93%
23	5g	76	97%
24	23	126	62% 34%
24	43	126	66% 34%
24	53	126	61% 39%
25	2B	225	11% 40% 59%
26	2A	255	11% 62% 36%
27	7	793	14% 26% 74%
28	E	357	83% 16%
29	B	2136	78% 21%
30	x	557	7% 93%
30	y	557	6% 93%
31	v	513	5% 93%
31	w	513	13% 92%
32	z	248	29% 70%
33	W	177	86% 10% 5%
34	5	117	33% 49% 16%
35	Q	144	97%

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Mol	Chain	Length	Quality of chain
36	D	142	96%
37	X	376	21% 78%
38	K	439	48% 52%
39	Z	347	7% 5% 87%
40	L	499	74% 25%
41	F	522	80% 17%
42	N	941	80% 16%
43	A	2335	94%
44	I	312	57% 41%
45	S	800	21% 79%
46	C	972	85% 13%
47	M	128	94%
48	T	1098	37% 62%
49	4	144	42% 37% 9% 12%
50	6	106	35% 42% 11% 11%
51	r	199	57% 43%
52	J	683	38% 62%
53	s	73	100%

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 87322 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 Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	B4	78	391	235	78	78	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	8	100	510	310	100	100	0	0
2	G	44	219	131	44	44	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	9	313	1569	943	313	313	0	0
3	H	70	351	211	70	70	0	0

- Molecule 4 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	B2	208	1072	656	208	208	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	B5	69	347	209	69	69	0	0

- Molecule 6 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	2	98	2071	926	349	698	98	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	97	A	G	conflict	GB 36516

- Molecule 7 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	B3	1174	5908	3560	1174	1174	0	0

- Molecule 8 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	BP	100	498	298	100	100	0	0

- Molecule 9 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	B1	870	4383	2643	870	870	0	0

- Molecule 10 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	B6	90	455	275	90	90	0	0

- Molecule 11 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	62	90	360	180	90	90	0	0

- Molecule 12 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	63	74	296	148	74	74	0	0

- Molecule 13 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	64	74	296	148	74	74	0	0

- Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	65	72	288	144	72	72	0	0

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	66	70	280	140	70	70	0	0

- Molecule 16 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	67	65	260	130	65	65	0	0

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	68	61	244	122	61	61	0	0

- Molecule 18 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	5b	86	344	172	86	86	0	0
18	2b	82	413	249	82	82	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	4b	82	413	249	82	82	0	0

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	51	82	328	164	82	82	0	0
19	21	80	402	242	80	80	0	0
19	41	81	407	245	81	81	0	0

- Molecule 20 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	52	97	388	194	97	97	0	0
20	22	95	482	292	95	95	0	0
20	42	92	463	279	92	92	0	0

- Molecule 21 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	5f	74	296	148	74	74	0	0
21	2f	72	359	215	72	72	0	0
21	4f	72	359	215	72	72	0	0

- Molecule 22 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	5e	79	316	158	79	79	0	0
22	2e	81	403	241	81	81	0	0
22	4e	76	378	226	76	76	0	0

- Molecule 23 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	5g	74	296	148	74	74	0	0
23	2g	73	364	218	73	73	0	0
23	4g	74	369	221	74	74	0	0

- Molecule 24 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	53	77	308	154	77	77	0	0
24	23	83	415	249	83	83	0	0
24	43	83	415	249	83	83	0	0

- Molecule 25 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	2B	92	461	277	92	92	0	0

- Molecule 26 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	2A	162	816	492	162	162	0	0

- Molecule 27 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	7	204	1028	620	204	204	0	0

- Molecule 28 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

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

- Molecule 29 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	B	1693	8538	5154	1693	1691	0	0

- Molecule 30 is a protein called Protein Red.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	x	39	197	119	39	39	0	0
30	y	37	187	113	37	37	0	0

- Molecule 31 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	v	496	2478	1486	496	496	0	0
31	w	495	2474	1484	495	495	0	0

- Molecule 32 is a protein called Serine/arginine-rich splicing factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	z	74	368	220	74	74	0	0

- Molecule 33 is a protein called Peptidyl-prolyl cis-trans isomerase H.

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

- Molecule 34 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
34	5	115	2420	1084	403	818	115	0	0

- Molecule 35 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	Q	142	713	429	142	142	0	0

- Molecule 36 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	D	141	708	426	141	141	0	0

- Molecule 37 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	X	81	408	246	81	81	0	0

- Molecule 38 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	K	212	1057	633	212	212	0	0

- Molecule 39 is a RNA chain called MINX pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	Z	46	977	438	175	319	45	0	0

- Molecule 40 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	L	373	1873	1127	373	373	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	F	431	2155	1293	431	431	0	0

- Molecule 42 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	N	791	3990	2408	791	791	0	0

- Molecule 43 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	A	2234	11052	6584	2234	2234	0	0

- Molecule 44 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	I	184	925	557	184	184	0	0

- Molecule 45 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	S	171	854	512	171	171	0	0

- Molecule 46 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	C	843	4260	2574	843	843	0	0

- Molecule 47 is a protein called NHP2-like protein 1, N-terminally processed.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	M	124	627	379	124	124	0	0

- Molecule 48 is a protein called Transcription elongation regulator 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	T	412	2071	1247	412	412	0	0

- Molecule 49 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	4	127	2692	1203	467	895	127	0	0

- Molecule 50 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	6	94	1995	891	362	648	94	0	0

- Molecule 51 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	r	114	568	340	114	114	0	0

- Molecule 52 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	J	260	1314	794	260	260	0	0

- Molecule 53 is a protein called Ubiquitin-like protein 5.

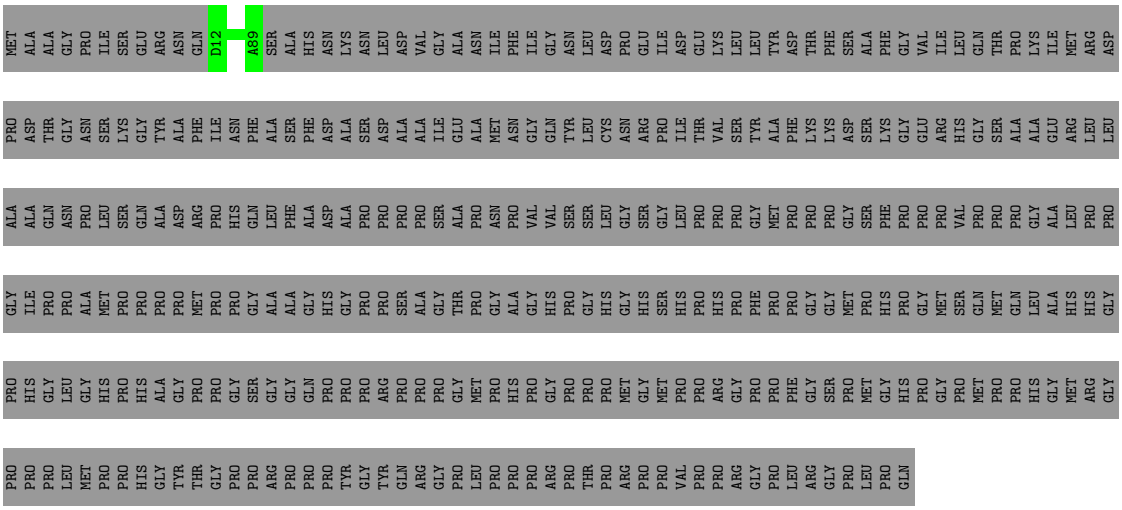
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	s	73	360	214	73	73	0	0

3 Residue-property plots (i)

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

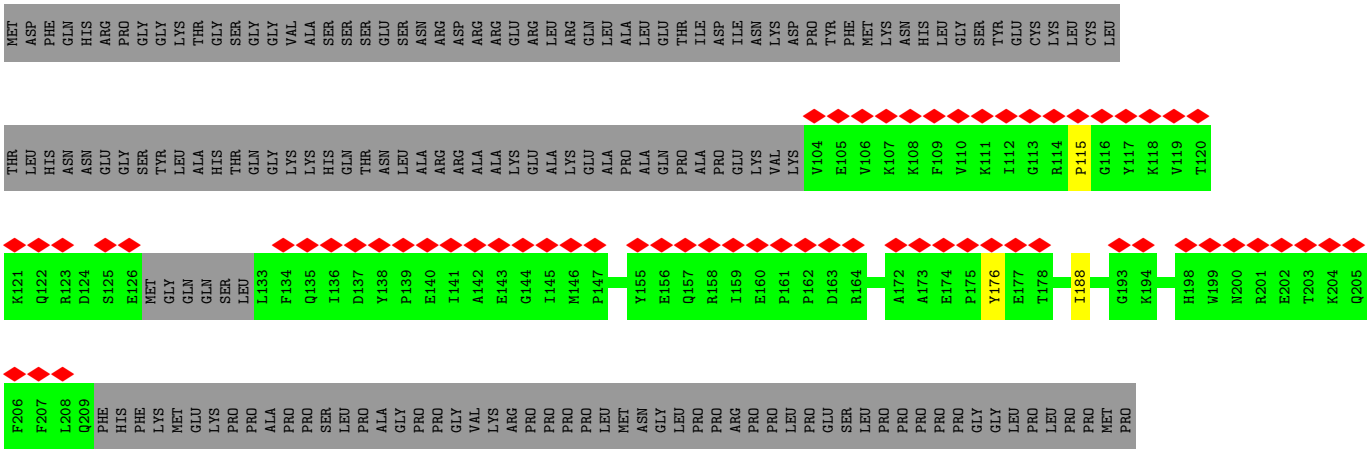
- Molecule 1: Splicing factor 3B subunit 4

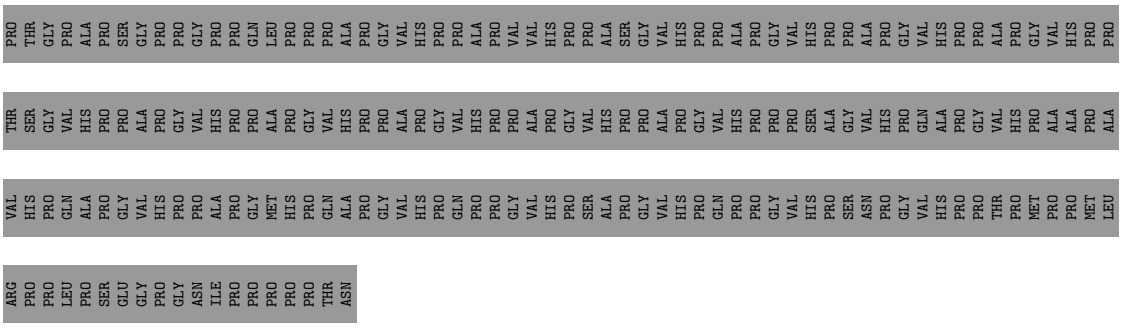
Chain B4:



- Molecule 2: Splicing factor 3A subunit 2

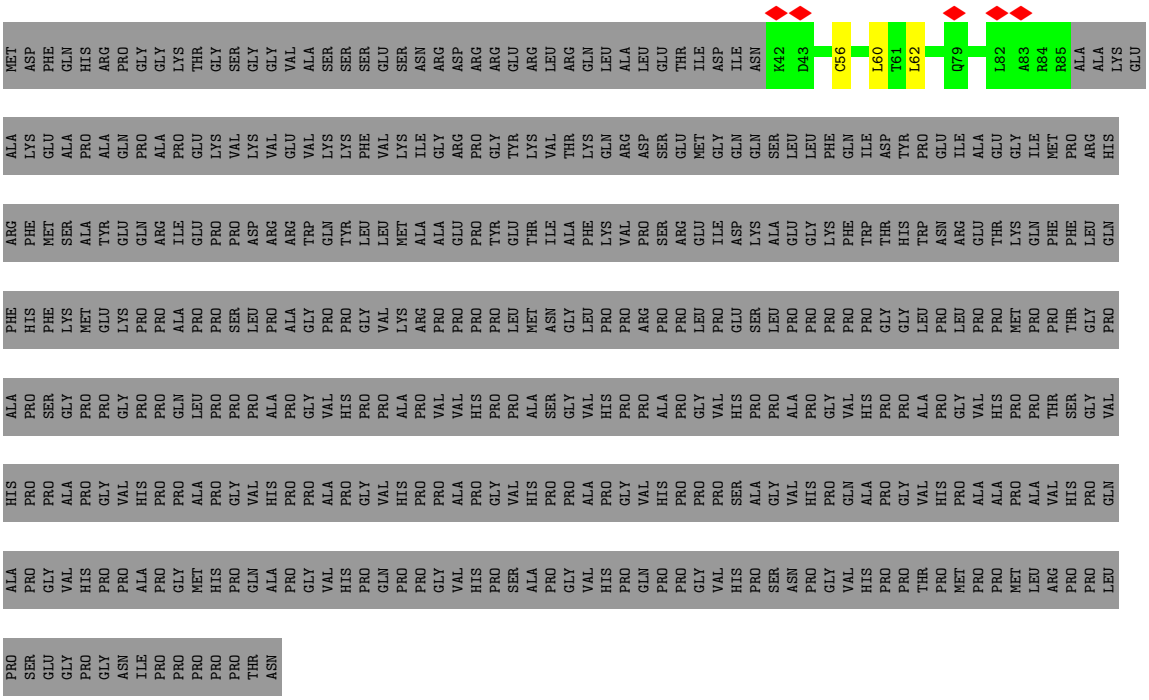
Chain 8:





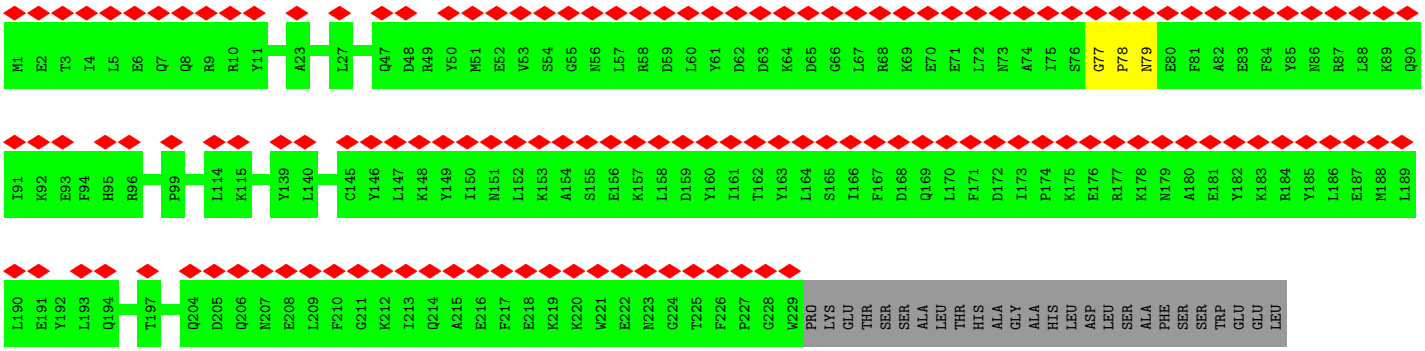
- Molecule 2: Splicing factor 3A subunit 2

Chain G:



- Molecule 3: Splicing factor 3A subunit 3

Chain 9:



ALA SER LEU GLY LEU ASP ARG LEU LYS SER ALA LEU LEU ALA LEU GLY LEU LYS CYS GLY GLY THR LEU E279 E280 R281 A282 Q283 R284 L285 F286 S287 T288 K289 G290 K291 S292 L293 E294 S295 L296 D297 T298 S299 L300 F301 A302 K303 N304 P305 K306 S307 K308 G309 T310 K311 R312 D313 T314 E315

R316 N317 K318 D319 I320 A321 F322 L323 E324 A325 Q326 I327 Y328 E329 Y330 V331 E332 I333 L334 G335 E336 Q337 R338 H339 L340 T341 H342 E343 N344 V345 Q346 R347 K348 Q349 A350 R351 T352 G353 E354 E355 R356 E357 E358 E359 E360 E361 E362 GLN ILE SER GLU SER GLU SER GLU ASP GLU GLU ASN GLU

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

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

LYS ARG GLN GLY LEU LEU

- Molecule 3: Splicing factor 3A subunit 3

Chain H: 14% 86%

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

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

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

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

GLY ALA HIS LEU ASP LEU SER ALA PHE SER SER TRP GLU GLU LEU ALA SER LEU GLY LEU ASP ARG LEU LYS SER ALA LEU LEU ALA LEU GLY LEU LYS CYS GLY GLY THR LEU GLU GLU ARG ALA GLN ARG LEU PHE SER THR LYS GLY LYS SER LEU GLU SER LEU ASP THR SER LEU

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

GLU GLU GLN ILE SER GLU SER GLU SER GLU ASP GLU GLU ASN GLU ILE ILE TYR ASN PRO LYS ASN LEU PRO LEU GLY TRP ASP GLY LYS PRO ILE P393 C411 G412 N413 Y414 T415 P419 K420 L462 LYS LEU GLN LYS ALA SER GLU ARG TRP GLN PRO ASP THR GLU GLU GLU

TYR GLU ASP SER SER GLY ASN VAL VAL ASN LYS LYS THR TYR GLU ASP LEU LYS ARG GLN GLY LEU LEU

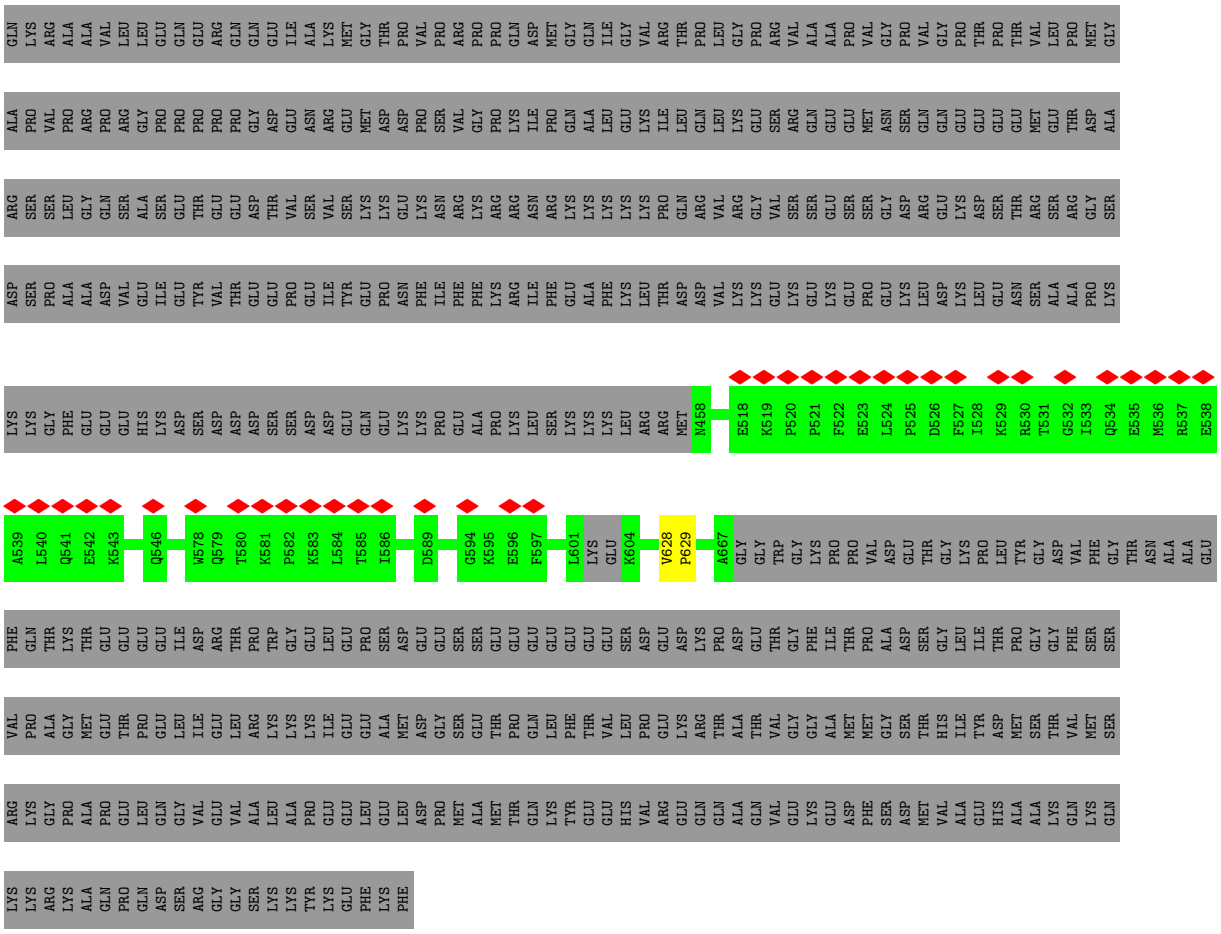
- Molecule 4: Splicing factor 3B subunit 2

Chain B2: 23% 77%

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

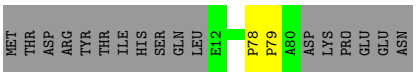
THR GLY ILE VAL LEU ASN ARG PRO VAL LEU ARG GLY GLU ASP GLY ASP LYS ALA ALA PRO PRO PRO MET SER ALA GLN LEU PRO GLY ILE PRO MET PRO PRO PRO LEU PRO LEU GLN PRO PRO PRO PRO PRO PRO PRO PRO GLY LEU GLY LEU PRO PRO PRO

MET ALA HIS PRO PRO ASN LEU GLY PRO PRO PRO LEU ARG VAL GLY GLU PRO VAL ALA LEU SER GLU GLU GLU ARG LEU LYS LEU ALA GLN GLN GLN ALA ALA LEU LEU MET GLN GLN GLU GLU ARG ALA LYS GLN GLN GLY ASP HIS SER LEU LYS GLU HIS GLU LEU LEU GLU GLN



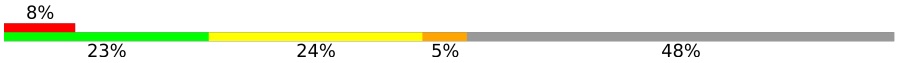
• Molecule 5: Splicing factor 3B subunit 5

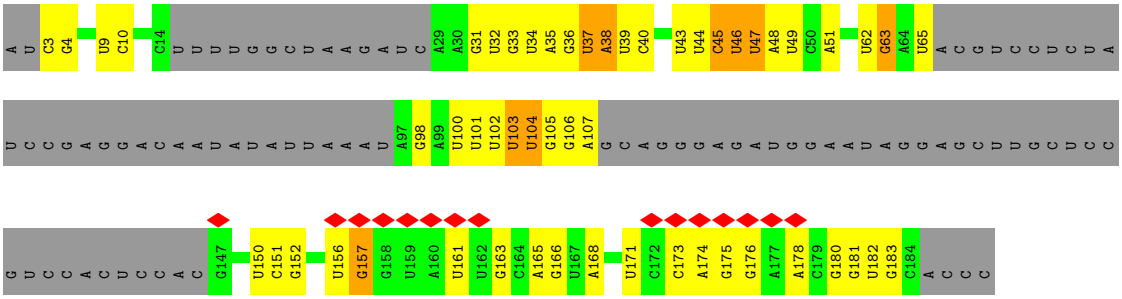
Chain B5:



• Molecule 6: U2 snRNA

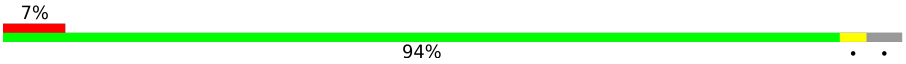
Chain 2:

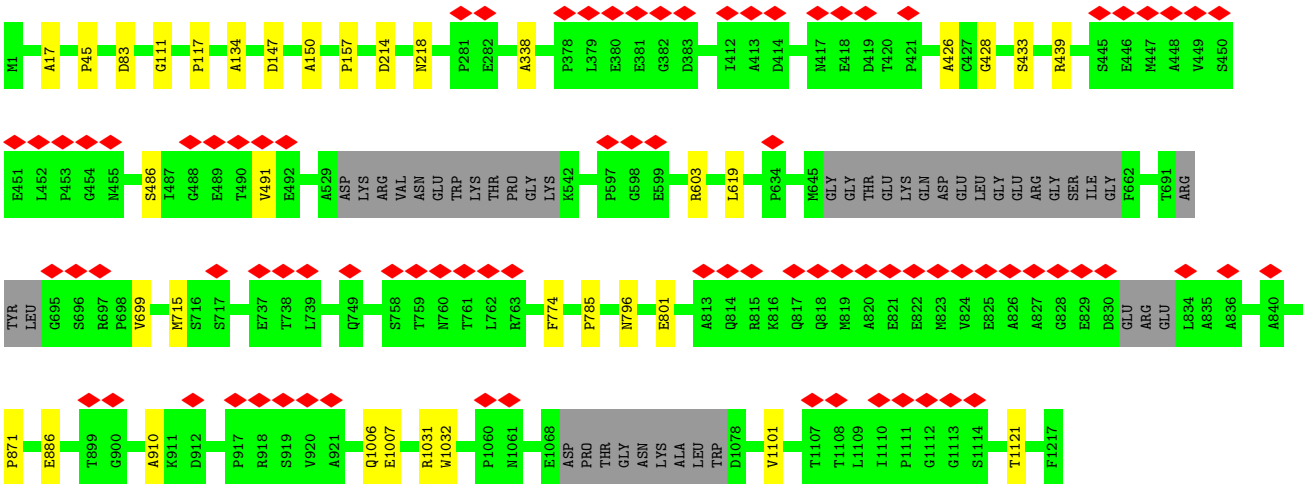




• Molecule 7: Splicing factor 3B subunit 3

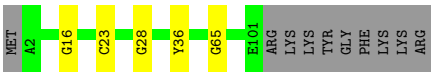
Chain B3:





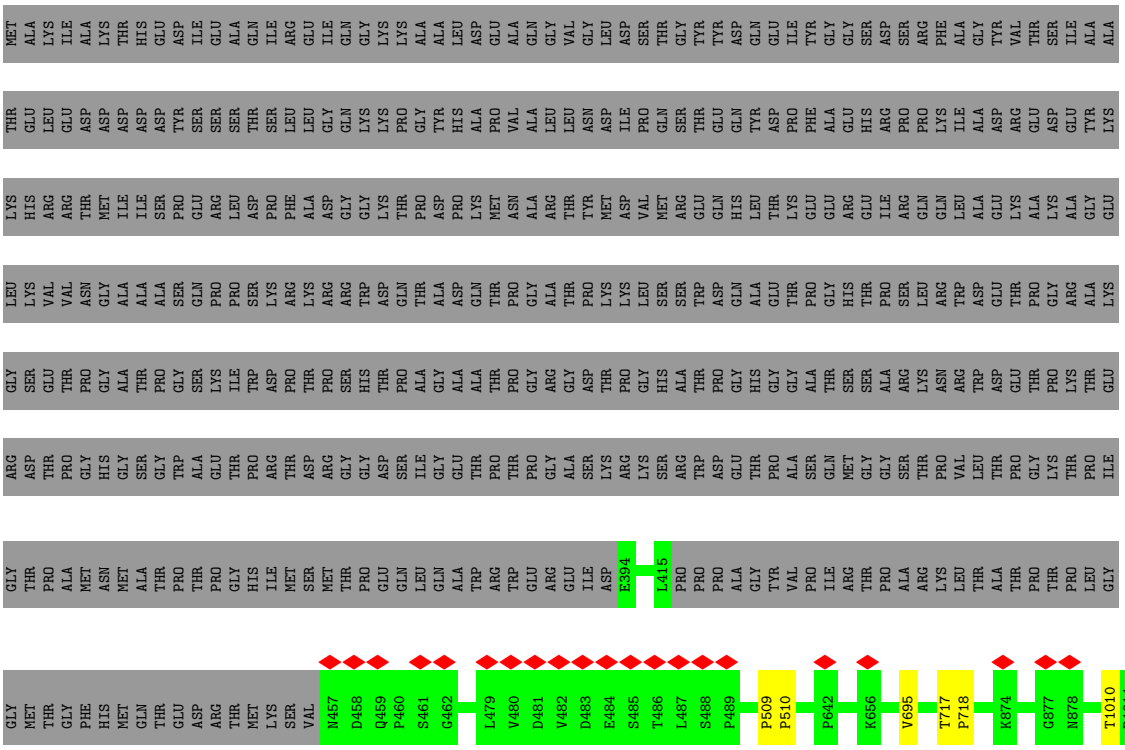
- Molecule 8: PHD finger-like domain-containing protein 5A

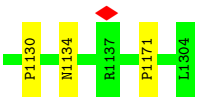
Chain BP:



- Molecule 9: Splicing factor 3B subunit 1

Chain B1:



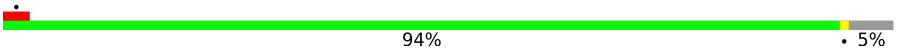


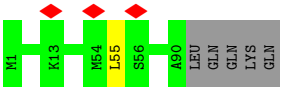
• Molecule 10: Splicing factor 3B subunit 6

Chain B6:

• Molecule 11: U6 snRNA-associated Sm-like protein LSm2

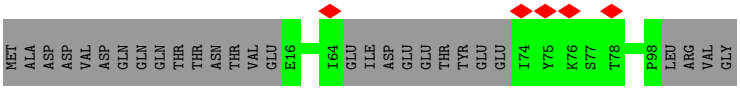
Chain 62:





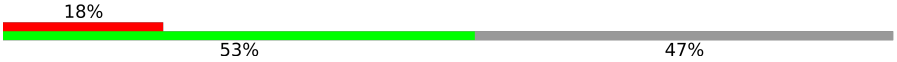
• Molecule 12: U6 snRNA-associated Sm-like protein LSm3

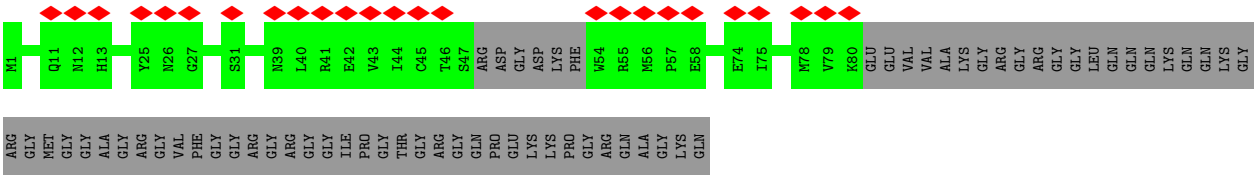
Chain 63:



• Molecule 13: U6 snRNA-associated Sm-like protein LSm4

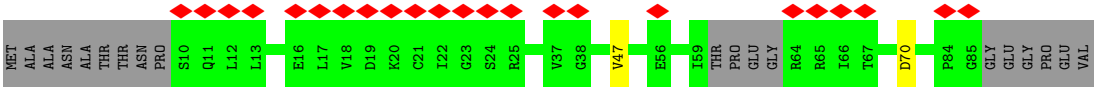
Chain 64:





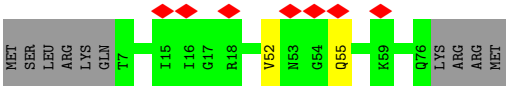
• Molecule 14: U6 snRNA-associated Sm-like protein LSm5

Chain 65:



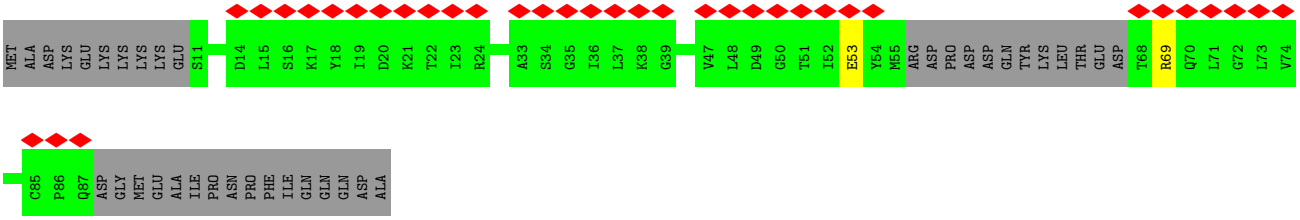
• Molecule 15: U6 snRNA-associated Sm-like protein LSm6

Chain 66:



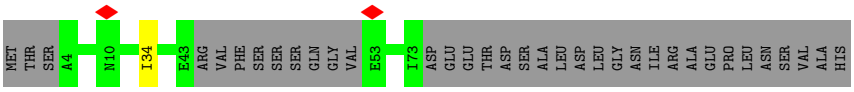
- Molecule 16: U6 snRNA-associated Sm-like protein LSm7

Chain 67:



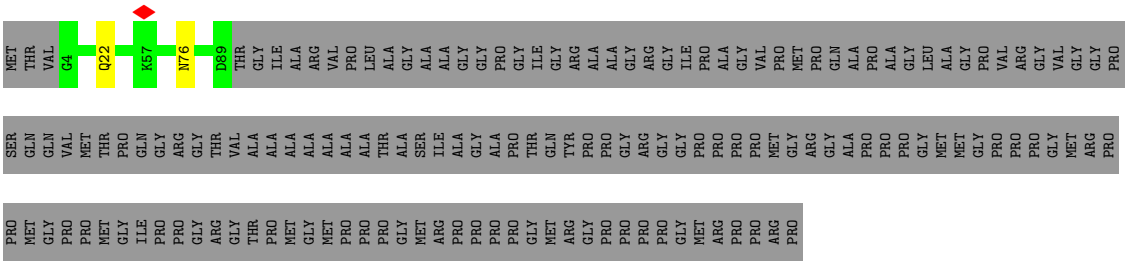
- Molecule 17: U6 snRNA-associated Sm-like protein LSm8

Chain 68:



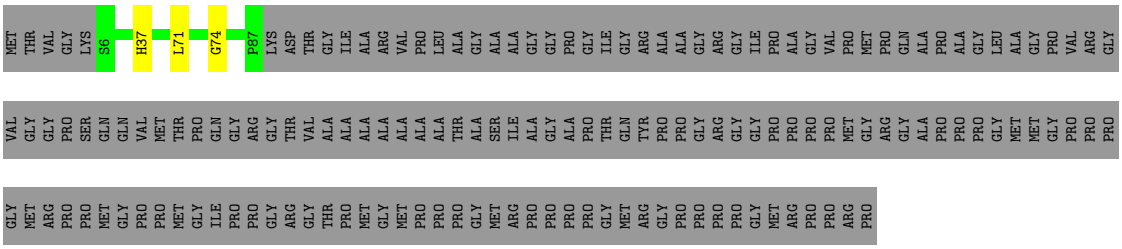
- Molecule 18: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain 5b:



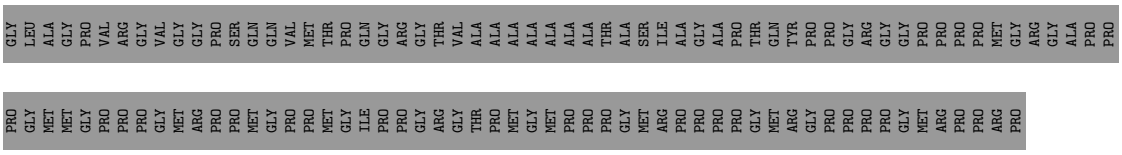
- Molecule 18: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain 2b:



- Molecule 18: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain 4b:

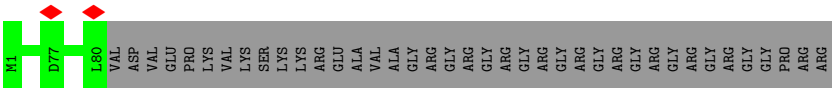


• Molecule 19: Small nuclear ribonucleoprotein Sm D1

Chain 51:

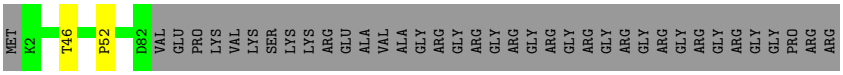
• Molecule 19: Small nuclear ribonucleoprotein Sm D1

Chain 21:



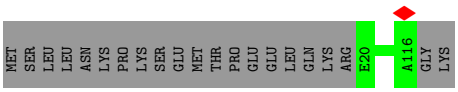
• Molecule 19: Small nuclear ribonucleoprotein Sm D1

Chain 41:



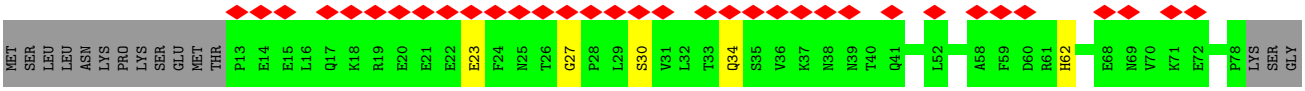
• Molecule 20: Small nuclear ribonucleoprotein Sm D2

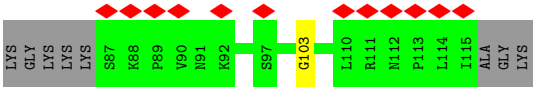
Chain 52:



• Molecule 20: Small nuclear ribonucleoprotein Sm D2

Chain 22:



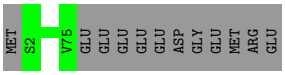


• Molecule 20: Small nuclear ribonucleoprotein Sm D2

Chain 42:

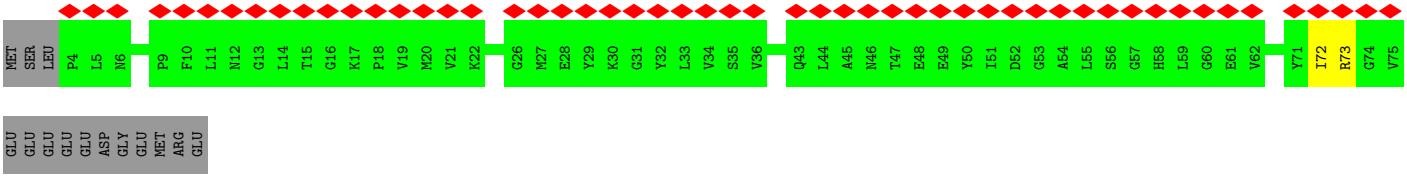
• Molecule 21: Small nuclear ribonucleoprotein F

Chain 5f:



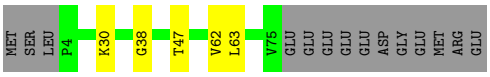
• Molecule 21: Small nuclear ribonucleoprotein F

Chain 2f:



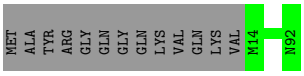
• Molecule 21: Small nuclear ribonucleoprotein F

Chain 4f:



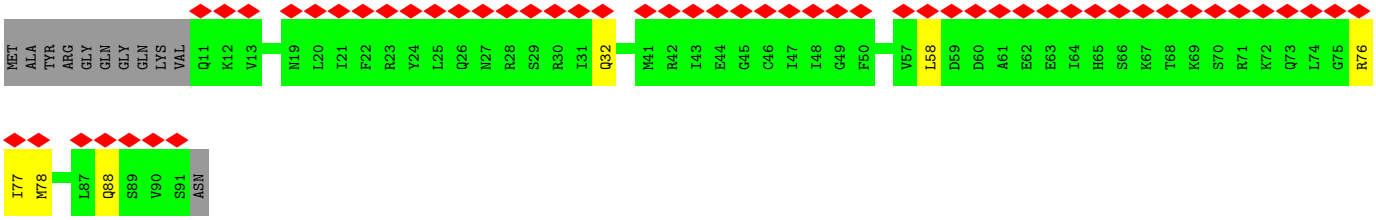
• Molecule 22: Small nuclear ribonucleoprotein E

Chain 5e:



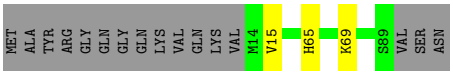
• Molecule 22: Small nuclear ribonucleoprotein E

Chain 2e:



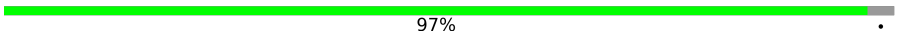
• Molecule 22: Small nuclear ribonucleoprotein E

Chain 4e:



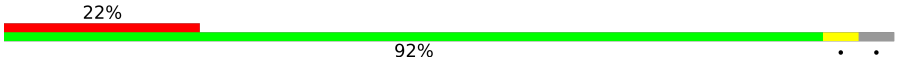
• Molecule 23: Small nuclear ribonucleoprotein G

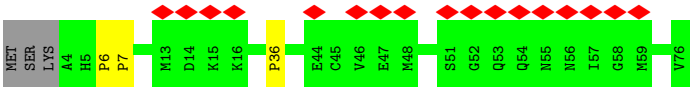
Chain 5g:



• Molecule 23: Small nuclear ribonucleoprotein G

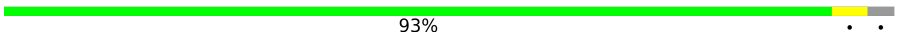
Chain 2g:





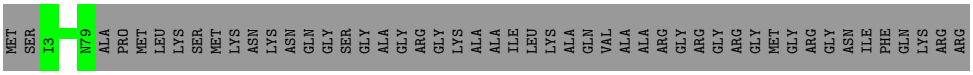
• Molecule 23: Small nuclear ribonucleoprotein G

Chain 4g:



• Molecule 24: Small nuclear ribonucleoprotein Sm D3

Chain 53:



• Molecule 24: Small nuclear ribonucleoprotein Sm D3

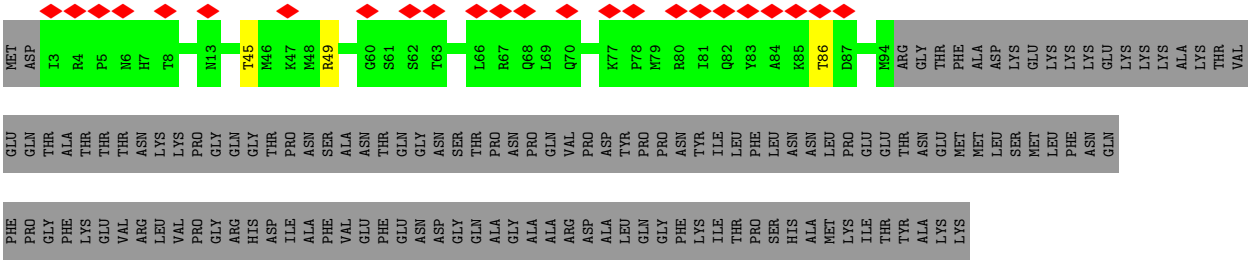
Chain 23:

• Molecule 24: Small nuclear ribonucleoprotein Sm D3

Chain 43:

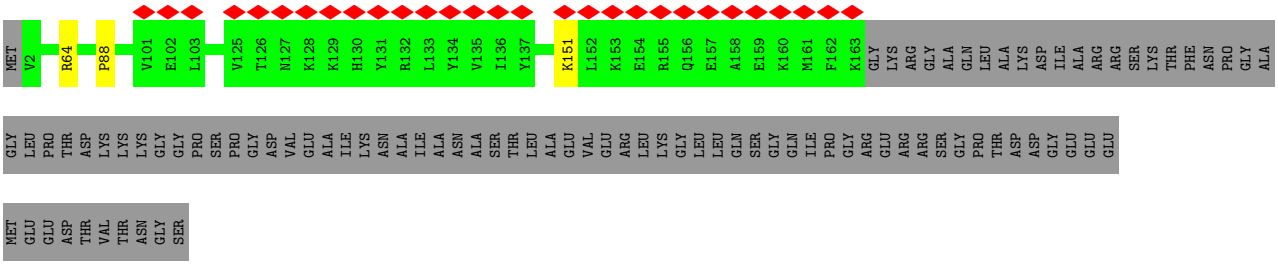
• Molecule 25: U2 small nuclear ribonucleoprotein B"

Chain 2B:



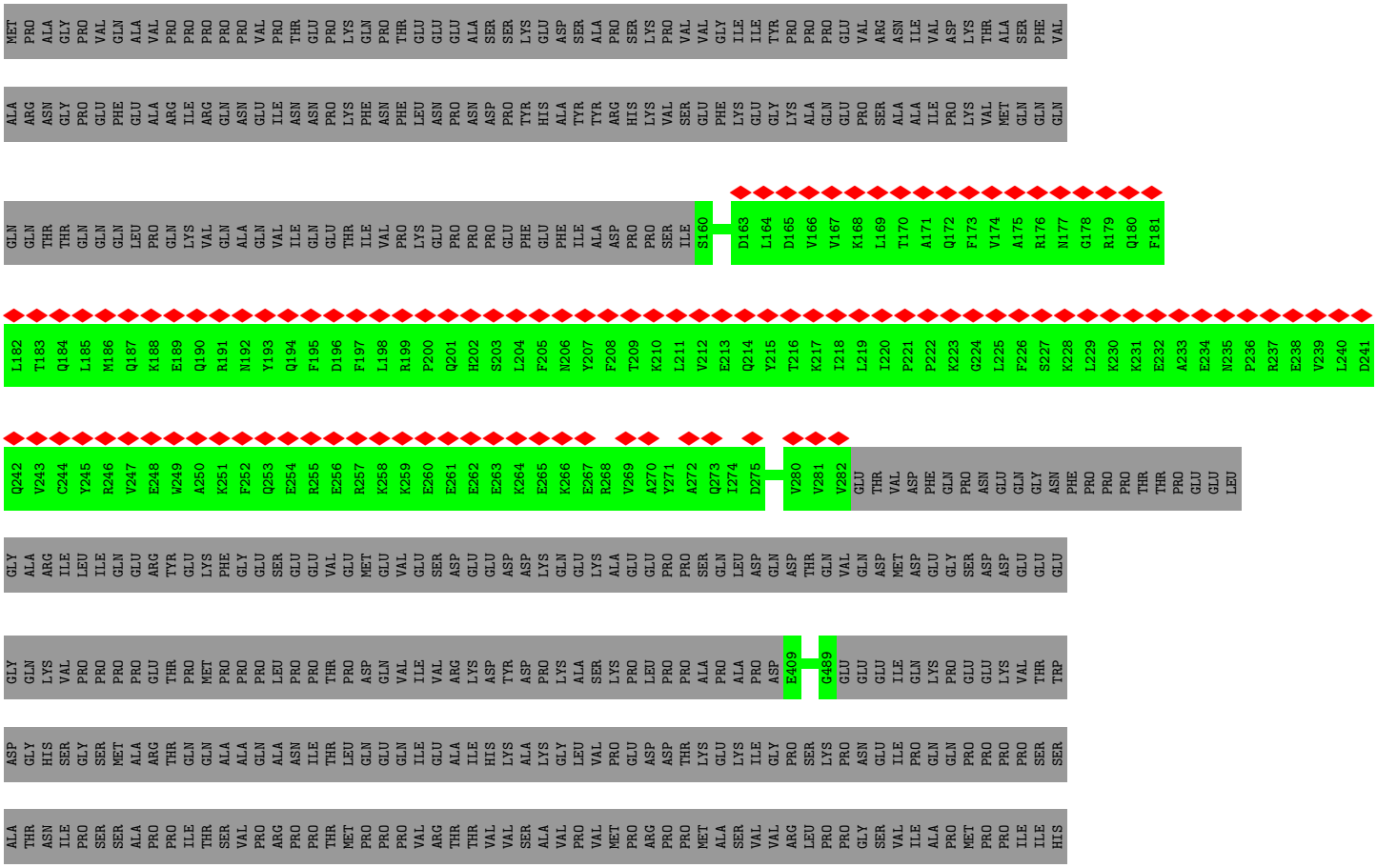
- Molecule 26: U2 small nuclear ribonucleoprotein A'

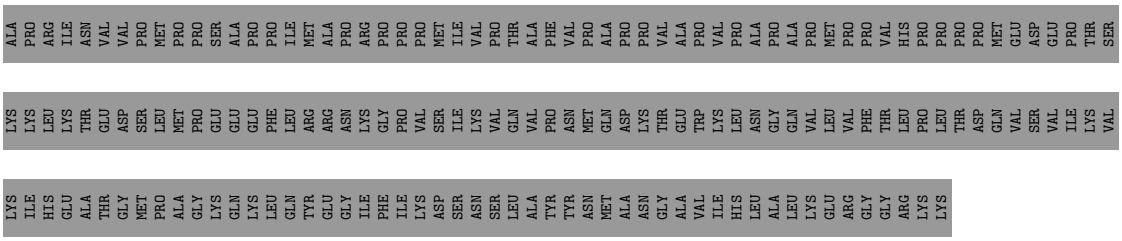
Chain 2A:



- Molecule 27: Splicing factor 3A subunit 1

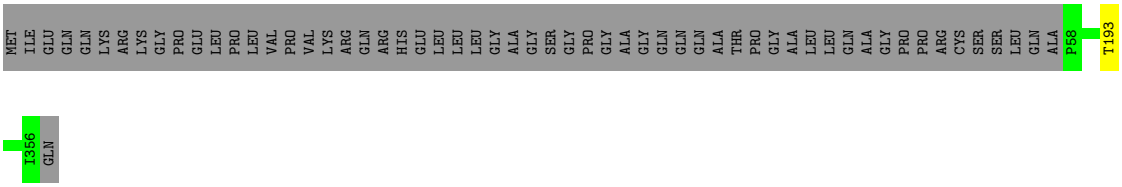
Chain 7:





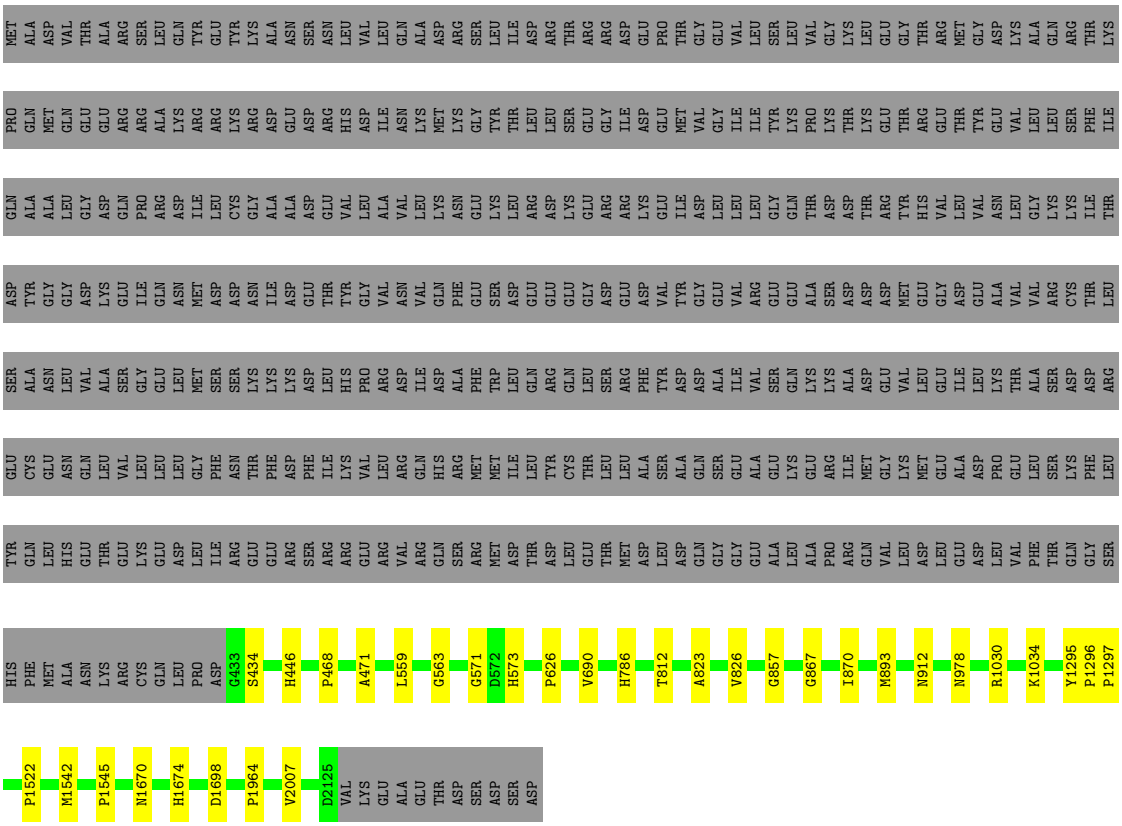
• Molecule 28: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E: 83% 16%



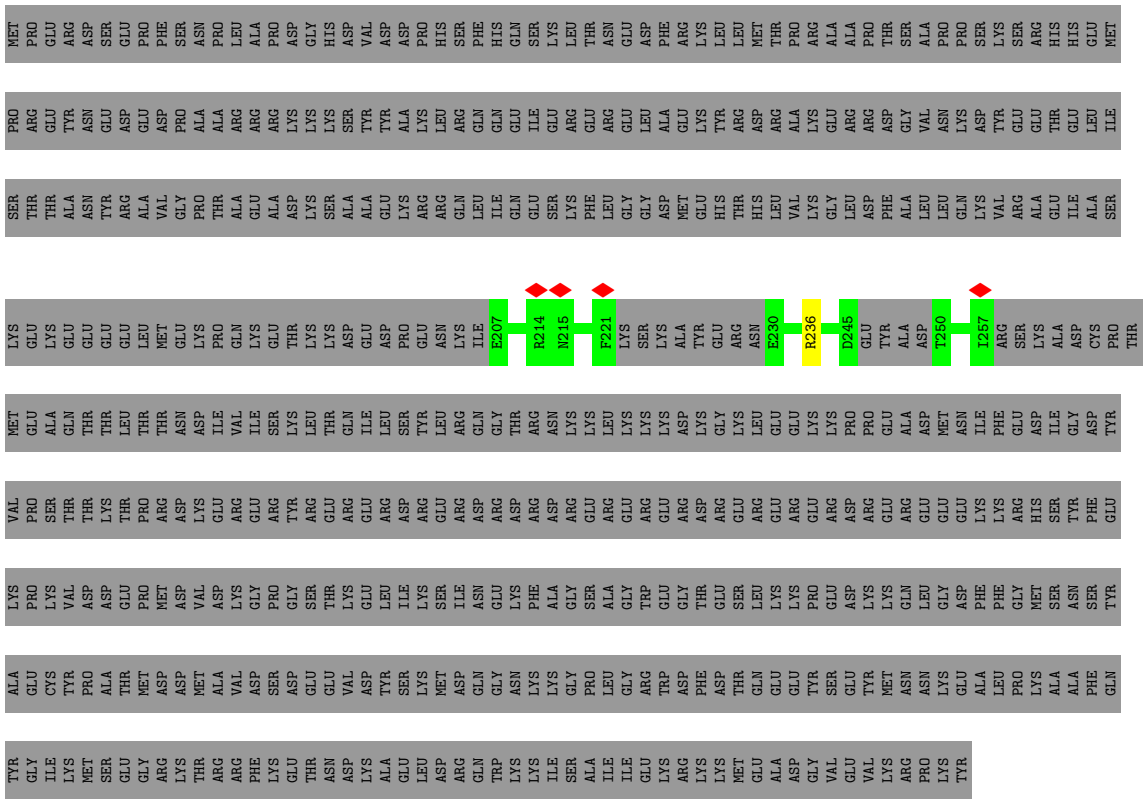
• Molecule 29: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain B: 78% • 21%



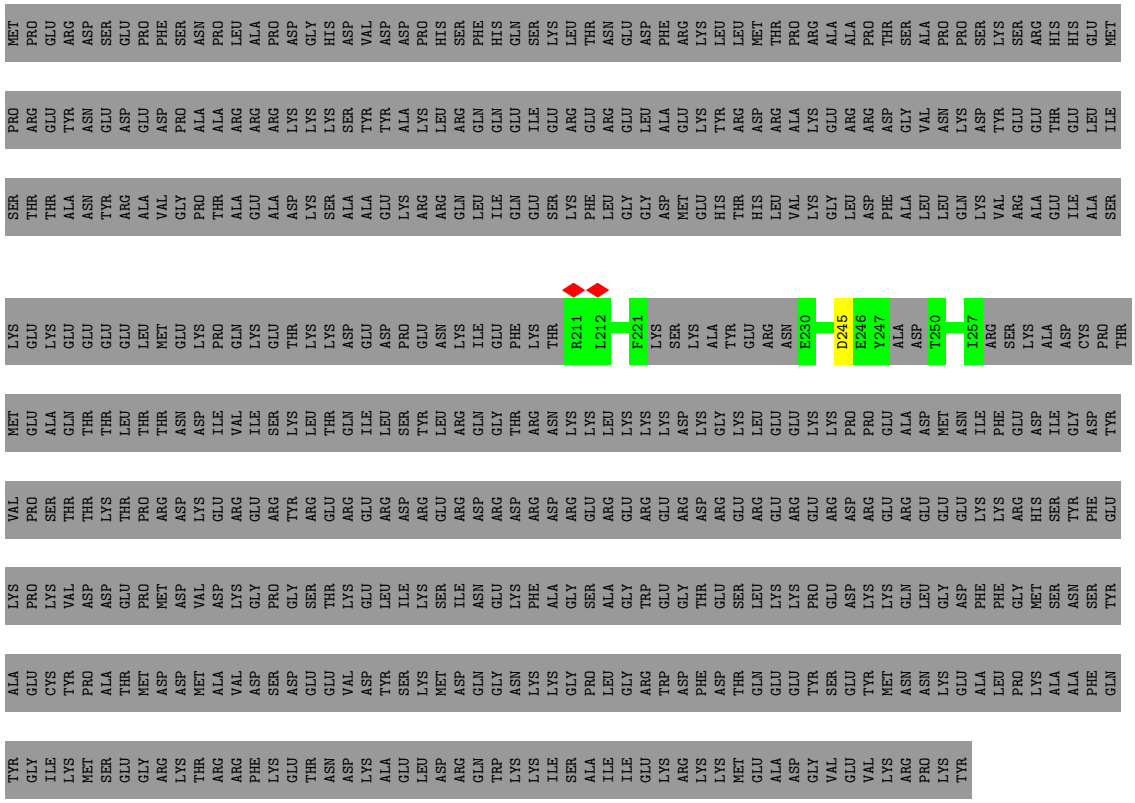
• Molecule 30: Protein Red

Chain x: • 7% 93%



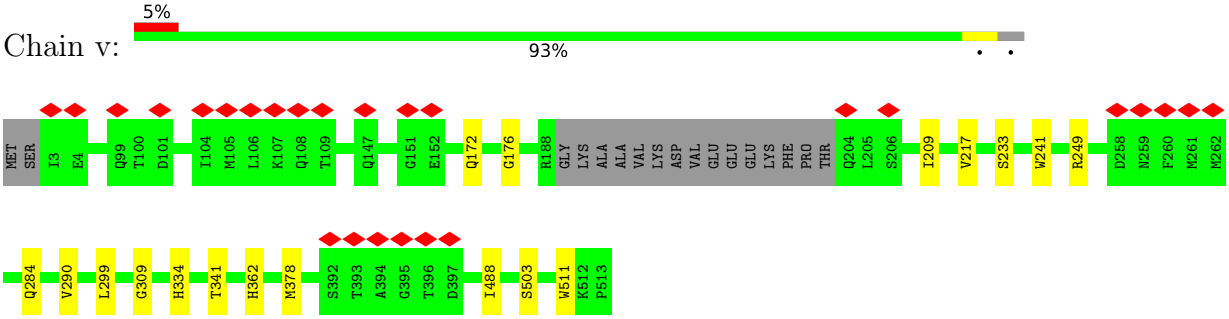
- Molecule 30: Protein Red

Chain y: 6% 93%



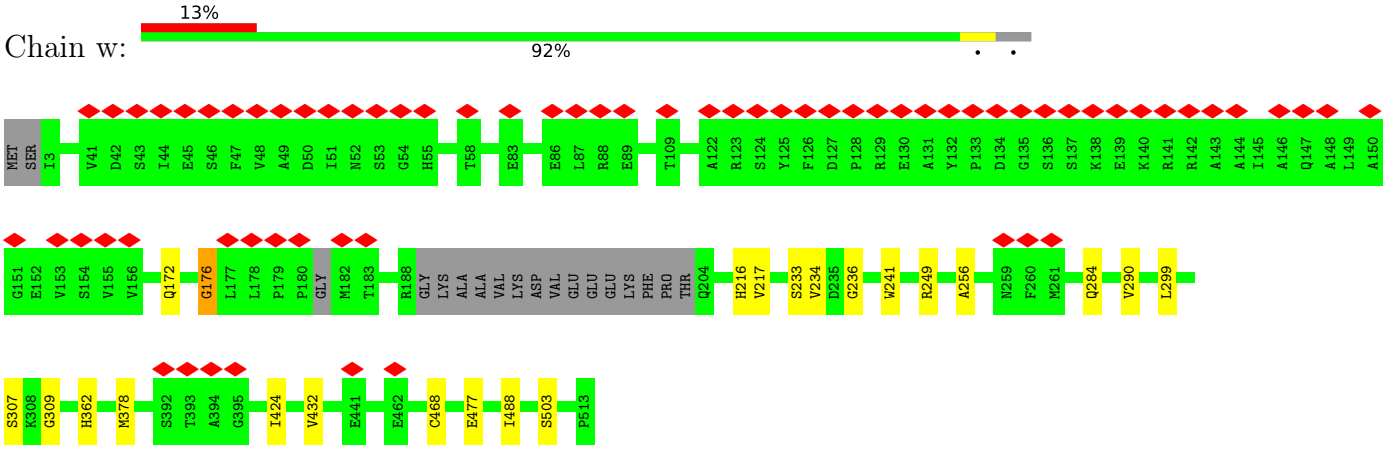
• Molecule 31: WD40 repeat-containing protein SMU1

Chain v:



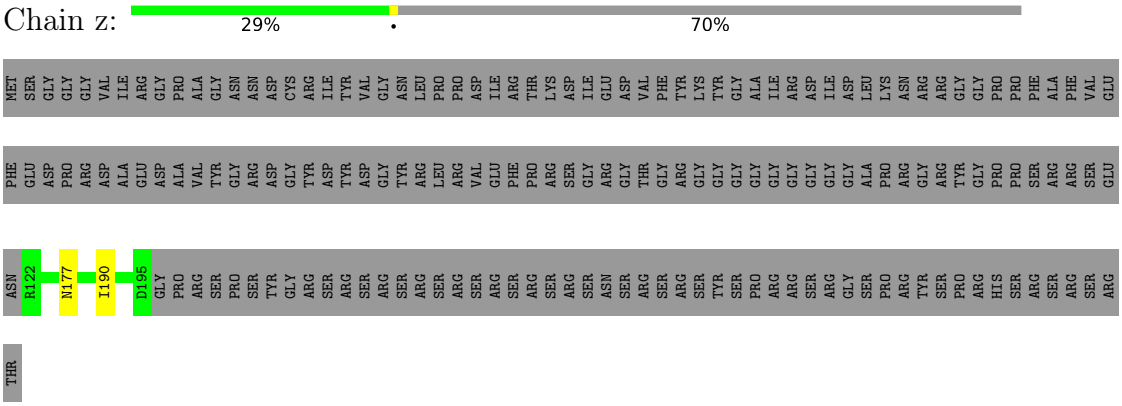
• Molecule 31: WD40 repeat-containing protein SMU1

Chain w:



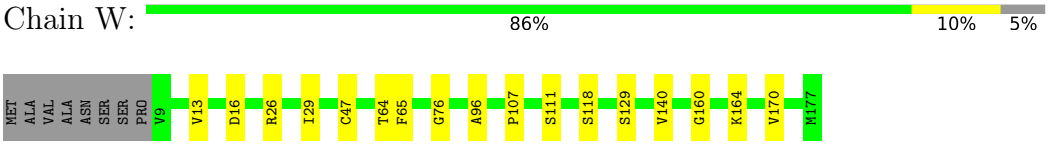
• Molecule 32: Serine/arginine-rich splicing factor 1

Chain z:



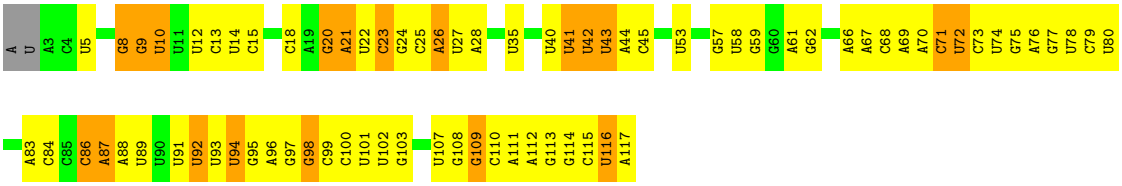
• Molecule 33: Peptidyl-prolyl cis-trans isomerase H

Chain W:



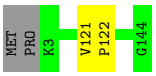
• Molecule 34: U5 snRNA

Chain 5:



- Molecule 35: Protein BUD31 homolog

Chain Q: 97%

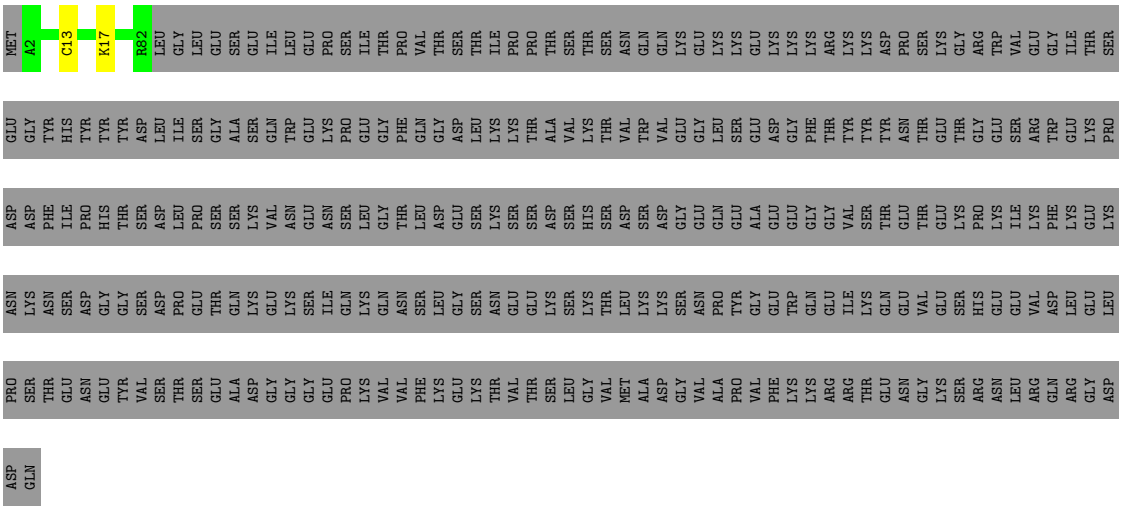


- Molecule 36: Thioredoxin-like protein 4A

Chain D: 96%

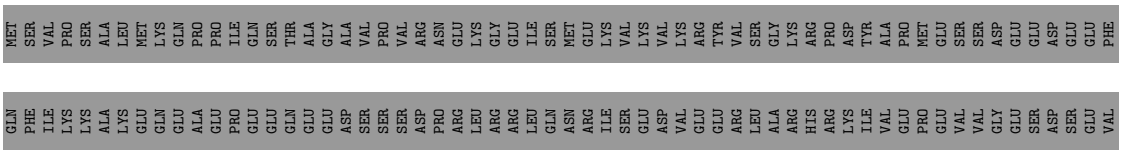
- Molecule 37: WW domain-binding protein 4

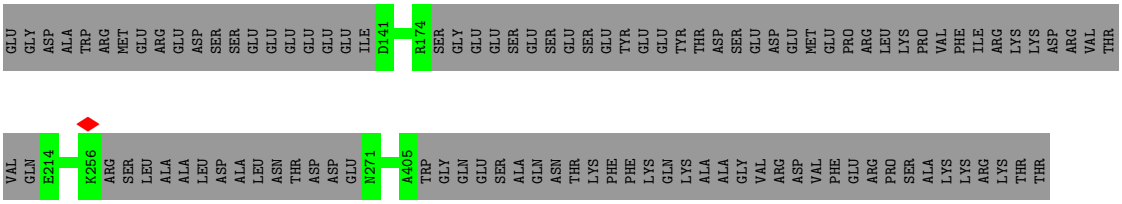
Chain X: 21% 78%



- Molecule 38: Microfibrillar-associated protein 1

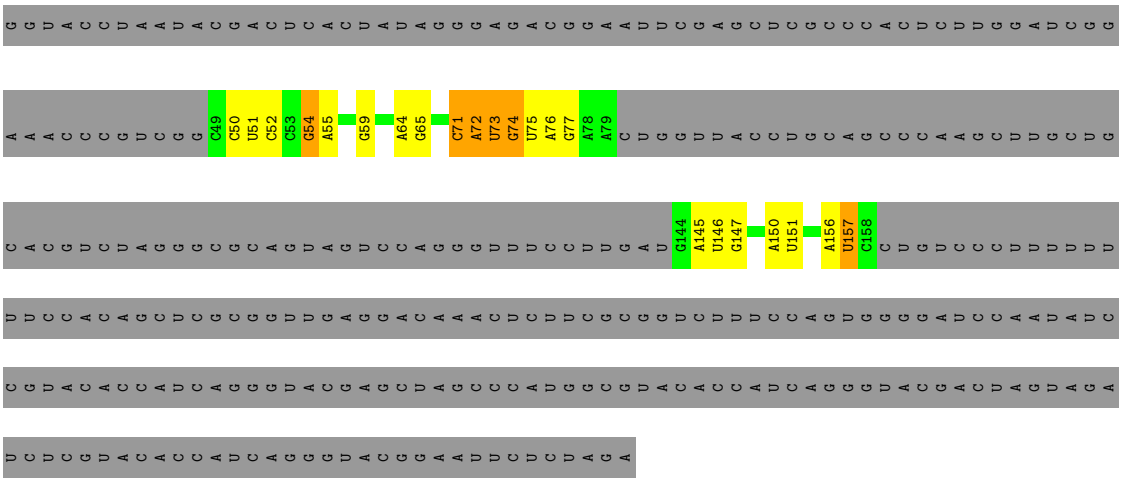
Chain K: 48% 52%





- Molecule 39: MINX pre-mRNA

Chain Z:



- Molecule 40: U4/U6 small nuclear ribonucleoprotein Prp31

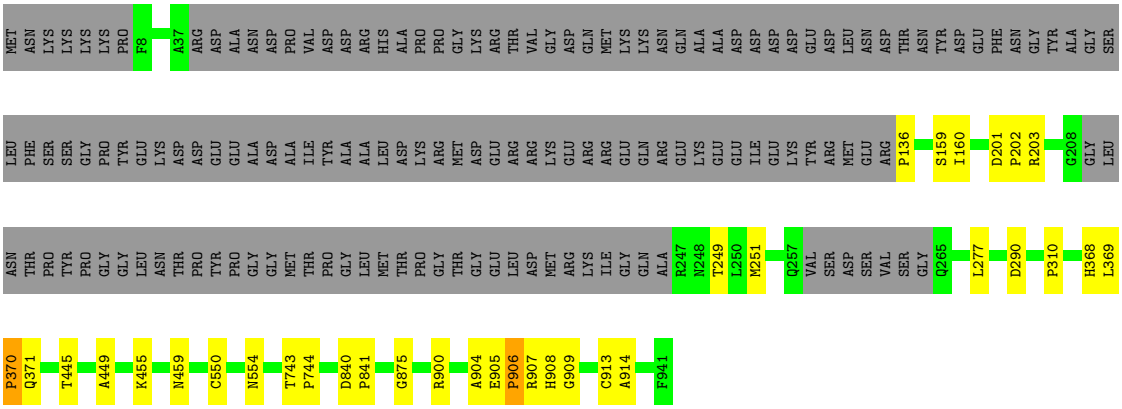
Chain L:

- Molecule 41: U4/U6 small nuclear ribonucleoprotein Prp4

Chain F:

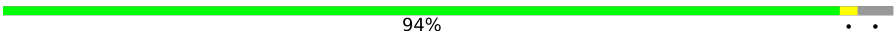
- Molecule 42: Pre-mRNA-processing factor 6

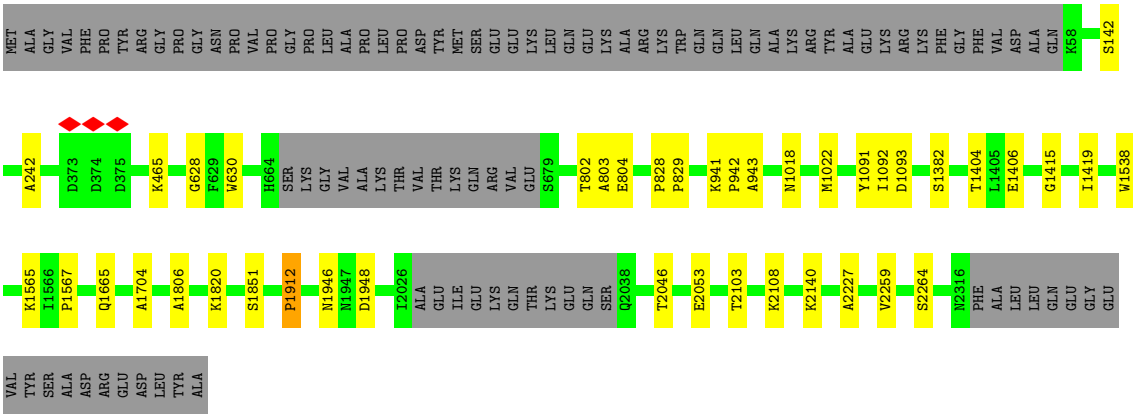
Chain N:



- Molecule 43: Pre-mRNA-processing-splicing factor 8

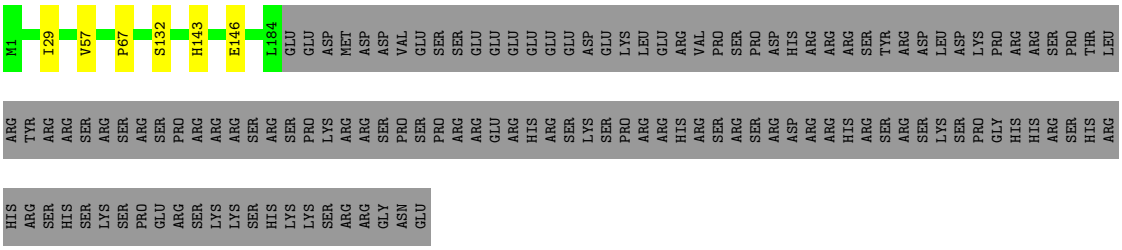
Chain A:





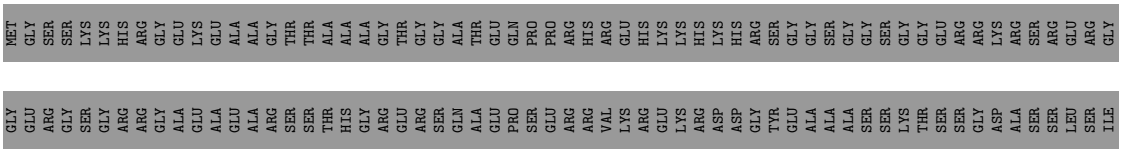
- Molecule 44: Pre-mRNA-splicing factor 38A

Chain I:



- Molecule 45: U4/U6.U5 tri-snRNP-associated protein 1

Chain S:



GLU GLU THR ASN LYS LEU ARG ALA LYS LEU GLY LEU LYS PRO LEU GLU VAL ASN ALA ILE LYS LYS GLU ALA GLY THR LYS E148 G191 GLU ASP ASP PRO TRP LEU D198 K219 ARG ALA LYS LEU LEU GLU GLU MET ASP GLN GLU PHE GLY VAL SER THR LEU VAL GLU GLU GLU

PHE GLY GLN ARG ARG GLN ASP LEU TYR SER A251 VAL P311 ASP TYR LEU PRO TYR ALA GLU ASP GLU SER VAL ASP ASP LEU ALA GLN GLN LYS PRO R331 ASP GLN THR GLN G343 GLU R345 P346 GLY ASP PHE GLY SER ARG LEU ARG GLY ARG GLY ARG ARG ARG VAL SER GLU VAL GLU GLU GLU LYS GLU

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

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

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

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

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

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

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

- Molecule 46: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C: 85% 13%

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

GLU ASP LYS LYS TYR TYR PRO THR ALA GLU GLU VAL TYR GLY PRO GLU VAL GLU THR ILE VAL GLN GLU GLU ASP THR GLN PRO LEU THR GLU PRO ILE ILE LYS PRO VAL LYS THR LYS LYS PHE THR LEU MET GLU GLN THR I109 V132 I202 V226 T254 A328

G332 V507 P568 N683 V795 I808 A812 M828 I906 K951 PHE PHE ASP ASP PRO MET LEU LEU GLU LEU ALA LYS GLN ASP VAL VAL LEU ASN TYR PRO MET

- Molecule 47: NHP2-like protein 1, N-terminally processed

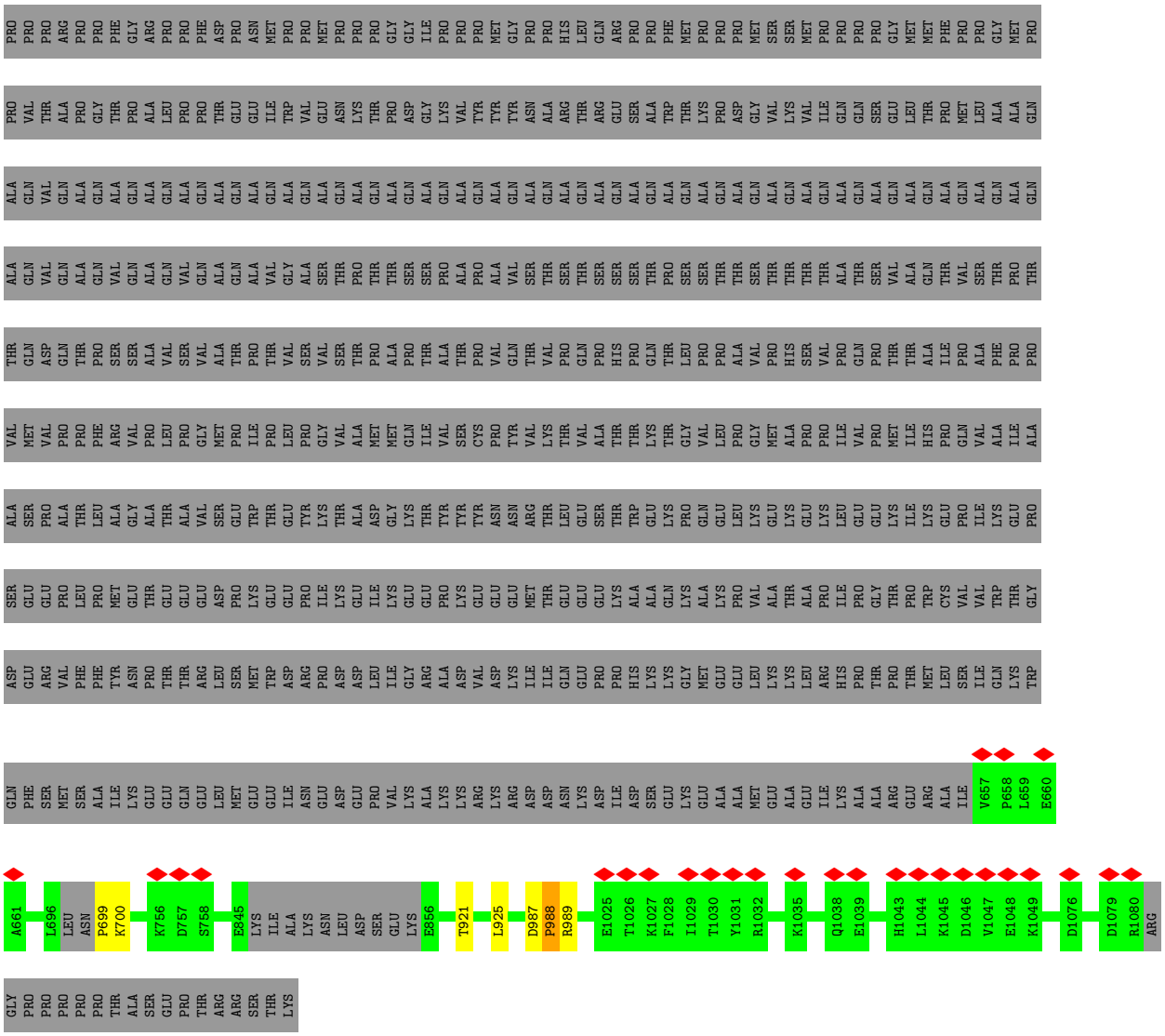
Chain M: 94%

MET THR GLU ALA D5 M56 L67 P70 F82 V128

- Molecule 48: Transcription elongation regulator 1

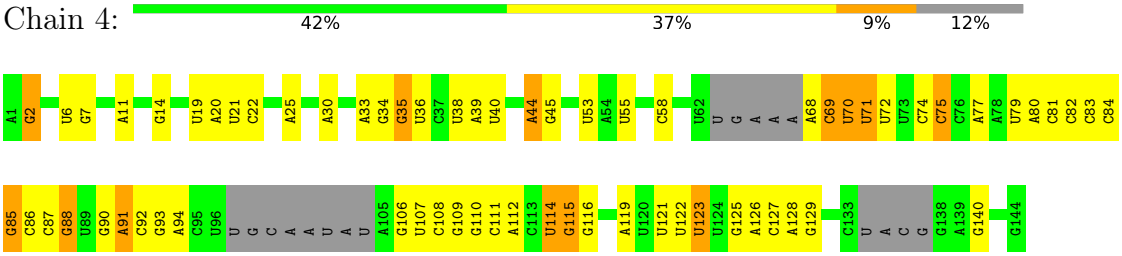
Chain T: 37% 62%

MET ALA GLU ARG GLY GLY ASP GLY GLY GLU SER GLU ARG PHE ASN PRO GLY GLU LEU ARG MET ALA GLN GLN GLN ALA LEU ARG PHE ARG GLY PRO ALA PRO PRO PRO ASN ALA VAL MET ARG GLY PRO PRO PRO LEU MET ARG PRO PRO PRO PRO PHE GLY MET MET ARG GLY PRO PRO



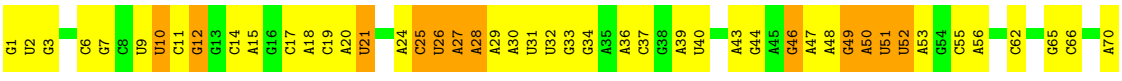
- Molecule 49: U4 snRNA

Chain 4:



- Molecule 50: U6 snRNA

Chain 6:



G71 G72 A73 U74 G75 A76 C77 A78 C G C A A A U85 U89 G90 U96 U C C A U A102 U103 U104 U105 U

• Molecule 51: Zinc finger matrin-type protein 2

Chain r: 57% 43%

MET ALA SER GLY SER GLY THR LYS ASN LEU ASP PHE ARG ARG LYS W16 P40 VAL GLN PRO VAL K45 M133 GLU GLU LYS GLN LYS ASP TYR ASP PHE GLU GLU ARG MET LYS GLU LEU ARG GLU GLU GLU GLU LYS ALA LYS ALA TYR LYS LYS GLU LYS GLN LYS GLU LYS LYS

ARG ARG ALA GLU GLU ASP LEU THR PHE GLU GLU GLU ASP ASP GLU MET ALA ALA VAL MET GLY PHE SER GLY PHE GLY SER THR LYS LYS SER TYR

• Molecule 52: U4/U6 small nuclear ribonucleoprotein Prp3

Chain J: 38% 62%

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

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

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

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

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

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

LYS THR GLY ILE HIS THR SER THR ARG LEU ALA LEU ILE ALA PRO LYS LYS GLU LEU LYS GLU GLY ASP ILE P385 I394 I395 PRO ASN GLY PHE ASP LEU THR GLU GLU ASN PRO LYS ARG GLU ASP TYR F412 P427 VAL ASP ASN D431 E606 GLN THR SER ASN THR LYS GLY

ASP ASP ASP GLU GLU SER ASP GLU GLU ALA VAL LYS LYS T627 D683

• Molecule 53: Ubiquitin-like protein 5

Chain s: 100%

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50321	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.141	Depositor
Minimum map value	-0.034	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	603.2, 603.2, 603.2	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.32, 2.32, 2.32	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	B4	0.13	0/394	0.34	0/549
2	8	0.23	0/515	0.58	1/721 (0.1%)
2	G	0.11	0/219	0.41	0/304
3	9	0.14	0/1575	0.39	0/2201
3	H	0.80	1/353 (0.3%)	1.16	3/491 (0.6%)
4	B2	0.17	0/1092	0.45	0/1536
5	B5	0.11	0/349	0.34	0/487
6	2	0.12	0/2307	0.31	0/3582
7	B3	0.14	0/5961	0.39	1/8335 (0.0%)
8	BP	0.12	0/501	0.43	0/697
9	B1	0.16	0/4421	0.47	3/6190 (0.0%)
10	B6	0.13	0/459	0.30	0/642
11	62	0.14	0/359	0.41	0/447
12	63	0.14	0/294	0.46	0/364
13	64	0.12	0/294	0.42	0/364
14	65	0.10	0/286	0.30	0/354
15	66	0.12	0/279	0.28	0/347
16	67	0.14	0/258	0.37	0/319
17	68	0.11	0/242	0.39	0/299
18	2b	0.13	0/416	0.41	0/581
18	4b	0.18	0/416	0.40	0/581
18	5b	0.15	0/343	0.44	0/427
19	21	0.13	0/404	0.37	0/564
19	41	0.15	0/409	0.36	0/571
19	51	0.14	0/327	0.31	0/407
20	22	0.13	0/485	0.32	0/677
20	42	0.15	0/466	0.39	0/651
20	52	0.14	0/387	0.38	0/482
21	2f	0.13	0/362	0.32	0/502
21	4f	0.16	0/362	0.37	0/502
21	5f	0.16	0/295	0.38	0/367
22	2e	0.13	0/403	0.36	0/561
22	4e	0.14	0/378	0.43	0/526
22	5e	0.14	0/315	0.35	0/392

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
23	2g	0.12	0/366	0.35	0/509
23	4g	0.13	0/371	0.37	0/516
23	5g	0.14	0/295	0.36	0/367
24	23	0.12	0/417	0.33	0/581
24	43	0.17	0/417	0.44	0/581
24	53	0.15	0/307	0.32	0/382
25	2B	0.11	0/463	0.28	0/646
26	2A	0.12	0/821	0.35	0/1149
27	7	0.21	0/1034	0.41	0/1446
28	E	0.15	0/1195	0.41	0/1492
29	B	0.17	0/8614	0.38	0/12072
30	x	0.17	0/196	0.87	2/270 (0.7%)
30	y	0.19	0/186	0.78	2/256 (0.8%)
31	v	0.13	0/2491	0.34	0/3477
31	w	0.14	0/2486	0.41	2/3469 (0.1%)
32	z	0.22	0/369	0.47	0/513
33	W	0.22	0/853	0.45	0/1188
34	5	0.65	0/2698	0.44	0/4195
35	Q	0.32	0/718	0.59	0/1003
36	D	0.53	0/712	0.63	0/995
37	X	0.29	0/409	0.48	0/572
38	K	0.32	0/1056	0.53	0/1471
39	Z	0.67	0/1089	0.57	0/1692
40	L	0.43	0/1884	0.58	0/2632
41	F	0.20	0/2170	0.43	0/3028
42	N	0.34	4/4021 (0.1%)	0.56	5/5630 (0.1%)
43	A	0.53	1/11156 (0.0%)	0.69	4/15500 (0.0%)
44	I	0.45	0/931	0.62	0/1302
45	S	0.52	3/853 (0.4%)	0.73	3/1184 (0.3%)
46	C	0.41	0/4308	0.57	0/6037
47	M	0.33	0/632	0.53	0/885
48	T	0.47	2/2075 (0.1%)	0.96	7/2903 (0.2%)
49	4	0.57	0/3002	0.41	0/4666
50	6	0.57	0/2230	0.45	0/3468
51	r	0.36	0/568	0.51	0/790
52	J	0.27	0/1323	0.42	0/1848
53	s	0.62	0/359	0.88	0/498
All	All	0.35	11/89001 (0.0%)	0.51	33/125233 (0.0%)

The worst 5 of 11 bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	419	PRO	CG-CD	-13.71	1.04	1.50
48	T	988	PRO	N-CA	13.66	1.66	1.47
45	S	346	PRO	N-CD	7.75	1.58	1.47
48	T	988	PRO	N-CD	-7.66	1.37	1.47
42	N	370	PRO	N-CD	6.84	1.57	1.47

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	T	988	PRO	N-CD-CG	-25.99	64.22	103.20
48	T	988	PRO	CA-CB-CG	-25.38	56.29	104.50
48	T	988	PRO	CB-CG-CD	23.09	179.99	106.10
3	H	419	PRO	N-CD-CG	-16.46	78.51	103.20
45	S	346	PRO	CA-N-CD	-14.80	91.28	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	B4	391	0	197	0	0
2	8	510	0	255	1	0
2	G	219	0	101	2	0
3	9	1569	0	721	2	0
3	H	351	0	181	2	0
4	B2	1072	0	563	1	0
5	B5	347	0	171	1	0
6	2	2071	0	1049	39	0
7	B3	5908	0	2954	18	0
8	BP	498	0	241	3	0
9	B1	4383	0	2195	5	0
10	B6	455	0	227	1	0
11	62	360	0	95	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	63	296	0	76	0	0
13	64	296	0	77	0	0
14	65	288	0	78	0	0
15	66	280	0	81	0	0
16	67	260	0	75	1	0
17	68	244	0	71	0	0
18	2b	413	0	194	2	0
18	4b	413	0	194	4	0
18	5b	344	0	93	1	0
19	21	402	0	184	0	0
19	41	407	0	183	1	0
19	51	328	0	89	1	0
20	22	482	0	220	3	0
20	42	463	0	211	4	0
20	52	388	0	102	0	0
21	2f	359	0	179	2	0
21	4f	359	0	179	4	0
21	5f	296	0	87	0	0
22	2e	403	0	173	4	0
22	4e	378	0	163	2	0
22	5e	316	0	85	0	0
23	2g	364	0	176	2	0
23	4g	369	0	178	2	0
23	5g	296	0	84	0	0
24	23	415	0	198	3	0
24	43	415	0	198	0	0
24	53	308	0	86	0	0
25	2B	461	0	218	2	0
26	2A	816	0	386	2	0
27	7	1028	0	487	0	0
28	E	1196	0	337	0	0
29	B	8538	0	4146	22	0
30	x	197	0	90	0	0
30	y	187	0	86	0	0
31	v	2478	0	1181	9	0
31	w	2474	0	1177	12	0
32	z	368	0	175	2	0
33	W	844	0	426	9	0
34	5	2420	0	1226	46	0
35	Q	713	0	337	1	0
36	D	708	0	328	2	0
37	X	408	0	205	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	K	1057	0	480	0	0
39	Z	977	0	498	16	0
40	L	1873	0	926	6	0
41	F	2155	0	1069	7	0
42	N	3990	0	2055	20	0
43	A	11052	0	5148	22	0
44	I	925	0	438	3	0
45	S	854	0	405	3	0
46	C	4260	0	2118	7	0
47	M	627	0	315	3	0
48	T	2071	0	935	6	0
49	4	2692	0	1367	34	0
50	6	1995	0	1006	33	0
51	r	568	0	245	0	0
52	J	1314	0	651	2	0
53	s	360	0	159	0	0
All	All	87322	0	41284	352	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 3.

The worst 5 of 352 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)
42:N:370:PRO:CG	42:N:370:PRO:CB	1.81	1.46
45:S:346:PRO:CG	45:S:346:PRO:CB	1.82	1.40
48:T:988:PRO:HD2	48:T:989:ARG:H	1.20	1.06
48:T:988:PRO:HD2	48:T:989:ARG:N	1.84	0.92
22:2e:58:LEU:O	22:2e:76:ARG:HA	1.69	0.91

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	B4	76/424 (18%)	76 (100%)	0	0	100	100
2	8	96/464 (21%)	91 (95%)	5 (5%)	0	100	100
2	G	42/464 (9%)	42 (100%)	0	0	100	100
3	9	309/501 (62%)	302 (98%)	6 (2%)	1 (0%)	36	71
3	H	68/501 (14%)	67 (98%)	1 (2%)	0	100	100
4	B2	204/895 (23%)	194 (95%)	10 (5%)	0	100	100
5	B5	67/86 (78%)	65 (97%)	2 (3%)	0	100	100
7	B3	1162/1217 (96%)	1117 (96%)	45 (4%)	0	100	100
8	BP	98/110 (89%)	94 (96%)	4 (4%)	0	100	100
9	B1	866/1304 (66%)	834 (96%)	32 (4%)	0	100	100
10	B6	88/125 (70%)	86 (98%)	2 (2%)	0	100	100
11	62	88/95 (93%)	86 (98%)	1 (1%)	1 (1%)	11	45
12	63	70/102 (69%)	65 (93%)	5 (7%)	0	100	100
13	64	70/139 (50%)	68 (97%)	2 (3%)	0	100	100
14	65	68/91 (75%)	63 (93%)	3 (4%)	2 (3%)	3	22
15	66	68/80 (85%)	64 (94%)	2 (3%)	2 (3%)	3	22
16	67	61/103 (59%)	58 (95%)	3 (5%)	0	100	100
17	68	57/96 (59%)	55 (96%)	1 (2%)	1 (2%)	6	32
18	2b	80/240 (33%)	76 (95%)	4 (5%)	0	100	100
18	4b	80/240 (33%)	77 (96%)	3 (4%)	0	100	100
18	5b	84/240 (35%)	80 (95%)	4 (5%)	0	100	100
19	21	78/119 (66%)	77 (99%)	1 (1%)	0	100	100
19	41	79/119 (66%)	76 (96%)	3 (4%)	0	100	100
19	51	80/119 (67%)	75 (94%)	5 (6%)	0	100	100
20	22	91/118 (77%)	89 (98%)	2 (2%)	0	100	100
20	42	90/118 (76%)	88 (98%)	2 (2%)	0	100	100
20	52	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
21	2f	70/86 (81%)	70 (100%)	0	0	100	100
21	4f	70/86 (81%)	68 (97%)	2 (3%)	0	100	100
21	5f	72/86 (84%)	68 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	2e	79/92 (86%)	78 (99%)	1 (1%)	0	100	100
22	4e	74/92 (80%)	72 (97%)	2 (3%)	0	100	100
22	5e	77/92 (84%)	74 (96%)	3 (4%)	0	100	100
23	2g	71/76 (93%)	70 (99%)	1 (1%)	0	100	100
23	4g	72/76 (95%)	69 (96%)	3 (4%)	0	100	100
23	5g	72/76 (95%)	71 (99%)	1 (1%)	0	100	100
24	23	81/126 (64%)	79 (98%)	2 (2%)	0	100	100
24	43	81/126 (64%)	78 (96%)	3 (4%)	0	100	100
24	53	75/126 (60%)	73 (97%)	2 (3%)	0	100	100
25	2B	90/225 (40%)	89 (99%)	1 (1%)	0	100	100
26	2A	160/255 (63%)	155 (97%)	5 (3%)	0	100	100
27	7	200/793 (25%)	187 (94%)	13 (6%)	0	100	100
28	E	297/357 (83%)	280 (94%)	16 (5%)	1 (0%)	36	71
29	B	1691/2136 (79%)	1622 (96%)	68 (4%)	1 (0%)	48	82
30	x	33/557 (6%)	27 (82%)	6 (18%)	0	100	100
30	y	31/557 (6%)	29 (94%)	2 (6%)	0	100	100
31	v	492/513 (96%)	477 (97%)	15 (3%)	0	100	100
31	w	489/513 (95%)	475 (97%)	14 (3%)	0	100	100
32	z	72/248 (29%)	66 (92%)	6 (8%)	0	100	100
33	W	167/177 (94%)	157 (94%)	10 (6%)	0	100	100
35	Q	140/144 (97%)	125 (89%)	15 (11%)	0	100	100
36	D	139/142 (98%)	132 (95%)	7 (5%)	0	100	100
37	X	79/376 (21%)	79 (100%)	0	0	100	100
38	K	206/439 (47%)	189 (92%)	17 (8%)	0	100	100
40	L	367/499 (74%)	342 (93%)	24 (6%)	1 (0%)	36	71
41	F	427/522 (82%)	411 (96%)	16 (4%)	0	100	100
42	N	783/941 (83%)	682 (87%)	100 (13%)	1 (0%)	48	82
43	A	2228/2335 (95%)	2044 (92%)	181 (8%)	3 (0%)	48	82
44	I	182/312 (58%)	173 (95%)	9 (5%)	0	100	100
45	S	161/800 (20%)	152 (94%)	9 (6%)	0	100	100
46	C	841/972 (86%)	794 (94%)	47 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	M	122/128 (95%)	119 (98%)	3 (2%)	0	100	100
48	T	406/1098 (37%)	386 (95%)	20 (5%)	0	100	100
51	r	110/199 (55%)	104 (94%)	6 (6%)	0	100	100
52	J	252/683 (37%)	236 (94%)	16 (6%)	0	100	100
53	s	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
All	All	15445/25362 (61%)	14624 (95%)	807 (5%)	14 (0%)	49	82

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	9	78	PRO
11	62	55	LEU
14	65	70	ASP
15	66	52	VAL
15	66	55	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B4	4/336 (1%)	4 (100%)	0	100	100
2	8	7/382 (2%)	7 (100%)	0	100	100
2	G	1/382 (0%)	1 (100%)	0	100	100
3	9	8/446 (2%)	8 (100%)	0	100	100
3	H	3/446 (1%)	3 (100%)	0	100	100
4	B2	22/776 (3%)	22 (100%)	0	100	100
5	B5	3/77 (4%)	3 (100%)	0	100	100
7	B3	59/1051 (6%)	59 (100%)	0	100	100
8	BP	4/95 (4%)	4 (100%)	0	100	100
9	B1	40/1104 (4%)	40 (100%)	0	100	100
10	B6	5/109 (5%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	2b	4/177 (2%)	4 (100%)	0	100	100
18	4b	4/177 (2%)	4 (100%)	0	100	100
19	21	3/101 (3%)	3 (100%)	0	100	100
19	41	3/101 (3%)	3 (100%)	0	100	100
20	22	5/110 (4%)	5 (100%)	0	100	100
20	42	4/110 (4%)	4 (100%)	0	100	100
21	2f	4/74 (5%)	4 (100%)	0	100	100
21	4f	4/74 (5%)	4 (100%)	0	100	100
22	2e	1/84 (1%)	1 (100%)	0	100	100
22	4e	1/84 (1%)	1 (100%)	0	100	100
23	2g	3/66 (4%)	3 (100%)	0	100	100
23	4g	3/66 (4%)	3 (100%)	0	100	100
24	23	3/101 (3%)	3 (100%)	0	100	100
24	43	3/101 (3%)	3 (100%)	0	100	100
25	2B	3/195 (2%)	3 (100%)	0	100	100
26	2A	6/218 (3%)	6 (100%)	0	100	100
27	7	8/709 (1%)	8 (100%)	0	100	100
29	B	77/1908 (4%)	77 (100%)	0	100	100
30	x	2/498 (0%)	2 (100%)	0	100	100
30	y	2/498 (0%)	2 (100%)	0	100	100
31	v	15/450 (3%)	15 (100%)	0	100	100
31	w	15/450 (3%)	15 (100%)	0	100	100
32	z	2/203 (1%)	2 (100%)	0	100	100
33	W	10/148 (7%)	10 (100%)	0	100	100
35	Q	6/130 (5%)	6 (100%)	0	100	100
36	D	5/130 (4%)	5 (100%)	0	100	100
37	X	2/333 (1%)	2 (100%)	0	100	100
38	K	2/395 (0%)	2 (100%)	0	100	100
40	L	14/424 (3%)	14 (100%)	0	100	100
41	F	17/442 (4%)	17 (100%)	0	100	100
42	N	35/792 (4%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	A	107/2108 (5%)	107 (100%)	0	100	100
44	I	7/293 (2%)	7 (100%)	0	100	100
45	S	4/681 (1%)	4 (100%)	0	100	100
46	C	49/866 (6%)	49 (100%)	0	100	100
47	M	6/111 (5%)	6 (100%)	0	100	100
48	T	7/956 (1%)	7 (100%)	0	100	100
51	r	2/181 (1%)	2 (100%)	0	100	100
52	J	13/599 (2%)	13 (100%)	0	100	100
All	All	617/20348 (3%)	617 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	5	114/117 (97%)	46 (40%)	2 (1%)
39	Z	44/347 (12%)	12 (27%)	1 (2%)
49	4	123/144 (85%)	38 (30%)	3 (2%)
50	6	90/106 (84%)	26 (28%)	4 (4%)
6	2	94/188 (50%)	22 (23%)	4 (4%)
All	All	465/902 (51%)	144 (30%)	14 (3%)

5 of 144 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	2	31	G
6	2	38	A
6	2	40	C
6	2	45	C
6	2	46	U

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
49	4	44	A

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Mol	Chain	Res	Type
49	4	80	A
50	6	77	C
50	6	39	A
50	6	52	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 (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
43	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	461:HIS	C	462:ARG	N	1.18

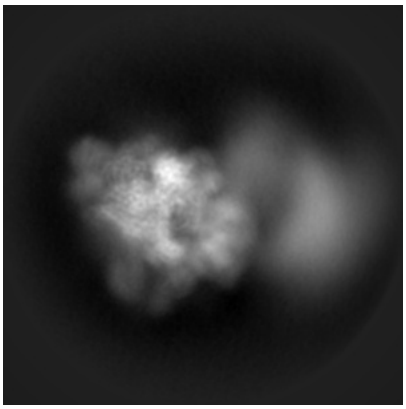
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-18529. These allow visual inspection of the internal detail of the map and identification of artifacts.

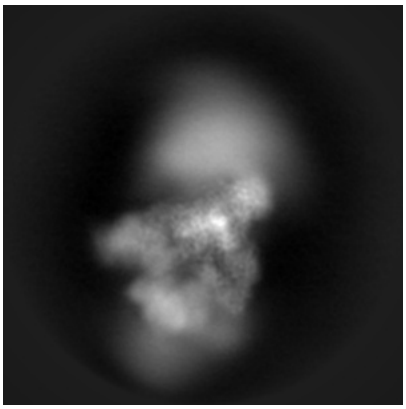
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

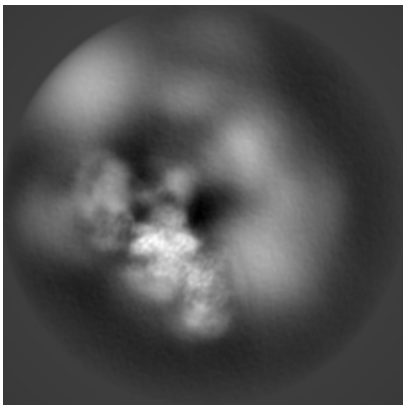
6.1.1 Primary map



X

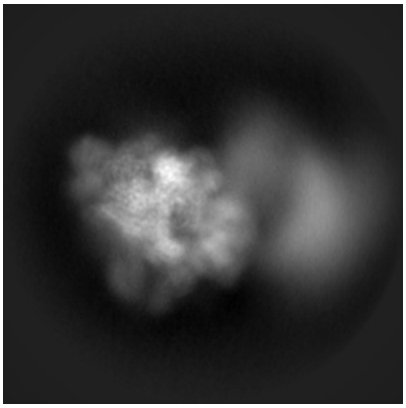


Y

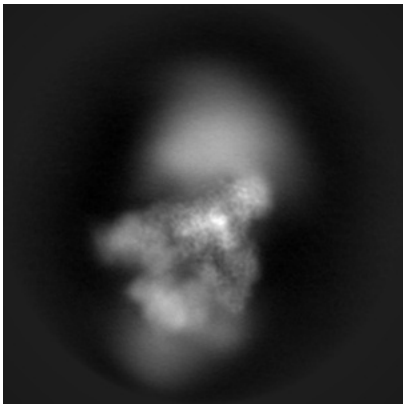


Z

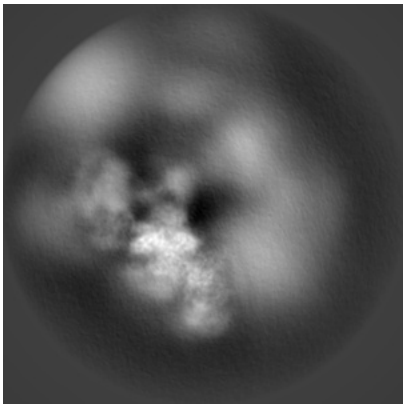
6.1.2 Raw map



X



Y

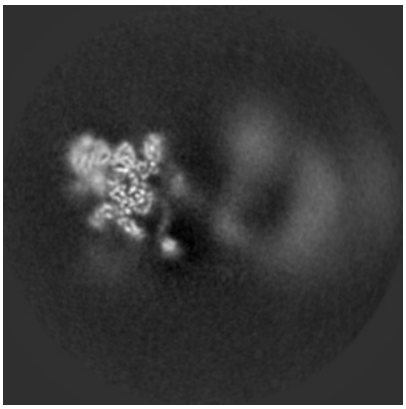


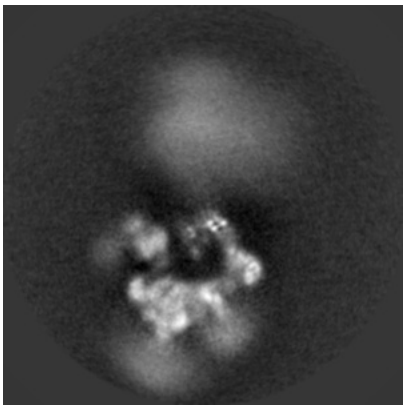
Z

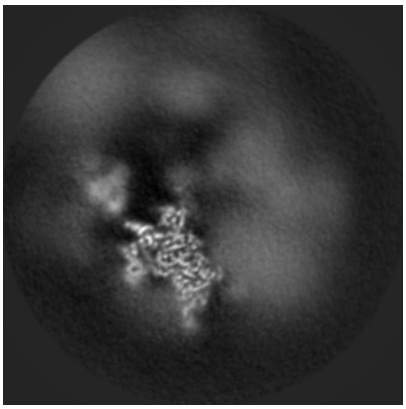
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

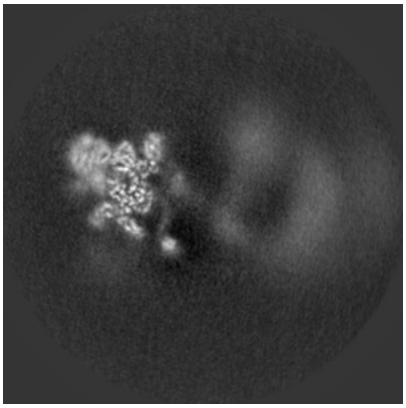
6.2.1 Primary map

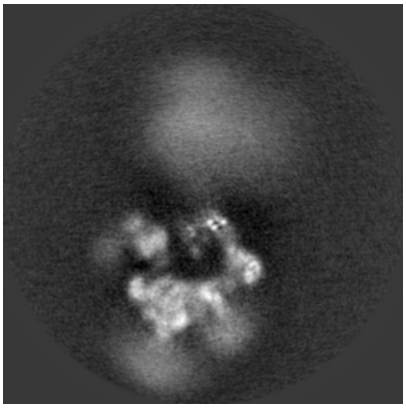

X Index: 130

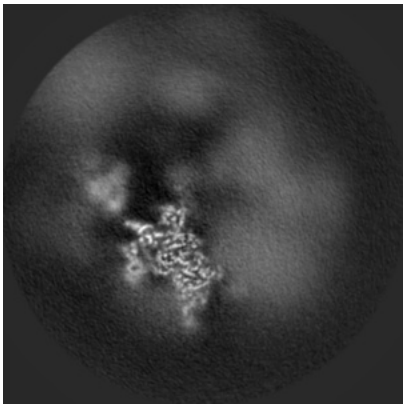

Y Index: 130


Z Index: 130

6.2.2 Raw map


X Index: 130

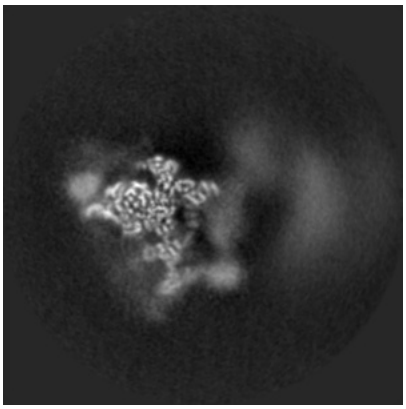

Y Index: 130

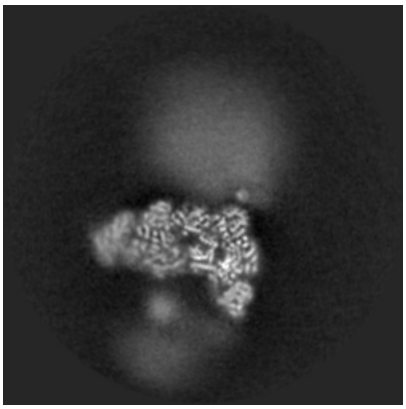

Z Index: 130

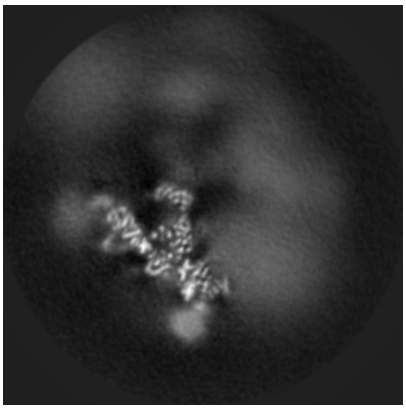
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

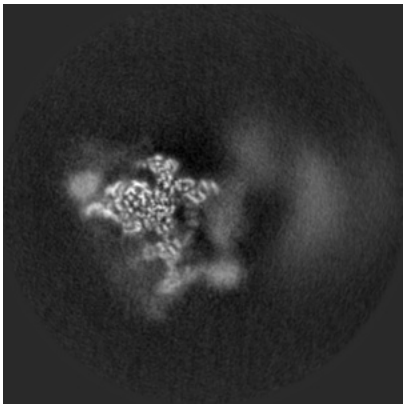
6.3.1 Primary map

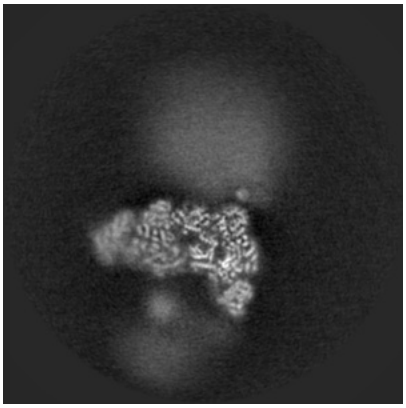

X Index: 118

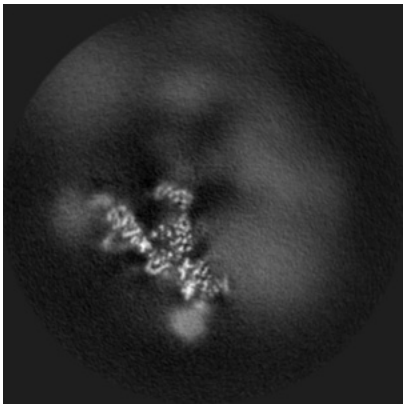

Y Index: 106


Z Index: 141

6.3.2 Raw map


X Index: 118

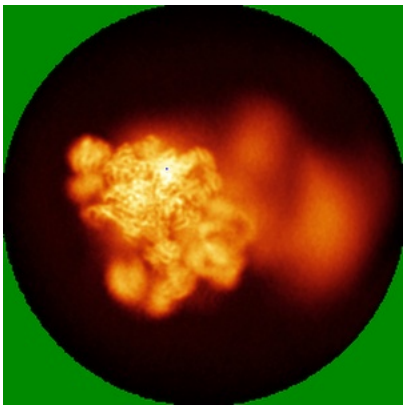

Y Index: 106

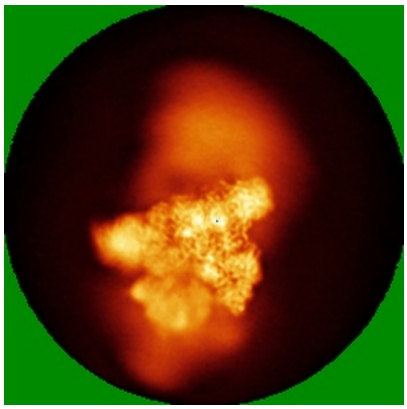

Z Index: 141

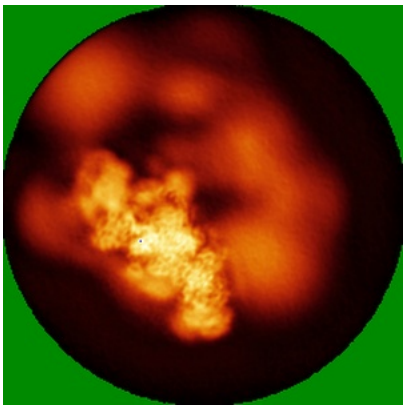
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

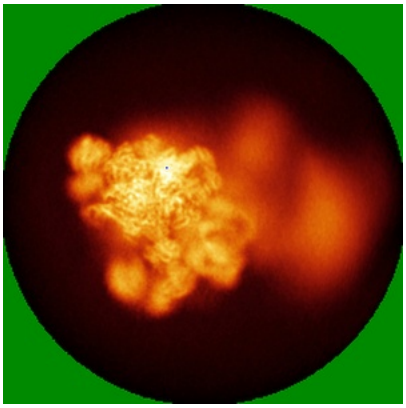
6.4.1 Primary map

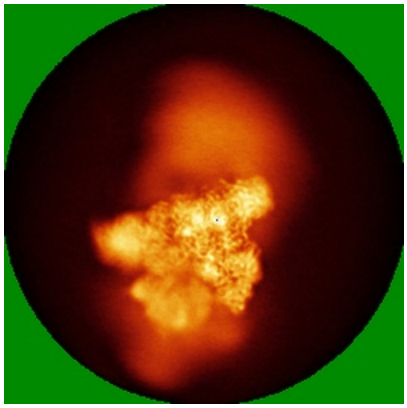

X

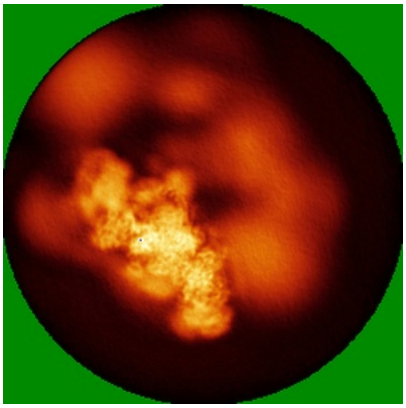

Y


Z

6.4.2 Raw 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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

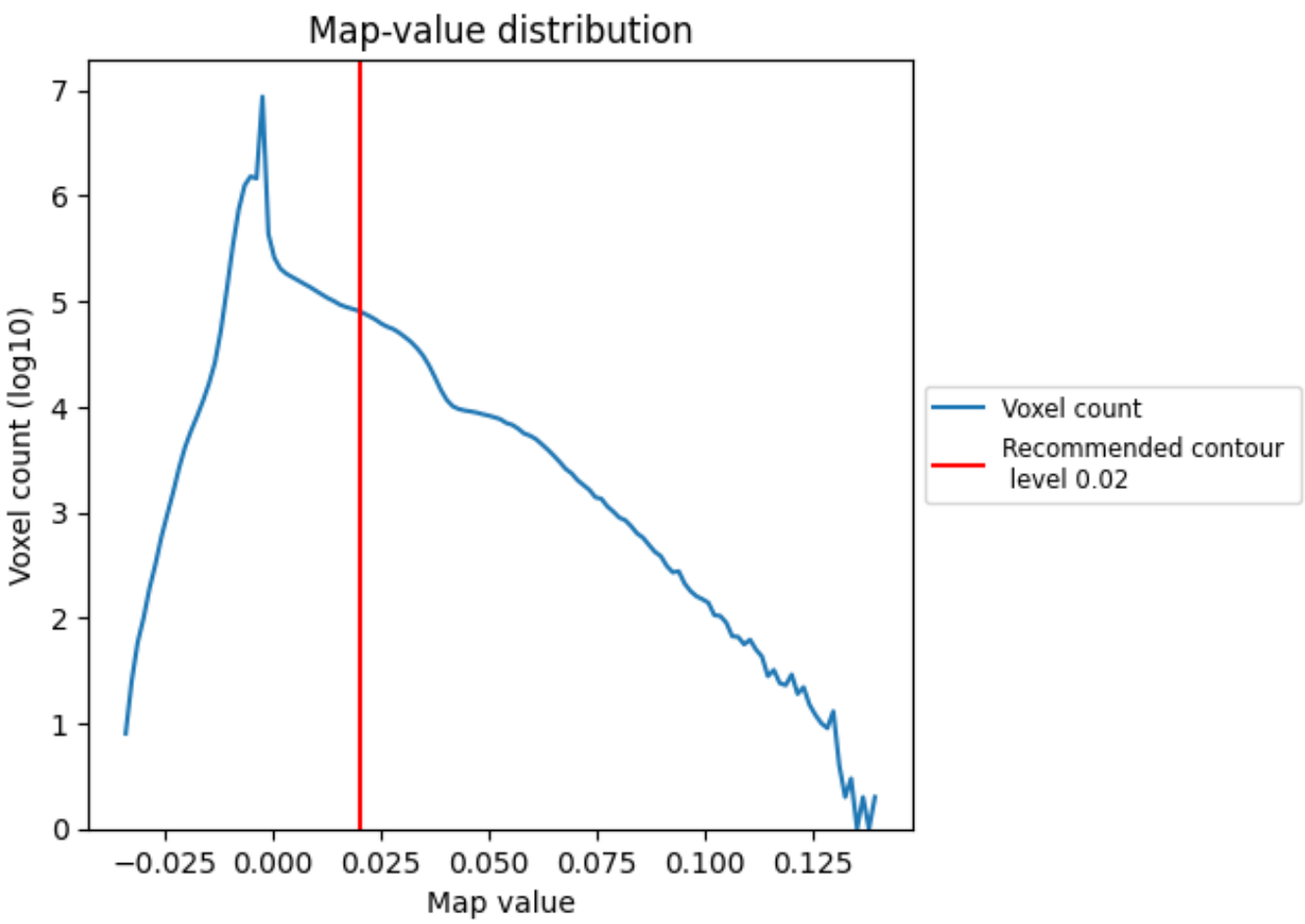
6.6 Mask visualisation (i)

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

7 Map analysis (i)

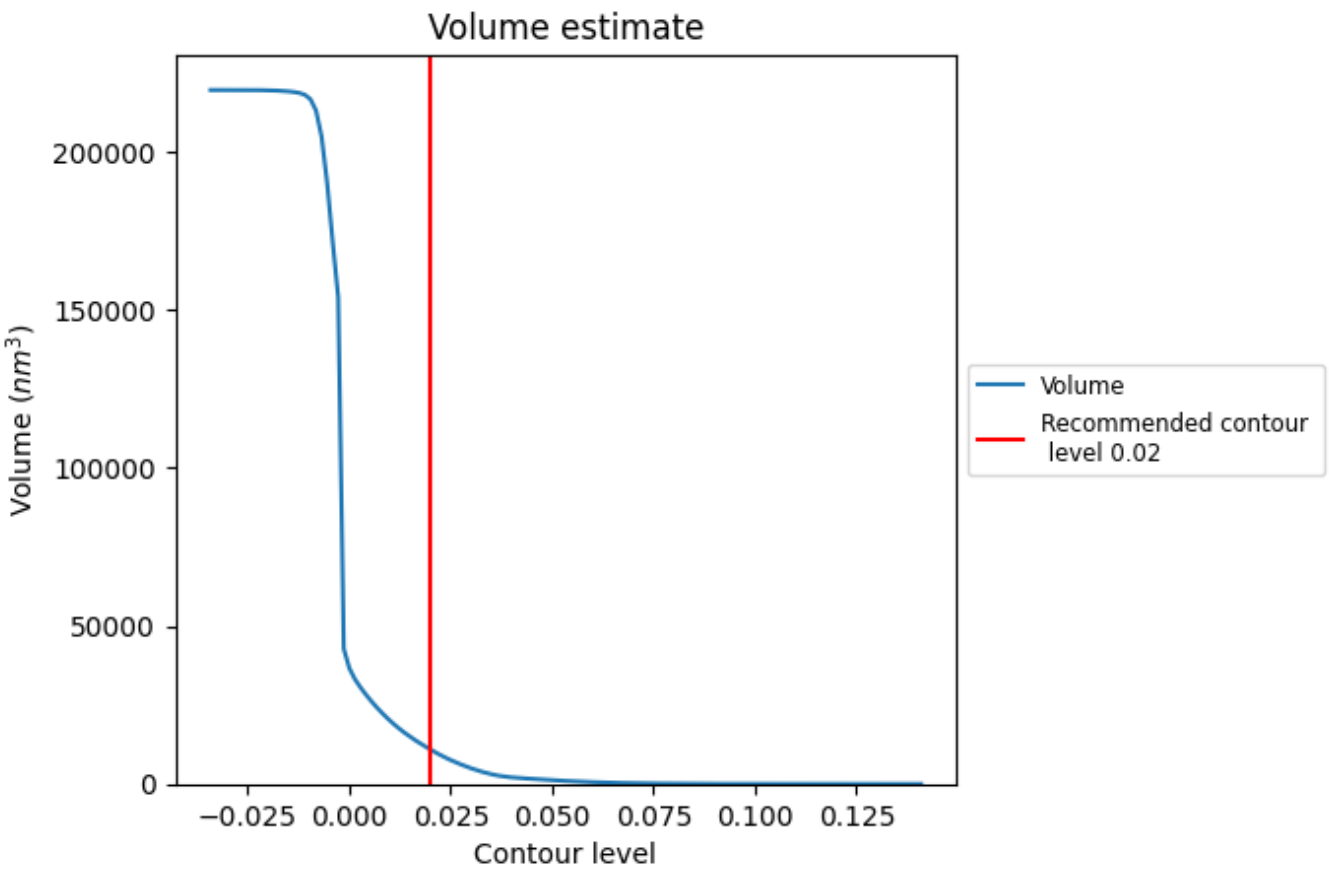
This section contains the results of statistical analysis of the map.

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.

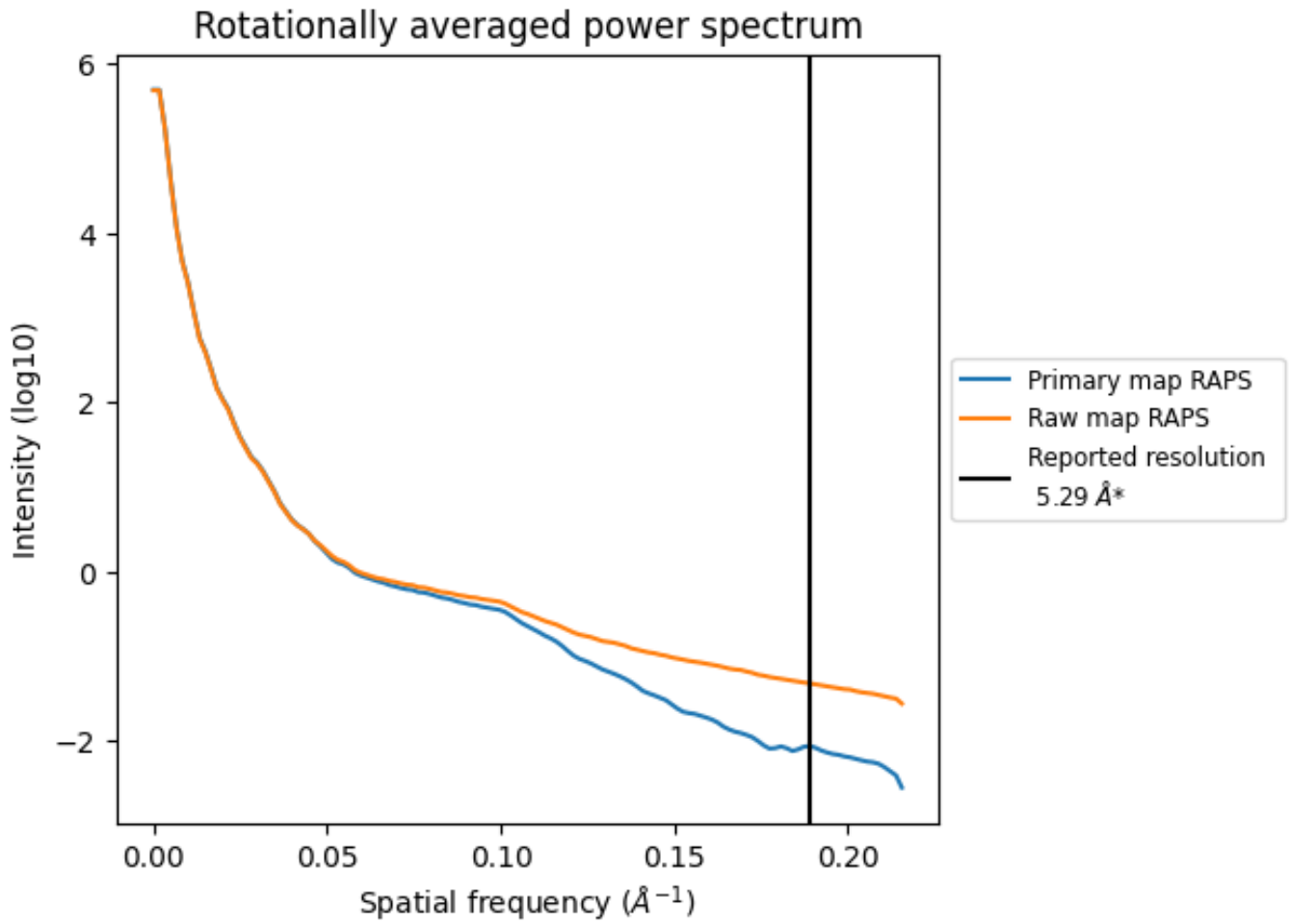
7.2 Volume estimate (i)



The volume at the recommended contour level is 10940 nm^3; this corresponds to an approximate mass of 9883 kDa.

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

7.3 Rotationally averaged power spectrum (i)

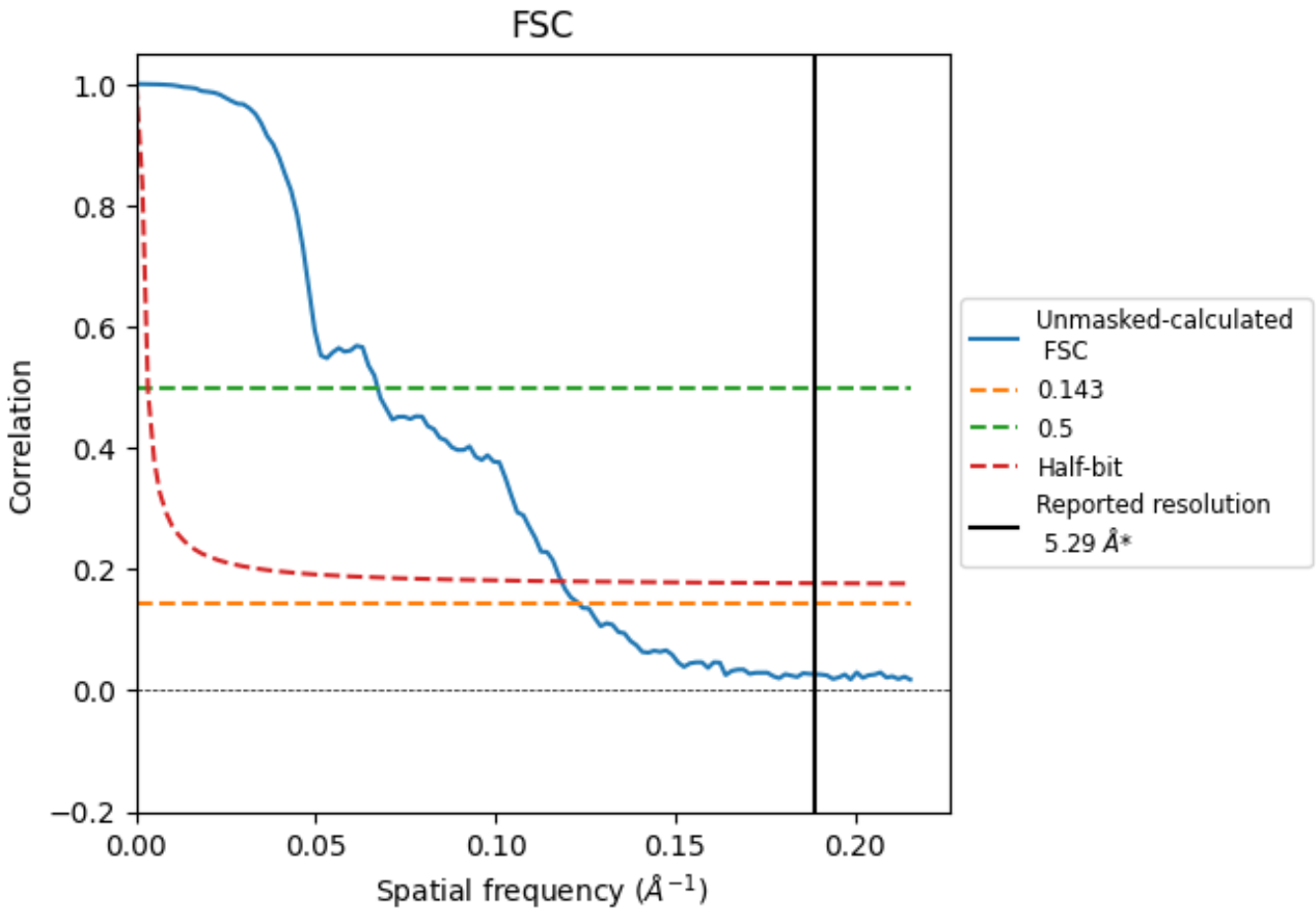


*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

8.2 Resolution estimates (i)

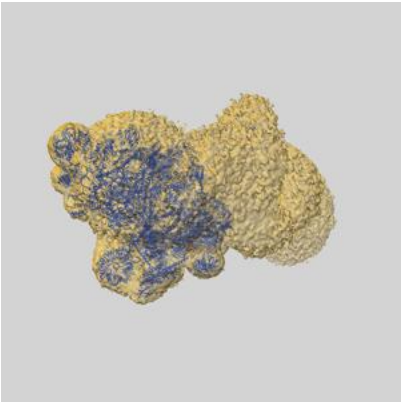
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.29	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.12	14.88	8.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.12 differs from the reported value 5.29 by more than 10 %

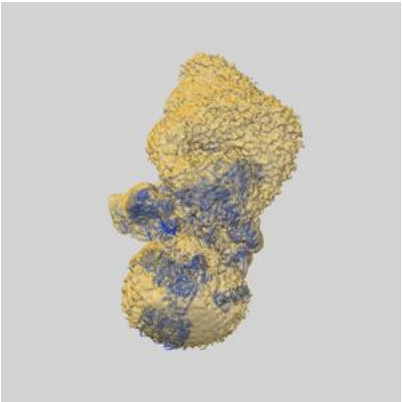
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-18529 and PDB model 8QO9. Per-residue inclusion information can be found in section 3 on page 15.

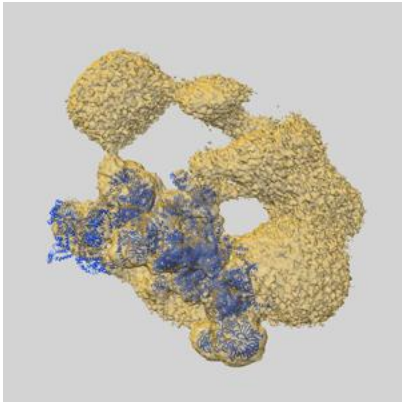
9.1 Map-model overlay (i)



X



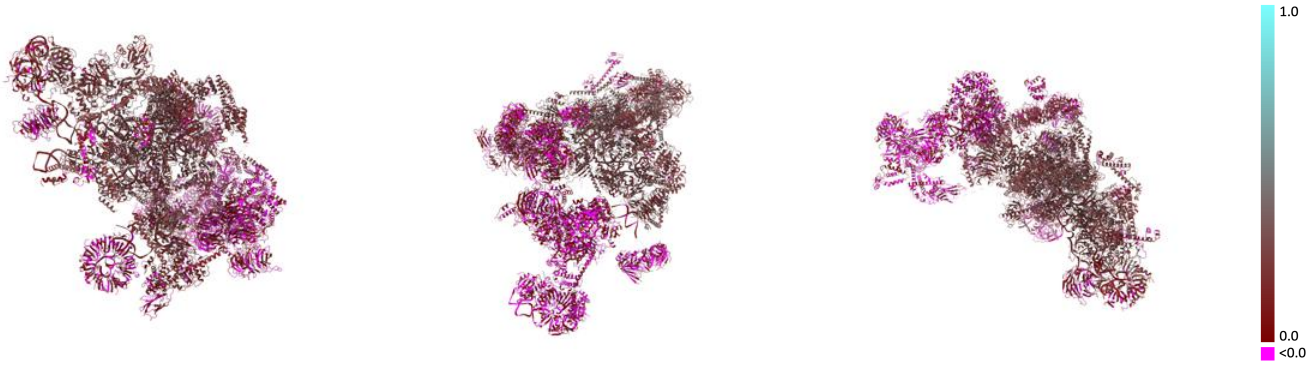
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

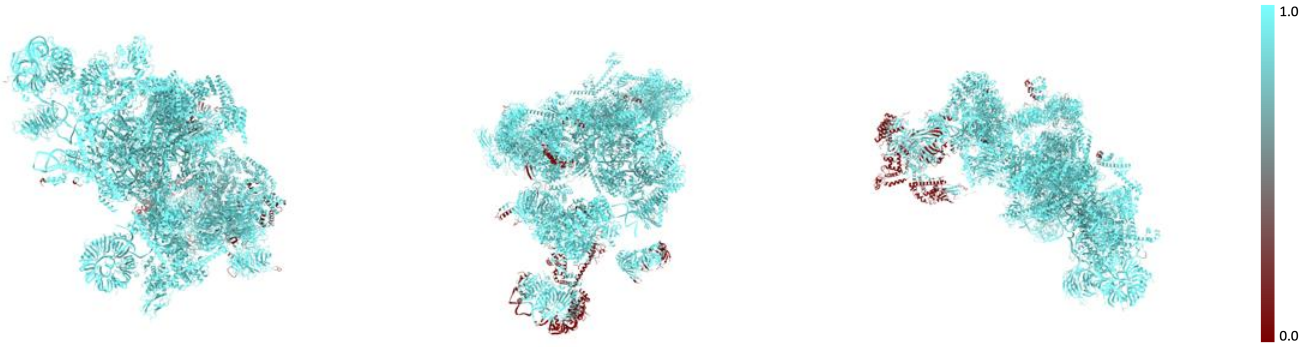
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

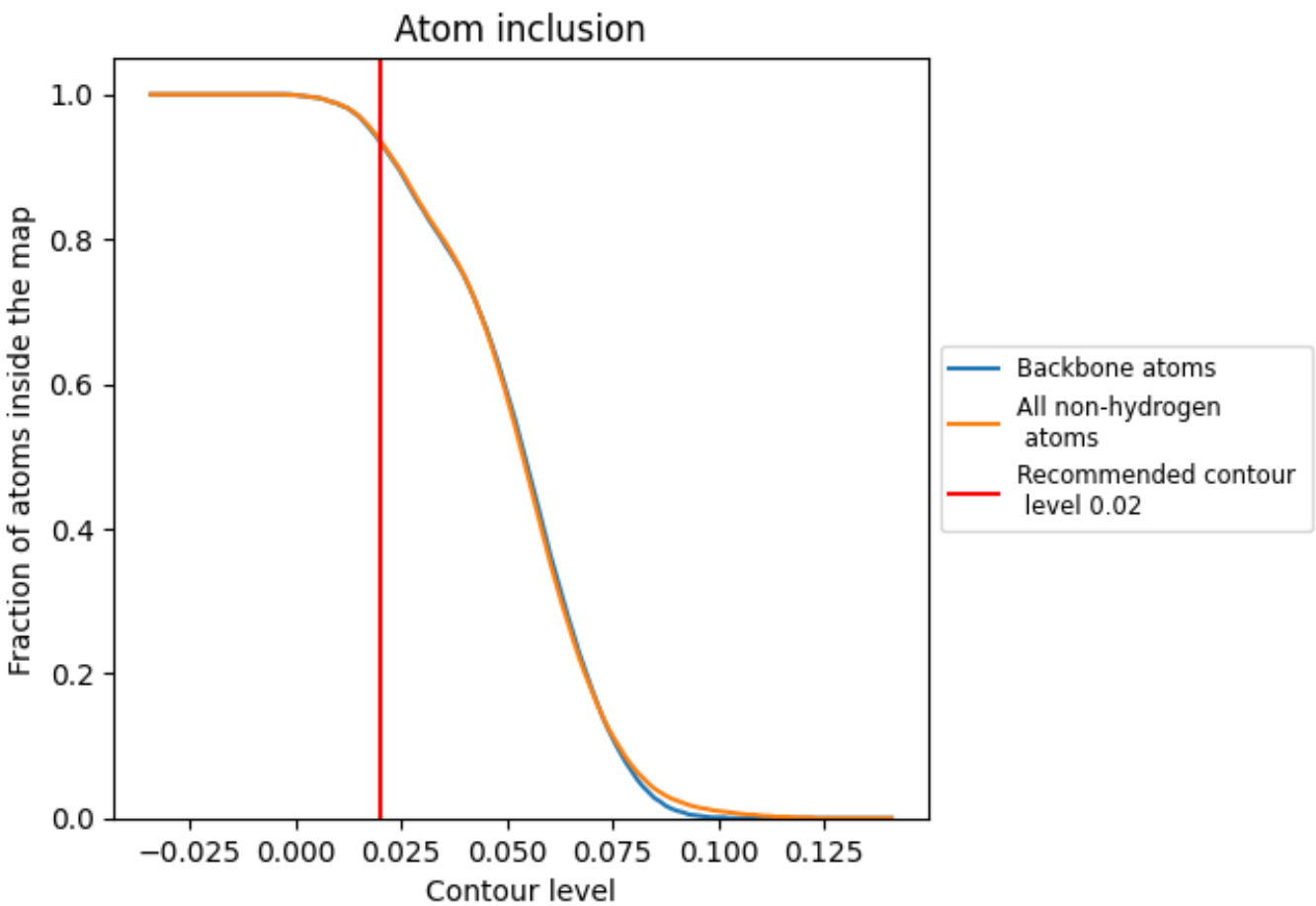
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9370	0.1580
2	0.8310	0.0270
21	0.9550	0.0410
22	0.5140	0.0130
23	1.0000	0.0220
2A	0.8200	0.0220
2B	0.7570	0.0160
2b	1.0000	0.0020
2e	0.3570	0.0210
2f	0.2590	0.0420
2g	0.7640	0.0410
4	0.9990	0.1710
41	1.0000	0.0340
42	0.9980	0.0600
43	1.0000	0.0350
4b	1.0000	0.0530
4e	1.0000	0.0510
4f	1.0000	0.0540
4g	1.0000	0.0230
5	1.0000	0.1840
51	1.0000	0.2060
52	0.9920	0.1130
53	1.0000	0.2640
5b	0.9860	0.1870
5e	1.0000	0.1950
5f	1.0000	0.1230
5g	1.0000	0.2370
6	1.0000	0.2000
62	0.9420	0.0120
63	0.9190	0.0070
64	0.6280	-0.0180
65	0.6420	0.0370
66	0.8860	-0.0100
67	0.4190	0.0540
68	0.9470	0.0500

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Chain	Atom inclusion	Q-score
7	0.4450	0.0960
8	0.3390	0.0500
9	0.2770	0.0100
A	0.9980	0.2880
B	1.0000	0.1950
B1	0.9710	0.0360
B2	0.8320	0.0190
B3	0.9230	0.0570
B4	1.0000	0.0240
B5	1.0000	0.0650
B6	1.0000	0.0630
BP	1.0000	0.0440
C	1.0000	0.2540
D	1.0000	0.2890
E	0.9980	0.0590
F	1.0000	0.2480
G	0.8720	0.0660
H	0.9200	0.0570
I	1.0000	0.2780
J	1.0000	0.2610
K	0.9920	0.2360
L	1.0000	0.2850
M	1.0000	0.2950
N	1.0000	0.2430
Q	1.0000	0.2340
S	0.9910	0.2670
T	0.9340	0.1530
W	1.0000	0.2050
X	1.0000	0.2490
Z	1.0000	0.1570
r	1.0000	0.2650
s	1.0000	0.2980
v	0.9460	0.0550
w	0.8530	0.0470
x	0.8830	0.0250
y	0.9470	-0.0010
z	1.0000	0.0640