



Full wwPDB EM Validation Report ⓘ

May 25, 2024 – 10:25 am BST

PDB ID : 8QZS
EMDB ID : EMD-18781
Title : Cryo-EM structure of the cross-exon B-like complex
Authors : Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.
Deposited on : 2023-10-29
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

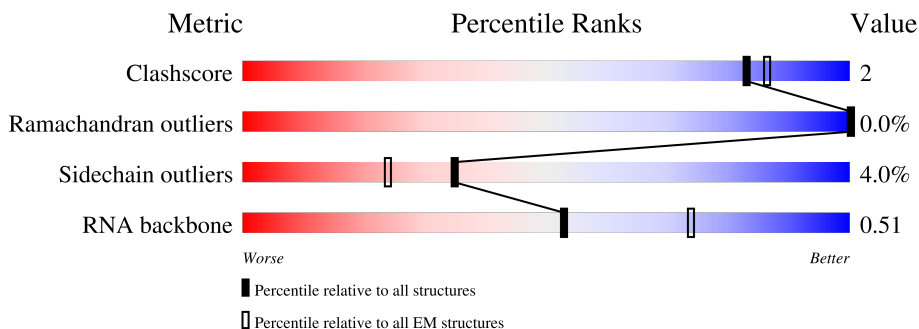
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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.



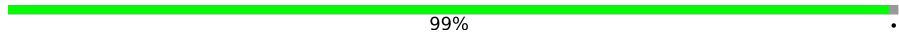


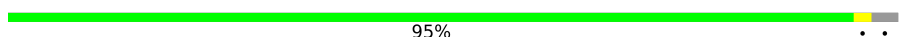

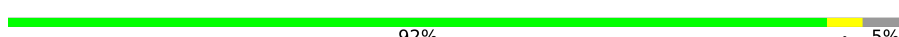







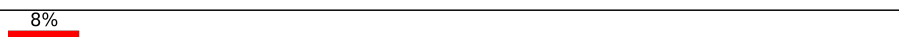
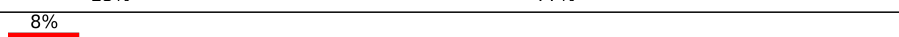
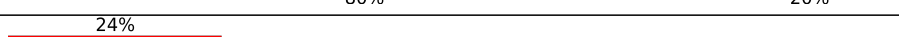
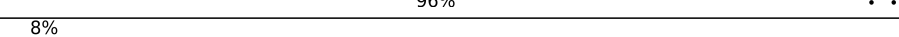


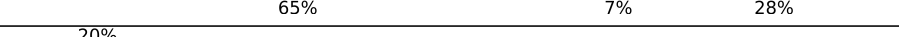
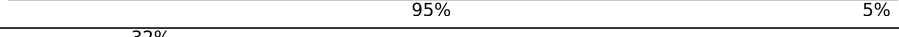




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	2335	95% (Green), 2% (Grey), 2% (Grey)
2	B	2136	79% (Green), 21% (Grey), 1% (Grey)
3	5	117	48% (Green), 32% (Yellow), 13% (Orange), 7% (Red), 1% (Grey)
4	2	188	32% (Green), 16% (Yellow), 48% (Grey), 3% (Red), 3% (Red)
5	6	106	32% (Green), 16% (Yellow), 8% (Orange), 44% (Grey), 1% (Red)
6	4	144	54% (Green), 38% (Yellow), 6% (Orange), 1% (Red)
7	C	972	85% (Green), 14% (Grey), 1% (Grey)

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Mol	Chain	Length	Quality of chain
8	D	142	 99%
9	E	357	 84% 16%
10	I	312	 58% 41%
11	M	128	 95%
12	U	565	 80% 19%
13	W	177	 92% 5%
14	X	376	 21% 79%
15	Z	15	 87% 13%
16	7	793	 14% 26% 74%
17	r	199	 57% 43%
18	B4	424	 18% 82%
19	8	464	 22% 30% 69%
20	9	501	 62% 69% 30%
21	B2	895	 8% 23% 77%
22	B5	86	 8% 80% 20%
23	B3	1217	 24% 96%
24	BP	110	 8% 88% 9%
25	B1	1304	 19% 66% 33%
26	B6	125	 65% 7% 28%
27	62	95	 20% 95% 5%
28	63	102	 32% 73% 27%
29	64	139	 13% 53% 47%
30	65	91	 77% 77% 21%
31	66	80	 79% 88% 12%
32	67	103	 42% 63% 37%

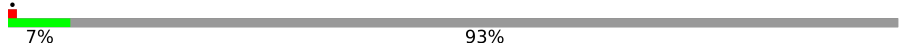

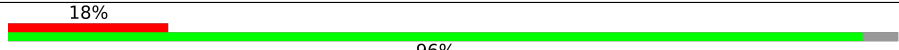


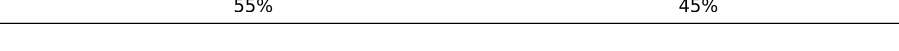

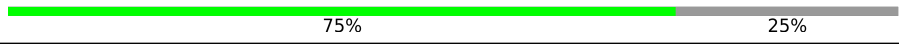


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Mol	Chain	Length	Quality of chain
33	68	96	61% 36%
34	22	118	72% 81% 19%
34	42	118	60% 37%
34	52	118	6% 48% 33% 17%
35	2f	86	81% 84% 16%
35	4f	86	83% 17%
35	5f	86	83% 15%
36	2e	92	78% 88% 12%
36	4e	92	85% 15%
36	5e	92	84% 16%
37	2g	76	64% 96%
37	4g	76	96%
37	5g	76	72% 25%
38	23	126	55% 64% 34%
38	43	126	56% 44%
38	53	126	55% 12% 33%
39	2b	240	31% 34% 66%
39	4b	240	27% 73%
39	5b	240	30% 70%
40	21	119	61% 67% 33%
40	41	119	69% 31%
40	51	119	38% 26% 32%
41	2B	225	41% 40% 59%
42	2A	255	64% 64% 36%
43	x	557	6% 7% 93%

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Mol	Chain	Length	Quality of chain
43	y	557	 7% 93%
44	v	513	 24% 97%
44	w	513	 18% 96%
45	K	439	 25% 75%
46	z1	11	 55% 45%
47	z2	4	 100%
48	J	683	 33% 67%
49	L	499	 75% 25%
50	F	522	 75% 23%
51	N	941	 87% 12%
52	S	800	 21% 79%

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 86145 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	2247	11389	6895	2247	2247	0	0

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

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

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	5	109	2296	1028	383	776	109	0	0

- Molecule 4 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	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 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	6	59	1251	558	230	404	59	0	0

- Molecule 6 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
6	4	136	2881	1288	498	959	136	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
7	C	836	4223	2551	836	836		0	0

- Molecule 8 is a protein called Thioredoxin-like protein 4A.

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

- Molecule 9 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

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

- Molecule 10 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
10	I	183	920	554	183	183		0	0

- Molecule 11 is a protein called NHP2-like protein 1, N-terminally processed.

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

- Molecule 12 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
12	U	456	2308	1396	456	456		0	0

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase H.

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

- Molecule 14 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	80	Total	C	N	O	0	0
			403	243	80	80		

- Molecule 15 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	15	Total	C	N	O	P	0	0
			314	141	51	107	15		

- Molecule 16 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	7	204	Total	C	N	O	0	0
			1028	620	204	204		

- Molecule 17 is a protein called Zinc finger matrin-type protein 2.

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

- Molecule 18 is a protein called Splicing factor 3B subunit 4.

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

- Molecule 19 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	8	144	Total	C	N	O	0	0
			729	441	144	144		

- Molecule 20 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	9	350	1755	1055	350	350	0	0

- Molecule 21 is a protein called Splicing factor 3B subunit 2.

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

- Molecule 22 is a protein called Splicing factor 3B subunit 5.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	B3	1186	5969	3597	1186	1186	0	0

- Molecule 24 is a protein called PHD finger-like domain-containing protein 5A.

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

- Molecule 25 is a protein called Splicing factor 3B subunit 1.

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

- Molecule 26 is a protein called Splicing factor 3B subunit 6.

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

- Molecule 27 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	62	90	360	180	90	90	0	0

- Molecule 28 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	63	74	296	148	74	74	0	0

- Molecule 29 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	64	74	296	148	74	74	0	0

- Molecule 30 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	65	72	288	144	72	72	0	0

- Molecule 31 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	66	70	280	140	70	70	0	0

- Molecule 32 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	67	65	260	130	65	65	0	0

- Molecule 33 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	68	61	244	122	61	61	0	0

- Molecule 34 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	42	74	Total	C	N	O	0	0
			300	152	74	74		
34	52	98	Total	C	N	O	S	0
			796	498	144	148	6	0
34	22	95	Total	C	N	O	0	0
			482	292	95	95		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	4f	71	Total	C	N	O	0	0
			292	150	71	71		
35	5f	73	Total	C	N	O	S	0
			567	367	94	101	5	0
35	2f	72	Total	C	N	O	0	0
			359	215	72	72		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	4e	78	Total	C	N	O	0	0
			314	158	78	78		
36	5e	77	Total	C	N	O	S	0
			638	405	113	115	5	0
36	2e	81	Total	C	N	O	0	0
			403	241	81	81		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	4g	73	Total	C	N	O	0	0
			298	152	73	73		
37	5g	74	Total	C	N	O	S	0
			577	364	104	103	6	0
37	2g	73	Total	C	N	O	0	0
			364	218	73	73		

- Molecule 38 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	43	71	Total	C	N	O	0	0
			288	146	71	71		

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Mol	Chain	Residues	Atoms					AltConf	Trace
38	53	84	Total	C	N	O	S	0	0
			657	412	116	123	6		
38	23	83	Total	C	N	O		0	0
			415	249	83	83			

- Molecule 39 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4b	64	Total	C	N	O		0	0
			256	128	64	64			
39	5b	73	Total	C	N	O	S	0	0
			594	376	108	103	7		
39	2b	82	Total	C	N	O		0	0
			413	249	82	82			

- Molecule 40 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	41	82	Total	C	N	O		0	0
			334	170	82	82			
40	51	81	Total	C	N	O	S	0	0
			641	408	112	118	3		
40	21	80	Total	C	N	O		0	0
			402	242	80	80			

- Molecule 41 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	2B	92	Total	C	N	O	0	0
			461	277	92	92		

- Molecule 42 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	2A	162	Total	C	N	O	0	0
			816	492	162	162		

- Molecule 43 is a protein called Protein Red.

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

- Molecule 44 is a protein called WD40 repeat-containing protein SMU1.

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

- Molecule 45 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	K	109	Total	C	N	O	0	0
			543	325	109	109		

- Molecule 46 is a RNA chain called Oligo 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	z1	11	Total	C	N	O	P	0	0
			239	107	46	75	11		

- Molecule 47 is a RNA chain called Oligo 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z2	4	Total	C	N	O	P	0	0
			90	40	20	26	4		

- Molecule 48 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	J	224	Total	C	N	O	0	0
			1125	677	224	224		

- Molecule 49 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	L	376	Total	C	N	O	0	0
			1887	1135	376	376		

- Molecule 50 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	F	404	2020	1212	404	404	0	0

- Molecule 51 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	N	831	4192	2530	831	831	0	0

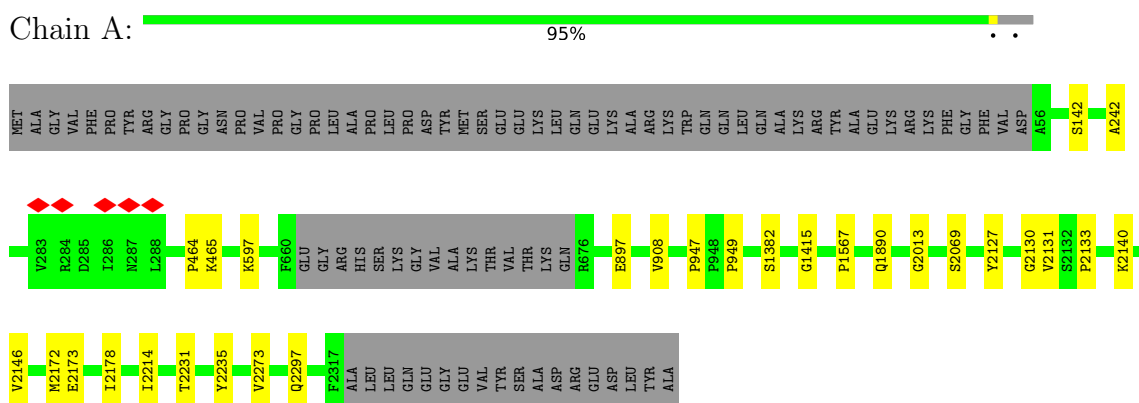
- Molecule 52 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	S	171	858	516	171	171	0	0

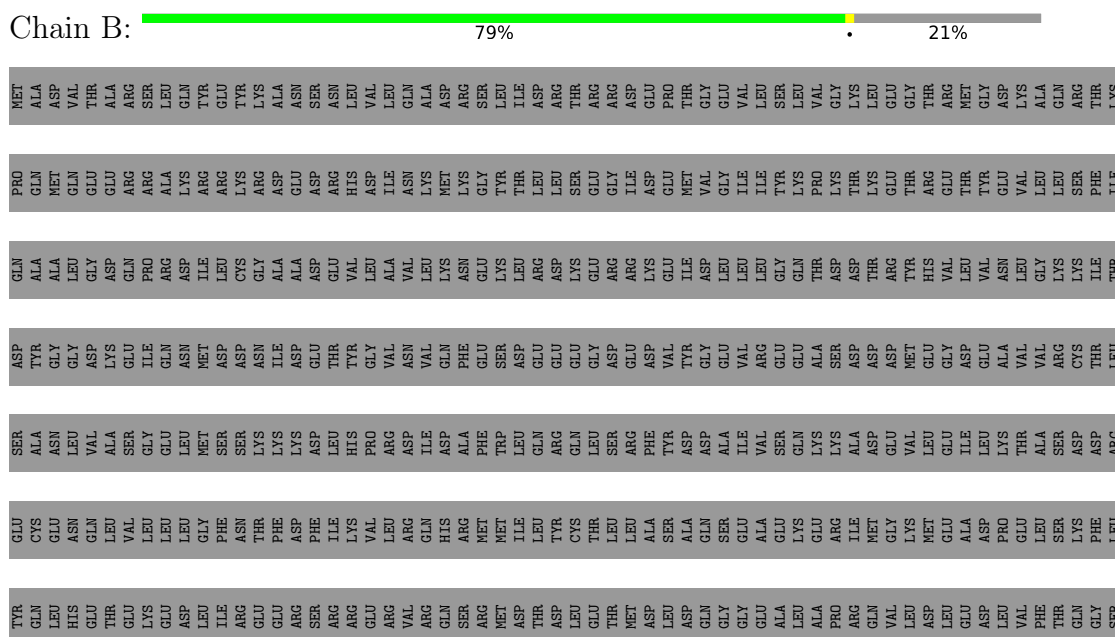
3 Residue-property plots

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

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

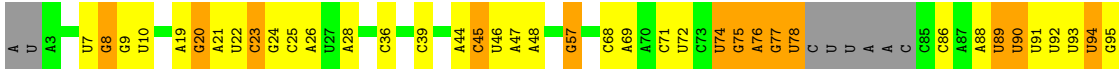


- Molecule 2: U5 small nuclear ribonucleoprotein 200 kDa helicase

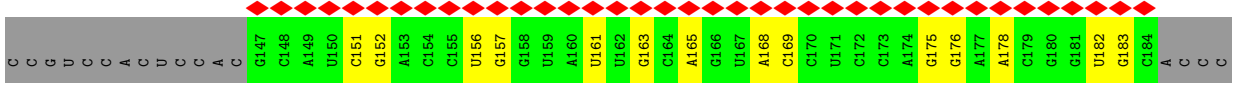
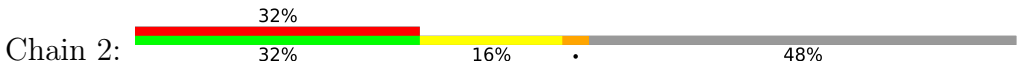




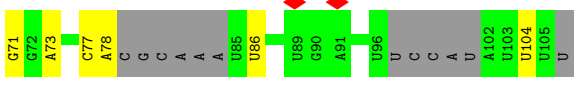
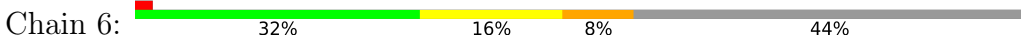
• Molecule 3: U5 snRNA



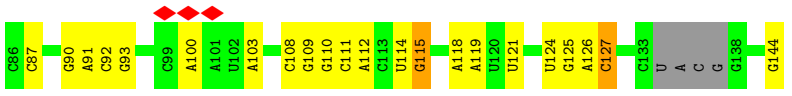
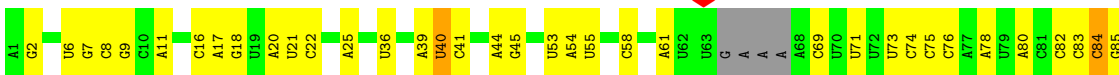
• Molecule 4: U2 snRNA



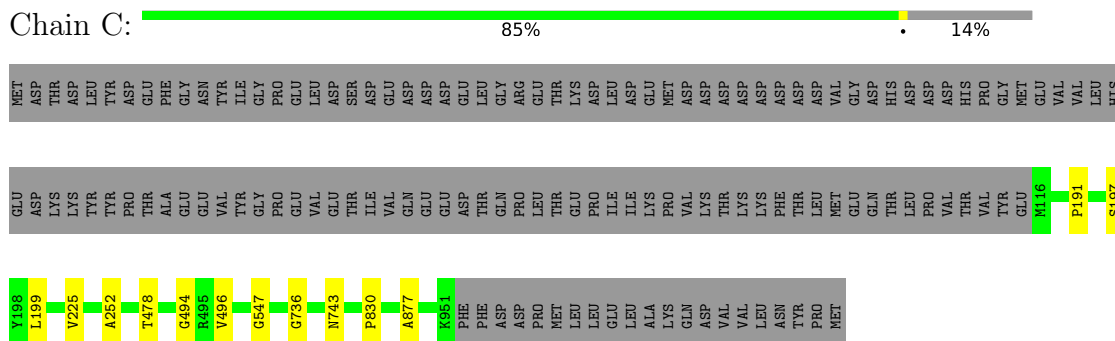
• Molecule 5: U6 snRNA



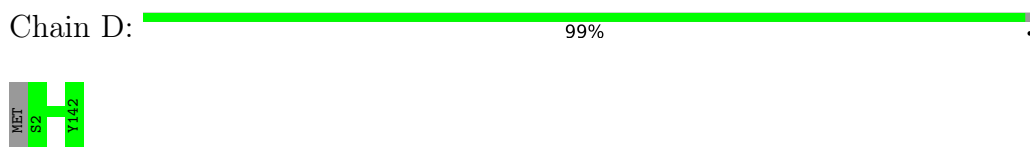
• Molecule 6: U4 snRNA



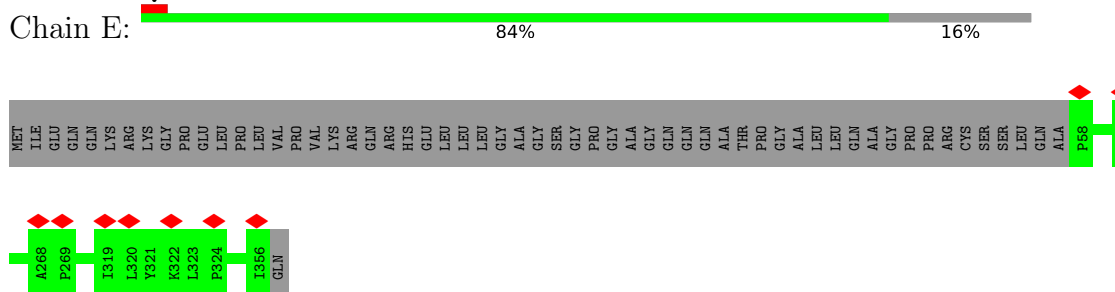
• Molecule 7: 116 kDa U5 small nuclear ribonucleoprotein component



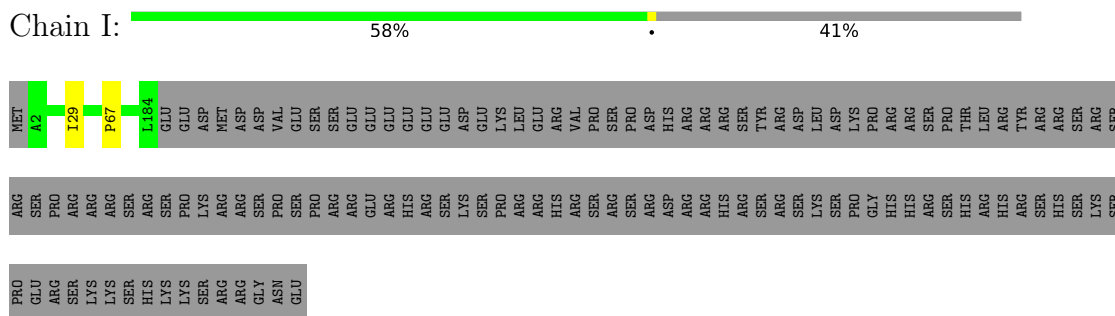
• Molecule 8: Thioredoxin-like protein 4A



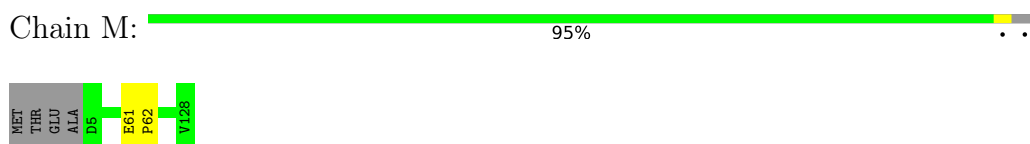
• Molecule 9: U5 small nuclear ribonucleoprotein 40 kDa protein

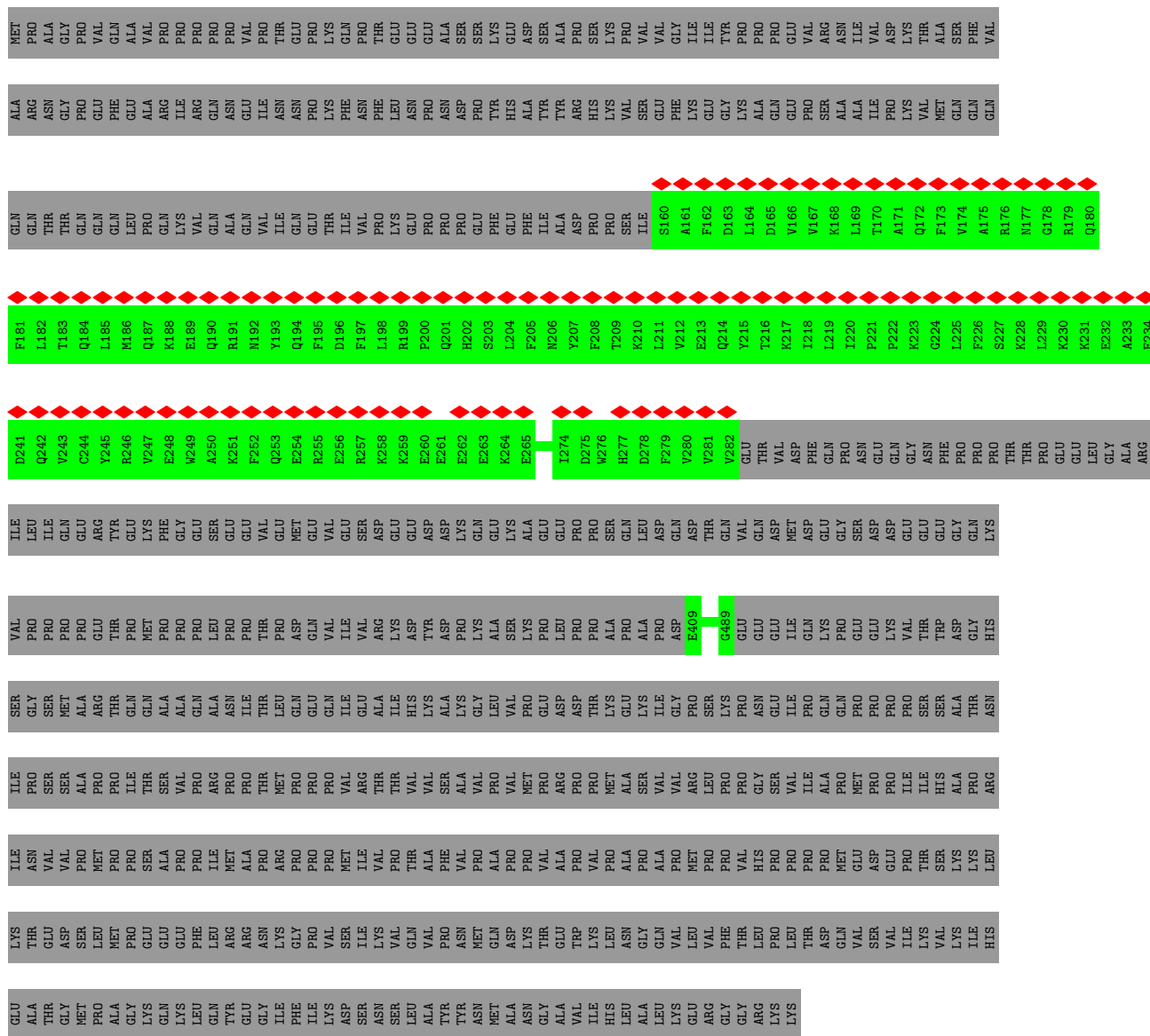


• Molecule 10: Pre-mRNA-splicing factor 38A

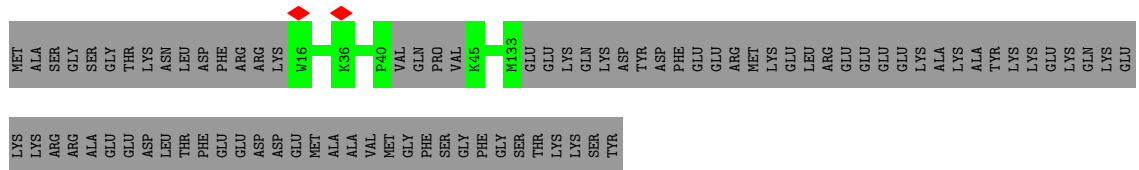


• Molecule 11: NHP2-like protein 1, N-terminally processed

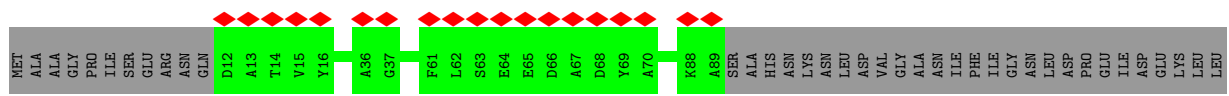


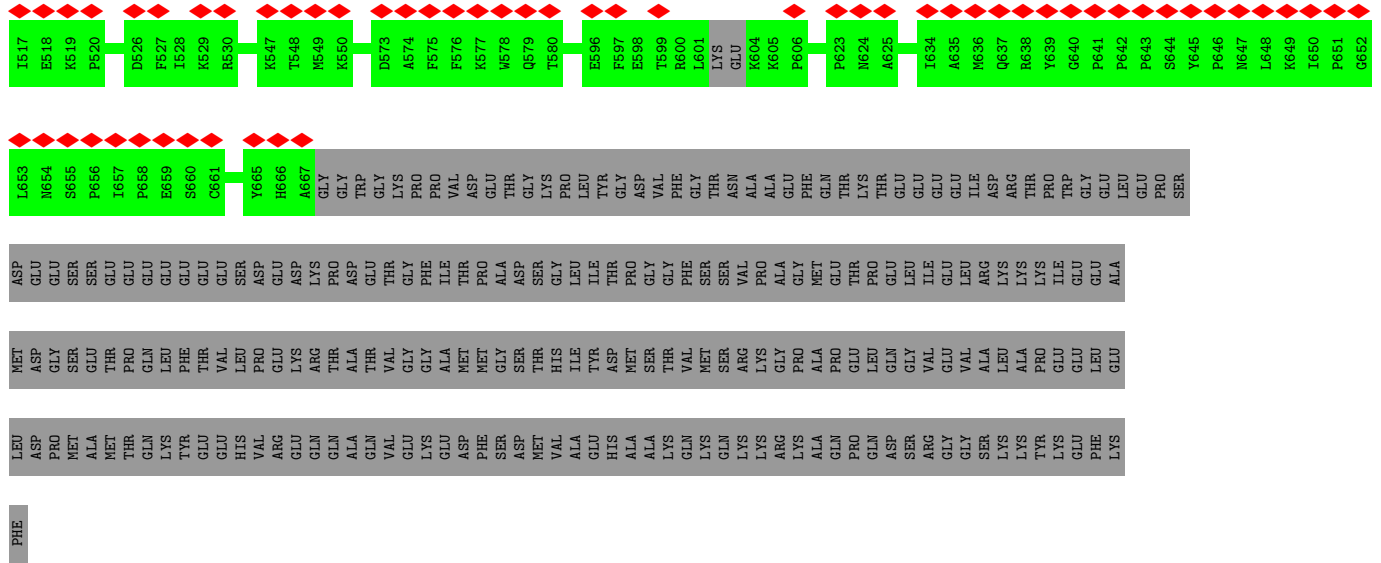


• Molecule 17: Zinc finger matrin-type protein 2

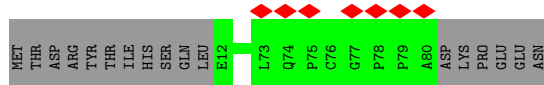
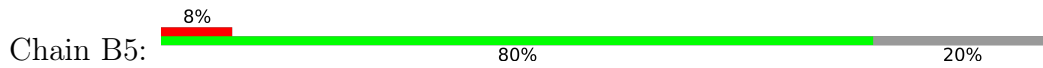


• Molecule 18: Splicing factor 3B subunit 4

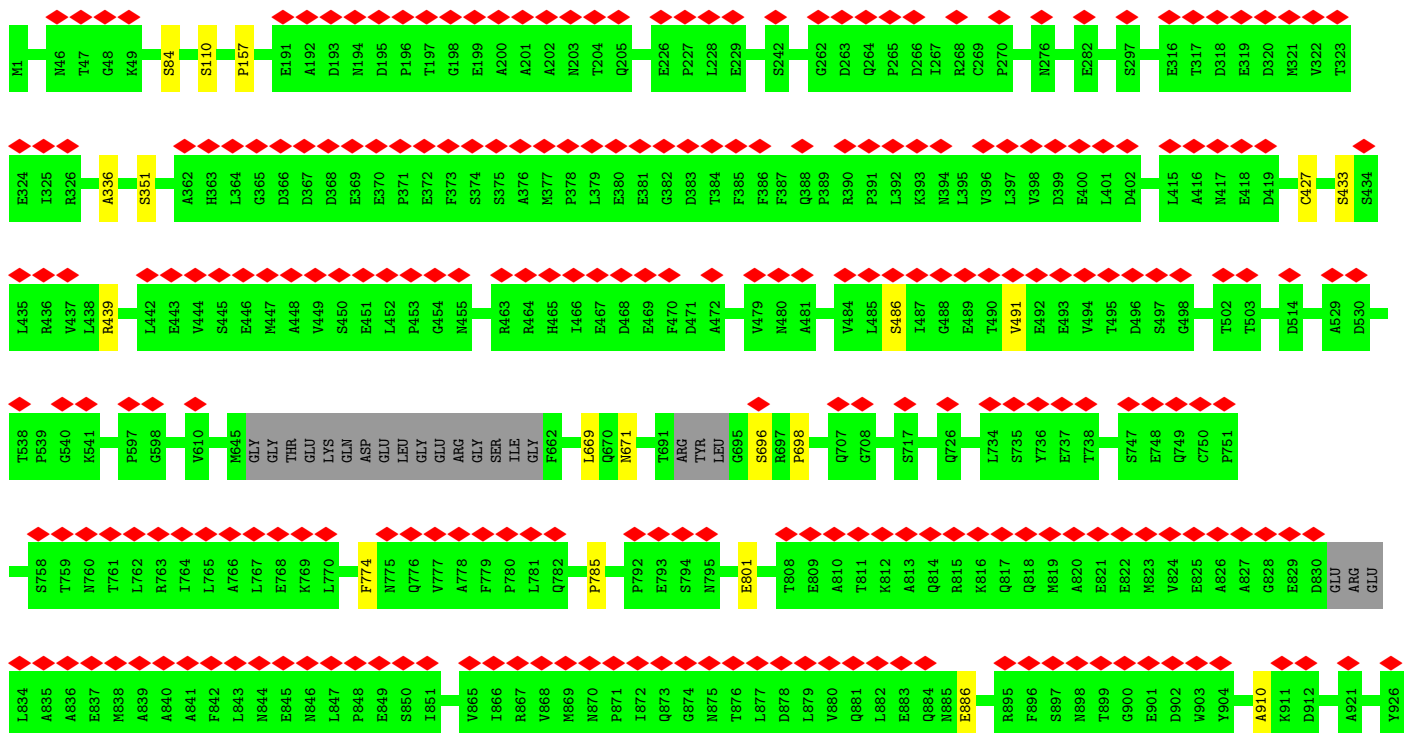


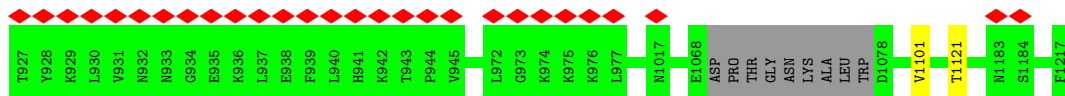


• Molecule 22: Splicing factor 3B subunit 5

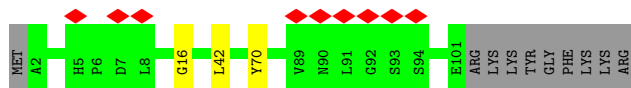
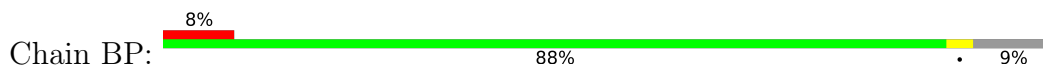


• Molecule 23: Splicing factor 3B subunit 3

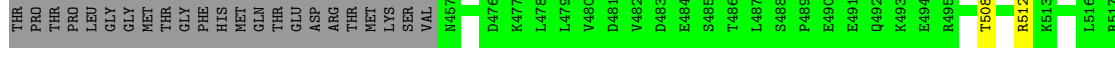
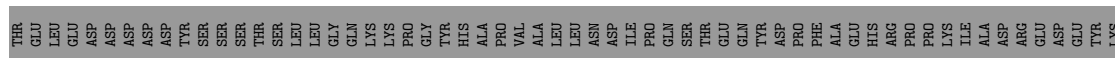
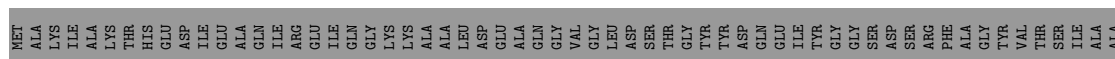


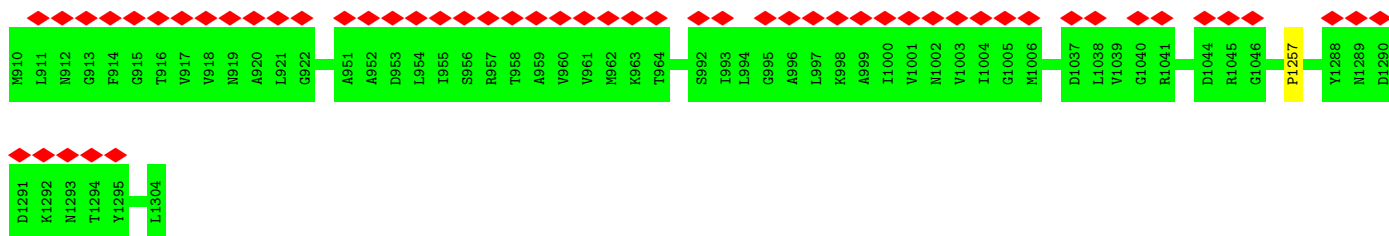


• Molecule 24: PHD finger-like domain-containing protein 5A

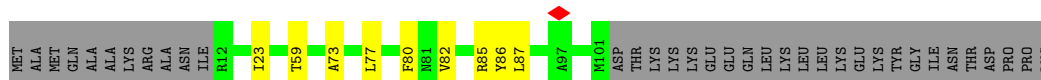


• Molecule 25: Splicing factor 3B subunit 1

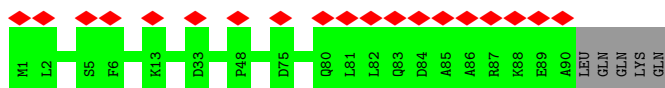




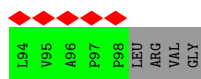
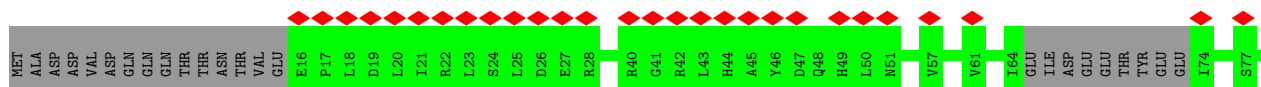
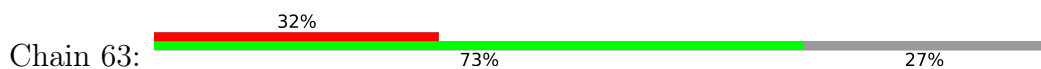
• Molecule 26: Splicing factor 3B subunit 6



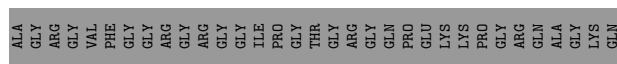
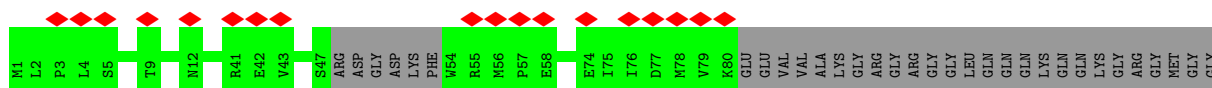
• Molecule 27: U6 snRNA-associated Sm-like protein LSm2



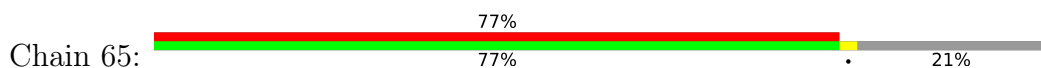
• Molecule 28: U6 snRNA-associated Sm-like protein LSm3

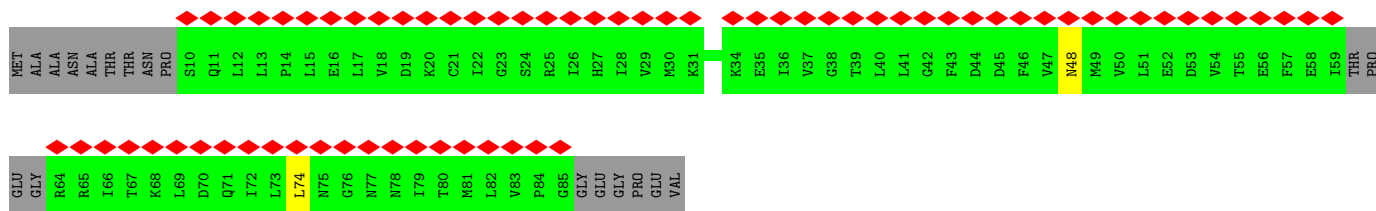


• Molecule 29: U6 snRNA-associated Sm-like protein LSm4

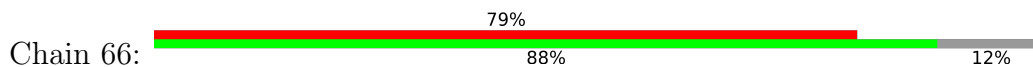


• Molecule 30: U6 snRNA-associated Sm-like protein LSm5

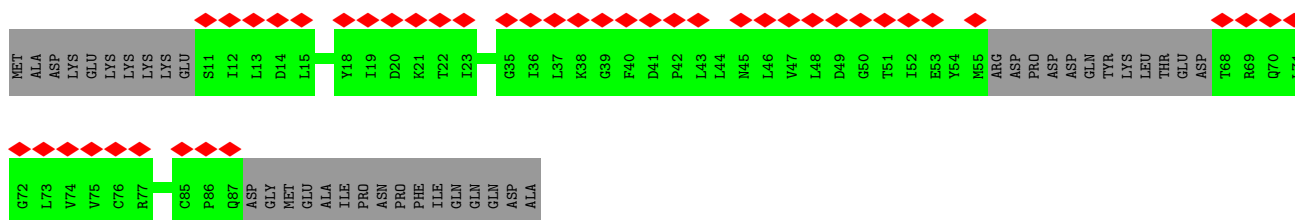
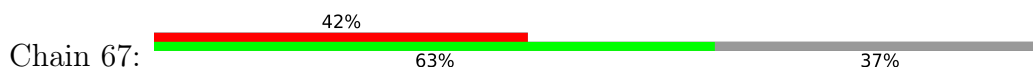




• Molecule 31: U6 snRNA-associated Sm-like protein LSM6



• Molecule 32: U6 snRNA-associated Sm-like protein LSM7



• Molecule 33: U6 snRNA-associated Sm-like protein LSM8

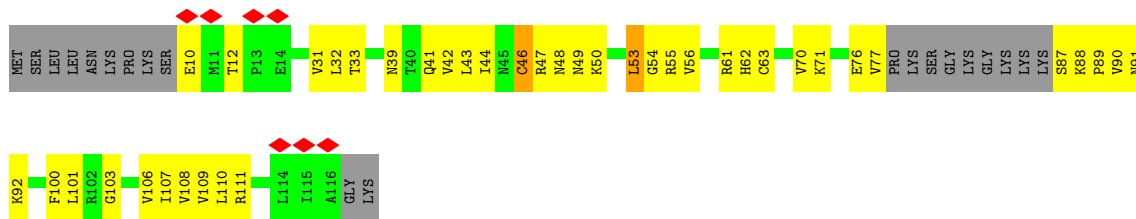


• Molecule 34: Small nuclear ribonucleoprotein Sm D2

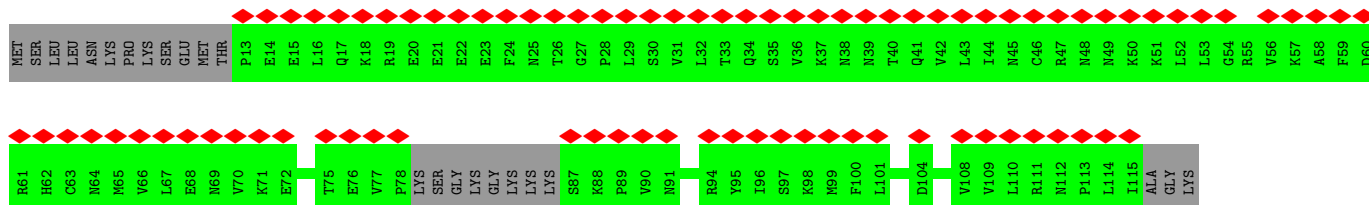
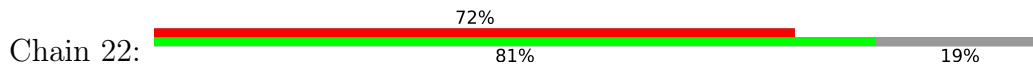


• Molecule 34: Small nuclear ribonucleoprotein Sm D2

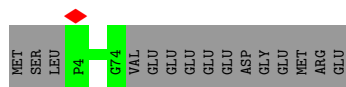
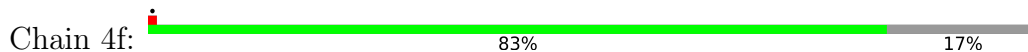




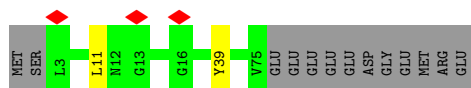
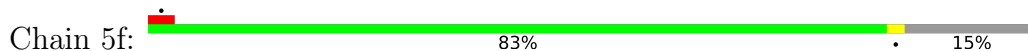
• Molecule 34: Small nuclear ribonucleoprotein Sm D2



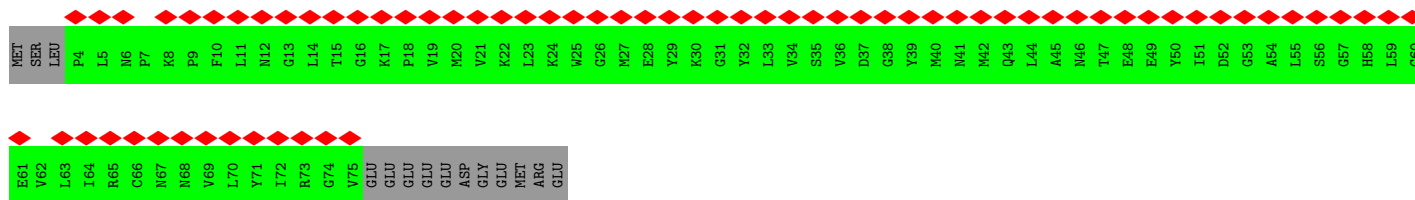
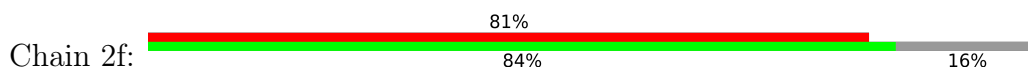
• Molecule 35: Small nuclear ribonucleoprotein F



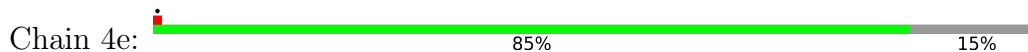
• Molecule 35: Small nuclear ribonucleoprotein F

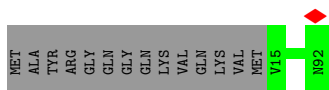


• Molecule 35: Small nuclear ribonucleoprotein F

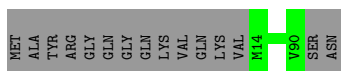
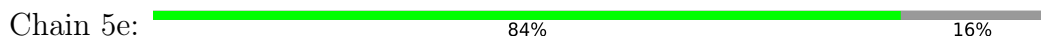


• Molecule 36: Small nuclear ribonucleoprotein E

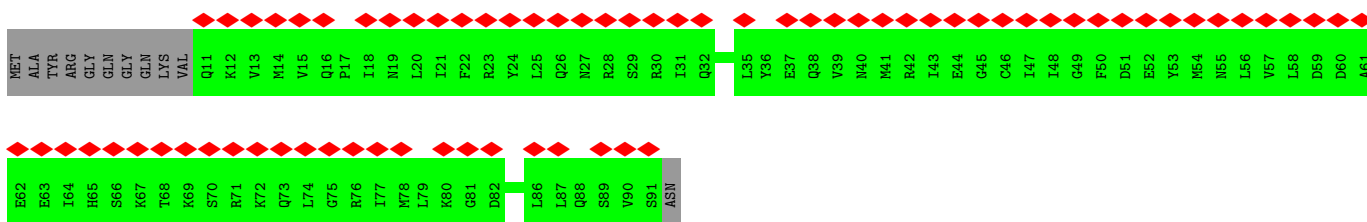
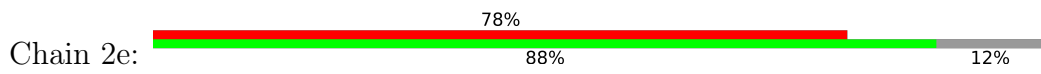




• Molecule 36: Small nuclear ribonucleoprotein E



• Molecule 36: Small nuclear ribonucleoprotein E



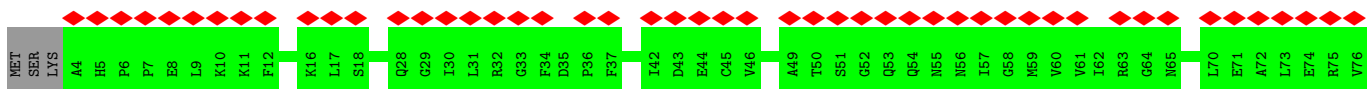
• Molecule 37: Small nuclear ribonucleoprotein G



• Molecule 37: Small nuclear ribonucleoprotein G

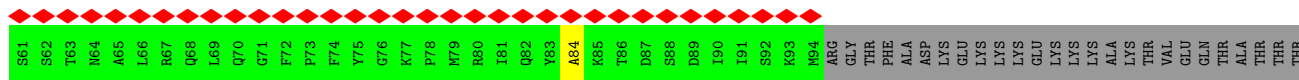


• Molecule 37: Small nuclear ribonucleoprotein G



• Molecule 38: Small nuclear ribonucleoprotein Sm D3

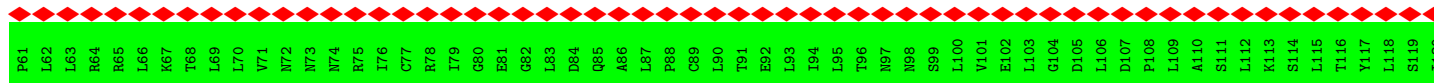
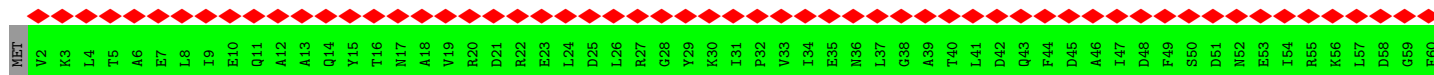




ASN	LYS	PRO	GLY	ARG	GLY	THR	ALA	ASN	PHE	VAL	GLN	GLY	ASP	ASN	THR	GLY	GLN	THR	THR	GLY	THR	GLN	VAL	GLU	THR	THR	THR	THR
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ARG	LEU	VAL	PRO	GLY	HIS	ILE	ALA	PHE	VAL	GLU	ASN	ASP	GLY	GLN	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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• Molecule 42: U2 small nuclear ribonucleoprotein A'



PHE	ASN	PRO	GLY	ALA	LEU	THR	ASP	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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ASP	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
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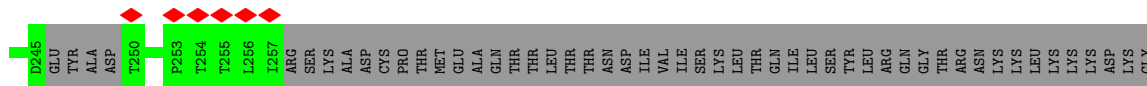
• Molecule 43: Protein Red



MET	PRO	GLU	ARG	THR	ALA	ASN	ASP	GLY	GLU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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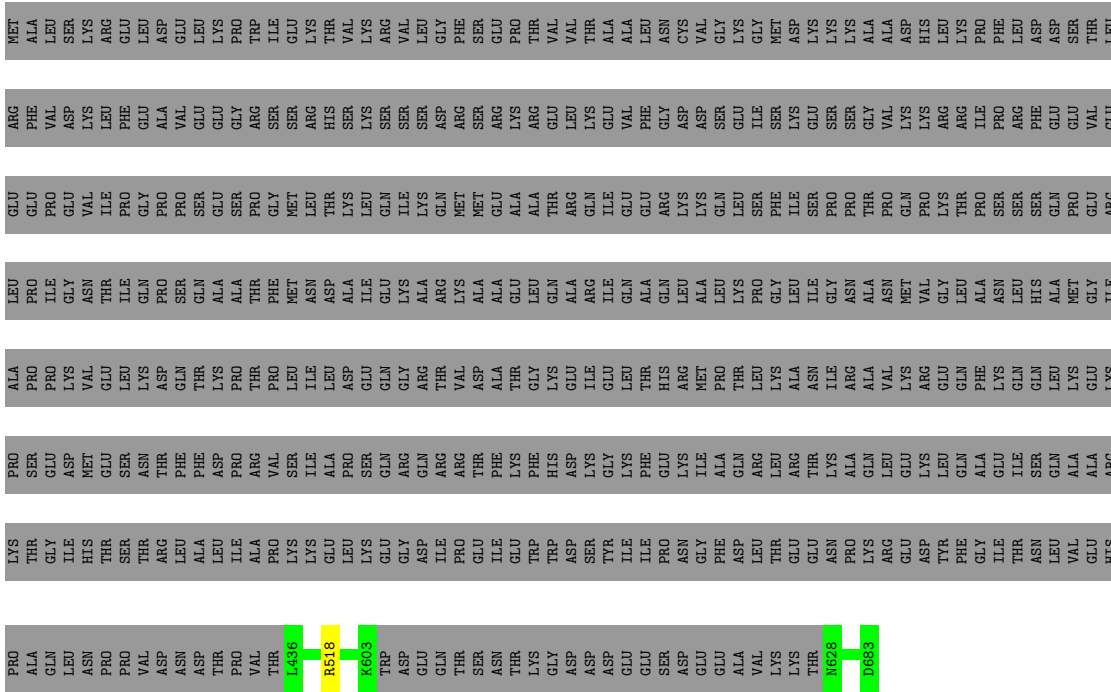
PRO	ARG	GLU	TYR	ASN	GLU	ASP	GLU	PRO	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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SER	THR	ALA	TYR	ASN	GLU	ASP	GLU	PRO	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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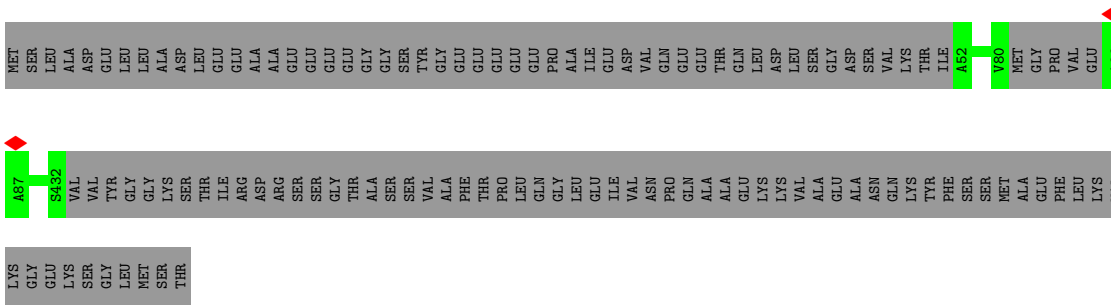


LYS	LEU	GLU	TYR	ASN	GLU	ASP	GLU	PRO	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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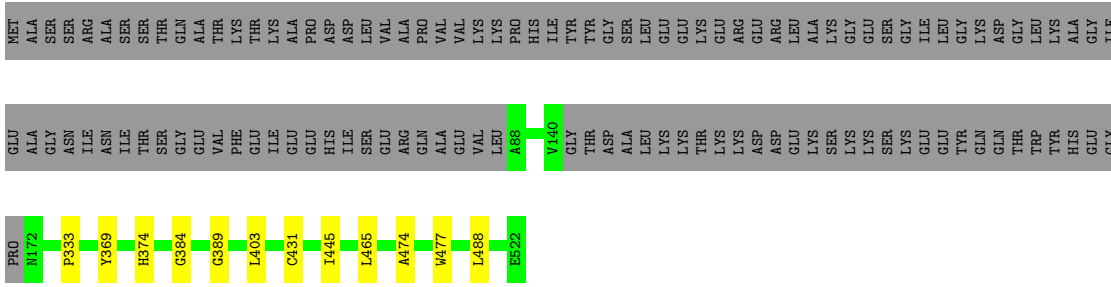
GLU	ARG	GLU	ARG	GLU	LYS	PRO	ASP	GLU	PRO	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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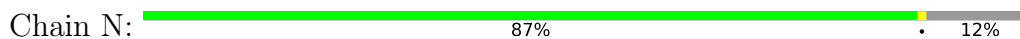
● Molecule 49: U4/U6 small nuclear ribonucleoprotein Prp31

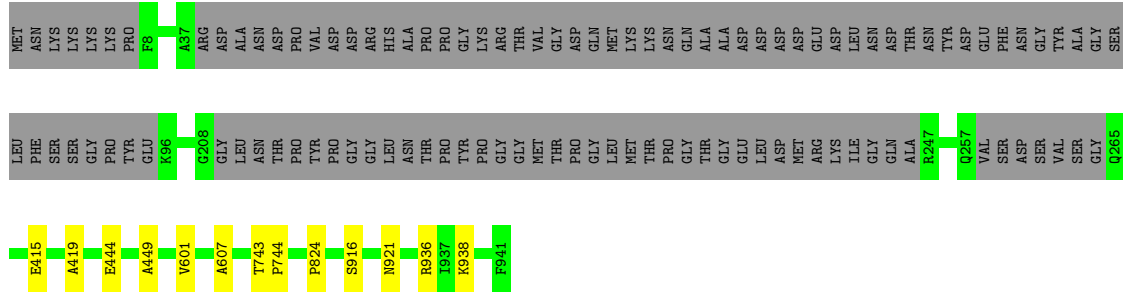


● Molecule 50: U4/U6 small nuclear ribonucleoprotein Prp4



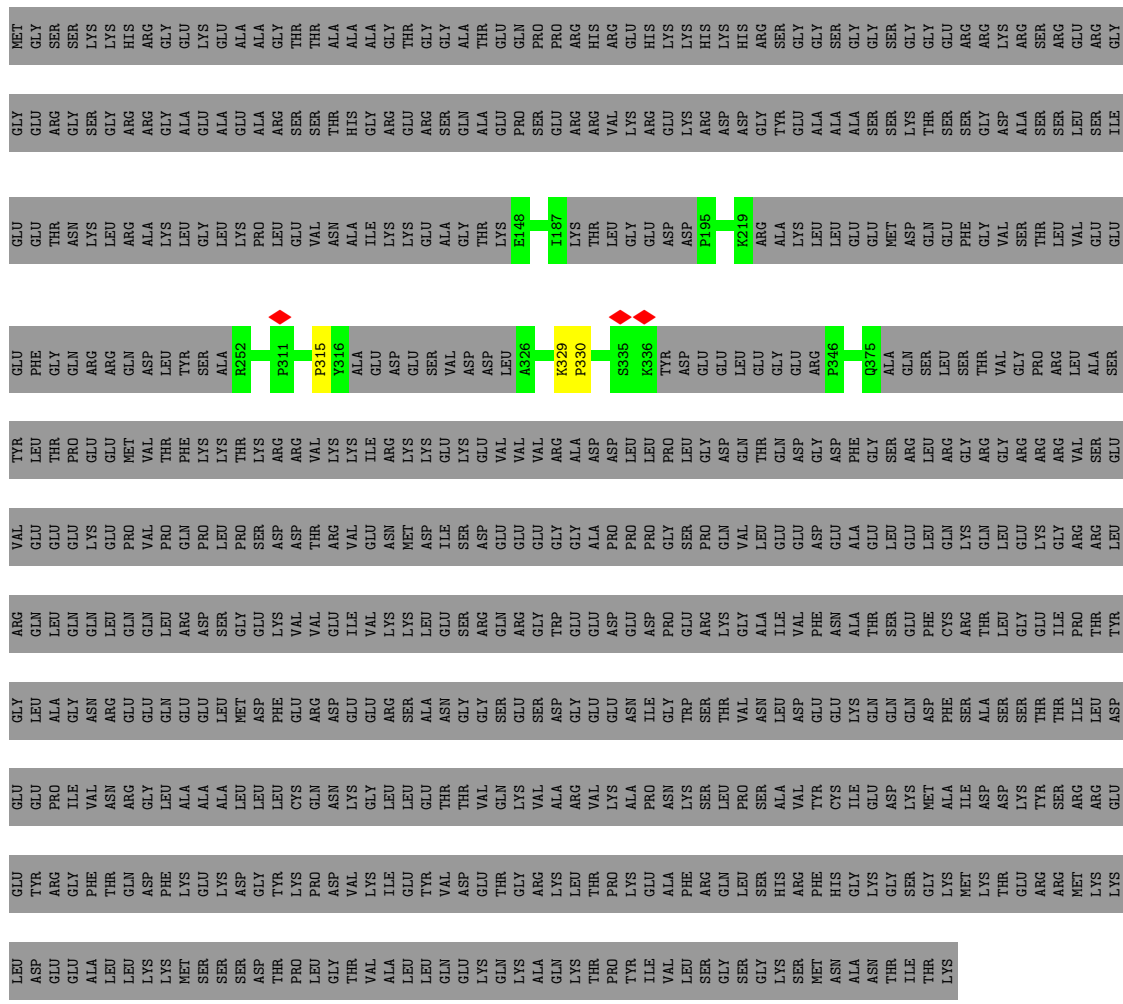
● Molecule 51: Pre-mRNA-processing factor 6





● Molecule 52: U4/U6.U5 tri-snRNP-associated protein 1

Chain S: 21% 79%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	334084	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 ($e^-/\text{\AA}^2$)	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	0.088	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size (\AA)	540.0, 540.0, 540.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.35, 1.35, 1.35	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	A	0.25	0/11512	0.42	0/16156
2	B	0.25	0/8614	0.43	0/12072
3	5	0.35	0/2559	1.02	22/3977 (0.6%)
4	2	0.32	0/2307	1.05	12/3582 (0.3%)
5	6	0.31	0/1398	0.90	6/2172 (0.3%)
6	4	0.25	0/3214	0.87	4/4998 (0.1%)
7	C	0.26	0/4270	0.44	0/5983
8	D	0.25	0/712	0.43	0/995
9	E	0.24	0/1195	0.50	0/1492
10	I	0.23	0/926	0.41	0/1295
11	M	0.24	0/632	0.41	0/885
12	U	0.24	0/2330	0.43	0/3268
13	W	0.25	0/853	0.47	0/1188
14	X	0.24	0/404	0.36	0/565
15	Z	0.28	0/349	1.03	0/540
16	7	0.24	0/1034	0.39	0/1446
17	r	0.23	0/568	0.39	0/790
18	B4	0.26	0/394	0.44	0/549
19	8	0.24	0/734	0.46	0/1025
20	9	0.24	0/1762	0.38	0/2460
21	B2	0.25	0/1092	0.43	0/1536
22	B5	0.24	0/349	0.36	0/487
23	B3	0.26	0/6024	0.48	0/8425
24	BP	0.25	0/501	0.45	0/697
25	B1	0.25	0/4421	0.43	0/6190
26	B6	0.31	0/459	0.43	0/642
27	62	0.23	0/359	0.44	0/447
28	63	0.23	0/294	0.49	0/364
29	64	0.23	0/294	0.45	0/364
30	65	0.23	0/286	0.49	0/354
31	66	0.24	0/279	0.49	0/347
32	67	0.24	0/258	0.51	0/319
33	68	0.22	0/242	0.49	0/299
34	22	0.24	0/485	0.44	0/677

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	42	0.23	0/298	0.48	0/370
34	52	0.43	0/805	0.71	1/1081 (0.1%)
35	2f	0.26	0/362	0.48	0/502
35	4f	0.24	0/291	0.52	0/363
35	5f	0.44	0/579	0.79	0/783
36	2e	0.24	0/403	0.45	0/561
36	4e	0.22	0/313	0.51	0/390
36	5e	0.37	0/646	0.70	0/867
37	2g	0.24	0/366	0.49	0/509
37	4g	0.25	0/297	0.53	0/371
37	5g	0.41	0/584	0.72	1/779 (0.1%)
38	23	0.26	0/417	0.48	0/581
38	43	0.24	0/287	0.51	0/358
38	53	0.44	0/665	0.56	0/896
39	2b	0.25	0/416	0.47	0/581
39	4b	0.22	0/254	0.50	0/314
39	5b	0.42	0/602	0.59	0/801
40	21	0.23	0/404	0.48	0/564
40	41	0.22	0/333	0.48	0/416
40	51	0.40	0/649	0.73	1/878 (0.1%)
41	2B	0.24	0/463	0.41	0/646
42	2A	0.24	0/821	0.46	0/1149
43	x	0.43	0/196	0.47	0/270
43	y	0.37	0/186	0.44	0/256
44	v	0.25	0/2491	0.45	0/3477
44	w	0.29	0/2486	0.46	0/3469
45	K	0.22	0/540	0.28	0/750
46	z1	0.25	0/268	0.77	0/416
47	z2	0.20	0/101	0.79	0/156
48	J	0.24	0/1131	0.39	0/1580
49	L	0.24	0/1899	0.38	0/2654
50	F	0.24	0/2034	0.45	0/2838
51	N	0.23	0/4224	0.39	0/5915
52	S	0.40	0/858	0.46	0/1191
All	All	0.27	0/87779	0.54	47/123318 (0.0%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	66	C	P-O3'-C3'	-10.19	107.47	119.70
5	6	67	G	P-O3'-C3'	-9.98	107.72	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	75	G	P-O3'-C3'	-9.83	107.90	119.70
3	5	76	A	P-O3'-C3'	-9.79	107.95	119.70
3	5	115	C	C2-N1-C1'	9.67	129.44	118.80
5	6	68	C	P-O3'-C3'	-9.35	108.48	119.70
5	6	65	G	P-O3'-C3'	-9.31	108.53	119.70
3	5	90	U	N1-C2-O2	8.57	128.80	122.80
6	4	87	C	N3-C2-O2	-7.97	116.32	121.90
3	5	90	U	N3-C2-O2	-7.80	116.74	122.20
3	5	110	C	C5-C6-N1	7.75	124.87	121.00
3	5	110	C	C6-N1-C2	-7.67	117.23	120.30
3	5	90	U	C2-N1-C1'	7.51	126.72	117.70
4	2	106	G	P-O3'-C3'	7.13	128.25	119.70
4	2	103	U	OP2-P-O3'	7.06	120.73	105.20
3	5	115	C	N1-C2-O2	6.99	123.10	118.90
3	5	115	C	C6-N1-C1'	-6.88	112.55	120.80
4	2	103	U	P-O3'-C3'	6.88	127.95	119.70
4	2	46	U	P-O3'-C3'	6.68	127.71	119.70
3	5	115	C	C5-C6-N1	6.65	124.33	121.00
5	6	64	U	P-O3'-C3'	-6.53	111.87	119.70
3	5	105	U	N1-C2-O2	6.50	127.35	122.80
3	5	96	A	N7-C8-N9	6.38	116.99	113.80
3	5	105	U	N3-C2-O2	-6.37	117.74	122.20
4	2	156	U	C2-N1-C1'	6.35	125.32	117.70
3	5	110	C	N1-C2-O2	6.19	122.61	118.90
3	5	74	U	P-O3'-C3'	-6.16	112.31	119.70
4	2	156	U	N1-C2-O2	6.01	127.01	122.80
3	5	115	C	C6-N1-C2	-5.97	117.91	120.30
6	4	87	C	N1-C2-O2	5.94	122.46	118.90
4	2	156	U	N3-C2-O2	-5.83	118.12	122.20
3	5	105	U	C2-N1-C1'	5.80	124.66	117.70
6	4	115	G	N3-C4-N9	5.77	129.46	126.00
37	5g	19	LEU	CB-CG-CD2	-5.76	101.22	111.00
3	5	96	A	C4-N9-C1'	5.65	136.47	126.30
4	2	40	C	N1-C2-O2	5.63	122.28	118.90
3	5	96	A	C8-N9-C4	-5.49	103.61	105.80
6	4	84	C	N1-C2-O2	5.47	122.18	118.90
4	2	58	U	N1-C2-O2	5.34	126.54	122.80
4	2	168	A	C4-N9-C1'	5.34	135.91	126.30
4	2	58	U	N3-C2-O2	-5.30	118.49	122.20
40	51	76	LEU	CA-CB-CG	5.27	127.41	115.30
4	2	168	A	C2-N3-C4	5.25	113.23	110.60
3	5	110	C	N3-C2-O2	-5.20	118.26	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	69	A	P-O3'-C3'	-5.20	113.46	119.70
34	52	53	LEU	CA-CB-CG	5.20	127.25	115.30
3	5	110	C	C2-N1-C1'	5.08	124.39	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11389	0	5553	17	0
2	B	8538	0	4146	7	0
3	5	2296	0	1163	29	0
4	2	2071	0	1049	11	0
5	6	1251	0	630	16	0
6	4	2881	0	1461	15	0
7	C	4223	0	2099	9	0
8	D	708	0	328	0	0
9	E	1196	0	337	0	0
10	I	920	0	433	1	0
11	M	627	0	315	1	0
12	U	2308	0	1104	3	0
13	W	844	0	426	9	0
14	X	403	0	200	6	0
15	Z	314	0	160	1	0
16	7	1028	0	487	0	0
17	r	568	0	245	0	0
18	B4	391	0	197	0	0
19	8	729	0	356	4	0
20	9	1755	0	823	1	0
21	B2	1072	0	563	1	0
22	B5	347	0	171	0	0
23	B3	5969	0	2985	14	0
24	BP	498	0	241	2	0
25	B1	4383	0	2195	2	0
26	B6	455	0	227	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	62	360	0	95	0	0
28	63	296	0	76	0	0
29	64	296	0	77	0	0
30	65	288	0	78	1	0
31	66	280	0	81	0	0
32	67	260	0	75	0	0
33	68	244	0	71	1	0
34	22	482	0	220	0	0
34	42	300	0	80	2	0
34	52	796	0	821	38	0
35	2f	359	0	179	0	0
35	4f	292	0	93	0	0
35	5f	567	0	575	0	0
36	2e	403	0	173	0	0
36	4e	314	0	86	0	0
36	5e	638	0	657	0	0
37	2g	364	0	176	0	0
37	4g	298	0	89	0	0
37	5g	577	0	603	0	0
38	23	415	0	198	1	0
38	43	288	0	84	0	0
38	53	657	0	675	10	0
39	2b	413	0	194	0	0
39	4b	256	0	70	0	0
39	5b	594	0	615	0	0
40	21	402	0	184	0	0
40	41	334	0	92	0	0
40	51	641	0	681	15	0
41	2B	461	0	218	1	0
42	2A	816	0	386	0	0
43	x	197	0	90	0	0
43	y	187	0	86	0	0
44	v	2478	0	1181	0	0
44	w	2474	0	1177	0	0
45	K	543	0	238	0	0
46	z1	239	0	119	0	0
47	z2	90	0	45	0	0
48	J	1125	0	551	1	0
49	L	1887	0	934	0	0
50	F	2020	0	1002	6	0
51	N	4192	0	2152	7	0
52	S	858	0	408	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	86145	0	43579	202	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 2.

All (202) 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)
13:W:153:LYS:HA	14:X:72:ALA:HB2	1.20	1.10
7:C:191:PRO:HA	7:C:197:SER:HA	1.45	0.97
13:W:153:LYS:CA	14:X:72:ALA:HB2	2.00	0.92
13:W:153:LYS:HA	14:X:72:ALA:CB	2.03	0.89
23:B3:886:GLU:HA	23:B3:910:ALA:O	1.73	0.88
38:23:48:VAL:O	38:23:55:VAL:HA	1.77	0.83
3:5:94:U:H2'	34:52:47:ARG:HH12	1.42	0.82
7:C:191:PRO:CA	7:C:197:SER:HA	2.15	0.76
34:52:77:VAL:HA	34:52:88:LYS:HA	1.69	0.75
23:B3:486:SER:O	23:B3:491:VAL:HA	1.87	0.74
7:C:191:PRO:HA	7:C:197:SER:CA	2.17	0.74
5:6:67:G:H5'	48:J:518:ARG:O	1.89	0.73
3:5:23:C:O2'	3:5:57:G:N2	2.23	0.71
38:53:48:VAL:O	38:53:55:VAL:HA	1.92	0.70
13:W:153:LYS:CA	14:X:72:ALA:CB	2.67	0.68
23:B3:671:ASN:HA	23:B3:696:SER:HA	1.75	0.68
34:52:76:GLU:HB2	34:52:89:PRO:HG2	1.76	0.68
2:B:434:SER:HA	2:B:446:HIS:O	1.94	0.67
3:5:96:A:H1'	34:52:47:ARG:HH21	1.57	0.67
3:5:76:A:H2'	3:5:77:G:C8	2.30	0.67
51:N:601:VAL:HA	51:N:607:ALA:HB3	1.77	0.67
1:A:465:LYS:O	3:5:23:C:N4	2.27	0.67
34:52:77:VAL:HA	34:52:88:LYS:HB3	1.76	0.66
12:U:411:PRO:HG2	12:U:469:THR:HA	1.78	0.66
34:52:48:ASN:O	34:52:50:LYS:N	2.30	0.65
34:52:77:VAL:HA	34:52:88:LYS:CB	2.27	0.64
34:52:42:VAL:O	34:52:53:LEU:HA	1.99	0.63
3:5:77:G:H4'	3:5:78:U:OP1	2.00	0.62
34:52:10:GLU:HG2	34:52:12:THR:H	1.64	0.62
3:5:74:U:H2'	3:5:75:G:C8	2.35	0.61
12:U:174:CYS:O	12:U:178:ASN:N	2.33	0.61
1:A:597:LYS:N	3:5:45:C:OP1	2.33	0.61
34:52:77:VAL:HA	34:52:88:LYS:CA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:F:369:TYR:H	50:F:384:GLY:HA2	1.66	0.60
23:B3:669:LEU:O	23:B3:698:PRO:HA	2.03	0.59
51:N:444:GLU:HA	51:N:449:ALA:HB3	1.84	0.59
5:6:66:C:H2'	5:6:67:G:C8	2.38	0.59
38:53:19:THR:HG23	38:53:72:ILE:HB	1.84	0.58
1:A:142:SER:HA	1:A:242:ALA:HB2	1.84	0.58
34:52:39:ASN:O	34:52:55:ARG:NH1	2.36	0.58
40:51:76:LEU:HA	40:51:79:LEU:HB2	1.84	0.58
13:W:153:LYS:CB	14:X:72:ALA:CB	2.82	0.58
23:B3:671:ASN:HA	23:B3:696:SER:CA	2.34	0.57
34:52:53:LEU:HD11	34:52:71:LYS:HD3	1.86	0.57
3:5:75:G:H2'	3:5:76:A:C8	2.40	0.57
23:B3:671:ASN:CA	23:B3:696:SER:HA	2.35	0.57
34:52:46:CYS:SG	34:52:50:LYS:HB2	2.45	0.56
26:B6:85:ARG:C	26:B6:87:LEU:H	2.09	0.56
34:52:76:GLU:HB2	34:52:89:PRO:CG	2.34	0.56
34:52:107:ILE:HG22	34:52:108:VAL:HG13	1.86	0.56
40:51:25:VAL:HG22	40:51:45:MET:HG3	1.86	0.56
3:5:94:U:C2'	34:52:47:ARG:HH12	2.17	0.56
3:5:96:A:H8	34:52:47:ARG:NH2	2.04	0.55
40:51:33:ASP:HB2	40:51:37:ASN:HB2	1.89	0.55
34:52:41:GLN:HE21	34:52:53:LEU:HD13	1.72	0.55
1:A:2130:GLY:N	1:A:2173:GLU:O	2.35	0.55
4:2:165:A:H61	41:2B:84:ALA:HB1	1.71	0.55
34:52:46:CYS:HA	34:52:106:VAL:HA	1.88	0.55
23:B3:1101:VAL:HA	23:B3:1121:THR:HA	1.88	0.55
50:F:474:ALA:O	50:F:488:LEU:N	2.39	0.54
1:A:2273:VAL:O	1:A:2297:GLN:N	2.34	0.54
1:A:1382:SER:HA	1:A:1415:GLY:HA2	1.89	0.53
34:52:44:ILE:HG23	34:52:106:VAL:HG23	1.90	0.53
3:5:91:U:O2'	40:51:61:ARG:NH1	2.42	0.53
34:52:32:LEU:HD22	34:52:56:VAL:HG11	1.90	0.53
5:6:69:A:H2'	5:6:70:A:O4'	2.09	0.53
10:I:29:ILE:HA	10:I:67:PRO:HG3	1.90	0.53
5:6:65:G:H2'	5:6:66:C:C6	2.44	0.53
7:C:478:THR:HA	7:C:494:GLY:HA3	1.90	0.52
3:5:46:U:O4	3:5:47:A:N6	2.42	0.52
3:5:76:A:H2'	3:5:77:G:H8	1.74	0.52
4:2:161:U:O2	4:2:163:G:N2	2.42	0.52
51:N:936:ARG:O	51:N:938:LYS:N	2.42	0.52
7:C:736:GLY:N	7:C:743:ASN:O	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:52:54:GLY:HA3	34:52:70:VAL:HG12	1.92	0.51
4:2:33:G:H1	15:Z:42:U:H3	1.58	0.51
3:5:96:A:C1'	34:52:47:ARG:HH21	2.22	0.51
5:6:51:U:O2'	5:6:52:U:OP1	2.27	0.51
40:51:29:ILE:HA	40:51:40:LEU:HD23	1.92	0.51
40:51:66:ARG:CZ	34:52:48:ASN:HB3	2.41	0.51
23:B3:336:ALA:HA	23:B3:351:SER:HA	1.92	0.51
1:A:2133:PRO:HA	1:A:2140:LYS:HA	1.93	0.51
5:6:44:G:O3'	5:6:45:A:H3'	2.11	0.51
6:4:17:A:H2'	6:4:18:G:H5''	1.94	0.50
30:65:48:ASN:CA	30:65:74:LEU:O	2.60	0.50
7:C:830:PRO:HG2	7:C:877:ALA:HB3	1.92	0.50
34:52:77:VAL:CA	34:52:88:LYS:HA	2.40	0.50
51:N:415:GLU:O	51:N:419:ALA:N	2.37	0.49
23:B3:785:PRO:HA	23:B3:801:GLU:HA	1.93	0.49
23:B3:439:ARG:O	23:B3:774:PHE:HA	2.12	0.49
23:B3:671:ASN:CB	23:B3:696:SER:HA	2.43	0.49
34:52:43:LEU:HB3	34:52:110:LEU:HD23	1.95	0.49
1:A:464:PRO:HB2	3:5:23:C:C4	2.47	0.49
3:5:19:A:H4'	3:5:20:G:C8	2.47	0.49
6:4:16:C:H2'	6:4:17:A:C8	2.48	0.48
3:5:96:A:C8	34:52:47:ARG:NH2	2.82	0.48
23:B3:157:PRO:HD2	24:BP:16:GLY:HA2	1.94	0.48
19:8:56:CYS:O	19:8:60:LEU:HA	2.13	0.48
4:2:3:C:H2'	4:2:4:G:H8	1.77	0.48
13:W:65:PHE:HA	13:W:76:GLY:HA3	1.94	0.48
34:52:62:HIS:O	34:52:103:GLY:HA3	2.14	0.48
5:6:40:U:H2'	5:6:41:A:C8	2.49	0.47
26:B6:80:PHE:C	26:B6:82:VAL:H	2.17	0.47
50:F:465:LEU:N	50:F:477:TRP:O	2.43	0.47
5:6:37:C:H2'	5:6:38:G:O4'	2.14	0.47
5:6:65:G:H2'	5:6:66:C:H6	1.79	0.47
38:53:23:ASN:O	38:53:69:ARG:NH2	2.46	0.47
34:52:32:LEU:HD11	34:52:109:VAL:HG11	1.95	0.47
3:5:47:A:O2'	3:5:48:A:H5''	2.15	0.47
4:2:12:G:H1	5:6:86:U:H3	1.62	0.47
40:51:68:PHE:HB2	34:52:100:PHE:HB3	1.96	0.47
51:N:916:SER:HA	51:N:921:ASN:H	1.80	0.47
33:68:35:ASN:CA	33:68:62:VAL:O	2.62	0.47
34:52:31:VAL:HG13	34:52:111:ARG:HE	1.80	0.47
38:53:16:HIS:HB3	38:53:74:PRO:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:F:333:PRO:HG2	50:F:374:HIS:O	2.16	0.46
19:8:115:PRO:HD2	19:8:176:TYR:HA	1.98	0.46
3:5:7:U:H3'	3:5:8:G:H8	1.80	0.46
3:5:89:U:O2'	38:53:64:ARG:NH2	2.48	0.46
3:5:109:G:O3'	40:51:49:ASN:ND2	2.48	0.46
40:51:19:LEU:HD21	40:51:60:ILE:HD13	1.98	0.46
6:4:91:A:H2	6:4:110:G:H22	1.62	0.46
6:4:108:C:H2'	6:4:109:G:C8	2.51	0.46
6:4:20:A:H2'	6:4:21:U:C6	2.51	0.45
40:51:67:TYR:HB3	34:52:101:LEU:HD12	1.98	0.45
5:6:66:C:H2'	5:6:67:G:H8	1.79	0.45
13:W:12:VAL:HA	13:W:30:GLU:HA	1.98	0.45
6:4:20:A:C5	6:4:54:A:H8	2.34	0.45
26:B6:73:ALA:O	26:B6:77:LEU:CB	2.64	0.45
34:52:32:LEU:HD23	34:52:32:LEU:HA	1.82	0.45
1:A:2131:VAL:HA	1:A:2172:MET:HA	1.98	0.44
4:2:32:U:H2'	4:2:33:G:H8	1.82	0.44
3:5:111:A:H2'	3:5:112:A:C8	2.53	0.44
34:52:90:VAL:O	34:52:92:LYS:N	2.50	0.44
3:5:75:G:C6	3:5:76:A:C6	3.05	0.44
3:5:71:C:H2'	3:5:72:U:C6	2.53	0.44
1:A:1567:PRO:HB2	5:6:47:A:H61	1.83	0.44
7:C:191:PRO:HA	7:C:197:SER:N	2.32	0.44
50:F:431:CYS:N	50:F:445:ILE:O	2.43	0.44
2:B:1670:ASN:O	2:B:1674:HIS:N	2.50	0.43
13:W:153:LYS:CB	14:X:72:ALA:HB2	2.45	0.43
1:A:2069:SER:C	52:S:315:PRO:CB	2.87	0.43
21:B2:482:ALA:HB2	25:B1:1257:PRO:HG3	2.00	0.43
4:2:175:G:H2'	4:2:176:G:H8	1.83	0.43
1:A:897:GLU:O	1:A:908:VAL:N	2.44	0.43
3:5:93:U:H4'	3:5:94:U:H5''	2.00	0.43
2:B:716:ALA:HB1	2:B:749:GLY:HA3	2.01	0.43
4:2:37:U:H2'	4:2:38:A:C8	2.54	0.43
23:B3:427:CYS:O	23:B3:433:SER:HA	2.19	0.43
38:53:64:ARG:NE	38:53:66:SER:OG	2.49	0.43
38:53:23:ASN:N	38:53:67:LYS:O	2.52	0.43
5:6:51:U:HO2'	5:6:52:U:P	2.40	0.43
2:B:1670:ASN:O	2:B:1674:HIS:HA	2.19	0.43
38:53:30:GLY:HA3	38:53:46:ILE:HD13	2.00	0.42
40:51:51:GLU:OE1	40:51:51:GLU:N	2.52	0.42
34:52:61:ARG:C	34:52:63:CYS:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:92:U:OP1	40:51:63:ASN:ND2	2.52	0.42
11:M:61:GLU:HA	11:M:62:PRO:HA	1.93	0.42
12:U:459:LYS:HA	12:U:464:VAL:HA	2.01	0.42
38:53:19:THR:HB	38:53:29:ARG:HG3	2.01	0.42
4:2:182:U:H2'	4:2:183:G:C8	2.55	0.42
6:4:40:U:O2'	51:N:824:PRO:O	2.23	0.42
52:S:329:LYS:N	52:S:330:PRO:HD2	2.34	0.42
1:A:2127:TYR:O	1:A:2146:VAL:N	2.30	0.42
3:5:75:G:H2'	3:5:76:A:H8	1.82	0.42
5:6:45:A:H2'	5:6:45:A:N3	2.34	0.42
26:B6:23:ILE:O	26:B6:59:THR:HA	2.19	0.42
40:51:66:ARG:NH1	34:52:48:ASN:H	2.18	0.42
1:A:2178:ILE:HA	1:A:2214:ILE:O	2.20	0.42
7:C:225:VAL:N	7:C:252:ALA:O	2.47	0.42
25:B1:508:THR:O	25:B1:512:ARG:N	2.49	0.42
1:A:1890:GLN:N	1:A:2013:GLY:HA3	2.35	0.42
20:9:408:CYS:O	20:9:413:ASN:HA	2.20	0.42
1:A:947:PRO:HB2	1:A:949:PRO:HD2	2.01	0.41
4:2:151:C:H2'	4:2:152:G:H8	1.84	0.41
5:6:73:A:H2	6:4:2:G:H22	1.68	0.41
19:8:147:PRO:HB3	19:8:173:ALA:HB2	2.03	0.41
6:4:20:A:N3	6:4:54:A:H1'	2.35	0.41
6:4:127:C:O2'	34:42:47:ARG:O	2.38	0.41
7:C:496:VAL:O	7:C:547:GLY:N	2.36	0.41
2:B:2018:GLU:CB	2:B:2042:GLU:O	2.68	0.41
4:2:3:C:H2'	4:2:4:G:C8	2.55	0.41
40:51:13:GLU:HG2	40:51:74:LEU:HD11	2.02	0.41
50:F:389:GLY:O	50:F:403:LEU:N	2.53	0.41
34:42:50:LYS:CA	34:42:73:MET:O	2.69	0.41
5:6:67:G:H1	6:4:8:C:H42	1.69	0.41
23:B3:84:SER:HA	23:B3:110:SER:HA	2.03	0.41
24:BP:42:LEU:HA	24:BP:70:TYR:HA	2.02	0.41
6:4:6:U:H2'	6:4:7:G:C8	2.56	0.41
6:4:108:C:H2'	6:4:109:G:H8	1.86	0.41
19:8:56:CYS:O	19:8:60:LEU:CA	2.69	0.41
38:53:48:VAL:HG21	38:53:58:LEU:HD12	2.03	0.41
40:51:16:THR:HA	40:51:25:VAL:O	2.20	0.41
2:B:1263:PRO:HA	2:B:1264:PRO:HD3	1.98	0.41
34:52:87:SER:O	34:52:89:PRO:HD3	2.20	0.41
2:B:1300:GLU:HA	2:B:1514:PHE:HA	2.03	0.40
6:4:92:C:H2'	6:4:93:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2231:THR:O	1:A:2235:TYR:N	2.46	0.40
3:5:94:U:O2'	34:52:47:ARG:NH2	2.45	0.40
6:4:111:C:H2'	6:4:112:A:H8	1.86	0.40
13:W:27:MET:HA	13:W:147:GLY:HA3	2.02	0.40
51:N:743:THR:N	51:N:744:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2243/2335 (96%)	2208 (98%)	35 (2%)	0	100	100
2	B	1691/2136 (79%)	1643 (97%)	47 (3%)	1 (0%)	51	84
7	C	834/972 (86%)	815 (98%)	18 (2%)	1 (0%)	51	84
8	D	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
9	E	297/357 (83%)	283 (95%)	14 (5%)	0	100	100
10	I	181/312 (58%)	176 (97%)	5 (3%)	0	100	100
11	M	122/128 (95%)	122 (100%)	0	0	100	100
12	U	454/565 (80%)	447 (98%)	7 (2%)	0	100	100
13	W	167/177 (94%)	163 (98%)	4 (2%)	0	100	100
14	X	78/376 (21%)	78 (100%)	0	0	100	100
16	7	200/793 (25%)	197 (98%)	3 (2%)	0	100	100
17	r	110/199 (55%)	109 (99%)	1 (1%)	0	100	100
18	B4	76/424 (18%)	76 (100%)	0	0	100	100
19	8	138/464 (30%)	136 (99%)	2 (1%)	0	100	100
20	9	344/501 (69%)	336 (98%)	8 (2%)	0	100	100
21	B2	204/895 (23%)	200 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	B5	67/86 (78%)	66 (98%)	1 (2%)	0	100	100
23	B3	1176/1217 (97%)	1131 (96%)	45 (4%)	0	100	100
24	BP	98/110 (89%)	96 (98%)	2 (2%)	0	100	100
25	B1	866/1304 (66%)	840 (97%)	26 (3%)	0	100	100
26	B6	88/125 (70%)	86 (98%)	1 (1%)	1 (1%)	14	50
27	62	88/95 (93%)	84 (96%)	4 (4%)	0	100	100
28	63	70/102 (69%)	66 (94%)	4 (6%)	0	100	100
29	64	70/139 (50%)	66 (94%)	4 (6%)	0	100	100
30	65	68/91 (75%)	64 (94%)	4 (6%)	0	100	100
31	66	68/80 (85%)	63 (93%)	5 (7%)	0	100	100
32	67	61/103 (59%)	59 (97%)	2 (3%)	0	100	100
33	68	57/96 (59%)	55 (96%)	2 (4%)	0	100	100
34	22	91/118 (77%)	90 (99%)	1 (1%)	0	100	100
34	42	70/118 (59%)	67 (96%)	3 (4%)	0	100	100
34	52	94/118 (80%)	86 (92%)	6 (6%)	2 (2%)	7	38
35	2f	70/86 (81%)	68 (97%)	2 (3%)	0	100	100
35	4f	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
35	5f	71/86 (83%)	64 (90%)	7 (10%)	0	100	100
36	2e	79/92 (86%)	79 (100%)	0	0	100	100
36	4e	76/92 (83%)	75 (99%)	1 (1%)	0	100	100
36	5e	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
37	2g	71/76 (93%)	70 (99%)	1 (1%)	0	100	100
37	4g	71/76 (93%)	65 (92%)	6 (8%)	0	100	100
37	5g	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
38	23	81/126 (64%)	79 (98%)	2 (2%)	0	100	100
38	43	69/126 (55%)	68 (99%)	1 (1%)	0	100	100
38	53	82/126 (65%)	77 (94%)	5 (6%)	0	100	100
39	2b	80/240 (33%)	80 (100%)	0	0	100	100
39	4b	60/240 (25%)	58 (97%)	2 (3%)	0	100	100
39	5b	69/240 (29%)	67 (97%)	2 (3%)	0	100	100
40	21	78/119 (66%)	76 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	41	80/119 (67%)	78 (98%)	2 (2%)	0	100	100
40	51	79/119 (66%)	75 (95%)	4 (5%)	0	100	100
41	2B	90/225 (40%)	90 (100%)	0	0	100	100
42	2A	160/255 (63%)	157 (98%)	3 (2%)	0	100	100
43	x	33/557 (6%)	29 (88%)	4 (12%)	0	100	100
43	y	31/557 (6%)	28 (90%)	3 (10%)	0	100	100
44	v	492/513 (96%)	484 (98%)	8 (2%)	0	100	100
44	w	489/513 (95%)	478 (98%)	10 (2%)	1 (0%)	47	80
45	K	103/439 (24%)	103 (100%)	0	0	100	100
48	J	220/683 (32%)	217 (99%)	3 (1%)	0	100	100
49	L	372/499 (74%)	364 (98%)	8 (2%)	0	100	100
50	F	400/522 (77%)	386 (96%)	14 (4%)	0	100	100
51	N	823/941 (88%)	799 (97%)	24 (3%)	0	100	100
52	S	161/800 (20%)	160 (99%)	1 (1%)	0	100	100
All	All	15016/23399 (64%)	14624 (97%)	386 (3%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	52	49	ASN
34	52	91	ASN
44	w	177	LEU
2	B	1292	PRO
7	C	199	LEU
26	B6	86	TYR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	125/2108 (6%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	77/1908 (4%)	77 (100%)	0	100	100
7	C	48/866 (6%)	48 (100%)	0	100	100
8	D	5/130 (4%)	5 (100%)	0	100	100
10	I	7/293 (2%)	7 (100%)	0	100	100
11	M	6/111 (5%)	6 (100%)	0	100	100
12	U	23/511 (4%)	23 (100%)	0	100	100
13	W	10/148 (7%)	10 (100%)	0	100	100
14	X	2/333 (1%)	2 (100%)	0	100	100
16	7	8/709 (1%)	8 (100%)	0	100	100
17	r	2/181 (1%)	2 (100%)	0	100	100
18	B4	4/336 (1%)	4 (100%)	0	100	100
19	8	8/382 (2%)	8 (100%)	0	100	100
20	9	10/446 (2%)	10 (100%)	0	100	100
21	B2	22/776 (3%)	22 (100%)	0	100	100
22	B5	3/77 (4%)	3 (100%)	0	100	100
23	B3	60/1051 (6%)	60 (100%)	0	100	100
24	BP	4/95 (4%)	4 (100%)	0	100	100
25	B1	40/1104 (4%)	40 (100%)	0	100	100
26	B6	5/109 (5%)	5 (100%)	0	100	100
34	22	5/110 (4%)	5 (100%)	0	100	100
34	52	93/110 (84%)	91 (98%)	2 (2%)	52	71
35	2f	4/74 (5%)	4 (100%)	0	100	100
35	5f	61/74 (82%)	59 (97%)	2 (3%)	38	62
36	2e	1/84 (1%)	1 (100%)	0	100	100
36	5e	72/84 (86%)	72 (100%)	0	100	100
37	2g	3/66 (4%)	3 (100%)	0	100	100
37	5g	64/66 (97%)	46 (72%)	18 (28%)	0	3
38	23	3/101 (3%)	3 (100%)	0	100	100
38	53	73/101 (72%)	73 (100%)	0	100	100
39	2b	4/177 (2%)	4 (100%)	0	100	100
39	5b	67/177 (38%)	65 (97%)	2 (3%)	41	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	21	3/101 (3%)	3 (100%)	0	100	100
40	51	76/101 (75%)	55 (72%)	21 (28%)	0	3
41	2B	3/195 (2%)	3 (100%)	0	100	100
42	2A	6/218 (3%)	6 (100%)	0	100	100
43	x	2/498 (0%)	2 (100%)	0	100	100
43	y	2/498 (0%)	2 (100%)	0	100	100
44	v	15/450 (3%)	15 (100%)	0	100	100
44	w	15/450 (3%)	15 (100%)	0	100	100
48	J	8/599 (1%)	8 (100%)	0	100	100
49	L	14/424 (3%)	14 (100%)	0	100	100
50	F	16/442 (4%)	16 (100%)	0	100	100
51	N	36/792 (4%)	36 (100%)	0	100	100
52	S	5/681 (1%)	5 (100%)	0	100	100
All	All	1120/18347 (6%)	1075 (96%)	45 (4%)	35	57

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	5f	11	LEU
35	5f	39	TYR
40	51	2	LYS
40	51	4	VAL
40	51	8	MET
40	51	10	LEU
40	51	11	SER
40	51	16	THR
40	51	28	THR
40	51	33	ASP
40	51	35	SER
40	51	44	LYS
40	51	47	LEU
40	51	48	LYS
40	51	51	GLU
40	51	53	VAL
40	51	54	GLN
40	51	55	LEU
40	51	56	GLU

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Mol	Chain	Res	Type
40	51	57	THR
40	51	74	LEU
40	51	76	LEU
40	51	81	VAL
39	5b	16	ARG
39	5b	61	ARG
34	52	33	THR
34	52	46	CYS
37	5g	3	LYS
37	5g	10	LYS
37	5g	11	LYS
37	5g	15	LYS
37	5g	27	VAL
37	5g	35	ASP
37	5g	43	ASP
37	5g	44	GLU
37	5g	46	VAL
37	5g	47	GLU
37	5g	50	THR
37	5g	51	SER
37	5g	59	MET
37	5g	62	ILE
37	5g	66	SER
37	5g	70	LEU
37	5g	71	GLU
37	5g	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
36	5e	32	GLN
36	5e	38	GLN
36	5e	88	GLN
38	53	42	GLN
35	5f	6	ASN
35	5f	68	ASN
40	51	63	ASN
40	51	64	ASN
39	5b	22	GLN
34	52	34	GLN
34	52	41	GLN
37	5g	5	HIS

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Mol	Chain	Res	Type
37	5g	26	HIS
37	5g	55	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	Z	14/15 (93%)	1 (7%)	0
3	5	107/117 (91%)	34 (31%)	3 (2%)
4	2	94/188 (50%)	18 (19%)	4 (4%)
46	z1	10/11 (90%)	5 (50%)	0
47	z2	3/4 (75%)	0	0
5	6	55/106 (51%)	11 (20%)	3 (5%)
6	4	133/144 (92%)	39 (29%)	0
All	All	416/585 (71%)	108 (25%)	10 (2%)

All (108) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	5	8	G
3	5	9	G
3	5	10	U
3	5	20	G
3	5	21	A
3	5	22	U
3	5	23	C
3	5	24	G
3	5	25	C
3	5	26	A
3	5	28	A
3	5	36	C
3	5	39	C
3	5	44	A
3	5	45	C
3	5	57	G
3	5	68	C
3	5	69	A
3	5	78	U
3	5	86	C
3	5	88	A
3	5	89	U
3	5	90	U

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Mol	Chain	Res	Type
3	5	94	U
3	5	95	G
3	5	97	G
3	5	98	G
3	5	102	U
3	5	104	C
3	5	105	U
3	5	106	U
3	5	107	U
3	5	108	G
3	5	109	G
4	2	30	A
4	2	38	A
4	2	40	C
4	2	42	G
4	2	47	U
4	2	48	A
4	2	49	U
4	2	100	U
4	2	101	U
4	2	102	U
4	2	103	U
4	2	104	U
4	2	105	G
4	2	106	G
4	2	107	A
4	2	157	G
4	2	169	C
4	2	178	A
5	6	45	A
5	6	46	G
5	6	47	A
5	6	49	G
5	6	51	U
5	6	52	U
5	6	53	A
5	6	71	G
5	6	77	C
5	6	78	A
5	6	104	U
6	4	9	G
6	4	11	A

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Mol	Chain	Res	Type
6	4	22	C
6	4	25	A
6	4	36	U
6	4	39	A
6	4	40	U
6	4	41	C
6	4	44	A
6	4	45	G
6	4	53	U
6	4	55	U
6	4	58	C
6	4	61	A
6	4	69	C
6	4	71	U
6	4	73	U
6	4	74	C
6	4	75	C
6	4	76	C
6	4	78	A
6	4	80	A
6	4	82	C
6	4	83	C
6	4	84	C
6	4	85	G
6	4	90	G
6	4	100	A
6	4	103	A
6	4	114	U
6	4	115	G
6	4	118	A
6	4	119	A
6	4	121	U
6	4	124	U
6	4	125	G
6	4	126	A
6	4	127	C
6	4	144	G
15	Z	41	A
46	z1	-2	A
46	z1	1	G
46	z1	2	U
46	z1	4	A

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Mol	Chain	Res	Type
46	z1	5	G

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	5	77	G
3	5	96	A
3	5	105	U
4	2	37	U
4	2	46	U
4	2	103	U
4	2	106	G
5	6	45	A
5	6	51	U
5	6	77	C

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 monosaccharides 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](#)

There are no chain breaks in this entry.

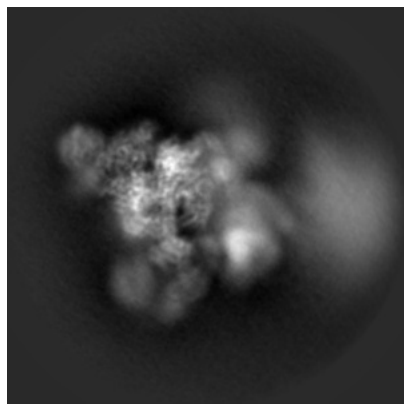
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18781. These allow visual inspection of the internal detail of the map and identification of artifacts.

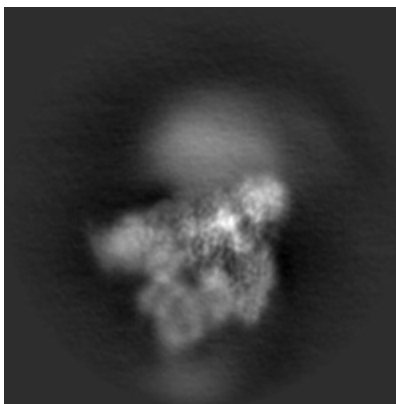
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

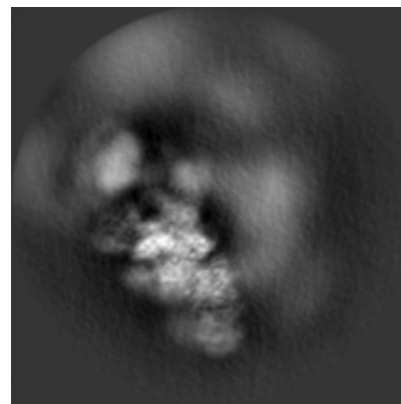
6.1.1 Primary map



X

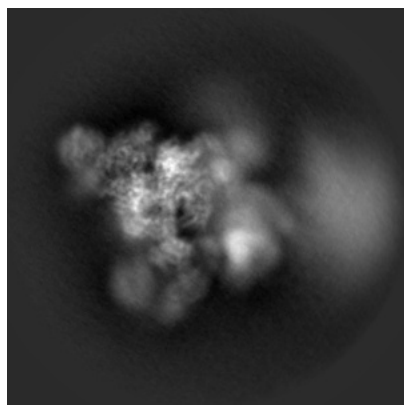


Y

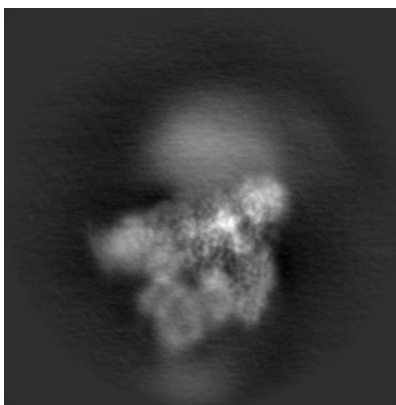


Z

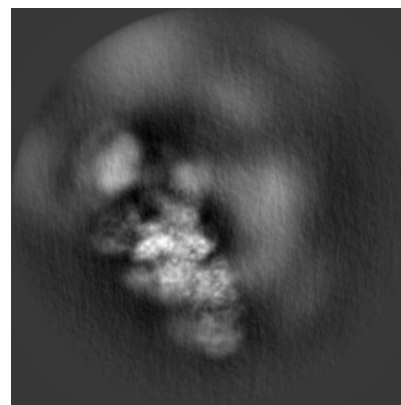
6.1.2 Raw map



X



Y

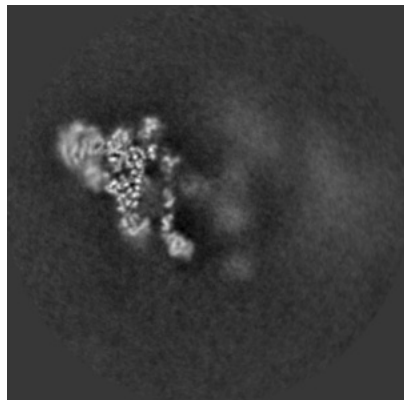


Z

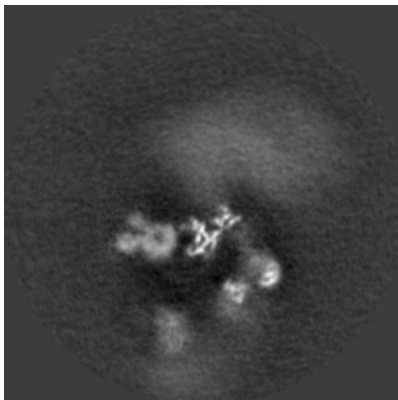
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

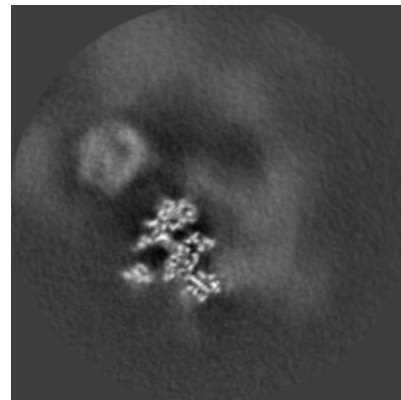
6.2.1 Primary map



X Index: 200

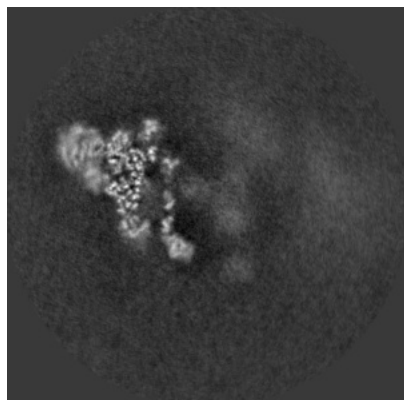


Y Index: 200

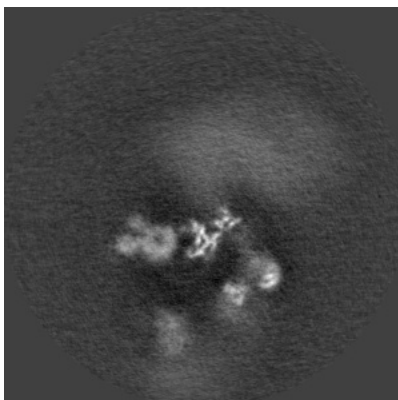


Z Index: 200

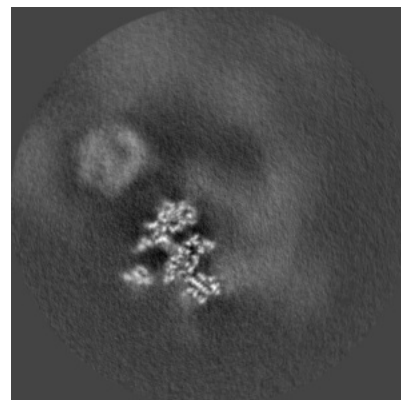
6.2.2 Raw map



X Index: 200



Y Index: 200

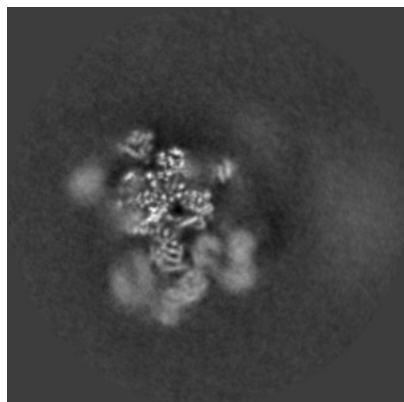


Z Index: 200

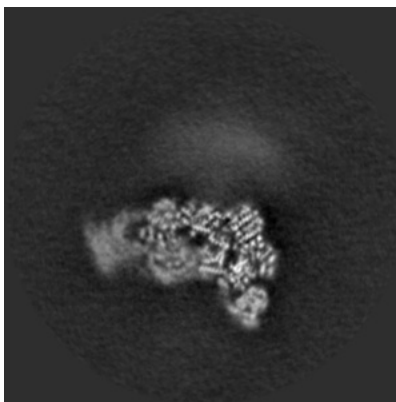
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

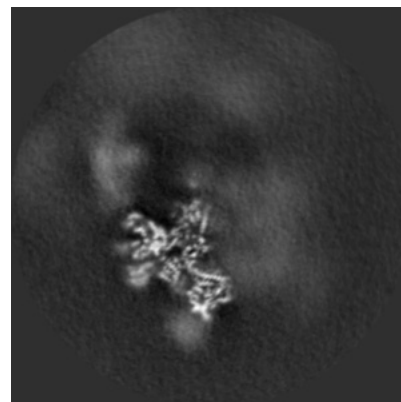
6.3.1 Primary map



X Index: 171

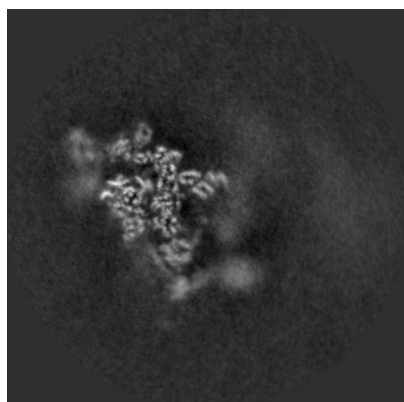


Y Index: 164

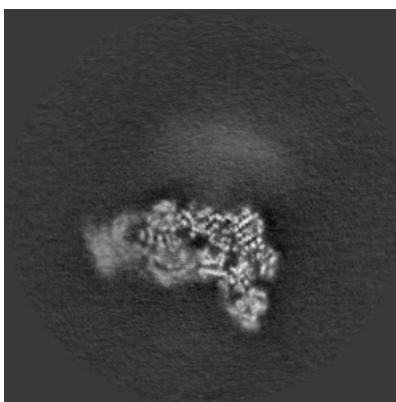


Z Index: 216

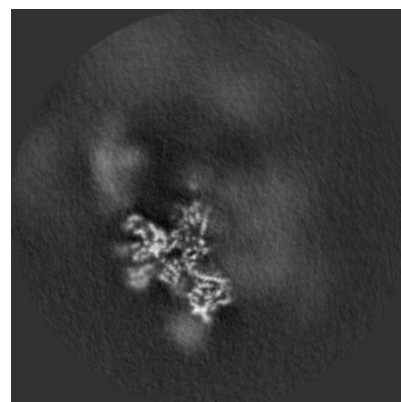
6.3.2 Raw map



X Index: 187



Y Index: 165

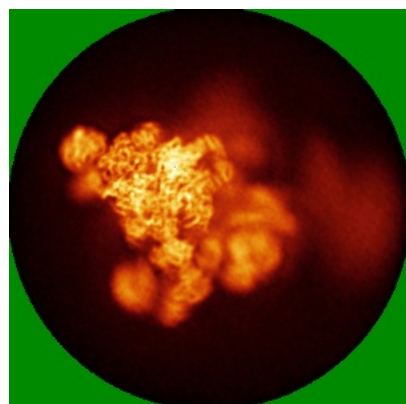


Z Index: 216

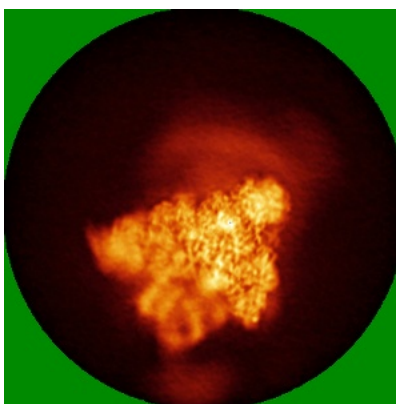
The images above show the largest variance slices of the map in three orthogonal directions.

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

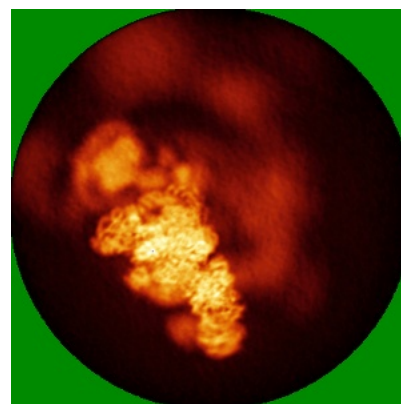
6.4.1 Primary map



X

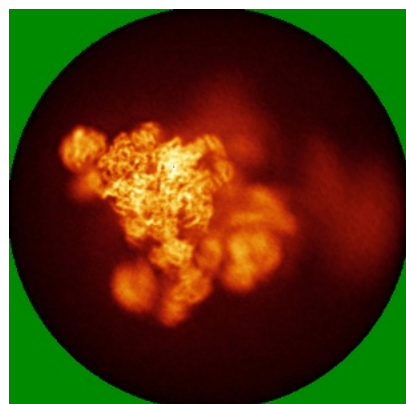


Y

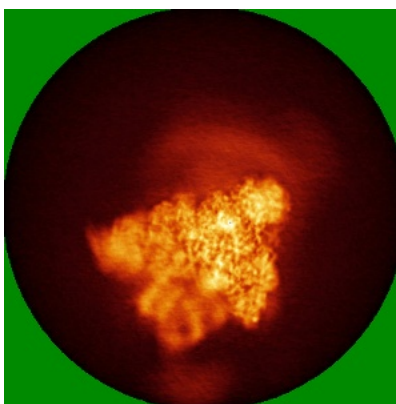


Z

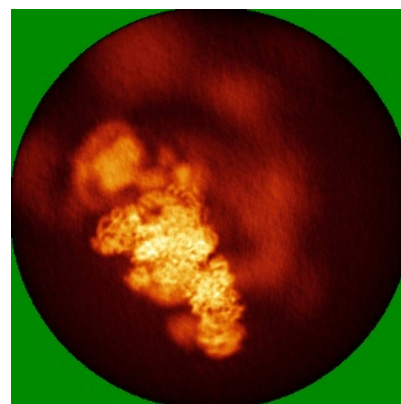
6.4.2 Raw map



X



Y

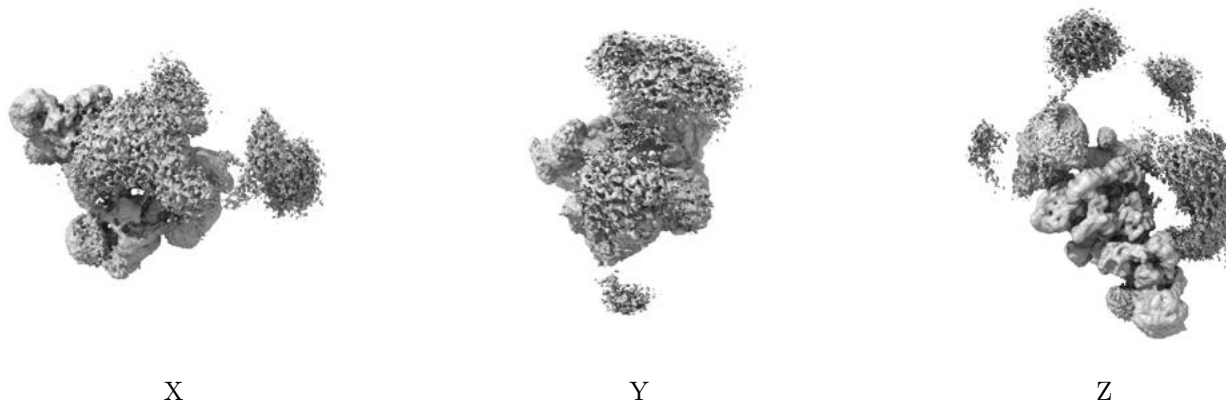


Z

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.

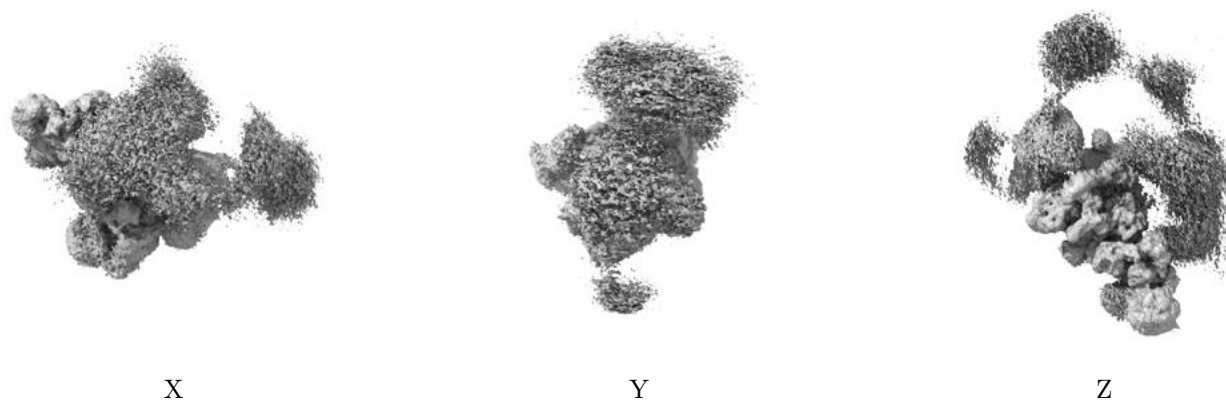
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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



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.

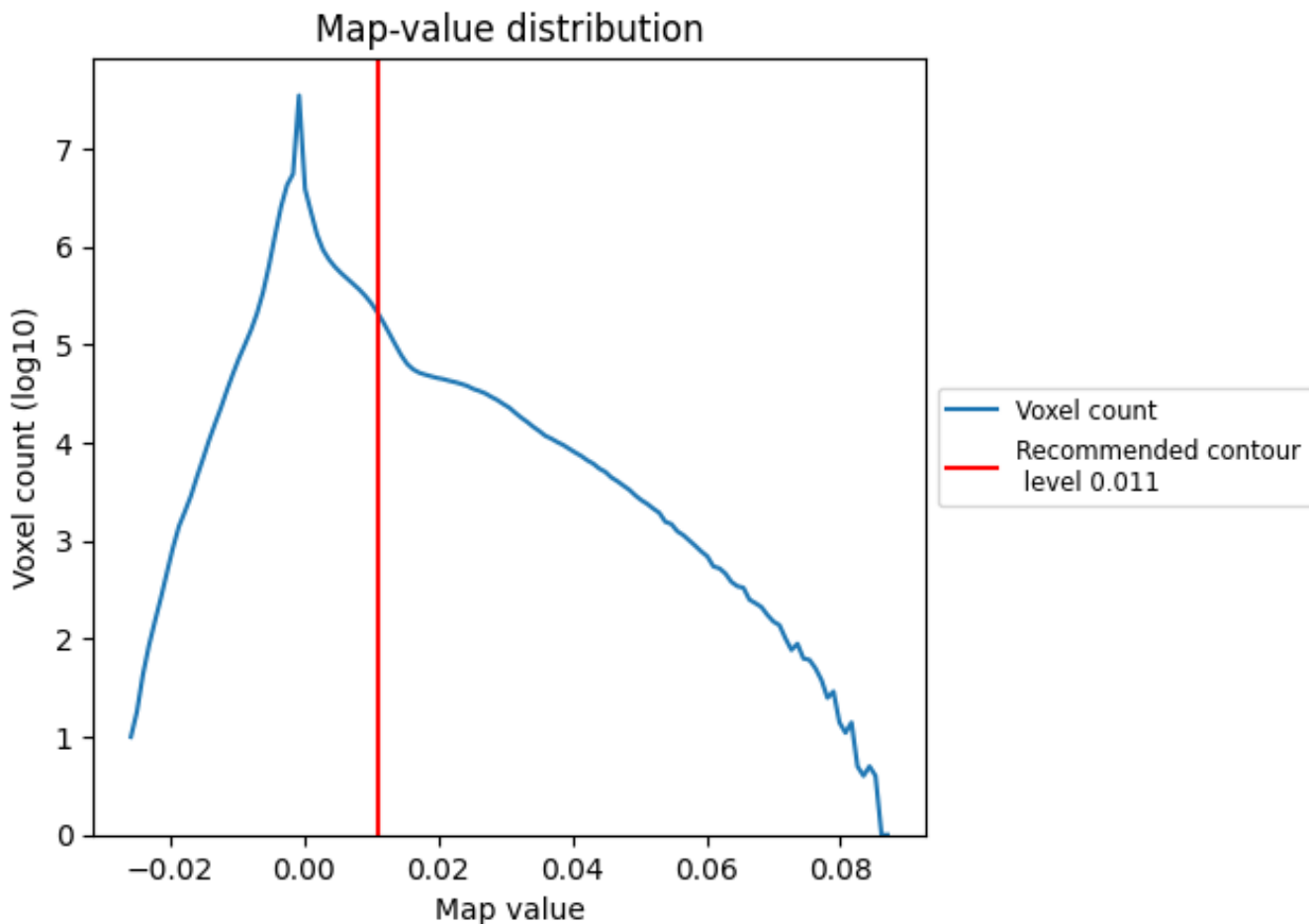
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

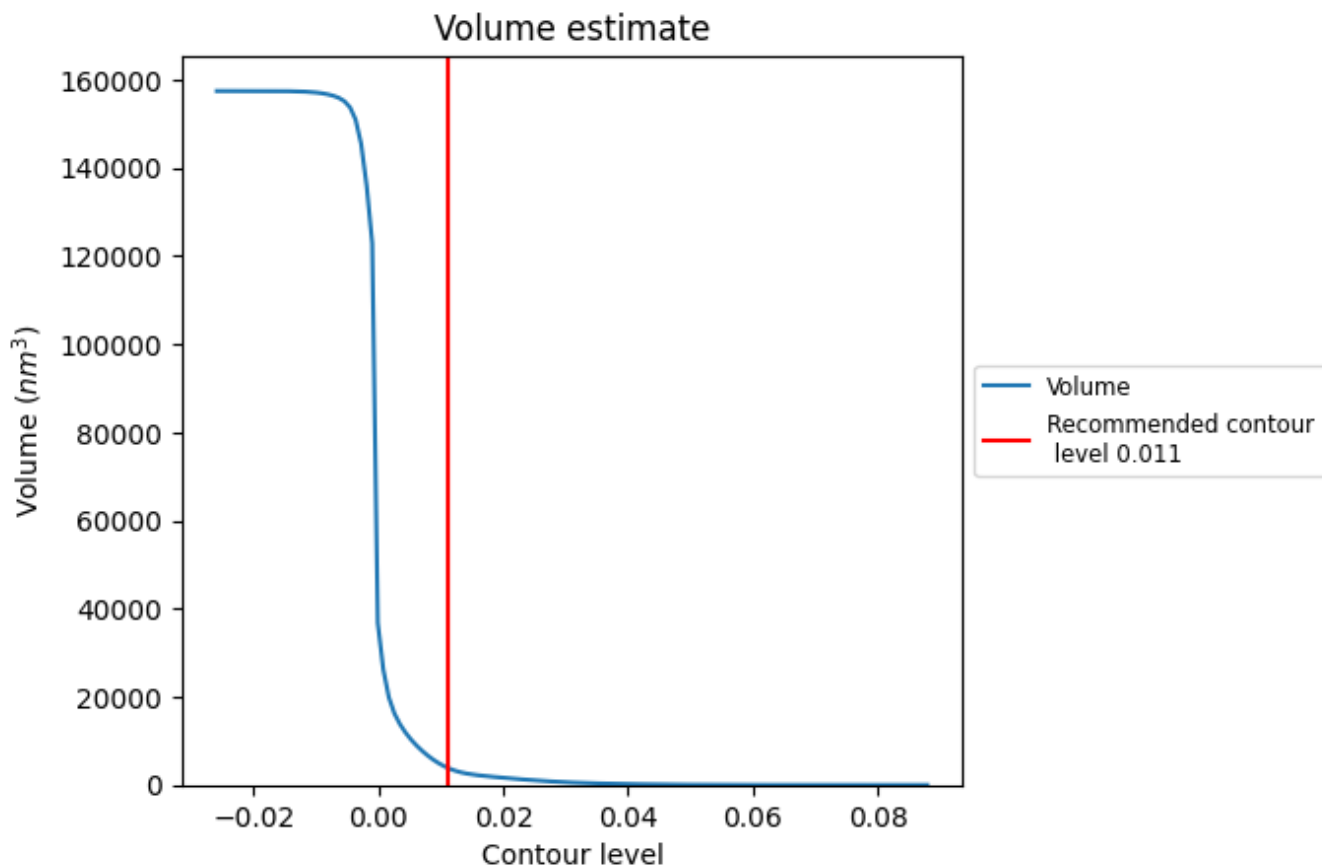
This section contains the results of statistical analysis of the map.

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.

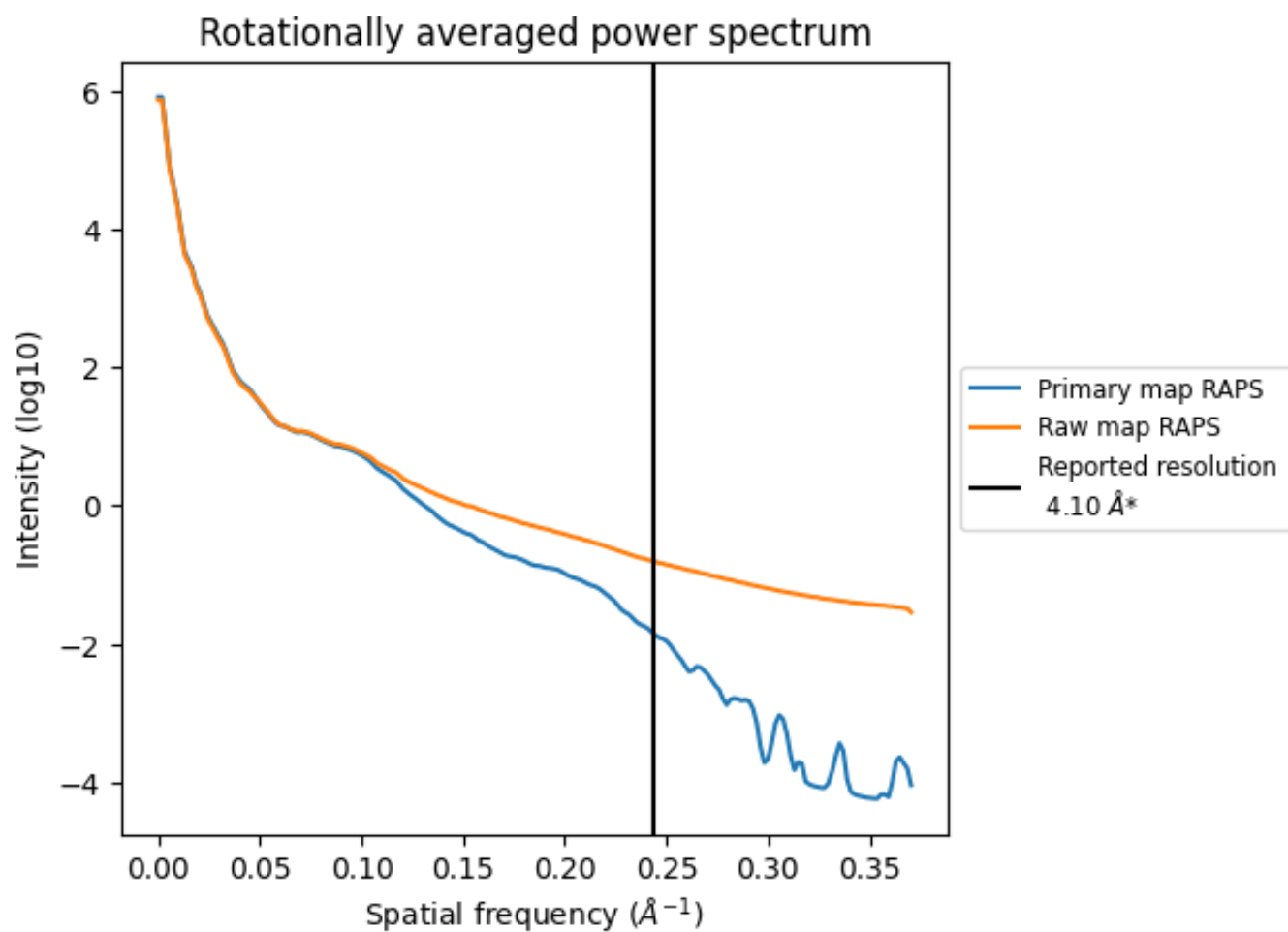
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3969 nm^3 ; this corresponds to an approximate mass of 3585 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

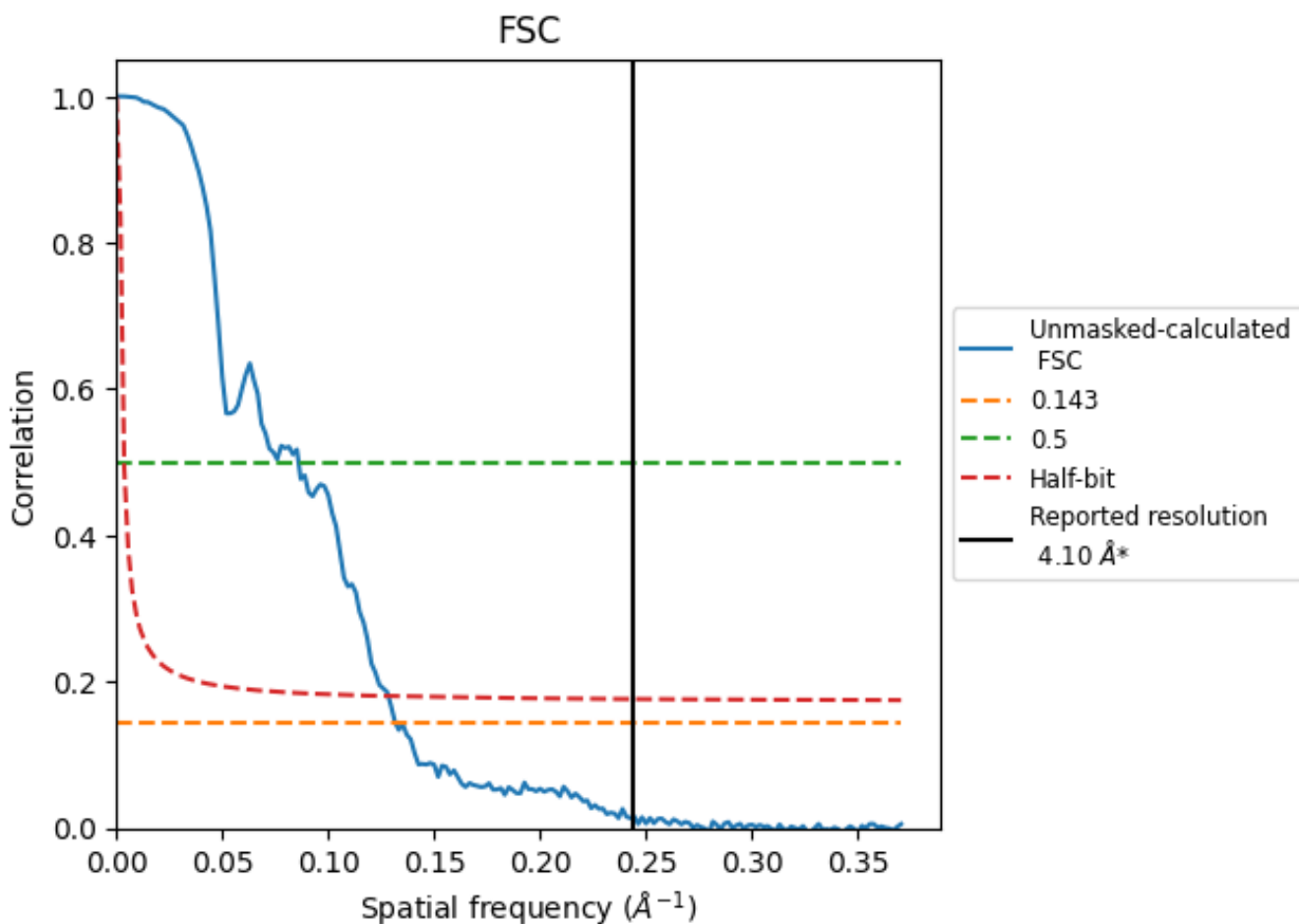


*Reported resolution corresponds to spatial frequency of 0.244 \AA^{-1}

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

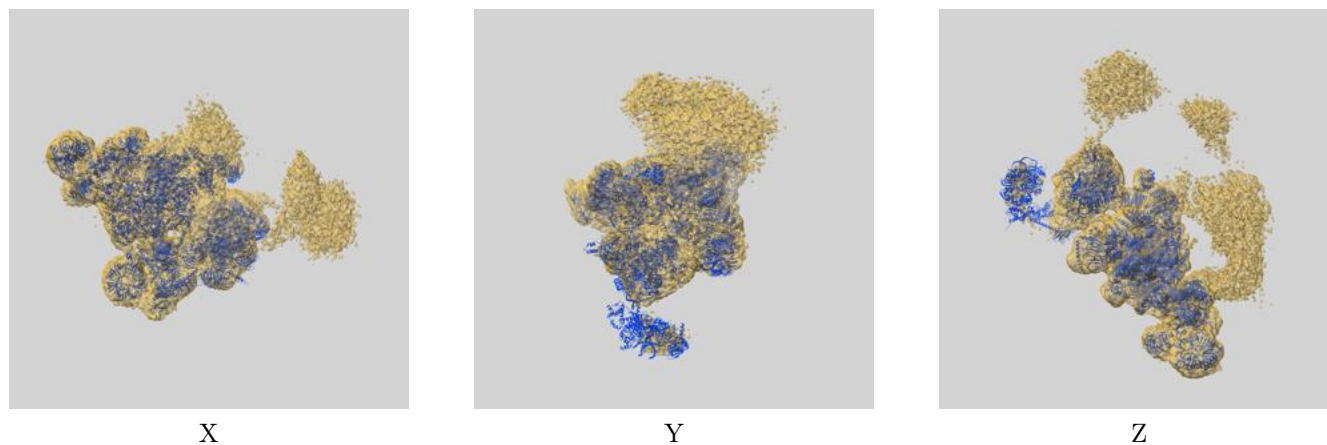
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.59	11.63	7.79

*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 7.59 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

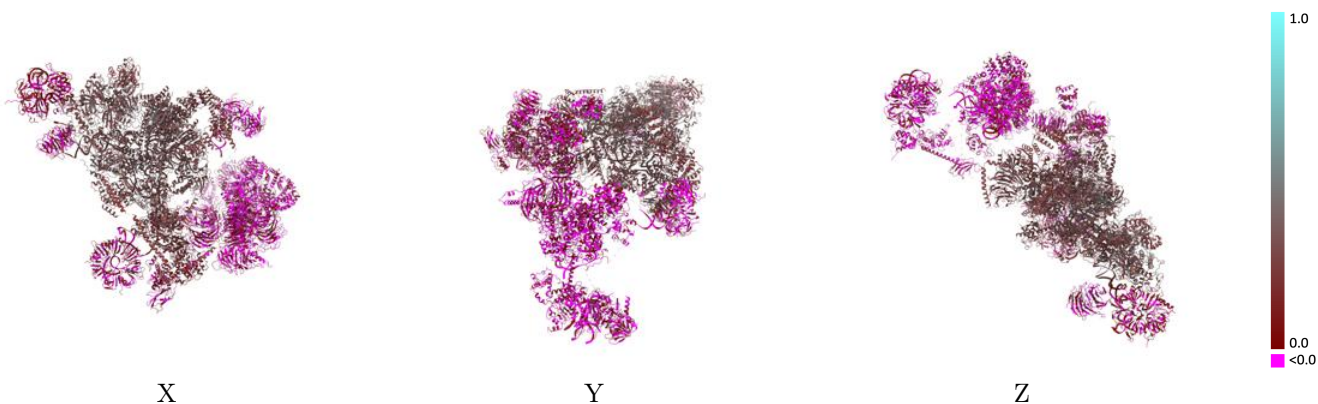
This section contains information regarding the fit between EMDB map EMD-18781 and PDB model 8QZS. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



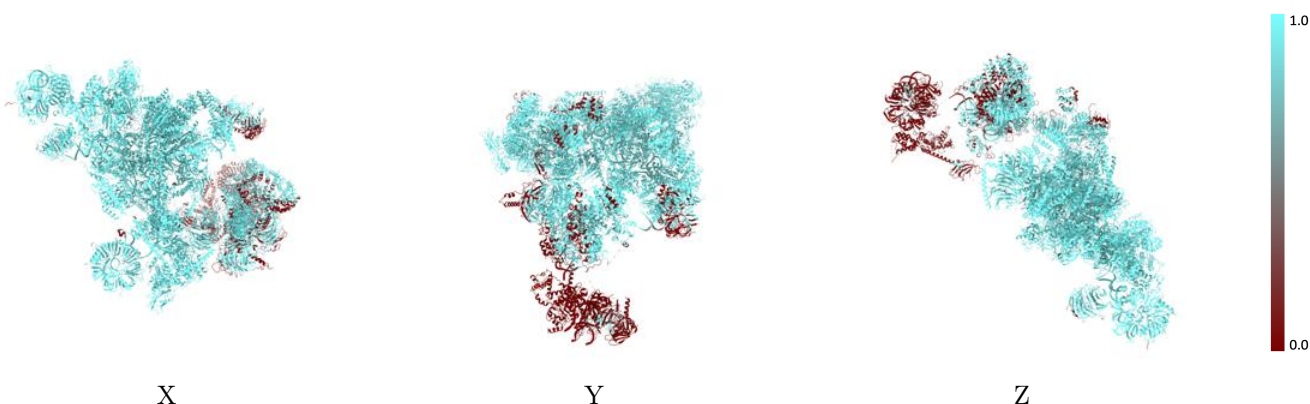
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



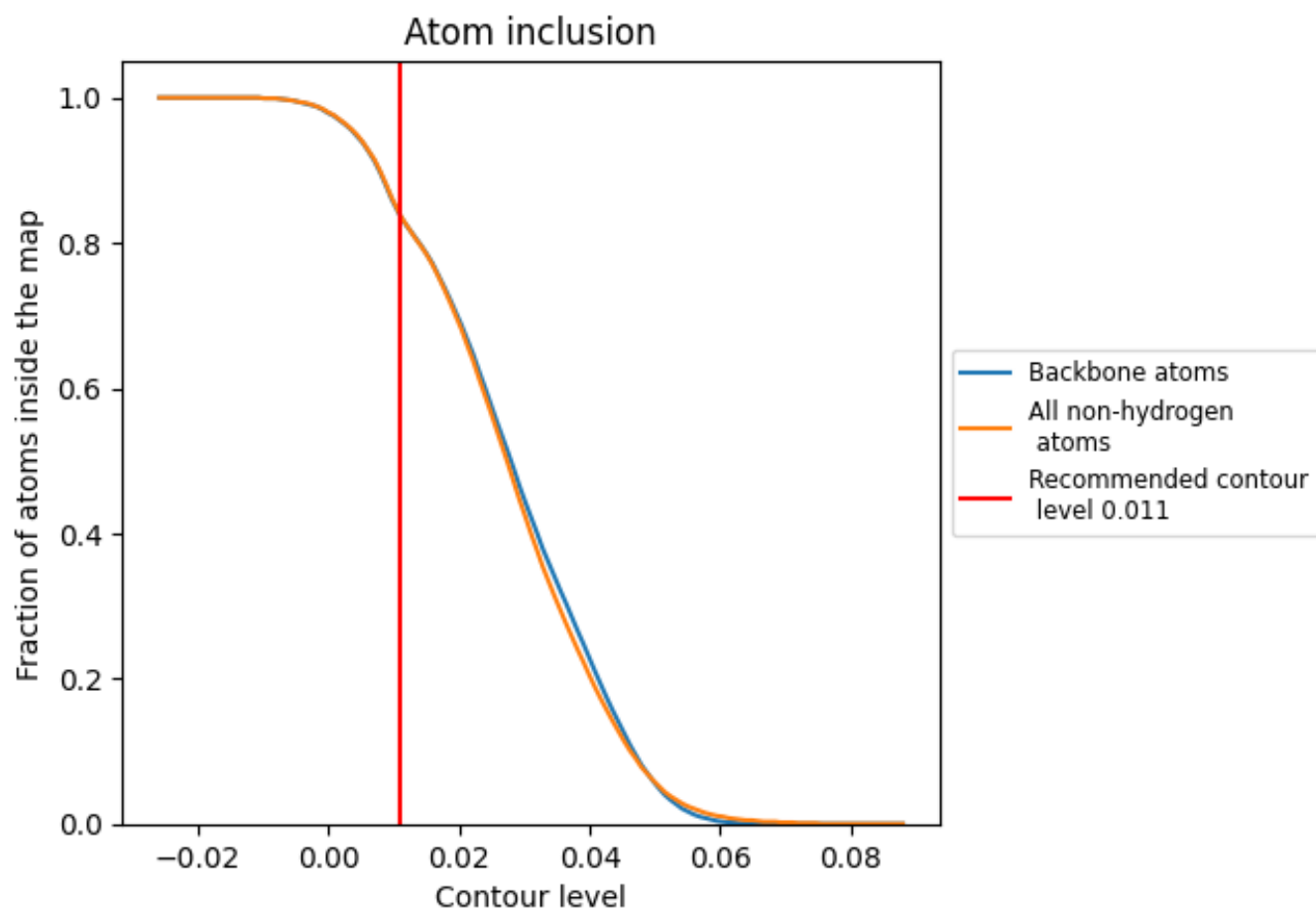
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.1680
2	 0.3540	 -0.0190
21	 0.0900	 0.0130
22	 0.0980	 0.0220
23	 0.1730	 0.0220
2A	 0.0040	 -0.0060
2B	 0.0090	 0.0360
2b	 0.1190	 -0.0180
2e	 0.1090	 -0.0070
2f	 0.0470	 0.0470
2g	 0.3430	 0.0280
4	 0.9500	 0.1680
41	 1.0000	 0.0610
42	 1.0000	 0.0610
43	 0.9970	 0.0530
4b	 0.9920	 0.0540
4e	 0.9840	 0.0580
4f	 0.9830	 0.0330
4g	 0.9730	 0.0790
5	 0.9980	 0.2060
51	 1.0000	 0.0990
52	 0.9230	 0.0950
53	 0.9810	 0.0860
5b	 0.9930	 0.0910
5e	 0.9700	 0.0730
5f	 0.9610	 0.0810
5g	 0.9820	 0.0570
6	 0.9190	 0.2200
62	 0.7610	 0.0080
63	 0.5340	 0.0060
64	 0.6930	 0.0110
65	 0.0210	 -0.0540
66	 0.0790	 -0.0320
67	 0.3000	 0.0020
68	 0.9550	 -0.0080



Continued on next page...

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Chain	Atom inclusion	Q-score
7	0.4520	0.1340
8	0.3060	0.0100
9	0.1180	0.0150
A	0.9970	0.3450
B	0.9950	0.2040
B1	0.7250	-0.0010
B2	0.6230	-0.0080
B3	0.7530	0.0100
B4	0.7750	0.0500
B5	0.8700	0.0380
B6	0.9870	0.0020
BP	0.9020	-0.0080
C	1.0000	0.3320
D	1.0000	0.3700
E	0.9580	0.0470
F	1.0000	0.2960
I	0.9990	0.3150
J	1.0000	0.3140
K	0.9820	0.2080
L	0.9940	0.3270
M	1.0000	0.3490
N	0.9990	0.2840
S	0.9710	0.2950
U	0.9580	0.3090
W	1.0000	0.2400
X	1.0000	0.3080
Z	0.9780	-0.0170
r	0.9790	0.3070
v	0.7610	0.0240
w	0.8150	0.0420
x	0.1880	-0.0090
y	0.8400	-0.0060
z1	1.0000	0.3250
z2	1.0000	0.2400