



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 02:07 pm GMT

PDB ID : 5MPS
EMDB ID : EMD-3539
Title : Structure of a spliceosome remodeled for exon ligation
Authors : Fica, S.M.; Oubridge, C.; Galej, W.P.; Wilkinson, M.E.; Newman, A.J.; Bai, X.-C.; Nagai, K.
Deposited on : 2016-12-18
Resolution : 3.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

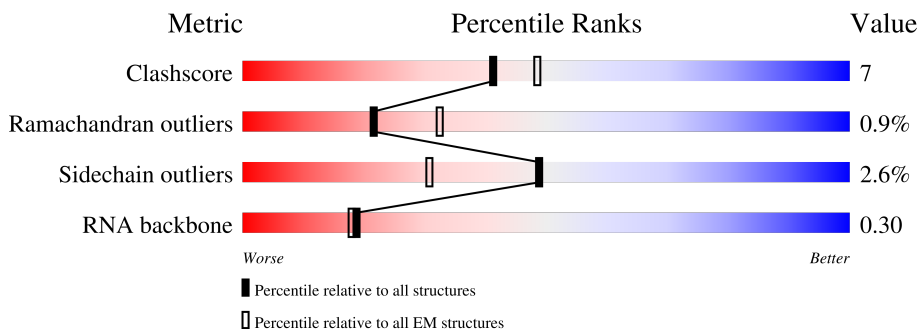
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.85 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	I	95	
2	E	20	
3	2	1175	
4	6	112	
5	5	179	
6	A	2413	
7	C	1008	

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Mol	Chain	Length	Quality of chain
8	H	577	
9	J	451	
10	K	379	
11	L	157	
12	M	339	
13	N	364	
14	O	590	
15	P	175	
16	R	135	
17	S	687	
18	T	877	
19	a	251	
20	c	382	
21	o	455	
22	X	68	
23	y	215	
24	b	196	
25	d	101	
26	e	94	
27	f	86	
28	g	77	
29	h	146	
30	j	110	

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 58929 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called Yeast UBC4 gene for ubiquitin-conjugating enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	I	34	714	321	118	241	34	0	0

- Molecule 2 is a RNA chain called UBC4 gene exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	E	16	346	155	66	109	16	0	0

- Molecule 3 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	49	1025	459	161	356	49	0	0

- Molecule 4 is a RNA chain called Saccharomyces cerevisiae strain T.52_2H chromosome XII sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	6	99	2108	944	375	690	99	0	0

- Molecule 5 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	5	141	2999	1342	530	986	141	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	1914	15199	9832	2669	2645	53	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	874	6562	4265	1104	1168	25	0	0

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	401	3261	2104	544	595	18	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	342	2690	1699	475	506	10	0	0

- Molecule 10 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	187	1458	908	269	276	5	0	0

- Molecule 11 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	155	1162	737	217	198	10	0	0

- Molecule 12 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	252	2016	1281	356	368	11	0	0

- Molecule 13 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	227	1798	1139	309	335	15	0	0

- Molecule 14 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	211	Total	C	N	O	S	0	0
			1755	1102	320	327	6		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	69	Total	C	N	O	S	0	0
			565	358	112	94	1		

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	R	108	Total	C	N	O	0	0
			614	369	121	124		

- Molecule 17 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	468	Total	C	N	O	S	0	0
			3229	2025	599	598	7		

- Molecule 18 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	T	338	Total	C	N	O	0	0
			1684	1008	338	338		

- Molecule 19 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	137	Total	C	N	O	S	0	0
			1119	726	194	196	3		

- Molecule 20 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	103	Total	C	N	O	S	0	0
			786	498	142	144	2		

- Molecule 21 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	o	313	2425	1537	429	451	8	0	0

- Molecule 22 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	X	68	338	202	68	68	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	y	83	679	420	125	133	1	0	0

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	b	80	631	403	114	111	3	0	0

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	d	82	625	399	109	115	2	0	0

- Molecule 26 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	e	75	575	379	92	101	3	0	0

- Molecule 27 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	f	72	573	368	101	103	1	0	0

- Molecule 28 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		

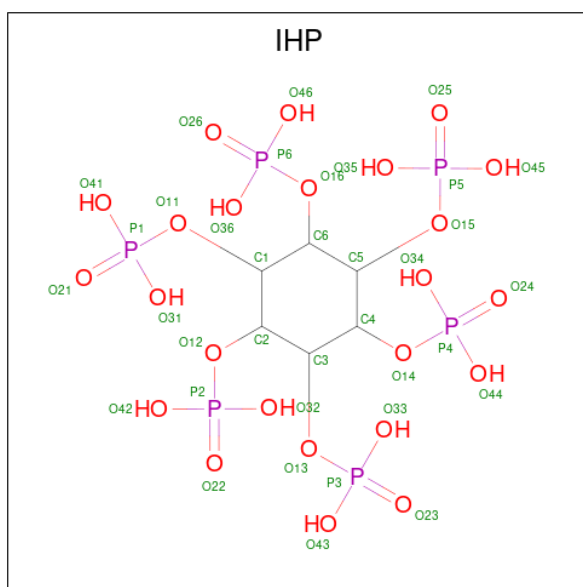
- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
31	6	3	Total	Mg	0
			3	3	

- Molecule 32 is POTASSIUM ION (three-letter code: K) (formula: K).

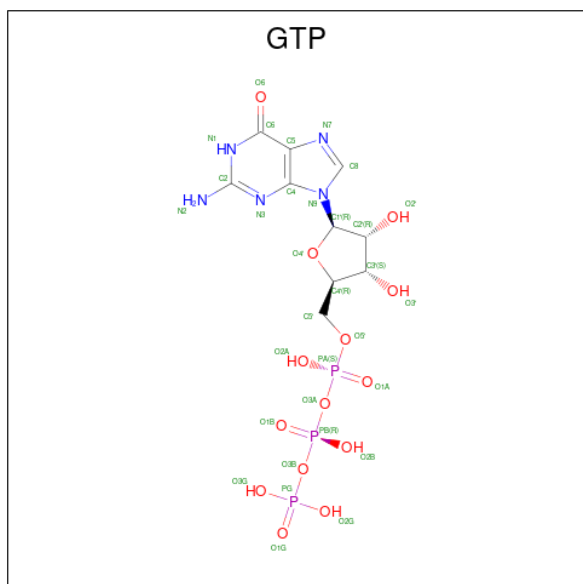
Mol	Chain	Residues	Atoms		AltConf
32	6	2	Total	K	0
			2	2	

- Molecule 33 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



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

- Molecule 34 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

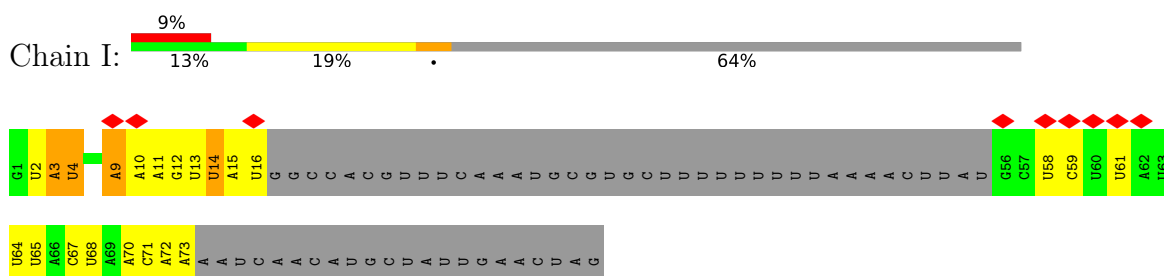
- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
35	L	3	Total 3	Zn 3	0
35	M	1	Total 1	Zn 1	0
35	N	2	Total 2	Zn 2	0

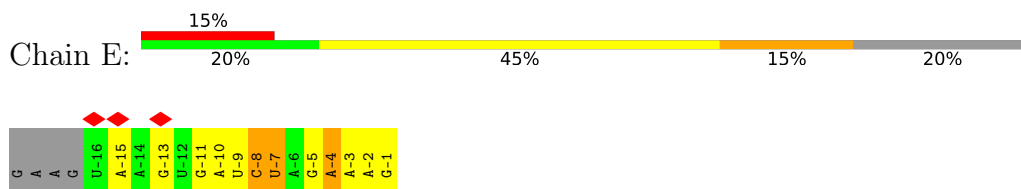
3 Residue-property plots [i](#)

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.

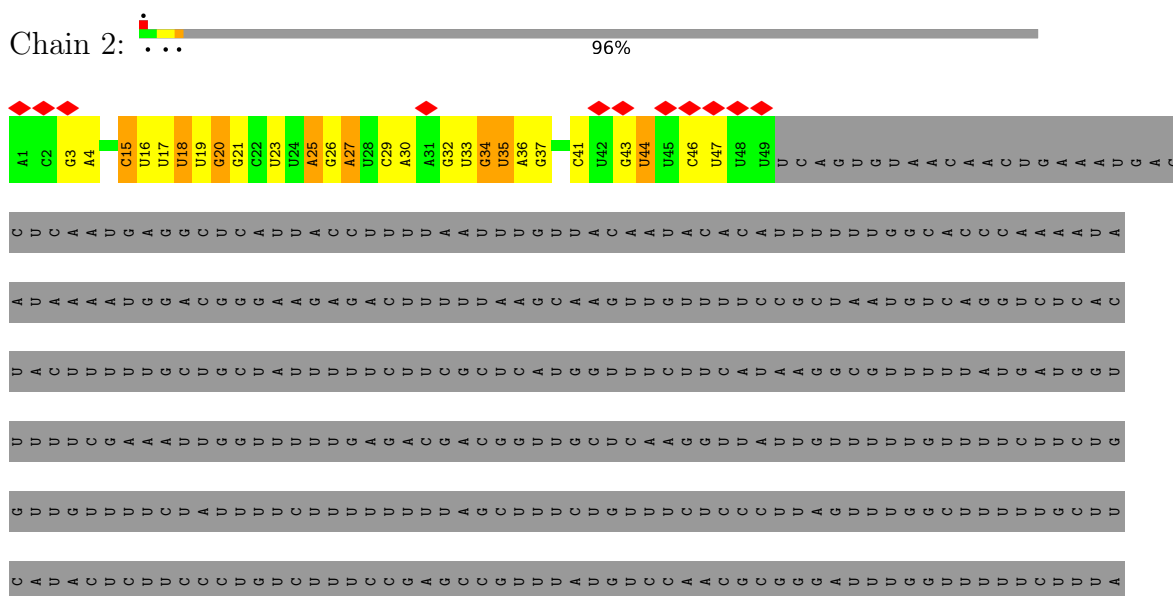
- Molecule 1: Yeast UBC4 gene for ubiquitin-conjugating enzyme

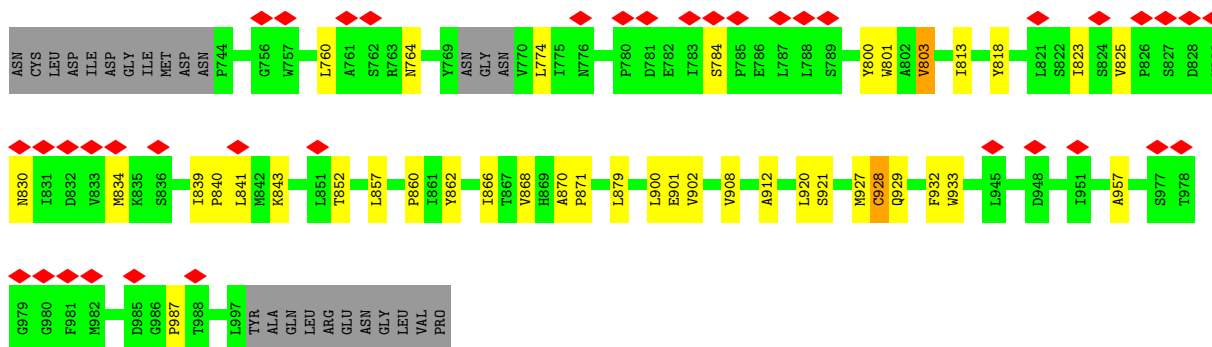


- Molecule 2: UBC4 gene exon

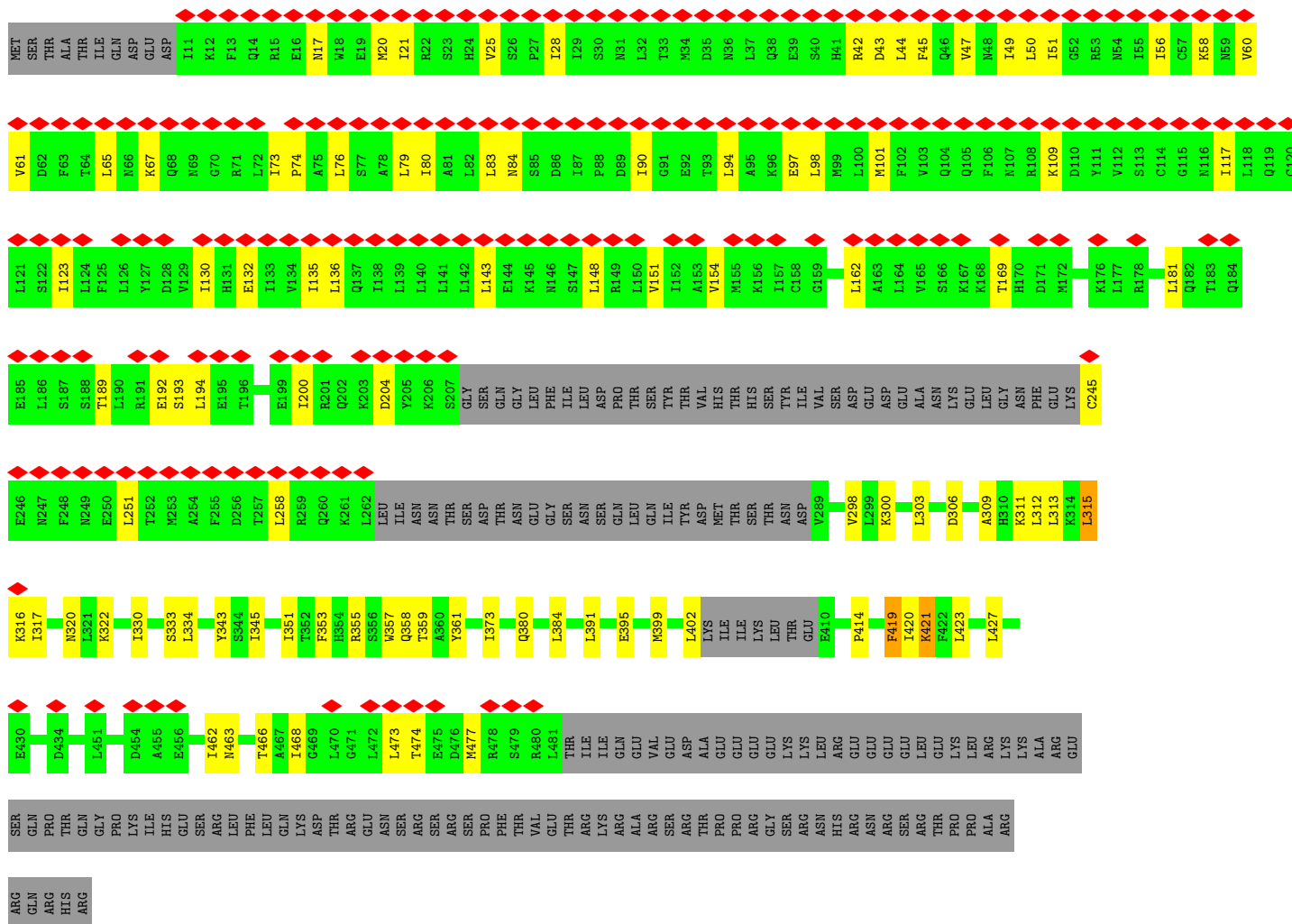


- Molecule 3: U2 snRNA



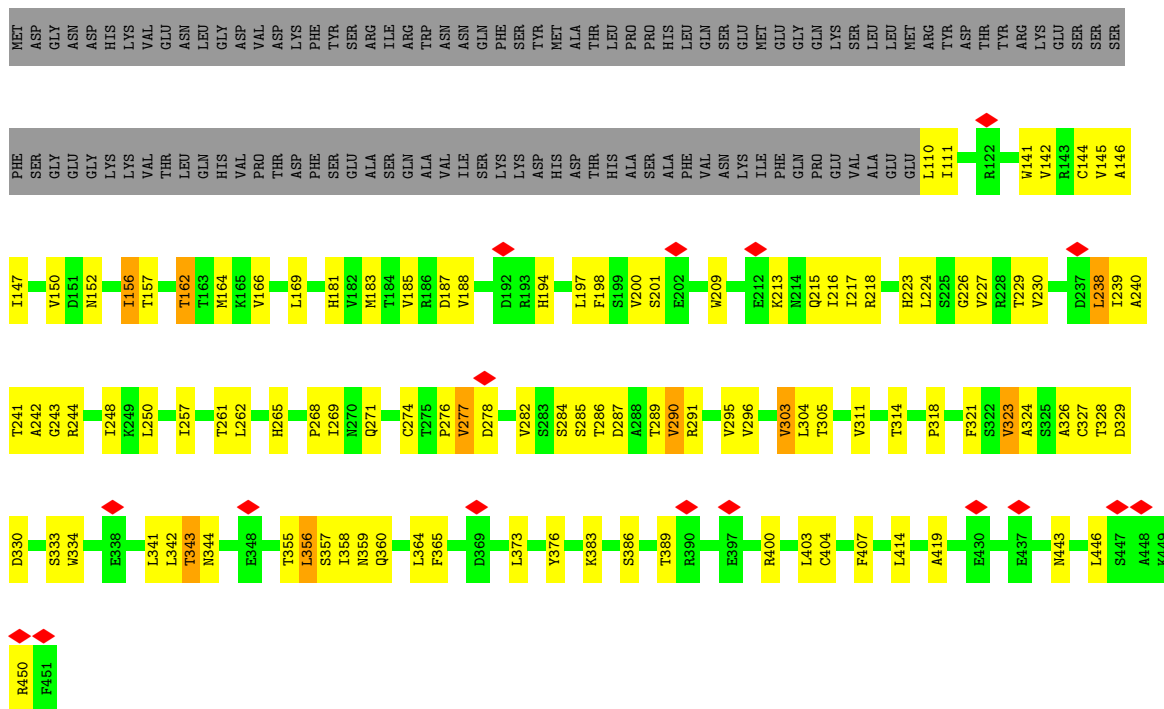


• Molecule 8: Pre-mRNA-splicing factor CWC22

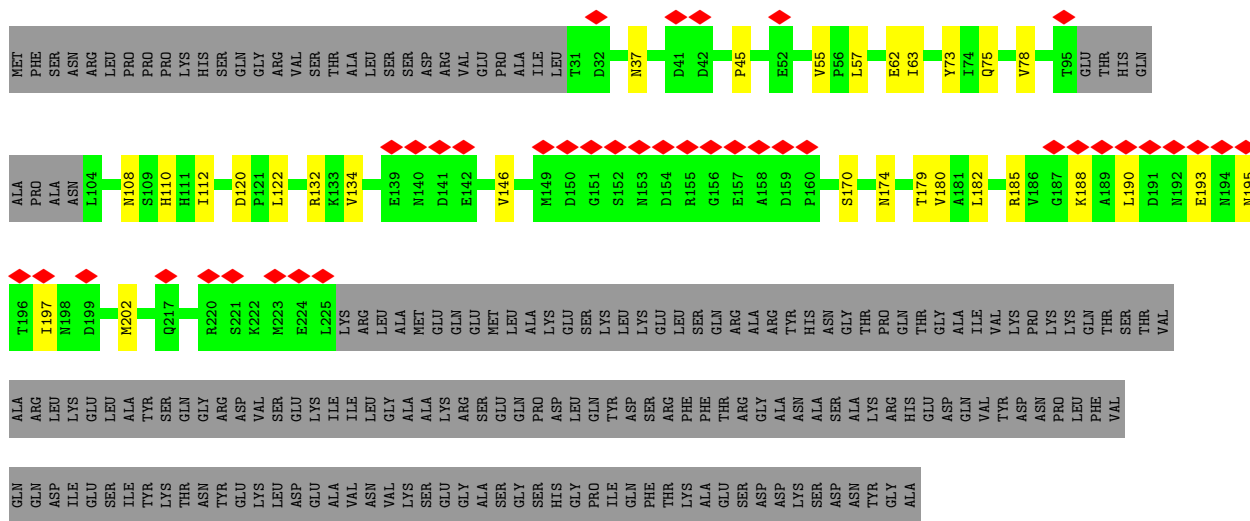
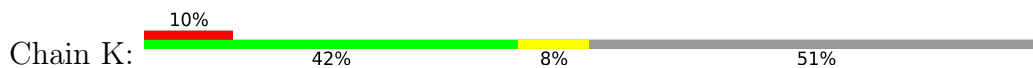


• Molecule 9: Pre-mRNA-splicing factor PRP46

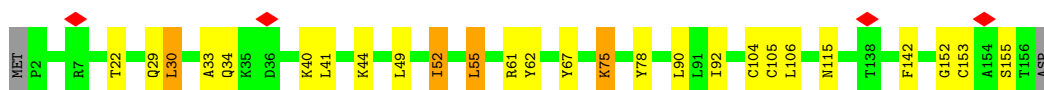
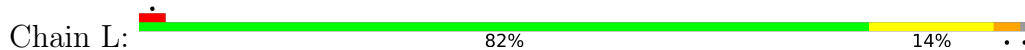




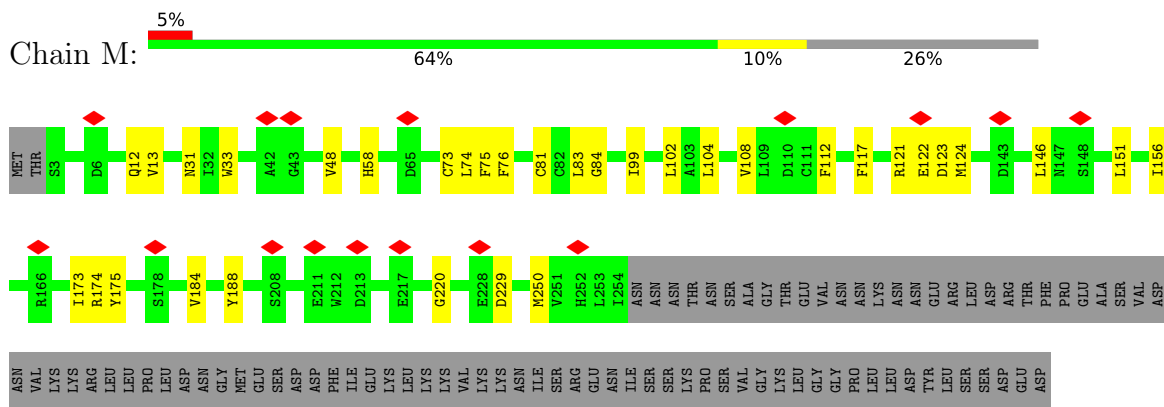
• Molecule 10: Pre-mRNA-processing protein 45



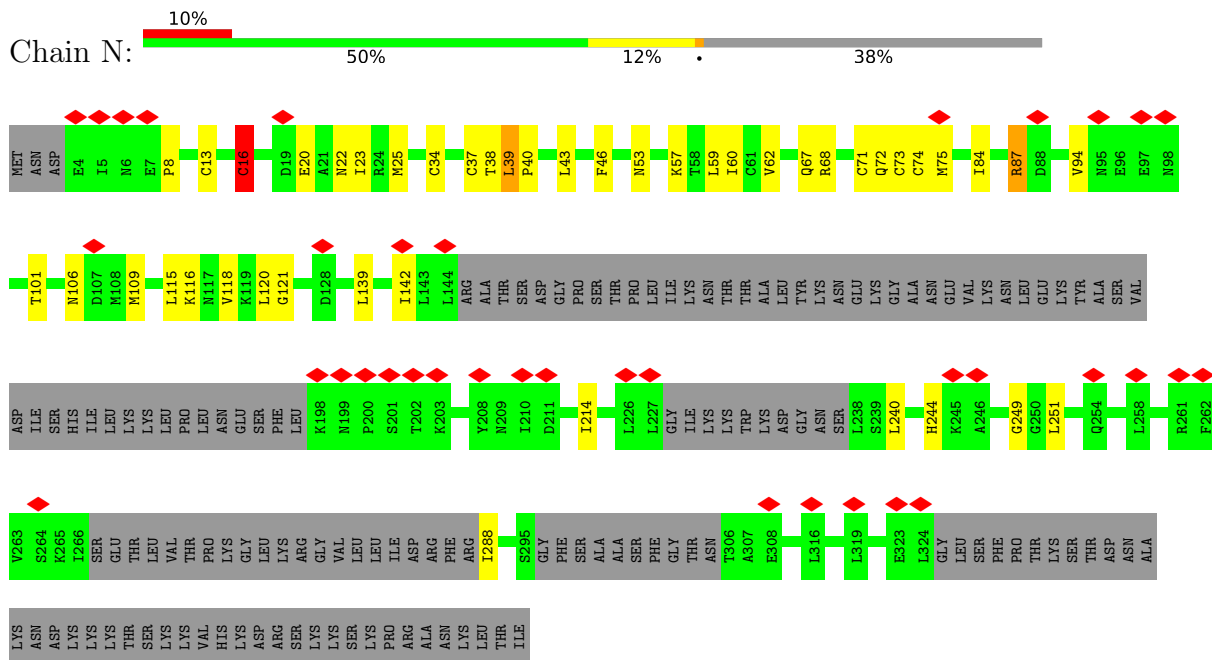
• Molecule 11: Pre-mRNA-splicing factor BUD31



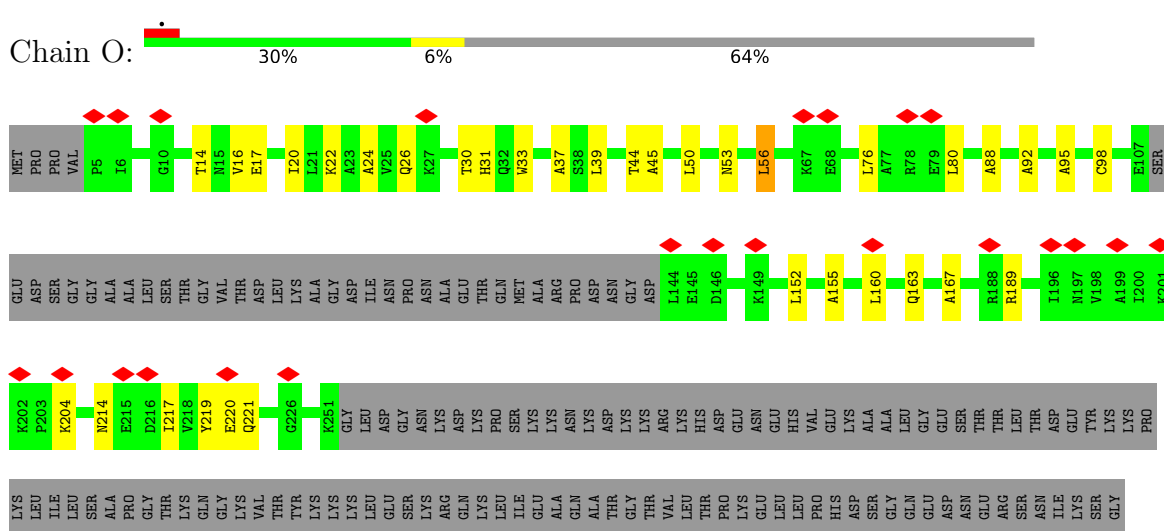
• Molecule 12: Pre-mRNA-splicing factor CWC2

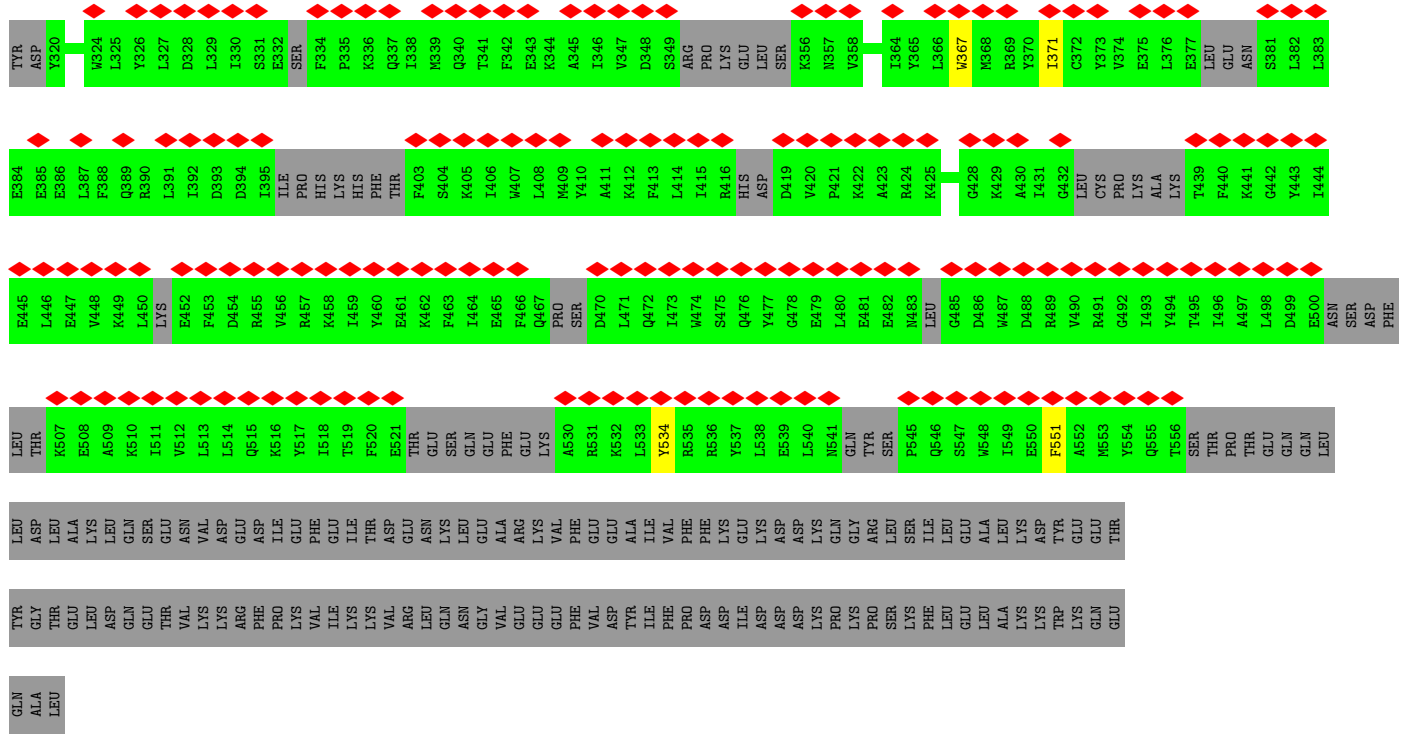


• Molecule 13: Pre-mRNA-splicing factor SLT11

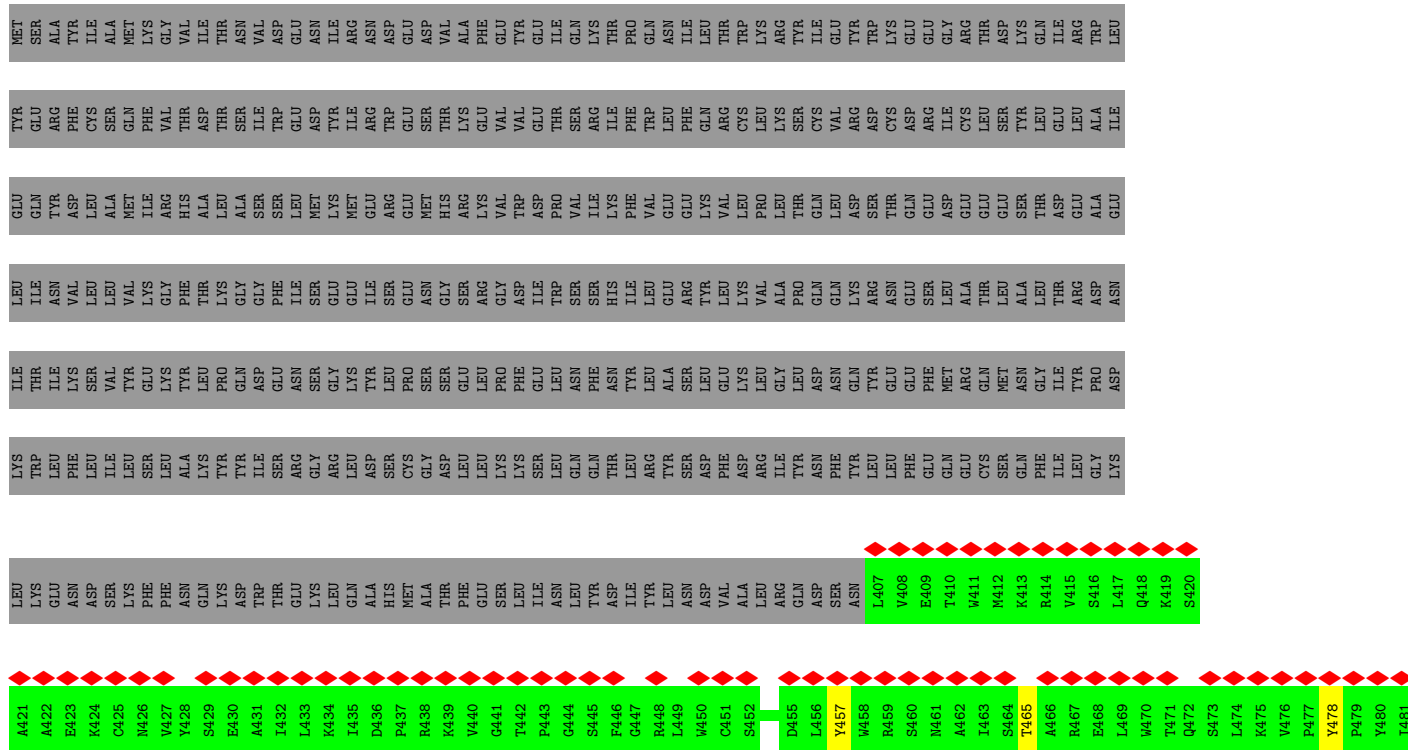


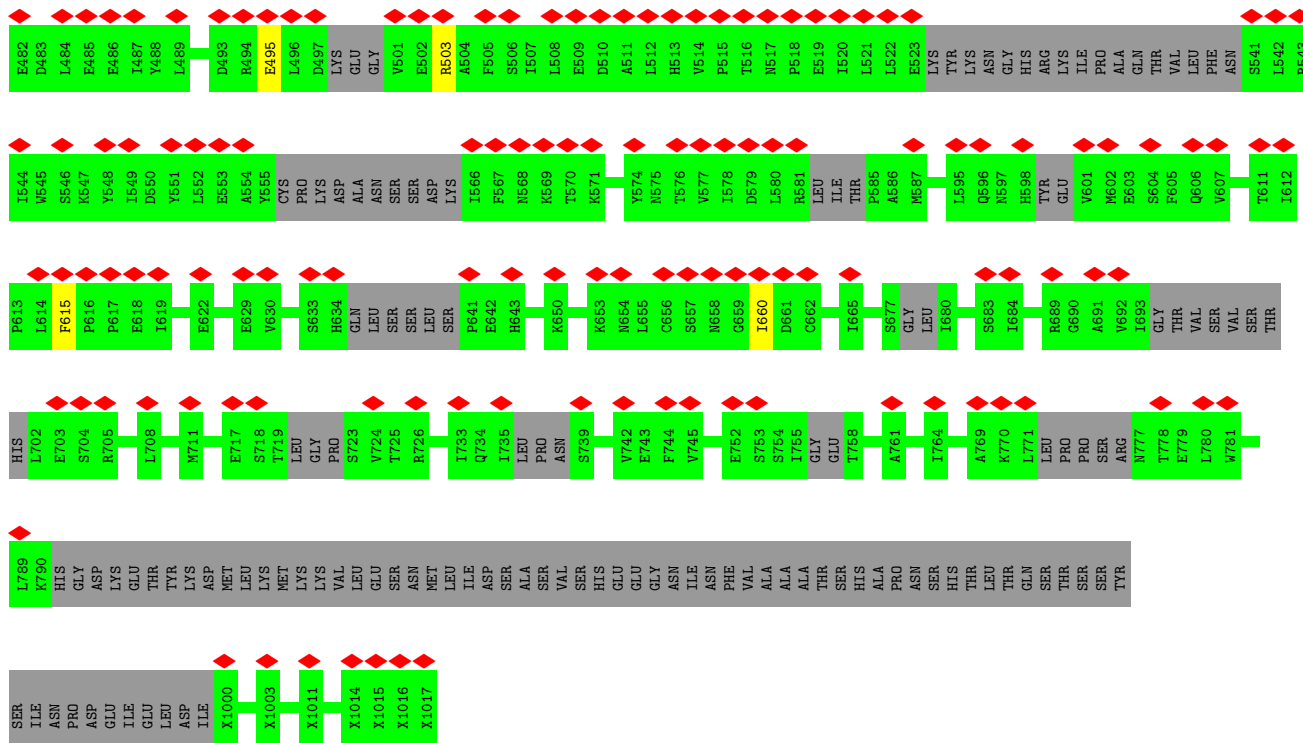
• Molecule 14: Pre-mRNA-splicing factor CEF1



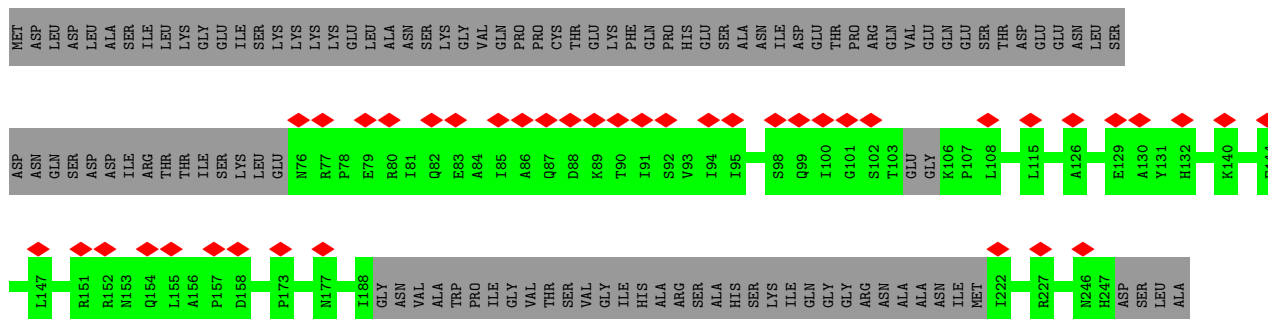


● Molecule 18: Pre-mRNA-splicing factor SYF1

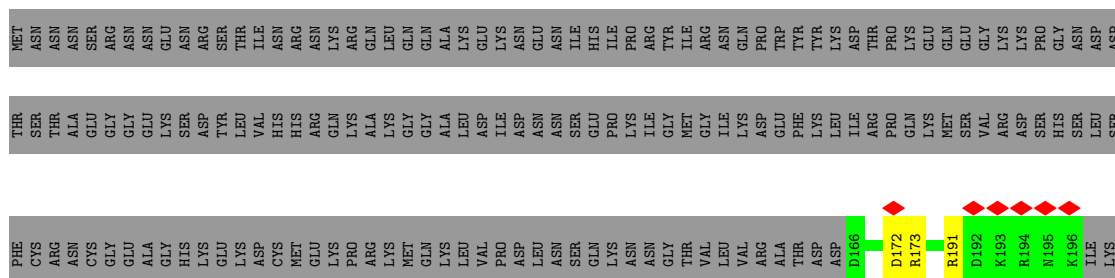


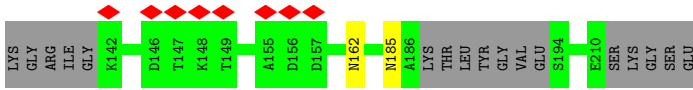
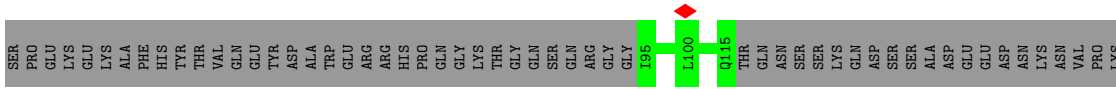


● Molecule 19: Pre-mRNA-splicing factor 18

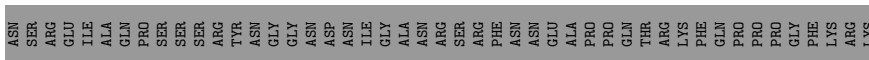
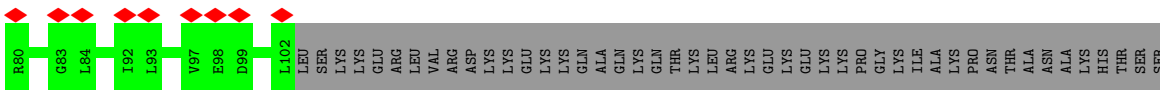
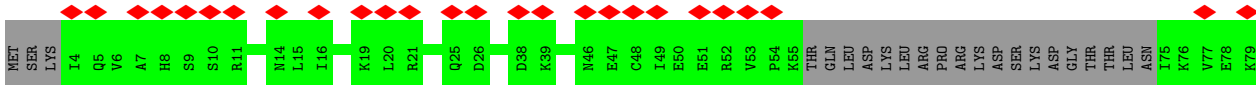


● Molecule 20: Pre-mRNA-splicing factor SLU7

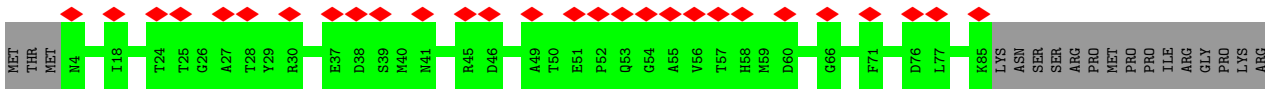
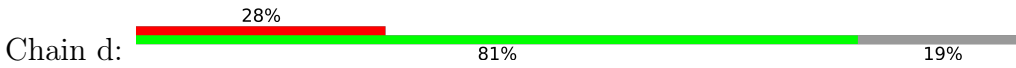




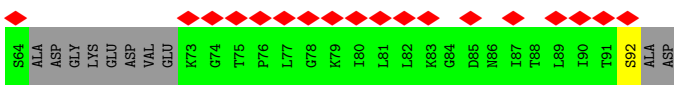
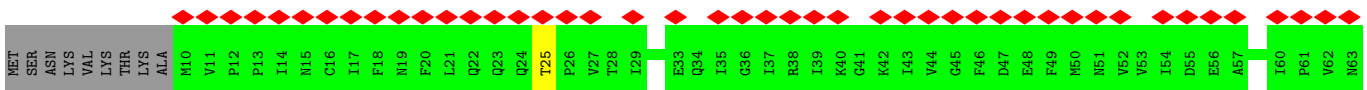
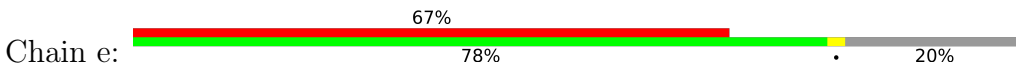
• Molecule 24: Small nuclear ribonucleoprotein-associated protein B



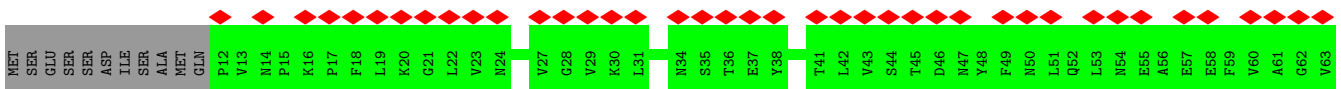
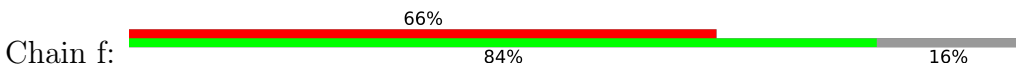
• Molecule 25: Small nuclear ribonucleoprotein Sm D3

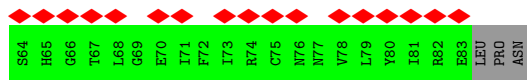


• Molecule 26: Small nuclear ribonucleoprotein E

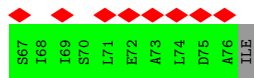
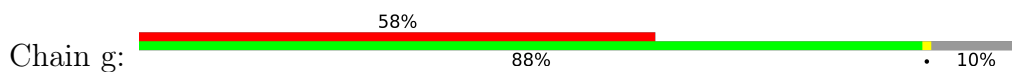


• Molecule 27: Small nuclear ribonucleoprotein F

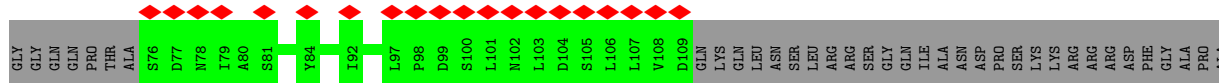
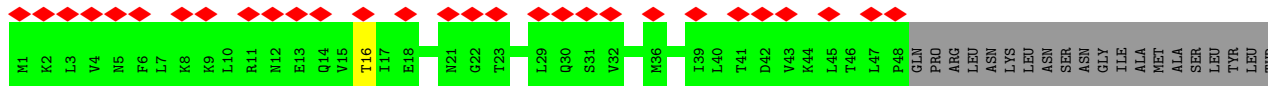




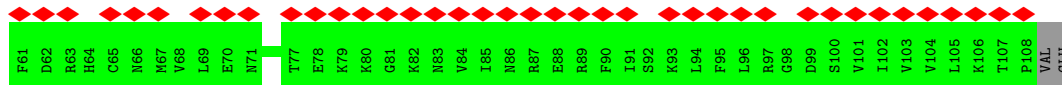
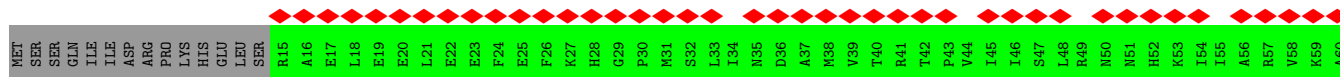
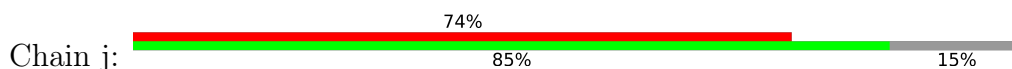
• Molecule 28: Small nuclear ribonucleoprotein G



• Molecule 29: Small nuclear ribonucleoprotein Sm D1



• Molecule 30: Small nuclear ribonucleoprotein Sm D2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65824	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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	589.16, 589.16, 589.16	wwPDB
Map dimensions	412, 412, 412	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: K, GTP, MG, IHP, ZN

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	I	0.33	0/795	0.83	1/1231 (0.1%)
2	E	0.34	0/388	0.78	0/603
3	2	0.31	0/1140	0.75	0/1770
4	6	0.33	0/2357	0.72	1/3667 (0.0%)
5	5	0.32	0/3351	0.73	0/5213
6	A	0.46	0/15598	0.73	0/21212
7	C	0.42	0/6703	0.69	0/9138
8	H	0.48	0/3314	0.77	0/4463
9	J	0.47	0/2749	0.74	0/3735
10	K	0.44	0/1480	0.75	0/2000
11	L	0.46	0/1186	0.71	0/1606
12	M	0.41	0/2062	0.66	0/2772
13	N	0.41	0/1823	0.71	1/2456 (0.0%)
14	O	0.46	0/1781	0.79	0/2385
15	P	0.39	0/580	0.66	0/776
16	R	0.40	0/617	0.68	0/848
17	S	0.47	0/3269	0.76	0/4446
18	T	0.44	0/1583	0.65	0/2192
19	a	0.38	0/1141	0.61	0/1546
20	c	0.45	1/798 (0.1%)	0.60	0/1074
21	o	0.41	0/2491	0.64	0/3384
23	y	0.34	0/681	0.54	0/902
24	b	0.36	0/636	0.63	0/856
25	d	0.35	0/634	0.56	0/859
26	e	0.41	0/585	0.61	0/795
27	f	0.40	0/585	0.57	0/791
28	g	0.50	0/532	0.61	0/715
29	h	0.37	0/649	0.54	0/880
30	j	0.36	0/753	0.57	0/1013
All	All	0.43	1/60261 (0.0%)	0.71	3/83328 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	1
9	J	0	1
15	P	0	1
21	o	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	230	SER	C-O	6.11	1.34	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	6	45	A	C2'-C3'-O3'	7.14	125.22	109.50
1	I	9	A	C4'-C3'-O3'	5.26	123.51	113.00
13	N	16	CYS	CA-CB-SG	5.00	123.00	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	C	105	ILE	Peptide
9	J	194	HIS	Peptide
15	P	5	HIS	Peptide
21	o	239	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	714	0	361	6	0
2	E	346	0	173	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	1025	0	518	12	0
4	6	2108	0	1063	28	0
5	5	2999	0	1515	34	0
6	A	15199	0	14954	264	0
7	C	6562	0	6486	107	0
8	H	3261	0	3323	90	0
9	J	2690	0	2690	85	0
10	K	1458	0	1468	20	0
11	L	1162	0	1111	19	0
12	M	2016	0	1985	32	0
13	N	1798	0	1842	38	0
14	O	1755	0	1794	23	0
15	P	565	0	555	7	0
16	R	614	0	390	8	0
17	S	3229	0	2573	37	0
18	T	1684	0	716	2	0
19	a	1119	0	1164	0	0
20	c	786	0	719	0	0
21	o	2425	0	2253	0	0
22	X	338	0	70	1	0
23	y	679	0	706	0	0
24	b	631	0	670	0	0
25	d	625	0	647	0	0
26	e	575	0	597	0	0
27	f	573	0	572	0	0
28	g	529	0	557	0	0
29	h	644	0	686	0	0
30	j	741	0	778	0	0
31	6	3	0	0	0	0
32	6	2	0	0	0	0
33	A	36	0	6	0	0
34	C	32	0	12	0	0
35	L	3	0	0	0	0
35	M	1	0	0	0	0
35	N	2	0	0	0	0
All	All	58929	0	52954	722	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 7.

The worst 5 of 722 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)
8:H:312:LEU:HA	8:H:315:LEU:CD2	1.64	1.27
8:H:311:LYS:O	8:H:315:LEU:CD2	1.85	1.24
8:H:311:LYS:O	8:H:315:LEU:HD22	1.38	1.24
8:H:312:LEU:CA	8:H:315:LEU:HD23	1.72	1.19
12:M:108:VAL:CG1	13:N:59:LEU:HD22	1.72	1.19

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	
6	A	1906/2413 (79%)	1733 (91%)	161 (8%)	12 (1%)	25	62
7	C	864/1008 (86%)	771 (89%)	87 (10%)	6 (1%)	22	59
8	H	393/577 (68%)	353 (90%)	36 (9%)	4 (1%)	15	51
9	J	340/451 (75%)	295 (87%)	39 (12%)	6 (2%)	8	41
10	K	183/379 (48%)	163 (89%)	17 (9%)	3 (2%)	9	43
11	L	153/157 (98%)	136 (89%)	16 (10%)	1 (1%)	22	59
12	M	250/339 (74%)	236 (94%)	12 (5%)	2 (1%)	19	56
13	N	217/364 (60%)	191 (88%)	22 (10%)	4 (2%)	8	41
14	O	207/590 (35%)	193 (93%)	11 (5%)	3 (1%)	11	45
15	P	63/175 (36%)	56 (89%)	7 (11%)	0	100	100
16	R	104/135 (77%)	91 (88%)	12 (12%)	1 (1%)	15	51
17	S	438/687 (64%)	415 (95%)	20 (5%)	3 (1%)	22	59
18	T	294/877 (34%)	279 (95%)	12 (4%)	3 (1%)	15	51
19	a	131/251 (52%)	123 (94%)	8 (6%)	0	100	100
20	c	97/382 (25%)	87 (90%)	8 (8%)	2 (2%)	7	38
21	o	305/455 (67%)	251 (82%)	46 (15%)	8 (3%)	5	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	y	77/215 (36%)	76 (99%)	1 (1%)	0	100	100
24	b	76/196 (39%)	74 (97%)	2 (3%)	0	100	100
25	d	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
26	e	71/94 (76%)	62 (87%)	9 (13%)	0	100	100
27	f	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
28	g	65/77 (84%)	63 (97%)	2 (3%)	0	100	100
29	h	78/146 (53%)	71 (91%)	7 (9%)	0	100	100
30	j	92/110 (84%)	83 (90%)	9 (10%)	0	100	100
All	All	6554/10265 (64%)	5936 (91%)	560 (8%)	58 (1%)	21	53

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	487	ASN
6	A	742	VAL
6	A	1620	TYR
7	C	568	SER
7	C	901	GLU

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	
6	A	1577/2182 (72%)	1550 (98%)	27 (2%)	60	77
7	C	681/910 (75%)	662 (97%)	19 (3%)	43	66
8	H	366/538 (68%)	357 (98%)	9 (2%)	47	68
9	J	299/397 (75%)	280 (94%)	19 (6%)	17	47
10	K	159/328 (48%)	152 (96%)	7 (4%)	28	56
11	L	112/141 (79%)	105 (94%)	7 (6%)	18	47
12	M	214/296 (72%)	210 (98%)	4 (2%)	57	75
13	N	211/332 (64%)	205 (97%)	6 (3%)	43	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	187/525 (36%)	181 (97%)	6 (3%)	39	63
15	P	56/151 (37%)	54 (96%)	2 (4%)	35	61
16	R	25/121 (21%)	24 (96%)	1 (4%)	31	58
17	S	230/633 (36%)	221 (96%)	9 (4%)	32	59
18	T	1/786 (0%)	1 (100%)	0	100	100
19	a	125/225 (56%)	125 (100%)	0	100	100
20	c	71/346 (20%)	68 (96%)	3 (4%)	30	57
21	o	256/413 (62%)	247 (96%)	9 (4%)	36	61
23	y	76/193 (39%)	74 (97%)	2 (3%)	46	68
24	b	70/176 (40%)	70 (100%)	0	100	100
25	d	69/89 (78%)	69 (100%)	0	100	100
26	e	65/83 (78%)	63 (97%)	2 (3%)	40	64
27	f	63/77 (82%)	63 (100%)	0	100	100
28	g	58/66 (88%)	57 (98%)	1 (2%)	60	77
29	h	77/129 (60%)	76 (99%)	1 (1%)	69	81
30	j	79/103 (77%)	79 (100%)	0	100	100
All	All	5127/9240 (56%)	4993 (97%)	134 (3%)	49	68

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	S	266	LEU
21	o	156	ARG
26	e	25	THR
8	H	193	SER
8	H	130	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
9	J	271	GLN
12	M	12	GLN
21	o	330	GLN
9	J	443	ASN
10	K	192	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	32/95 (33%)	14 (43%)	4 (12%)
2	E	15/20 (75%)	5 (33%)	1 (6%)
3	2	48/1175 (4%)	19 (39%)	2 (4%)
4	6	98/112 (87%)	37 (37%)	3 (3%)
5	5	138/179 (77%)	61 (44%)	3 (2%)
All	All	331/1581 (20%)	136 (41%)	13 (3%)

5 of 136 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	2	U
1	I	3	A
1	I	4	U
1	I	10	A
1	I	11	A

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	6	16	C
4	6	45	A
5	5	45	A
5	5	27	G
5	5	39	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	IHP	A	3001	-	36,36,36	0.71	0	54,60,60	1.08	4 (7%)
34	GTP	C	1101	-	26,34,34	0.83	1 (3%)	32,54,54	1.83	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	IHP	A	3001	-	-	0/30/54/54	0/1/1/1
34	GTP	C	1101	-	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	1101	GTP	C6-N1	-2.05	1.34	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	1101	GTP	PB-O3B-PG	-5.83	112.83	132.83
34	C	1101	GTP	PA-O3A-PB	-4.09	118.80	132.83
34	C	1101	GTP	C5-C6-N1	2.85	118.99	113.95
33	A	3001	IHP	C3-C2-C1	2.84	116.63	110.41
34	C	1101	GTP	O6-C6-C5	-2.50	119.49	124.37

There are no chirality outliers.

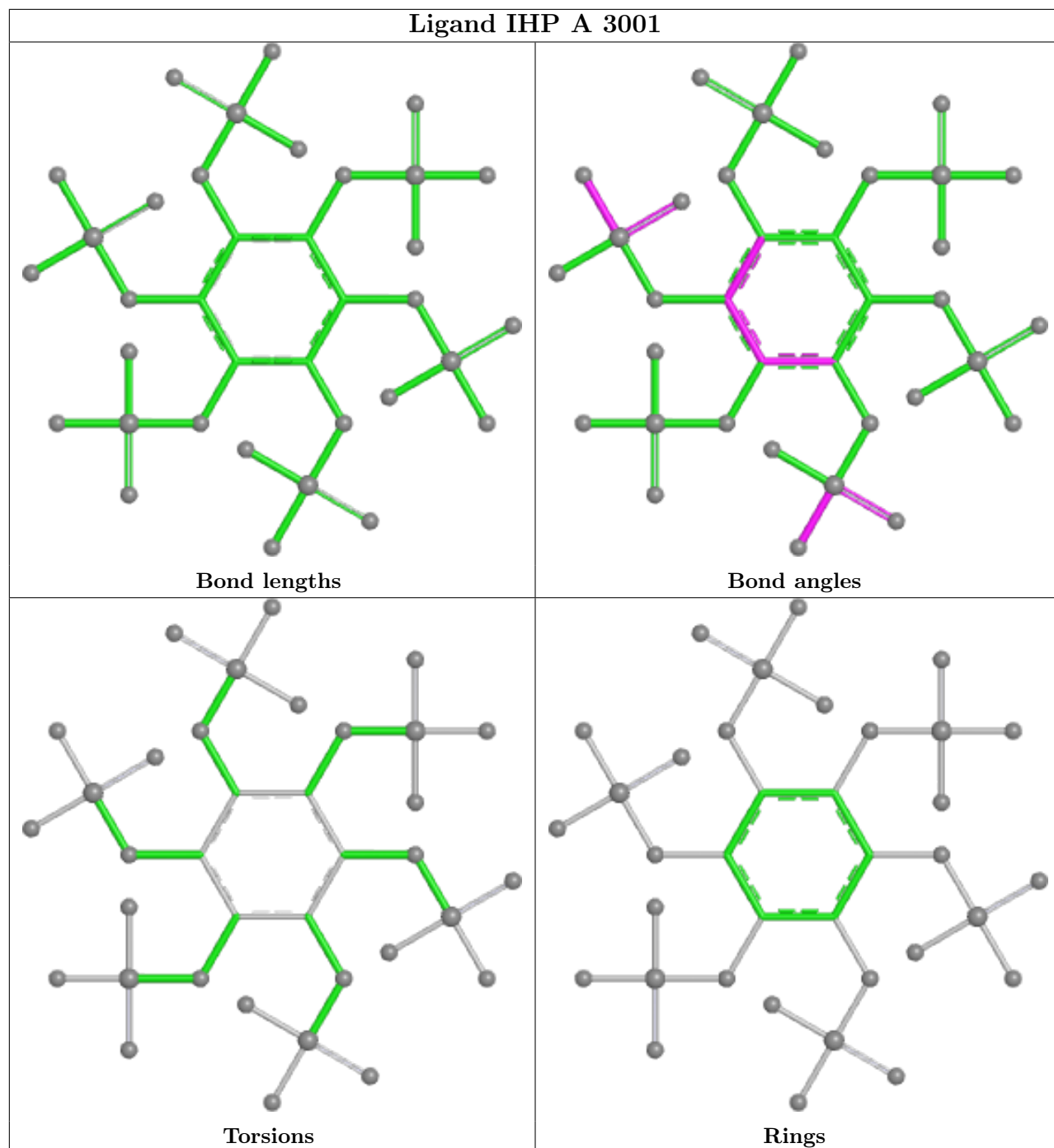
5 of 6 torsion outliers are listed below:

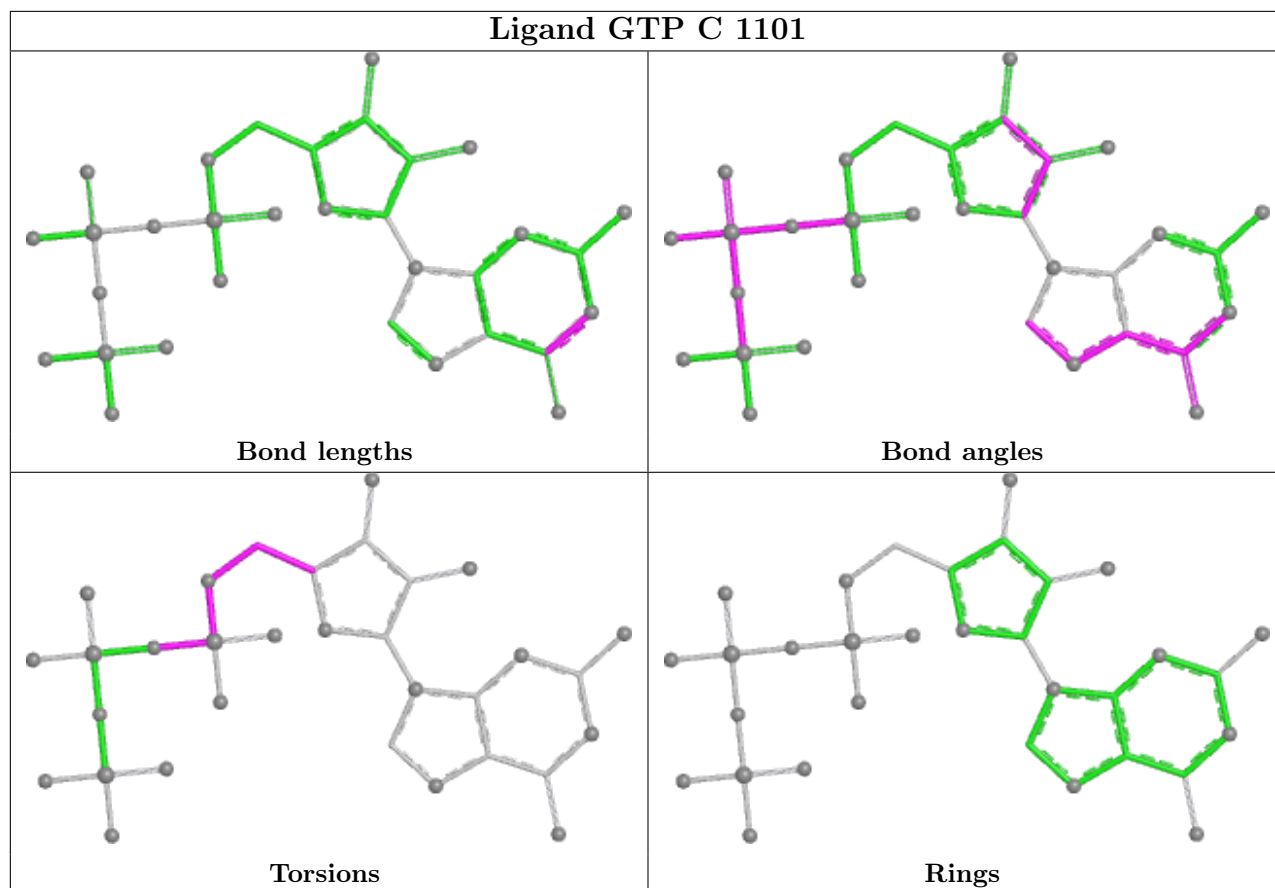
Mol	Chain	Res	Type	Atoms
34	C	1101	GTP	C5'-O5'-PA-O1A
34	C	1101	GTP	O4'-C4'-C5'-O5'
34	C	1101	GTP	C3'-C4'-C5'-O5'
34	C	1101	GTP	C4'-C5'-O5'-PA
34	C	1101	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	o	1
22	X	1
7	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	423:LYS	C	428:PRO	N	10.32
1	X	27:UNK	C	86:UNK	N	8.48
1	C	770:VAL	C	774:LEU	N	6.52

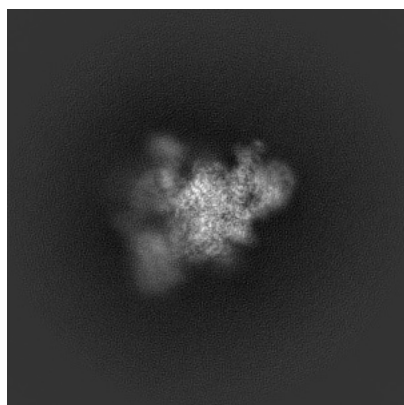
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3539. These allow visual inspection of the internal detail of the map and identification of artifacts.

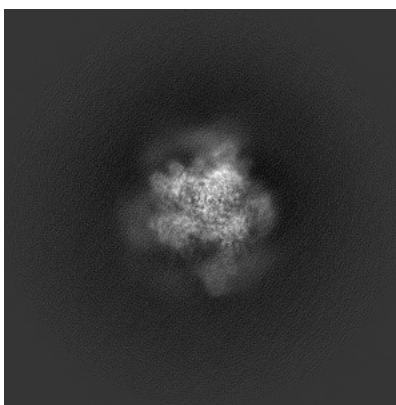
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

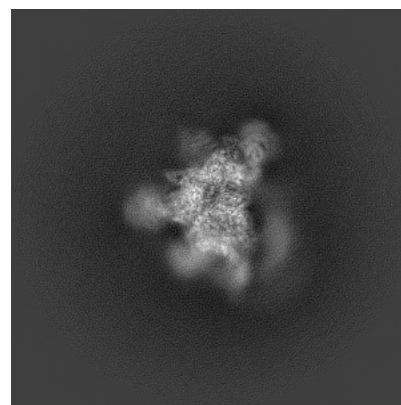
6.1.1 Primary map



X



Y

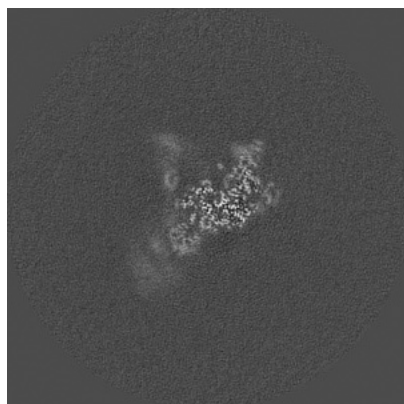


Z

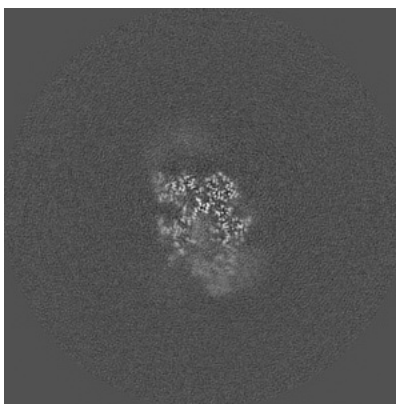
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

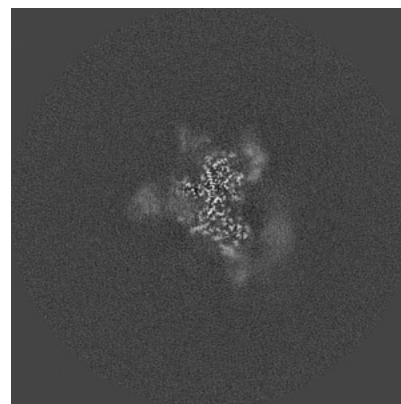
6.2.1 Primary map



X Index: 206



Y Index: 206

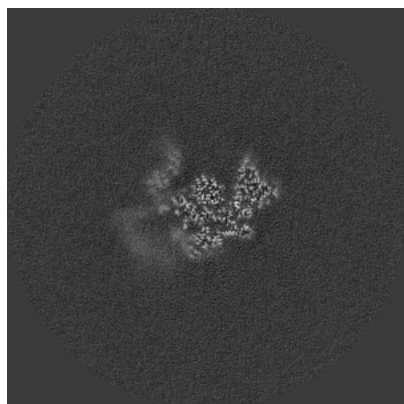


Z Index: 206

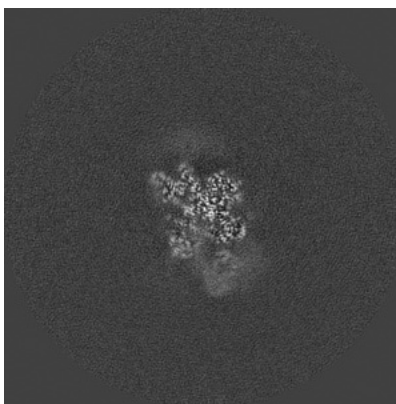
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

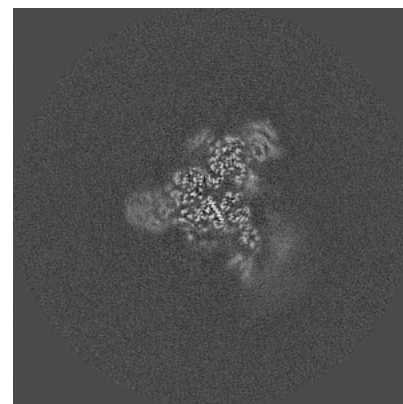
6.3.1 Primary map



X Index: 225



Y Index: 201



Z Index: 224

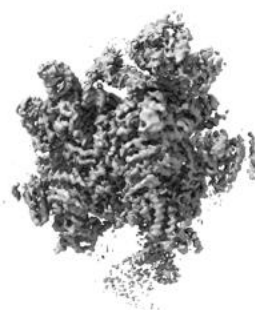
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

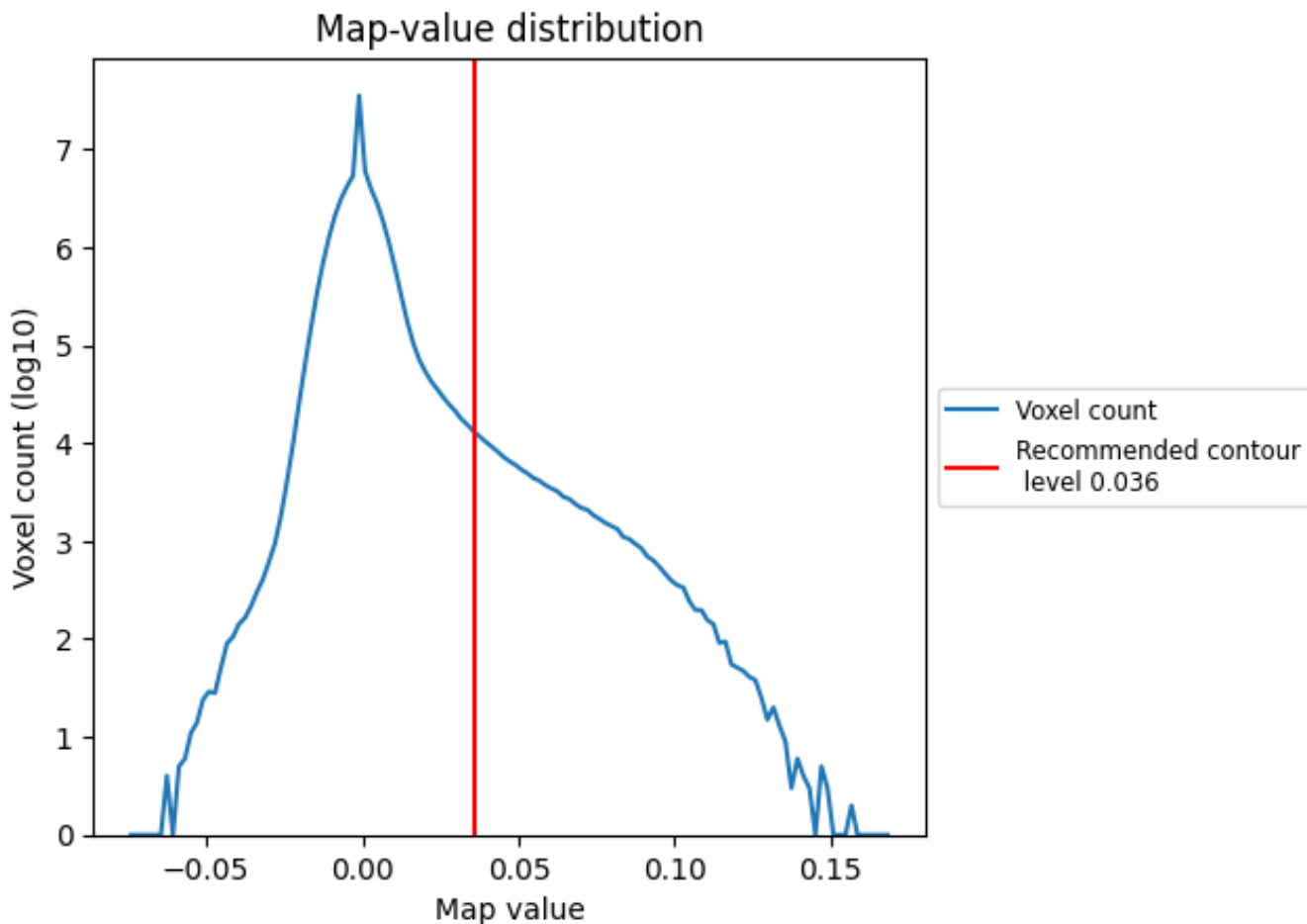
6.5 Mask visualisation

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

7 Map analysis [i](#)

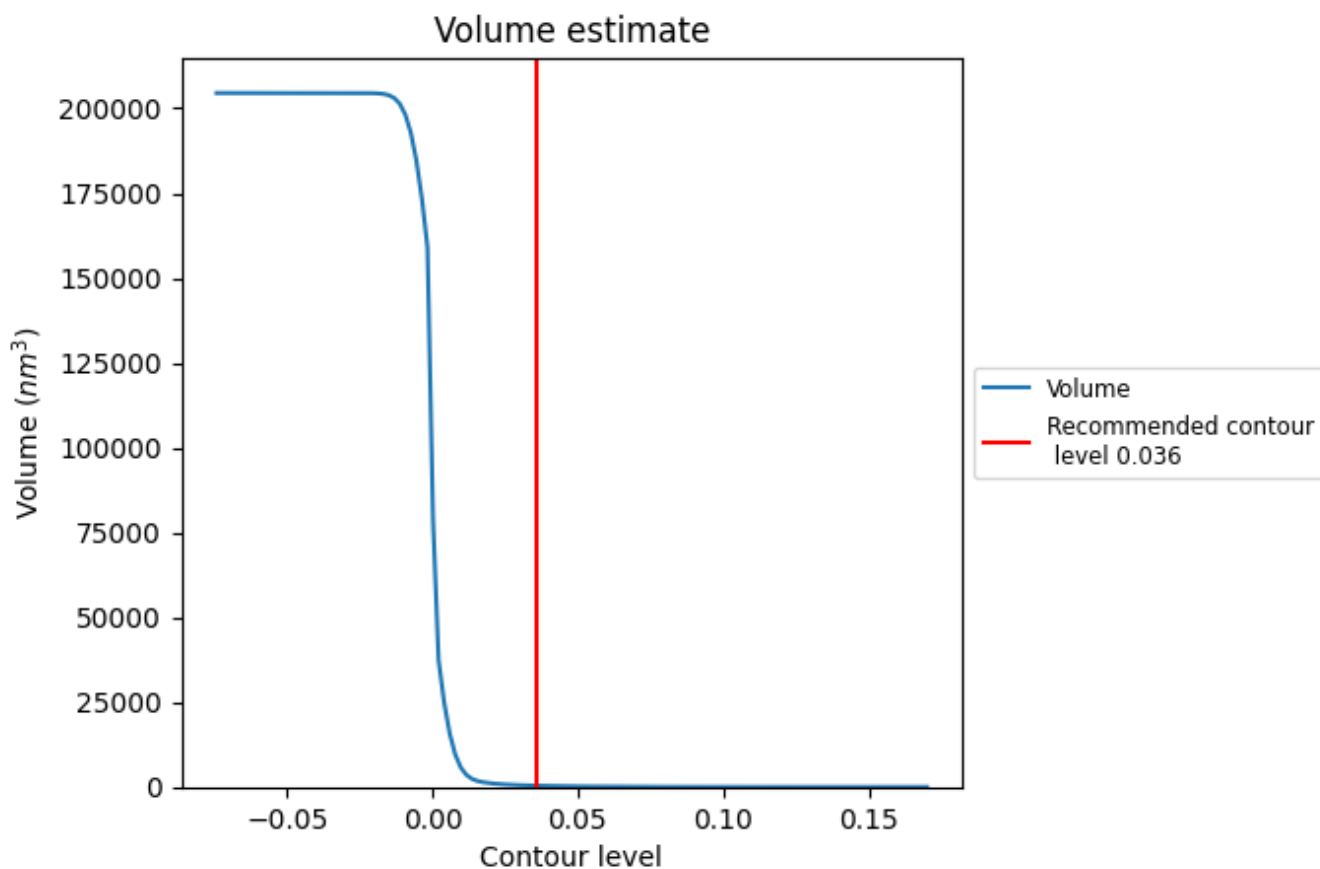
This section contains the results of statistical analysis of the map.

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.

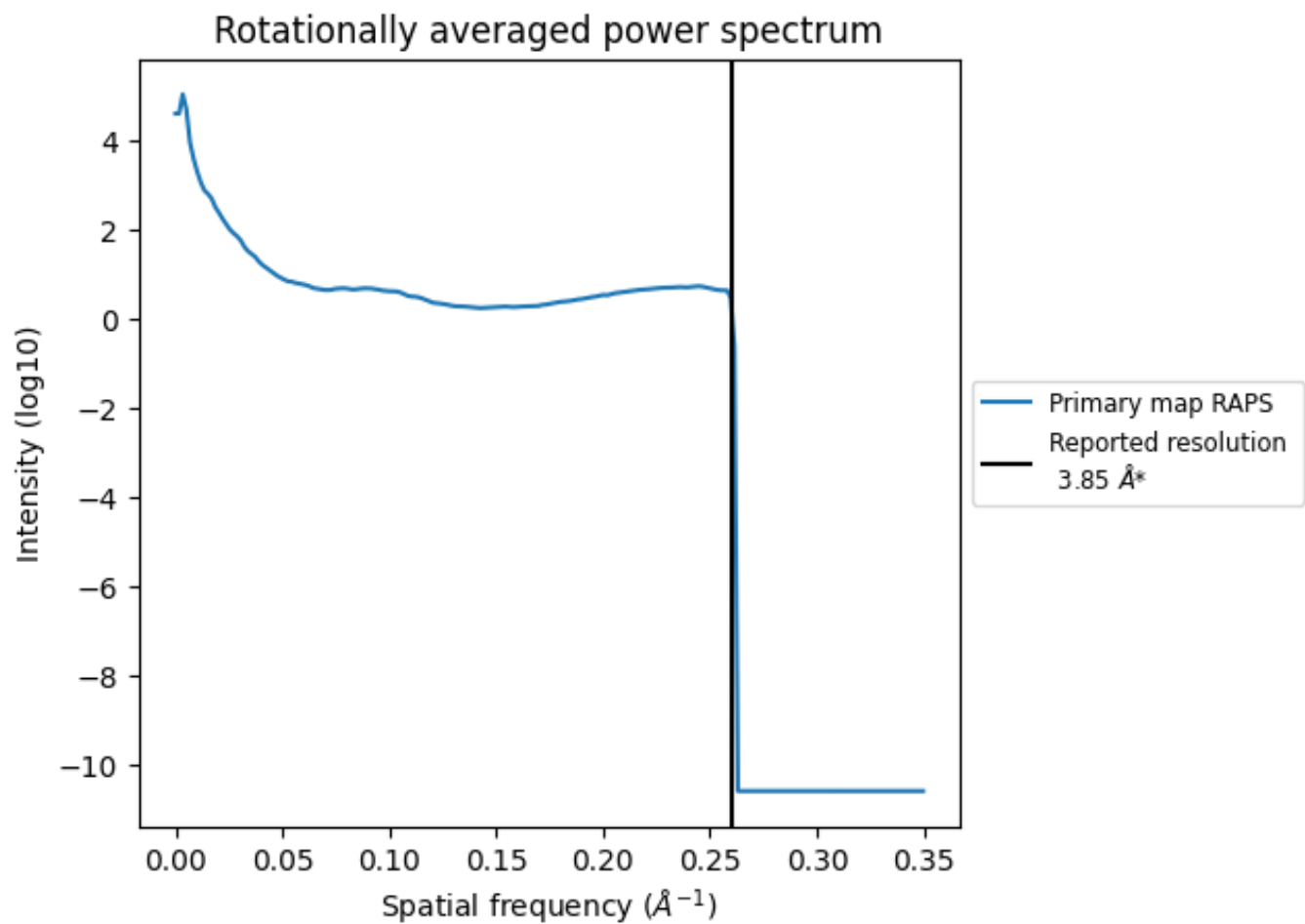
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 372 nm³; this corresponds to an approximate mass of 336 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 [\(i\)](#)

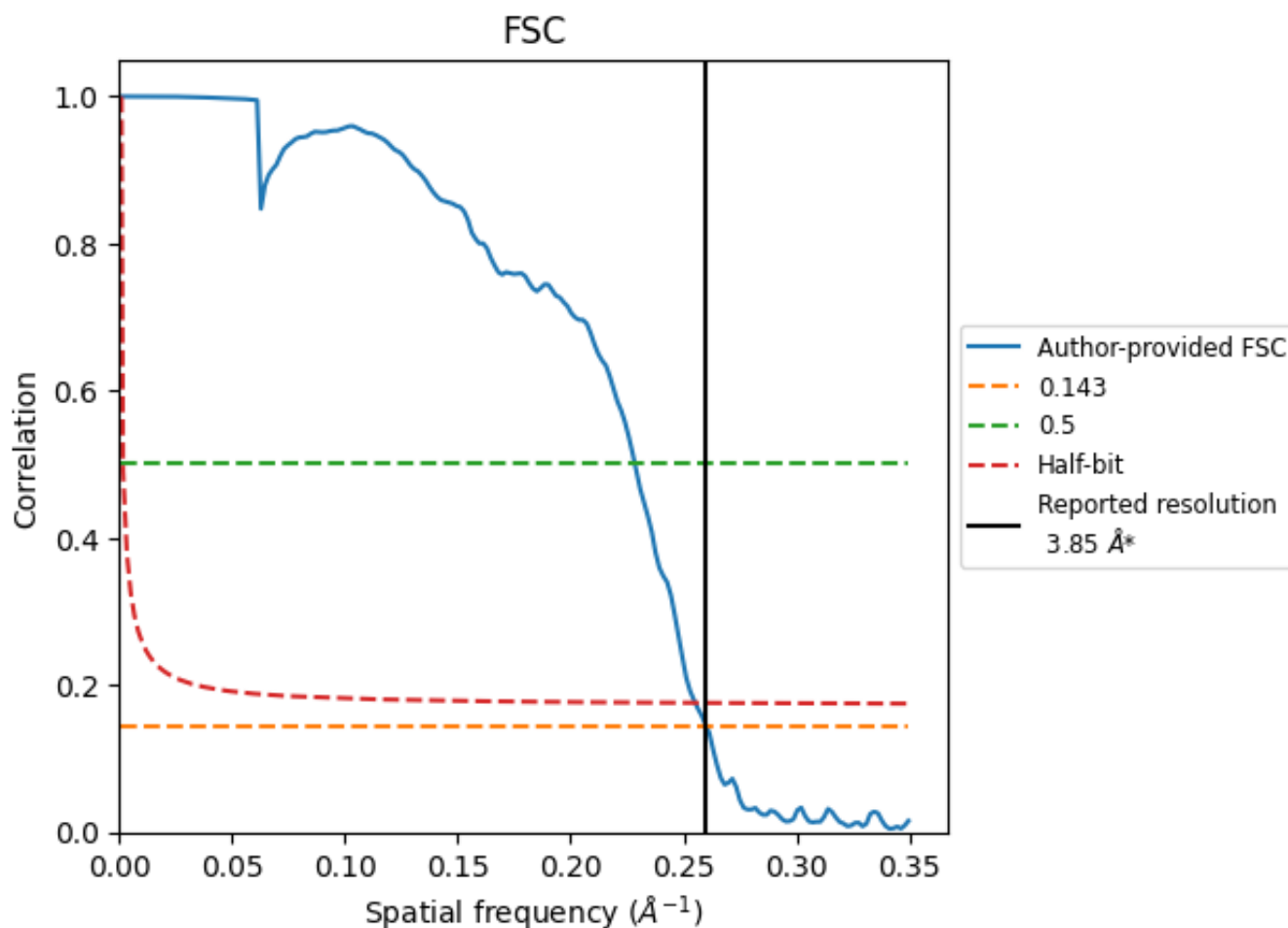


*Reported resolution corresponds to spatial frequency of 0.260 Å⁻¹

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 0.260 Å⁻¹

8.2 Resolution estimates [i](#)

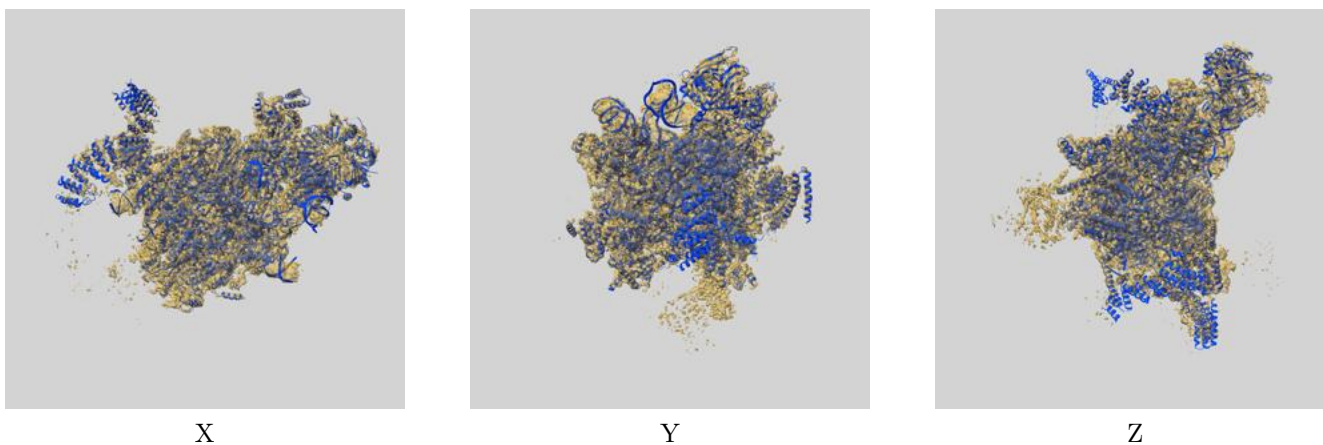
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	3.84	4.38	3.92
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

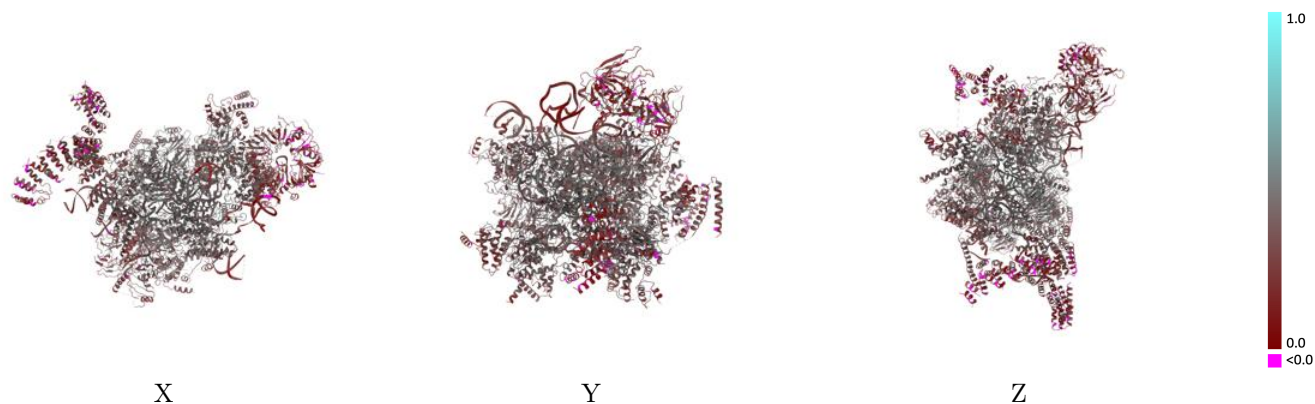
This section contains information regarding the fit between EMDB map EMD-3539 and PDB model 5MPS. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



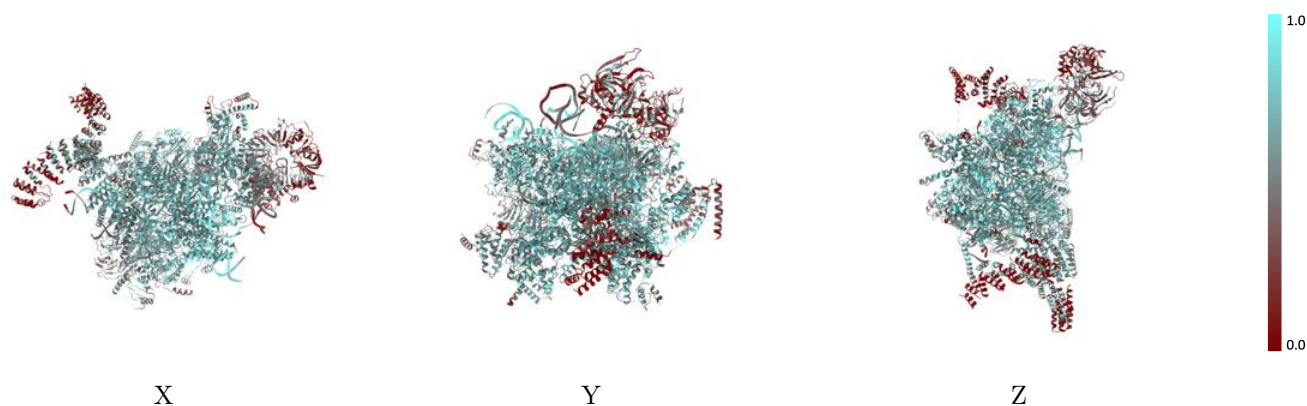
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



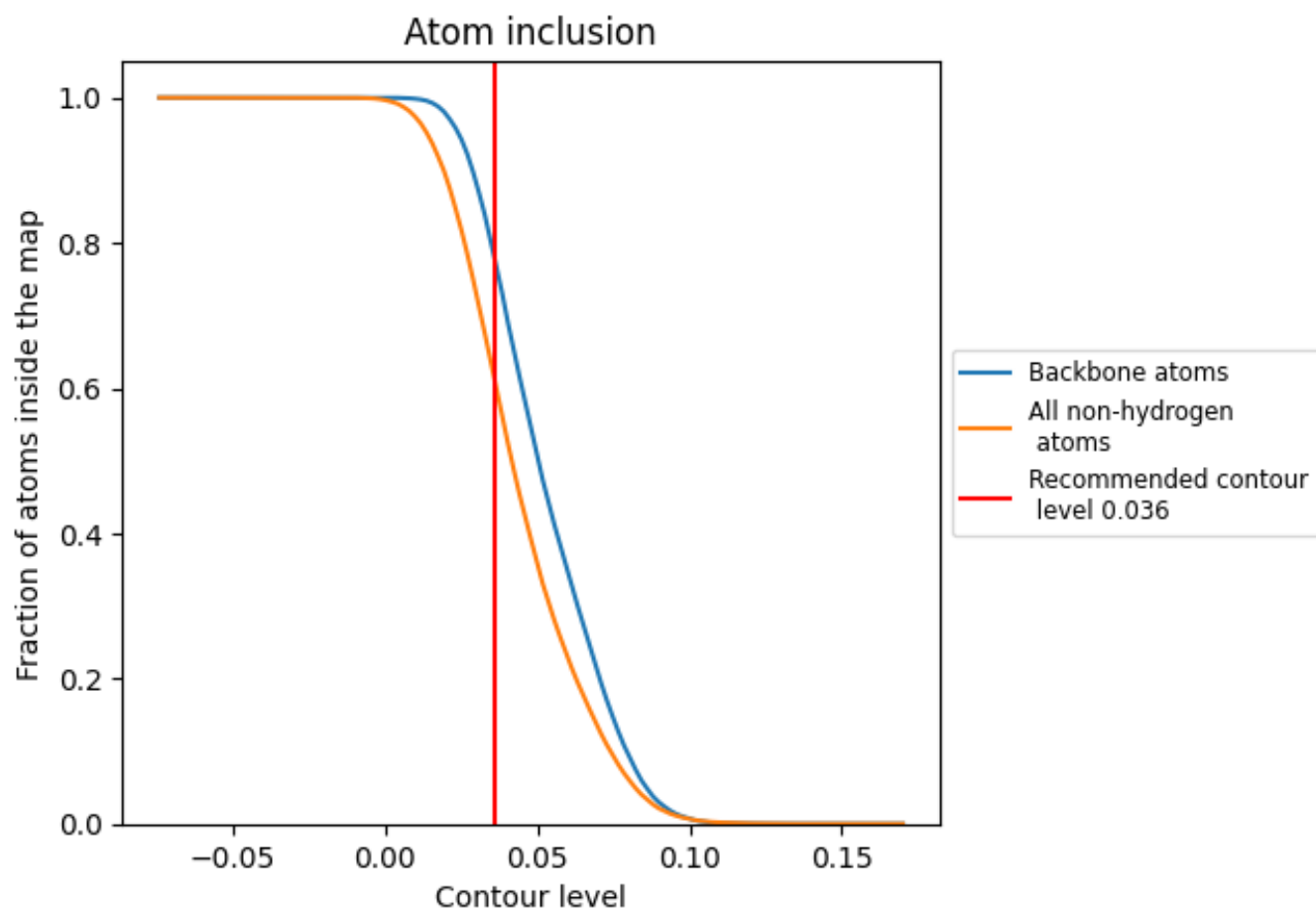
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 61% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6098	 0.3560
2	 0.6468	 0.3100
5	 0.7209	 0.3090
6	 0.8348	 0.3890
A	 0.7022	 0.4130
C	 0.6745	 0.3940
E	 0.6936	 0.4080
H	 0.3798	 0.2640
I	 0.6218	 0.3090
J	 0.7020	 0.4300
K	 0.5730	 0.3780
L	 0.7678	 0.4020
M	 0.6650	 0.3780
N	 0.6016	 0.3560
O	 0.6169	 0.3700
P	 0.6410	 0.4360
R	 0.4276	 0.3020
S	 0.4935	 0.3020
T	 0.3990	 0.2400
X	 0.5503	 0.3240
a	 0.5260	 0.2860
b	 0.4279	 0.2850
c	 0.5477	 0.3150
d	 0.4871	 0.3460
e	 0.2063	 0.1840
f	 0.2402	 0.1840
g	 0.3455	 0.2640
h	 0.3491	 0.2450
j	 0.2058	 0.1900
o	 0.5177	 0.3300
y	 0.6111	 0.3410

