



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 08:28 PM UTC

PDB ID : 5LJ3 / pdb_00005lj3
EMDB ID : EMD-4055
Title : Structure of the core of the yeast spliceosome immediately after branching
Authors : Galej, W.P.; Wilkinson, M.F.; Fica, S.M.; Oubridge, C.; Newman, A.J.; Nagai, K.
Deposited on : 2016-07-17
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

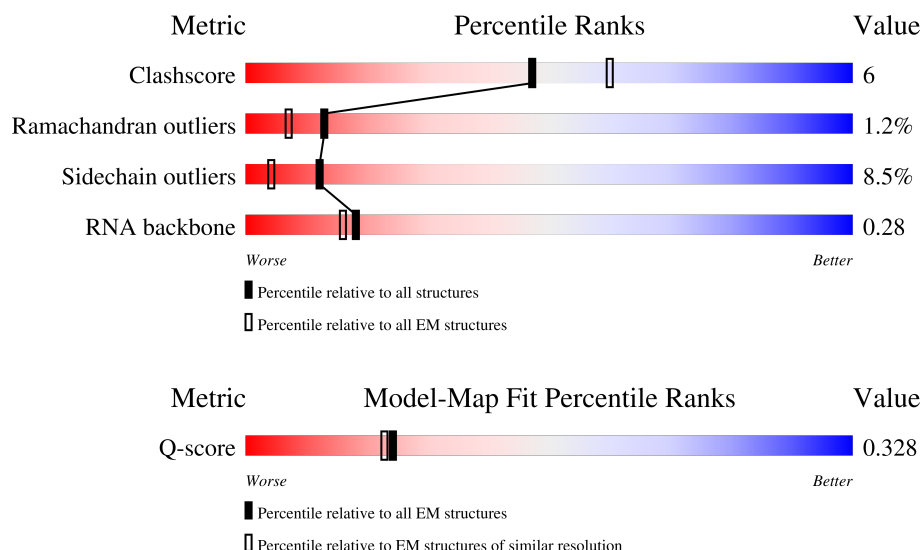
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



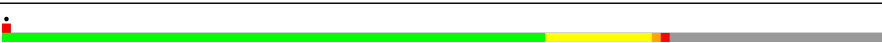
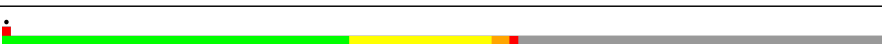
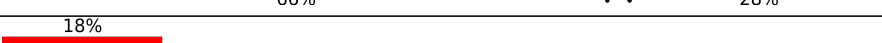
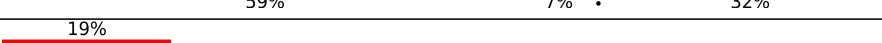
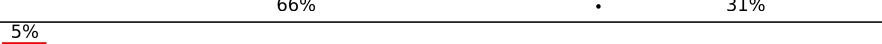
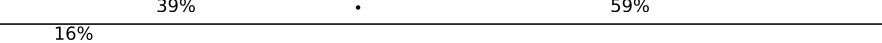
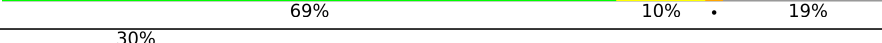
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	U	179	
2	E	16	
3	I	76	

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Mol	Chain	Length	Quality of chain
4	Z	1175	
5	V	112	
6	A	2413	
7	D	278	
8	F	179	
9	C	1008	
10	G	235	
11	H	591	
12	J	451	
13	K	379	
14	L	157	
15	M	339	
16	N	364	
17	O	590	
18	P	175	
19	R	135	
20	S	687	
21	T	859	
22	b	196	
22	k	196	
23	d	101	
23	n	101	
24	e	94	
24	p	94	
25	f	86	

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Mol	Chain	Length	Quality of chain
25	q	86	
26	g	77	
26	r	77	
27	h	146	
27	l	146	
28	j	110	
28	m	110	
29	W	238	
30	Y	111	
31	x	132	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	ZN	N	401	-	-	X	-
33	ZN	N	402	-	-	X	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 63161 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 U5 snRNA (small nuclear RNA).

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

- Molecule 2 is a RNA chain called Exon 1 (5' exon) of UBC4 pre-mRNA.

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

- Molecule 3 is a RNA chain called Intron of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	33	Total	C	N	O	P	0	0
			693	312	116	232	33		

- Molecule 4 is a RNA chain called U2 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	171	Total	C	N	O	P	0	0
			3610	1614	604	1221	171		

- Molecule 5 is a RNA chain called U6 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	97	Total	C	N	O	P	0	0
			2066	925	368	676	97		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1922	Total	C	N	O	S	0	0
			15704	10112	2720	2814	58		

- Molecule 7 is a protein called Protein CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	114	Total	C	N	O	S	0	0
			912	577	165	162	8		

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC25.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	F	46	Total	C	N	O	0	0
			321	203	61	57		

- Molecule 9 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	882	Total	C	N	O	S	0	0
			6756	4393	1133	1203	27		

- Molecule 10 is a protein called ISY1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	97	Total	C	N	O	S	0	0
			823	513	154	155	1		

- Molecule 11 is a protein called CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	399	Total	C	N	O	S	0	0
			2639	1657	468	506	8		

- Molecule 12 is a protein called PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	326	Total	C	N	O	S	0	0
			2556	1616	454	476	10		

- Molecule 13 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	163	Total	C	N	O	S	0	0
			1289	808	236	240	5		

- Molecule 14 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	155	Total	C	N	O	S	0	0
			1270	797	238	225	10		

- Molecule 15 is a protein called CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	252	Total	C	N	O	S	0	0
			2010	1275	354	370	11		

- Molecule 16 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	209	Total	C	N	O	S	0	0
			1658	1055	287	301	15		

- Molecule 17 is a protein called CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	198	Total	C	N	O	S	0	0
			1645	1032	300	307	6		

- Molecule 18 is a protein called CWC15.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	36	Total	C	N	O	0	0
			275	176	53	46		

- Molecule 19 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	R	97	Total	C	N	O	0	0
			550	328	109	113		

- Molecule 20 is a protein called CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	464	Total	C	N	O	S	0	0
			3120	1948	581	584	7		

- Molecule 21 is a protein called SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	592	Total	C	N	O	0	0
			2946	1762	592	592		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
22	k	80	Total	C	N	O		0	0
			396	236	80	80			

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
23	n	82	Total	C	N	O		0	0
			404	240	82	82			

- Molecule 24 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
24	p	75	Total	C	N	O		0	0
			369	219	75	75			

- Molecule 25 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
25	q	72	Total	C	N	O		0	0
			354	210	72	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
26	r	69	Total	C	N	O		0	0
			340	202	69	69			

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
27	l	79	Total	C	N	O		0	0
			392	234	79	79			

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
28	m	94	Total	C	N	O		0	0
			467	279	94	94			

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	W	164	Total	C	N	O	0	0
			816	488	164	164		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Y	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 31 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	x	132	Total	C	N	O	0	0
			660	396	132	132		

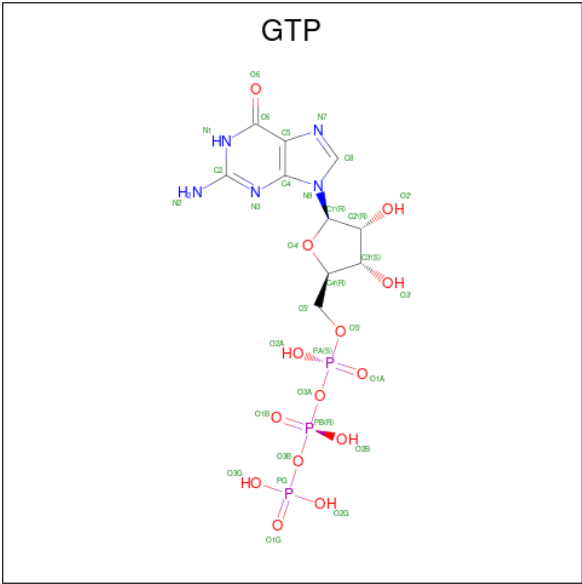
- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	E	1	Total	Mg	0
			1	1	
32	V	1	Total	Mg	0
			1	1	

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

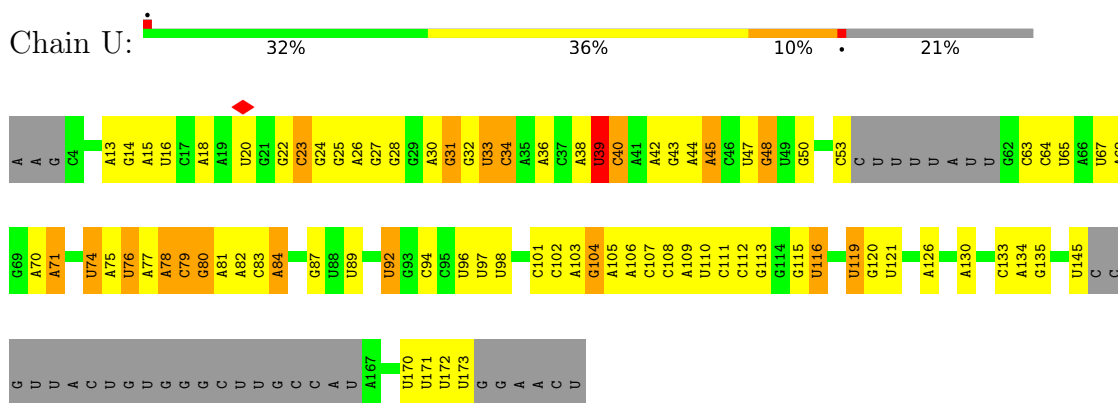
- Molecule 34 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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.

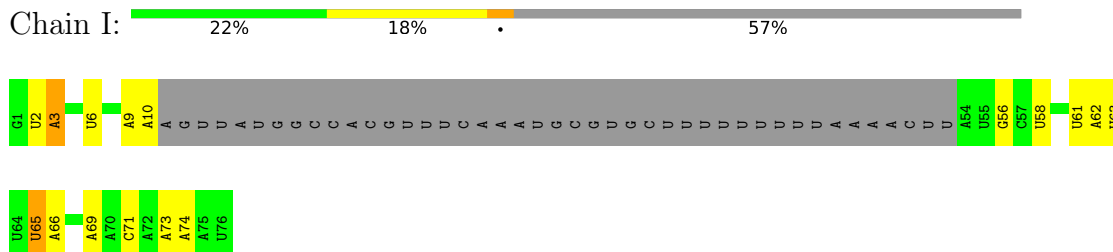
- Molecule 1: U5 snRNA (small nuclear RNA)



- Molecule 2: Exon 1 (5' exon) of UBC4 pre-mRNA

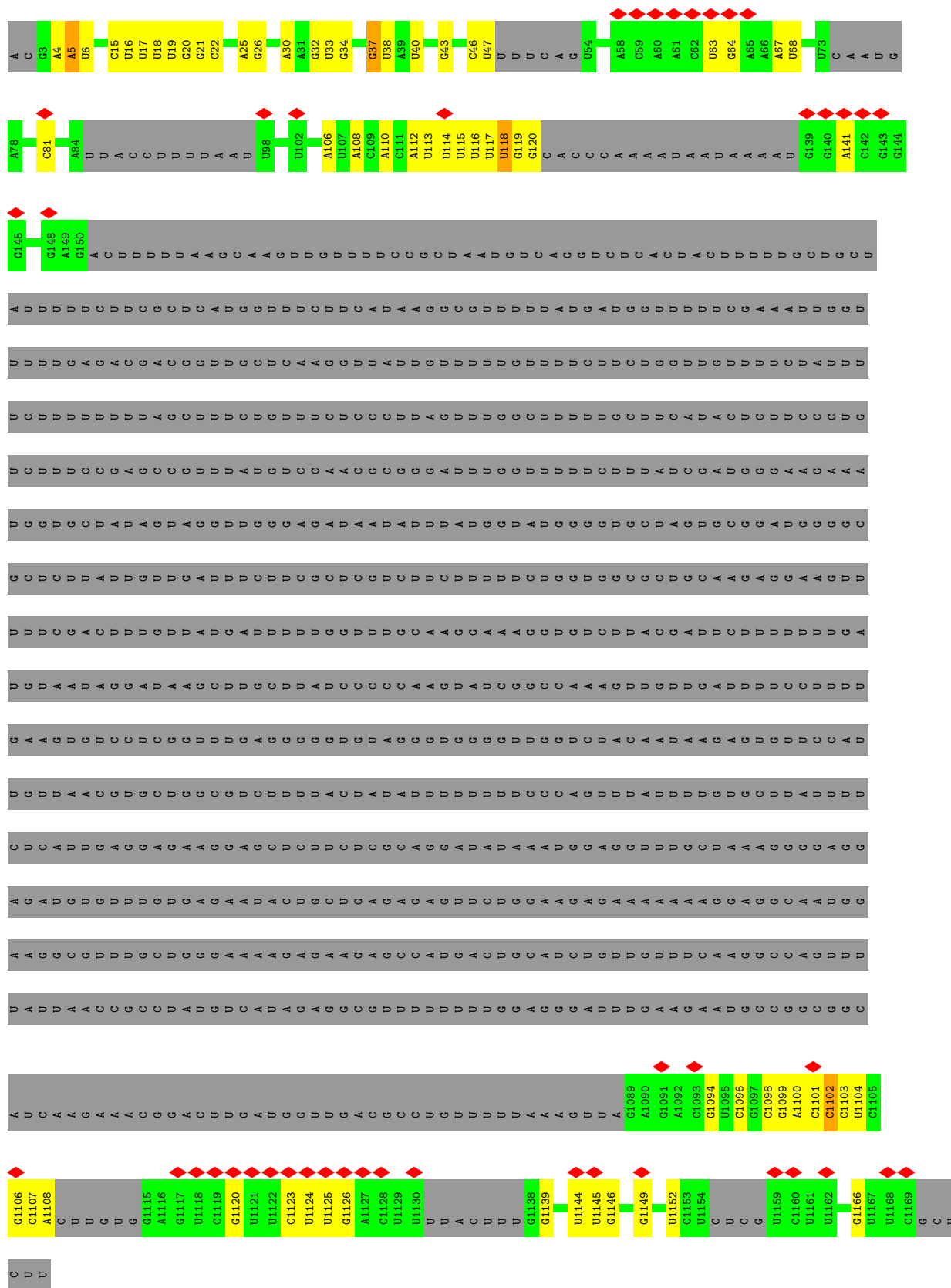


- Molecule 3: Intron of UBC4 pre-mRNA

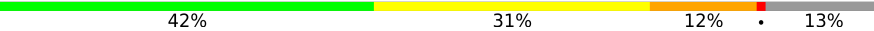


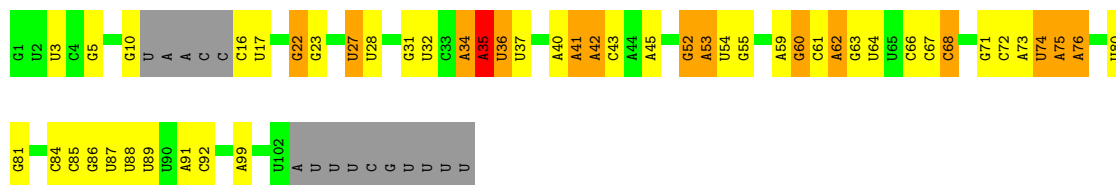
- Molecule 4: U2 snRNA (small nuclear RNA)





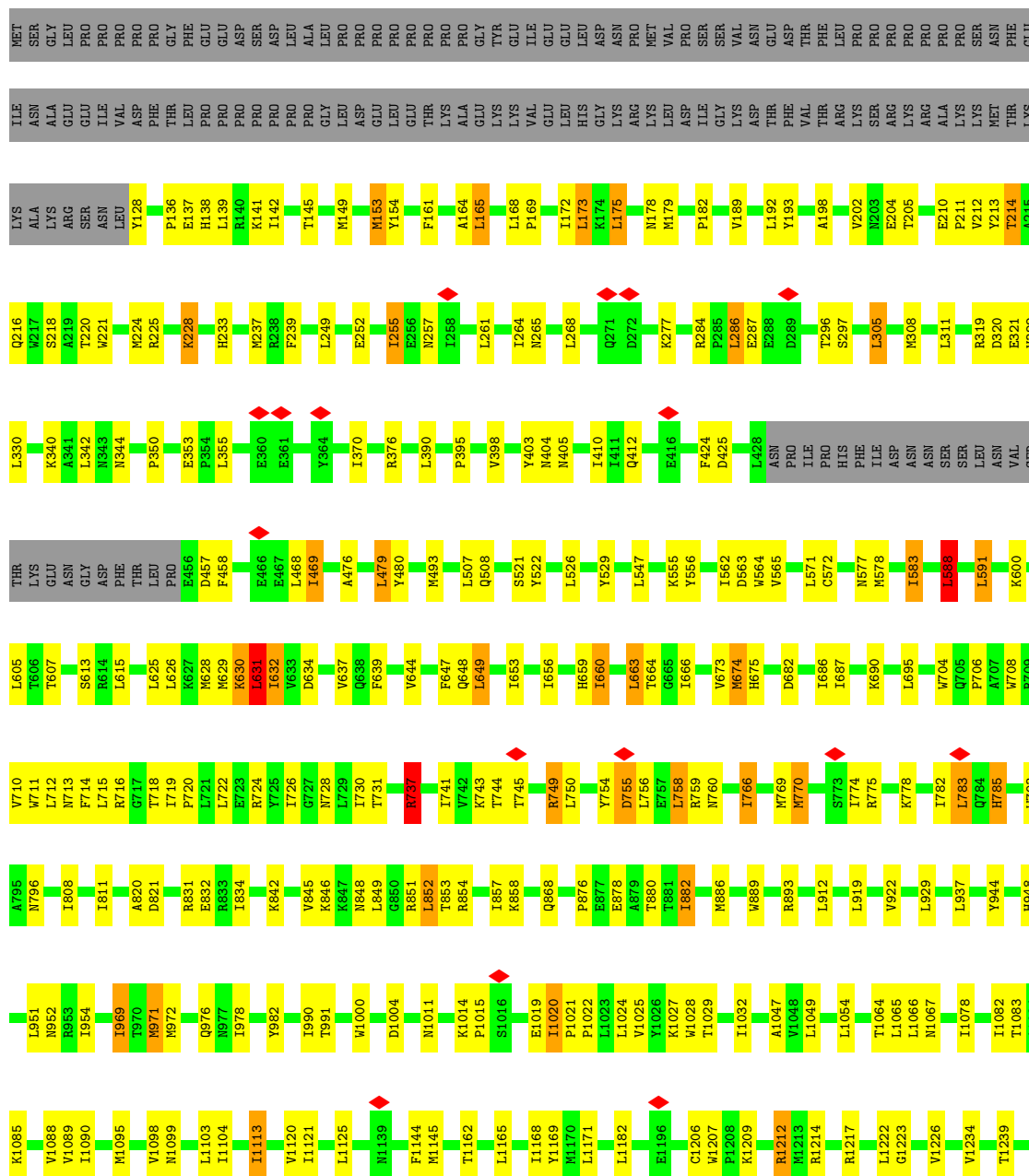
- Molecule 5: U6 snRNA (small nuclear RNA)

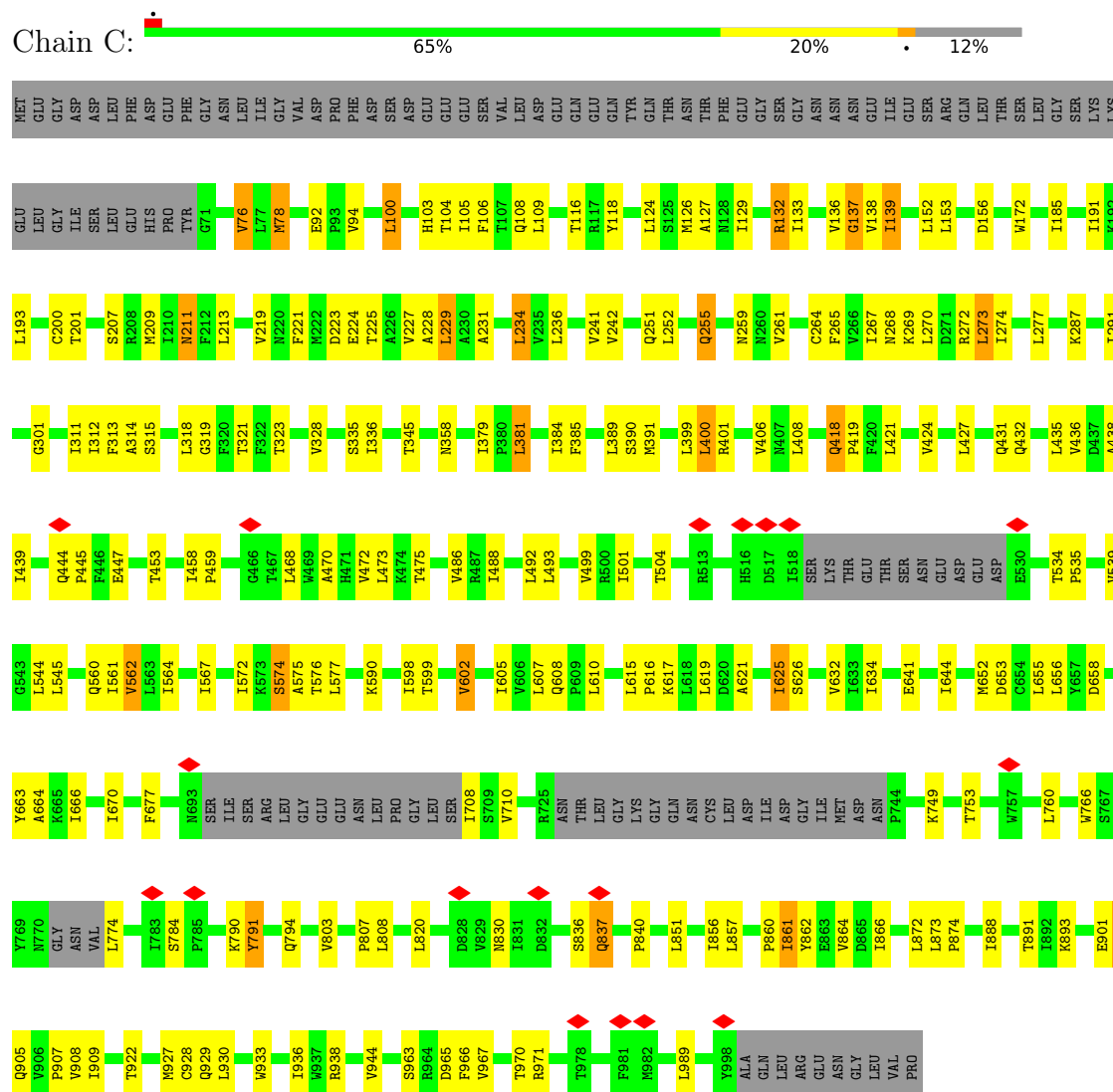
Chain V:  42% 31% 12% 13%



• Molecule 6: Pre-mRNA-splicing factor 8

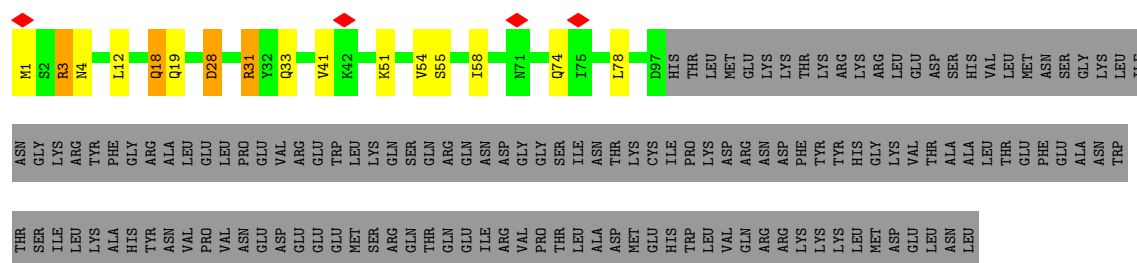
Chain A:  61% 16% 20%



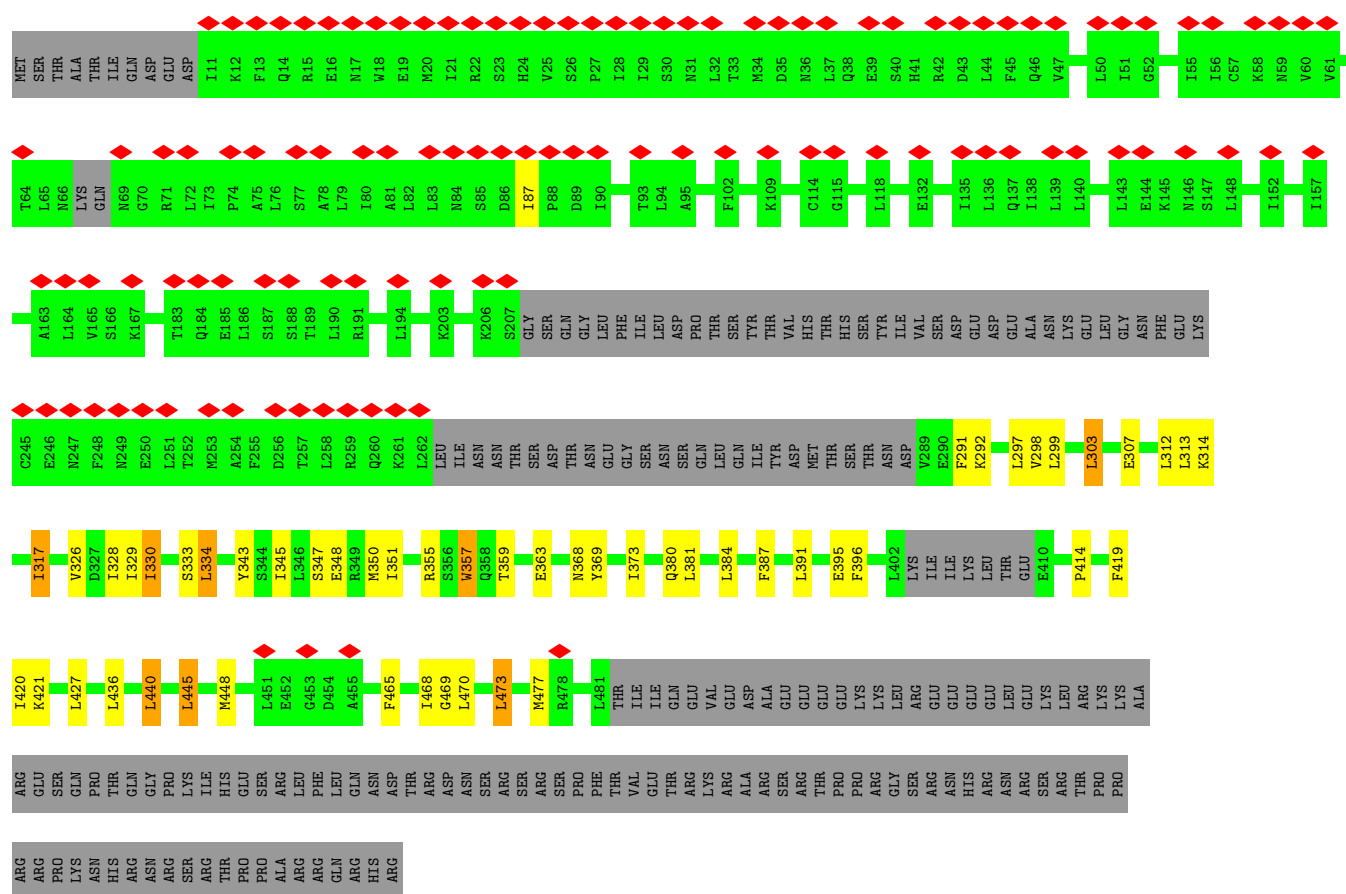


- Molecule 10: ISY1

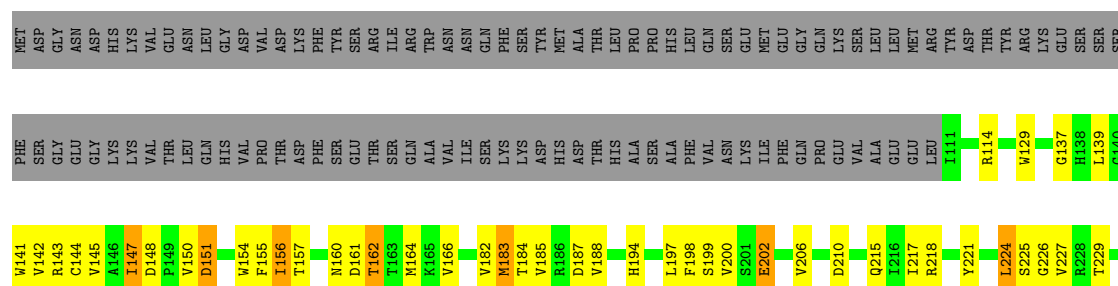


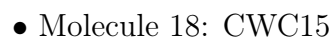


• Molecule 11: CWC22



• Molecule 12: PRP46





ILE	LYS	GLY	GLU	HIS	ALA	THR	LYS	LYS	LYS	SER	SER	ALA	ALA	SER	LEU	GLN	TYR	ILE	ASN	ASP	VAL	THR	MET	THR	SER	SER	GLU	TYR	HIS	GLN	GLU	PHE	LEU	HIS	LYS	HIS	VAL	ARG						
THR	ARG	SER	GLU	LYS	ASP	GLN	LYS	LEU	SER	LEU	GLN	GLU	LEU	VAL	THR	GLN	LYS	ASN	LYS	VAL	ASP	GLU	ASP	GLU	LYS	GLY	GLU	GLN	GLN	GLY	GLU	ALA	ASN	GLY	GLY	ASN	LEU	GLN						
MET	THR	HIS	SER	ARG	P7	Q8	L9	R12	K16	R29	L30	L31	F42	LYS	GLU	GLU	GLU	ASN	LYS	ALA	ASN	CYS	ALA	GLN	GLU	ASP	ASN	ASN	LYS	LEU	GLU	VAL	VAL	ASN	GLU	LYS	ASP	VAL	GLY	SER	GLY	ASN	LEU	GLN

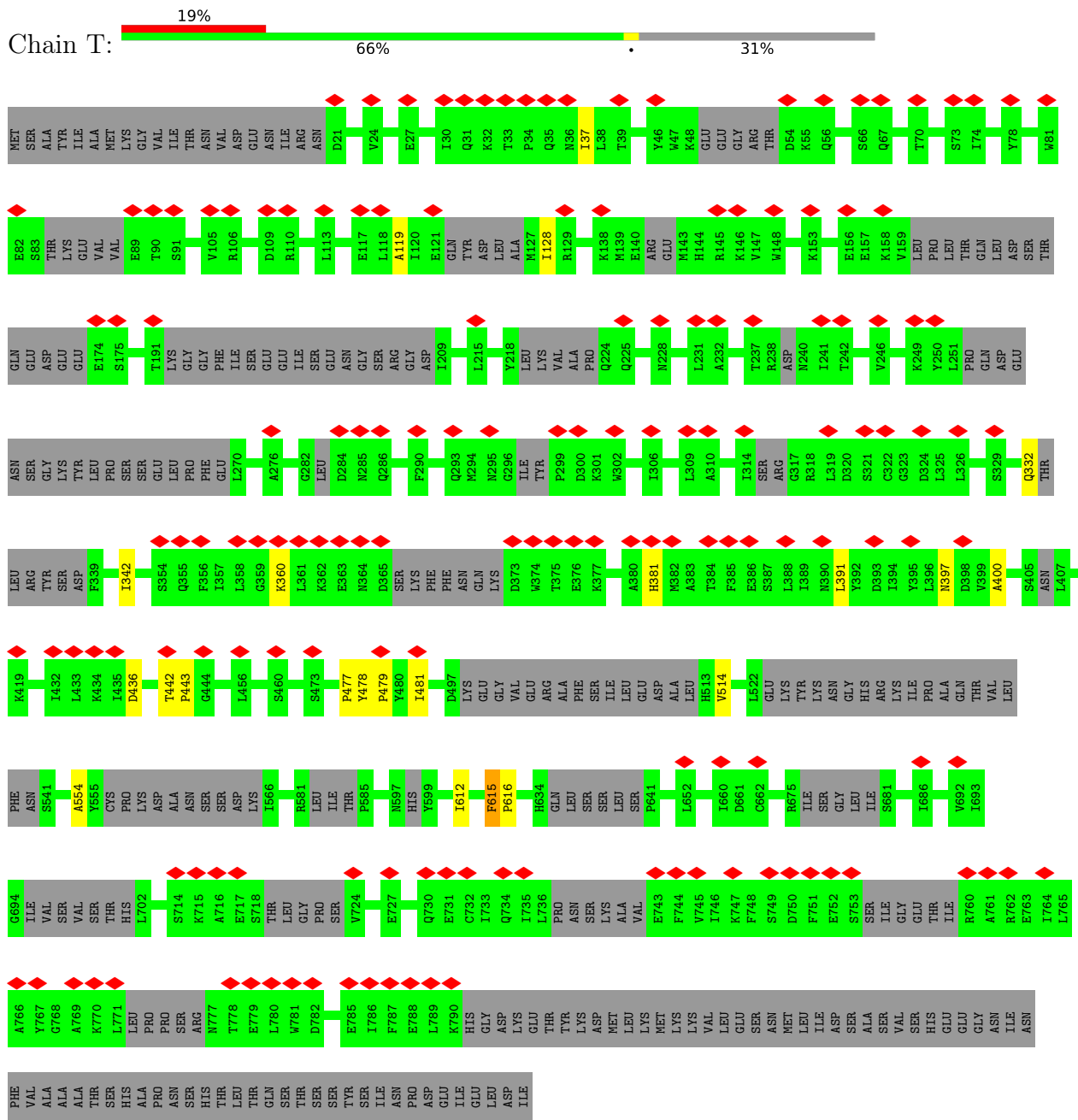
Chain R:

Figure 1: Schematic representation of the protein structure of the human Hsp70 protein. The protein is shown as a linear sequence of amino acids. The N-terminal region (residues 1-16) is highlighted in green. The C-terminal region (residues 164-211) is highlighted in green. The middle region (residues 17-163) is highlighted in grey. Red diamonds indicate the positions of the 16 amino acid substitutions. The substitutions are: S2, I6, G7, L8, K12, G13, S14, S15, T16, R29, R30, R31, P32, Q33, Q34, S35, Q36, Q37, Q38, R39, Q40, Q41, I46, S50, H51, A52, L53, S54, S55, P56, L57, L58, L59, A60, V61, G62, L63, L64, I65, R66, E67, S68, K69, A70, Q71, G72, G73, G74.

Chain S:

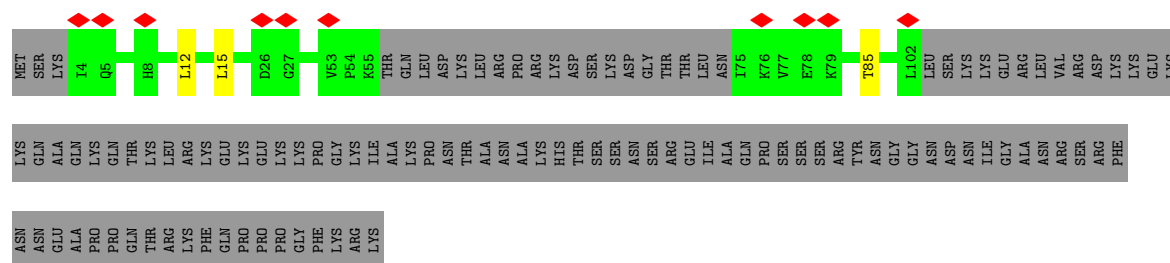
[illegible]

- Molecule 21: SYF1

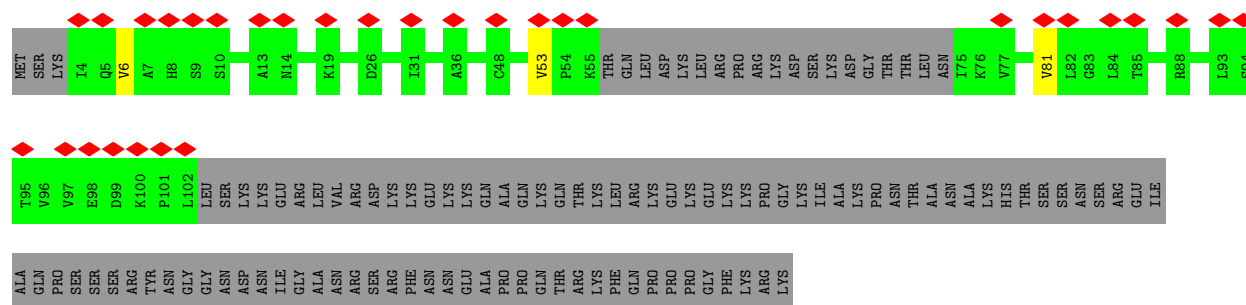


- Molecule 22: Small nuclear ribonucleoprotein-associated protein B

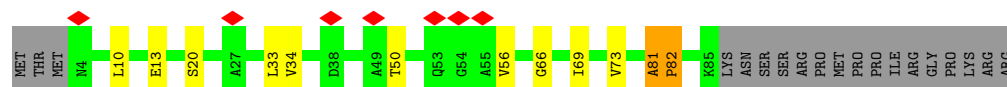




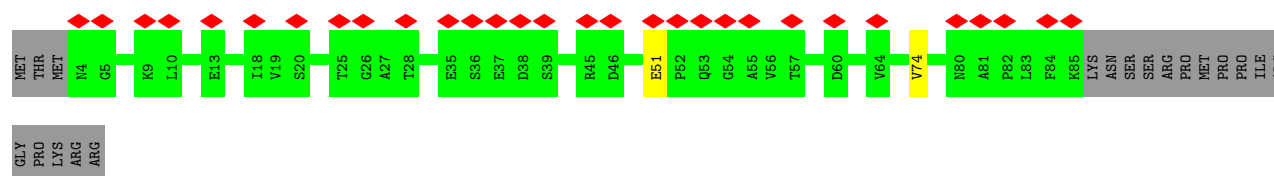
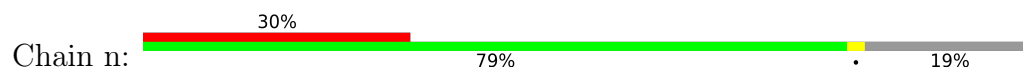
• Molecule 22: Small nuclear ribonucleoprotein-associated protein B



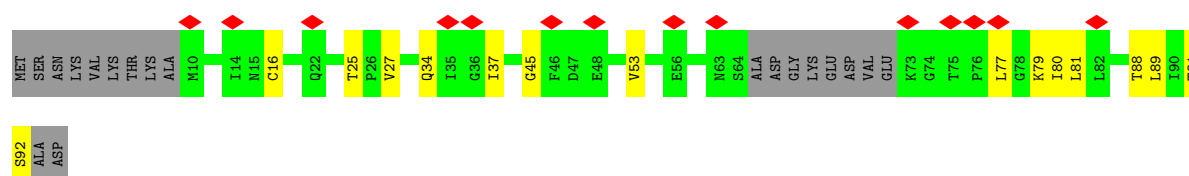
• Molecule 23: Small nuclear ribonucleoprotein Sm D3



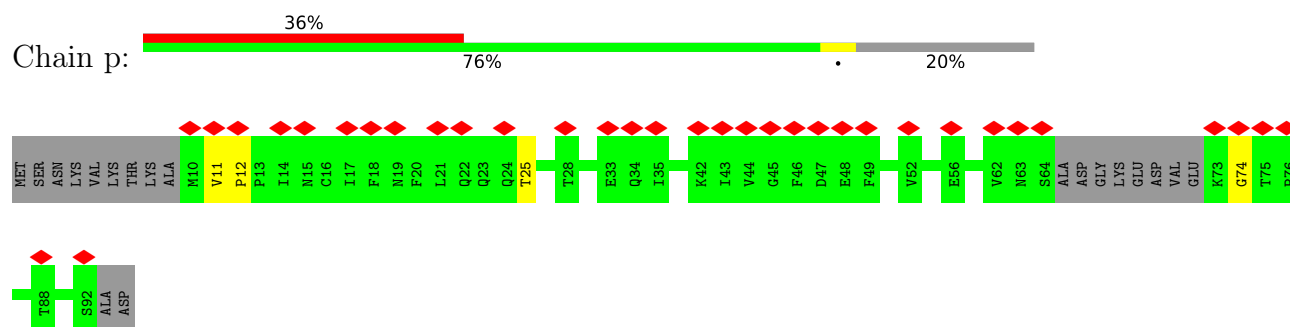
• Molecule 23: Small nuclear ribonucleoprotein Sm D3



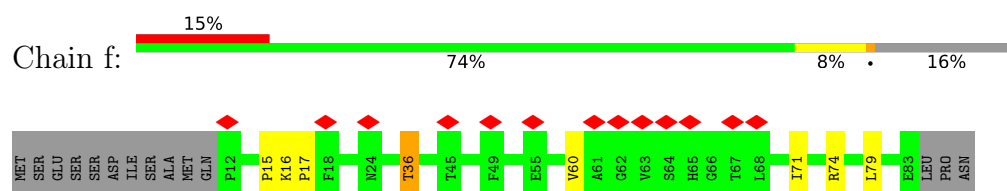
• Molecule 24: Small nuclear ribonucleoprotein E



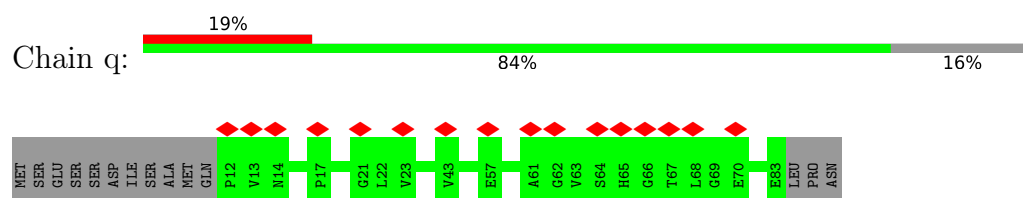
- Molecule 24: Small nuclear ribonucleoprotein E



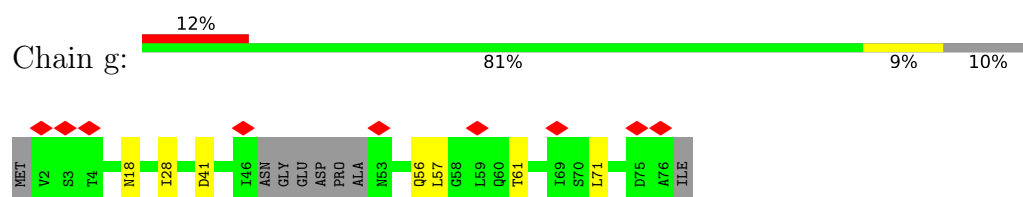
- Molecule 25: Small nuclear ribonucleoprotein F



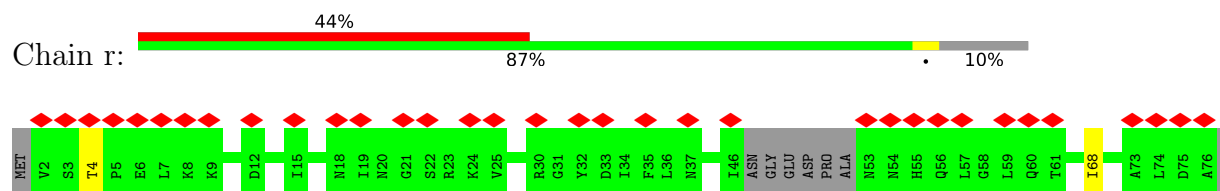
- Molecule 25: Small nuclear ribonucleoprotein F



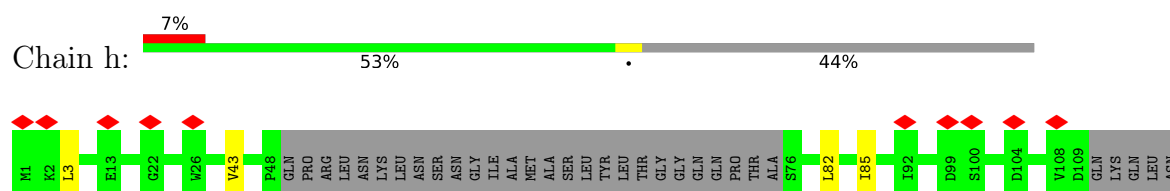
- Molecule 26: Small nuclear ribonucleoprotein G

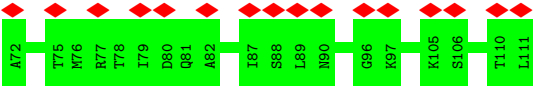
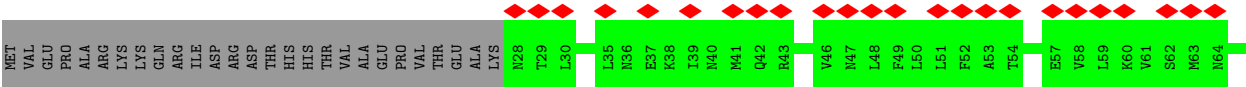


- Molecule 26: Small nuclear ribonucleoprotein G



- Molecule 27: Small nuclear ribonucleoprotein Sm D1





• Molecule 31: unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93106	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)	4000	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.091	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.027	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 ⓘ

5.1 Standard geometry ⓘ

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

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	U	0.41	0/3351	0.88	5/5213 (0.1%)
2	E	0.42	0/388	0.80	1/603 (0.2%)
3	I	0.40	0/772	0.81	1/1195 (0.1%)
4	Z	0.40	0/4018	0.76	1/6233 (0.0%)
5	V	0.40	0/2309	0.85	7/3590 (0.2%)
6	A	0.55	1/16107 (0.0%)	1.05	26/21845 (0.1%)
7	D	0.49	0/929	0.81	0/1243
8	F	0.53	0/325	1.20	0/442
9	C	0.55	0/6902	1.02	7/9386 (0.1%)
10	G	0.52	0/839	1.10	0/1126
11	H	0.55	0/2667	1.35	4/3630 (0.1%)
12	J	0.59	0/2613	0.88	2/3551 (0.1%)
13	K	0.53	0/1308	1.05	4/1765 (0.2%)
14	L	0.52	0/1294	1.05	2/1732 (0.1%)
15	M	0.52	0/2056	0.97	2/2766 (0.1%)
16	N	0.55	0/1680	1.03	2/2258 (0.1%)
17	O	0.55	0/1669	1.14	1/2236 (0.0%)
18	P	0.61	0/282	0.88	1/380 (0.3%)
19	R	0.52	0/550	1.29	1/752 (0.1%)
20	S	0.53	0/3154	1.32	2/4297 (0.0%)
21	T	0.48	0/2916	1.48	10/4026 (0.2%)
22	b	0.53	0/636	0.71	0/856
22	k	0.49	0/394	0.99	2/546 (0.4%)
23	d	0.53	0/634	0.88	2/859 (0.2%)
23	n	0.48	0/403	1.14	4/559 (0.7%)
24	e	0.61	0/585	0.84	0/795
24	p	0.49	0/367	1.28	6/507 (1.2%)
25	f	0.57	0/585	0.85	0/791
25	q	0.50	0/353	1.01	0/489
26	g	0.55	0/532	0.76	0/715
26	r	0.48	0/338	0.90	2/467 (0.4%)
27	h	0.50	0/649	0.77	0/880

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	l	0.52	0/390	1.23	4/541 (0.7%)
28	j	0.55	0/753	0.89	0/1013
28	m	0.50	0/466	1.18	4/649 (0.6%)
29	W	0.50	0/814	1.18	10/1134 (0.9%)
30	Y	0.49	0/415	1.08	0/577
All	All	0.52	1/64443 (0.0%)	1.05	113/89647 (0.1%)

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
6	A	0	2
10	G	0	1
15	M	0	1
17	O	0	1
20	S	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	632	ILE	N-CA	5.10	1.52	1.46

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	87	ILE	CA-C-N	14.31	134.45	118.85
11	H	87	ILE	C-N-CA	14.31	134.45	118.85
21	T	615	PHE	CA-C-N	10.69	131.39	120.38
21	T	615	PHE	C-N-CA	10.69	131.39	120.38
27	l	33	SER	CA-C-N	9.88	130.02	119.05

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	403	TYR	Peptide
10	G	3	ARG	Peptide

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Mol	Chain	Res	Type	Group
15	M	231	ASP	Peptide
17	O	83	GLN	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	U	2999	0	1515	23	0
2	E	346	0	173	5	0
3	I	693	0	351	3	0
4	Z	3610	0	1831	10	0
5	V	2066	0	1043	20	0
6	A	15704	0	15649	254	0
7	D	912	0	936	12	0
8	F	321	0	282	6	0
9	C	6756	0	6801	122	0
10	G	823	0	808	11	0
11	H	2639	0	2073	26	0
12	J	2556	0	2551	60	0
13	K	1289	0	1309	20	0
14	L	1270	0	1294	12	0
15	M	2010	0	1964	21	0
16	N	1658	0	1713	55	0
17	O	1645	0	1672	35	0
18	P	275	0	283	4	0
19	R	550	0	356	3	0
20	S	3120	0	2397	44	0
21	T	2946	0	1250	10	0
22	b	631	0	670	2	0
22	k	396	0	169	0	0
23	d	625	0	647	6	0
23	n	404	0	180	0	0
24	e	575	0	597	7	0
24	p	369	0	152	0	0
25	f	573	0	572	4	0
25	q	354	0	153	0	0
26	g	529	0	557	3	0
26	r	340	0	152	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	h	644	0	686	3	0
27	l	392	0	165	0	0
28	j	741	0	778	3	0
28	m	467	0	199	0	0
29	W	816	0	341	1	0
30	Y	416	0	182	0	0
31	x	660	0	142	7	0
32	E	1	0	0	0	0
32	V	1	0	0	0	0
33	D	1	0	0	1	0
33	L	3	0	0	0	0
33	M	1	0	0	0	0
33	N	2	0	0	4	0
34	C	32	0	12	0	0
All	All	63161	0	52605	692	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 6.

The worst 5 of 692 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)
16:N:34:CYS:SG	16:N:37:CYS:SG	1.40	1.39
1:U:45:A:N1	1:U:74:U:O4	1.65	1.30
16:N:16:CYS:SG	16:N:73:CYS:HB2	1.85	1.16
21:T:360:LYS:CB	21:T:381:HIS:CB	2.36	1.03
16:N:61:CYS:SG	33:N:401:ZN:ZN	1.54	0.94

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	1916/2413 (79%)	1762 (92%)	143 (8%)	11 (1%)	21	54
7	D	112/278 (40%)	93 (83%)	17 (15%)	2 (2%)	6	33
8	F	44/179 (25%)	41 (93%)	3 (7%)	0	100	100
9	C	872/1008 (86%)	777 (89%)	82 (9%)	13 (2%)	8	36
10	G	95/235 (40%)	89 (94%)	5 (5%)	1 (1%)	11	41
11	H	389/591 (66%)	362 (93%)	23 (6%)	4 (1%)	12	43
12	J	322/451 (71%)	263 (82%)	47 (15%)	12 (4%)	2	21
13	K	155/379 (41%)	146 (94%)	8 (5%)	1 (1%)	21	54
14	L	153/157 (98%)	136 (89%)	15 (10%)	2 (1%)	9	38
15	M	250/339 (74%)	228 (91%)	19 (8%)	3 (1%)	10	40
16	N	195/364 (54%)	178 (91%)	14 (7%)	3 (2%)	8	36
17	O	194/590 (33%)	173 (89%)	17 (9%)	4 (2%)	5	31
18	P	34/175 (19%)	28 (82%)	5 (15%)	1 (3%)	3	25
19	R	91/135 (67%)	80 (88%)	10 (11%)	1 (1%)	11	41
20	S	432/687 (63%)	416 (96%)	14 (3%)	2 (0%)	24	57
21	T	532/859 (62%)	504 (95%)	20 (4%)	8 (2%)	8	36
22	b	76/196 (39%)	70 (92%)	6 (8%)	0	100	100
22	k	76/196 (39%)	65 (86%)	9 (12%)	2 (3%)	4	27
23	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	9	38
23	n	80/101 (79%)	66 (82%)	14 (18%)	0	100	100
24	e	71/94 (76%)	68 (96%)	3 (4%)	0	100	100
24	p	71/94 (76%)	63 (89%)	7 (10%)	1 (1%)	9	37
25	f	70/86 (81%)	66 (94%)	3 (4%)	1 (1%)	9	37
25	q	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
26	g	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
26	r	65/77 (84%)	55 (85%)	9 (14%)	1 (2%)	8	36
27	h	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
27	l	75/146 (51%)	63 (84%)	10 (13%)	2 (3%)	4	27
28	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
28	m	92/110 (84%)	84 (91%)	8 (9%)	0	100	100
29	W	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	1	17
30	Y	82/111 (74%)	77 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7089/10809 (66%)	6428 (91%)	577 (8%)	84 (1%)	13	40

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	320	ASP
6	A	737	ARG
11	H	414	PRO
15	M	127	ILE
16	N	120	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	A	1701/2182 (78%)	1567 (92%)	134 (8%)	11	36
7	D	100/256 (39%)	90 (90%)	10 (10%)	7	28
8	F	26/163 (16%)	25 (96%)	1 (4%)	29	53
9	C	722/910 (79%)	662 (92%)	60 (8%)	10	34
10	G	89/216 (41%)	83 (93%)	6 (7%)	15	41
11	H	185/552 (34%)	167 (90%)	18 (10%)	8	29
12	J	283/398 (71%)	248 (88%)	35 (12%)	4	21
13	K	143/328 (44%)	119 (83%)	24 (17%)	2	13
14	L	138/141 (98%)	128 (93%)	10 (7%)	13	39
15	M	212/295 (72%)	195 (92%)	17 (8%)	11	36
16	N	194/332 (58%)	170 (88%)	24 (12%)	4	21
17	O	174/526 (33%)	156 (90%)	18 (10%)	7	27
18	P	26/152 (17%)	22 (85%)	4 (15%)	2	15
19	R	24/121 (20%)	20 (83%)	4 (17%)	2	13
20	S	208/633 (33%)	184 (88%)	24 (12%)	5	23
22	b	70/176 (40%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	d	69/89 (78%)	67 (97%)	2 (3%)	37	58
24	e	65/83 (78%)	61 (94%)	4 (6%)	16	42
25	f	63/77 (82%)	61 (97%)	2 (3%)	34	56
26	g	58/66 (88%)	56 (97%)	2 (3%)	32	55
27	h	77/129 (60%)	77 (100%)	0	100	100
28	j	79/103 (77%)	76 (96%)	3 (4%)	29	53
All	All	4706/7928 (59%)	4304 (92%)	402 (8%)	12	33

5 of 402 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	147	ILE
13	K	217	GLN
28	j	48	LEU
12	J	202	GLU
12	J	387	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
12	J	273	GLN
17	O	72	GLN
12	J	317	HIS
14	L	46	ASN
20	S	167	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	138/179 (77%)	68 (49%)	13 (9%)
2	E	15/16 (93%)	10 (66%)	2 (13%)
3	I	31/76 (40%)	15 (48%)	0
4	Z	162/1175 (13%)	58 (35%)	11 (6%)
5	V	96/112 (85%)	35 (36%)	5 (5%)
All	All	442/1558 (28%)	186 (42%)	31 (7%)

5 of 186 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	13	A
1	U	14	G
1	U	15	A
1	U	16	U
1	U	18	A

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	-9	U
5	V	53	A
4	Z	20	G
5	V	74	U
4	Z	1124	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	$\# Z > 2$
34	GTP	C	1101	-	33,34,34	1.09	3 (9%)	50,54,54	1.77	8 (16%)

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
34	GTP	C	1101	-	-	5/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	1101	GTP	C5-C4	2.70	1.46	1.38
34	C	1101	GTP	C5-N7	-2.61	1.33	1.39
34	C	1101	GTP	C6-N1	-2.39	1.34	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	1101	GTP	C5-C4-N3	-5.96	118.91	128.39
34	C	1101	GTP	C2-N3-C4	5.05	121.00	112.30
34	C	1101	GTP	N9-C4-N3	4.57	135.08	125.95
34	C	1101	GTP	C6-C5-N7	3.18	136.08	130.29
34	C	1101	GTP	O6-C6-C5	-2.83	119.07	126.53

There are no chirality outliers.

All (5) torsion outliers are listed below:

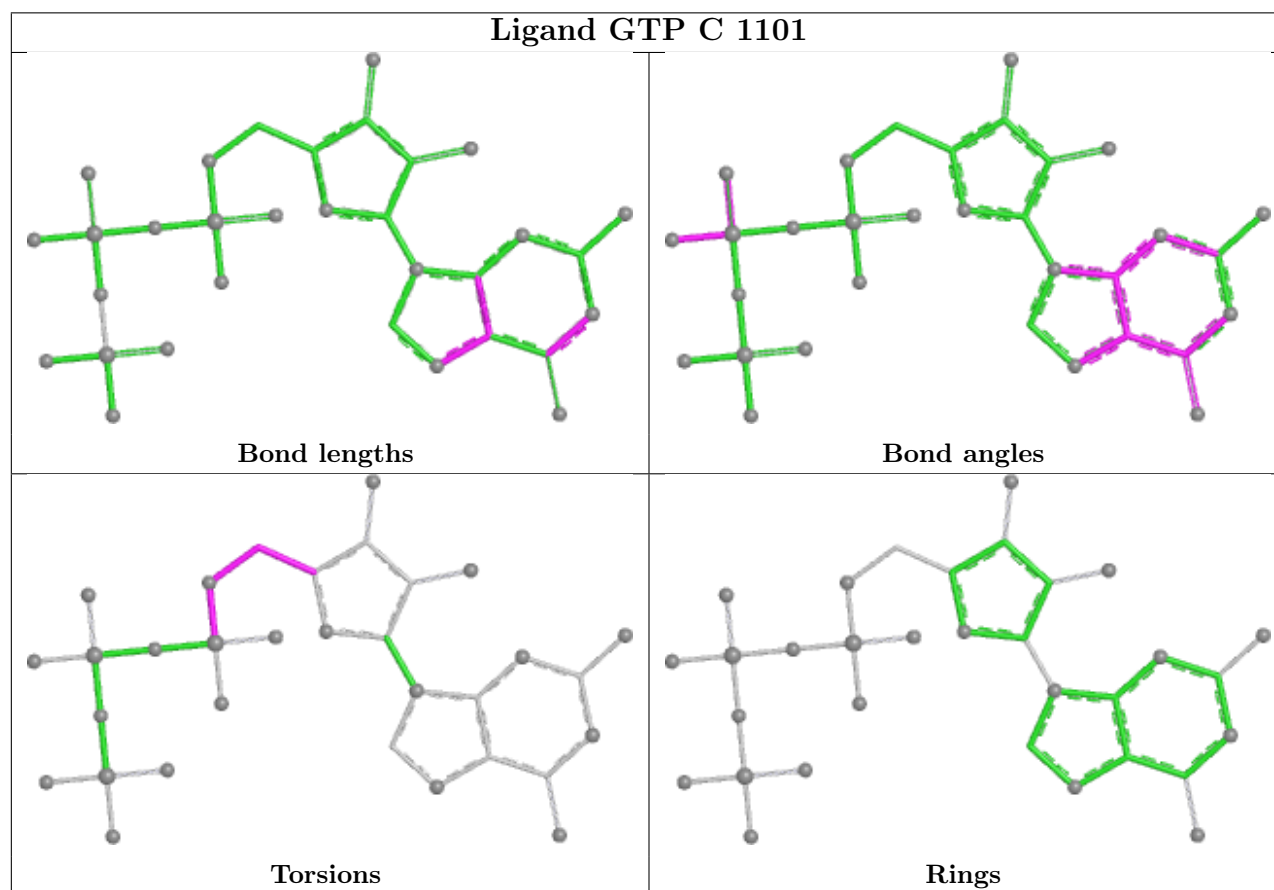
Mol	Chain	Res	Type	Atoms
34	C	1101	GTP	C5'-O5'-PA-O3A
34	C	1101	GTP	C5'-O5'-PA-O1A
34	C	1101	GTP	C3'-C4'-C5'-O5'
34	C	1101	GTP	O4'-C4'-C5'-O5'
34	C	1101	GTP	C4'-C5'-O5'-PA

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
31	x	4
21	T	2
19	R	1
5	V	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	54:UNK	C	55:UNK	N	111.76

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	110:UNK	C	111:UNK	N	53.94
1	x	36:UNK	C	37:UNK	N	49.39
1	x	87:UNK	C	88:UNK	N	31.03
1	T	419:LYS	C	420:SER	N	5.13

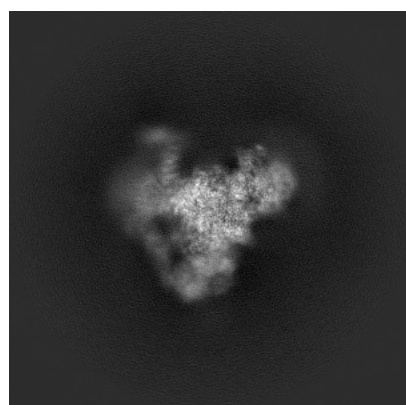
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4055. These allow visual inspection of the internal detail of the map and identification of artifacts.

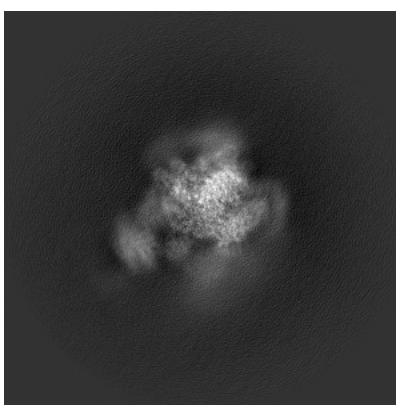
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

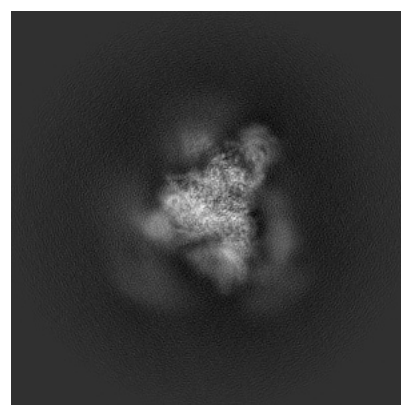
6.1.1 Primary map



X



Y

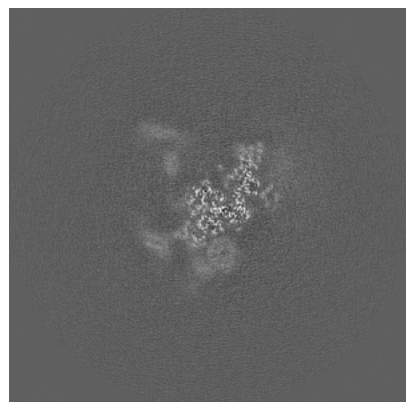


Z

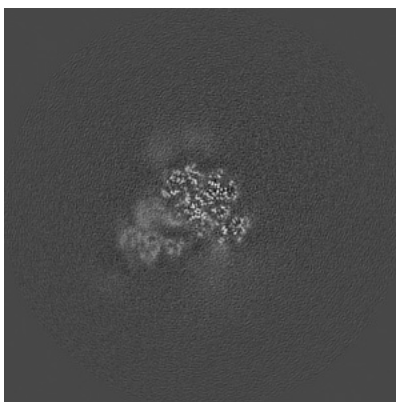
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

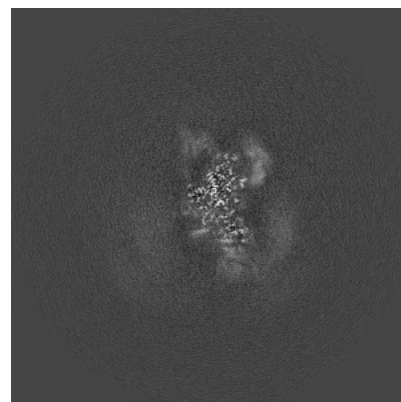
6.2.1 Primary map



X Index: 206



Y Index: 206

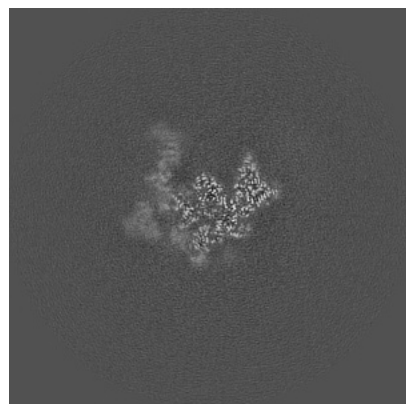


Z Index: 206

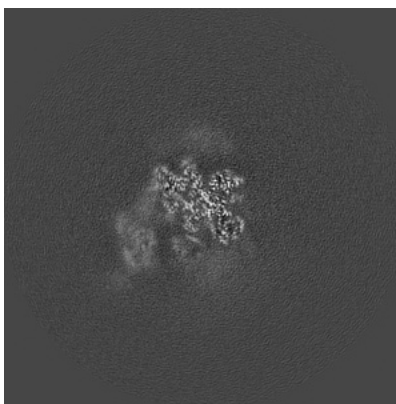
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

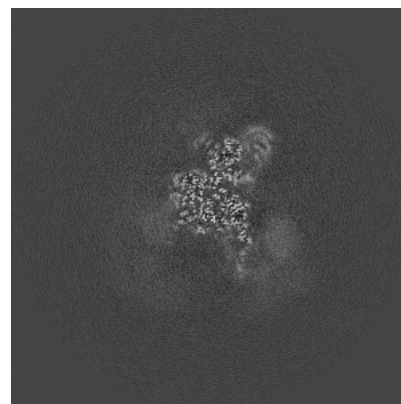
6.3.1 Primary map



X Index: 225



Y Index: 197

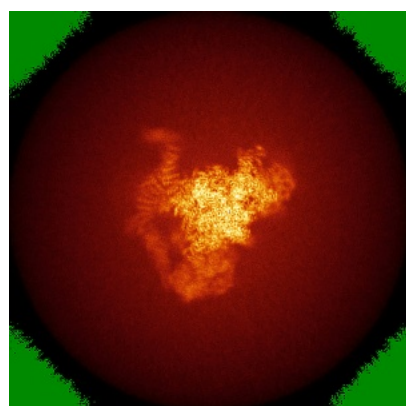


Z Index: 221

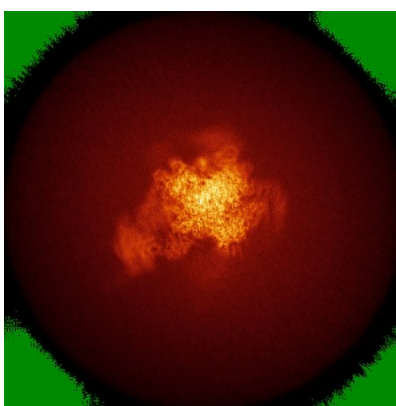
The images above show the largest variance slices of the map in three orthogonal directions.

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

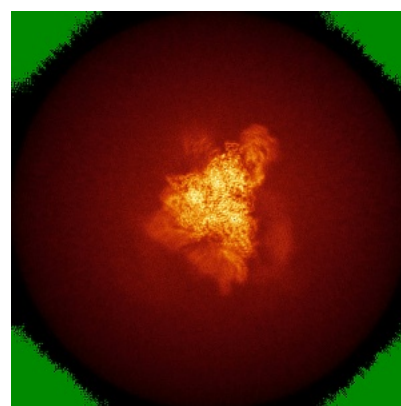
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

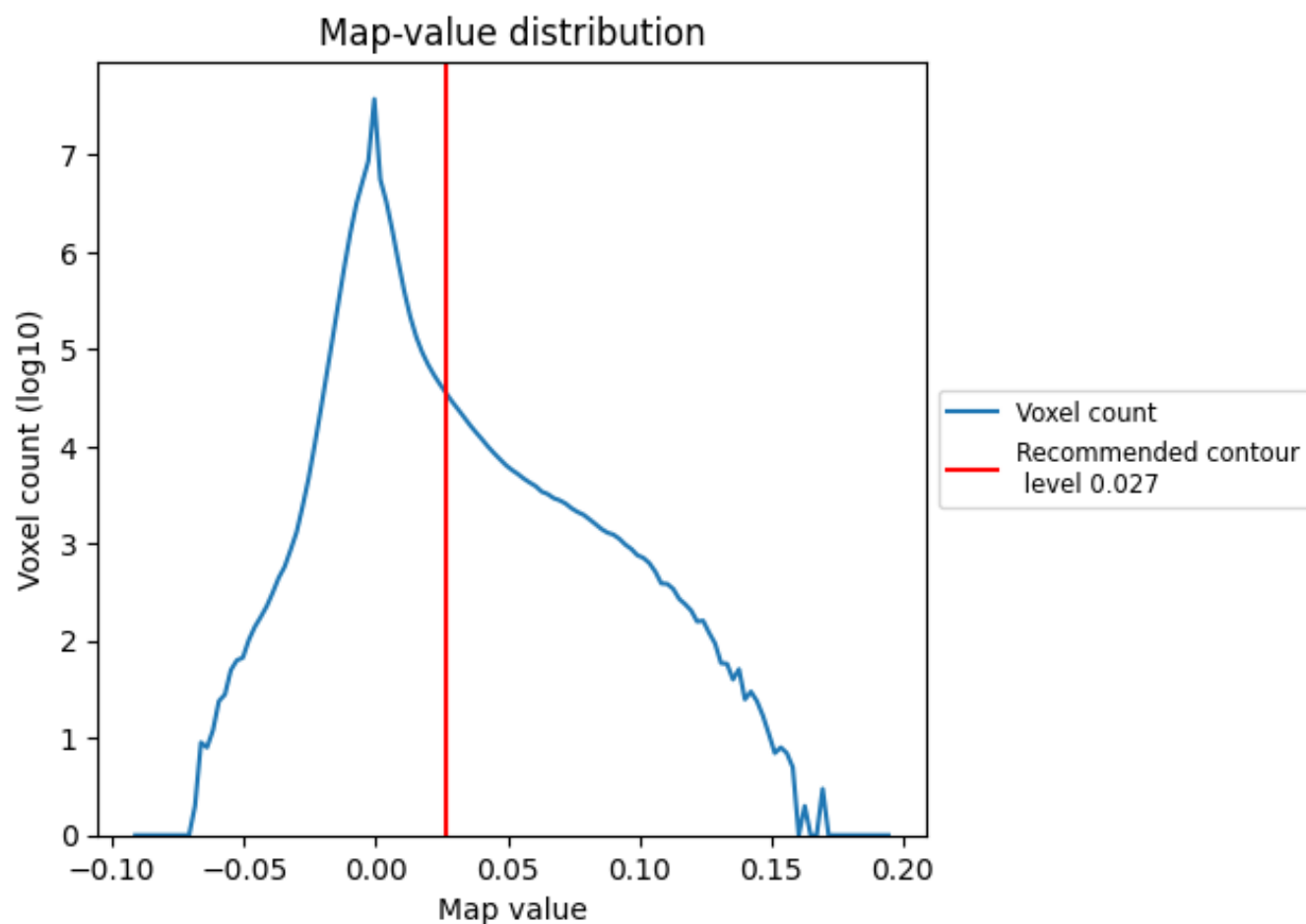
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

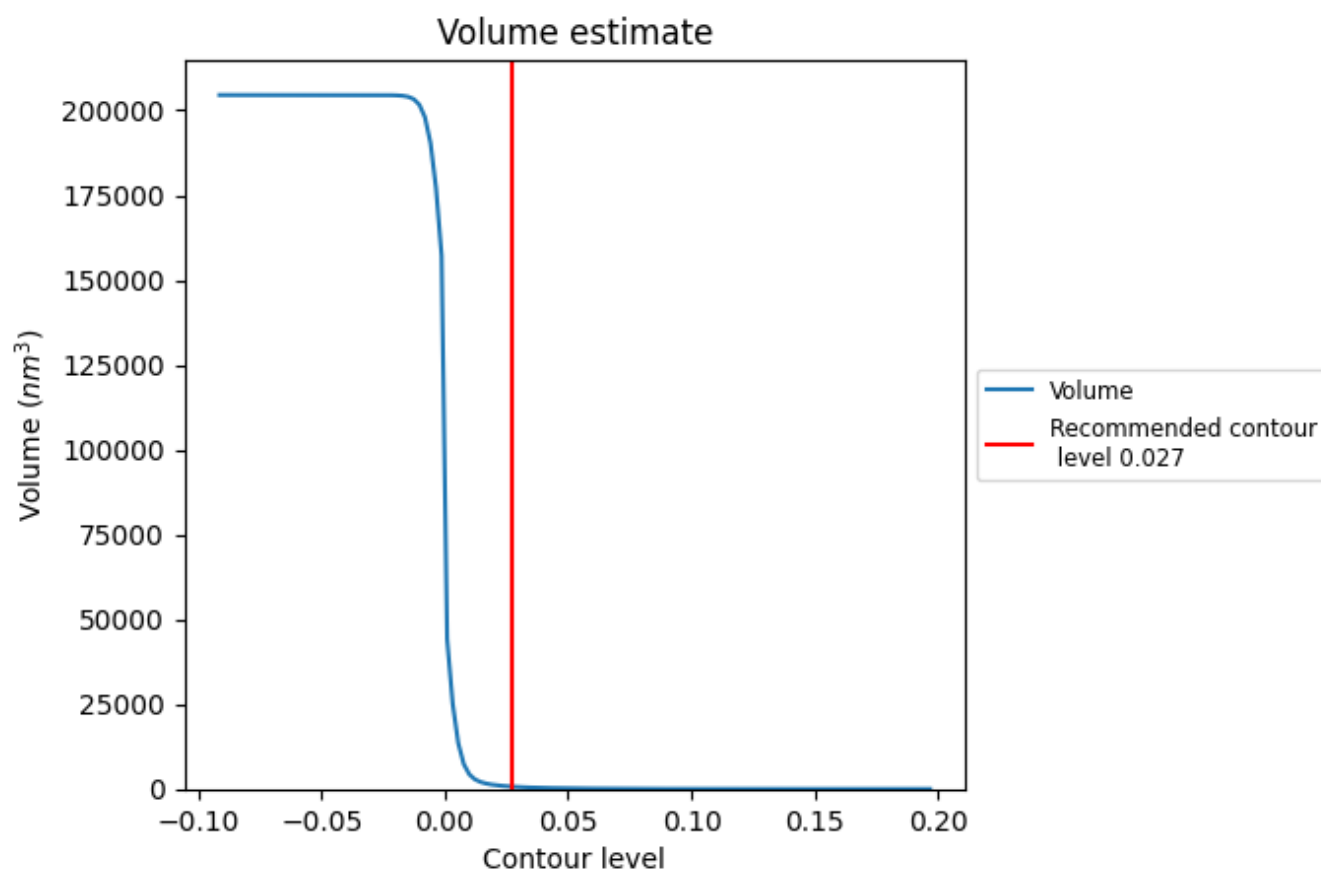
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

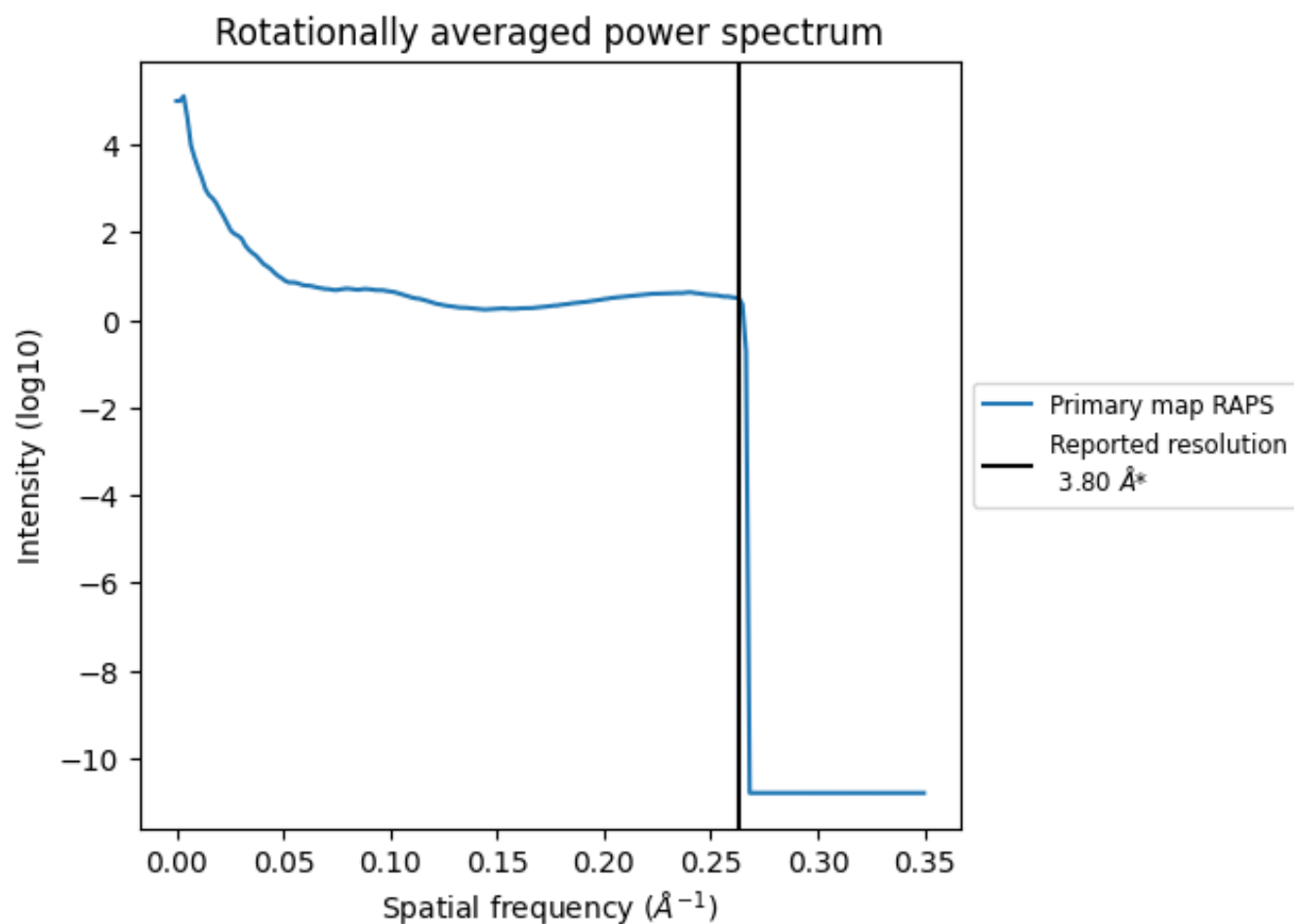
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm³; this corresponds to an approximate mass of 632 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

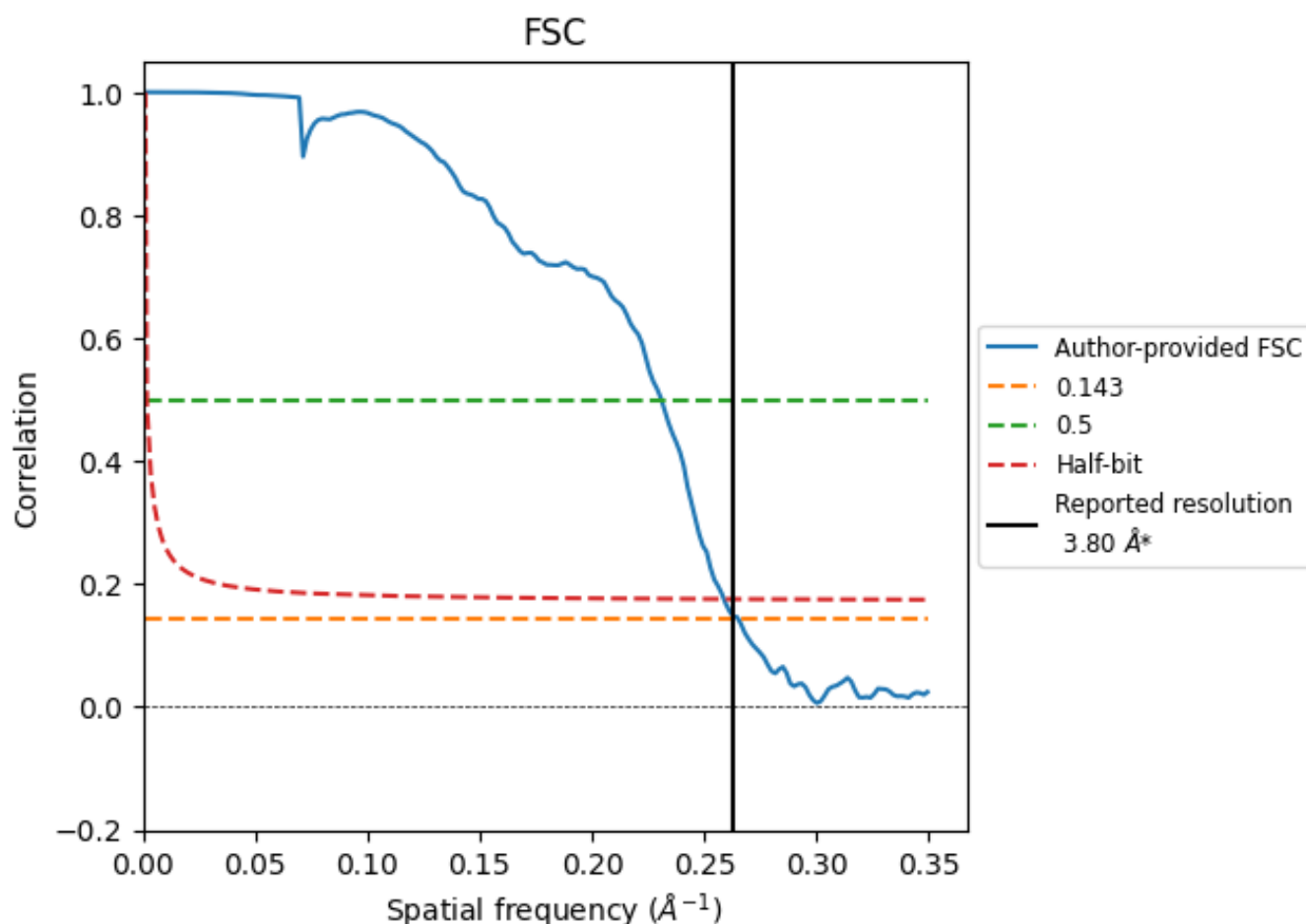


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.33	3.86
Unmasked-calculated*	-	-	-

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

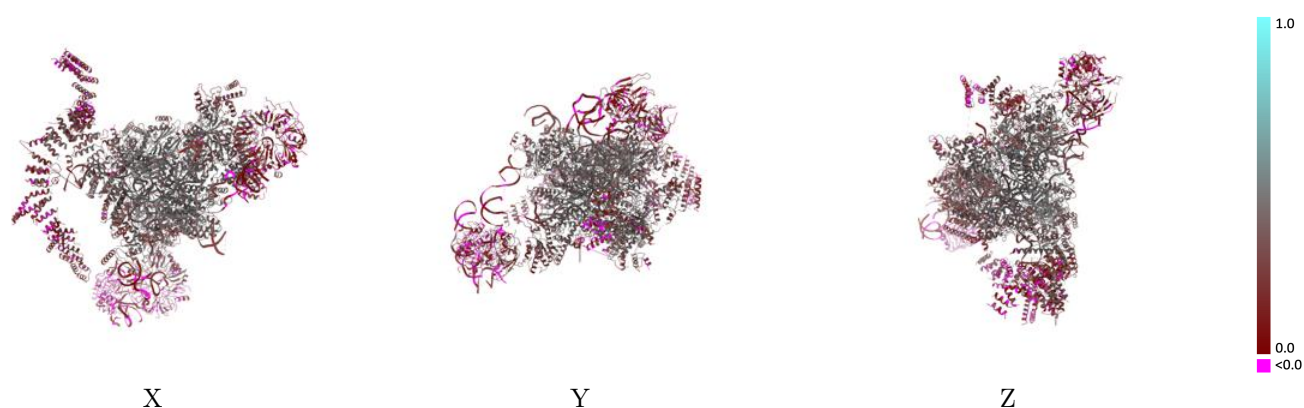
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4055 and PDB model 5LJ3. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

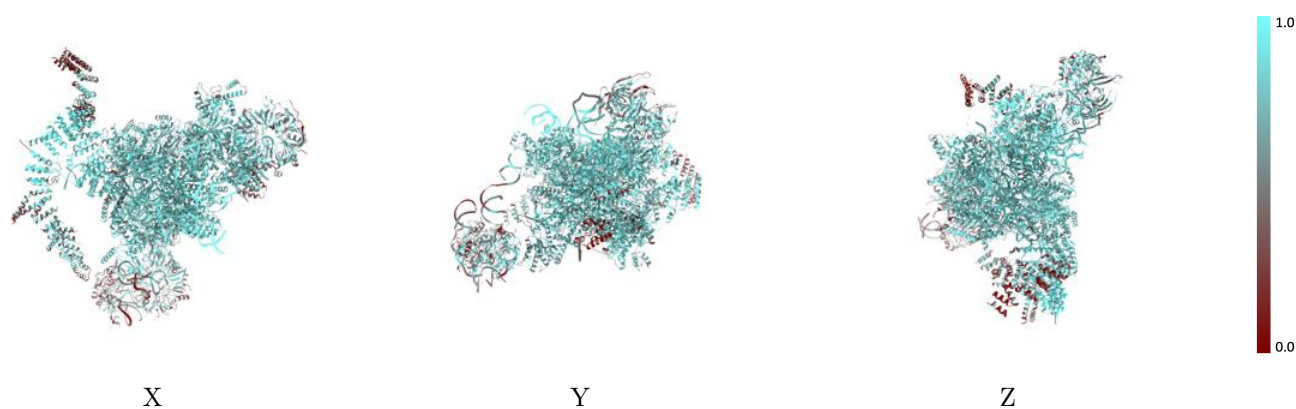
This section was not generated.

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



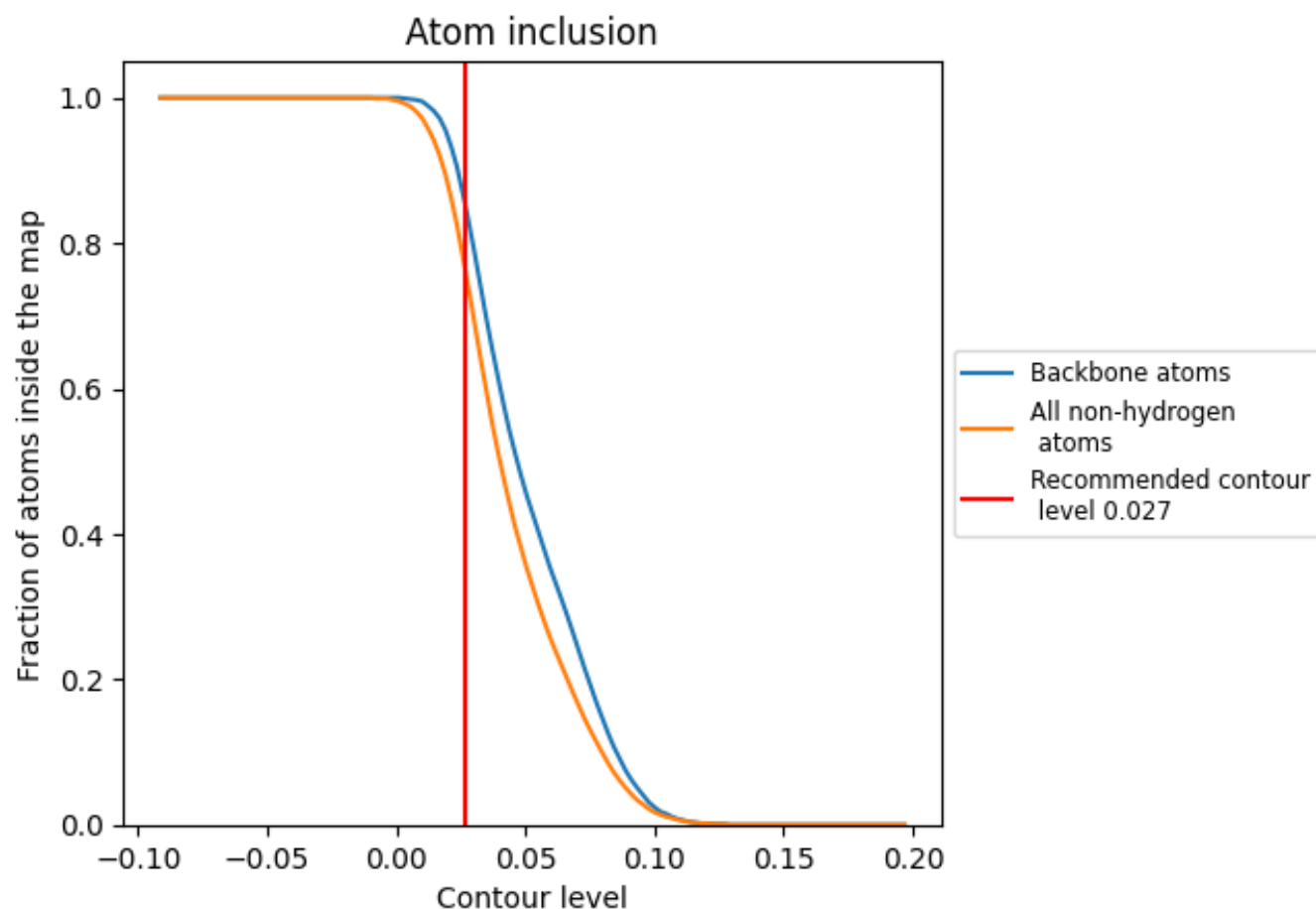
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 76% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.3280
A	 0.8060	 0.4030
C	 0.8210	 0.4000
D	 0.8160	 0.4470
E	 0.8730	 0.3790
F	 0.7540	 0.4070
G	 0.7620	 0.3730
H	 0.6400	 0.2920
I	 0.8460	 0.3550
J	 0.8530	 0.4480
K	 0.7530	 0.4000
L	 0.8500	 0.4130
M	 0.8270	 0.4050
N	 0.8050	 0.3720
O	 0.7520	 0.3480
P	 0.8910	 0.4710
R	 0.7720	 0.3030
S	 0.6930	 0.3080
T	 0.6800	 0.1940
U	 0.8720	 0.2820
V	 0.9360	 0.3840
W	 0.3480	 0.0310
Y	 0.4880	 0.0440
Z	 0.5860	 0.1400
b	 0.6580	 0.2180
d	 0.7200	 0.3150
e	 0.6290	 0.1410
f	 0.6170	 0.1160
g	 0.6540	 0.2000
h	 0.6180	 0.1670
j	 0.5950	 0.1050
k	 0.5830	 0.1470
l	 0.7400	 0.2760
m	 0.6940	 0.2170
n	 0.5520	 0.1460



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Chain	Atom inclusion	Q-score
p	 0.5090	 0.1000
q	 0.7230	 0.2400
r	 0.4760	 0.0880
x	 0.8470	 0.3030