



## wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 11:29 pm BST

PDB ID : 5LJ3  
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](mailto: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>.

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

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

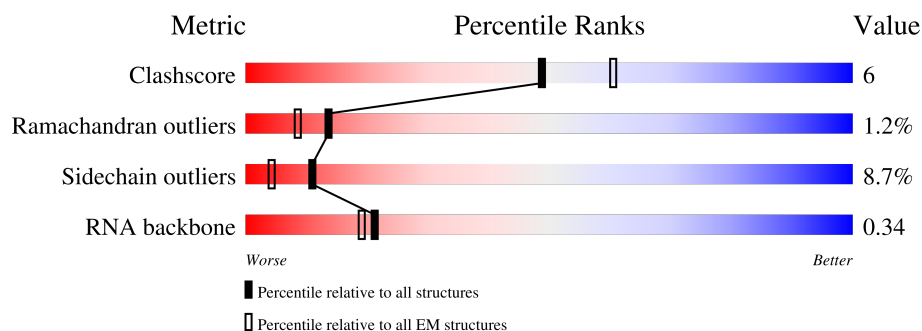
# 1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	
4	Z	1175	
5	V	112	
6	A	2413	
7	D	278	

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Mol	Chain	Length	Quality of chain
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	
25	q	86	
26	g	77	
26	r	77	
27	h	146	

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Mol	Chain	Length	Quality of chain
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		

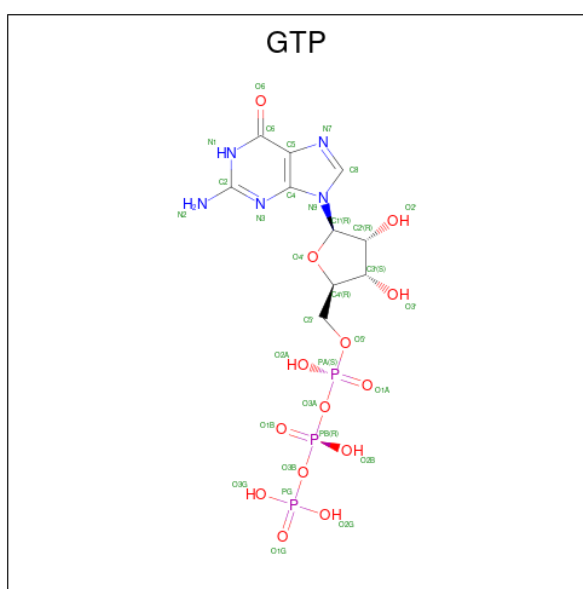
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: 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 (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

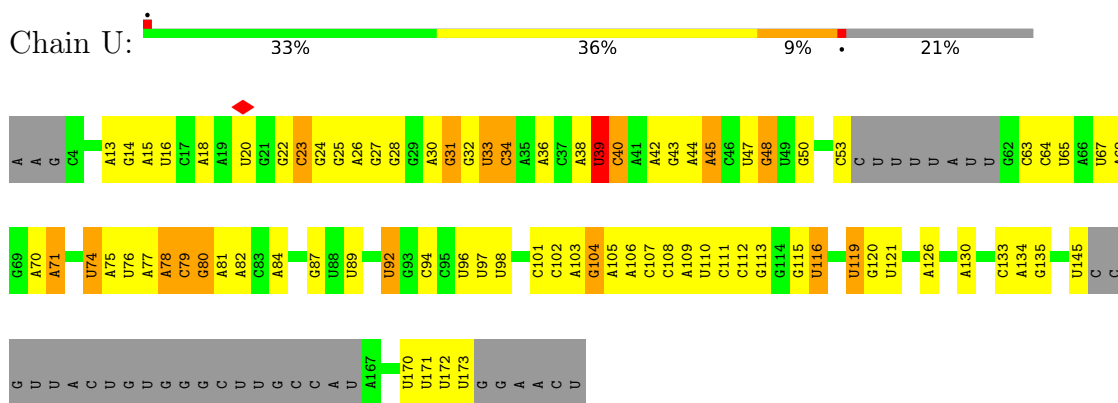


Mol	Chain	Residues	Atoms					AltConf
34	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

### 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.

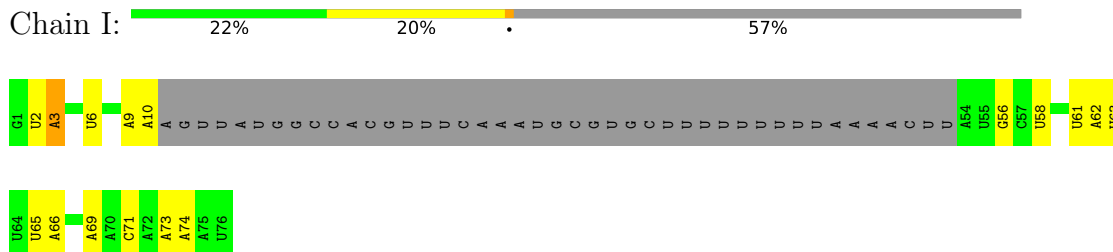
- Molecule 1: U5 snRNA (small nuclear RNA)



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

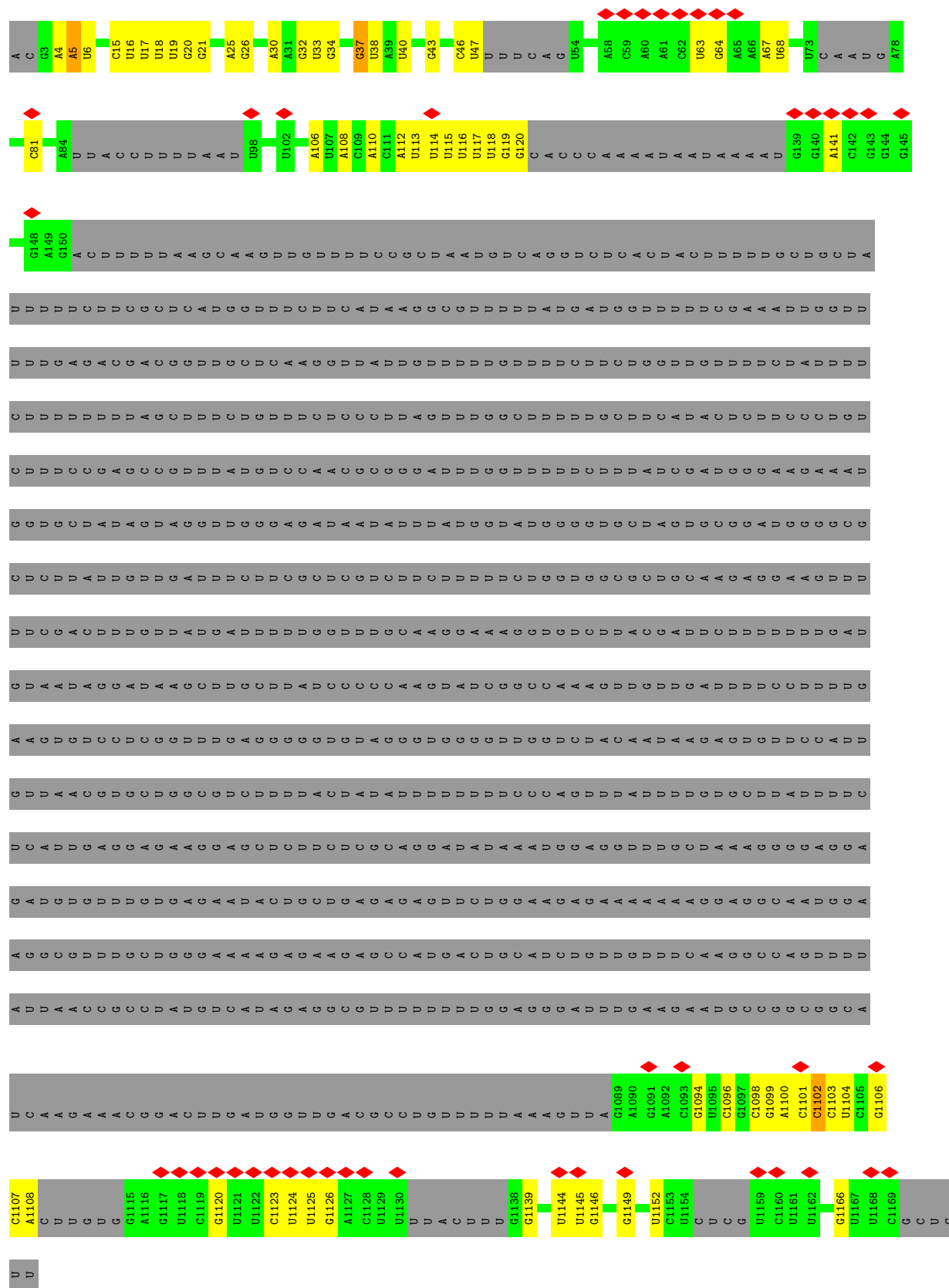


- Molecule 3: Intron of UBC4 pre-mRNA



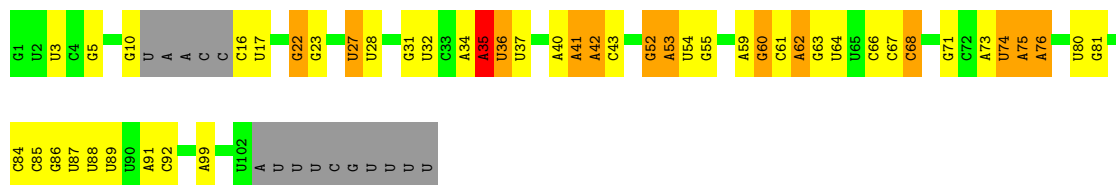
- Molecule 4: U2 snRNA (small nuclear RNA)





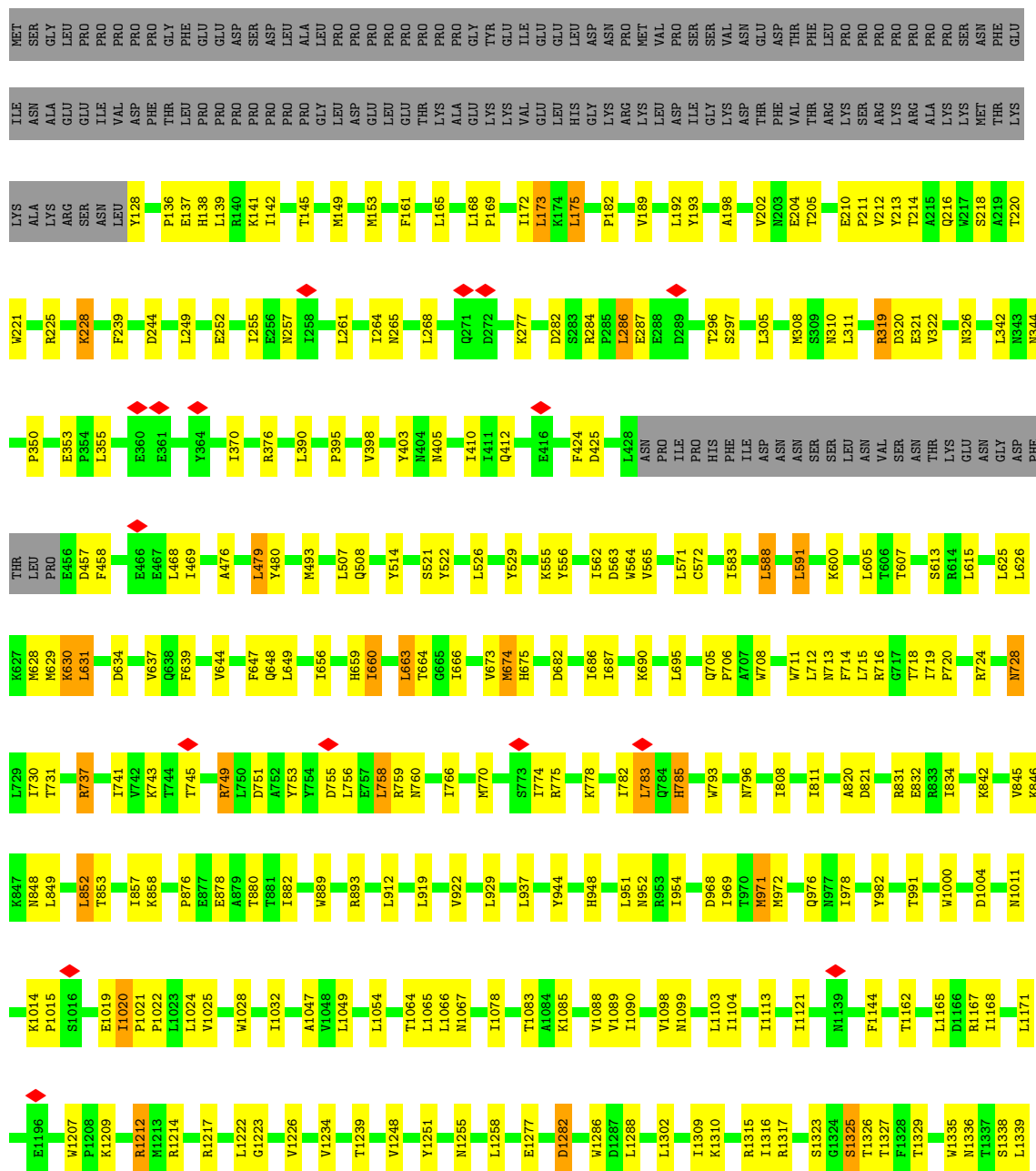
- Molecule 5: U6 snRNA (small nuclear RNA)

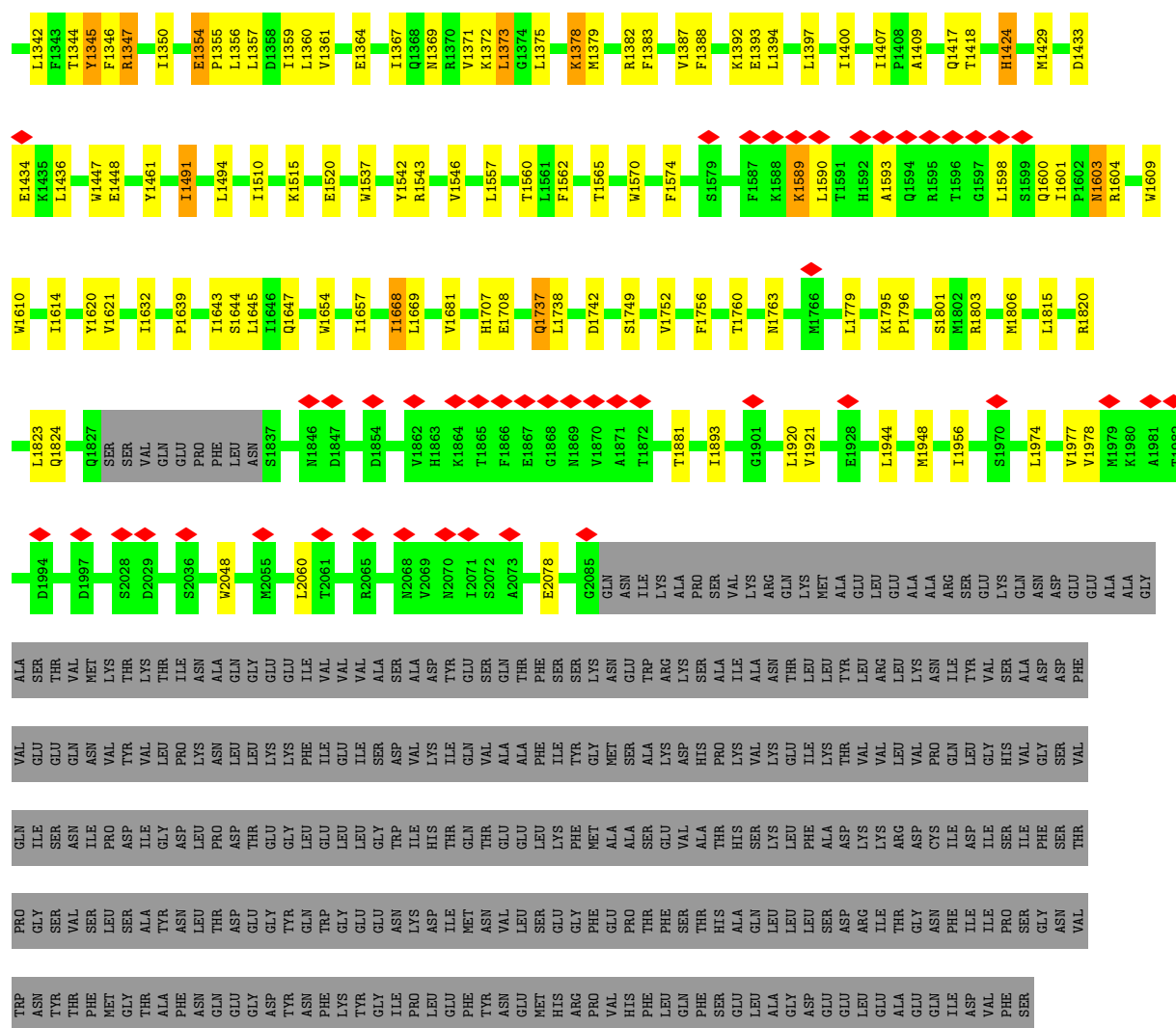
Chain V:  44% 30% 12% 13%



• Molecule 6: Pre-mRNA-splicing factor 8

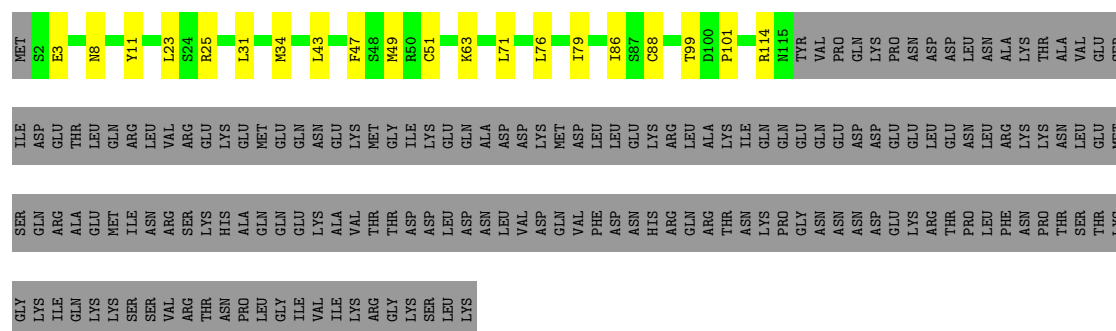
Chain A:  63% 15% 20%





### • Molecule 7: Protein CWC16

Chain D: 34% 7% 59%



### • Molecule 8: Pre-mRNA-splicing factor CWC25

Chain F: 23% 0% 74%



LEU	ILE	ASN	GLY	LYS	ARG	TYR	PHE	GLY	ARG	ASN	ALA	LEU	GLU	LEU	PRO	GLU	VAL	GLU	ASP	GLY	ARG	GLU	TRP	LEU	LYS	GLN	SER	GLN	ARG	GLN	ASN	GLN	ILE	SER	GLY	PRO	VAL	ASP	GLY	ASP	LEU	TRP	LYS	CYS	LYS	ASN	THR	ASP	ASP	LEU	GLN	VAL	ASP	ARG	ASN	ASP	PHE	LYS	TYR	LYS	LYS	LEU	HIS	GLY	MET	ASP	GLU	THR	ALA	ALA	ALA	LEU	LEU	THR	GLU	PHE	GLU	ALA
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• Molecule 11: CWC22



PRO	PRO	ALA	ARG	GLU	LYS	ASN	THR	GLN	ARG	ASN	ARG	THR	PRO	PRO	ALA	ARG	ARG	GLN	ARG	HIS	ARG	THR	PRO	PRO	THR	VAL	GLU	THR	ARG	LYS	ALA	ARG	ARG	SER	ARG	THR	PRO	PRO	PRO	ARG	LYS	LEU	ARG	GLY	SER	ARG	ASN	HIS	ARG	GLU	ASN	ARG	GLU	LEU	GLU	LYS	LEU	ARG	THR	LYS
F419	I420	K421	L427	L436	L440	K444	L445	M448	L451	E452	D453	A455	F465	I468	G469	L470	L473	R478	L481	THR	ILE	ILE	GLN	GLU	VAL	GLU	ALA	ASP	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	LYS	LYS	LEU	ARG	GLU	GLU	ASN	GLU	HIS	ARG	GLU	ASN	ARG	GLU	LEU	GLU	GLU	LYS	LEU	ARG	THR	LYS	
I317	V326	D327	I328	I329	I330	S333	L334	Y343	S344	I345	S347	E348	I351	R355	S356	Y357	Q358	T359	E363	Q367	N368	Y369	I373	Q380	L381	L384	F387	L391	E395	F396	M399	L402	LYS	ILE	ILE	LYS	LEU	THR	GLU	E410	P414																			
C246	E246	N247	F248	E250	L251	T252	M253	F255	D256	T257	L258	R259	Q260	K261	L262	LEU	ILE	ASN	ASN	THR	SER	ASP	THR	ASN	GLY	SER	THR	ILE	TYR	ASP	MET	THR	SER	THR	ASN	V289	E290	F291	K292	L297	V298	L299	L303	E307	L312	L313	K314													
A163	L164	V165	S166	K167	T183	Q184	E185	L186	S187	S188	T189	L190	E191	L194	K203	K206	GLY	SER	GLN	GLY	LEU	PHE	ILE	LEU	ASP	PRO	THR	SER	TYR	THR	VAL	HIS	THR	HIS	SER	THR	ASN	ASP	GLU	ASP	GLU	ALA	ASN	LYS	GLU	LEU	GLY	ASN	PHE	GLU	LYS									
T64	L65	N66	LYS	GLN	N69	G70	R71	L72	I73	P74	A75	L76	S77	A78	L79	I80	A81	L82	L83	N84	S85	D86	I87	P88	D89	I90	T93	L94	A95	F102	K109	C114	G115	L118	E132	I135	L136	Q137	I138	L139	L140	L143	E144	K145	N146	S147	L148	I152	I157											
MET	SER	THR	ALA	THR	ILE	GLN	ASP	GLU	ASP	I11	K12	F13	R14	R15	E16	N17	W18	E19	M20	I21	R22	S23	H24	V25	S26	P27	I28	I29	S30	N31	L32	L33	T32	S33	M34	D35	N36	L37	Q38	E39	S40	H41	R42	D43	L44	F45	Q46	V47	L50	I51	G52	I55	I56	C57	K58	N59	V60	V61		

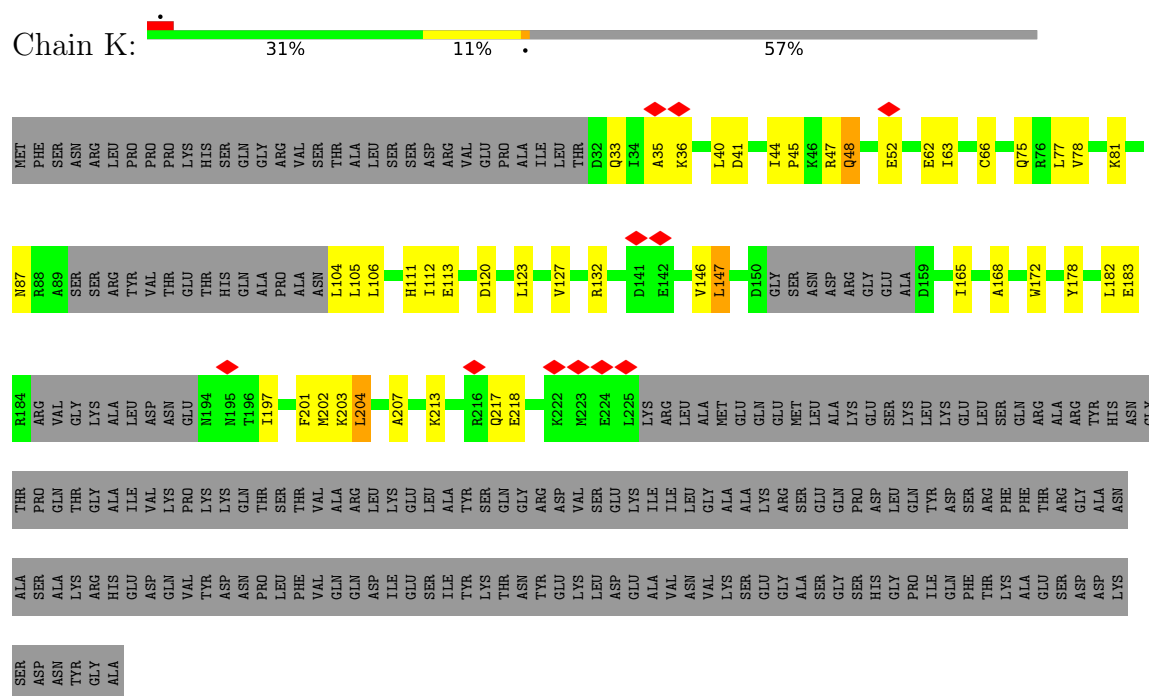
• Molecule 12: PRP46



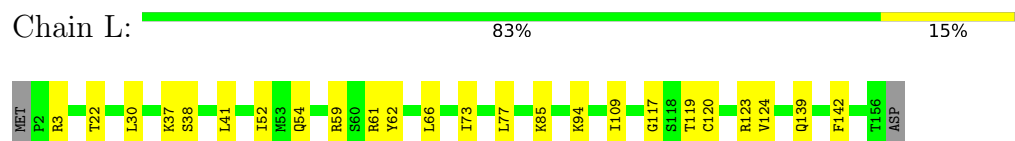
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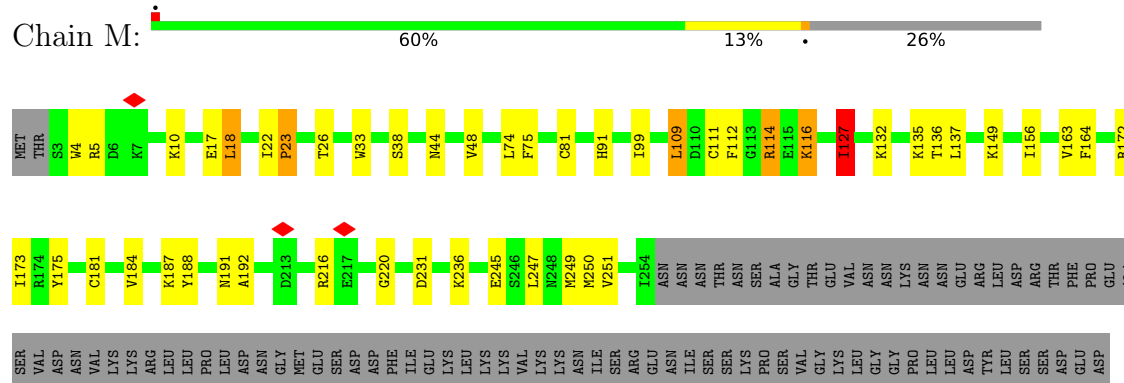
- Molecule 13: Pre-mRNA-processing protein 45



- Molecule 14: Pre-mRNA-splicing factor BUD31



- Molecule 15: CWC2



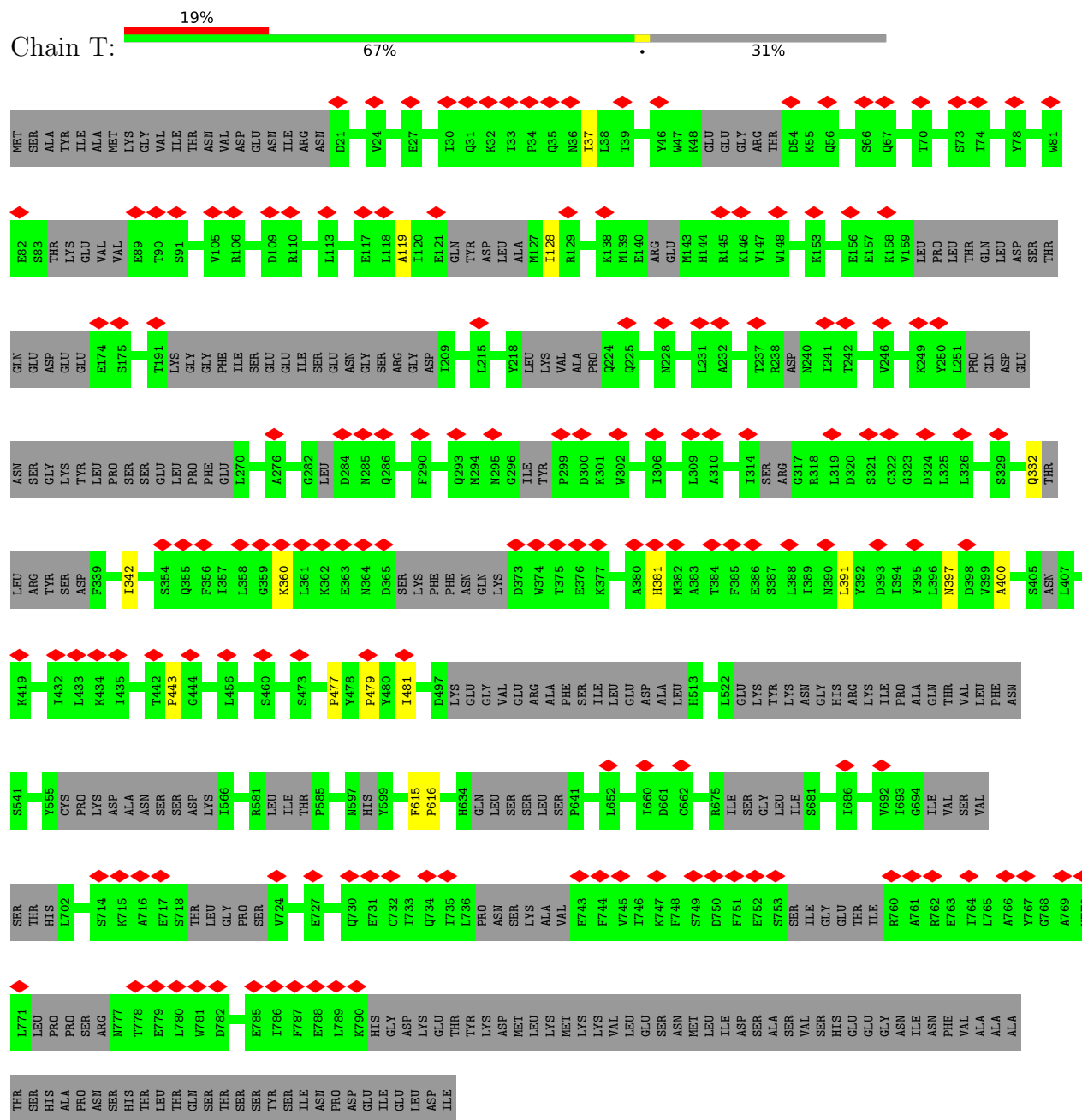
- Molecule 16: Pre-mRNA-splicing factor SLT11



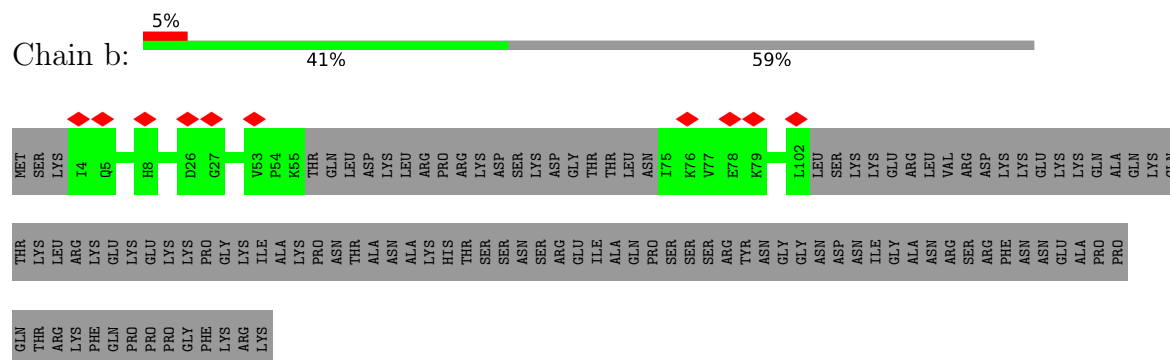




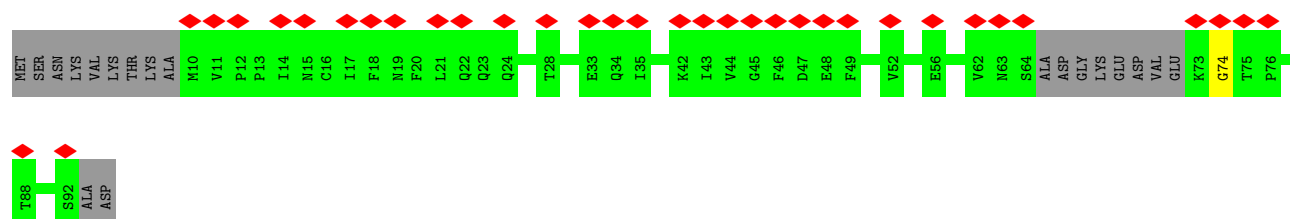
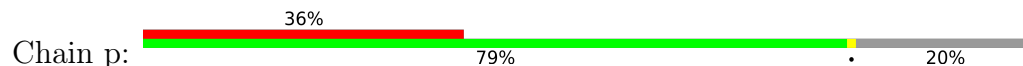
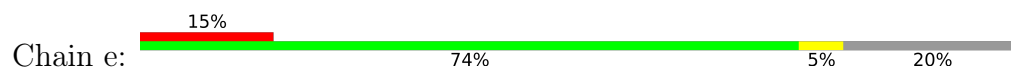
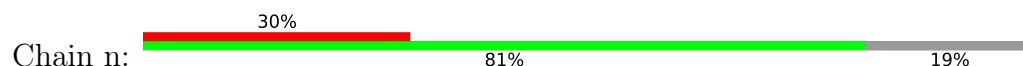
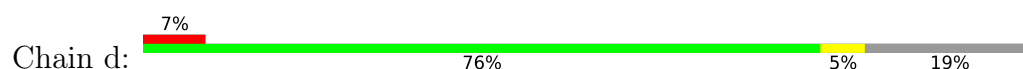
- Molecule 21: SYF1



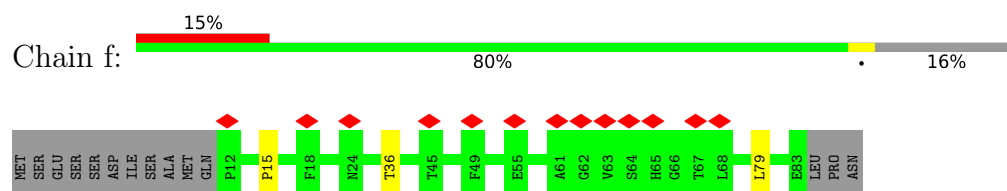
- Molecule 22: Small nuclear ribonucleoprotein-associated protein B



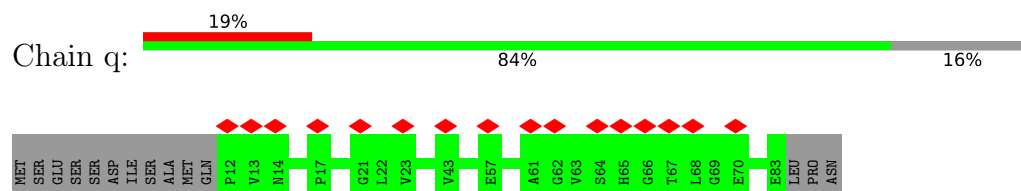
- Chain k: 



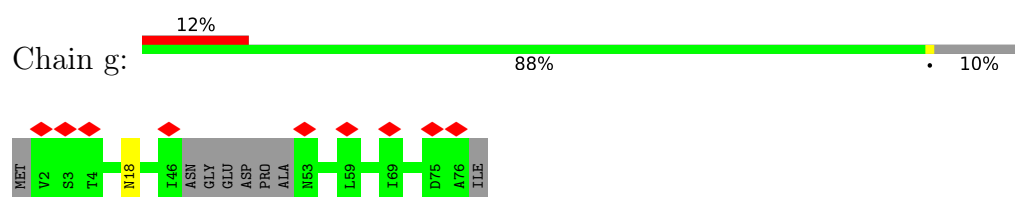
- Molecule 25: Small nuclear ribonucleoprotein F



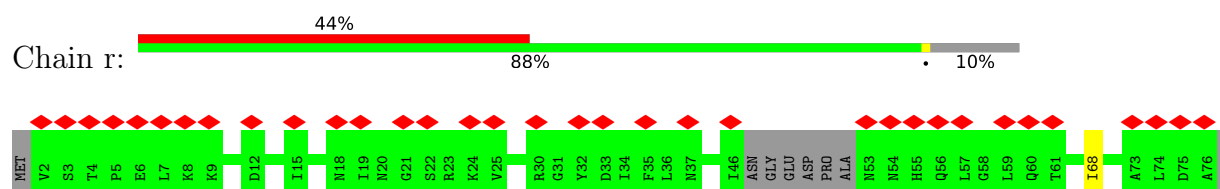
- Molecule 25: Small nuclear ribonucleoprotein F



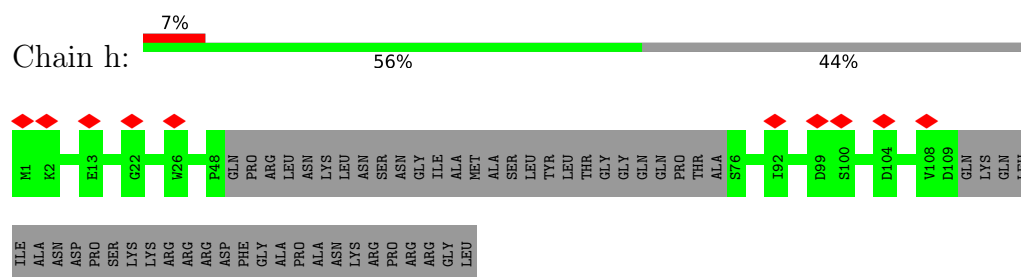
- Molecule 26: Small nuclear ribonucleoprotein G



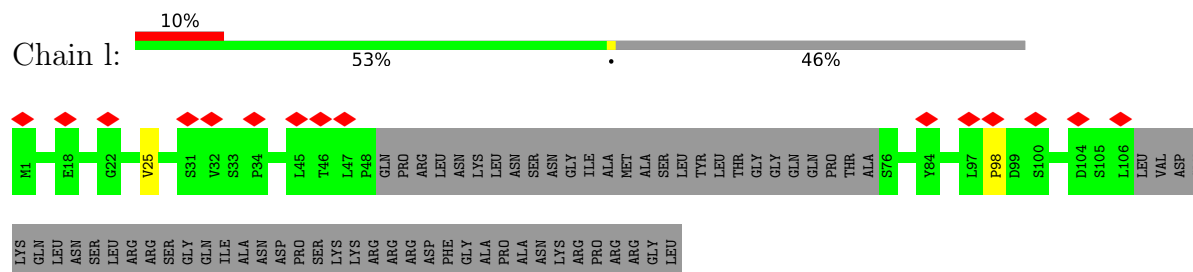
- Molecule 26: Small nuclear ribonucleoprotein G



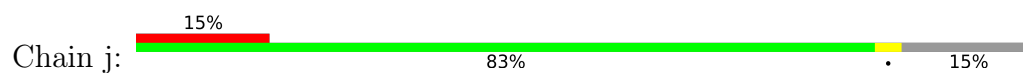
- Molecule 27: Small nuclear ribonucleoprotein Sm D1



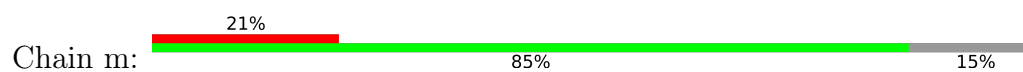
- Molecule 27: Small nuclear ribonucleoprotein Sm D1



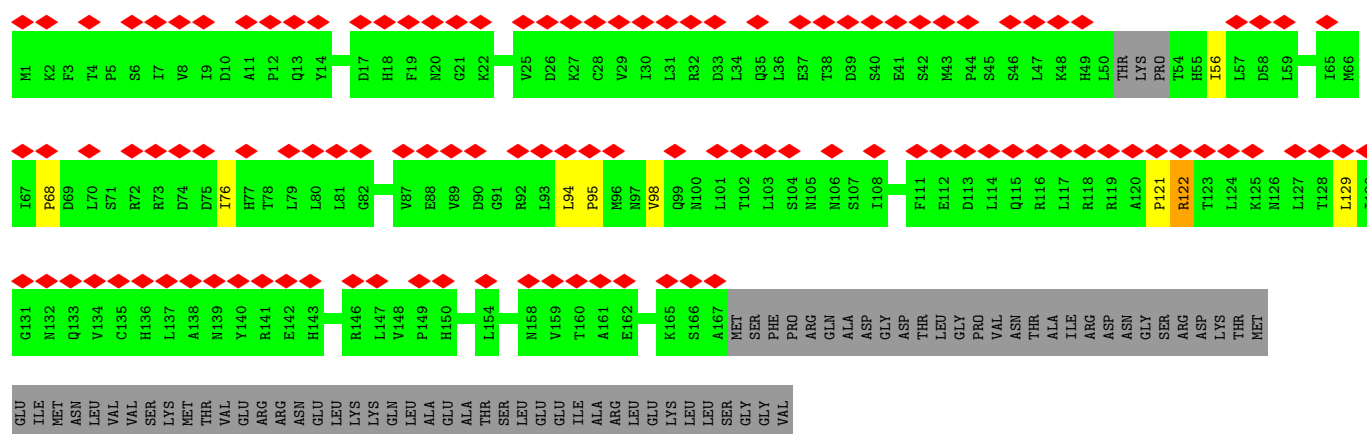
- Molecule 28: Small nuclear ribonucleoprotein Sm D2



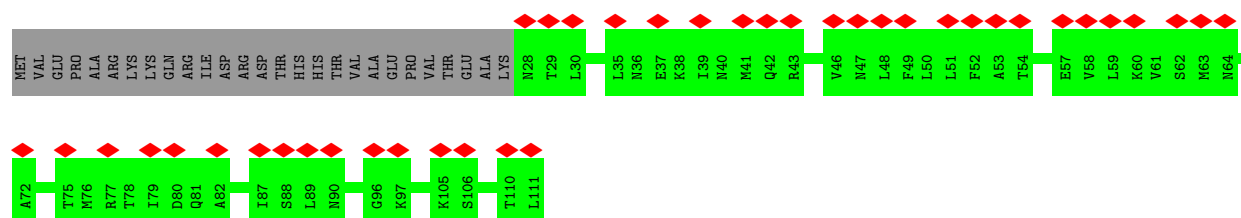
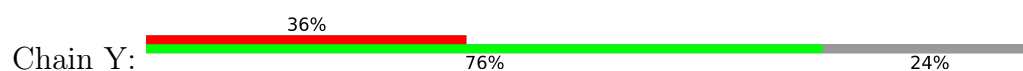
- Molecule 28: Small nuclear ribonucleoprotein Sm D2



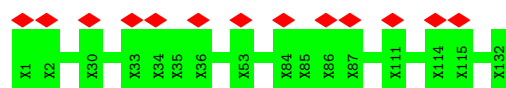
- Molecule 29: U2 small nuclear ribonucleoprotein A'



- Molecule 30: U2 small nuclear ribonucleoprotein B''



- 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: MG, ZN, GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	U	0.31	0/3351	0.75	1/5213 (0.0%)
2	E	0.36	0/388	0.69	0/603
3	I	0.28	0/772	0.71	0/1195
4	Z	0.26	0/4018	0.72	0/6233
5	V	0.31	0/2309	0.76	2/3590 (0.1%)
6	A	0.43	0/16107	0.75	0/21845
7	D	0.37	0/929	0.67	0/1243
8	F	0.42	0/325	0.74	0/442
9	C	0.41	0/6902	0.73	0/9386
10	G	0.42	0/839	0.74	0/1126
11	H	0.43	0/2667	0.80	1/3630 (0.0%)
12	J	0.45	0/2613	0.74	0/3551
13	K	0.40	0/1308	0.72	0/1765
14	L	0.40	0/1294	0.75	0/1732
15	M	0.42	0/2056	0.70	0/2766
16	N	0.41	0/1680	0.76	0/2258
17	O	0.43	0/1669	0.81	0/2236
18	P	0.43	0/282	0.69	0/380
19	R	0.40	0/550	0.76	0/752
20	S	0.44	0/3154	0.83	0/4297
21	T	0.38	0/2916	0.74	0/4026
22	b	0.34	0/636	0.59	0/856
22	k	0.28	0/394	0.50	0/546
23	d	0.36	0/634	0.62	1/859 (0.1%)
23	n	0.29	0/403	0.53	0/559
24	e	0.40	0/585	0.56	0/795
24	p	0.30	0/367	0.55	0/507
25	f	0.39	0/585	0.59	0/791
25	q	0.30	0/353	0.53	0/489
26	g	0.36	0/532	0.55	0/715
26	r	0.28	0/338	0.45	0/467
27	h	0.35	0/649	0.54	0/880

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
27	l	0.30	0/390	0.53	0/541
28	j	0.38	0/753	0.61	0/1013
28	m	0.31	0/466	0.54	0/649
29	W	0.31	0/814	0.53	0/1134
30	Y	0.32	0/415	0.55	0/577
All	All	0.39	0/64443	0.73	5/89647 (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
6	A	0	2
10	G	0	1
15	M	0	1
17	O	0	1
20	S	0	1
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	39	U	C2'-C3'-O3'	8.13	127.38	109.50
5	V	35	A	C5'-C4'-O4'	6.92	117.40	109.10
11	H	440	LEU	CA-CB-CG	6.54	130.33	115.30
23	d	81	ALA	C-N-CD	-6.46	106.39	120.60
5	V	35	A	O4'-C4'-C3'	5.43	110.44	106.10

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
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	24	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	21	0
6	A	15704	0	15649	227	0
7	D	912	0	936	11	0
8	F	321	0	282	3	0
9	C	6756	0	6801	117	0
10	G	823	0	808	10	0
11	H	2639	0	2073	25	0
12	J	2556	0	2551	54	0
13	K	1289	0	1309	17	0
14	L	1270	0	1294	12	0
15	M	2010	0	1964	20	0
16	N	1658	0	1713	49	0
17	O	1645	0	1672	32	0
18	P	275	0	283	4	0
19	R	550	0	356	2	0
20	S	3120	0	2397	39	0
21	T	2946	0	1250	6	0
22	b	631	0	670	0	0
22	k	396	0	169	0	0
23	d	625	0	647	0	0
23	n	404	0	180	0	0
24	e	575	0	597	0	0
24	p	369	0	152	0	0
25	f	573	0	572	0	0
25	q	354	0	153	0	0
26	g	529	0	557	0	0
26	r	340	0	152	0	0
27	h	644	0	686	0	0
27	l	392	0	165	0	0
28	j	741	0	778	0	0
28	m	467	0	199	0	0
29	W	816	0	341	1	0
30	Y	416	0	182	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	x	660	0	142	0	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	611	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 611 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%)	22	55
7	D	112/278 (40%)	93 (83%)	17 (15%)	2 (2%)	7	34
8	F	44/179 (25%)	41 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	C	872/1008 (86%)	777 (89%)	82 (9%)	13 (2%)	8	37
10	G	95/235 (40%)	89 (94%)	5 (5%)	1 (1%)	12	42
11	H	389/591 (66%)	362 (93%)	23 (6%)	4 (1%)	13	44
12	J	322/451 (71%)	263 (82%)	47 (15%)	12 (4%)	2	22
13	K	155/379 (41%)	146 (94%)	8 (5%)	1 (1%)	22	55
14	L	153/157 (98%)	136 (89%)	15 (10%)	2 (1%)	10	39
15	M	250/339 (74%)	228 (91%)	19 (8%)	3 (1%)	11	40
16	N	195/364 (54%)	178 (91%)	14 (7%)	3 (2%)	8	37
17	O	194/590 (33%)	173 (89%)	17 (9%)	4 (2%)	5	32
18	P	34/175 (19%)	28 (82%)	5 (15%)	1 (3%)	3	26
19	R	91/135 (67%)	80 (88%)	10 (11%)	1 (1%)	12	42
20	S	432/687 (63%)	416 (96%)	14 (3%)	2 (0%)	25	58
21	T	532/859 (62%)	504 (95%)	20 (4%)	8 (2%)	8	37
22	b	76/196 (39%)	70 (92%)	6 (8%)	0	100	100
22	k	76/196 (39%)	65 (86%)	9 (12%)	2 (3%)	4	28
23	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	10	39
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	37
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	18
30	Y	82/111 (74%)	77 (94%)	5 (6%)	0	100	100
All	All	7089/10809 (66%)	6428 (91%)	577 (8%)	84 (1%)	14	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%)	1580 (93%)	121 (7%)	12	36
7	D	100/256 (39%)	91 (91%)	9 (9%)	8	29
8	F	26/163 (16%)	25 (96%)	1 (4%)	28	52
9	C	722/910 (79%)	659 (91%)	63 (9%)	8	30
10	G	89/216 (41%)	81 (91%)	8 (9%)	8	29
11	H	185/552 (34%)	164 (89%)	21 (11%)	4	21
12	J	283/398 (71%)	250 (88%)	33 (12%)	4	20
13	K	143/328 (44%)	115 (80%)	28 (20%)	1	7
14	L	138/141 (98%)	129 (94%)	9 (6%)	14	39
15	M	212/295 (72%)	188 (89%)	24 (11%)	4	21
16	N	194/332 (58%)	175 (90%)	19 (10%)	6	25
17	O	174/526 (33%)	152 (87%)	22 (13%)	3	19
18	P	26/152 (17%)	21 (81%)	5 (19%)	1	7
19	R	24/121 (20%)	20 (83%)	4 (17%)	2	12
20	S	208/633 (33%)	181 (87%)	27 (13%)	3	18
22	b	70/176 (40%)	70 (100%)	0	100	100
23	d	69/89 (78%)	66 (96%)	3 (4%)	25	49
24	e	65/83 (78%)	60 (92%)	5 (8%)	10	34
25	f	63/77 (82%)	61 (97%)	2 (3%)	34	56
26	g	58/66 (88%)	57 (98%)	1 (2%)	56	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	h	77/129 (60%)	77 (100%)	0	100	100
28	j	79/103 (77%)	76 (96%)	3 (4%)	28	52
All	All	4706/7928 (59%)	4298 (91%)	408 (9%)	11	30

5 of 408 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	202	GLU
14	L	54	GLN
24	e	25	THR
12	J	269	ILE
13	K	48	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
13	K	33	GLN
20	S	61	ASN
13	K	174	ASN
15	M	44	ASN
20	S	79	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	138/179 (77%)	66 (47%)	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	95/112 (84%)	34 (35%)	5 (5%)
All	All	441/1558 (28%)	183 (41%)	31 (7%)

5 of 183 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

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Mol	Chain	Res	Type
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	-	26,34,34	0.88	1 (3%)	32,54,54	1.64	5 (15%)

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	-	-	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	-2.35	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	1101	GTP	PB-O3B-PG	-4.90	116.03	132.83
34	C	1101	GTP	PA-O3A-PB	-3.58	120.56	132.83
34	C	1101	GTP	C5-C6-N1	2.89	119.06	113.95
34	C	1101	GTP	O6-C6-C5	-2.72	119.07	124.37
34	C	1101	GTP	C8-N7-C5	2.53	107.81	102.99

There are no chirality outliers.

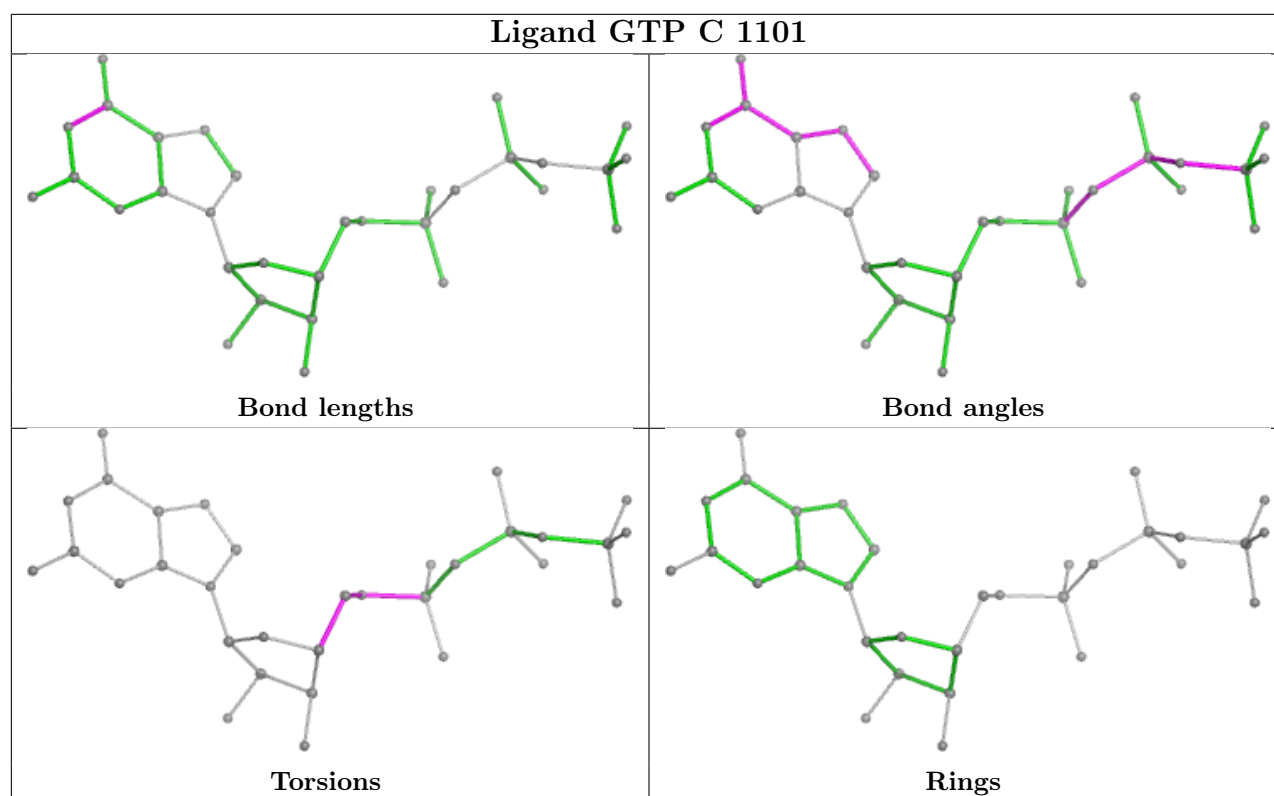
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	C	1101	GTP	C5'-O5'-PA-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
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

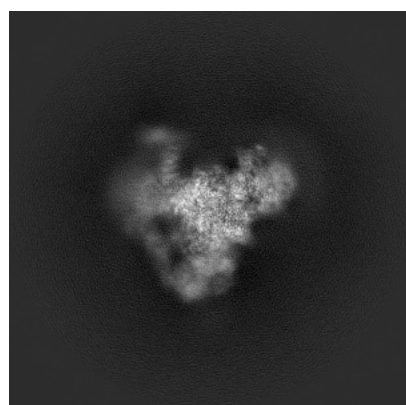
## 6 Map visualisation [i](#)

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.

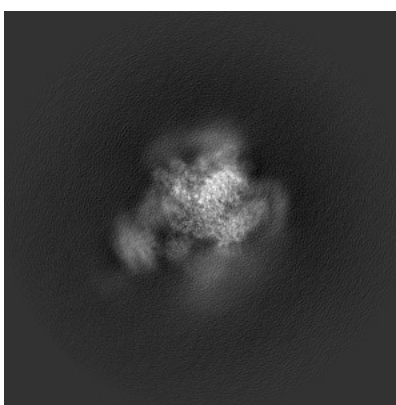
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

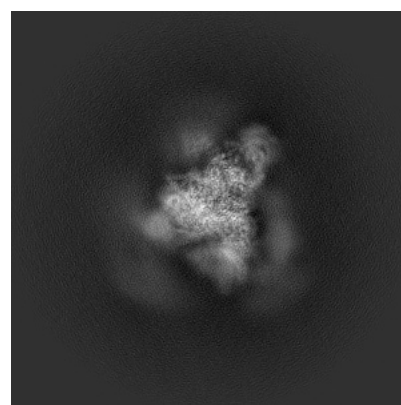
#### 6.1.1 Primary map



X



Y

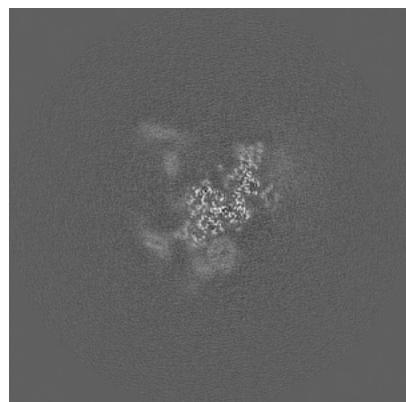


Z

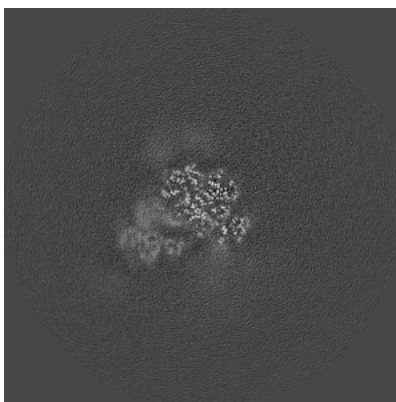
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

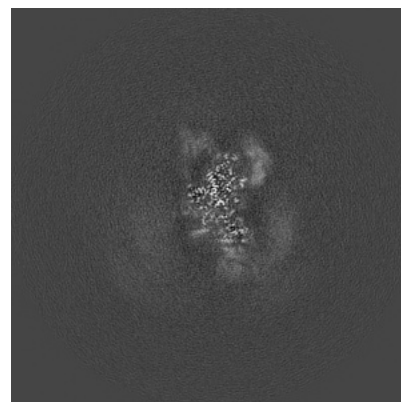
#### 6.2.1 Primary map



X Index: 206



Y Index: 206

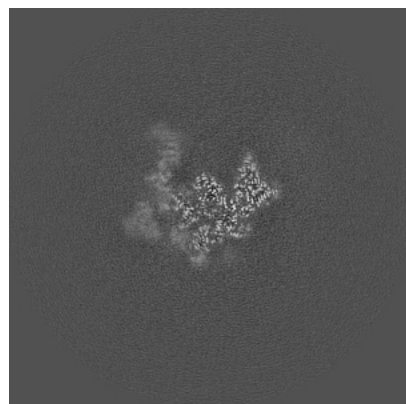


Z Index: 206

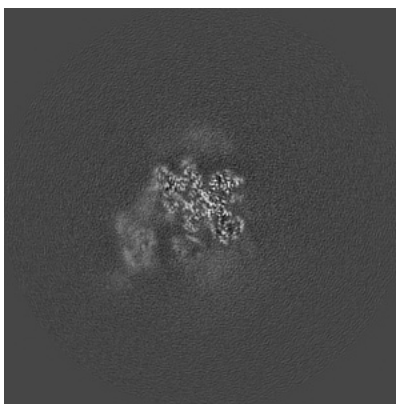
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

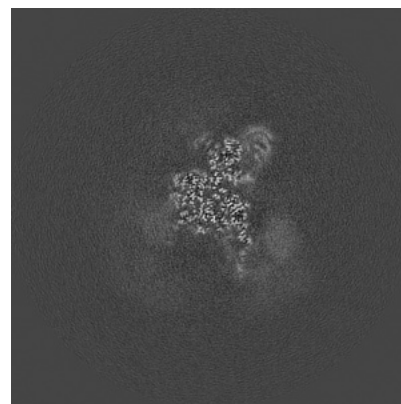
### 6.3.1 Primary map



X Index: 225



Y Index: 197

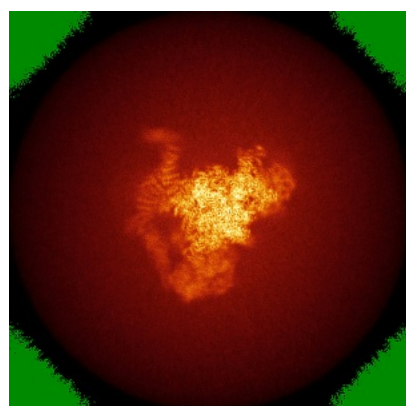


Z Index: 221

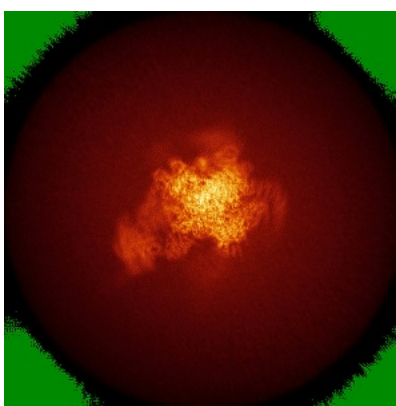
The images above show the largest variance slices of the map in three orthogonal directions.

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

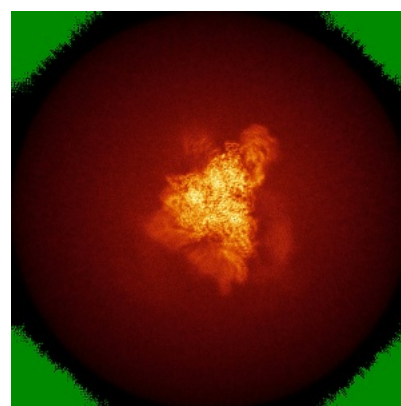
### 6.4.1 Primary map



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.

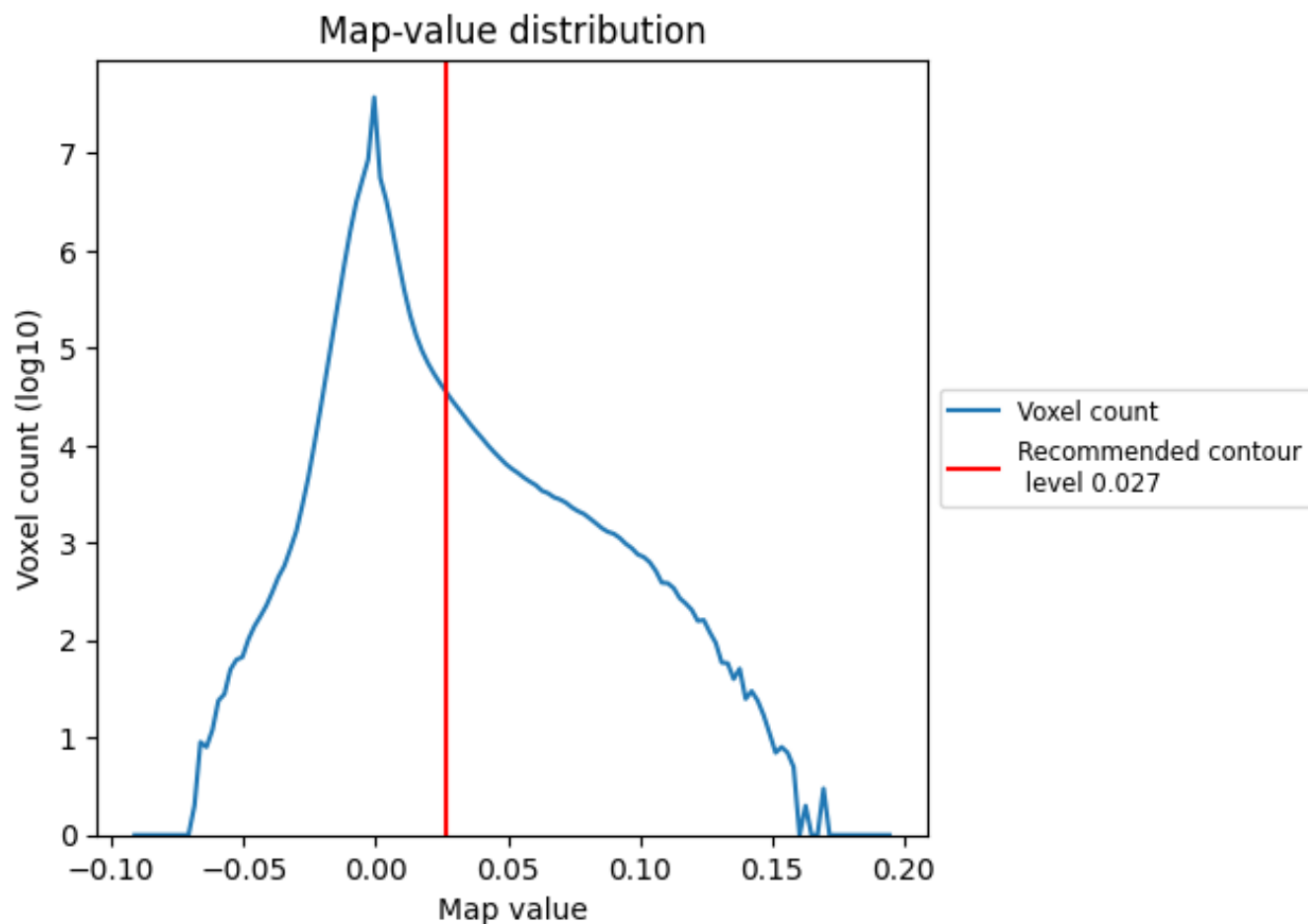
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

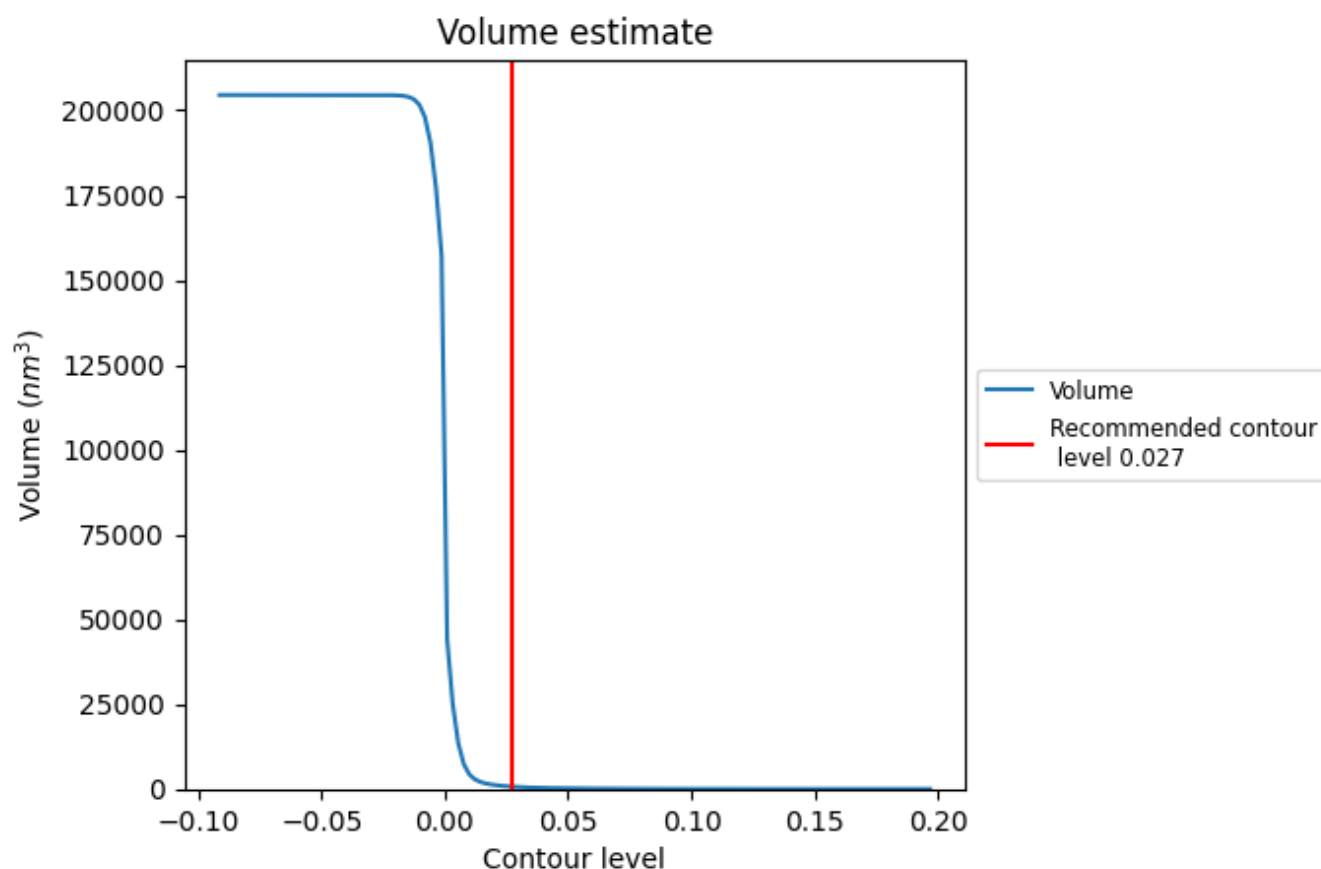
This section contains the results of statistical analysis of the map.

### 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.

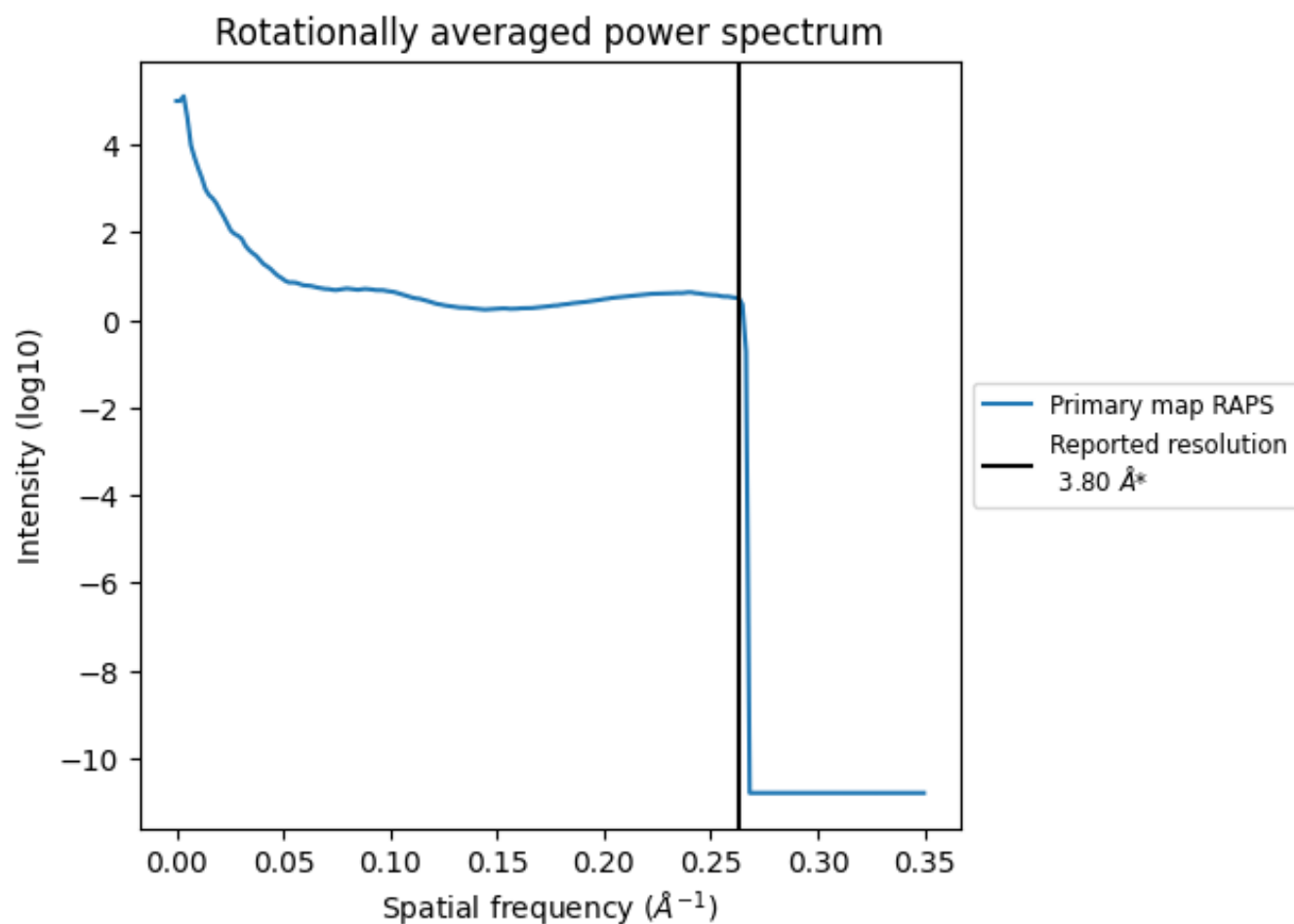
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699  $\text{nm}^3$ ; 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 ⓘ



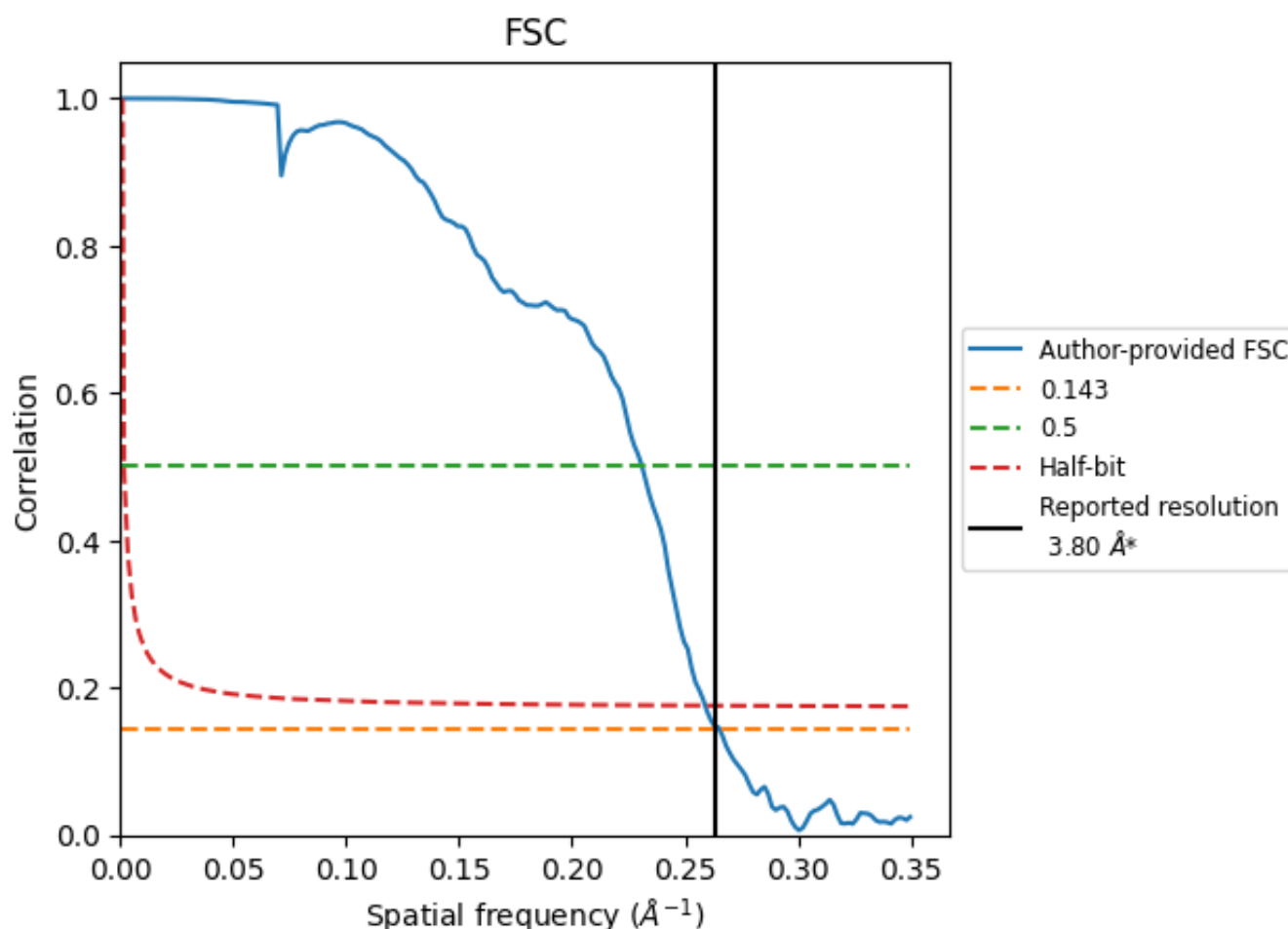
\*Reported resolution corresponds to spatial frequency of 0.263  $\text{\AA}^{-1}$



## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

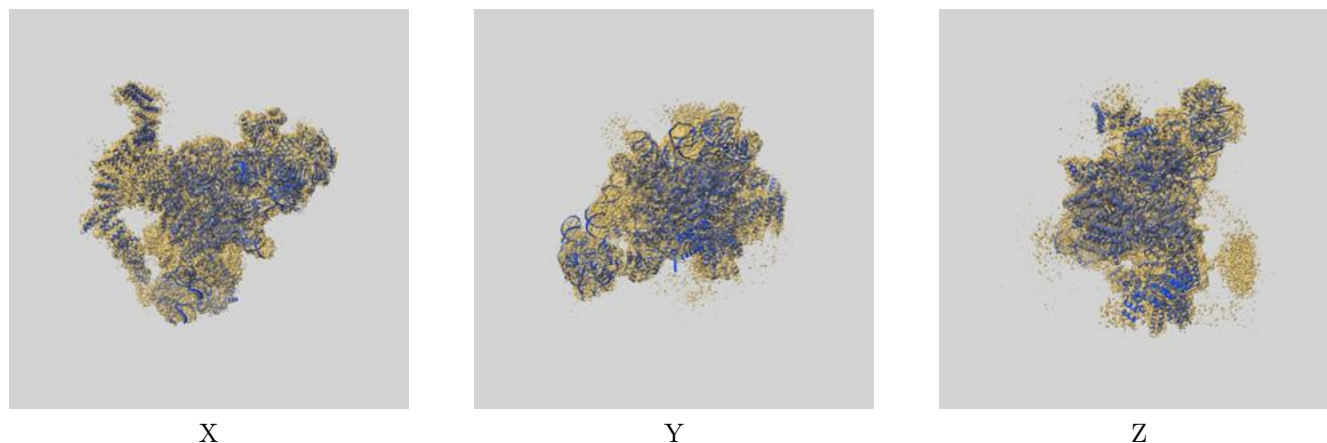
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.33	3.86
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

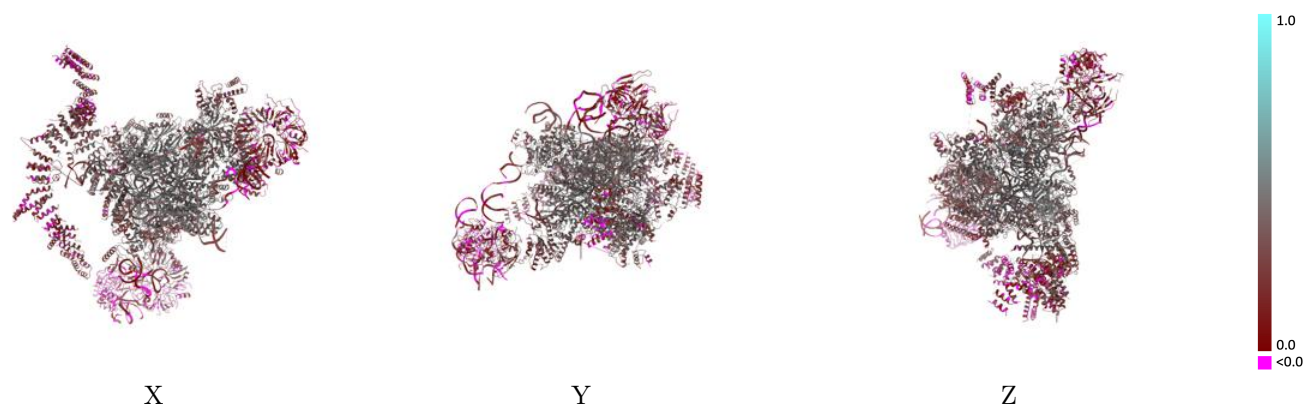
This section contains information regarding the fit between EMDB map EMD-4055 and PDB model 5LJ3. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

### 9.1 Map-model overlay [i](#)



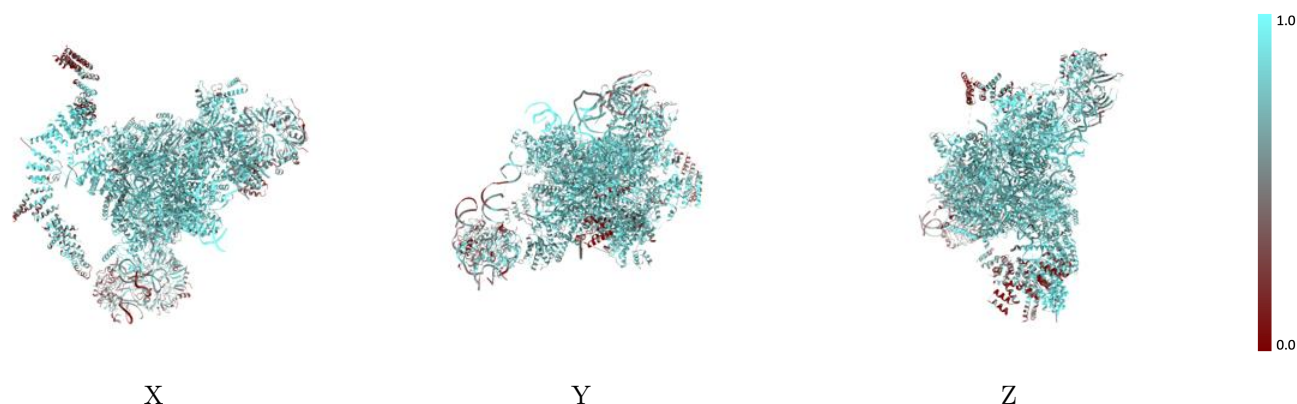
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



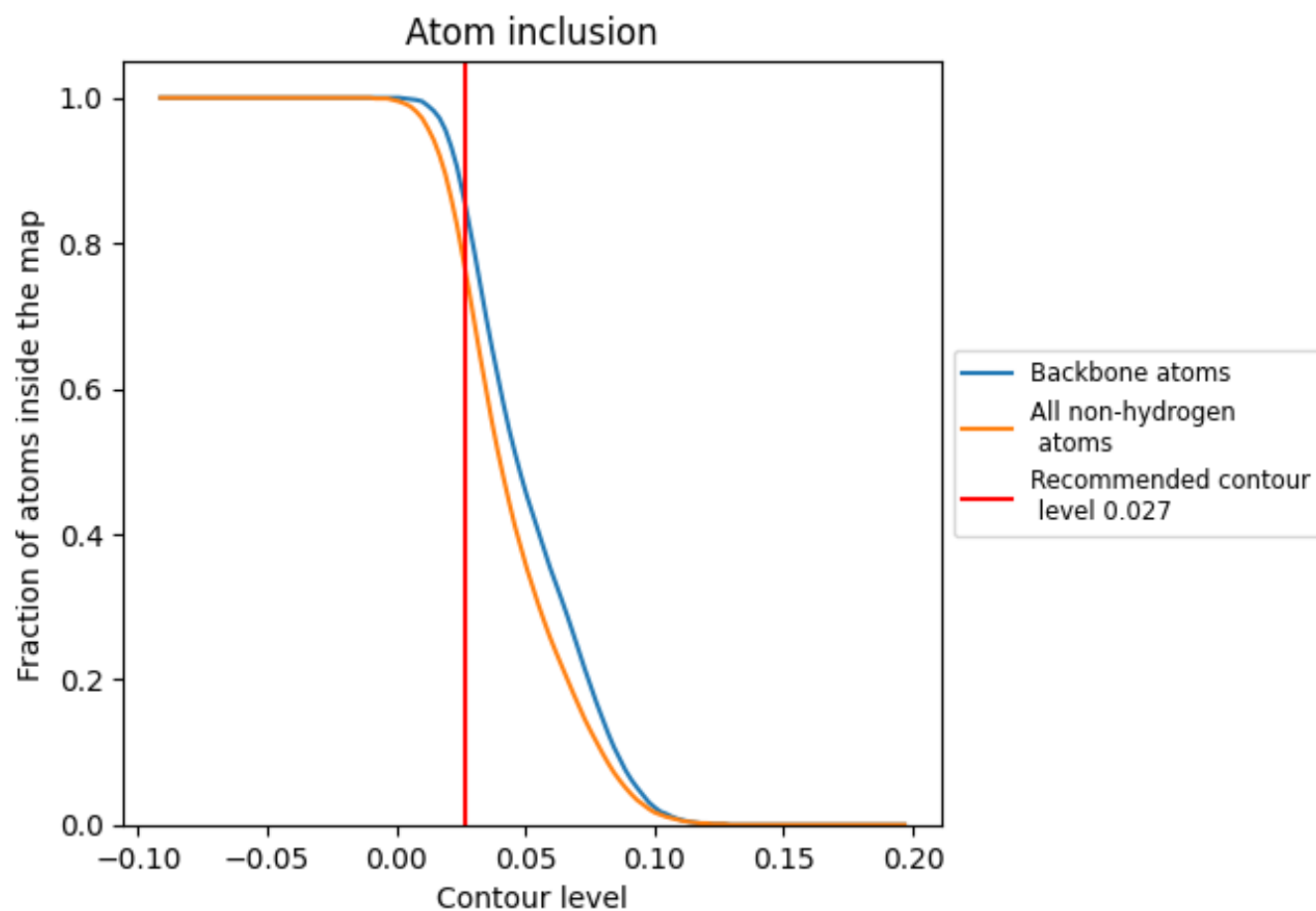
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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







































































## 9.4 Atom inclusion ⓘ



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