



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 10:49 PM UTC

PDB ID : 8I0R / pdb_00008i0r
EMDB ID : EMD-35107
Title : The cryo-EM structure of human Bact-I complex
Authors : Zhan, X.; Lu, Y.; Shi, Y.
Deposited on : 2023-01-11
Resolution : 3.00 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:

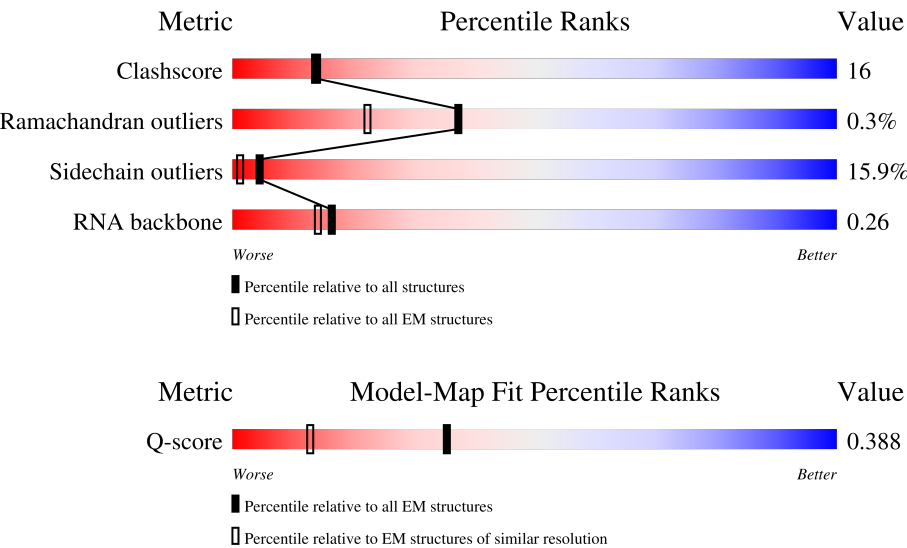
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	A	2335	56%32%7%.
2	B	117	28%44%11%16%
3	C	972	45%36%8%12%

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Mol	Chain	Length	Quality of chain
4	D	2136	
5	E	357	
6	F	107	
7	G	220	
8	H	188	
9	I	855	
10	J	848	
11	K	343	
12	L	802	
13	N	144	
14	O	420	
15	P	229	
16	Q	1485	
17	R	536	
18	S	1041	
19	T	514	
20	U	2752	
21	V	908	
22	W	122	
23	X	396	
24	Y	322	
25	Z	619	
26	1	1304	
27	3	1217	
28	p	225	

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Mol	Chain	Length	Quality of chain
29	w	501	
30	u	793	
31	2	895	
32	4	424	
33	6	125	
34	7	110	
35	5	86	
36	9	520	
37	8	904	
38	y	301	
39	v	464	
40	o	255	
41	c	118	
41	h	118	
42	d	86	
42	i	86	
43	a	240	
43	m	240	
44	g	126	
44	l	126	
45	f	76	
45	k	76	
46	e	92	
46	j	92	
47	b	119	

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Mol	Chain	Length	Quality of chain
47	n	119	30% 60% 8% 33%
48	z	472	23% 13% 62%

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 115060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2242	Total	C	N	O	S	0	0
			18543	11943	3241	3280	79		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	98	Total	C	N	O	P	0	0
			2066	925	347	696	98		

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	860	Total	C	N	O	S	0	0
			6724	4298	1122	1272	32		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1722	Total	C	N	O		0	0
			8528	5084	1722	1722			

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	299	Total	C	N	O	S	0	0
			2338	1470	410	445	13		

- Molecule 6 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 7 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	71	Total	C	N	O	P	0	0
			1481	663	243	504	71		

- Molecule 8 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	167	Total	C	N	O	P	0	0
			3539	1581	607	1184	167		

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	593	Total	C	N	O	0	0
			2991	1805	593	593		

- Molecule 10 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	249	Total	C	N	O	S	0	0
			2116	1355	380	375	6		

- Molecule 11 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	128	Total	C	N	O	S	0	0
			1059	660	190	204	5		

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	99	Total	C	N	O	S	0	0
			829	532	149	144	4		

- Molecule 13 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 14 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	290	Total	C	N	O	0	0
			1433	853	290	290		

- Molecule 15 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	42	Total	C	N	O	S	0	0
			362	231	63	66	2		

- Molecule 16 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	1329	Total	C	N	O	0	0
			6730	4072	1329	1329		

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	237	Total	C	N	O	S	0	0
			1889	1171	347	360	11		

- Molecule 18 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	643	Total	C	N	O	0	0
			3180	1894	643	643		

- Molecule 19 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	320	Total	C	N	O	S	0	0
			2507	1582	456	462	7		

- Molecule 20 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	72	Total	C	N	O	S	0	0
			422	257	82	82	1		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	468	Total	C	N	O	S	0	0
			3008	1873	546	576	13		

- Molecule 22 is a protein called Unknown polymer.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	43	Total	C	N	O	0	0
			229	140	46	43		

- Molecule 23 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	154	Total	C	N	O	S	0	0
			1279	819	231	227	2		

- Molecule 24 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	118	Total	C	N	O	S	0	0
			948	605	163	176	4		

- Molecule 25 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	137	Total	C	N	O	S	0	0
			1142	708	213	216	5		

- Molecule 26 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	993	Total	C	N	O	P	S	0	0
			7866	5018	1363	1438	1	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	1177	Total	C	N	O	S	0	0
			9220	5854	1566	1755	45		

- Molecule 28 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	p	169	Total	C	N	O	0	0
			851	513	169	169		

- Molecule 29 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	434	Total	C	N	O	S	0	0
			2275	1287	491	493	4		

- Molecule 30 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	u	187	Total	C	N	O	0	0
			834	460	187	187		

- Molecule 31 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2	250	Total	C	N	O	S	0	0
			1807	1134	340	326	7		

- Molecule 32 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	4	161	Total	C	N	O	0	0
			792	470	161	161		

- Molecule 33 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	109	Total	C	N	O	S	0	0
			906	582	157	163	4		

- Molecule 34 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	105	Total	C	N	O	S	0	0
			811	502	145	151	13		

- Molecule 35 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5	81	Total	C	N	O	S	0	0
			669	422	117	124	6		

- Molecule 36 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	379	Total	C	N	O	S	0	0
			2636	1633	479	516	8		

- Molecule 37 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	8	115	Total	C	N	O	S	0	0
			931	602	154	170	5		

- Molecule 38 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	y	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 39 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	v	173	Total	C	N	O	S	0	0
			1041	602	219	217	3		

- Molecule 40 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	o	162	Total	C	N	O	0	0
			816	492	162	162		

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	h	95	Total	C	N	O	0	0
			482	292	95	95		
41	c	97	Total	C	N	O	0	0
			388	194	97	97		

- Molecule 42 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	i	72	Total	C	N	O	0	0
			359	215	72	72		
42	d	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	m	82	Total	C	N	O	0	0
			413	249	82	82		
43	a	86	Total	C	N	O	0	0
			344	172	86	86		

- Molecule 44 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	l	83	Total	C	N	O	0	0
			415	249	83	83		
44	g	81	Total	C	N	O	0	0
			324	162	81	81		

- Molecule 45 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	k	73	Total	C	N	O	0	0
			364	218	73	73		
45	f	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 46 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	j	81	Total	C	N	O	0	0
			403	241	81	81		
46	e	79	Total	C	N	O	0	0
			316	158	79	79		

- Molecule 47 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	n	80	Total	C	N	O	0	0
			402	242	80	80		

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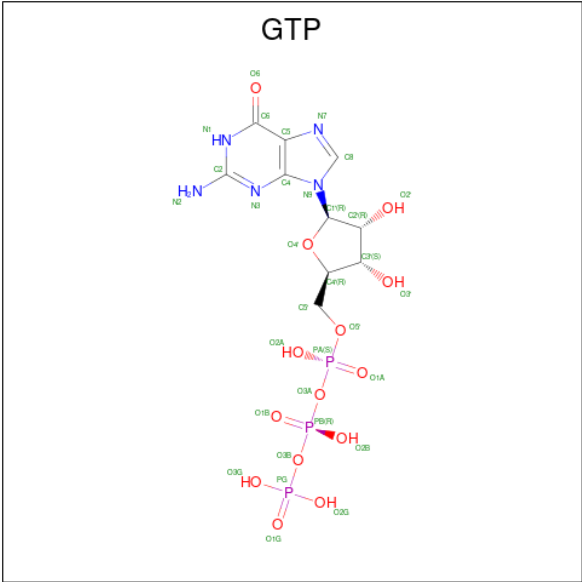
Mol	Chain	Residues	Atoms				AltConf	Trace
47	b	82	Total	C	N	O	0	0
			328	164	82	82		

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | z | 177 | Total | C | N | O | S | 1 | 0 |
| | | | 1402 | 884 | 243 | 270 | 5 | | |

-

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

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

- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	C	1	Total	Mg	0
			1	1	
51	F	5	Total	Mg	0
			5	5	

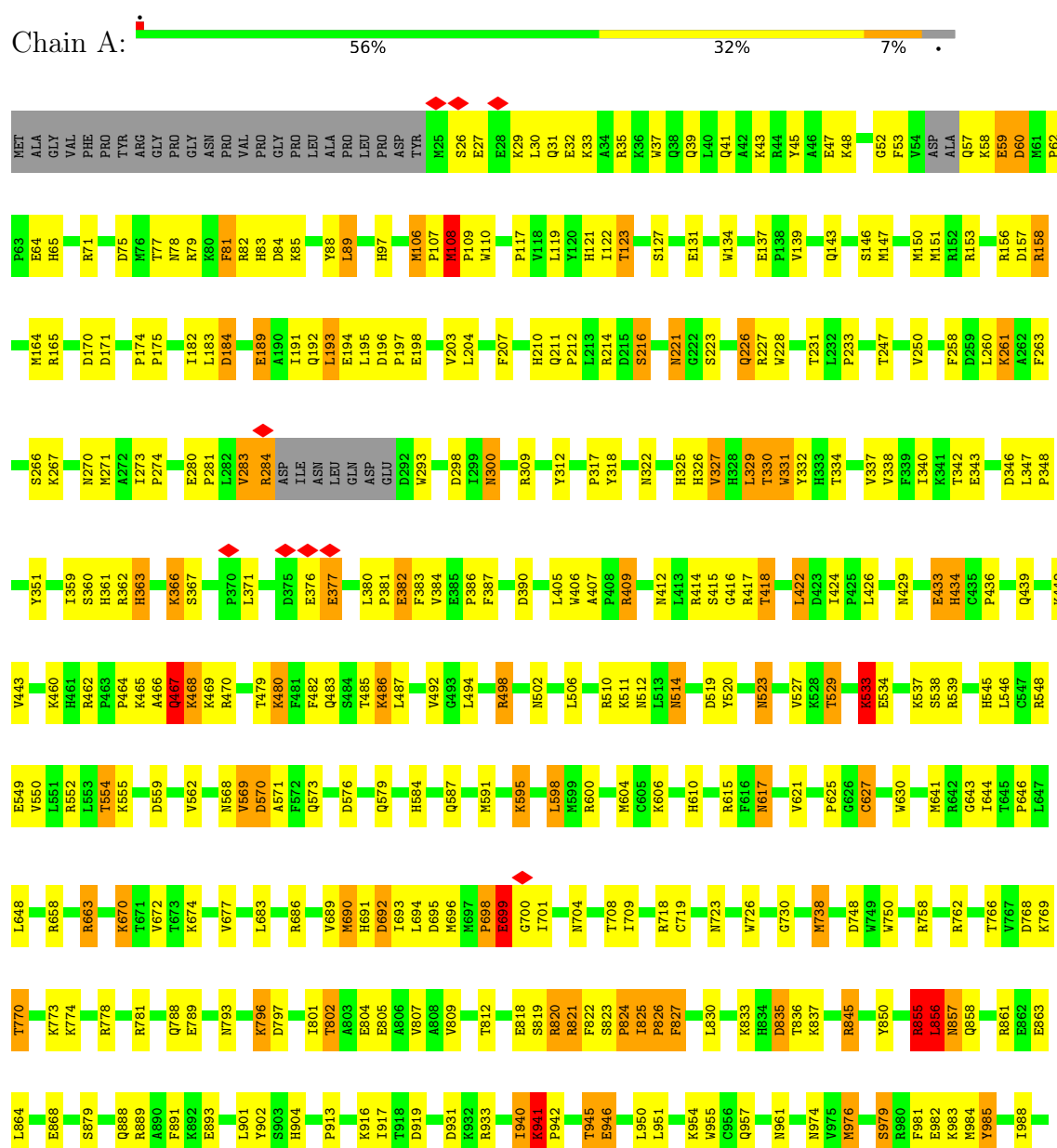
- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

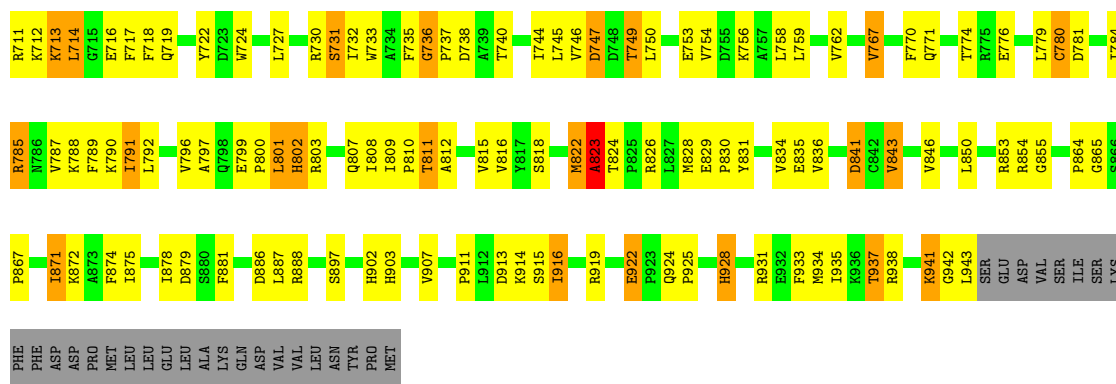
Mol	Chain	Residues	Atoms		AltConf
52	K	1	Total	Zn	0
			1	1	
52	N	3	Total	Zn	0
			3	3	
52	7	3	Total	Zn	0
			3	3	

3 Residue-property plots

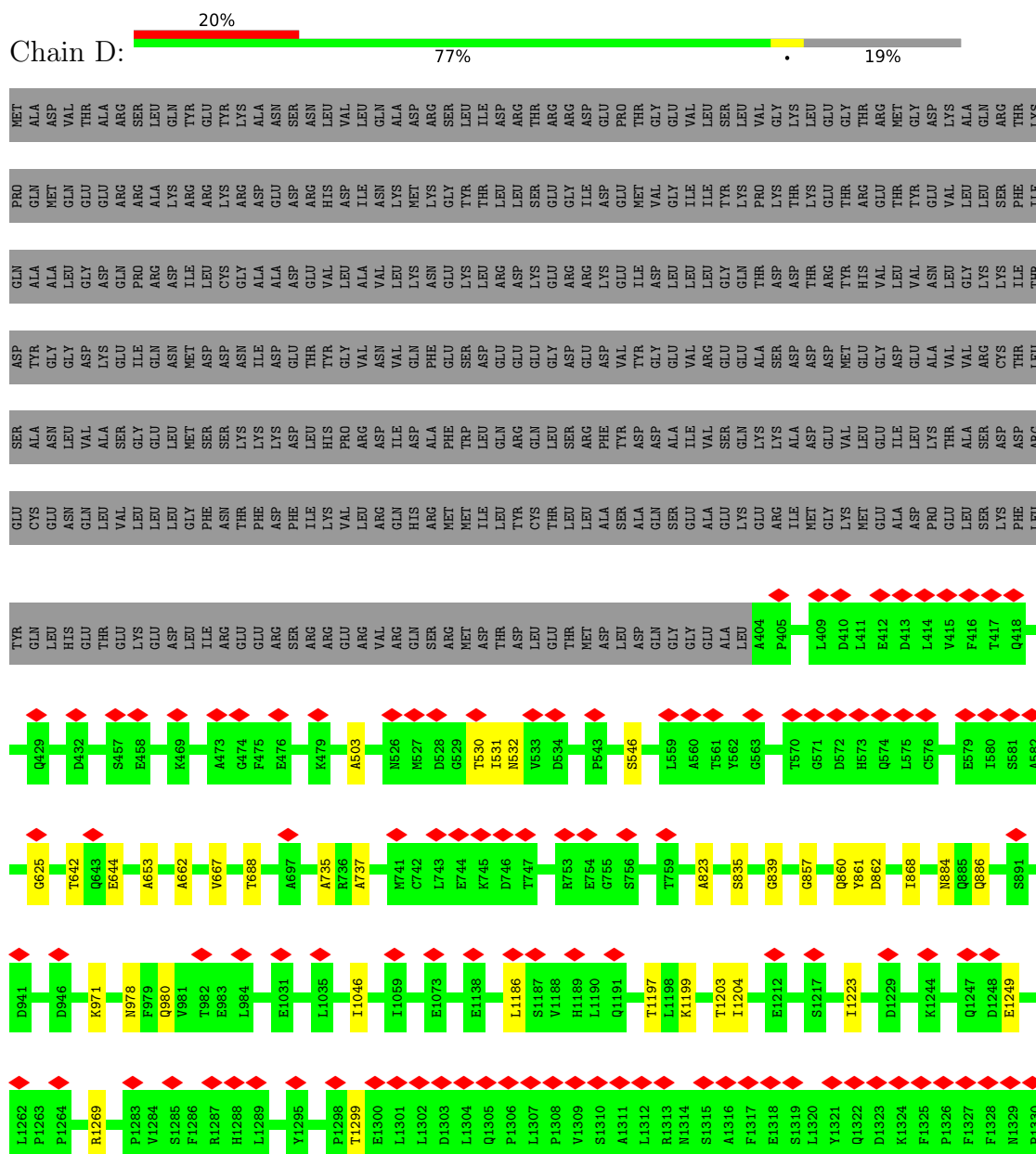
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

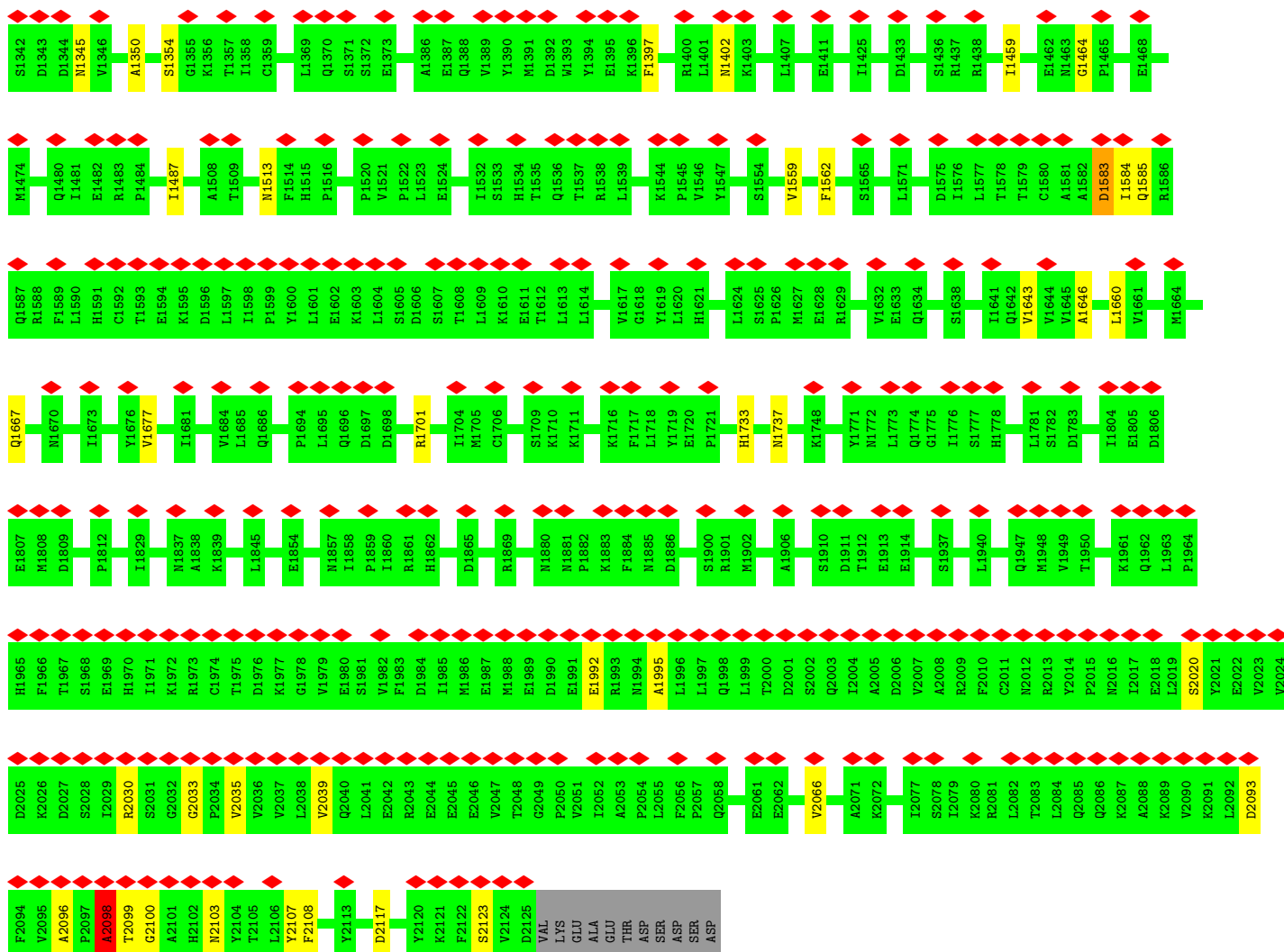
• Molecule 1: Pre-mRNA-processing-splicing factor 8



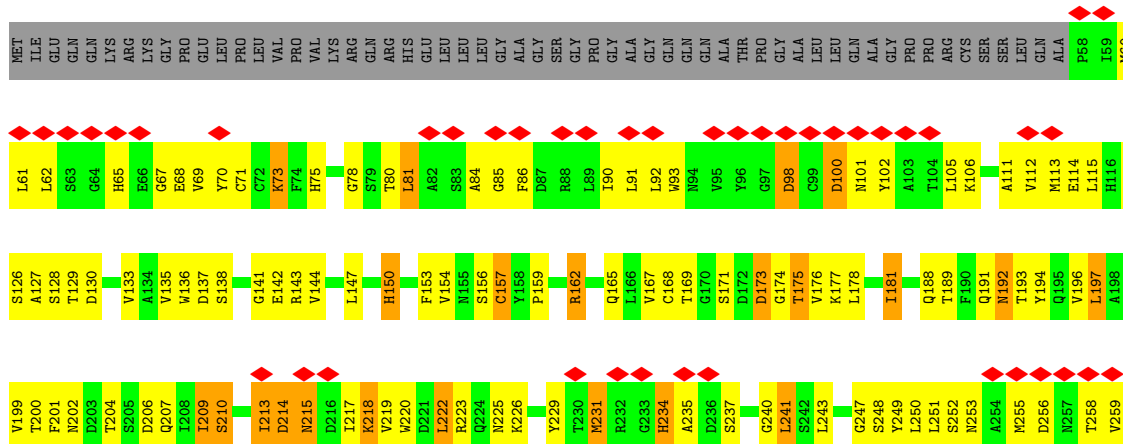


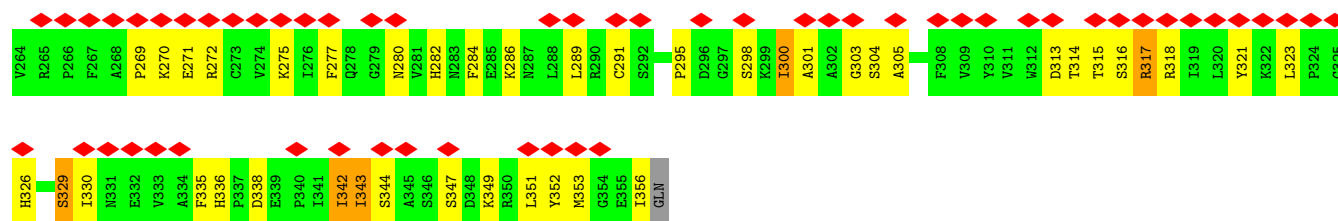
• Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase



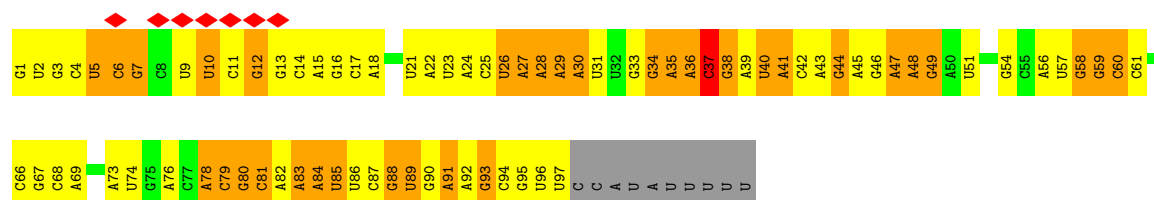
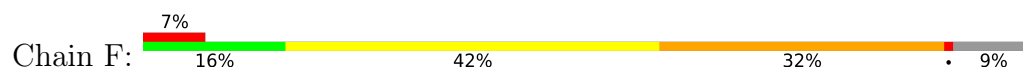


● Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

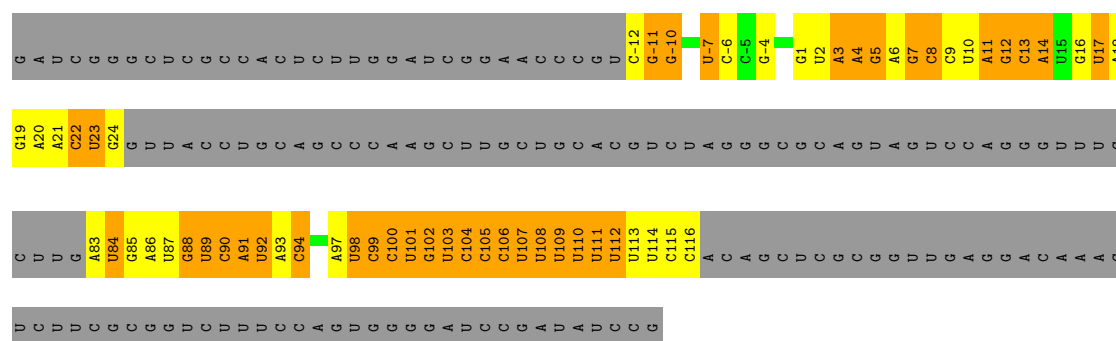




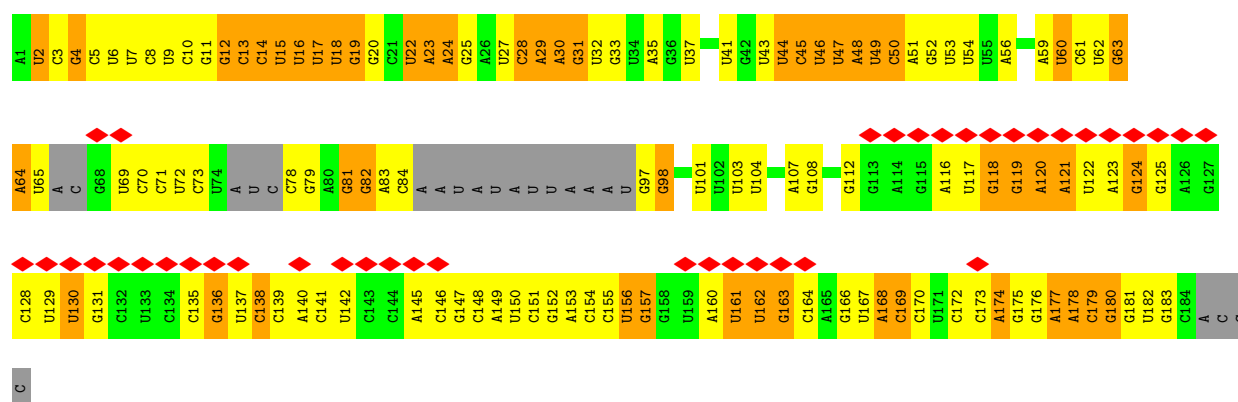
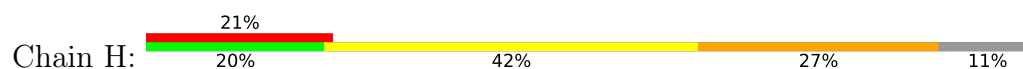
• Molecule 6: U6 snRNA



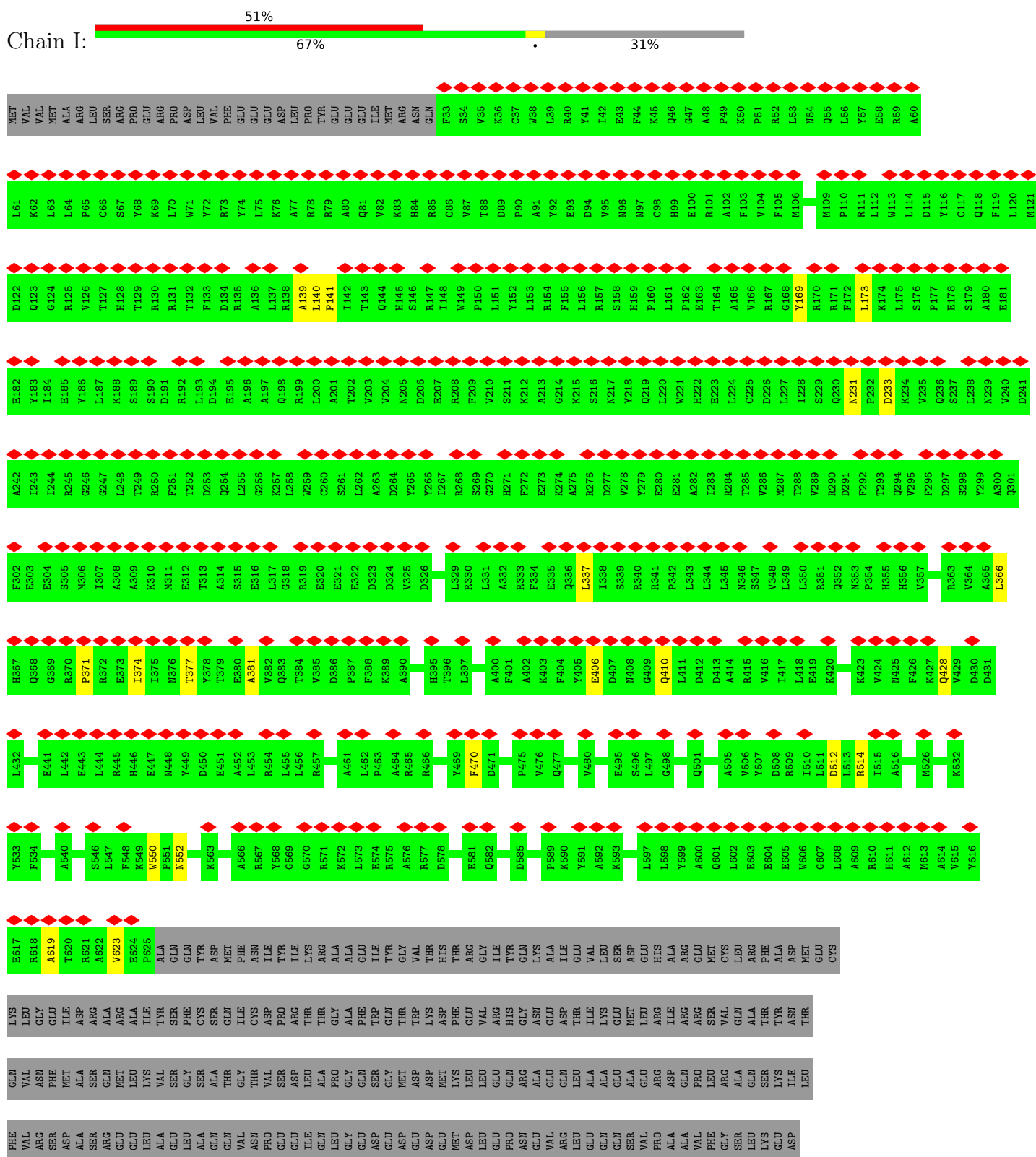
• Molecule 7: pre-mRNA



• Molecule 8: U2 snRNA



• Molecule 9: Pre-mRNA-splicing factor SYF1

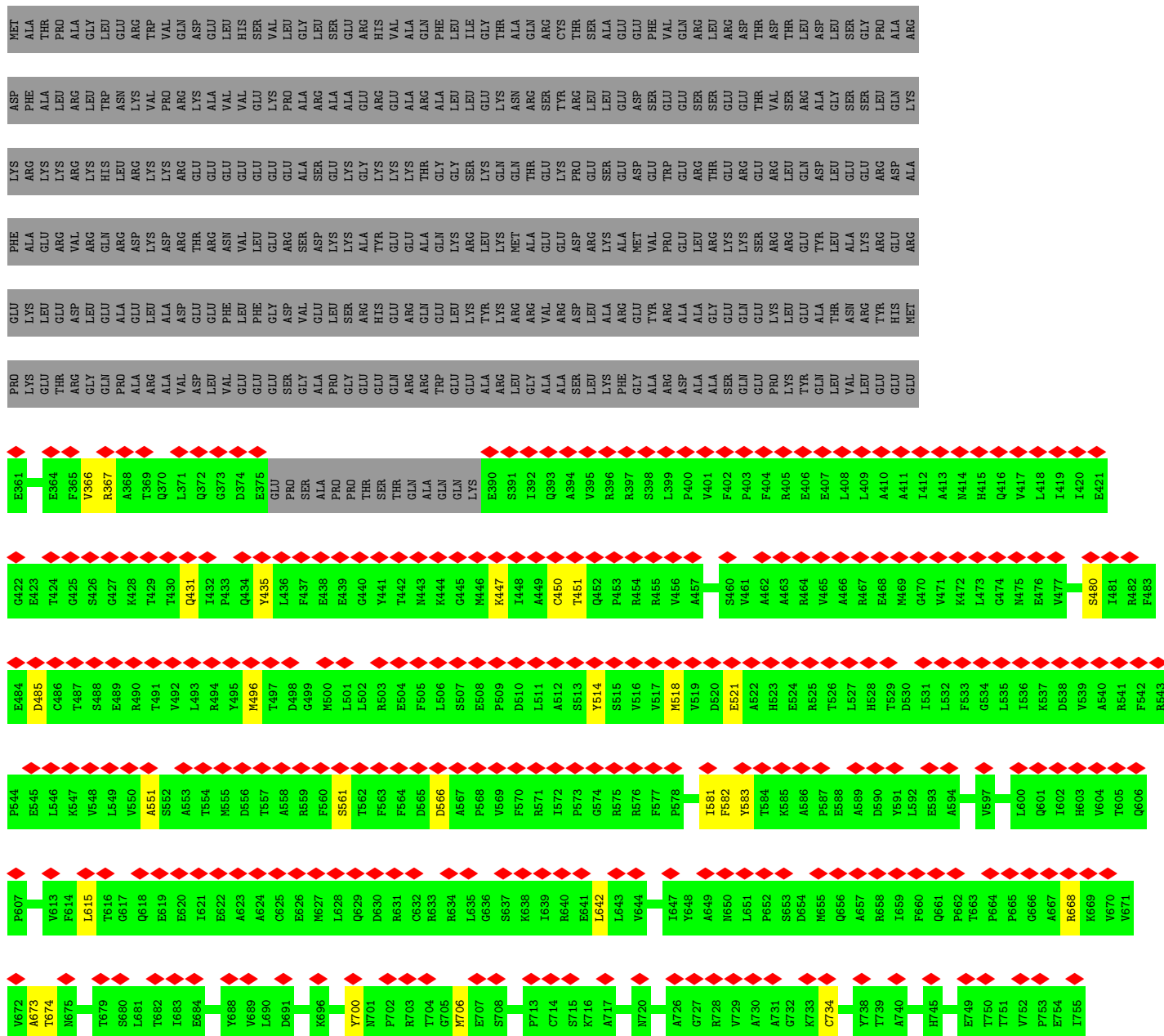


- Molecule 10: Crooked neck-like protein 1



R905	R906	E907	L908	L909	E910	E911	V912	R913	R914	L915	Q916	R917	S918	L919	Q920	V921	P922	G923	D924	A925	S926	Y927	T928	C929	E930	T931	G933	Y934	F935	F936	L937	Y938	Q939	V940	N941	S942	E943	W944	E945	E946	Y947	I948	S949	K950	V951	K952	N953	LYS	GLY	SER	LEU	P959	D960	V961	T962	E963	V964																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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- Molecule 18: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16

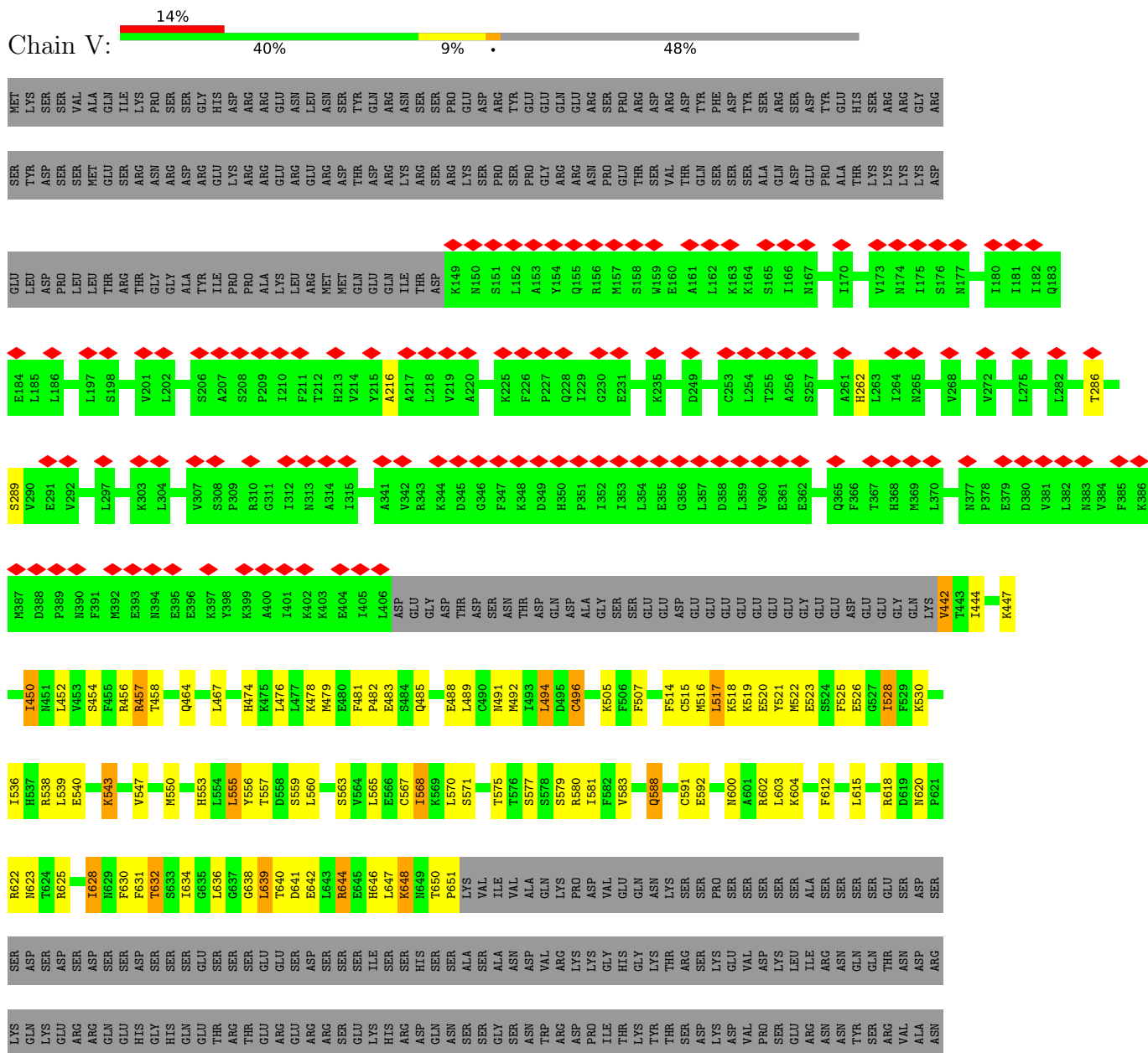




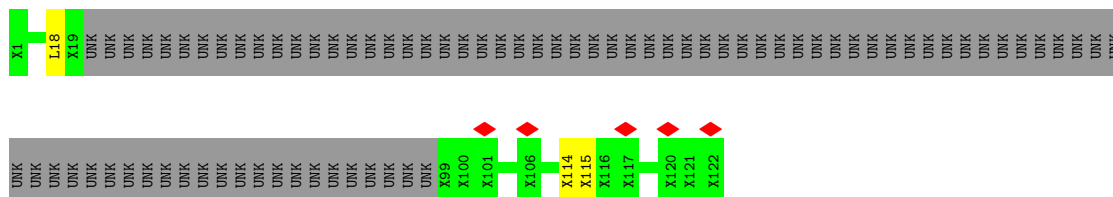




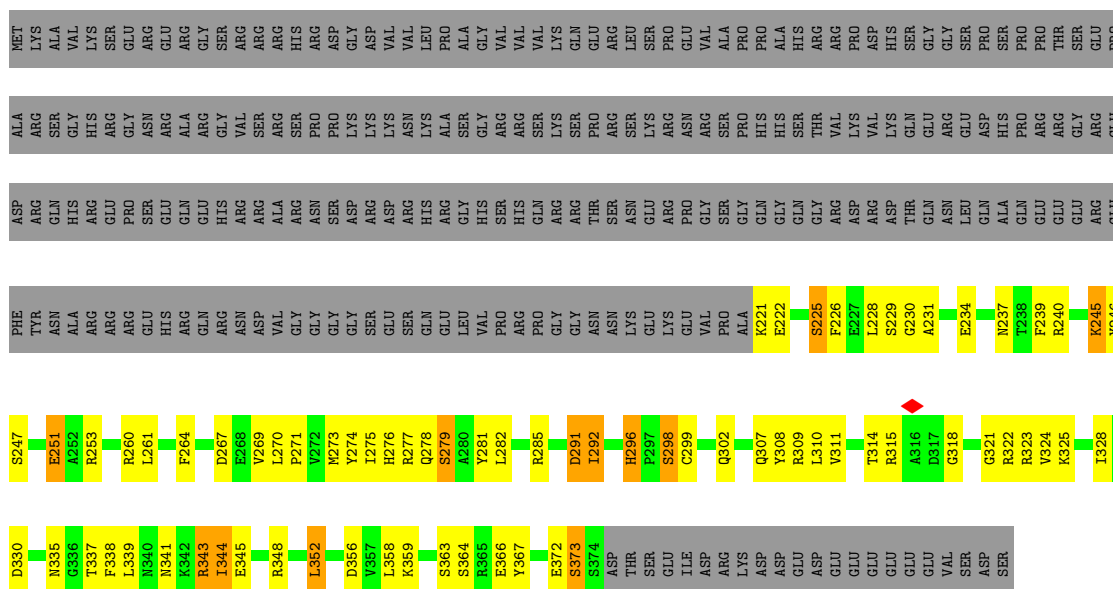
- Molecule 21: Pre-mRNA-splicing factor CWC22 homolog



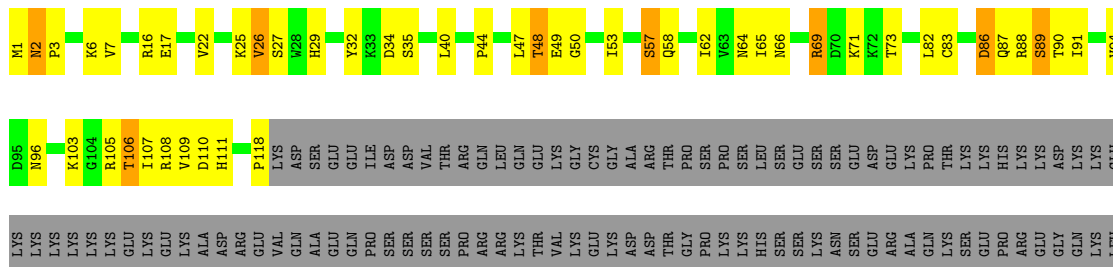
- Molecule 22: Unknown polymer



- Molecule 23: Smad nuclear-interacting protein 1



- Molecule 24: RNA-binding motif protein, X-linked 2



[illegible]

- Molecule 25: BUD13 homolog



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

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

The chart displays the distribution of 160 amino acids across four categories: ARG, ARG, ARG, and ARG. The segments are color-coded: yellow for the first 100, orange for the next 40, and green for the last 20. The segments are labeled with their respective amino acid codes (e.g., N557, K558, R559, etc.). The chart shows that the distribution is not uniform, with some amino acids appearing more frequently than others.

- Molecule 26: Splicing factor 3B subunit 1

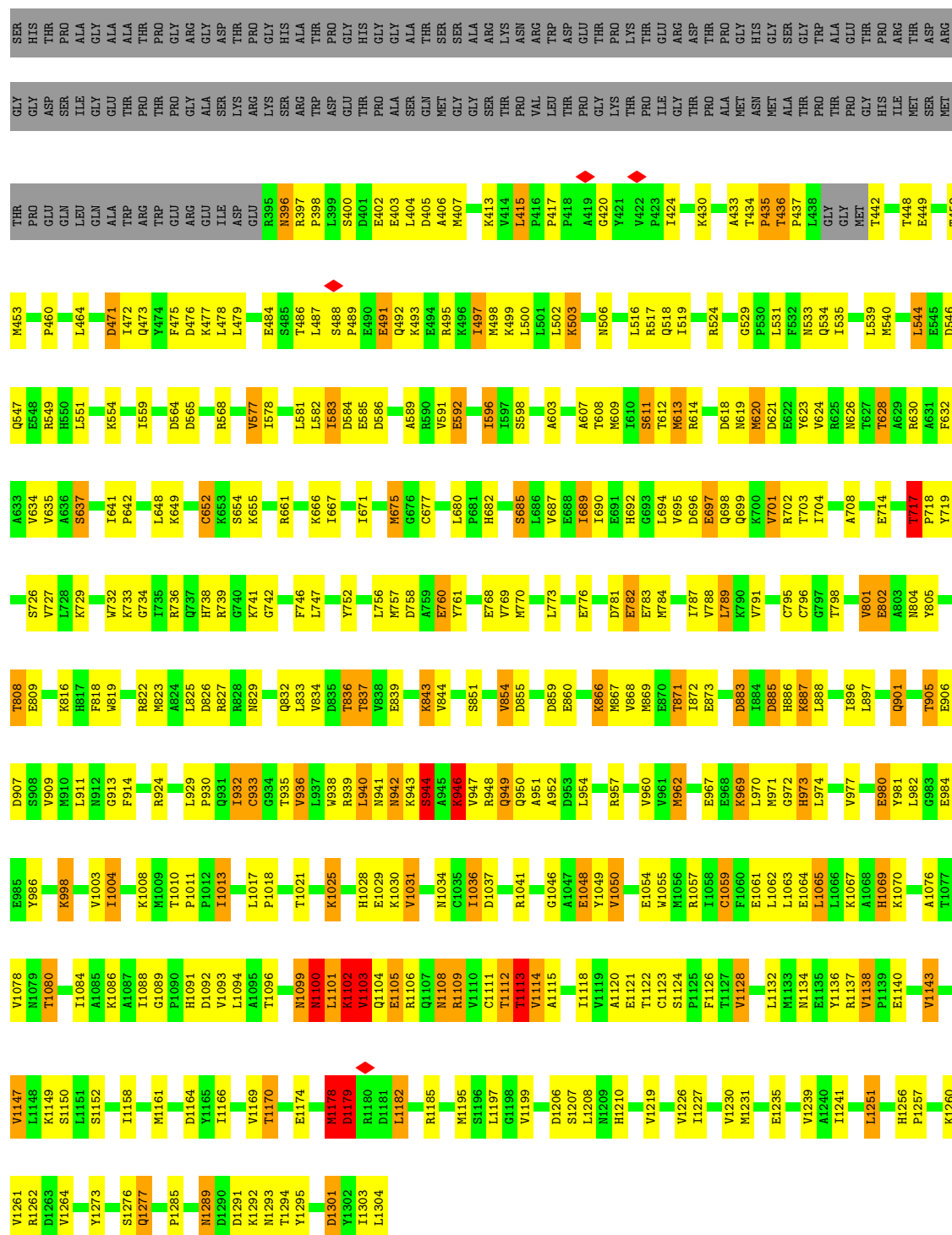


MET	ALA	LYS	ILE	ALA	LYS	THR	HIS	GLU	ASP	ILE	GLU	ALA	GLN	ILE	ARG	GLU	ILE	GLN	LYS	LYS	ALA	ALA	LEU	ASP	GLU	GLN	ALA	GLN	GLY	VAL	GLY	LEU	ASP	SER	THR	GLY	TYR	TYR	ASP	ASP	GLN	GLU	ILE	TYR	GLY	GLY	SER	SER	ARG	PHE	ALA	GLY	GLY	TYR	VAL	THR	SER	ILE	ALA	ALA
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THR	GLU	GLU	GLU	ASP	ASP	ASP	ASP	TYR	SER	SER	SER	THR	THR	GLU	GLN	Y101	D102	P103	E106	K111	I112	D117	E118	Y119	K120	K121	I122	K123	R124	T125	M126	I127	I128
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P130	D134	P135	D138	K141	T142	P145	K146	R150	T151	Y152	M153	D154	M155	R156	R157	E158	L161	T162	K163	E164	E165	R166	R169	Q170	Q171	L172	A173	E174	K175	A176	L178	L179	GLY	ALA	GLY	GLU	LEU	LYS	VAL	VAL	ASN	GLY	GLY	ALA	ALA	ALA	SER	GLN	PRO	PRO	SER	SER	LYS	ARG	LYS	PRO
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ARG ASP GLN THR ALA ASP GLN THR PRO LYS LYS LEU SER TRP ASP GLN GLU THR PRO GLY HIS PRO SER LEU ARG TRP ASP GLU THR PRO GLY GLY ARG ALG LYS GLY SER GLU THL THR PRO GLY ALA THR PRO GLY LYS LLE ASP TRP PRO



• Molecule 27: Splicing factor 3B subunit 3

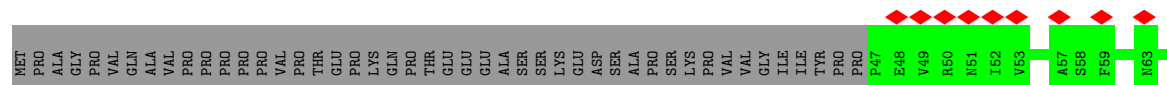
Chain 3: 47% 42% 7%



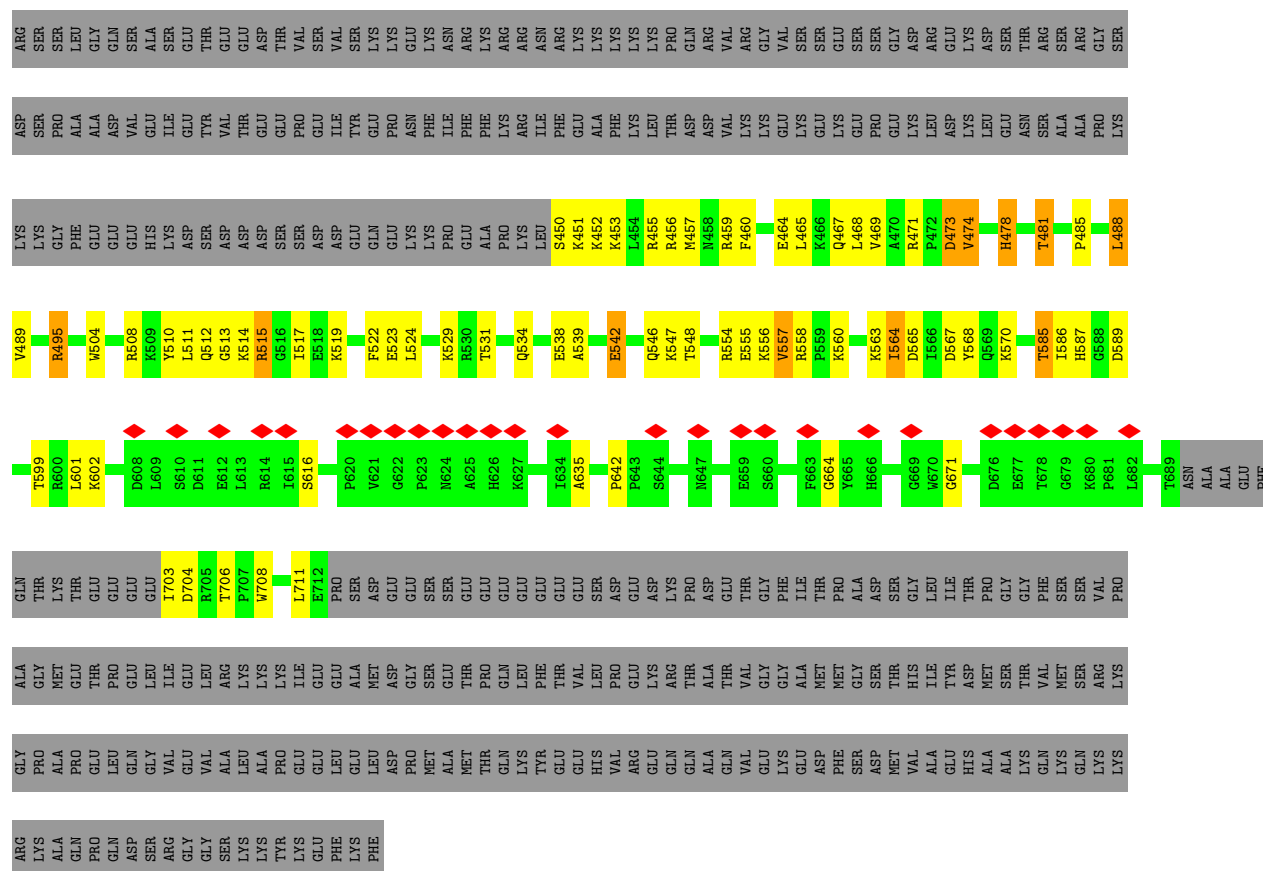
L1122	L1123	I1128	T1133	S1134	H1135	E1136	D1137	F1140	V1144	M1146	C1156	G1157	R1158	D1159	H1160	L1161	S1162	S1165	P1169	V1170	I1174	D1175	E1186	P1187	K1188	N1189	Q1190	S1194	R1199	T1200	E1203	K1207	D1210	R1214	Y1215	A1216	F1217																													
Y92	Q93	P94	S95	K96	E100	K101	H103	G108	A200	K109	S110	M187	D188	Y189	E190	E191	M194	D195	P196	T197	G198	E199	A200	K201	A202	R1114	I1115	T204	Q205	Q206	T209	E212	G127	R128	D214	L215	N218	H219	V220	K137	Q138	R222	K223	Y224	S225	R146	D147	R151	L152	T153	I154	S155	S156	E159	A160	H161	K162	T165	D174	V175	E178	T257	Y258	K259	N260	E186
D263	Q264	P265	D266	L267	P272	R275	L278	D280	P281	A282	Q285	Q286	S290	H293	K294	T295	M298	F299	F300	Q304	T305	E306	Q307	G308	D309	I310	F311	T314	L315	E316	T317	I236	T237	G240	P245	S246	L249	S252	E253	I256	T257	Y258	K259	N260	E186																					
L342	L347	S351	E352	F353	G354	H356	Y357	G365	E370	P371	R372	F373	S374	L379	E380	GLU	GLY	T384	F385	F386	F387	Q388	P389	R390	K393	N394	D399	E400	L401	D402	S403	L404	F405	P406	I407	F409	C410	Q411	I412	N417	E418	D419	T420	L423	Y424	A426																				
C427	G428	R429	G430	S433	S434	L438	L442	E443	M447	E451	R452	L452	M455	P456	M457	A458	V459	W460	T461	V462	R463	F464	H465	Q466	P467	D468	E469	F470	D471	A472	Y473	I474	I475	V476	S477	F478	V479	M480	A481	T482	L483	V484	L485	S486	I487	G488	R489	T490	K491	E492	E493	F499														
L506	S507	C508	L511	G512	A515	L516	V517	Q518	V519	Y520	P521	I524	R525	H526	I527	R528	W536	V537	E538	F539	N550	Q551	R552	Q553	V554	F555	I556	A557	Y473	I474	I475	V476	S477	F478	V479	M480	A481	T482	L483	V484	L485	S486	I487	G488	R489	T490	K491	E492	E493	F499																
V588	C589	M590	S591	L592	V595	E599	Q600	R601	F604	L605	A606	V607	G608	L609	V610	D611	M612	T613	V614	R615	L616	L617	S618	P619	L620	P621	L622	S623	M630	Q631	A632	L633	P634	A635	Q636	P637	E638	S639	L640	C641	I642	V643	E644	R645	GLY	THR	GLY	LYS	GLN	ASP	GLU															
LEU	GLY	ARG	GLY	SER	ILE	GLY	F662	L663	R664	L665	P666	L667	G668	L669	G670	N671	G672	V673	L674	L675	R676	T677	V678	L679	D680	P681	V682	T683	G684	D685	Q626	P627	L628	S629	M630	Q631	A632	L633	P634	A635	Q636	P637	E638	S639	L640	C641	I642	V643	E644	R645	GLY	THR	GLY	LYS	GLN	ASP	GLU									
S716	S717	R718	S719	W720	L721	S722	Y725	Q726	L731	T732	P733	L734	S735	Y736	L739	E740	F741	A742	S743	F744	R745	A746	S747	E748	Q749	C750	G753	L754	V755	A756	L757	S758	T761	L762	E768	R769	L770	F774	W775	L781	Q782	K783	F788	H791																						
S794	H795	N796	L799	I800	E801	H804	N805	A806	Y807	T811	R815	K816	Q817	Q818	E821	E822	R823	V824	G828	E833	ASP	GLU	ARG	GLU	L834	A835	A836	E837	N838	F842	L843	N844	E845	N846	L847	P848	T851	F852	K856	A857	G858	N859	Q860	Q861	S864	V865	I866	R867																		
H870	P871	I872	Q873	H874	G875	R876	L877	D878	L879	E883	O884	N885	E886	F889	S890	V893	C894	R895	F896	T899	G900	E901	D902	V905	L906	V907	G908	V909	A910	K911	N912	L913	I914	L915	N916	P917	R918	S919	V920	A921	G922	Y926	T927	Y928	K929	L930	V931	N932	N933	G934	E935	K936														
F939	L940	H941	K942	T943	E946	E947	V948	G957	R958	V959	L960	I961	K965	L966	L967	R968	D971	L972	K976	L977	L978	R979	K980	C981	E982	L983	K984	N988	Y989	I990	S991	T995	I996	G997	H998	I1001	V1002	S1003	S1008	F1009	R1013	Y1014	K1015	R1016	N1017	E1018	N1019	D1026																		
D1027	T1028	T1035	A1036	S1037	G1046	A1047	D1048	K1049	I1053	G1054	V1055	V1056	R1057	L1058	T1062	N1063	D1064	E1065	V1066	D1067	ASP	PRO	THR	GLY	ASN	LYS	ALA	LEU	TRP	ASP	ARG	GLY	N1083	G1084	K1088	M1093	L1102	Q1105	K1106	T1107	T1108	S1114	V1118	Y1119	T1120	T1121																				

• Molecule 28: U2 small nuclear ribonucleoprotein B”



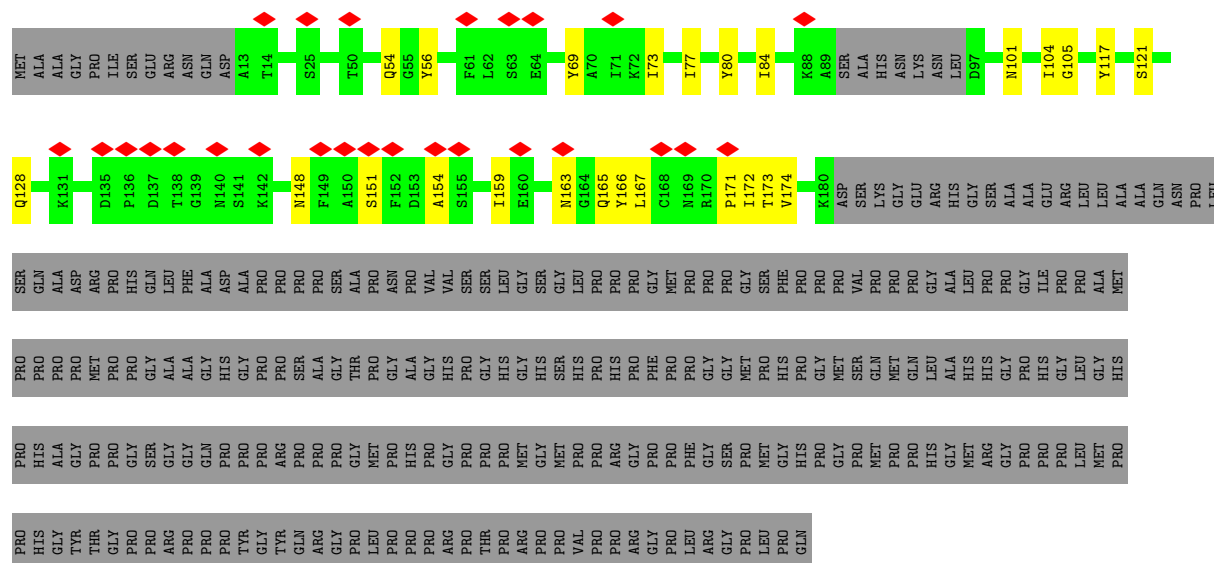






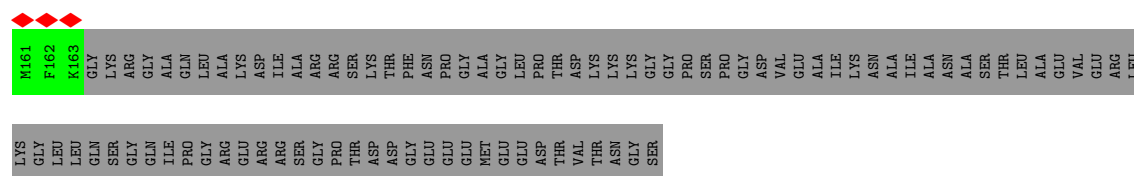
• Molecule 32: Splicing factor 3B subunit 4

Chain 4: 6% 32% 6% 62%

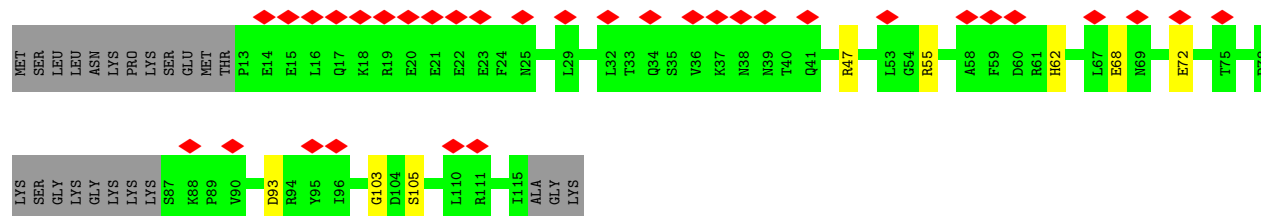
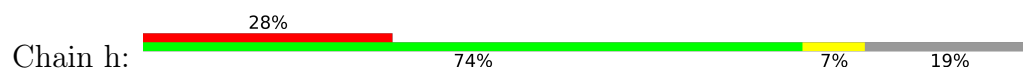


• Molecule 33: Splicing factor 3B subunit 6

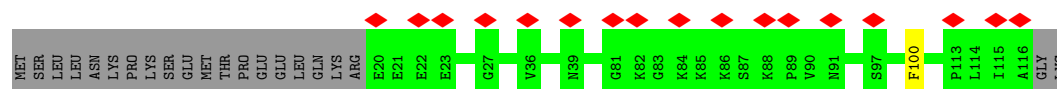
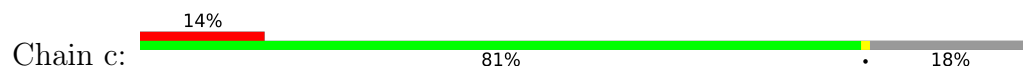
Chain 6: 37% 41% 10% 13%



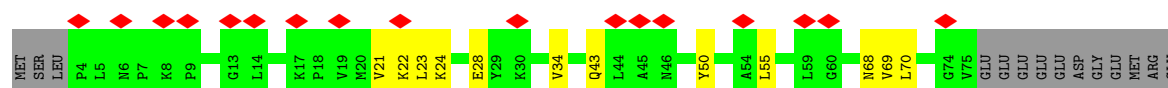
• Molecule 41: Small nuclear ribonucleoprotein Sm D2



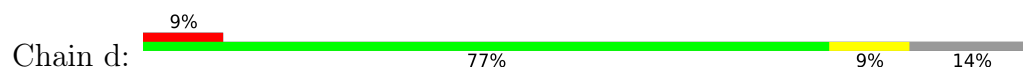
• Molecule 41: Small nuclear ribonucleoprotein Sm D2



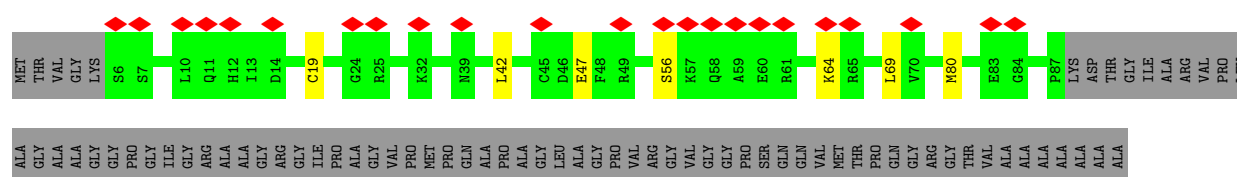
• Molecule 42: Small nuclear ribonucleoprotein F



• Molecule 42: Small nuclear ribonucleoprotein F

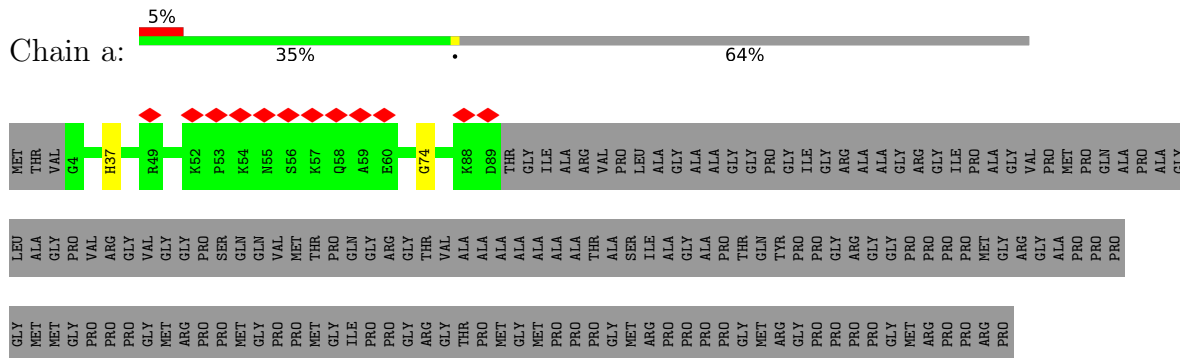


• Molecule 43: Small nuclear ribonucleoprotein-associated proteins B and B'

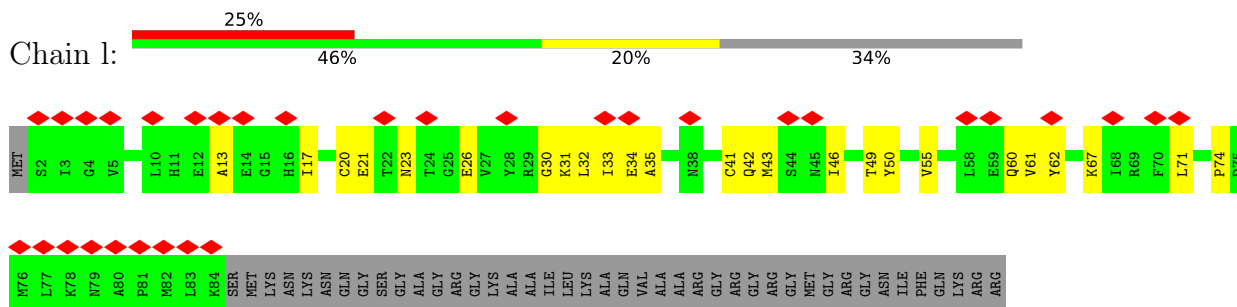




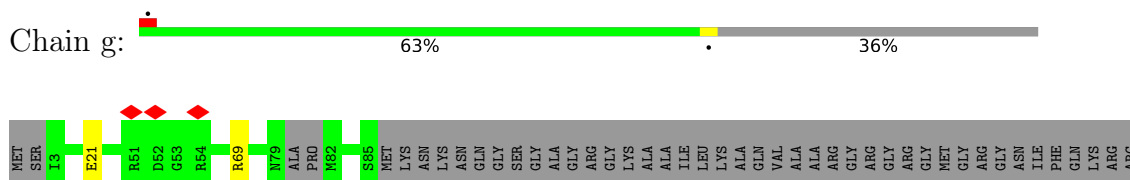
- Molecule 43: Small nuclear ribonucleoprotein-associated proteins B and B'



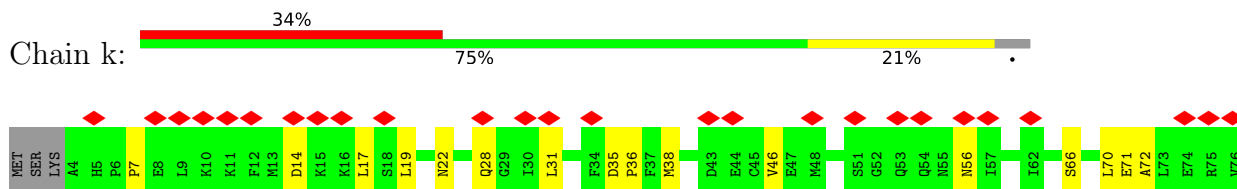
- Molecule 44: Small nuclear ribonucleoprotein Sm D3



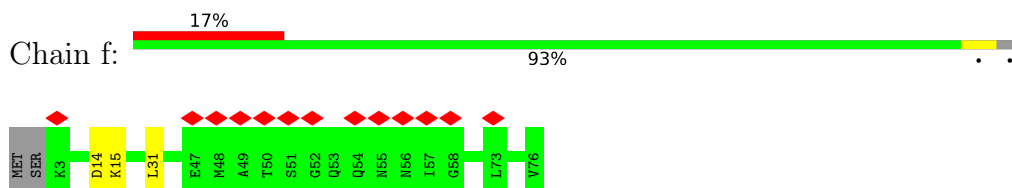
- Molecule 44: Small nuclear ribonucleoprotein Sm D3



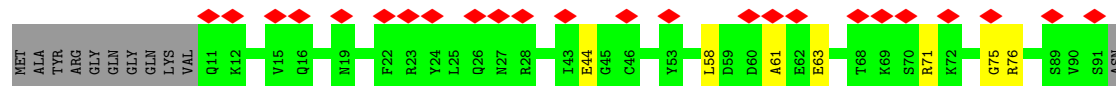
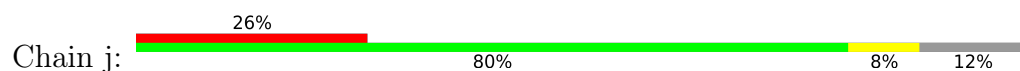
- Molecule 45: Small nuclear ribonucleoprotein G



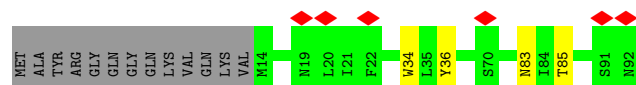
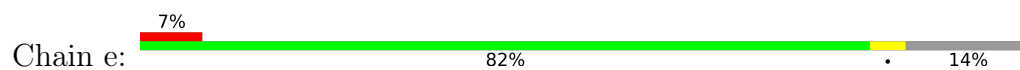
- Molecule 45: Small nuclear ribonucleoprotein G



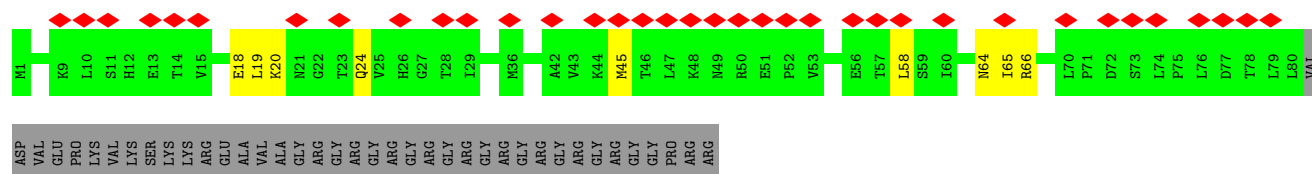
- Molecule 46: Small nuclear ribonucleoprotein E



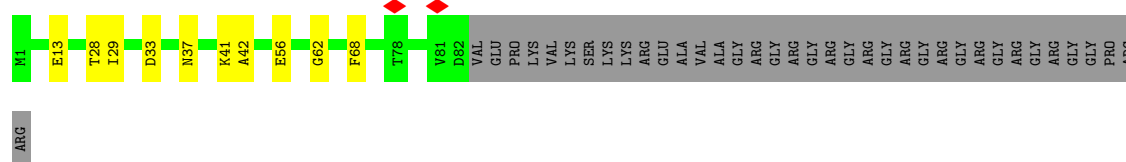
- Molecule 46: Small nuclear ribonucleoprotein E



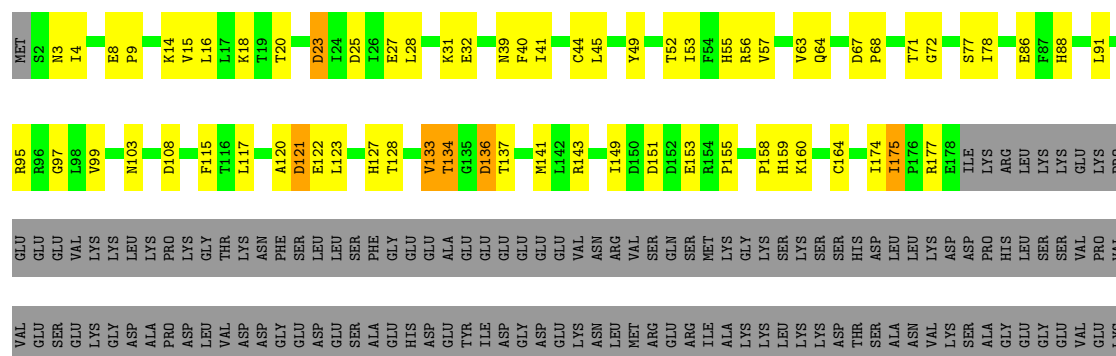
- Molecule 47: Small nuclear ribonucleoprotein Sm D1



- Molecule 47: Small nuclear ribonucleoprotein Sm D1



- Molecule 48: Peptidyl-prolyl cis-trans isomerase CWC27 homolog



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136665	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.781	Depositor
Minimum map value	-1.945	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.24	Depositor
Map size ($\text{\AA}$)	516.96, 516.96, 516.96	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.077, 1.077, 1.077	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, GTP, ZN, SEP, IHP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	10/19056 (0.1%)	0.75	20/25857 (0.1%)
2	B	0.53	0/2303	0.46	0/3579
3	C	0.40	0/6873	0.67	4/9346 (0.0%)
4	D	0.18	0/8527	0.48	0/11887
5	E	0.24	0/2392	0.63	0/3242
6	F	0.58	0/2323	0.58	1/3619 (0.0%)
7	G	0.48	0/1648	0.60	0/2558
8	H	0.37	0/3947	0.50	0/6138
9	I	0.20	0/3013	0.53	0/4223
10	J	0.26	0/2171	0.60	0/2929
11	K	0.54	0/1081	0.63	1/1447 (0.1%)
12	L	0.61	0/850	0.67	0/1146
13	N	0.27	0/1210	0.62	0/1622
14	O	0.20	0/1432	0.48	0/1993
15	P	0.72	0/369	0.76	0/489
16	Q	0.18	0/6796	0.43	0/9527
17	R	0.50	0/1920	0.68	0/2576
18	S	0.18	0/3178	0.46	0/4425
19	T	0.92	5/2574 (0.2%)	0.79	0/3511
20	U	0.36	0/424	0.82	2/582 (0.3%)
21	V	0.34	0/3043	0.54	0/4156
22	W	0.73	0/33	0.75	0/42
23	X	0.33	0/1312	0.59	0/1769
24	Y	0.55	0/966	0.59	0/1303
25	Z	0.39	0/1166	0.64	0/1559
26	1	0.80	30/8004 (0.4%)	0.82	18/10830 (0.2%)
27	3	0.55	0/9408	0.71	4/12767 (0.0%)
28	p	0.19	0/857	0.46	0/1196
29	w	0.23	0/2311	0.48	0/3008
30	u	0.15	0/842	0.38	0/1110
31	2	0.50	0/1837	0.75	3/2473 (0.1%)
32	4	0.21	0/790	0.49	0/1095

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.29	0/925	0.61	0/1247
34	7	0.43	0/825	0.62	0/1106
35	5	0.68	0/688	0.74	0/930
36	9	0.32	0/2675	0.61	0/3631
37	8	0.33	0/946	0.54	0/1270
38	y	0.20	0/389	0.45	0/540
39	v	0.45	0/1054	0.61	0/1385
40	o	0.18	0/821	0.53	0/1149
41	c	0.17	0/387	0.52	0/482
41	h	0.18	0/485	0.41	0/677
42	d	0.18	0/295	0.49	0/367
42	i	0.19	0/362	0.47	0/502
43	a	0.18	0/343	0.53	0/427
43	m	0.19	0/416	0.51	0/581
44	g	0.17	0/322	0.48	0/399
44	l	0.21	0/417	0.54	0/581
45	f	0.16	0/295	0.45	0/367
45	k	0.19	0/366	0.50	0/509
46	e	0.16	0/315	0.50	0/392
46	j	0.20	0/403	0.46	0/561
47	b	0.18	0/327	0.47	0/407
47	n	0.21	0/404	0.50	0/564
48	z	0.53	0/1436	0.61	0/1945
All	All	0.51	45/117552 (0.0%)	0.63	53/162023 (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
1	A	0	16
3	C	0	7
4	D	0	2
9	I	0	1
13	N	0	1
15	P	0	2
16	Q	0	2
17	R	0	1
23	X	0	1
26	1	0	5
27	3	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	2	0	1
48	z	0	1
All	All	0	42

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	827	PHE	C-N	14.66	1.50	1.33
19	T	307	SER	C-O	-13.31	1.09	1.23
1	A	826	PRO	C-O	-13.10	1.07	1.23
1	A	824	PRO	C-O	-9.99	1.12	1.23
19	T	307	SER	CA-CB	-9.89	1.40	1.53

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	827	PHE	CA-C-N	14.20	135.00	120.38
1	A	827	PHE	C-N-CA	14.20	135.00	120.38
26	1	1108	ASN	CB-CA-C	-11.62	91.49	110.79
26	1	935	THR	CB-CA-C	-9.57	95.85	110.88
26	1	942	ASN	CB-CA-C	-9.23	94.57	109.80

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	433	GLU	Peptide
1	A	467	GLN	Peptide
1	A	699	GLU	Peptide
1	A	700	GLY	Peptide
1	A	81	PHE	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	A	18543	0	18403	647	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2066	0	1047	57	0
3	C	6724	0	6696	317	0
4	D	8528	0	3745	45	0
5	E	2338	0	2275	130	0
6	F	2075	0	1048	103	0
7	G	1481	0	755	81	0
8	H	3539	0	1791	130	0
9	I	2991	0	1473	12	0
10	J	2116	0	1977	105	0
11	K	1059	0	1012	38	0
12	L	829	0	837	29	0
13	N	1184	0	1193	52	0
14	O	1433	0	621	18	0
15	P	362	0	356	16	0
16	Q	6730	0	3268	33	0
17	R	1889	0	1866	75	0
18	S	3180	0	1441	20	0
19	T	2507	0	2451	81	0
20	U	422	0	291	16	0
21	V	3008	0	2288	93	0
22	W	229	0	86	3	0
23	X	1279	0	1284	65	0
24	Y	948	0	954	36	0
25	Z	1142	0	1112	38	0
26	1	7866	0	7964	292	0
27	3	9220	0	9139	426	0
28	p	851	0	423	7	0
29	w	2275	0	1347	53	0
30	u	834	0	325	0	0
31	2	1807	0	1622	60	0
32	4	792	0	367	16	0
33	6	906	0	913	51	0
34	7	811	0	790	29	0
35	5	669	0	631	20	0
36	9	2636	0	2228	130	0
37	8	931	0	960	46	0
38	y	390	0	190	5	0
39	v	1041	0	800	30	0
40	o	816	0	386	4	0
41	c	388	0	102	1	0
41	h	482	0	220	5	0
42	d	296	0	87	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	i	359	0	179	6	0
43	a	344	0	93	1	0
43	m	413	0	194	5	0
44	g	324	0	89	1	0
44	l	415	0	198	15	0
45	f	296	0	84	2	0
45	k	364	0	176	10	0
46	e	316	0	85	3	0
46	j	403	0	173	4	0
47	b	328	0	89	6	0
47	n	402	0	184	5	0
48	z	1402	0	1336	39	0
49	A	36	0	6	2	0
50	C	32	0	12	3	0
51	C	1	0	0	0	0
51	F	5	0	0	0	0
52	7	3	0	0	0	0
52	K	1	0	0	0	0
52	N	3	0	0	0	0
All	All	115060	0	89662	3208	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 16.

The worst 5 of 3208 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)
26:1:933:CYS:SG	26:1:970:LEU:HD21	1.63	1.38
26:1:933:CYS:SG	26:1:970:LEU:HD11	1.74	1.27
26:1:933:CYS:SG	26:1:970:LEU:CD2	2.35	1.13
26:1:933:CYS:SG	26:1:970:LEU:CD1	2.43	1.06
21:V:580:ARG:HE	25:Z:545:MET:HB2	1.19	1.04

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2232/2335 (96%)	2012 (90%)	205 (9%)	15 (1%)	18	53
3	C	854/972 (88%)	748 (88%)	99 (12%)	7 (1%)	16	50
4	D	1720/2136 (80%)	1598 (93%)	118 (7%)	4 (0%)	43	76
5	E	297/357 (83%)	268 (90%)	28 (9%)	1 (0%)	36	70
9	I	591/855 (69%)	492 (83%)	98 (17%)	1 (0%)	43	76
10	J	245/848 (29%)	229 (94%)	15 (6%)	1 (0%)	30	65
11	K	124/343 (36%)	115 (93%)	9 (7%)	0	100	100
12	L	97/802 (12%)	89 (92%)	8 (8%)	0	100	100
13	N	141/144 (98%)	119 (84%)	20 (14%)	2 (1%)	9	36
14	O	288/420 (69%)	271 (94%)	17 (6%)	0	100	100
15	P	40/229 (18%)	30 (75%)	9 (22%)	1 (2%)	4	23
16	Q	1319/1485 (89%)	1237 (94%)	82 (6%)	0	100	100
17	R	227/536 (42%)	208 (92%)	18 (8%)	1 (0%)	30	65
18	S	639/1041 (61%)	600 (94%)	39 (6%)	0	100	100
19	T	318/514 (62%)	295 (93%)	23 (7%)	0	100	100
20	U	68/2752 (2%)	59 (87%)	9 (13%)	0	100	100
21	V	464/908 (51%)	438 (94%)	26 (6%)	0	100	100
22	W	4/122 (3%)	4 (100%)	0	0	100	100
23	X	152/396 (38%)	136 (90%)	16 (10%)	0	100	100
24	Y	116/322 (36%)	111 (96%)	5 (4%)	0	100	100
25	Z	135/619 (22%)	126 (93%)	8 (6%)	1 (1%)	18	53
26	1	984/1304 (76%)	910 (92%)	68 (7%)	6 (1%)	21	56
27	3	1165/1217 (96%)	1058 (91%)	104 (9%)	3 (0%)	36	70
28	p	165/225 (73%)	155 (94%)	10 (6%)	0	100	100
29	w	428/501 (85%)	393 (92%)	35 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	u	183/793 (23%)	175 (96%)	8 (4%)	0	100	100
31	2	246/895 (28%)	221 (90%)	25 (10%)	0	100	100
32	4	157/424 (37%)	143 (91%)	14 (9%)	0	100	100
33	6	107/125 (86%)	99 (92%)	8 (8%)	0	100	100
34	7	103/110 (94%)	95 (92%)	8 (8%)	0	100	100
35	5	79/86 (92%)	69 (87%)	10 (13%)	0	100	100
36	9	373/520 (72%)	336 (90%)	35 (9%)	2 (0%)	24	60
37	8	113/904 (12%)	106 (94%)	7 (6%)	0	100	100
38	y	77/301 (26%)	73 (95%)	4 (5%)	0	100	100
39	v	165/464 (36%)	156 (94%)	9 (6%)	0	100	100
40	o	160/255 (63%)	145 (91%)	15 (9%)	0	100	100
41	c	95/118 (80%)	84 (88%)	11 (12%)	0	100	100
41	h	91/118 (77%)	85 (93%)	6 (7%)	0	100	100
42	d	72/86 (84%)	66 (92%)	6 (8%)	0	100	100
42	i	70/86 (81%)	66 (94%)	4 (6%)	0	100	100
43	a	84/240 (35%)	78 (93%)	6 (7%)	0	100	100
43	m	80/240 (33%)	74 (92%)	6 (8%)	0	100	100
44	g	77/126 (61%)	70 (91%)	7 (9%)	0	100	100
44	l	81/126 (64%)	74 (91%)	7 (9%)	0	100	100
45	f	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
45	k	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
46	e	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
46	j	79/92 (86%)	71 (90%)	8 (10%)	0	100	100
47	b	80/119 (67%)	75 (94%)	5 (6%)	0	100	100
47	n	78/119 (66%)	70 (90%)	8 (10%)	0	100	100
48	z	176/472 (37%)	163 (93%)	13 (7%)	0	100	100
All	All	15859/28446 (56%)	14501 (91%)	1313 (8%)	45 (0%)	37	70

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	802	THR
1	A	856	LEU

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Mol	Chain	Res	Type
3	C	801	LEU
3	C	824	THR
13	N	40	LYS

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	
1	A	2012/2108 (95%)	1687 (84%)	325 (16%)	2	12
3	C	747/866 (86%)	619 (83%)	128 (17%)	2	11
5	E	256/300 (85%)	214 (84%)	42 (16%)	2	12
9	I	23/749 (3%)	23 (100%)	0	100	100
10	J	205/751 (27%)	178 (87%)	27 (13%)	4	18
11	K	111/294 (38%)	93 (84%)	18 (16%)	2	12
12	L	86/709 (12%)	74 (86%)	12 (14%)	3	16
13	N	130/130 (100%)	110 (85%)	20 (15%)	2	13
15	P	40/203 (20%)	36 (90%)	4 (10%)	7	29
16	Q	71/1336 (5%)	71 (100%)	0	100	100
17	R	200/459 (44%)	166 (83%)	34 (17%)	2	11
19	T	273/441 (62%)	232 (85%)	41 (15%)	3	14
20	U	21/2432 (1%)	20 (95%)	1 (5%)	23	57
21	V	194/838 (23%)	167 (86%)	27 (14%)	3	17
22	W	4/4 (100%)	4 (100%)	0	100	100
23	X	139/349 (40%)	119 (86%)	20 (14%)	3	15
24	Y	105/291 (36%)	90 (86%)	15 (14%)	3	16
25	Z	118/545 (22%)	101 (86%)	17 (14%)	3	15
26	1	840/1103 (76%)	674 (80%)	166 (20%)	1	8
27	3	1018/1051 (97%)	838 (82%)	180 (18%)	2	10
28	p	8/195 (4%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	w	112/446 (25%)	101 (90%)	11 (10%)	7	30
30	u	10/709 (1%)	10 (100%)	0	100	100
31	2	152/776 (20%)	130 (86%)	22 (14%)	3	15
33	6	97/109 (89%)	80 (82%)	17 (18%)	2	10
34	7	90/95 (95%)	76 (84%)	14 (16%)	2	13
35	5	72/77 (94%)	64 (89%)	8 (11%)	6	25
36	9	218/456 (48%)	180 (83%)	38 (17%)	2	10
37	8	104/831 (12%)	92 (88%)	12 (12%)	5	24
39	v	78/382 (20%)	66 (85%)	12 (15%)	2	13
40	o	6/218 (3%)	6 (100%)	0	100	100
41	h	5/110 (4%)	5 (100%)	0	100	100
42	i	4/74 (5%)	4 (100%)	0	100	100
43	m	4/177 (2%)	4 (100%)	0	100	100
44	l	3/101 (3%)	3 (100%)	0	100	100
45	k	3/66 (4%)	3 (100%)	0	100	100
46	j	1/84 (1%)	1 (100%)	0	100	100
47	n	3/101 (3%)	3 (100%)	0	100	100
48	z	152/416 (36%)	132 (87%)	20 (13%)	4	18
All	All	7715/20382 (38%)	6484 (84%)	1231 (16%)	4	12

5 of 1231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	3	153	THR
35	5	33	VAL
27	3	347	LEU
27	3	152	LEU
27	3	931	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 159 such sidechains are listed below:

Mol	Chain	Res	Type
26	1	1218	ASN
33	6	109	GLN
27	3	206	GLN

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Mol	Chain	Res	Type
27	3	861	GLN
36	9	327	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	27 (28%)	3 (3%)
6	F	96/107 (89%)	49 (51%)	6 (6%)
7	G	69/220 (31%)	43 (62%)	9 (13%)
8	H	163/188 (86%)	73 (44%)	7 (4%)
All	All	424/632 (67%)	192 (45%)	25 (5%)

5 of 192 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	G	101	U
7	G	108	U
8	H	47	U
7	G	106	C
8	H	12	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
26	SEP	1	129	26	8,9,10	1.52	1 (12%)	7,12,14	1.08	0

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
26	SEP	1	129	26	-	2/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	129	SEP	P-O1P	3.27	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	1	129	SEP	N-CA-CB-OG
26	1	129	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 13 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	$\# Z > 2$
49	IHP	A	2401	-	36,36,36	1.47	8 (22%)	60,60,60	1.90	15 (25%)
50	GTP	C	1500	51	33,34,34	0.93	1 (3%)	50,54,54	1.73	10 (20%)

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
49	IHP	A	2401	-	-	3/30/54/54	0/1/1/1
50	GTP	C	1500	51	-	6/22/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	A	2401	IHP	P1-O31	-2.91	1.44	1.54
49	A	2401	IHP	P5-O35	-2.62	1.45	1.54
49	A	2401	IHP	P5-O45	-2.40	1.45	1.54
50	C	1500	GTP	C5-N7	-2.27	1.34	1.39
49	A	2401	IHP	P6-O46	-2.18	1.46	1.54

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C	1500	GTP	C5'-C4'-N3	-5.29	119.97	128.39
49	A	2401	IHP	O15-C5-C4	5.19	119.81	108.76
50	C	1500	GTP	C2-N3-C4	4.81	120.59	112.30
49	A	2401	IHP	C5-C4-C3	4.47	120.24	110.43
49	A	2401	IHP	O14-C4-C5	4.25	117.80	108.76

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	C	1500	GTP	C5'-O5'-PA-O1A
50	C	1500	GTP	O4'-C4'-C5'-O5'
50	C	1500	GTP	C3'-C4'-C5'-O5'
49	A	2401	IHP	C2-O12-P2-O22

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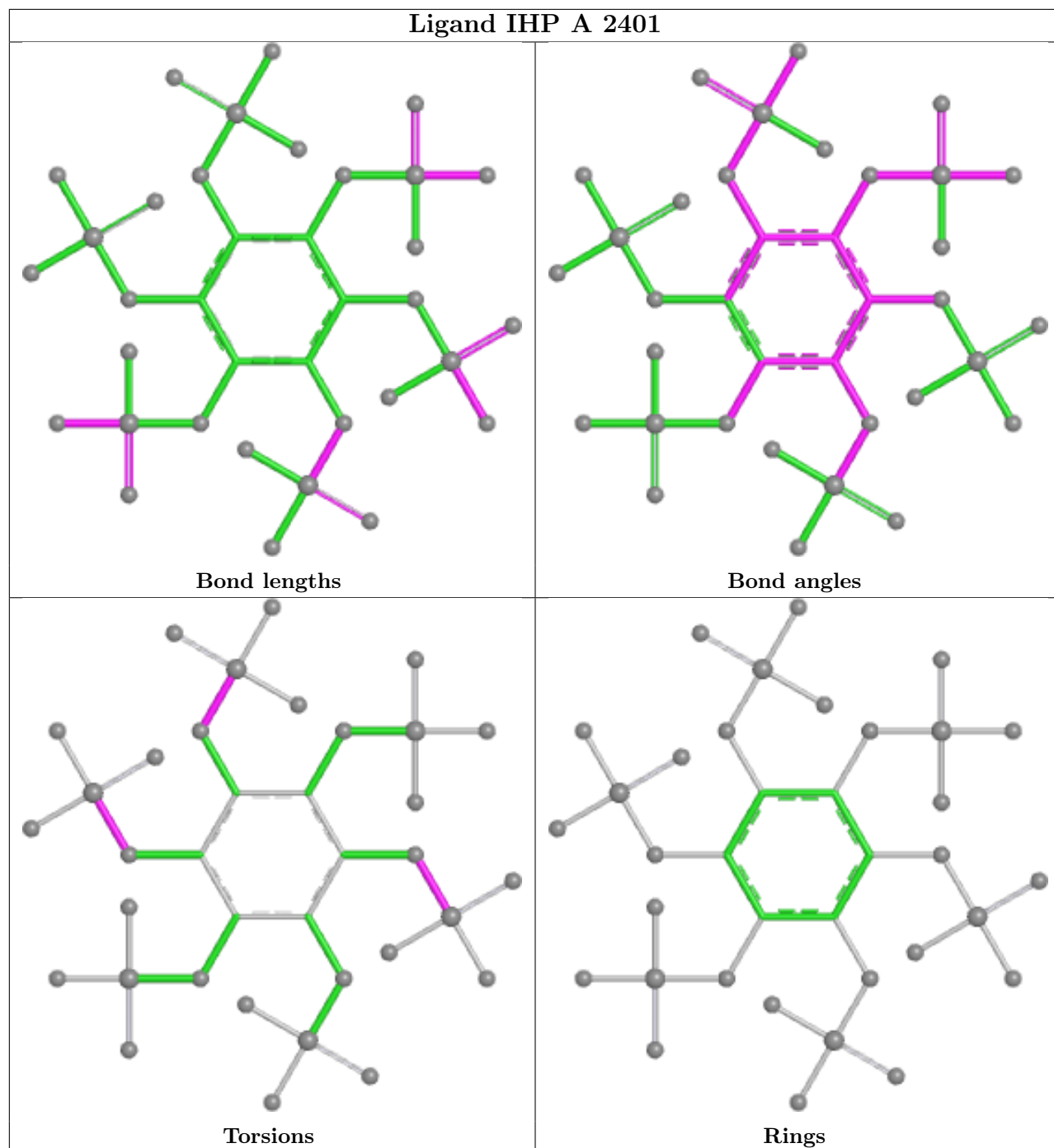
Mol	Chain	Res	Type	Atoms
50	C	1500	GTP	C5'-O5'-PA-O3A

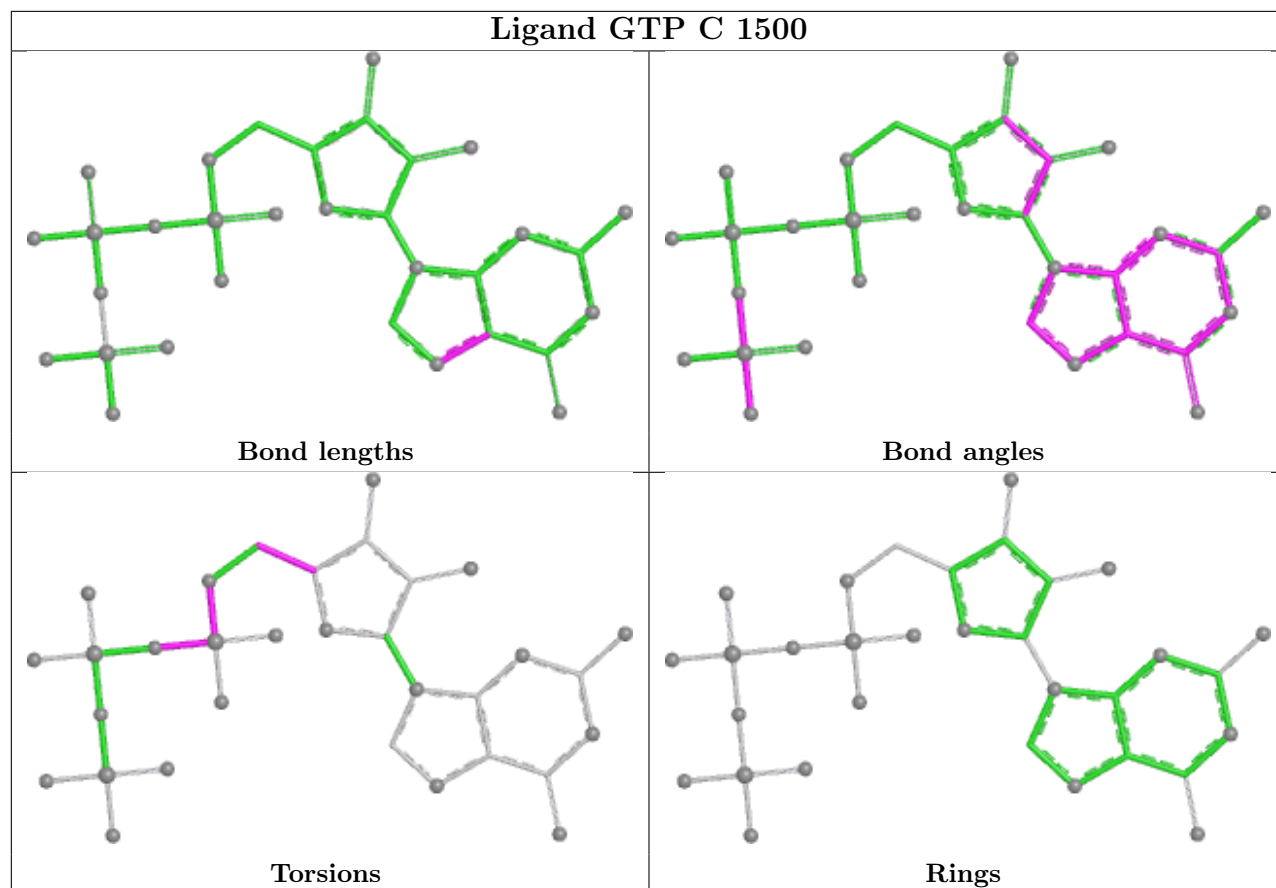
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	A	2401	IHP	2	0
50	C	1500	GTP	3	0

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](#)

There are no chain breaks in this entry.

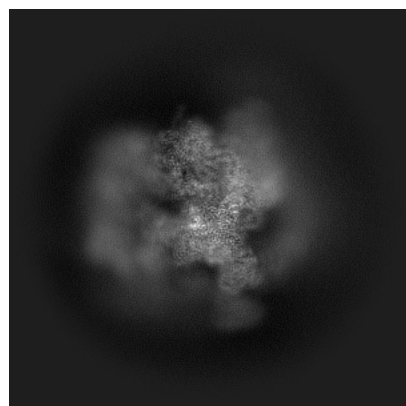
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35107. These allow visual inspection of the internal detail of the map and identification of artifacts.

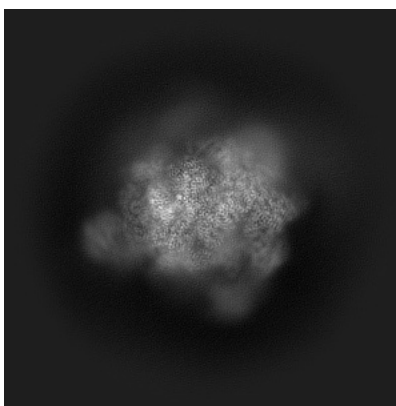
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

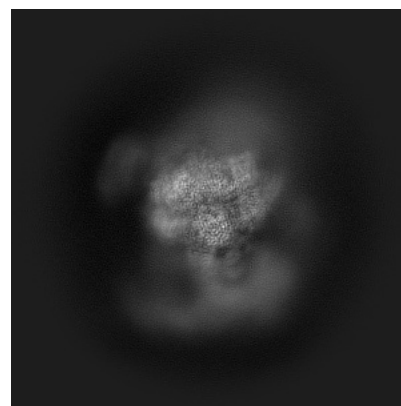
6.1.1 Primary map



X

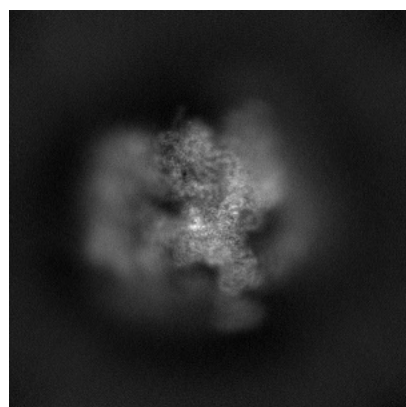


Y

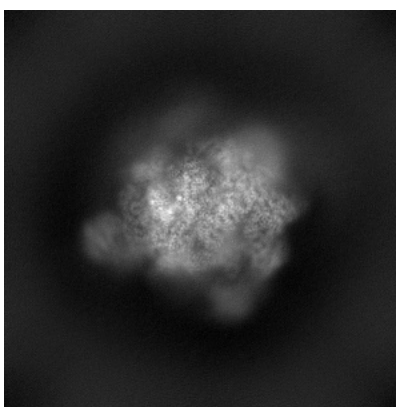


Z

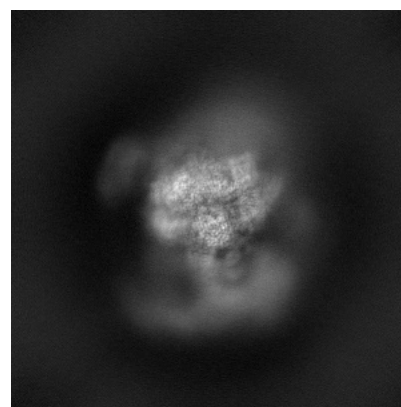
6.1.2 Raw map



X



Y

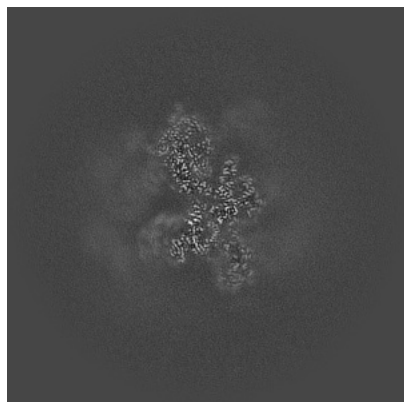


Z

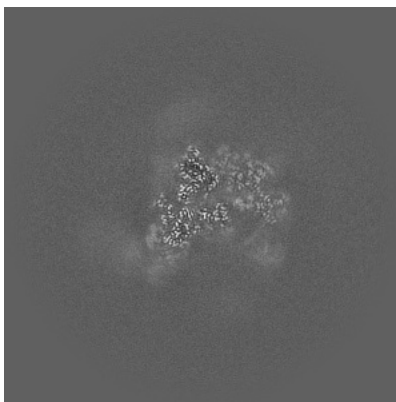
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

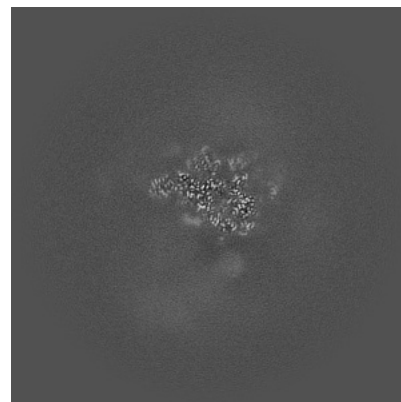
6.2.1 Primary map



X Index: 240

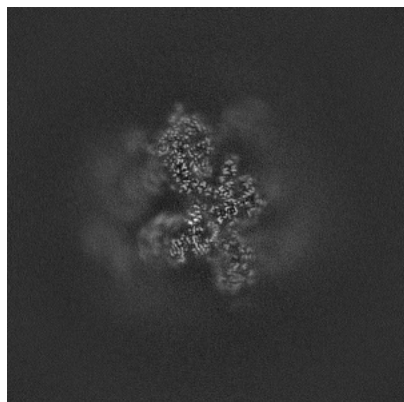


Y Index: 240

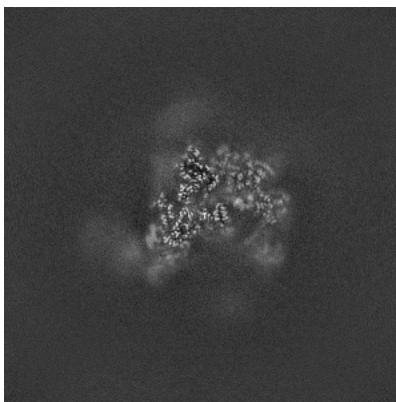


Z Index: 240

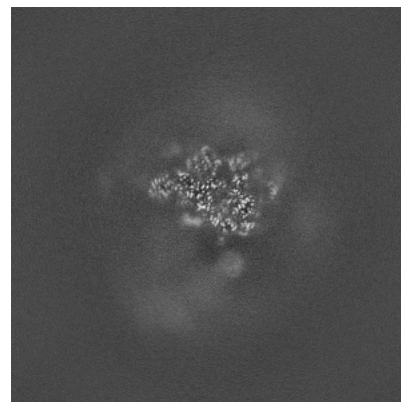
6.2.2 Raw map



X Index: 240



Y Index: 240

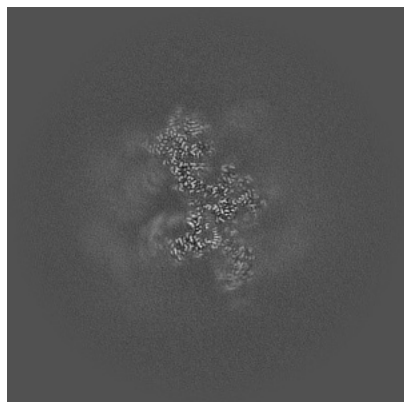


Z Index: 240

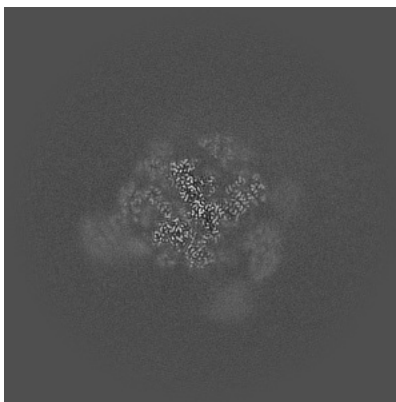
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

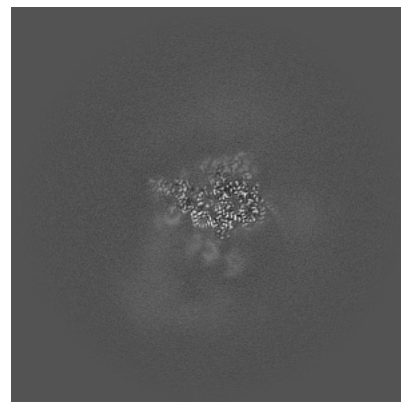
6.3.1 Primary map



X Index: 237

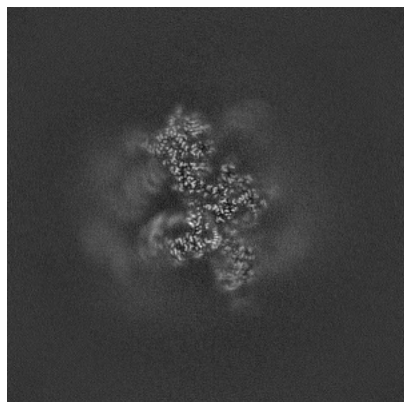


Y Index: 262

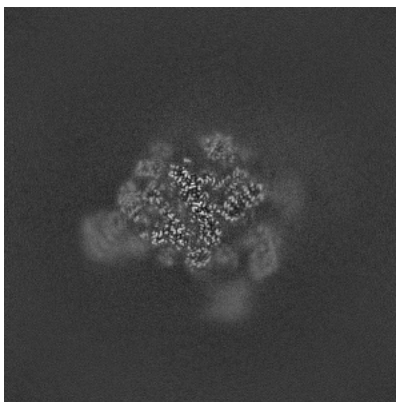


Z Index: 220

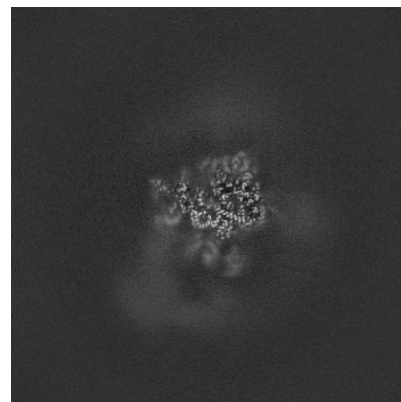
6.3.2 Raw map



X Index: 237



Y Index: 266

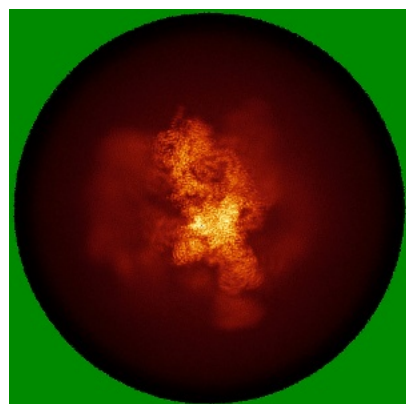


Z Index: 219

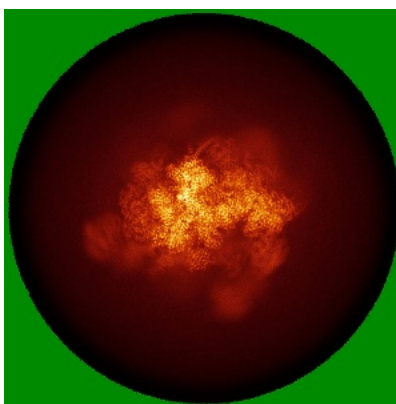
The images above show the largest variance slices of the map in three orthogonal directions.

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

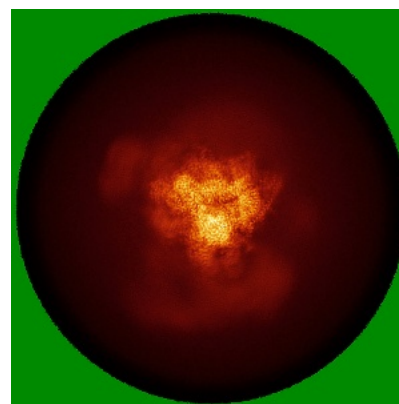
6.4.1 Primary map



X

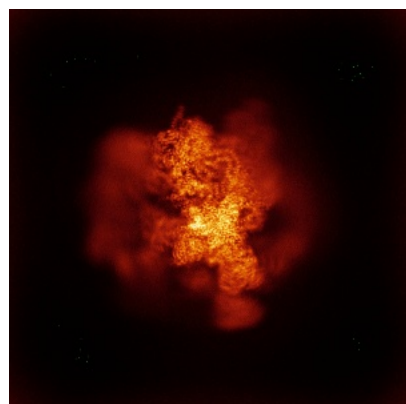


Y

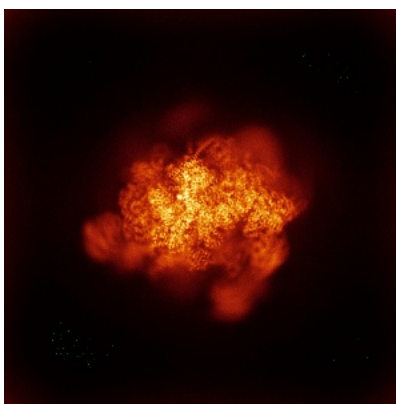


Z

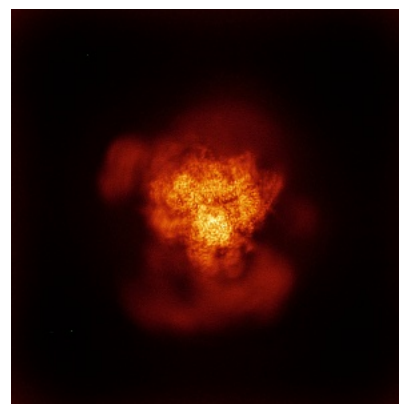
6.4.2 Raw map



X



Y

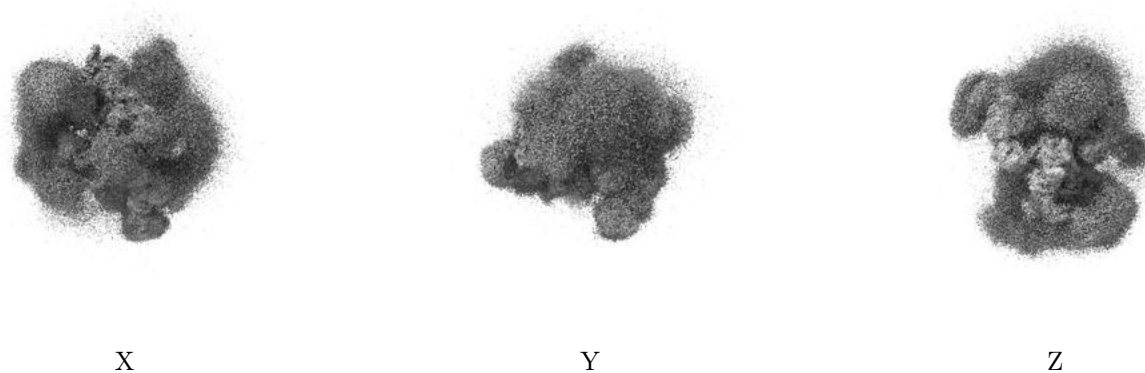


Z

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

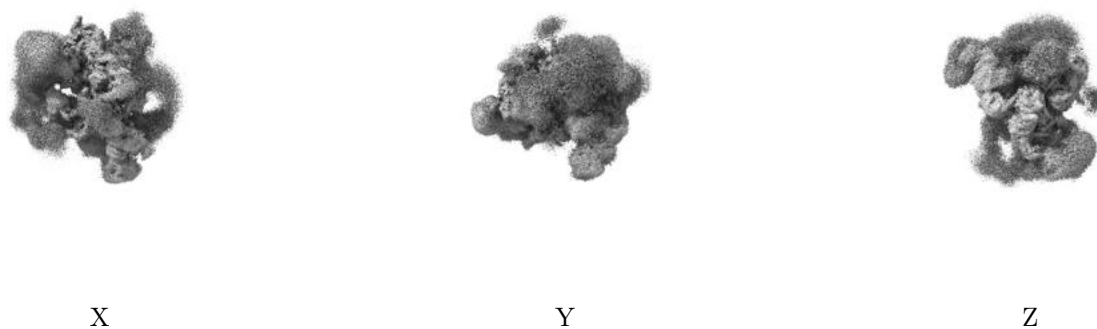
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

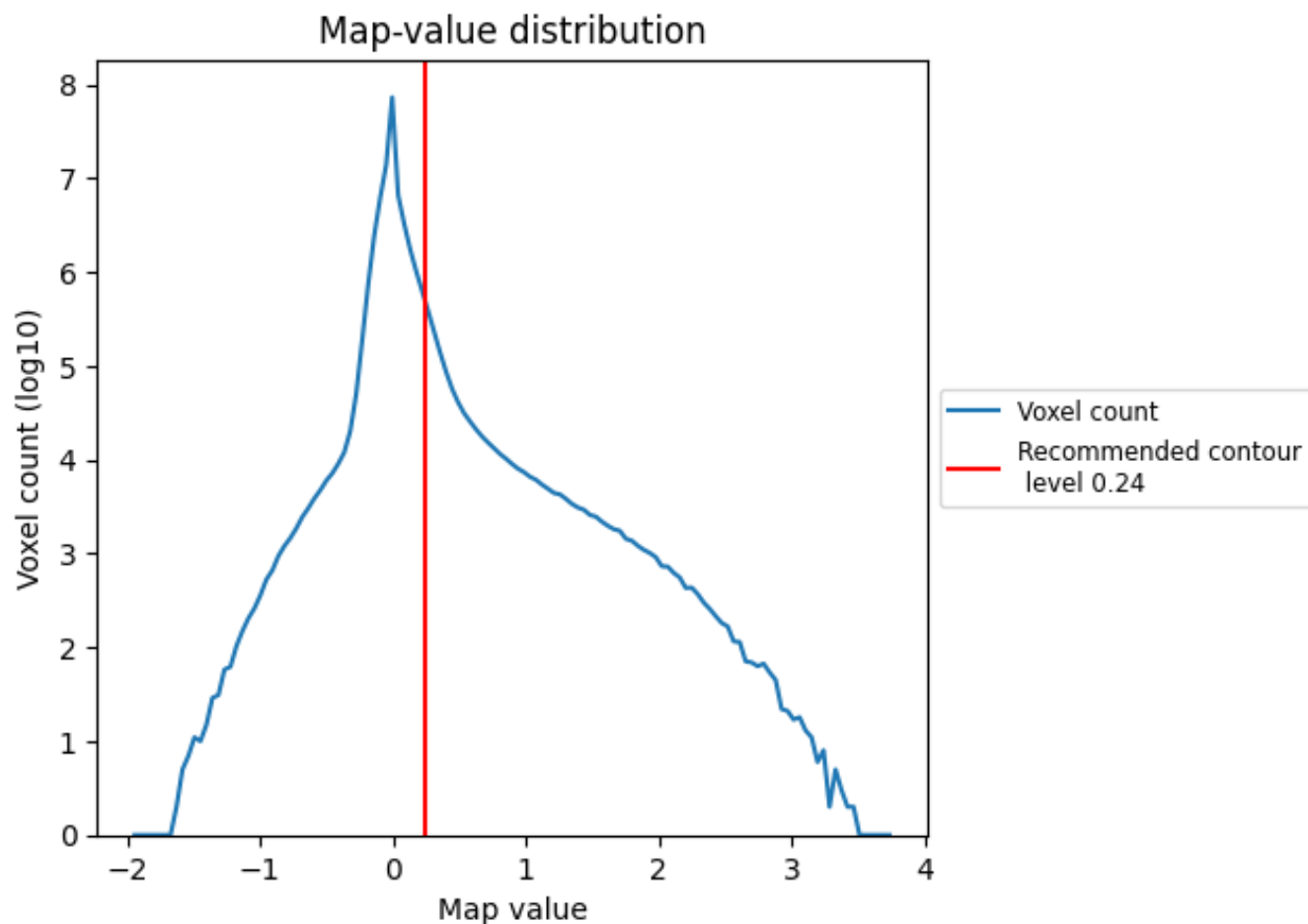
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

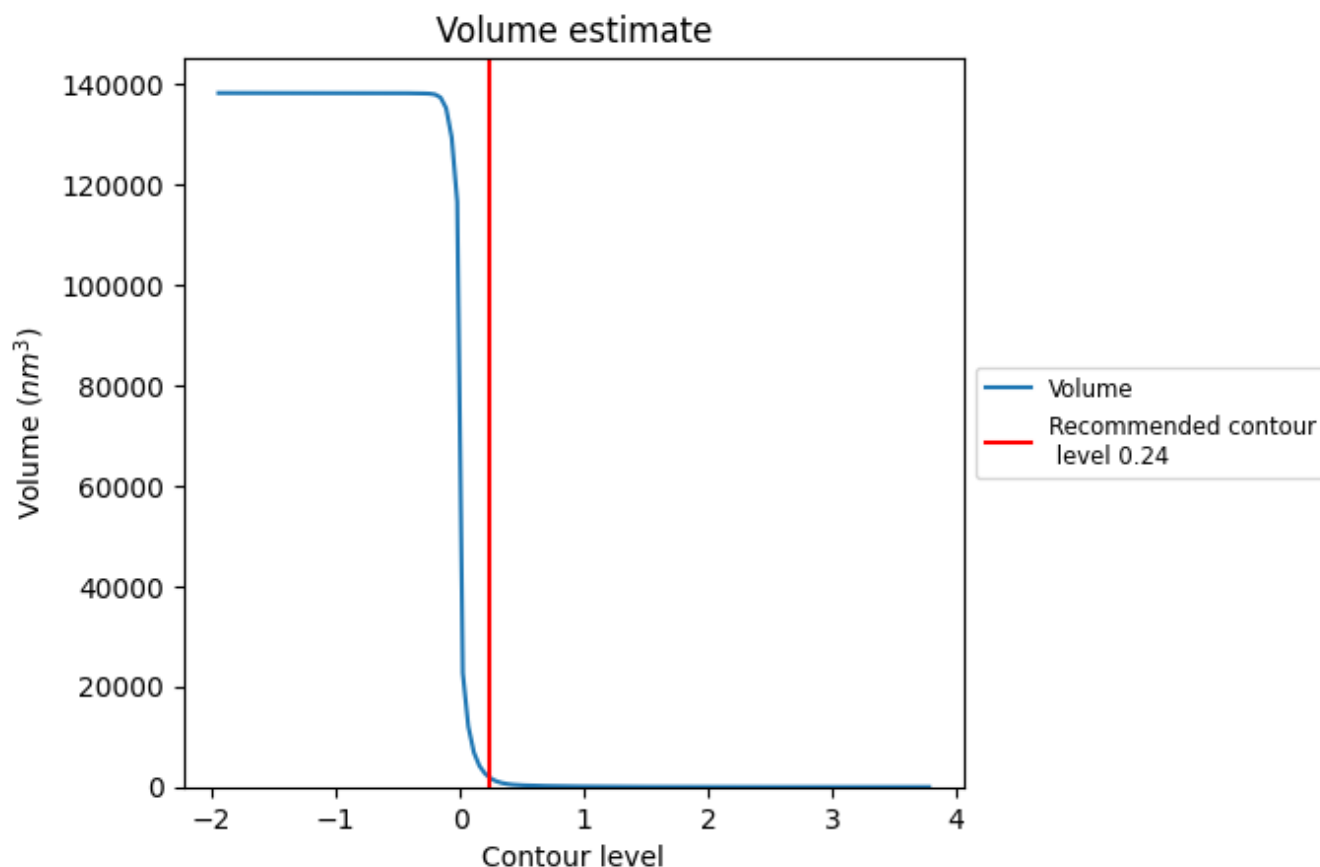
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

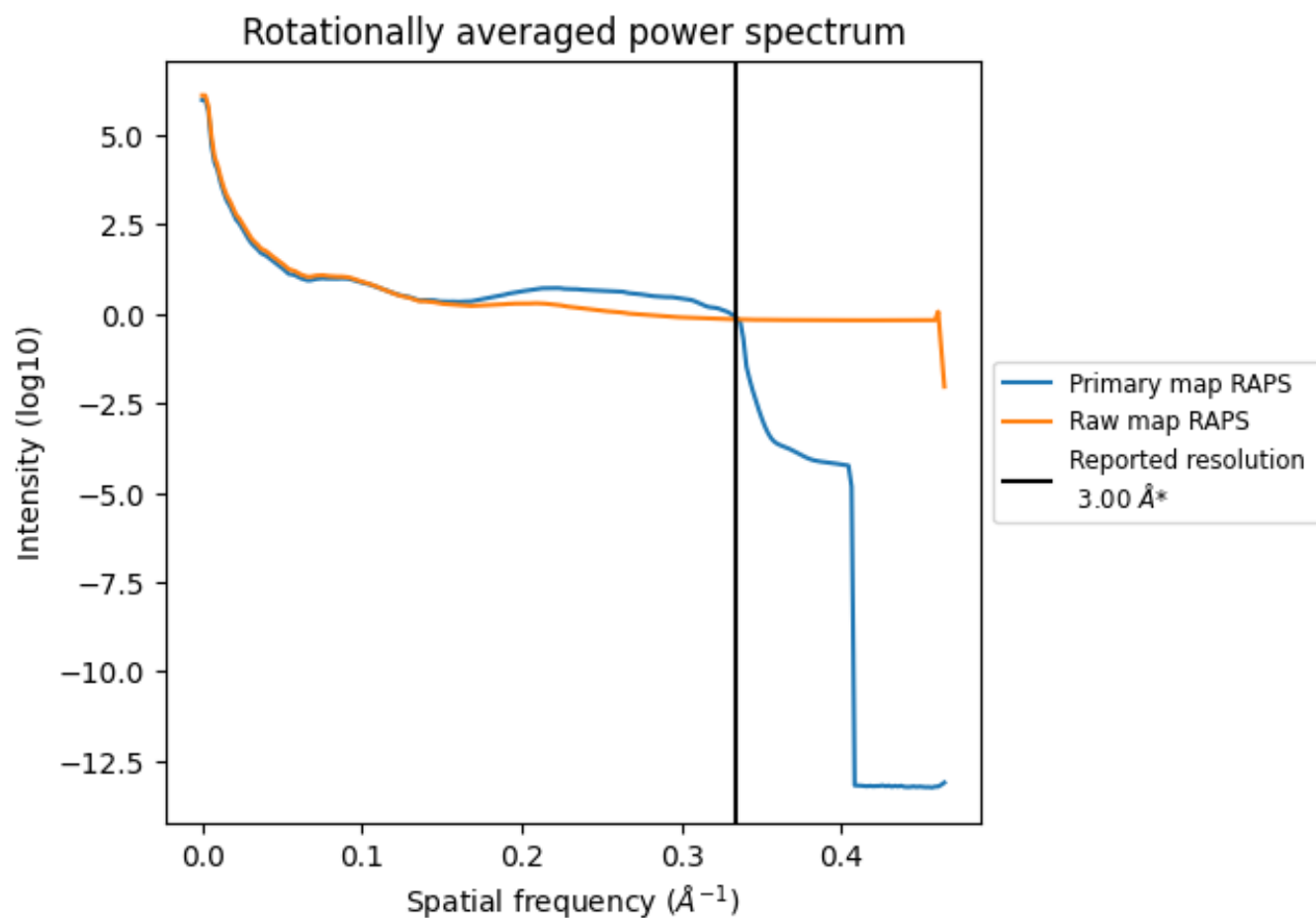
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1878 nm^3 ; this corresponds to an approximate mass of 1697 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 ⓘ

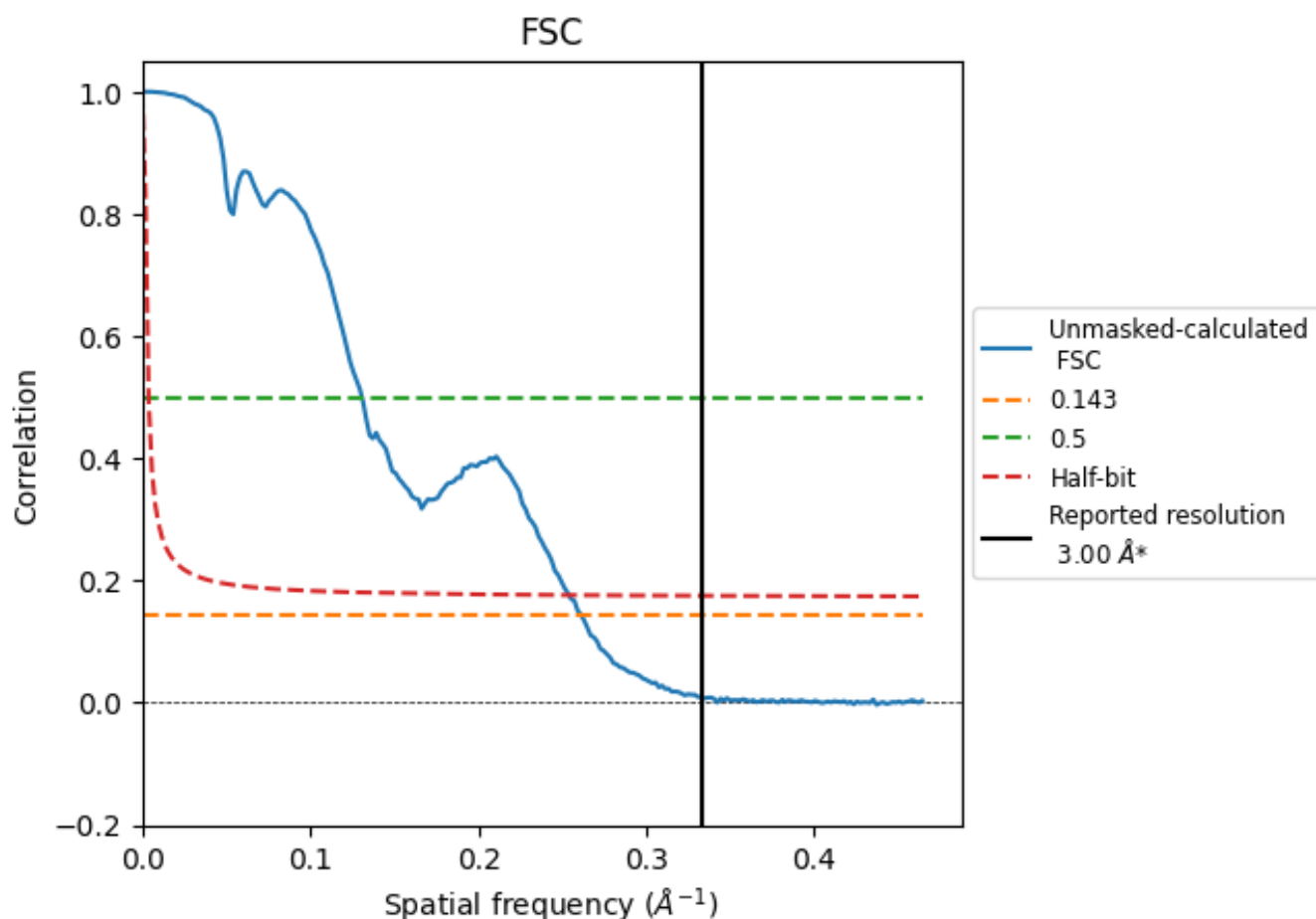


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

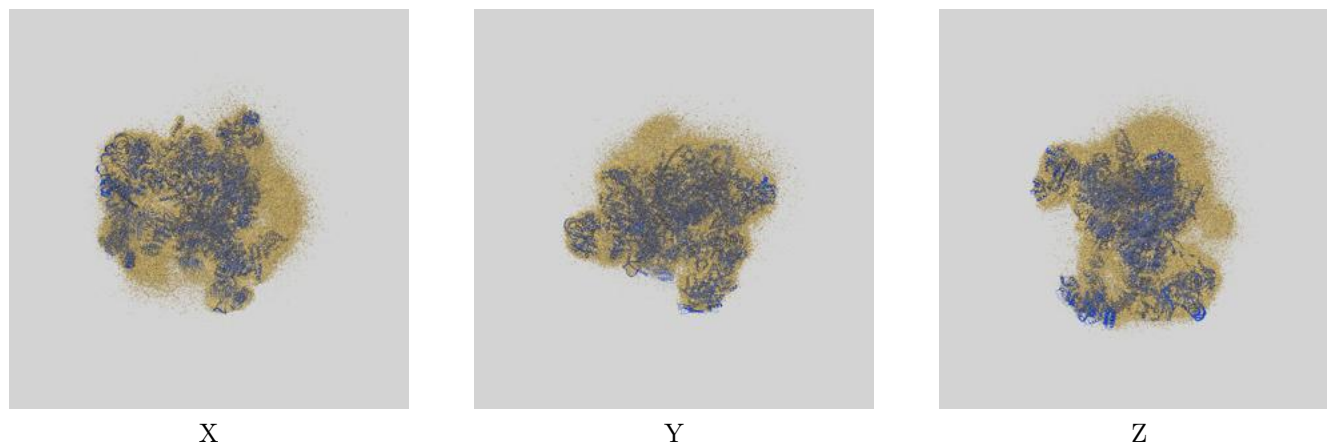
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	7.65	3.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

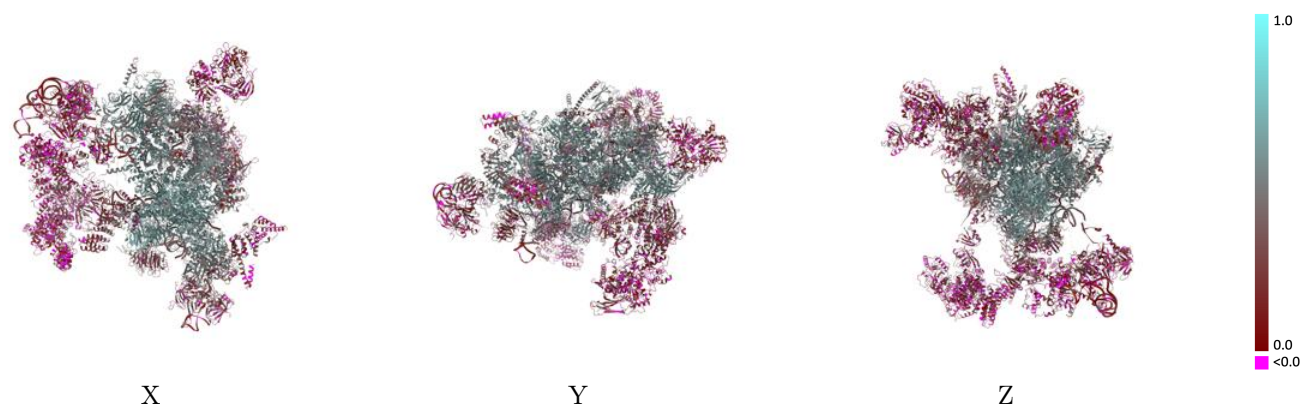
This section contains information regarding the fit between EMDB map EMD-35107 and PDB model 8I0R. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



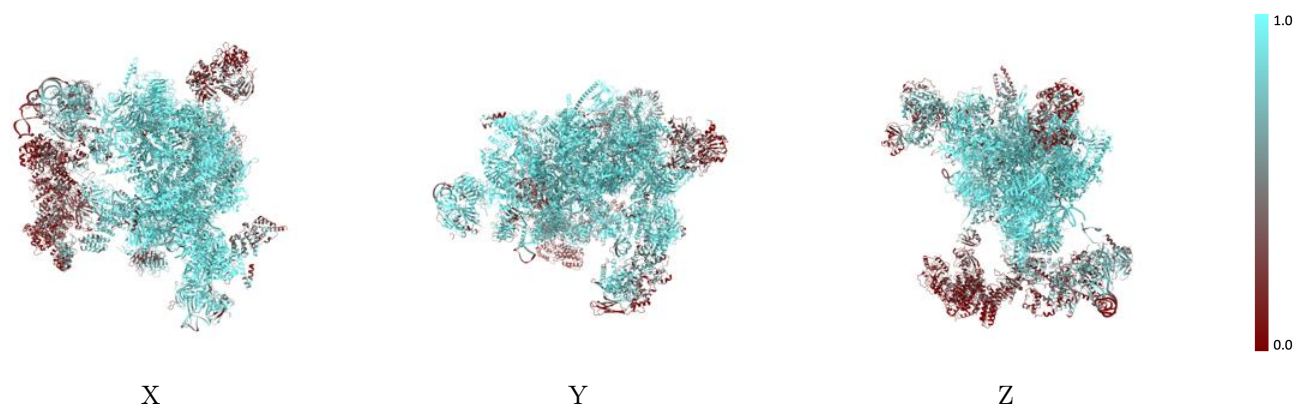
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



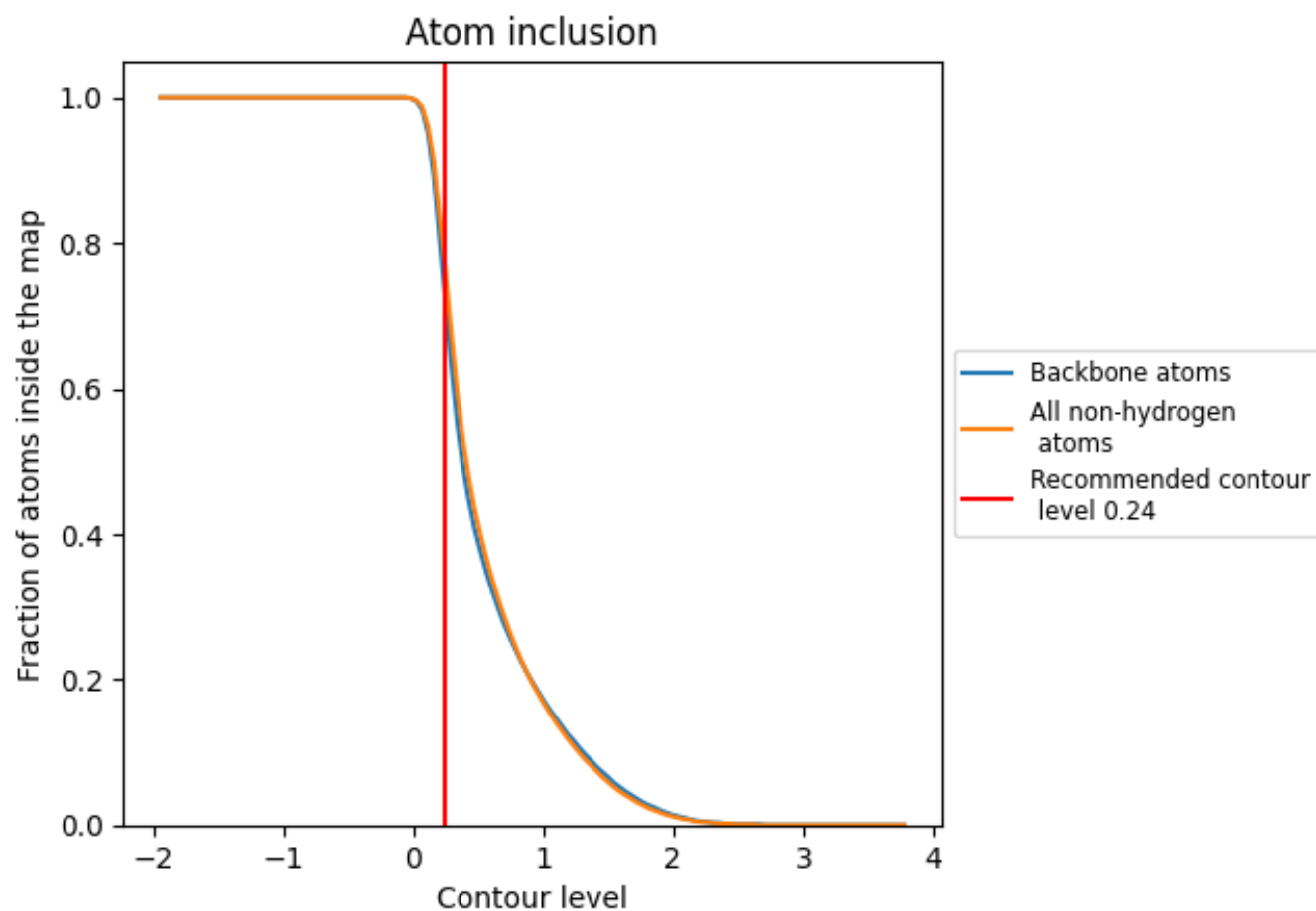
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).

9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 78% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.3880
1	 0.9580	 0.5450
2	 0.8750	 0.4670
3	 0.9680	 0.4970
4	 0.7370	 0.2210
5	 0.9130	 0.5330
6	 0.9390	 0.4230
7	 0.9170	 0.5070
8	 0.9470	 0.4500
9	 0.8880	 0.3600
A	 0.9370	 0.5370
B	 0.9000	 0.3820
C	 0.9660	 0.4770
D	 0.6980	 0.2090
E	 0.5950	 0.2590
F	 0.8920	 0.3750
G	 0.9370	 0.3900
H	 0.6720	 0.2550
I	 0.3100	 0.1380
J	 0.8480	 0.2900
K	 0.9090	 0.5550
L	 0.9780	 0.5670
N	 0.9300	 0.4500
O	 0.6680	 0.2620
P	 0.9550	 0.5210
Q	 0.1020	 0.1460
R	 0.9300	 0.4930
S	 0.2830	 0.1640
T	 0.9920	 0.6000
U	 0.6610	 0.2900
V	 0.7560	 0.3430
W	 0.8680	 0.4140
X	 0.9540	 0.4960
Y	 0.9690	 0.5740
Z	 0.8500	 0.4850



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Chain	Atom inclusion	Q-score
a	 0.7670	 0.2450
b	 0.8720	 0.2450
c	 0.7420	 0.2020
d	 0.8040	 0.2300
e	 0.8130	 0.2130
f	 0.7330	 0.3120
g	 0.8980	 0.3170
h	 0.6140	 0.1890
i	 0.6680	 0.1730
j	 0.6650	 0.2140
k	 0.5880	 0.1740
l	 0.5570	 0.1680
m	 0.6370	 0.2450
n	 0.5450	 0.1990
o	 0.4720	 0.1700
p	 0.6100	 0.1980
u	 0.2810	 0.1830
v	 0.7100	 0.4520
w	 0.5330	 0.2690
y	 0.2800	 0.1760
z	 0.9840	 0.5600