



## wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 04:47 am GMT

PDB ID : 7AOR  
EMDB ID : EMD-11846  
Title : mt-SSU from Trypanosoma cruzi in complex with mt-IF-3.  
Authors : Soufari, H.; Waltz, F.; Parrot, C.; Bochler, A.; Hashem, Y.  
Deposited on : 2020-10-15  
Resolution : 3.50 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:

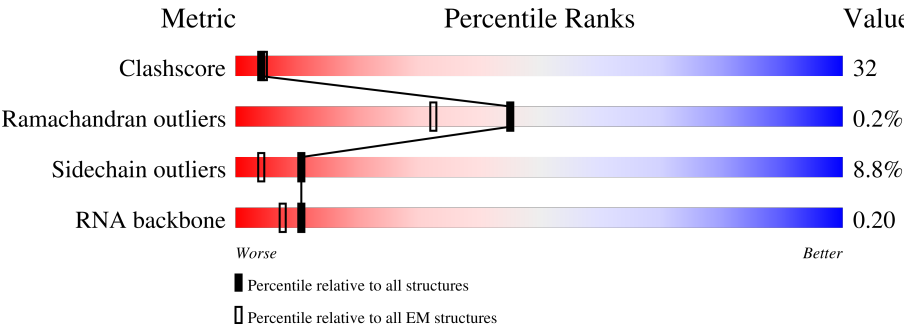
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.50 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.








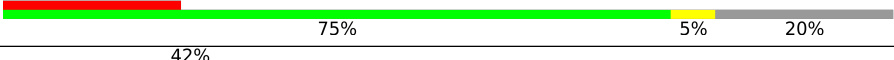




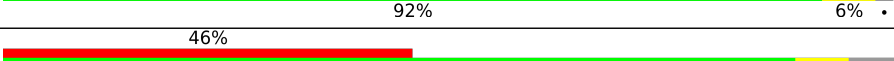
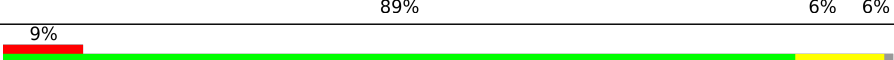
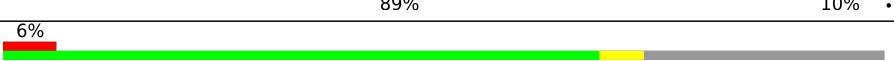
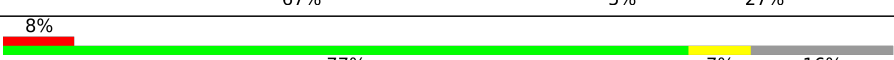
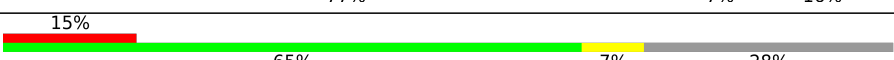
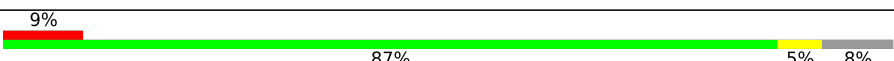
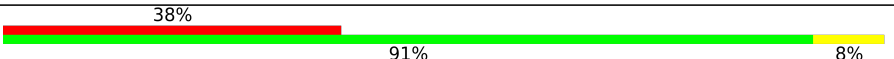
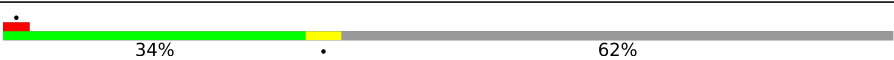



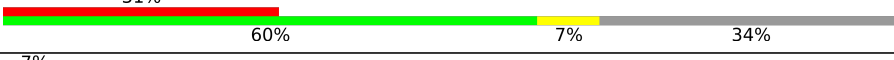
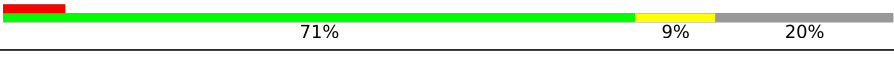
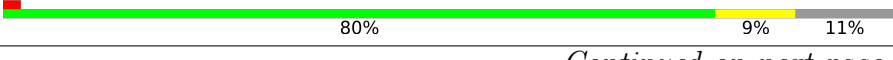

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	874	<div> <div>44%</div> <div>74%</div> <div>6%</div> <div>20%</div> </div>
2	s	180	<div> <div>24%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
3	r	500	<div> <div>41%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>
4	n	172	<div> <div>22%</div> <div>76%</div> <div>7%</div> <div>17%</div> </div>
5	h	166	<div> <div>16%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
6	e	818	<div> <div>38%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
7	az	163	<div> <div>22%</div> <div>91%</div> <div>.</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
8	ay	218	
9	ax	172	
10	aw	186	
11	au	247	
12	ak	314	
13	aj	396	
14	ag	581	
15	af	677	
16	ae	678	
17	l	714	
18	ac	1152	
19	ab	1175	
20	ad	810	
21	m	319	
22	i	429	
23	f	325	
24	c	285	
25	d	445	
26	ba	217	
27	av	237	
28	at	259	
29	ar	268	
30	aq	299	
31	ap	277	
32	ao	283	

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Mol	Chain	Length	Quality of chain
33	ai	410	
34	an	293	
35	z	1181	
36	y	449	
37	x	345	
38	w	186	
39	v	215	
40	bb	238	
41	t	256	
42	al	308	
43	q	442	
44	p	308	
45	Ca	603	
46	g	193	
47	j	189	
48	b	160	
49	bd	90	
50	a	434	
51	bc	376	
52	aa	1827	
53	k	309	
54	be	82	
55	as	261	
56	2	8129	
56	A	8129	

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 173743 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 mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	u	697	Total	C	N	O	S	0	0
			5597	3524	1014	1035	24		

- Molecule 2 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	s	165	Total	C	N	O	S	0	0
			1351	851	249	242	9		

- Molecule 3 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	r	465	Total	C	N	O	S	0	0
			3806	2451	655	681	19		

- Molecule 4 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	142	Total	C	N	O	S	0	0
			1169	760	203	201	5		

- Molecule 5 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	157	Total	C	N	O	S	0	0
			1324	842	252	222	8		

- Molecule 6 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	810	Total	C	N	O	S	0	0
			6577	4157	1153	1237	30		

- Molecule 7 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	az	154	Total	C	N	O	S	0	0
			1292	828	243	217	4		

- Molecule 8 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	ay	141	Total	C	N	O	S	0	0
			1200	765	229	202	4		

- Molecule 9 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	ax	161	Total	C	N	O	S	0	0
			1366	868	263	228	7		

- Molecule 10 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aw	160	Total	C	N	O	S	0	0
			1338	851	251	232	4		

- Molecule 11 is a protein called Rhodanese domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	au	239	Total	C	N	O	S	0	0
			2069	1331	371	357	10		

- Molecule 12 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	ak	230	Total	C	N	O	S	0	0
			1865	1174	345	338	8		

- Molecule 13 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	aj	315	Total	C	N	O	S	0	0
			2590	1667	450	459	14		

- Molecule 14 is a protein called mS55.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	ag	548	Total	C	N	O	S	0	0
			4472	2804	838	806	24		

- Molecule 15 is a protein called mS54.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	af	558	Total	C	N	O	S	0	0
			4590	2897	829	838	26		

- Molecule 16 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	ae	574	Total	C	N	O	S	0	0
			4634	2918	862	833	21		

- Molecule 17 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	l	588	Total	C	N	O	S	0	0
			4821	3070	855	880	16		

- Molecule 18 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	ac	1125	Total	C	N	O	S	0	0
			8864	5568	1581	1682	33		

- Molecule 19 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	ab	1110	Total	C	N	O	S	0	0
			9094	5669	1697	1697	31		

- Molecule 20 is a protein called mS51.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ad	801	Total	C	N	O	S	0	0
			6610	4182	1197	1186	45		

- Molecule 21 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	232	Total	C	N	O	S	0	0
			1940	1234	356	344	6		

- Molecule 22 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	360	Total	C	N	O	S	0	0
			2970	1890	543	522	15		

- Molecule 23 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	f	233	Total	C	N	O	S	0	0
			1917	1195	358	354	10		

- Molecule 24 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	c	263	Total	C	N	O	S	0	0
			2169	1358	417	384	10		

- Molecule 25 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	445	Total	C	N	O	S	0	0
			3538	2229	635	657	17		

- Molecule 26 is a protein called mS73.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	ba	83	Total	C	N	O	S	0	0
			706	460	115	127	4		

- Molecule 27 is a protein called mS68.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	av	213	Total	C	N	O	S	0	0
			1752	1102	310	333	7		

- Molecule 28 is a protein called mS66.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	at	242	Total	C	N	O	S	0	0
			1946	1216	364	352	14		

- Molecule 29 is a protein called AKAP7\_NLS domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	ar	255	Total	C	N	O	S	0	0
			2061	1303	382	368	8		

- Molecule 30 is a protein called mS63.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	aq	198	Total	C	N	O	S	0	0
			1701	1092	304	297	8		

- Molecule 31 is a protein called mS62.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	ap	222	Total	C	N	O	S	0	0
			1796	1109	329	344	14		

- Molecule 32 is a protein called mS61.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	ao	252	Total	C	N	O	S	0	0
			2062	1305	383	362	12		

- Molecule 33 is a protein called mS56.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	ai	390	Total	C	N	O	S	0	0
			3205	2046	554	592	13		

- Molecule 34 is a protein called mS60.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	an	293	Total	C	N	O	S	0	0
			2422	1533	458	419	12		

- Molecule 35 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	1071	Total	C	N	O	S	0	0
			8630	5428	1553	1612	37		

- Molecule 36 is a protein called Sod\_Fe\_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	y	253	Total	C	N	O	S	0	0
			1983	1260	360	350	13		

- Molecule 37 is a protein called Superoxide dismutase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	x	252	Total	C	N	O	S	0	0
			2016	1294	353	364	5		

- Molecule 38 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	175	Total	C	N	O	S	0	0
			1479	945	261	267	6		

- Molecule 39 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	v	196	Total	C	N	O	S	0	0
			1567	964	306	288	9		

- Molecule 40 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	bb	110	Total	C	N	O	S	0	0
			905	580	182	141	2		

- Molecule 41 is a protein called Trafficking protein particle complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	226	Total	C	N	O	S	0	0
			1797	1138	317	336	6		

- Molecule 42 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	al	292	Total	C	N	O	S	0	0
			2372	1500	444	415	13		

- Molecule 43 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	214	Total	C	N	O	S	0	0
			1840	1169	335	330	6		

- Molecule 44 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	242	Total	C	N	O	S	0	0
			1998	1264	362	364	8		

- Molecule 45 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ca	592	Total	C	N	O	S	0	0
			5070	3247	913	890	20		

- Molecule 46 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	g	184	Total	C	N	O	S	0	0
			1544	975	300	258	11		

- Molecule 47 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	j	180	Total	C	N	O	S	0	0
			1501	963	280	251	7		

- Molecule 48 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	b	150	Total	C	N	O	S	0	0
			1271	810	228	227	6		

- Molecule 49 is a protein called MURF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	bd	50	Total	C	N	O	S	0	0
			430	296	65	68	1		

- Molecule 50 is a protein called Ribosomal\_S5\_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	a	425	Total	C	N	O	S	0	0
			3436	2177	633	610	16		

- Molecule 51 is a protein called mt-iF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	bc	151	Total	C	N	O	S	0	0
			1247	792	229	220	6		

- Molecule 52 is a protein called mS48.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	aa	1558	Total	C	N	O	S	0	0
			12549	7926	2247	2337	39		

- Molecule 53 is a protein called 30S Ribosomal protein S17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	k	190	Total	C	N	O	S	0	0
			1577	1009	301	258	9		

- Molecule 54 is a protein called Ribosome protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	be	79	Total	C	N	O	S	0	0
			665	459	101	97	8		

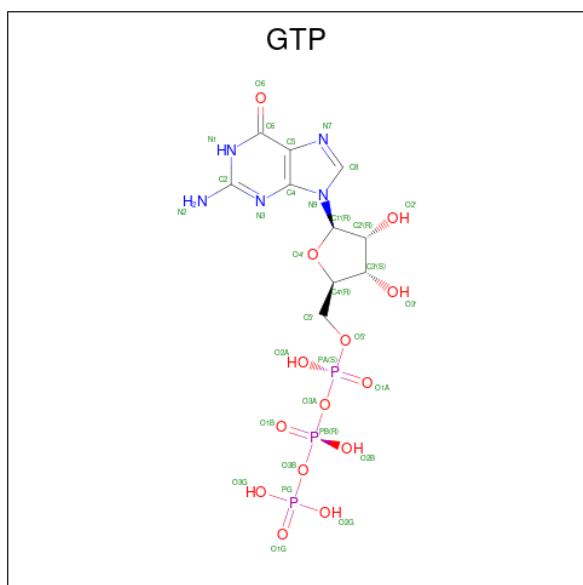
- Molecule 55 is a protein called mS65.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	as	252	Total	C	N	O	S	0	0
			2024	1305	356	353	10		

- Molecule 56 is a RNA chain called RNA (478-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	A	143	Total 3030	C 1364	N 522	O 1001	P 143	0	0
56	2	470	Total 9932	C 4470	N 1690	O 3302	P 470	0	0

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$ ).

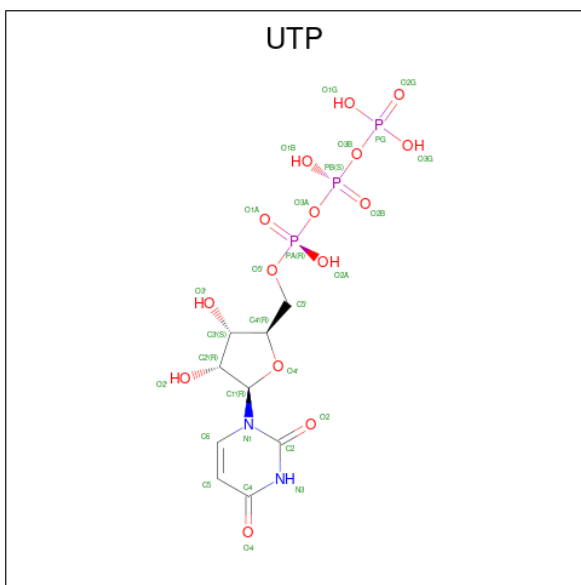


Mol	Chain	Residues	Atoms					AltConf
57	r	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
58	r	1	Total Mg 1 1	0

- Molecule 59 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula:  $\text{C}_9\text{H}_{15}\text{N}_2\text{O}_{15}\text{P}_3$ ) (labeled as "Ligand of Interest" by depositor).

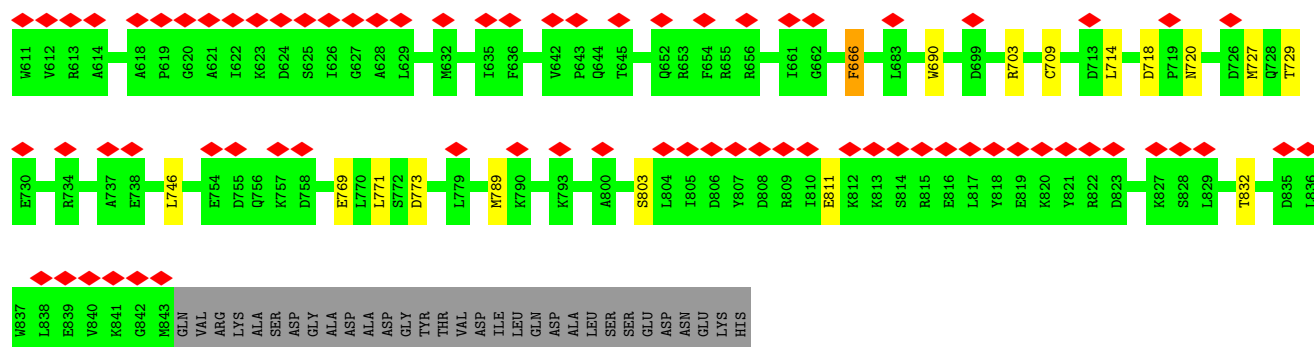


Mol	Chain	Residues	Atoms					AltConf
59	aj	1	Total	C	N	O	P	0
			29	9	2	15	3	

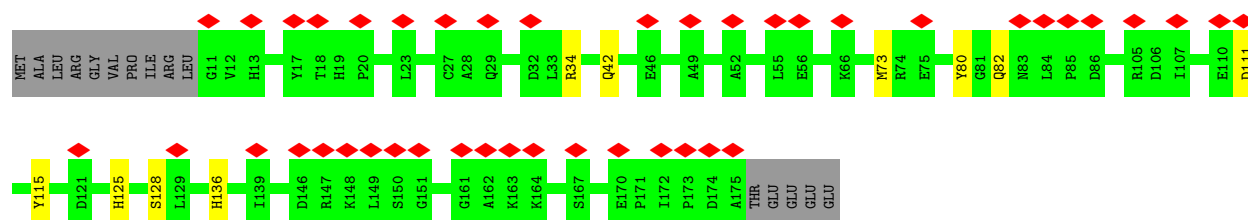
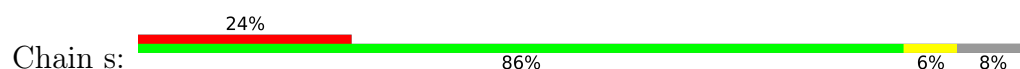
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
60	at	2	Total Zn 2 2	0
60	y	1	Total Zn 1 1	0
60	aa	1	Total Zn 1 1	0

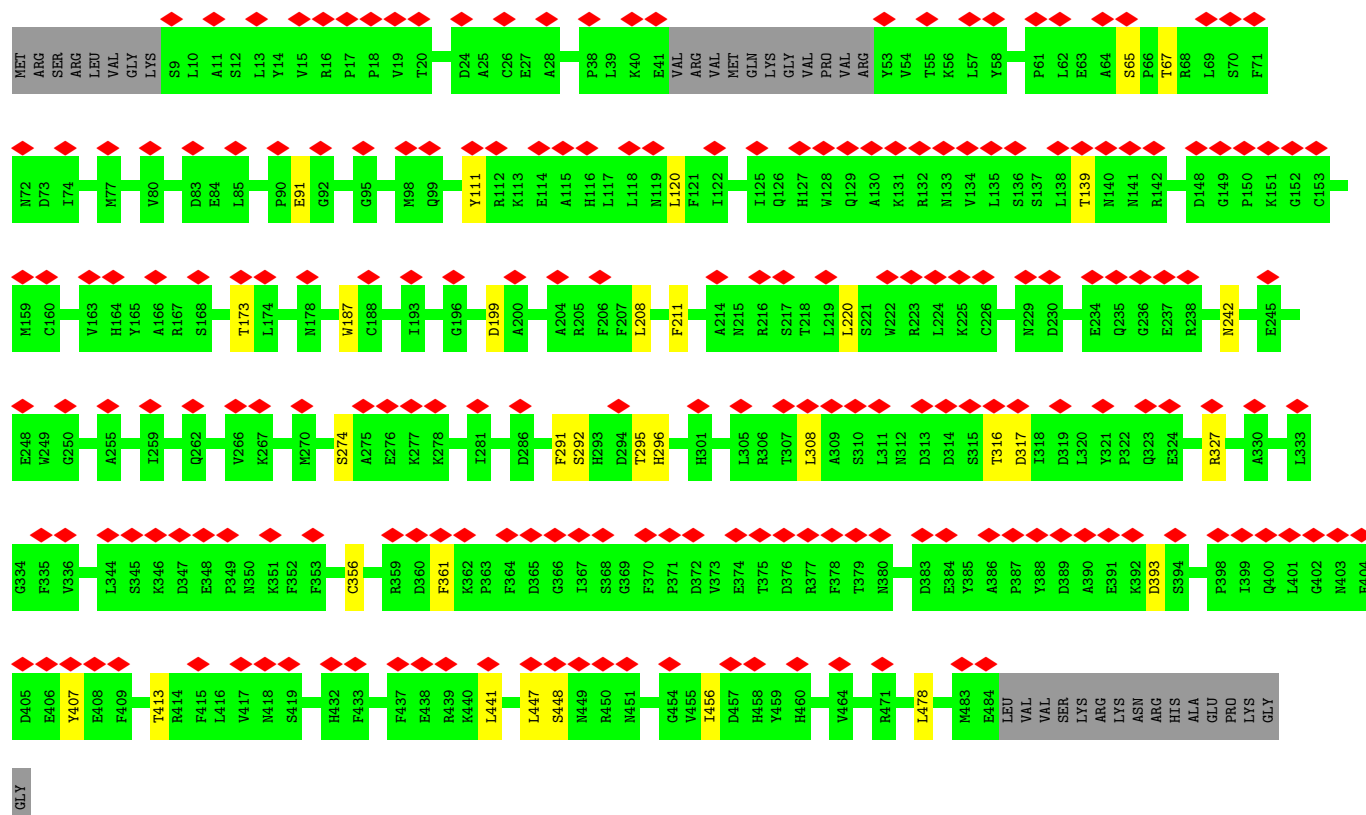
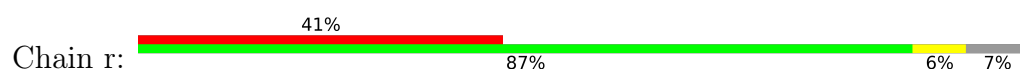




• Molecule 2: mS33

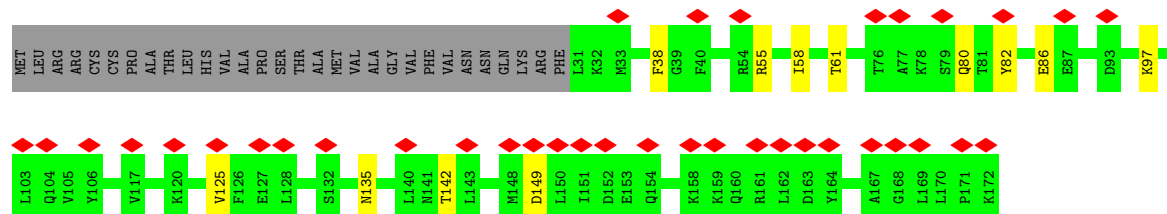
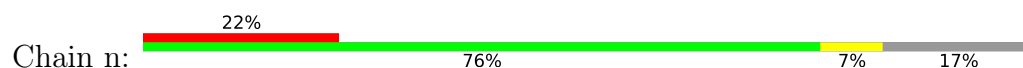


• Molecule 3: mS29

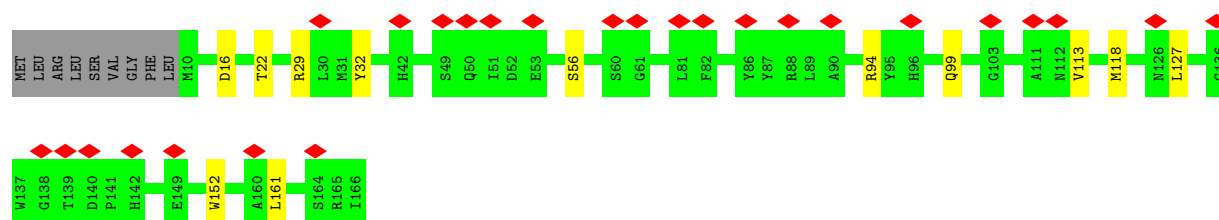
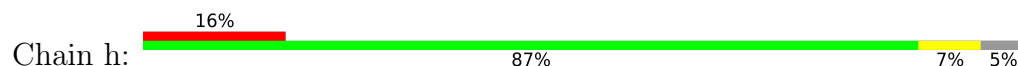




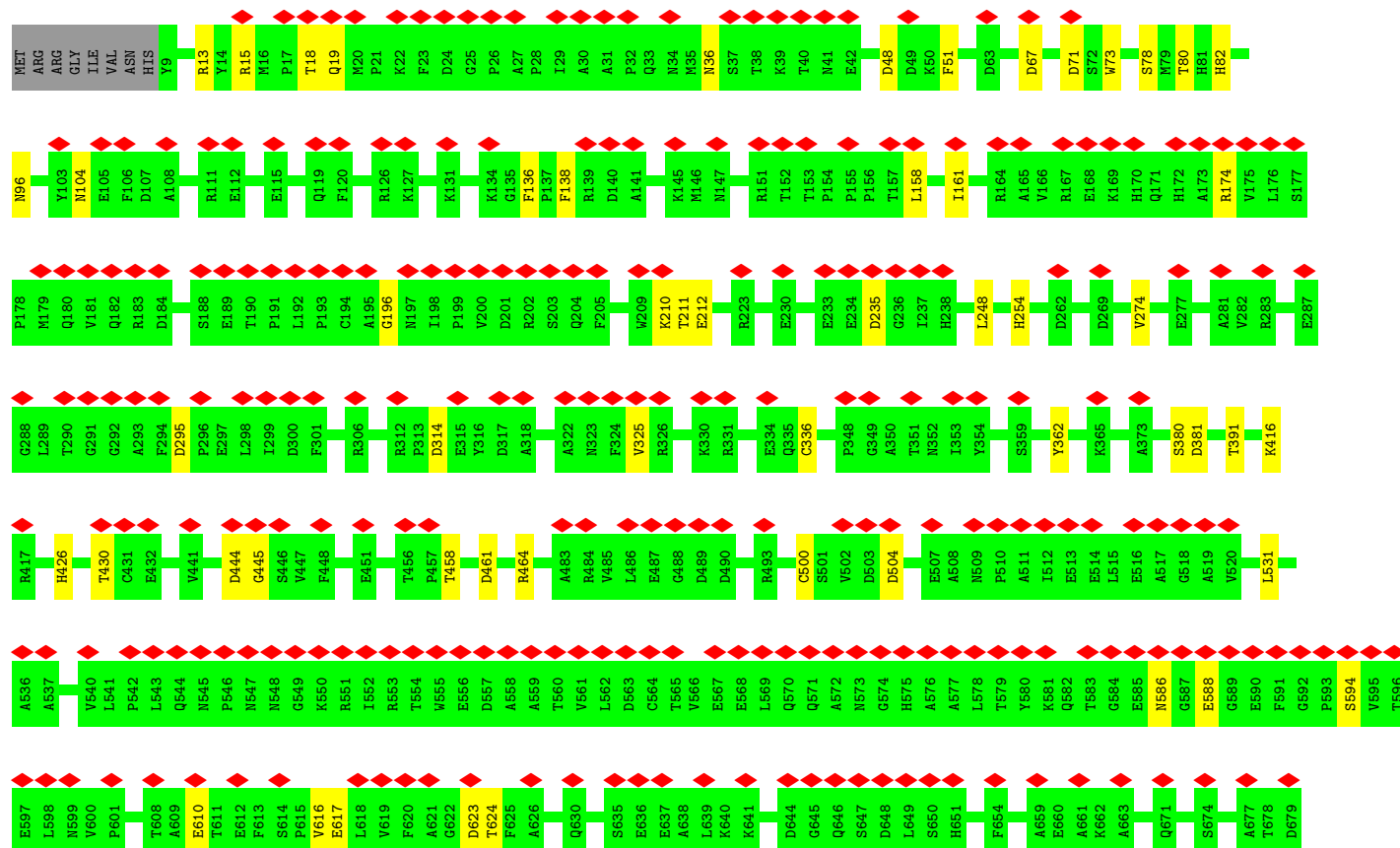
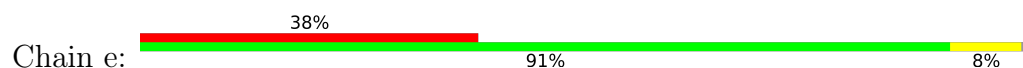
- Molecule 4: uS19

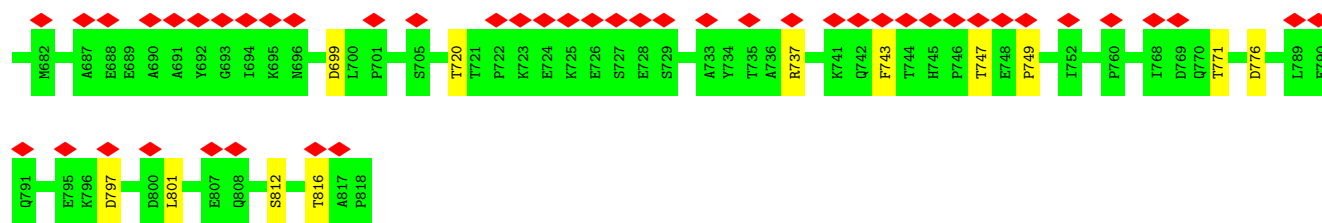


- Molecule 5: uS14m

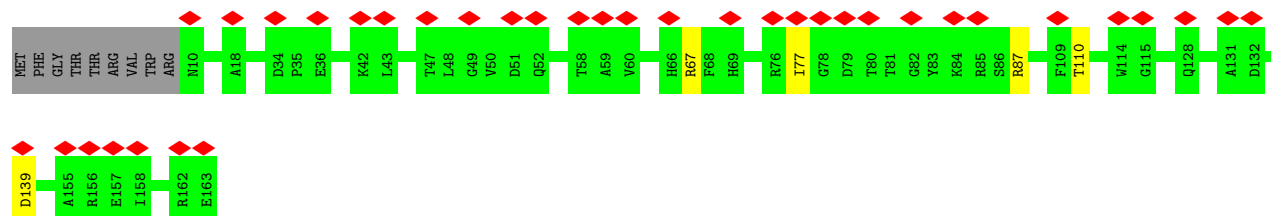


- Molecule 6: uS10m

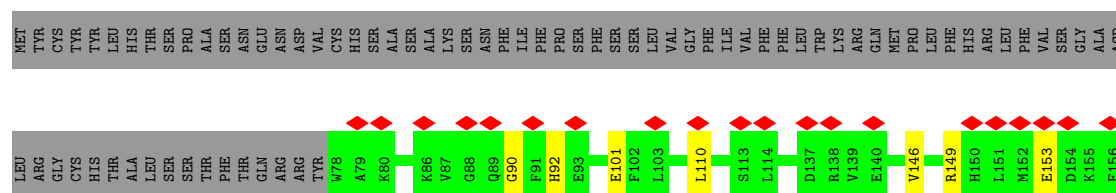




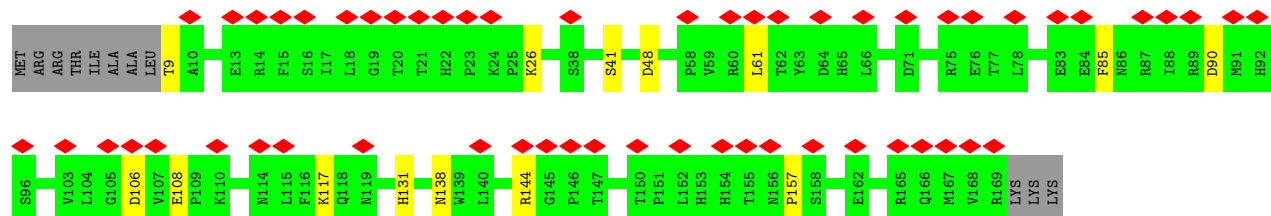
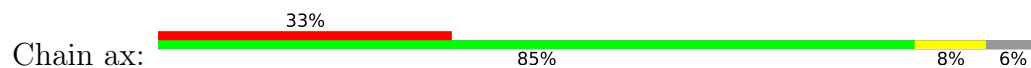
• Molecule 7: mS72



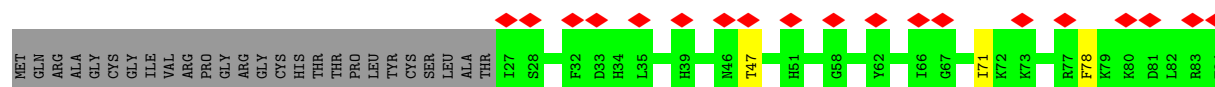
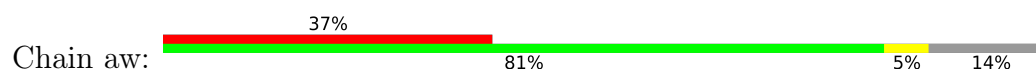
• Molecule 8: mS71

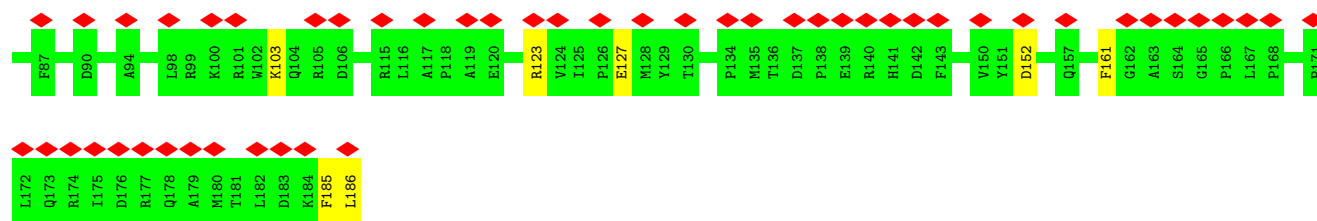


• Molecule 9: mS70

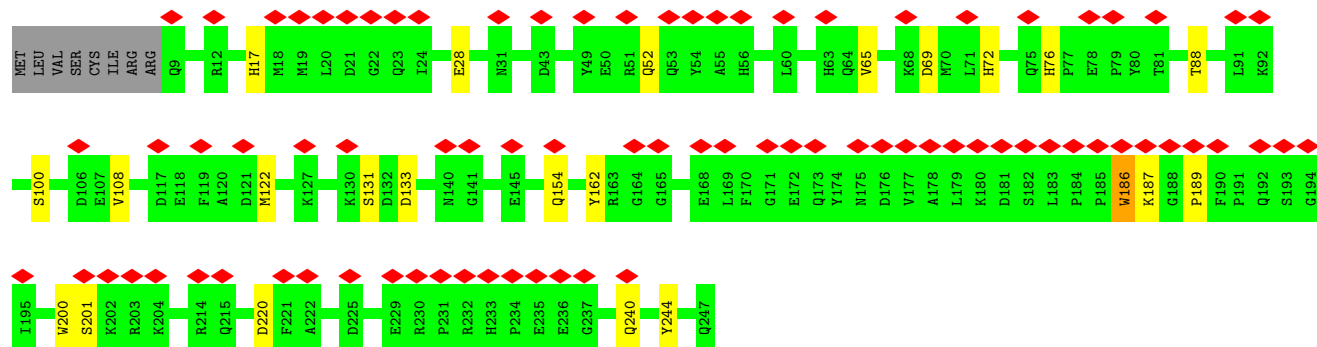
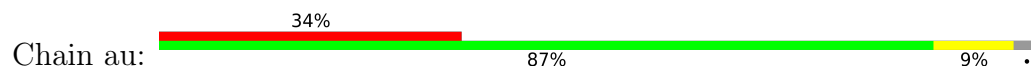


• Molecule 10: mS69

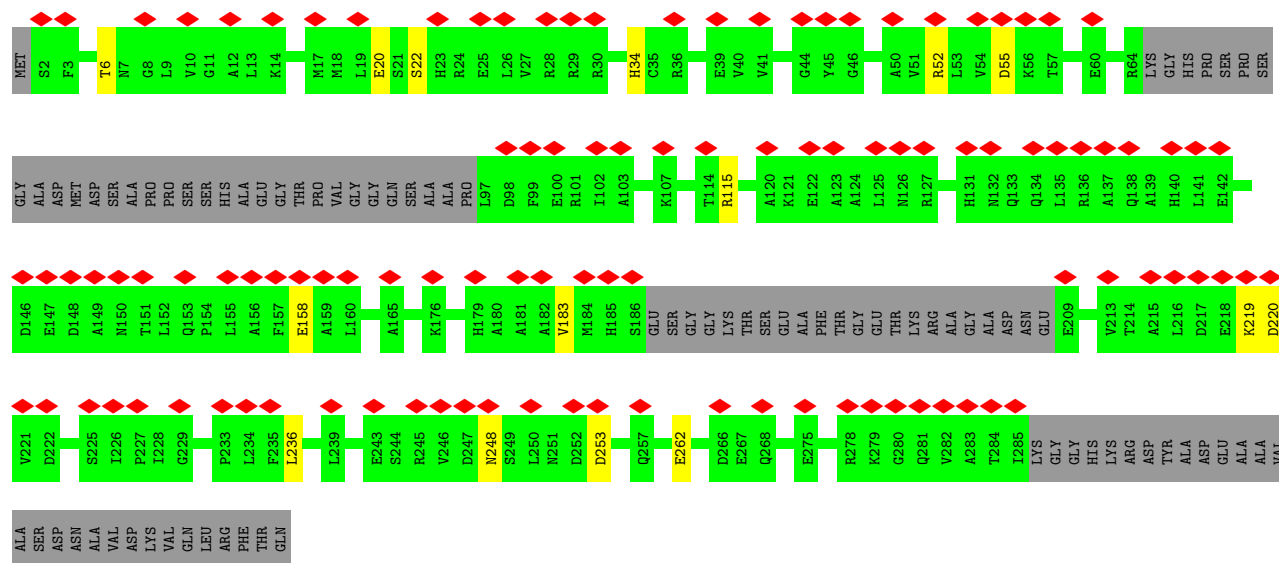




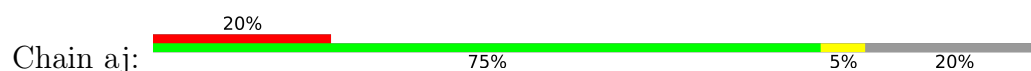
• Molecule 11: Rhodanese domain-containing protein

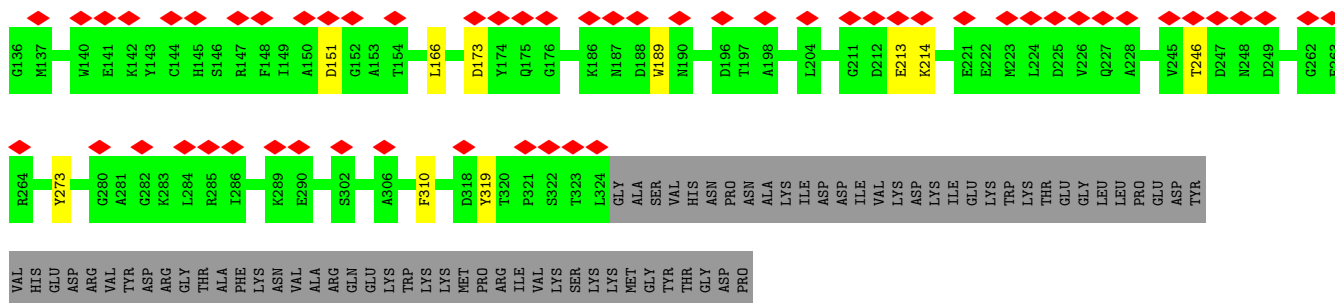


• Molecule 12: mS58

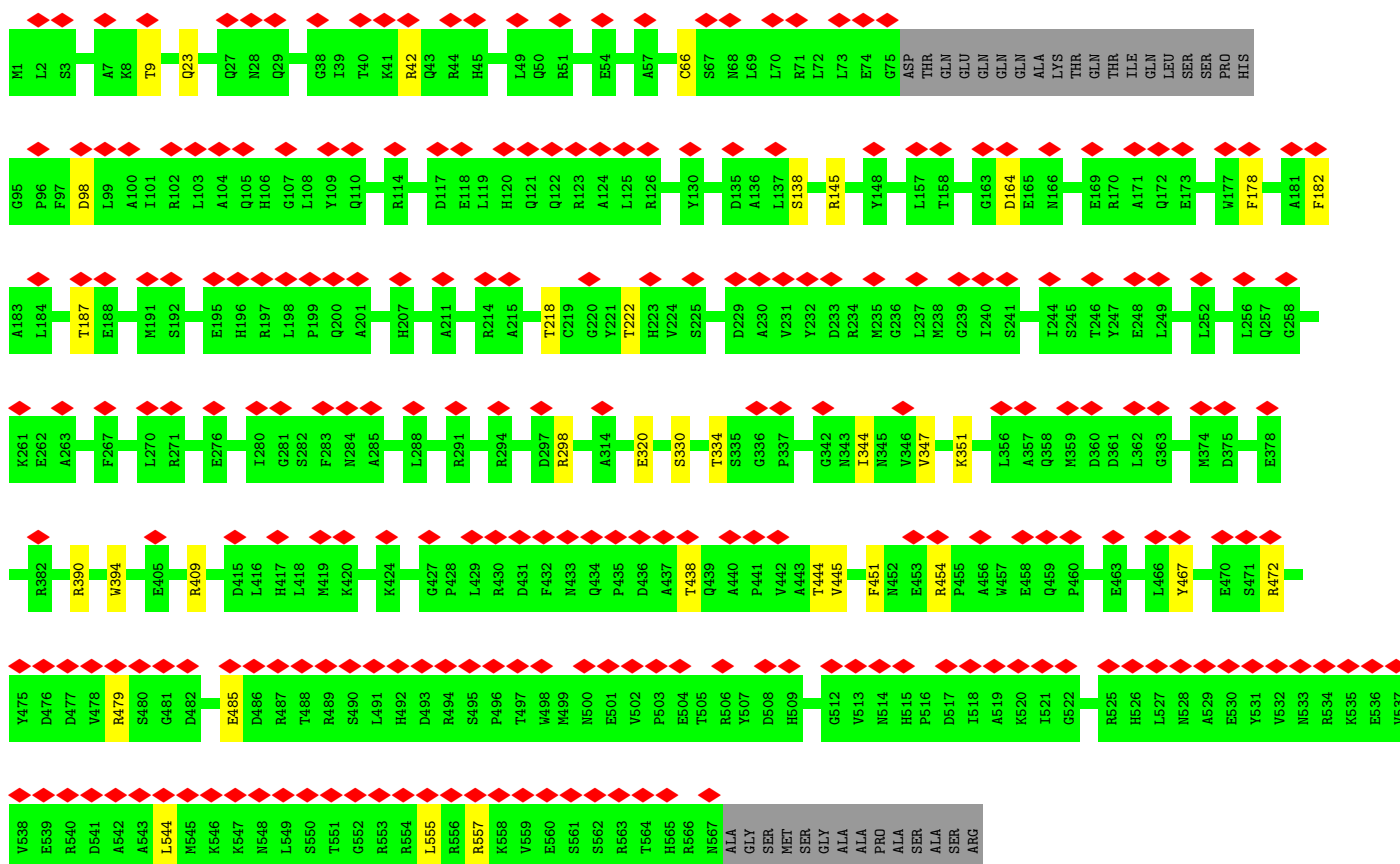
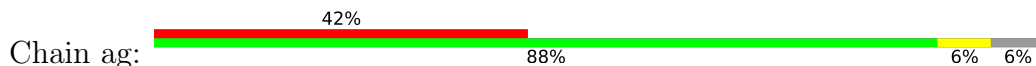


• Molecule 13: mS57

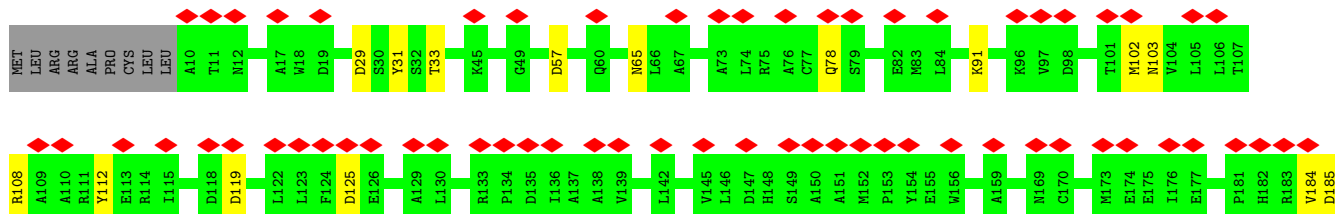
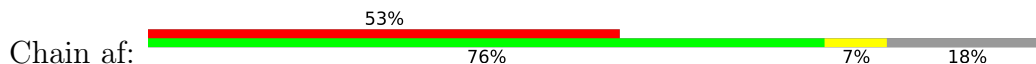


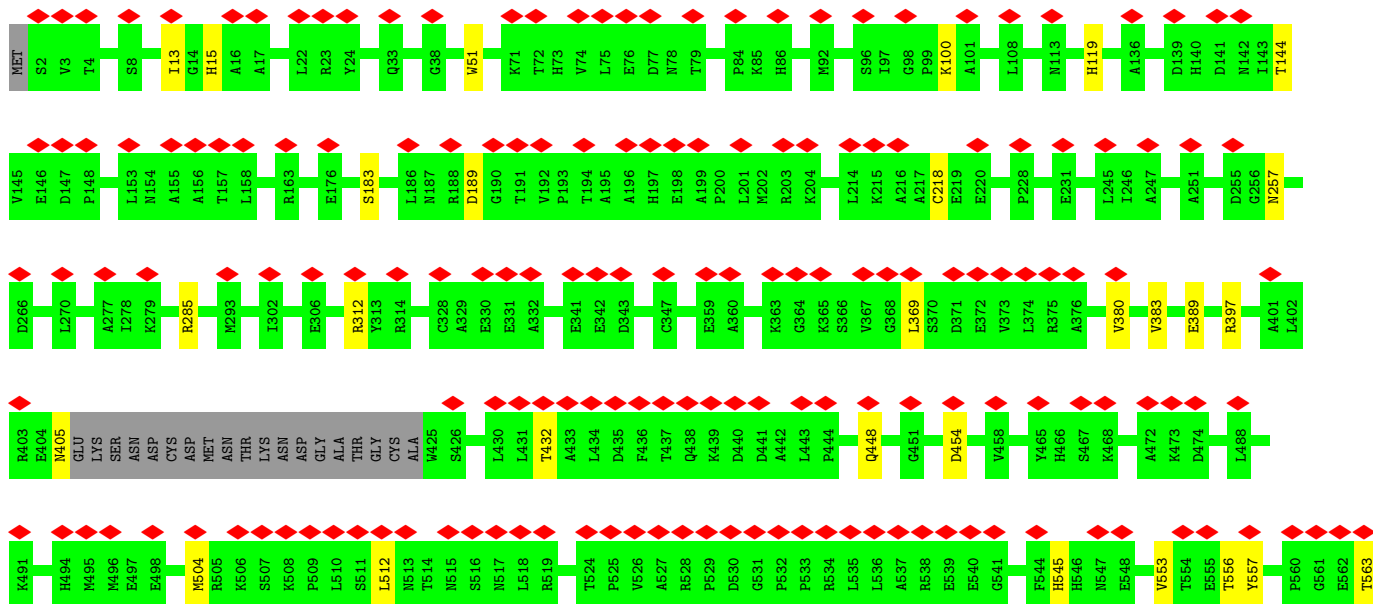


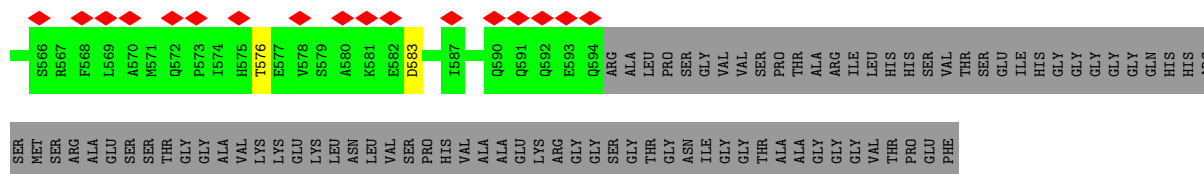
• Molecule 14: mS55



• Molecule 15: mS54

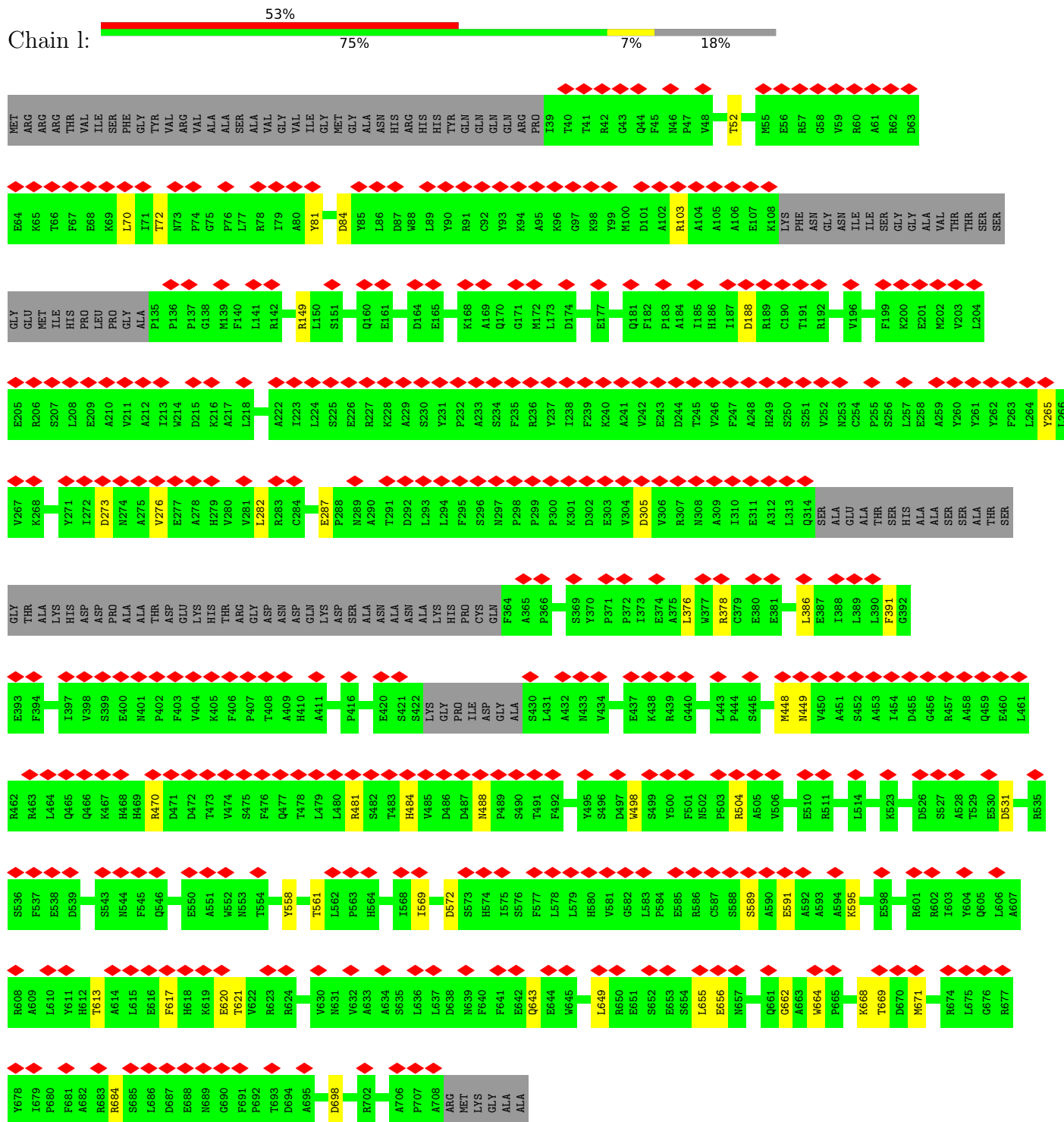






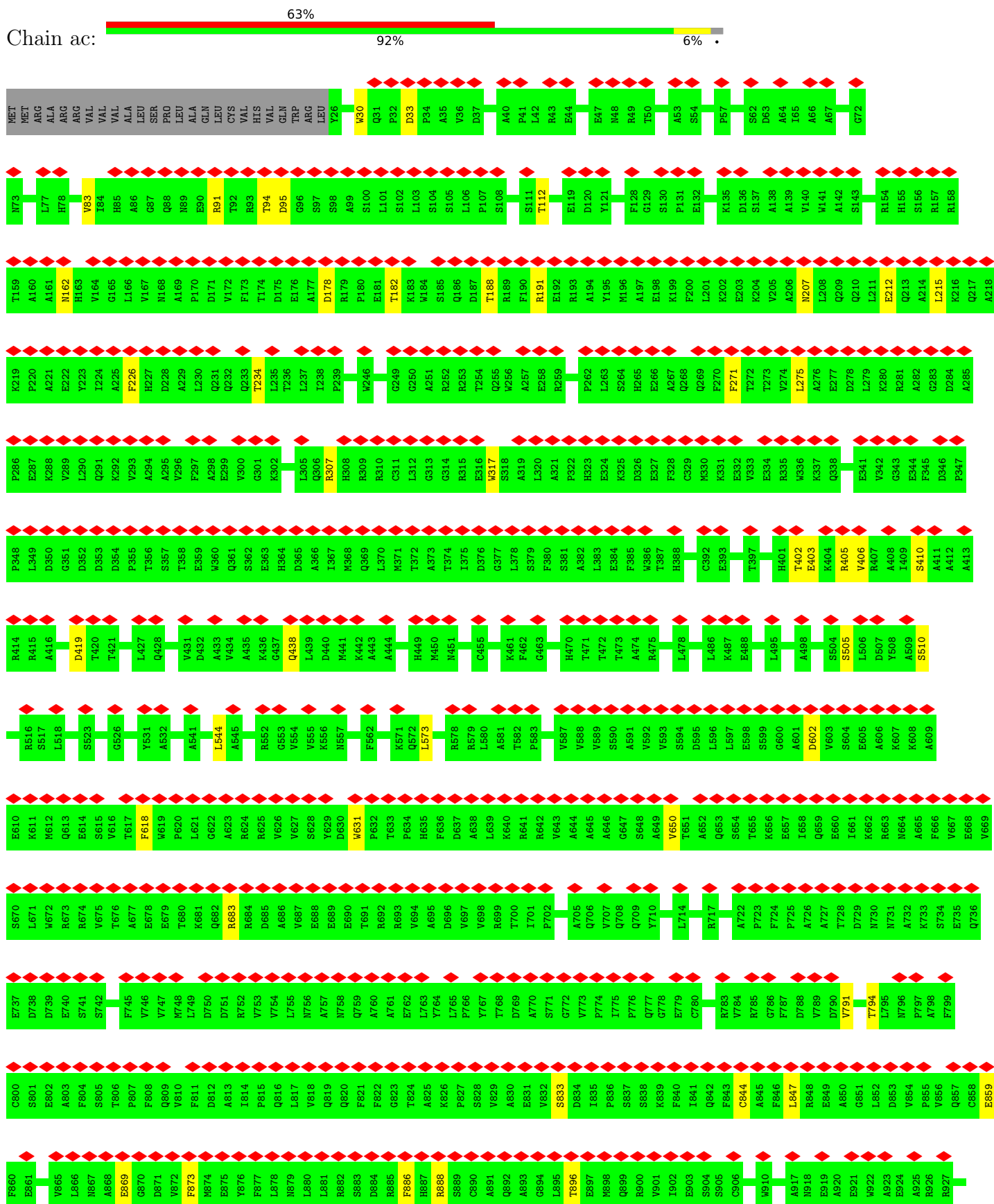
• Molecule 17: mS52

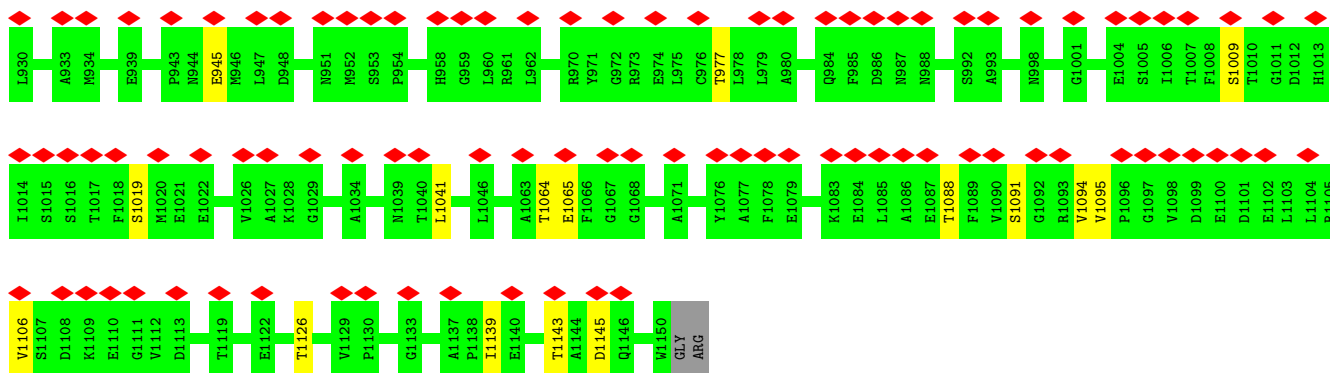
Chain 1:



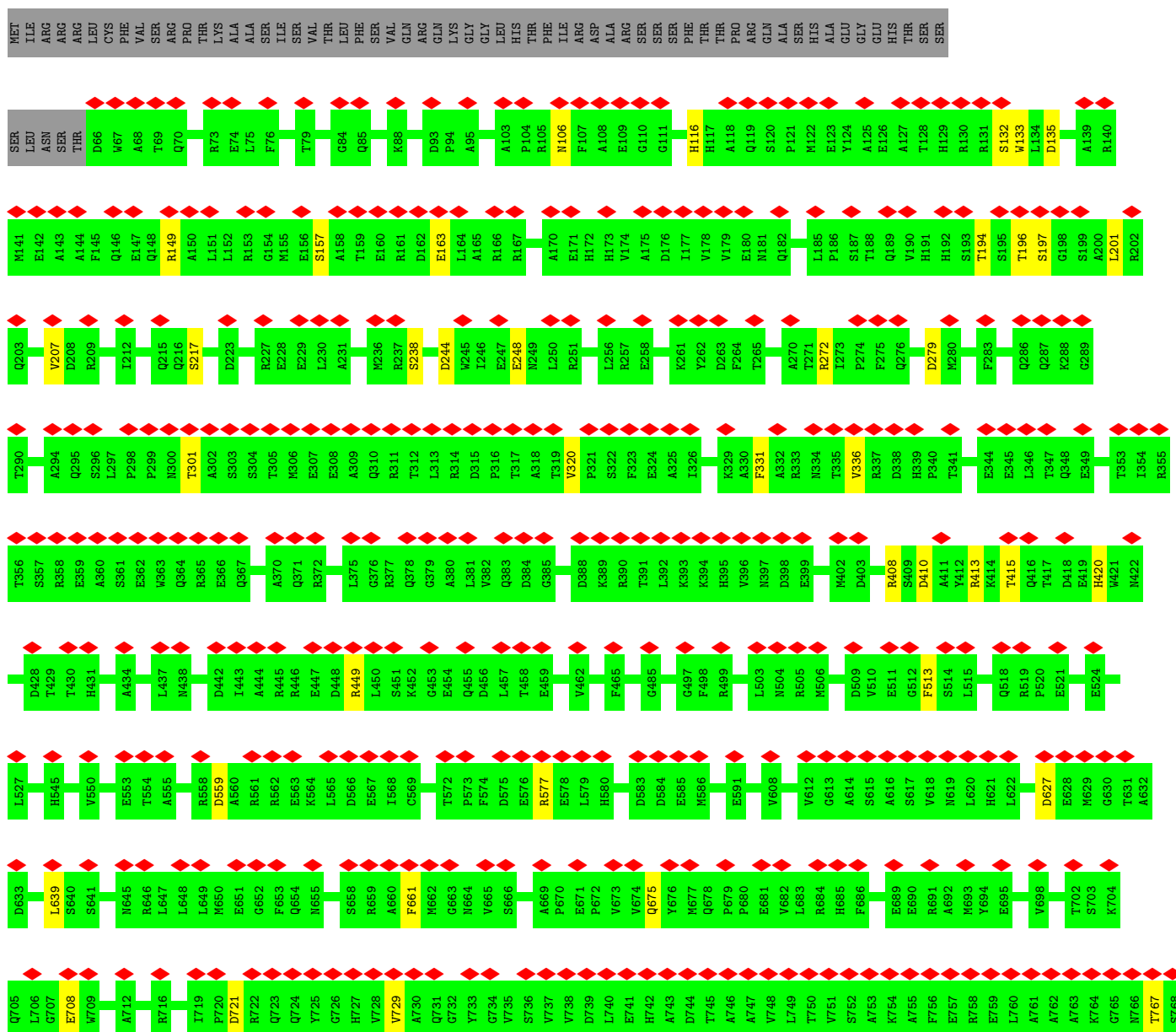
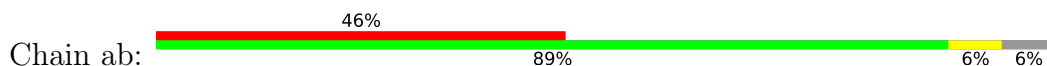
• Molecule 18: mS50

Chain ac:

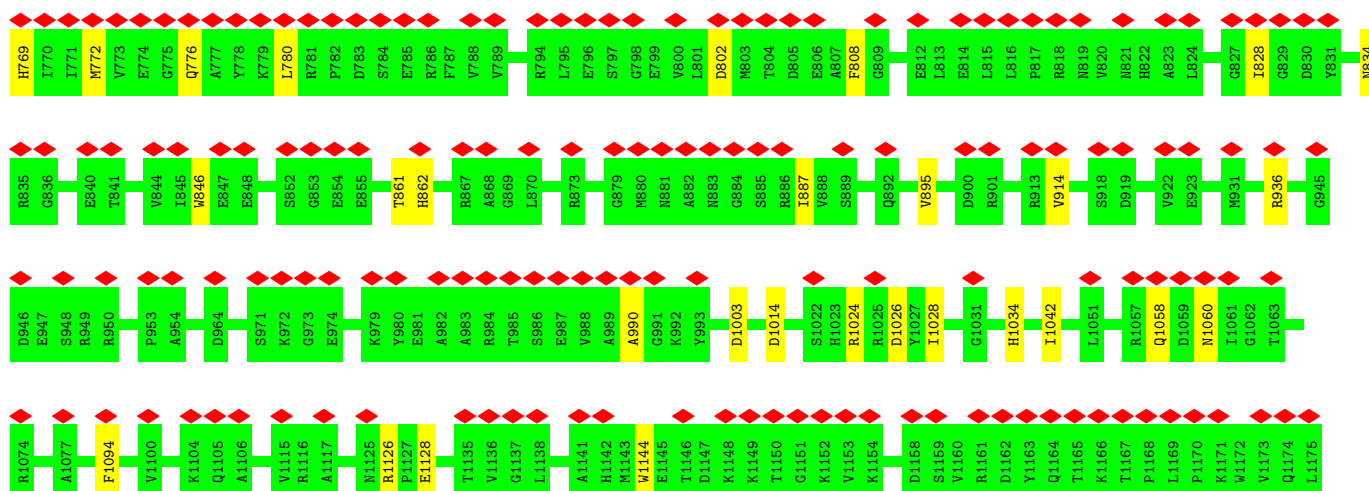




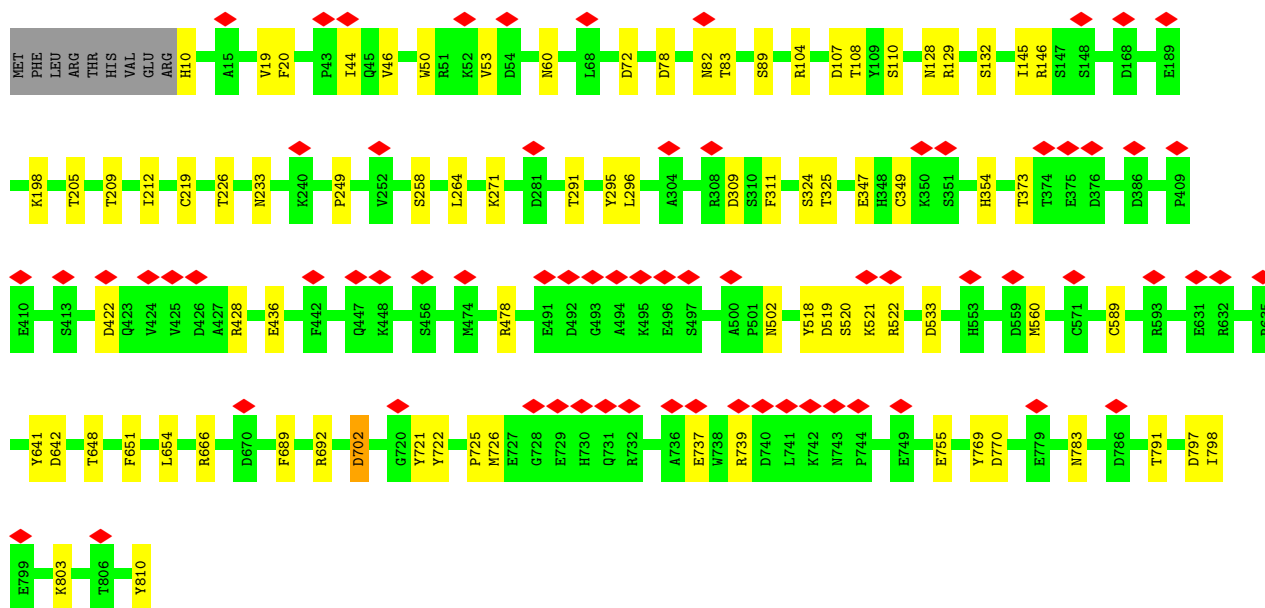
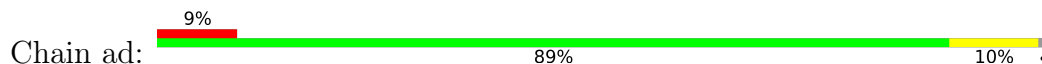
• Molecule 19: mS49



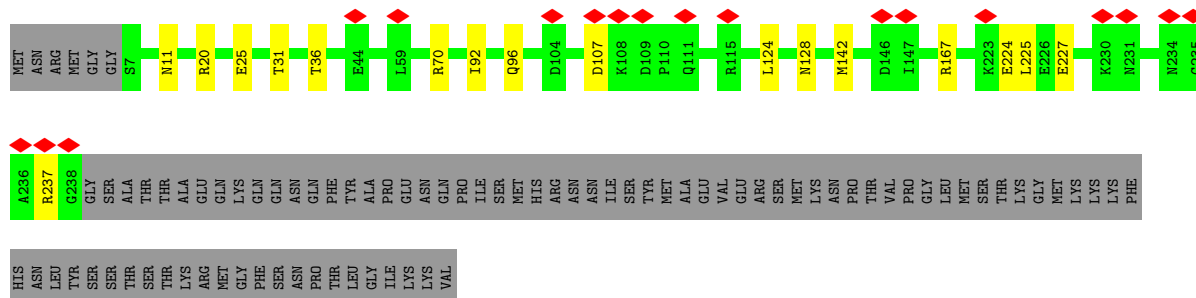




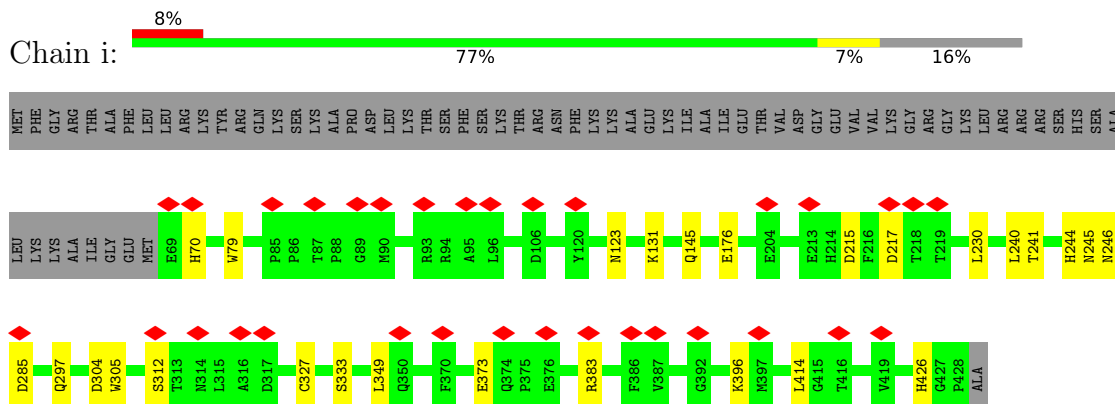
• Molecule 20: mS51



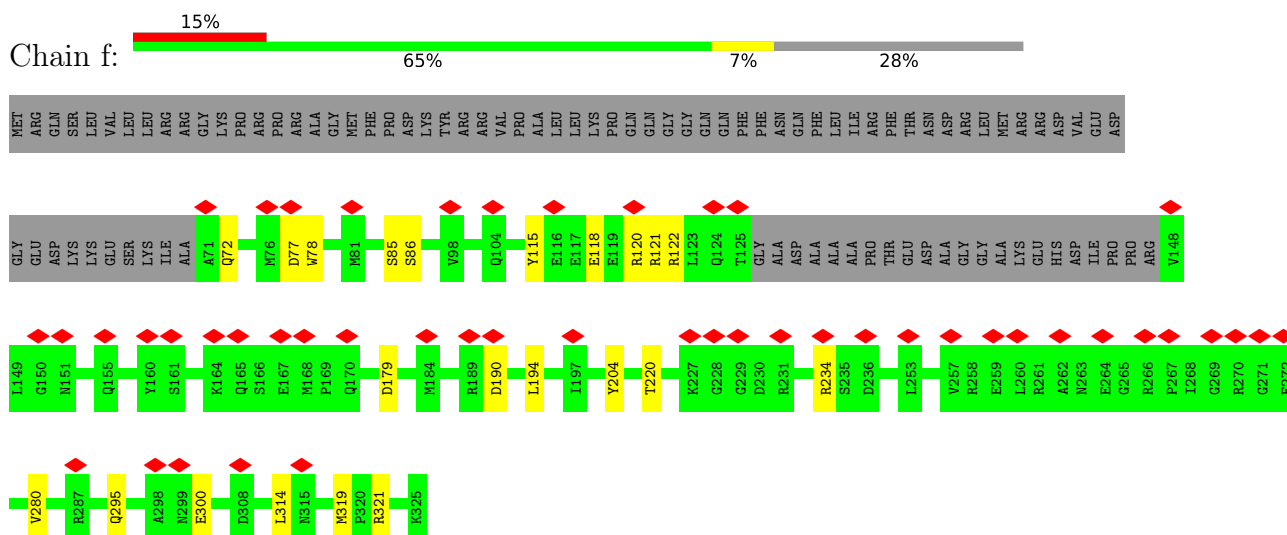
• Molecule 21: bS18m



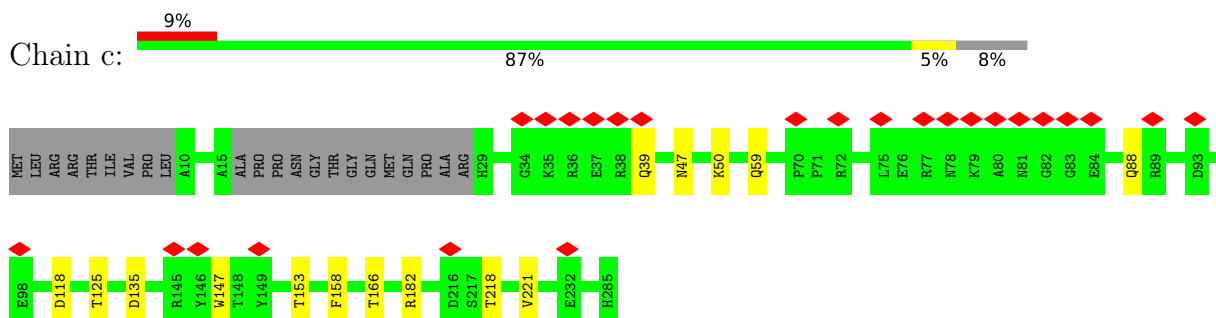
- Molecule 22: uS15m



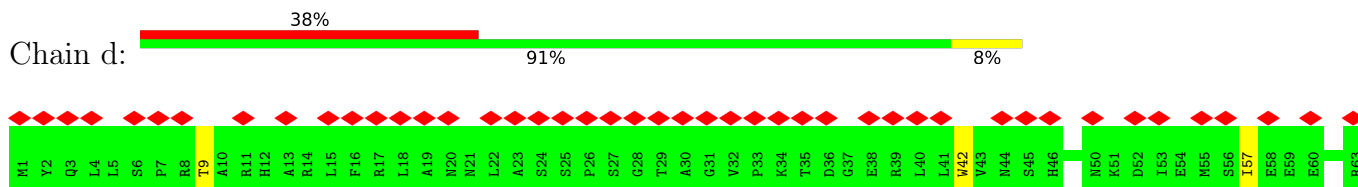
- Molecule 23: uS11m



- Molecule 24: uS8m

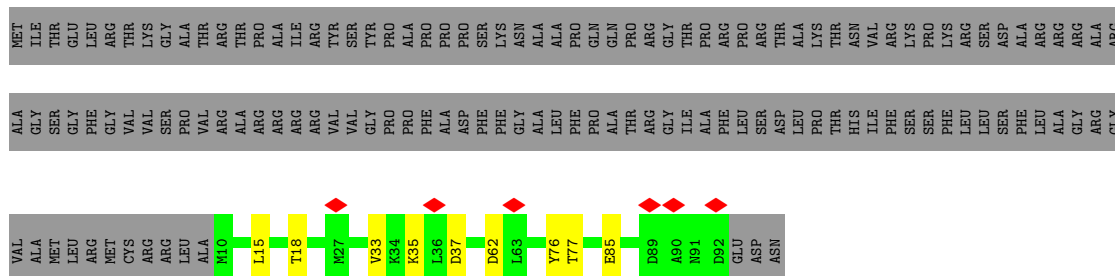


- Molecule 25: uS9m



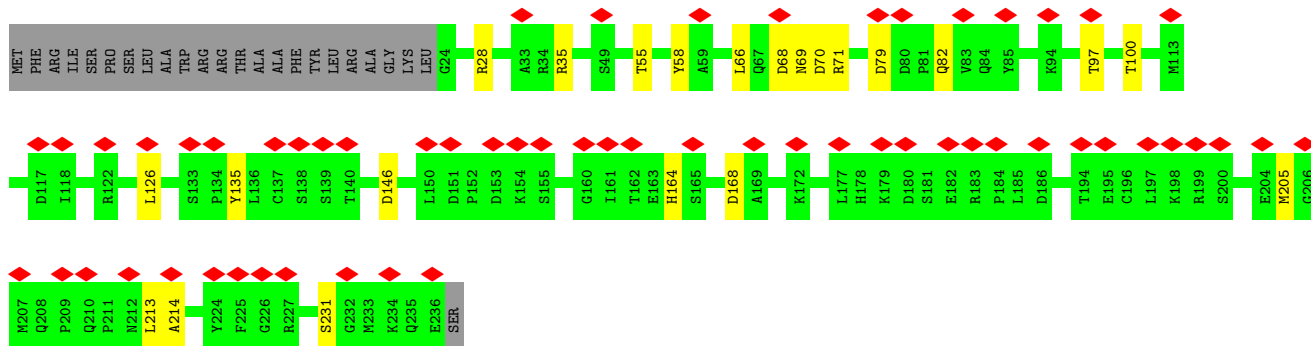
- Molecule 26: mS73

Chain ba:



- Molecule 27: mS68

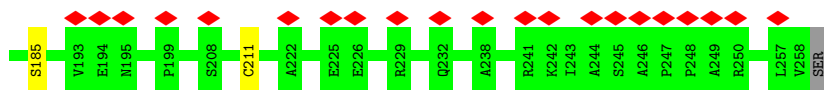
Chain av:



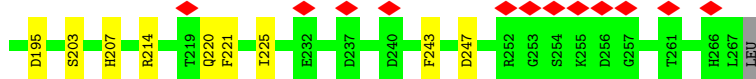
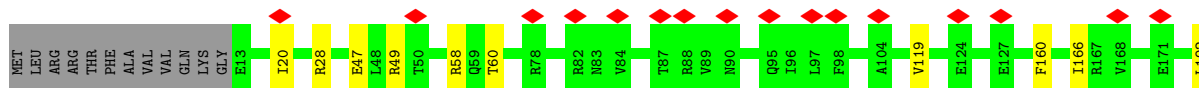
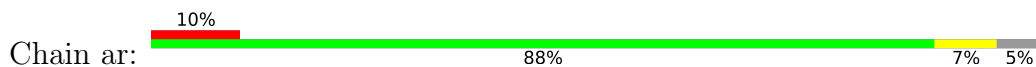
- Molecule 28: mS66

Chain at:

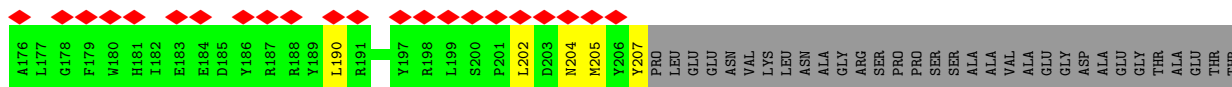
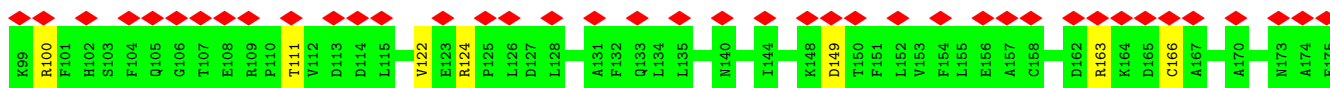
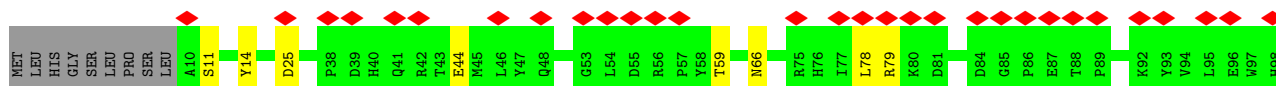




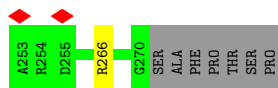
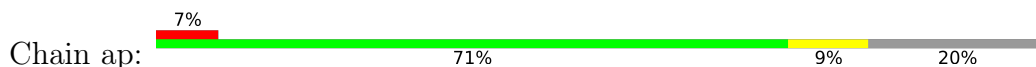
- Molecule 29: AKAP7\_NLS domain-containing protein



- Molecule 30: mS63

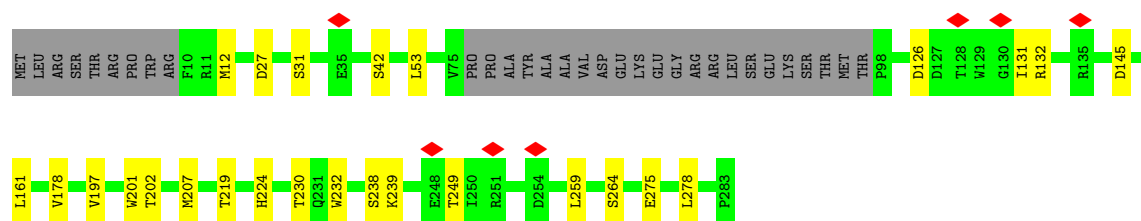


- Molecule 31: mS62

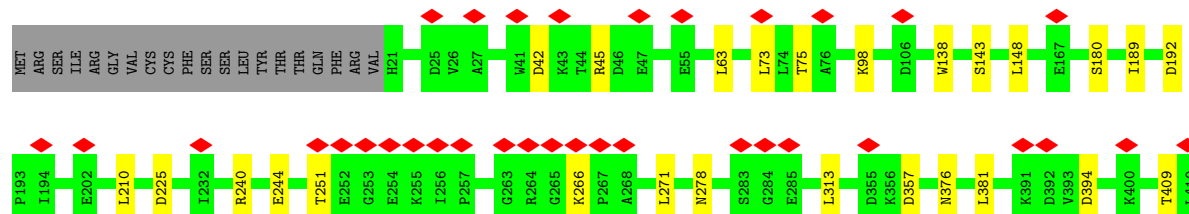


- Molecule 32: mS61

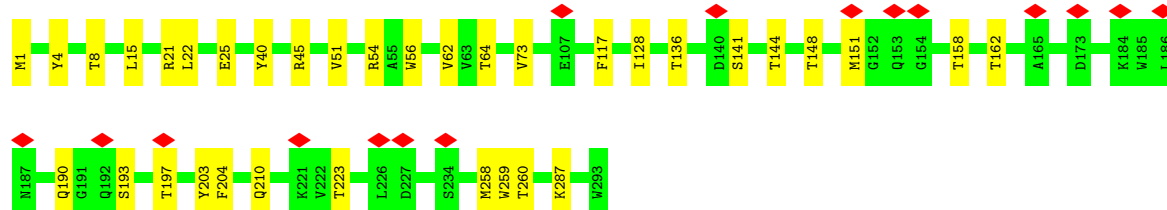
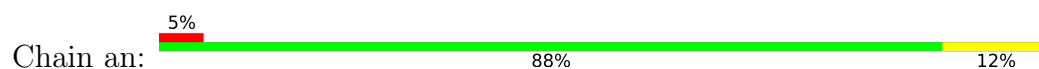




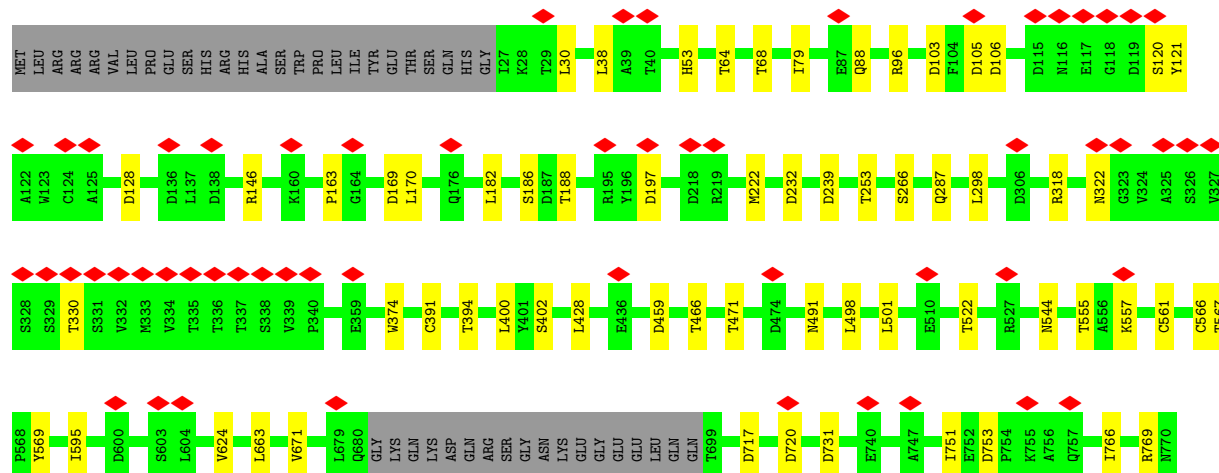
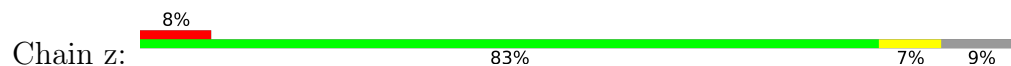
• Molecule 33: mS56

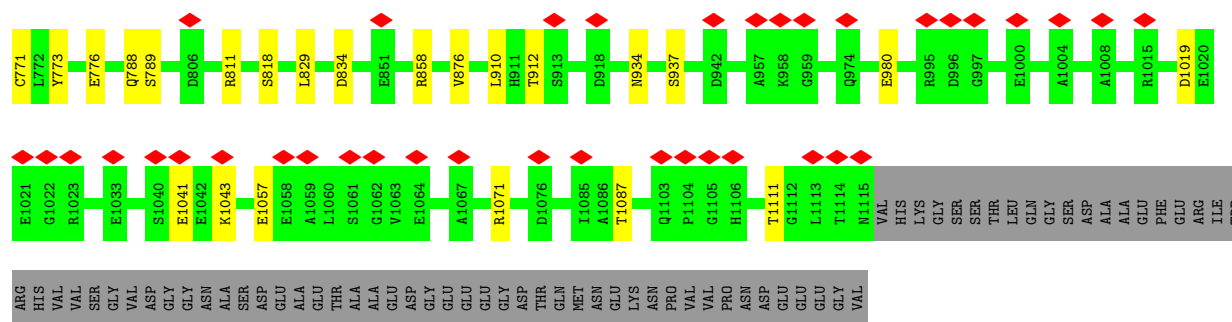


• Molecule 34: mS60

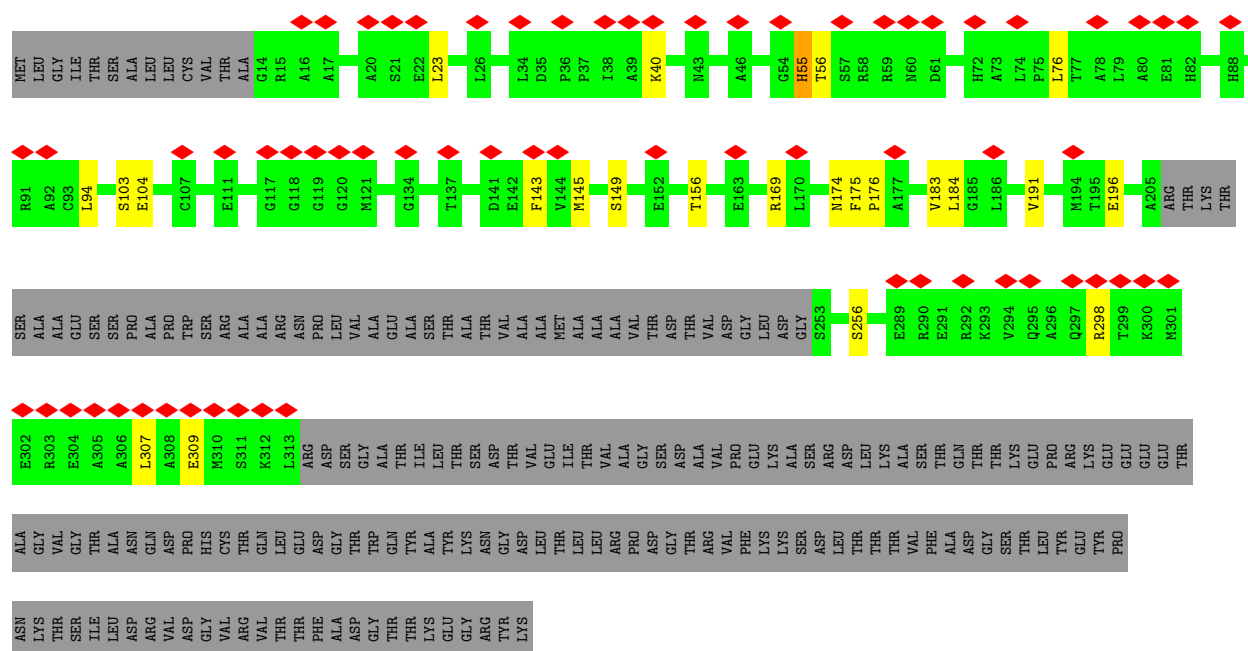


• Molecule 35: mS47

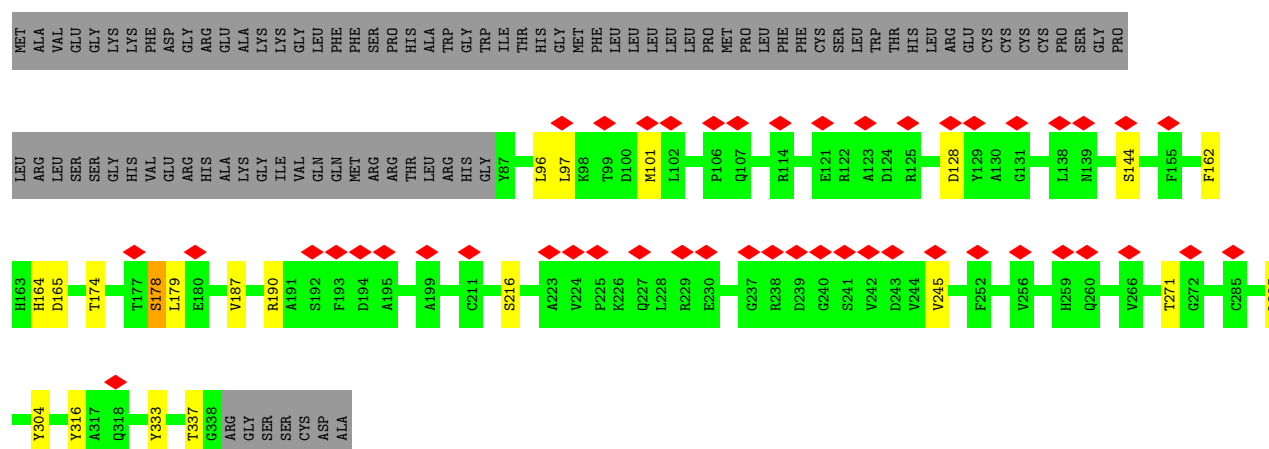




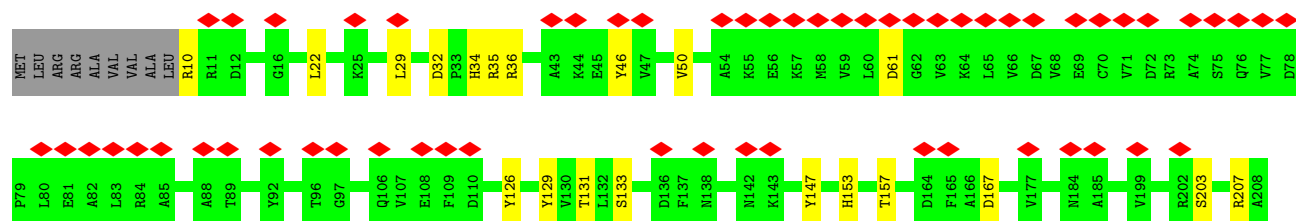
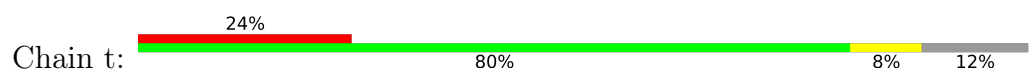
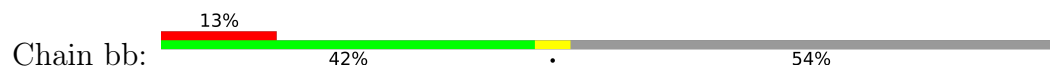
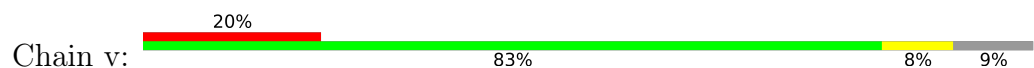
• Molecule 36: Sod\_Fe\_C domain-containing protein



• Molecule 37: Superoxide dismutase, putative



Chain w: 20% 88% 6% 6%

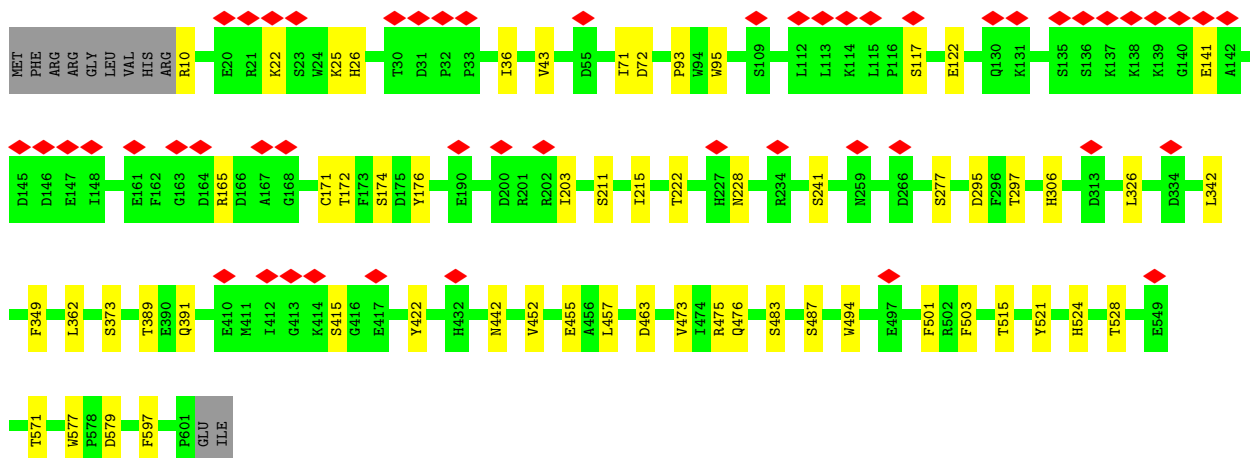
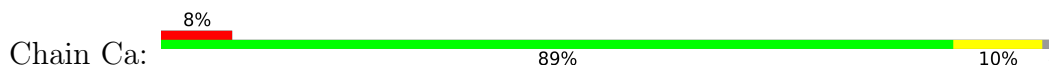




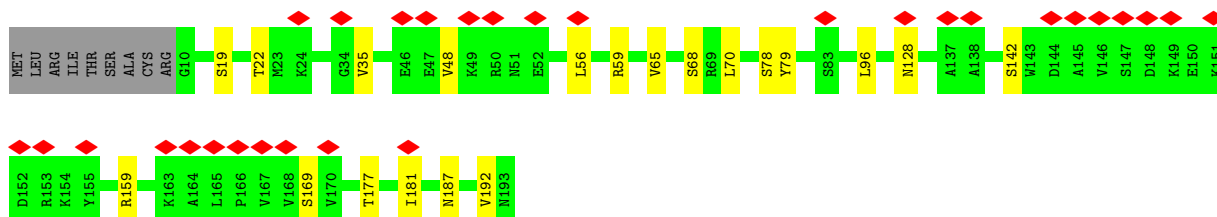
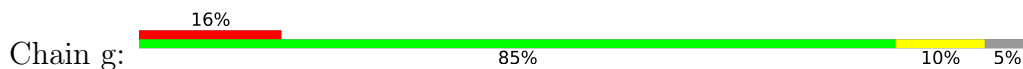




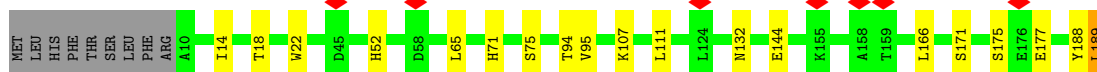
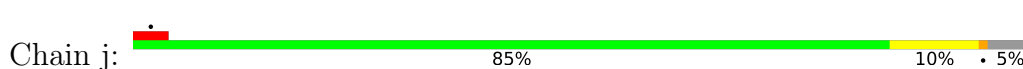
• Molecule 45: mS22



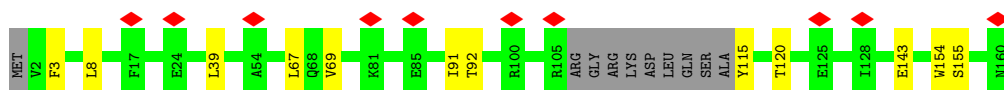
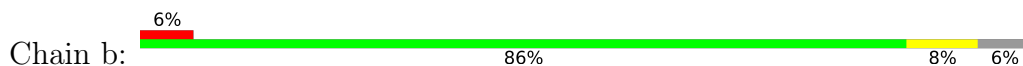
• Molecule 46: bS21m



• Molecule 47: bS16m

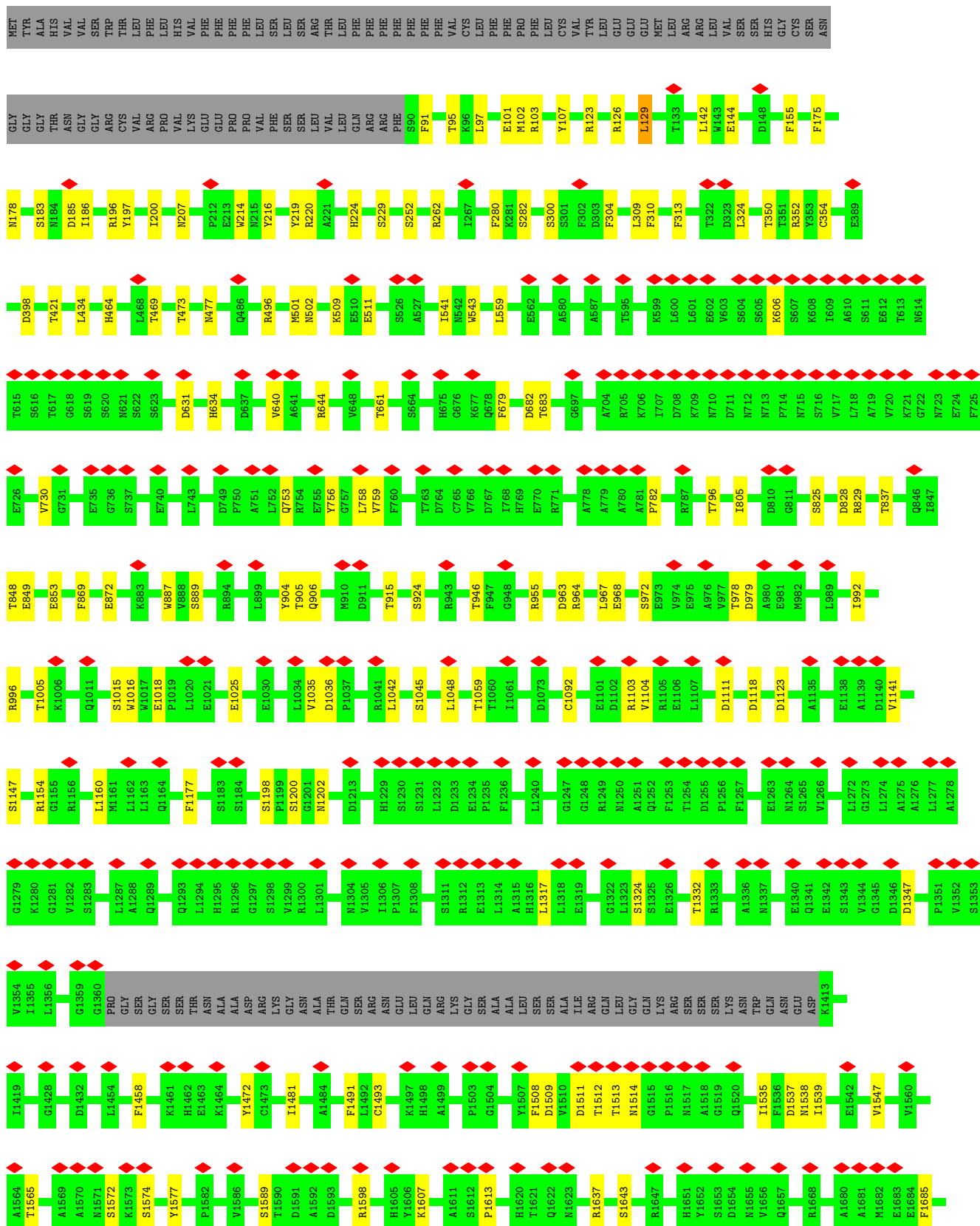


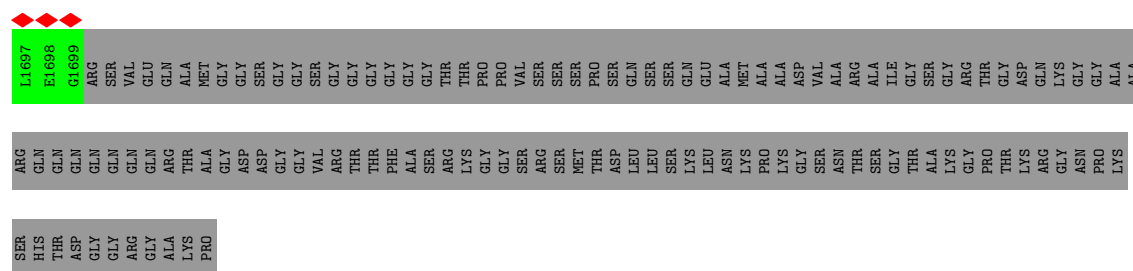
• Molecule 48: bS6m



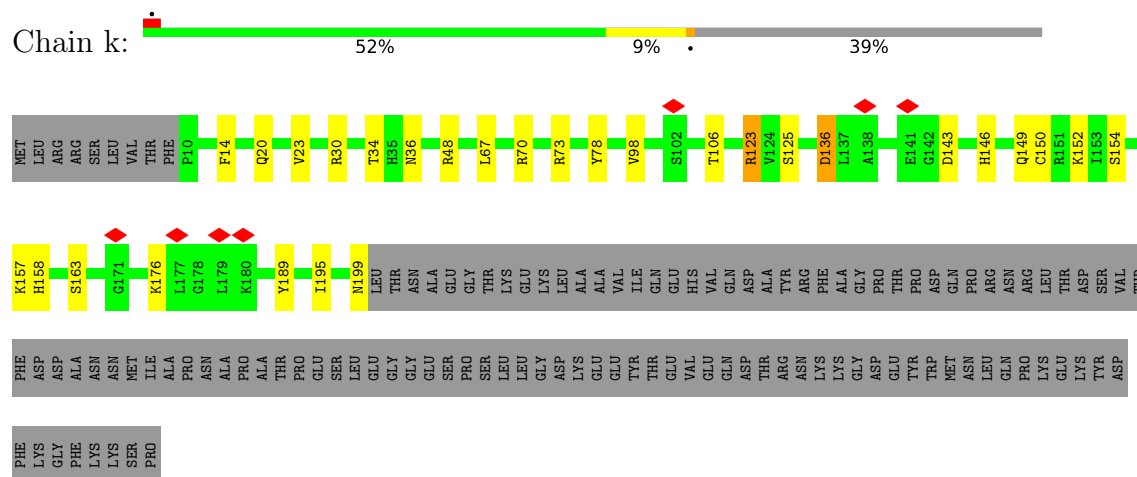
• Molecule 49: MURF5



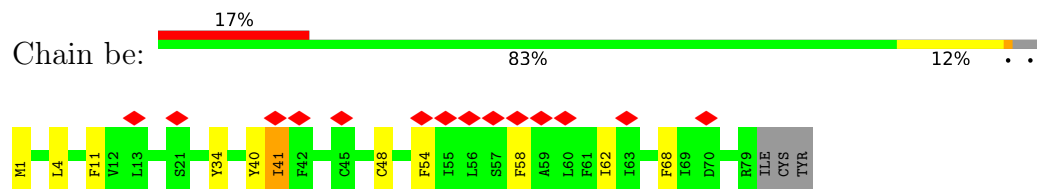




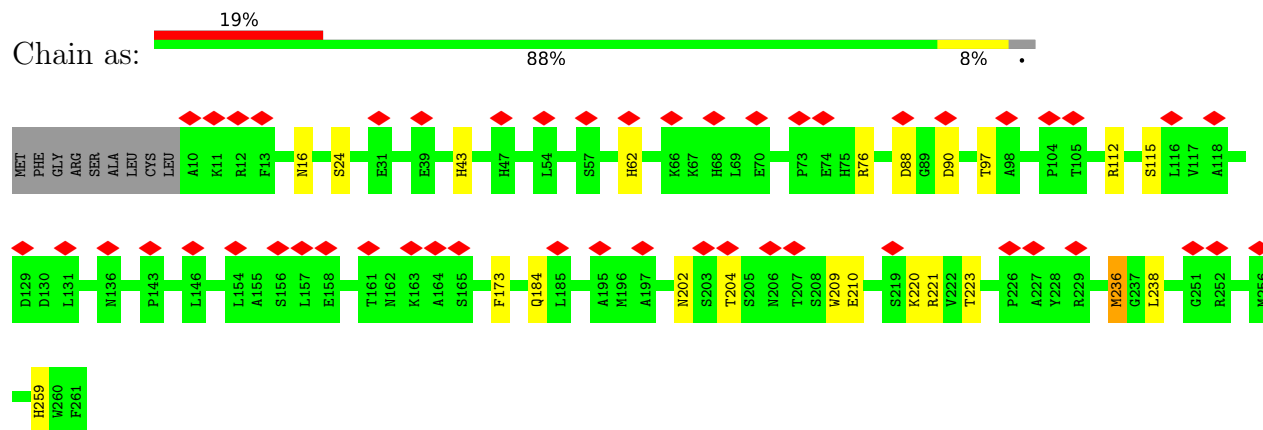
• Molecule 53: 30S Ribosomal protein S17-like protein



• Molecule 54: Ribosome protein S12



• Molecule 55: mS65



• Molecule 56: RNA (478-MER)



U U U A A G G G G A A U U U U A A A G C C A A A G U A A U U G A A U U A G G A A C A G A A U U C C A A G  
U C C C U A A U U G C G A U U U A U U G U C U U A A G A A U C U U U G A G G A U A G A A C A A U U A C C A A G U C C C  
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A A A U G C U U U C G A U U U G A  
U U G A A C A A A U U U G G A A A U U U G G U A A G G U A A U U U A A U U U A  
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G U U U A  
A A U C U U G C A  
A U U U A  
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C C A A U U C C A A A A A C U U U G A A A A C A  
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A U U U G A A U U A A G U U A  
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U U U A A A A A A C U C C A  
U A G G C A U A G U U C U A  
G A U U U G G U U G G A  
A G C U U U A  
A A U G G G U U G U A  
A U A A U U U A





A A U U U C C U U U G G A A C A A A G A A C A A G A A A A G U U U U U G G G C G A G C A G G C A A U U U C A A G G A A U U C U U  
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G U U U G A  
A U A C G A  
A U A  
U G A  
U C U A C A U U A A U U U A U G A G U U C U G A A U U C U G A A U U U A A A A G





[illegible]

- Molecule 56: RNA (478-MER)

Chain 2:  94%

[illegible]











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	148180	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.306	Depositor
Minimum map value	-0.176	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	428.40002, 428.40002, 428.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	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, UTP

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	1.21	6/5704 (0.1%)	0.55	2/7702 (0.0%)
2	s	0.48	0/1391	0.54	0/1880
3	r	0.41	0/3925	0.52	0/5331
4	n	0.43	0/1202	0.54	0/1618
5	h	0.52	0/1364	0.51	0/1842
6	e	0.60	2/6771 (0.0%)	0.59	2/9218 (0.0%)
7	az	0.43	0/1334	0.58	0/1811
8	ay	0.40	0/1236	0.50	0/1663
9	ax	0.35	0/1415	0.51	0/1923
10	aw	0.44	0/1376	0.53	0/1862
11	au	0.48	0/2151	0.54	0/2920
12	ak	0.38	0/1905	0.52	0/2572
13	aj	0.42	0/2665	0.52	1/3618 (0.0%)
14	ag	0.43	0/4572	0.54	0/6180
15	af	0.38	0/4689	0.54	0/6342
16	ae	0.41	0/4746	0.53	0/6439
17	l	0.37	0/4950	0.52	0/6705
18	ac	0.35	0/9073	0.51	0/12323
19	ab	0.41	0/9319	0.53	0/12610
20	ad	0.63	1/6805 (0.0%)	0.60	1/9217 (0.0%)
21	m	0.69	1/1998 (0.1%)	0.59	0/2707
22	i	0.56	0/3048	0.59	0/4110
23	f	0.48	0/1958	0.59	0/2631
24	c	0.79	1/2216 (0.0%)	0.63	0/2984
25	d	0.50	0/3611	0.57	1/4871 (0.0%)
26	ba	0.78	0/734	0.60	0/996
27	av	0.51	0/1795	0.61	0/2432
28	at	0.51	1/1992 (0.1%)	0.56	0/2686
29	ar	0.49	0/2109	0.56	0/2852
30	aq	0.42	0/1751	0.55	0/2374
31	ap	0.51	0/1826	0.56	0/2453
32	ao	0.65	1/2119 (0.0%)	0.61	0/2871

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	ai	0.59	0/3273	0.58	0/4412
34	an	0.64	0/2484	0.60	0/3357
35	z	0.73	3/8856 (0.0%)	0.66	5/12020 (0.0%)
36	y	0.44	0/2030	0.58	0/2751
37	x	0.60	0/2075	0.62	0/2825
38	w	0.50	0/1524	0.55	0/2066
39	v	0.66	0/1603	0.65	1/2154 (0.0%)
40	bb	0.53	0/926	0.59	0/1230
41	t	2.02	6/1846 (0.3%)	0.58	0/2511
42	al	0.62	0/2430	0.60	0/3275
43	q	0.65	0/1892	0.59	0/2551
44	p	0.66	0/2047	0.58	0/2762
45	Ca	1.33	9/5233 (0.2%)	0.61	1/7083 (0.0%)
46	g	0.57	0/1580	0.57	1/2113 (0.0%)
47	j	0.61	0/1546	0.67	1/2090 (0.0%)
48	b	0.58	0/1299	0.59	0/1751
49	bd	0.46	0/441	0.66	0/601
50	a	0.75	0/3523	0.61	0/4759
51	bc	0.36	0/1278	0.53	0/1711
52	aa	0.52	0/12863	0.56	0/17416
53	k	0.76	1/1624 (0.1%)	0.66	0/2192
54	be	0.56	0/690	0.65	0/934
55	as	0.66	1/2088 (0.0%)	0.67	1/2844 (0.0%)
56	2	0.98	2/11110 (0.0%)	1.28	84/17276 (0.5%)
56	A	0.69	0/3392	1.11	19/5275 (0.4%)
All	All	0.67	35/179403 (0.0%)	0.66	120/245702 (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	u	0	1
6	e	0	2
11	au	0	3
15	af	0	1
17	l	0	2
20	ad	0	3
25	d	0	2
27	av	0	1
29	ar	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	ao	0	2
33	ai	0	1
39	v	0	2
45	Ca	0	2
49	bd	0	2
52	aa	0	1
53	k	0	3
54	be	0	1
All	All	0	30

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Ca	95	TRP	CE3-CZ3	56.27	2.34	1.38
1	u	666	PHE	CE2-CZ	45.16	2.23	1.37
41	t	46	TYR	CD1-CE1	44.28	2.05	1.39
41	t	46	TYR	CD2-CE2	43.84	2.05	1.39
1	u	666	PHE	CD2-CE2	37.86	2.15	1.39

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	z	1071	ARG	CD-NE-CZ	21.92	154.28	123.60
6	e	444	ASP	C-N-CA	20.46	165.26	122.30
55	as	236	MET	CG-SD-CE	17.31	127.90	100.20
35	z	1071	ARG	NE-CZ-NH1	17.25	128.93	120.30
56	2	556	C	C5-C6-N1	8.72	125.36	121.00

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	au	154	GLN	Peptide
11	au	186	TRP	Peptide
6	e	15	ARG	Peptide
6	e	18	THR	Peptide
1	u	229	SER	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	5597	0	5628	0	0
2	s	1351	0	1315	0	0
3	r	3806	0	3680	0	0
4	n	1169	0	1188	0	0
5	h	1324	0	1304	0	0
6	e	6577	0	6289	0	0
7	az	1292	0	1287	0	0
8	ay	1200	0	1190	0	0
9	ax	1366	0	1342	0	0
10	aw	1338	0	1322	0	0
11	au	2069	0	1936	0	0
12	ak	1865	0	1836	0	0
13	aj	2590	0	2552	0	0
14	ag	4472	0	4434	0	0
15	af	4590	0	4545	0	0
16	ae	4634	0	4582	0	0
17	l	4821	0	4706	0	0
18	ac	8864	0	8621	0	0
19	ab	9094	0	8739	0	0
20	ad	6610	0	6371	0	0
21	m	1940	0	1881	0	0
22	i	2970	0	2976	0	0
23	f	1917	0	1854	0	0
24	c	2169	0	2146	0	0
25	d	3538	0	3515	0	0
26	ba	706	0	645	0	0
27	av	1752	0	1705	0	0
28	at	1946	0	1927	0	0
29	ar	2061	0	2058	0	0
30	aq	1701	0	1658	0	0
31	ap	1796	0	1747	0	0
32	ao	2062	0	2042	0	0
33	ai	3205	0	3206	0	0
34	an	2422	0	2434	0	0
35	z	8630	0	8339	0	0
36	y	1983	0	1989	0	0
37	x	2016	0	1932	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	w	1479	0	1458	0	0
39	v	1567	0	1500	0	0
40	bb	905	0	968	0	0
41	t	1797	0	1752	0	0
42	al	2372	0	2374	0	0
43	q	1840	0	1783	0	0
44	p	1998	0	1965	0	0
45	Ca	5070	0	4897	0	0
46	g	1544	0	1564	0	0
47	j	1501	0	1517	0	0
48	b	1271	0	1263	0	0
49	bd	430	0	448	0	0
50	a	3436	0	3427	0	0
51	bc	1247	0	1249	0	0
52	aa	12549	0	12207	0	0
53	k	1577	0	1587	0	0
54	be	665	0	668	0	0
55	as	2024	0	2025	0	0
56	2	9932	0	4972	313	0
56	A	3030	0	1513	72	0
57	r	32	0	11	0	0
58	r	1	0	0	0	0
59	aj	29	0	10	0	0
60	aa	1	0	0	0	0
60	at	2	0	0	0	0
60	y	1	0	0	0	0
All	All	173743	0	164079	383	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 32.

The worst 5 of 383 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)
56:2:590:A:H2'	56:2:591:A:C8	2.07	0.90
56:2:125:U:O2	56:2:127:G:N2	2.06	0.89
56:A:517:U:OP1	56:A:519:U:N3	2.04	0.89
56:2:337:U:H5'	56:2:356:U:H4'	1.54	0.89
56:2:236:G:HO2'	56:2:251:U:HO2'	1.20	0.87

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	u	693/874 (79%)	638 (92%)	55 (8%)	0	100	100
2	s	163/180 (91%)	138 (85%)	23 (14%)	2 (1%)	11	43
3	r	461/500 (92%)	408 (88%)	53 (12%)	0	100	100
4	n	140/172 (81%)	122 (87%)	18 (13%)	0	100	100
5	h	155/166 (93%)	143 (92%)	12 (8%)	0	100	100
6	e	808/818 (99%)	712 (88%)	94 (12%)	2 (0%)	44	75
7	az	152/163 (93%)	138 (91%)	14 (9%)	0	100	100
8	ay	139/218 (64%)	127 (91%)	11 (8%)	1 (1%)	19	53
9	ax	159/172 (92%)	148 (93%)	10 (6%)	1 (1%)	22	56
10	aw	158/186 (85%)	135 (85%)	23 (15%)	0	100	100
11	au	237/247 (96%)	205 (86%)	31 (13%)	1 (0%)	30	64
12	ak	224/314 (71%)	205 (92%)	19 (8%)	0	100	100
13	aj	313/396 (79%)	274 (88%)	38 (12%)	1 (0%)	37	68
14	ag	544/581 (94%)	500 (92%)	43 (8%)	1 (0%)	44	75
15	af	552/677 (82%)	505 (92%)	46 (8%)	1 (0%)	44	75
16	ae	570/678 (84%)	518 (91%)	52 (9%)	0	100	100
17	l	580/714 (81%)	520 (90%)	60 (10%)	0	100	100
18	ac	1123/1152 (98%)	1022 (91%)	101 (9%)	0	100	100
19	ab	1108/1175 (94%)	994 (90%)	113 (10%)	1 (0%)	48	79
20	ad	799/810 (99%)	692 (87%)	102 (13%)	5 (1%)	22	56
21	m	230/319 (72%)	201 (87%)	29 (13%)	0	100	100
22	i	358/429 (83%)	306 (86%)	51 (14%)	1 (0%)	37	68
23	f	229/325 (70%)	196 (86%)	33 (14%)	0	100	100
24	c	259/285 (91%)	228 (88%)	31 (12%)	0	100	100
25	d	443/445 (100%)	398 (90%)	44 (10%)	1 (0%)	44	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	ba	81/217 (37%)	68 (84%)	13 (16%)	0	100	100
27	av	211/237 (89%)	174 (82%)	35 (17%)	2 (1%)	14	49
28	at	240/259 (93%)	201 (84%)	38 (16%)	1 (0%)	30	64
29	ar	253/268 (94%)	220 (87%)	33 (13%)	0	100	100
30	aq	196/299 (66%)	177 (90%)	19 (10%)	0	100	100
31	ap	220/277 (79%)	196 (89%)	24 (11%)	0	100	100
32	ao	248/283 (88%)	209 (84%)	39 (16%)	0	100	100
33	ai	388/410 (95%)	333 (86%)	55 (14%)	0	100	100
34	an	291/293 (99%)	248 (85%)	41 (14%)	2 (1%)	19	53
35	z	1067/1181 (90%)	901 (84%)	163 (15%)	3 (0%)	37	68
36	y	249/449 (56%)	196 (79%)	51 (20%)	2 (1%)	16	51
37	x	250/345 (72%)	213 (85%)	36 (14%)	1 (0%)	30	64
38	w	173/186 (93%)	150 (87%)	22 (13%)	1 (1%)	22	56
39	v	194/215 (90%)	153 (79%)	37 (19%)	4 (2%)	5	32
40	bb	108/238 (45%)	95 (88%)	12 (11%)	1 (1%)	14	49
41	t	224/256 (88%)	193 (86%)	30 (13%)	1 (0%)	30	64
42	al	290/308 (94%)	257 (89%)	32 (11%)	1 (0%)	37	68
43	q	212/442 (48%)	185 (87%)	26 (12%)	1 (0%)	25	59
44	p	236/308 (77%)	206 (87%)	30 (13%)	0	100	100
45	Ca	590/603 (98%)	509 (86%)	80 (14%)	1 (0%)	44	75
46	g	182/193 (94%)	163 (90%)	19 (10%)	0	100	100
47	j	178/189 (94%)	140 (79%)	38 (21%)	0	100	100
48	b	146/160 (91%)	123 (84%)	23 (16%)	0	100	100
49	bd	48/90 (53%)	41 (85%)	7 (15%)	0	100	100
50	a	423/434 (98%)	363 (86%)	59 (14%)	1 (0%)	44	75
51	bc	149/376 (40%)	138 (93%)	11 (7%)	0	100	100
52	aa	1554/1827 (85%)	1363 (88%)	186 (12%)	5 (0%)	37	68
53	k	188/309 (61%)	156 (83%)	32 (17%)	0	100	100
54	be	77/82 (94%)	67 (87%)	9 (12%)	1 (1%)	10	41
55	as	250/261 (96%)	211 (84%)	39 (16%)	0	100	100
All	All	19513/22991 (85%)	17122 (88%)	2345 (12%)	46 (0%)	45	75

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
54	be	41	ILE
13	aj	36	GLN
37	x	178	SER
39	v	94	THR
2	s	42	GLN

### 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	u	613/762 (80%)	562 (92%)	51 (8%)	9	32
2	s	144/157 (92%)	136 (94%)	8 (6%)	17	45
3	r	413/443 (93%)	381 (92%)	32 (8%)	10	34
4	n	127/152 (84%)	115 (91%)	12 (9%)	7	29
5	h	142/150 (95%)	130 (92%)	12 (8%)	8	32
6	e	712/719 (99%)	652 (92%)	60 (8%)	9	32
7	az	136/144 (94%)	131 (96%)	5 (4%)	29	58
8	ay	126/195 (65%)	114 (90%)	12 (10%)	7	28
9	ax	149/158 (94%)	136 (91%)	13 (9%)	8	31
10	aw	144/164 (88%)	134 (93%)	10 (7%)	13	39
11	au	220/228 (96%)	200 (91%)	20 (9%)	7	30
12	ak	197/257 (77%)	182 (92%)	15 (8%)	11	35
13	aj	280/351 (80%)	264 (94%)	16 (6%)	17	45
14	ag	477/502 (95%)	443 (93%)	34 (7%)	12	38
15	af	490/583 (84%)	447 (91%)	43 (9%)	8	31
16	ae	492/567 (87%)	462 (94%)	30 (6%)	15	43
17	l	514/606 (85%)	467 (91%)	47 (9%)	7	30
18	ac	934/957 (98%)	870 (93%)	64 (7%)	13	39
19	ab	954/1011 (94%)	886 (93%)	68 (7%)	12	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	ad	703/712 (99%)	631 (90%)	72 (10%)	6	26
21	m	202/278 (73%)	186 (92%)	16 (8%)	10	34
22	i	314/371 (85%)	286 (91%)	28 (9%)	8	31
23	f	201/276 (73%)	179 (89%)	22 (11%)	5	24
24	c	228/246 (93%)	214 (94%)	14 (6%)	15	43
25	d	373/373 (100%)	338 (91%)	35 (9%)	7	29
26	ba	73/180 (41%)	64 (88%)	9 (12%)	4	20
27	av	191/210 (91%)	172 (90%)	19 (10%)	6	27
28	at	212/227 (93%)	201 (95%)	11 (5%)	19	47
29	ar	227/238 (95%)	209 (92%)	18 (8%)	10	34
30	aq	181/253 (72%)	161 (89%)	20 (11%)	5	24
31	ap	189/233 (81%)	165 (87%)	24 (13%)	3	18
32	ao	225/252 (89%)	202 (90%)	23 (10%)	6	26
33	ai	351/370 (95%)	326 (93%)	25 (7%)	12	38
34	an	250/250 (100%)	217 (87%)	33 (13%)	3	18
35	z	920/1011 (91%)	840 (91%)	80 (9%)	8	31
36	y	209/366 (57%)	186 (89%)	23 (11%)	5	24
37	x	206/284 (72%)	185 (90%)	21 (10%)	6	26
38	w	163/174 (94%)	152 (93%)	11 (7%)	13	40
39	v	164/181 (91%)	152 (93%)	12 (7%)	11	37
40	bb	92/197 (47%)	84 (91%)	8 (9%)	8	31
41	t	193/220 (88%)	174 (90%)	19 (10%)	6	27
42	al	247/262 (94%)	229 (93%)	18 (7%)	11	37
43	q	196/390 (50%)	187 (95%)	9 (5%)	23	52
44	p	213/258 (83%)	202 (95%)	11 (5%)	19	47
45	Ca	534/544 (98%)	483 (90%)	51 (10%)	7	28
46	g	163/171 (95%)	144 (88%)	19 (12%)	4	21
47	j	159/168 (95%)	140 (88%)	19 (12%)	4	21
48	b	138/146 (94%)	126 (91%)	12 (9%)	8	31
49	bd	48/86 (56%)	36 (75%)	12 (25%)	0	3
50	a	364/372 (98%)	327 (90%)	37 (10%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	bc	134/327 (41%)	124 (92%)	10 (8%)	11	35
52	aa	1340/1552 (86%)	1189 (89%)	151 (11%)	4	22
53	k	169/272 (62%)	142 (84%)	27 (16%)	2	12
54	be	70/73 (96%)	60 (86%)	10 (14%)	2	16
55	as	221/228 (97%)	199 (90%)	22 (10%)	6	26
All	All	17127/19857 (86%)	15624 (91%)	1503 (9%)	11	31

5 of 1503 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	z	79	ILE
45	Ca	172	THR
35	z	394	THR
35	z	68	THR
37	x	295	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 431 such sidechains are listed below:

Mol	Chain	Res	Type
21	m	28	ASN
32	ao	262	HIS
52	aa	284	HIS
22	i	237	ASN
25	d	89	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
56	2	468/8129 (5%)	249 (53%)	8 (1%)
56	A	142/8129 (1%)	90 (63%)	2 (1%)
All	All	610/16258 (3%)	339 (55%)	10 (1%)

5 of 339 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
56	A	397	U
56	A	398	U
56	A	399	A

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Mol	Chain	Res	Type
56	A	400	U
56	A	401	A

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
56	2	262	A
56	2	324	A
56	2	366	U
56	2	87	U
56	2	97	U

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 5 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	$\# Z  > 2$
59	UTP	aj	401	-	22,30,30	4.42	6 (27%)	27,47,47	1.32	4 (14%)
57	GTP	r	901	58	26,34,34	3.64	13 (50%)	32,54,54	1.90	12 (37%)

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
59	UTP	aj	401	-	-	4/20/38/38	0/2/2/2
57	GTP	r	901	58	-	5/18/38/38	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	aj	401	UTP	O4'-C1'	14.35	1.61	1.41
59	aj	401	UTP	C2'-C1'	-12.42	1.34	1.53
57	r	901	GTP	C3'-C4'	-9.63	1.28	1.53
57	r	901	GTP	O4'-C4'	7.36	1.61	1.45
57	r	901	GTP	O4'-C1'	-7.19	1.31	1.41

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	r	901	GTP	C5-C6-N1	3.92	120.87	113.95
57	r	901	GTP	O6-C6-C5	-3.83	116.89	124.37
57	r	901	GTP	C3'-C2'-C1'	-3.57	95.60	100.98
59	aj	401	UTP	PB-O3B-PG	-3.43	121.04	132.83
57	r	901	GTP	C2-N1-C6	-3.21	119.19	125.10

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

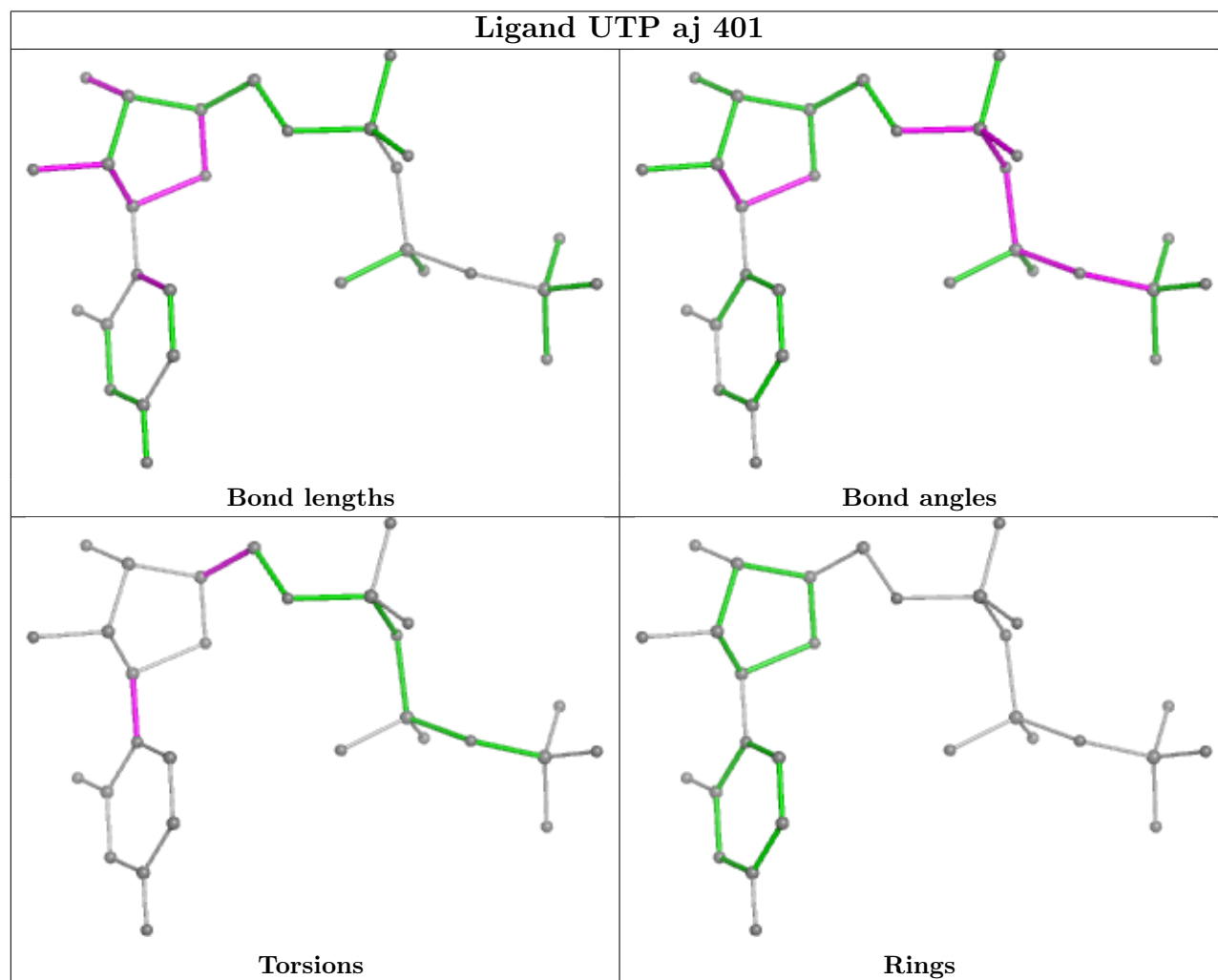
Mol	Chain	Res	Type	Atoms
57	r	901	GTP	C5'-O5'-PA-O3A
57	r	901	GTP	C5'-O5'-PA-O1A
57	r	901	GTP	C5'-O5'-PA-O2A
59	aj	401	UTP	O4'-C4'-C5'-O5'
59	aj	401	UTP	O4'-C1'-N1-C6

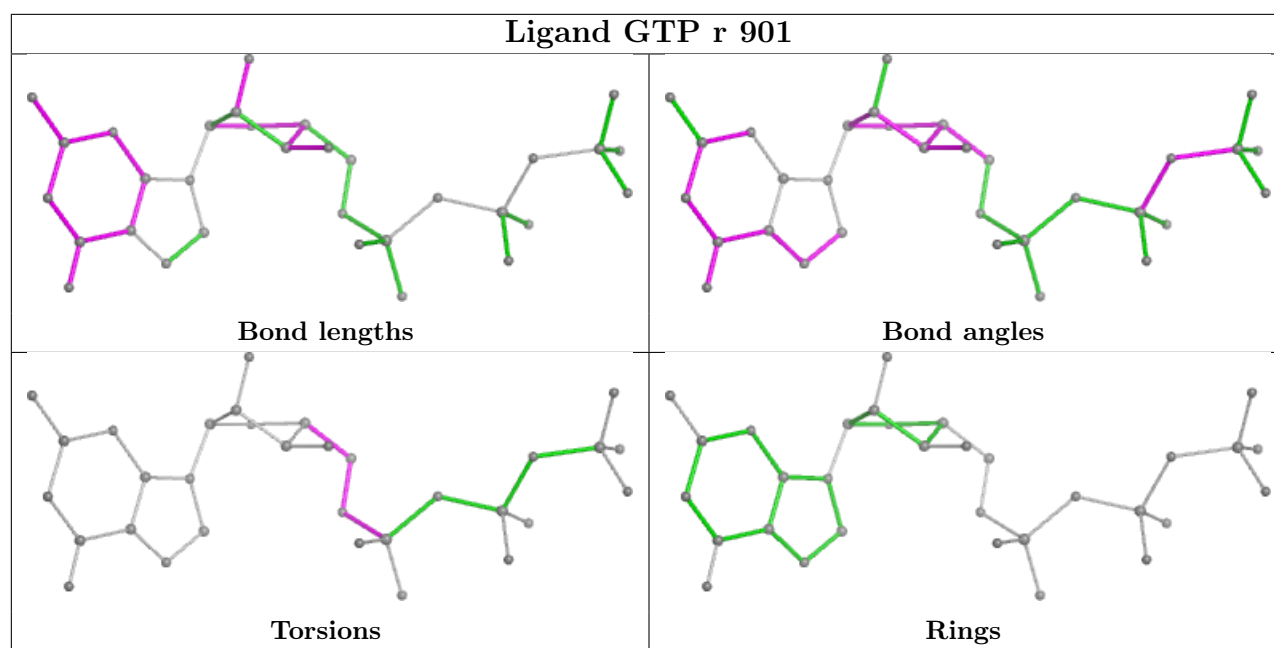
There are no ring outliers.

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
6	e	1
21	m	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	444:ASP	C	445:GLY	N	1.67
1	m	70:ARG	C	71:PHE	N	1.17

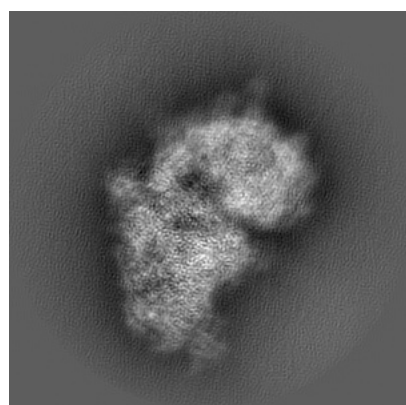
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11846. These allow visual inspection of the internal detail of the map and identification of artifacts.

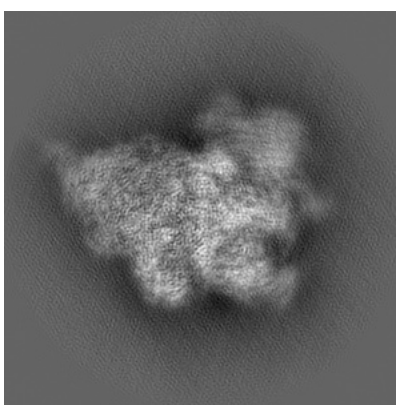
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

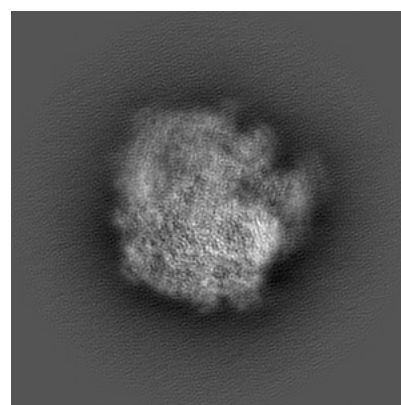
#### 6.1.1 Primary map



X



Y

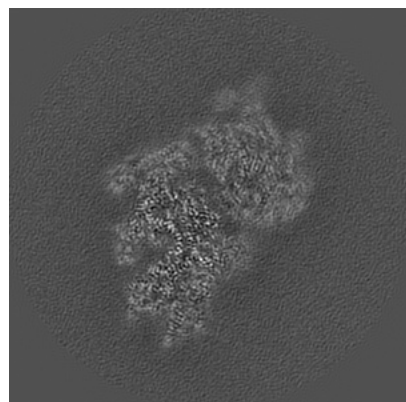


Z

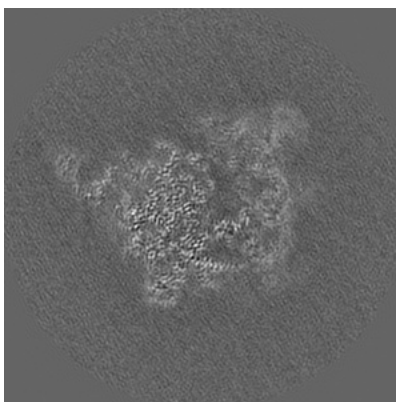
The images above show the map projected in three orthogonal directions.

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

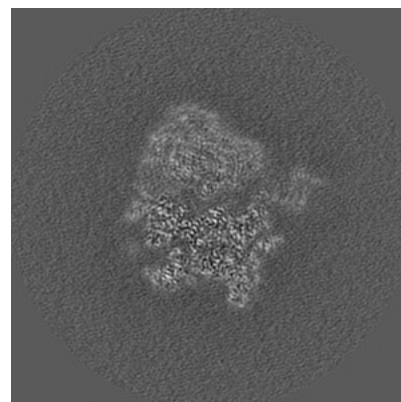
#### 6.2.1 Primary map



X Index: 180



Y Index: 180



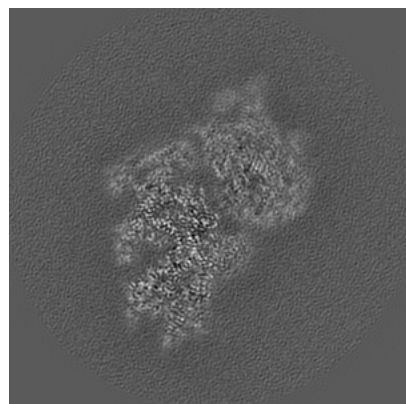
Z Index: 180



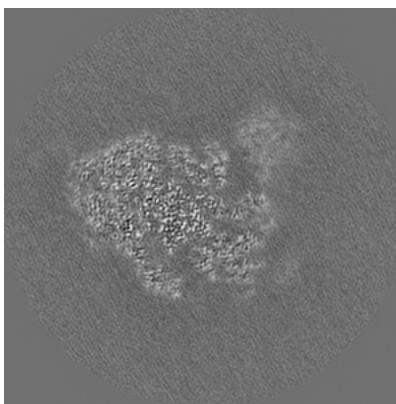
The images above show central slices of the map in three orthogonal directions.

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

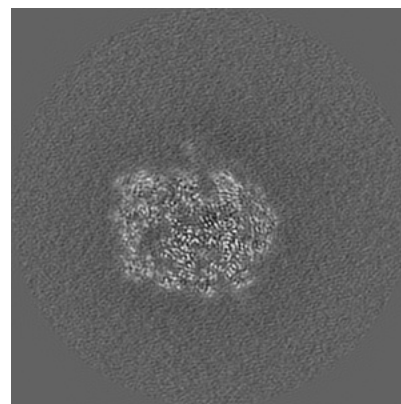
### 6.3.1 Primary map



X Index: 181



Y Index: 155

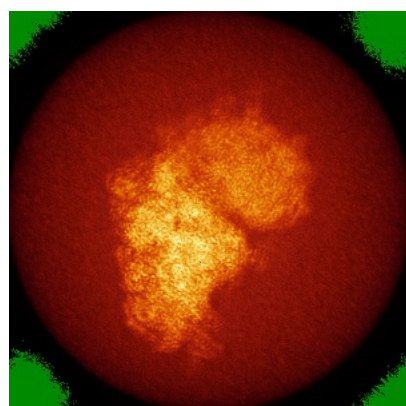


Z Index: 155

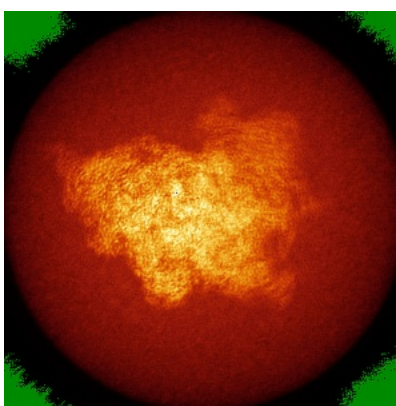
The images above show the largest variance slices of the map in three orthogonal directions.

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

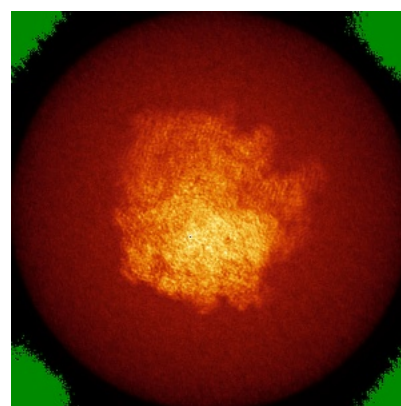
### 6.4.1 Primary map



X



Y



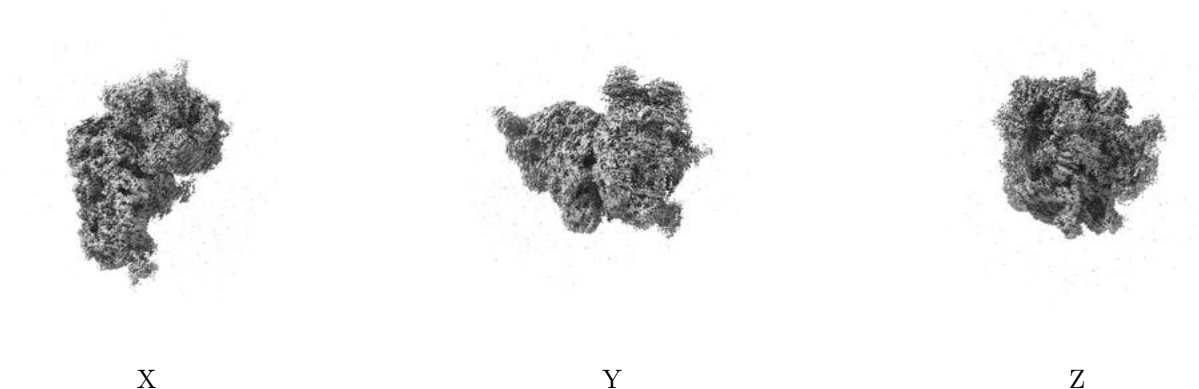
Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

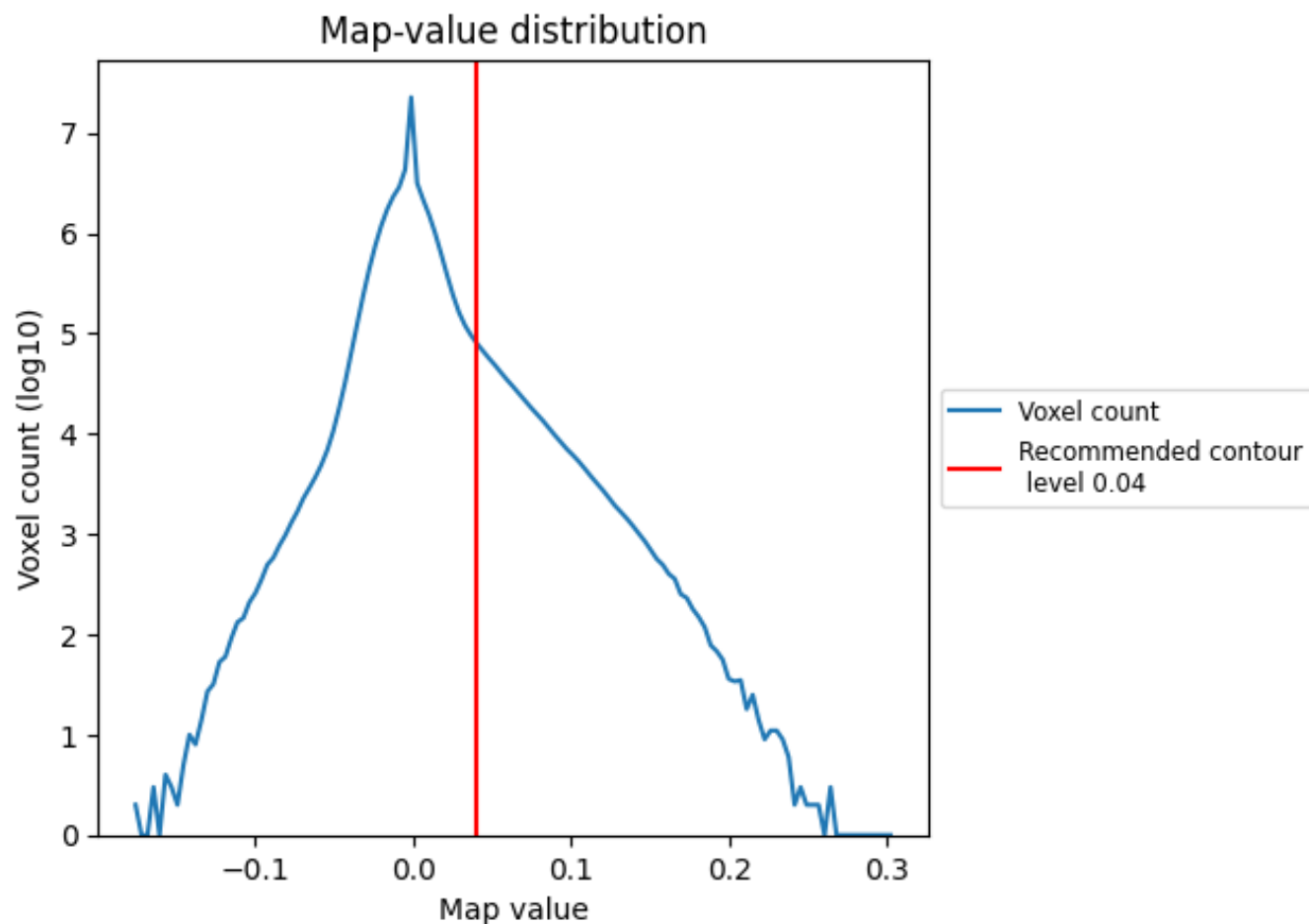
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

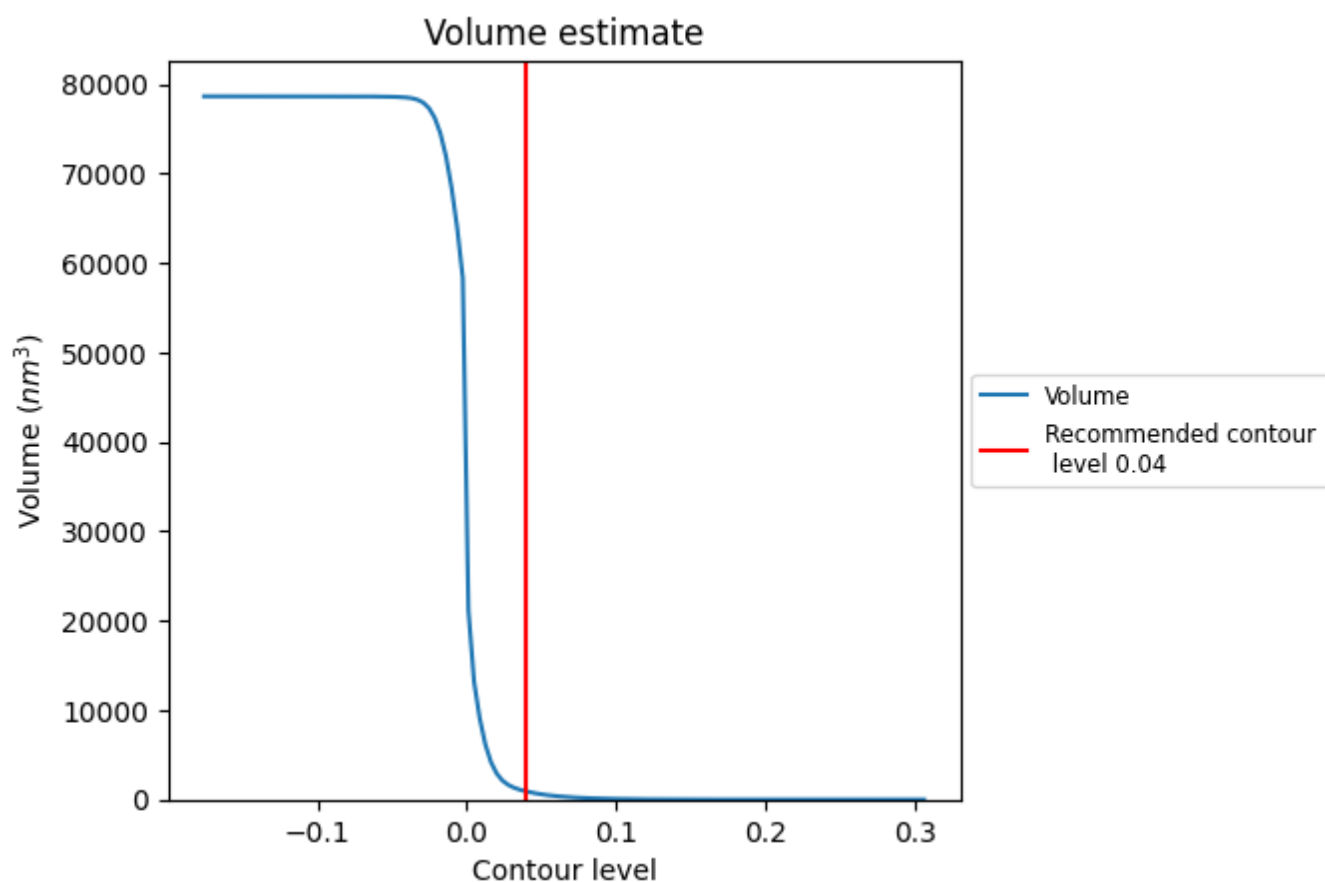
This section contains the results of statistical analysis of the map.

### 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.

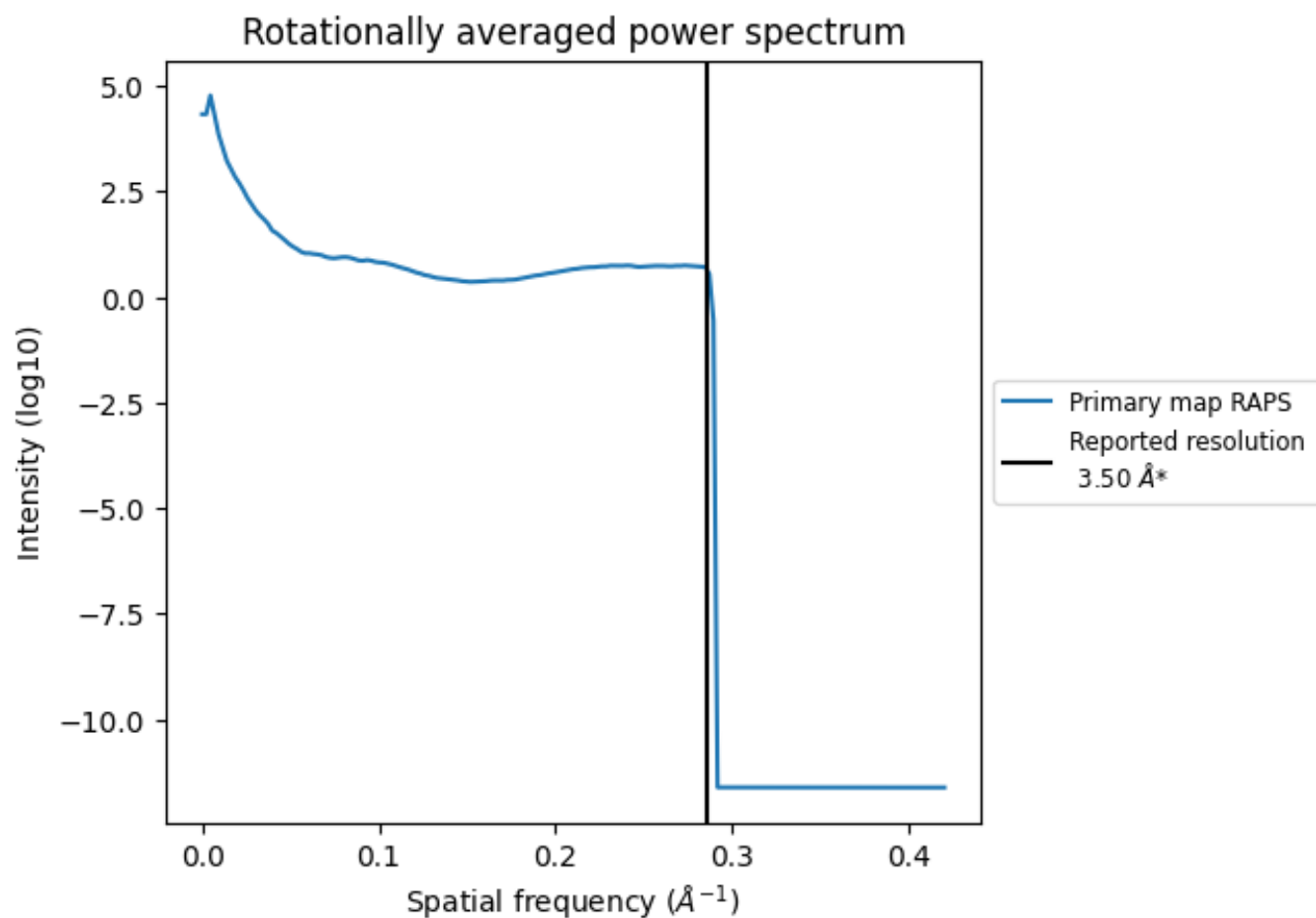
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 906 nm<sup>3</sup>; this corresponds to an approximate mass of 819 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 0.286  $\text{\AA}^{-1}$

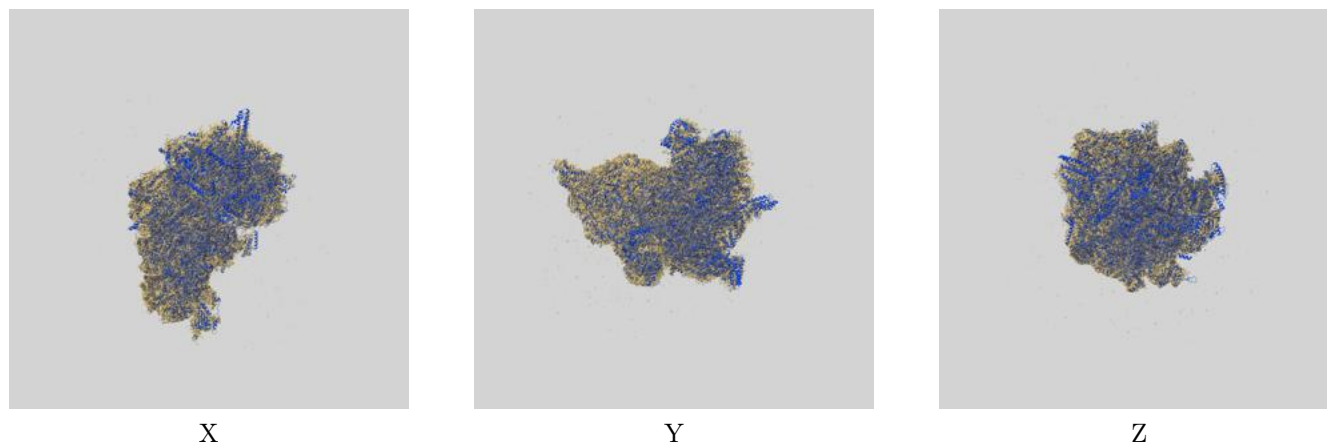
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

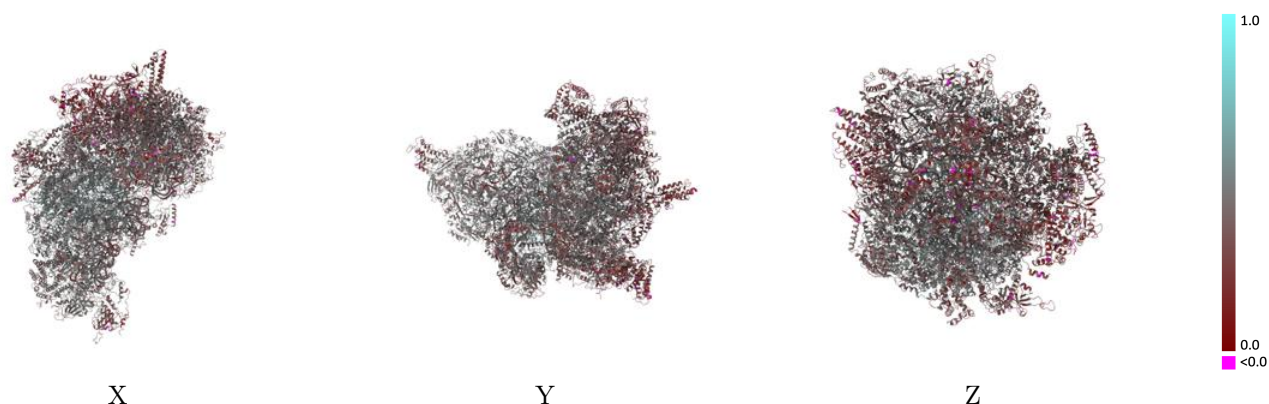
This section contains information regarding the fit between EMDB map EMD-11846 and PDB model 7AOR. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

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



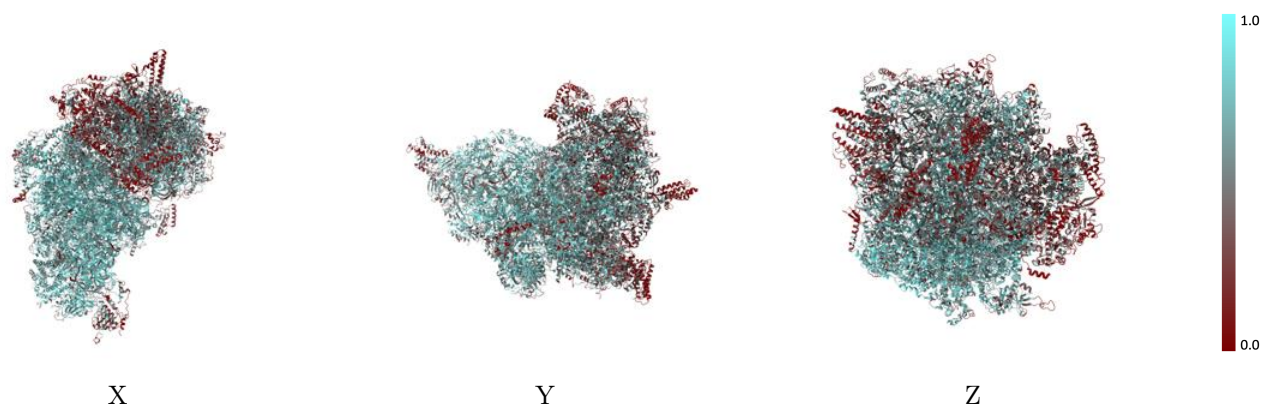
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



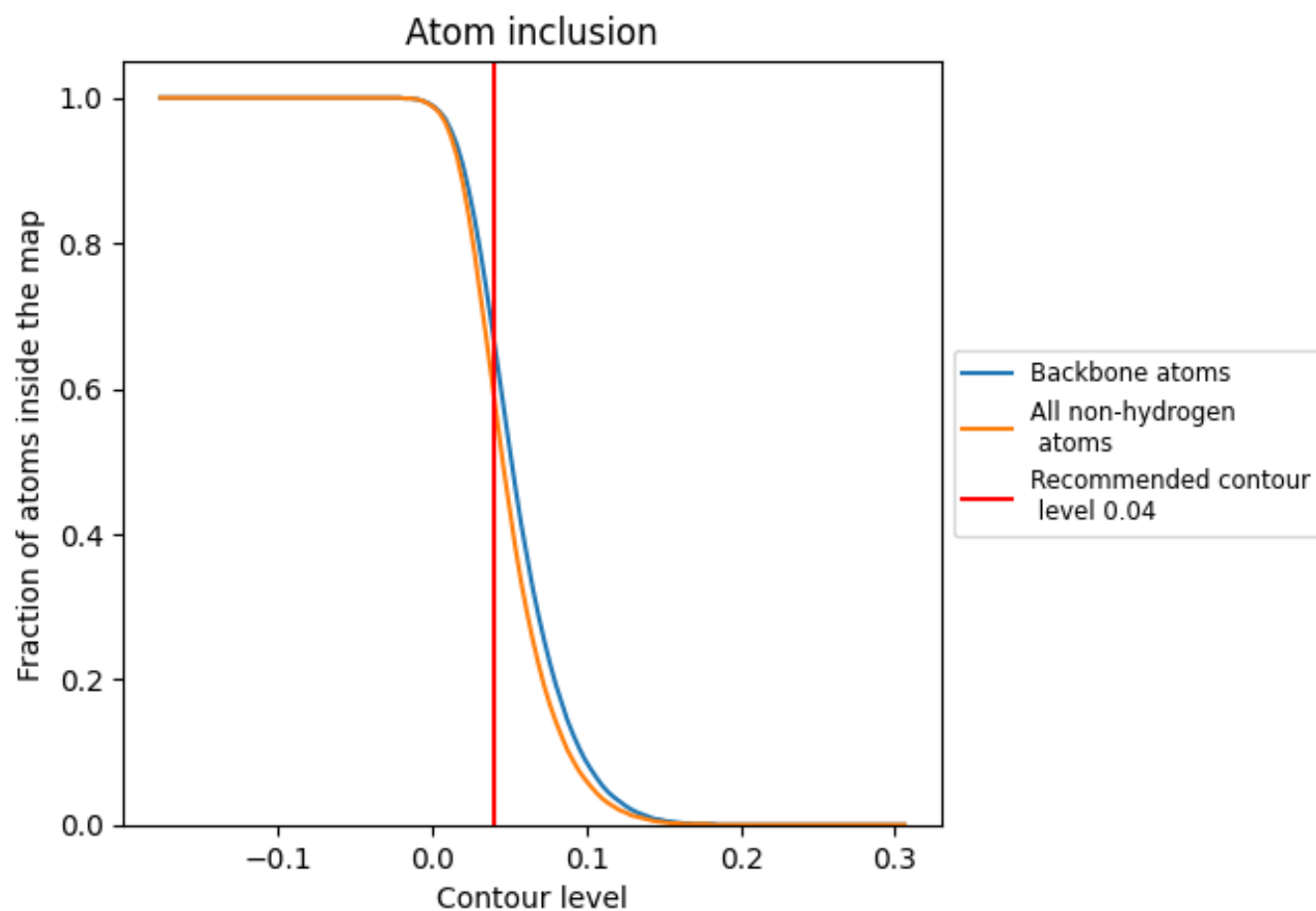
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 67% of all backbone atoms, 59% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5920	 0.4160
2	 0.7410	 0.4140
A	 0.6600	 0.3980
Ca	 0.7420	 0.4910
a	 0.7320	 0.4960
aa	 0.6640	 0.4110
ab	 0.4430	 0.3700
ac	 0.3200	 0.3360
ad	 0.7430	 0.4560
ae	 0.5340	 0.3860
af	 0.3260	 0.3100
ag	 0.4690	 0.4070
ai	 0.7240	 0.4790
aj	 0.5950	 0.4130
ak	 0.4270	 0.3980
al	 0.6320	 0.4760
an	 0.7690	 0.4550
ao	 0.7900	 0.5040
ap	 0.7140	 0.4600
aq	 0.4730	 0.3900
ar	 0.7100	 0.4430
as	 0.6550	 0.4210
at	 0.6870	 0.4310
au	 0.5240	 0.4330
av	 0.5850	 0.4390
aw	 0.4640	 0.4270
ax	 0.5110	 0.3730
ay	 0.5850	 0.3680
az	 0.5990	 0.3830
b	 0.7190	 0.4210
ba	 0.7380	 0.5020
bb	 0.5980	 0.4280
bc	 0.2980	 0.3440
bd	 0.3990	 0.3240
be	 0.6450	 0.4130



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Chain	Atom inclusion	Q-score
c	 0.7270	 0.5110
d	 0.4970	 0.4040
e	 0.5110	 0.4220
f	 0.6000	 0.4110
g	 0.6660	 0.4350
h	 0.6420	 0.4530
i	 0.7040	 0.4490
j	 0.7670	 0.4550
k	 0.7950	 0.4860
l	 0.3250	 0.3050
m	 0.7270	 0.4820
n	 0.5820	 0.4020
p	 0.6470	 0.4570
q	 0.7380	 0.4480
r	 0.4620	 0.3730
s	 0.5790	 0.4350
t	 0.6100	 0.4240
u	 0.3920	 0.3530
v	 0.6630	 0.4600
w	 0.6220	 0.4190
x	 0.6450	 0.4280
y	 0.5930	 0.3770
z	 0.7460	 0.4810