Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 02:10 pm GMT

PDB ID	:	5MC6
EMDB ID	:	EMD-3461
Title	:	Cryo-EM structure of a native ribosome-Ski2-Ski3-Ski8 complex from S. cerevisiae
Authors	:	Schmidt, C.; Kowalinski, E.; Shanmuganathan, V.; Defenouillere, Q.; Braunger, K.; Heuer, A.; Pech, M.; Namane, A.; Berninghausen, O.; Fromont-Racine, M.; Jacquier, A.; Conti, E.; Becker, T.; Beckmann, R.
Deposited on	:	2016-11-09
Resolution	:	3.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

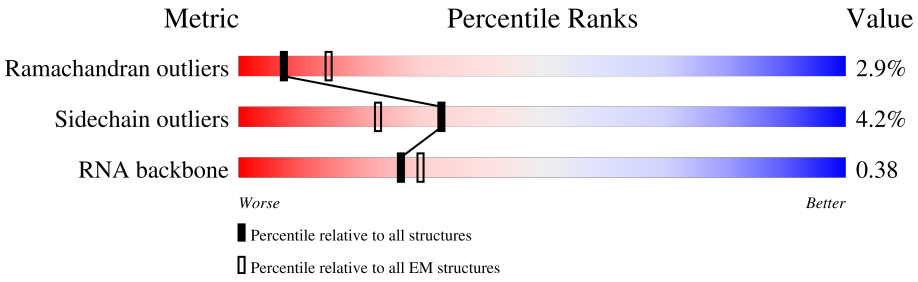
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2	1800	12% 56% 41%
2	A	240	27% 89% 7%
3	B	225	39% 83% 8% 8%
4	C	105	27% 81% 10% 9%
5	D	143	64% 75% 10% 15%
6	E	142	41% 80% 7% 13%
7	F	143	22% 92% 6%
8	G	136	20% 61% 5% 33%

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Mol	Chain	Length	Quality of chain
9	H	146	40% 89% 10%
10	I	144	42% 85% 13%
11	J	121	28% 83% 6% 12%
12	K	108	29% 57% 7% 35%
13	L	67	61% 91% 6%
14	M	56	12% 89% 5% 5%
15	N	152	24% 31% 66%
16	O	319	38% 95%
17	P	252	21% 76% 5% 18%
18	Q	255	41% 76% 7% 16%
19	R	254	15% 83% 13%
20	S	261	44% 95% 5%
21	T	236	43% 89% 6%
22	U	190	61% 89% 7%
23	V	200	37% 74% 16% 6%
24	W	197	32% 87% 10%
25	X	156	38% 93% 6%
26	Y	151	34% 93% 6%
27	Z	137	32% 85% 7% 7%
28	a	87	30% 94% 5%
29	b	130	23% 95%
30	c	145	30% 96%
31	d	135	42% 87% 9%
32	e	119	35% 68% 13% 18%
33	f	82	40% 93% 6%

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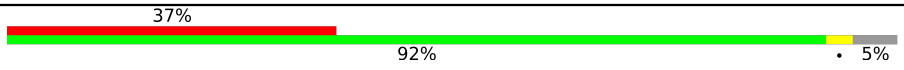
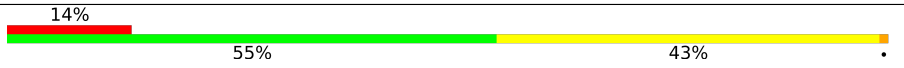
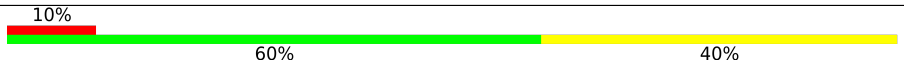
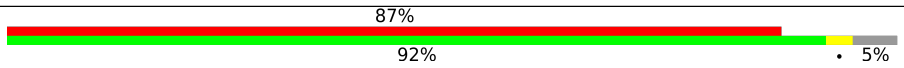
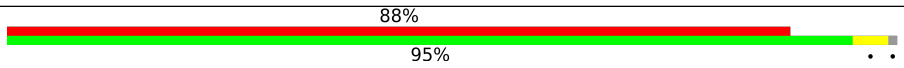
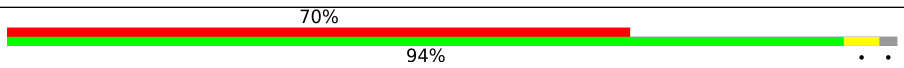
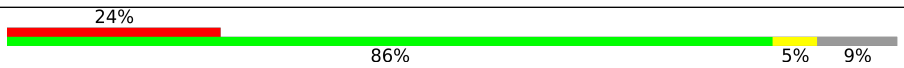
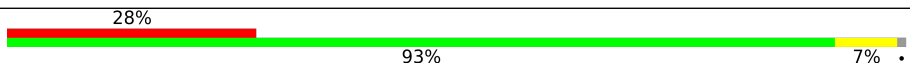
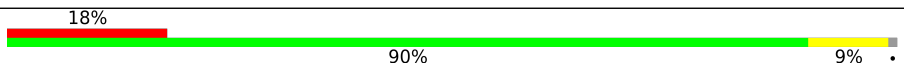
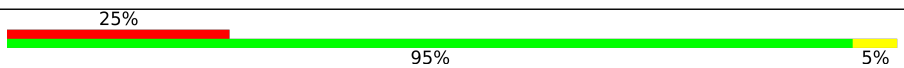
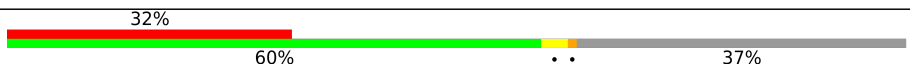
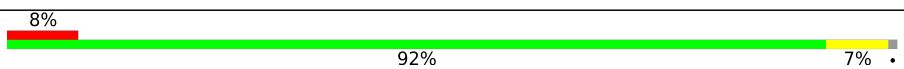
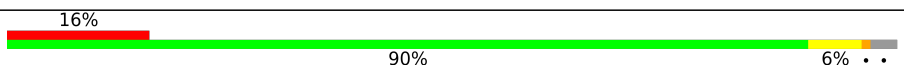
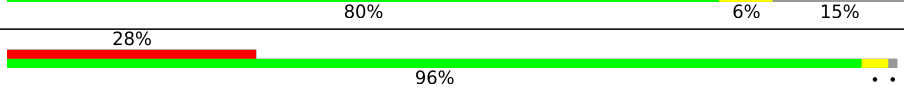
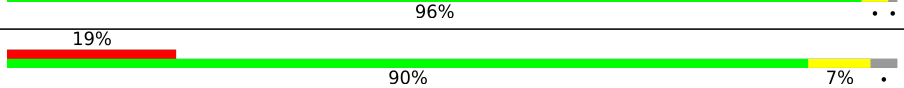
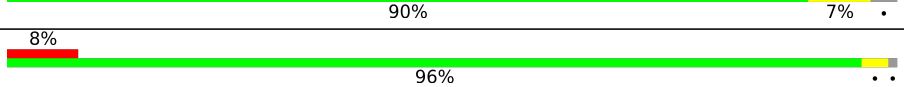
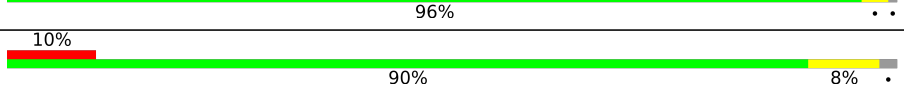
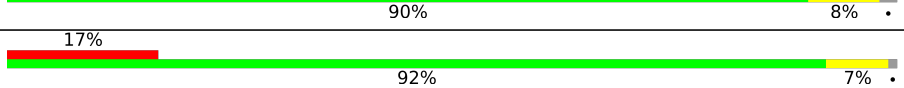
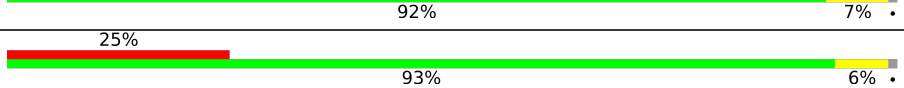
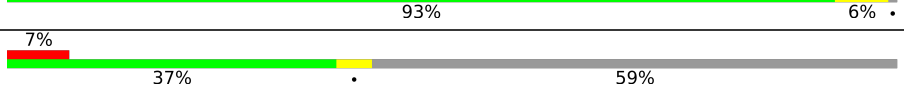
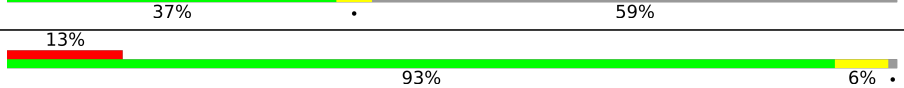
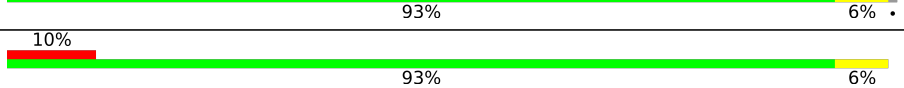
Mol	Chain	Length	Quality of chain
34	g	63	
35	l	34	
36	m	76	
37	n	77	
38	h	1287	
39	i	1432	
40	j	397	
40	k	397	
41	AA	256	
42	AB	137	
43	AC	100	
44	AD	191	
45	AE	155	
46	AF	88	
47	AG	174	
48	AH	142	
49	AI	78	
50	AJ	199	
51	AK	127	
52	AL	51	
53	AM	138	
54	AN	136	
55	AO	128	
56	AP	106	
57	AQ	204	

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Mol	Chain	Length	Quality of chain
58	AR	149	11% 90% 7%
59	AS	25	56% 92% 8%
60	AT	92	24% 96%
61	AU	199	13% 95%
62	AV	59	27% 97%
63	AW	254	15% 96%
64	AX	184	12% 93% 6%
65	AY	105	29% 89% 8%
66	AZ	210	91% 100%
67	BA	387	15% 93% 7%
68	BB	186	11% 95% 5%
69	BC	113	19% 88% 8%
70	BD	221	25% 89% 10%
71	BE	362	12% 93% 7%
72	BF	189	21% 95%
73	BG	130	12% 94%
74	BH	172	19% 95% 5%
75	BI	297	19% 94% 5%
76	BJ	160	19% 91% 8%
77	BK	107	12% 94% 5%
78	BL	121	18% 79% 17%
79	BM	176	23% 83% 5% 11%
80	BN	121	12% 89% 7%
81	BO	244	9% 87% 9%
82	BP	120	12% 96%

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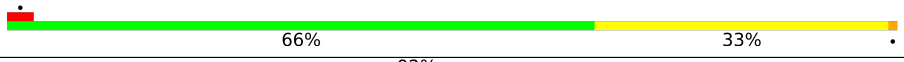
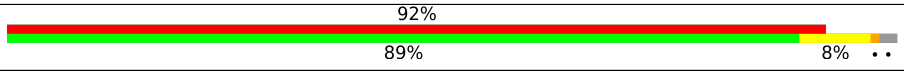
Mol	Chain	Length	Quality of chain
83	BQ	3396	
84	BR	121	
85	BS	158	
86	BT	157	

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 229285 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1767	37645	16830	6656	12392	1767	0	0

- Molecule 2 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	223	1734	1101	313	314	6	0	0

- Molecule 3 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	206	1609	1007	300	299	3	0	0

- Molecule 4 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	96	813	527	133	151	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	121	877	552	153	170	2	0	0

- Molecule 6 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	124	977	622	182	166	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	F	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 8 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	91	Total	C	N	O	S	0	0
			746	467	144	133	2		

- Molecule 9 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 10 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 11 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 12 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	K	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 13 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 14 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 15 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	51	Total	C	N	O	S	0	0
			397	249	73	71	4		

- Molecule 16 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	318	Total	C	N	O	S	0	0
			2436	1541	418	469	8		

- Molecule 17 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 18 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 19 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	220	Total	C	N	O	S	0	0
			1671	1072	297	300	2		

- Molecule 20 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 21 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 22 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 23 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 24 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	178	Total	C	N	O	S	0	0
			1434	905	276	252	1		

- Molecule 25 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 26 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 27 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 28 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 29 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 30 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 31 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	d	132	Total	C	N	O	0	0
			1060	669	206	185		

- Molecule 32 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 33 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 34 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	60	Total	C	N	O	S	0	0
			473	297	98	77	1		

- Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	34	Total	C	N	O	P	0	0
			692	311	84	263	34		

- Molecule 36 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	76	Total	C	N	O	P	0	0
			1611	721	281	534	75		

- Molecule 37 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	77	Total	C	N	O	P	0	0
			1644	731	290	546	77		

- Molecule 38 is a protein called Antiviral helicase SKI2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	1121	Total	C	N	O	S	0	0
			8814	5643	1504	1625	42		

- Molecule 39 is a protein called Superkiller protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	1365	Total	C	N	O	S	0	0
			9827	6302	1663	1825	37		

- Molecule 40 is a protein called Antiviral protein SKI8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	392	Total	C	N	O	S	0	0
			2933	1861	500	558	14		
40	k	388	Total	C	N	O	S	0	0
			2919	1851	502	552	14		

- Molecule 41 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AA	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 42 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AB	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 43 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AC	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 44 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AD	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 45 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AE	98	Total	C	N	O	S	0	0
			699	443	137	118	1		

- Molecule 46 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AF	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 47 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AG	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 48 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AH	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 49 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	AI	77	Total 612	C 391	N 115	O 106	0	0

- Molecule 50 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	AJ	193	Total 1543	C 962	N 315	O 266	0	0

- Molecule 51 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	AK	126	Total 993	C 625	N 192	O 176	0	0

- Molecule 52 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AL	50	Total 436	C 272	N 97	O 65	S 2	0	0

- Molecule 53 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AM	136	Total 1053	C 675	N 199	O 177	S 2	0	0

- Molecule 54 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	AN	135	Total 1092	C 710	N 202	O 180	0	0

- Molecule 55 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AO	52	Total 417	C 259	N 86	O 67	S 5	0	0

- Molecule 56 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AP	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 57 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AQ	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 58 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AR	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 59 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AS	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 60 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AT	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 61 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AU	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 62 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	AV	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 63 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AW	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 64 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	AX	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 65 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AY	97	Total	C	N	O	S	0	0
			742	479	124	138	1		

- Molecule 66 is a protein called uL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	AZ	210	Total	C	N	O	0	0
			1050	630	210	210		

- Molecule 67 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BA	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 68 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	BB	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 69 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	BC	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 70 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BD	220	Total	C	N	O	S	0	0
			1770	1121	335	307	7		

- Molecule 71 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	BE	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 72 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	BF	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 73 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	BG	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 74 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	BH	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 75 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	BI	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 76 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	BJ	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 77 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	BK	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 78 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	BL	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 79 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	BM	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 80 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	BN	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 81 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	BO	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 82 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	BP	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 83 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	BQ	3165	Total	C	N	O	P	0	0
			67695	30238	12201	22091	3165		

- Molecule 84 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	BR	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 85 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	BS	158	Total	C	N	O	P	0	0
			3352	1500	586	1108	158		

- Molecule 86 is a protein called Eukaryotic translation initiation factor 5A-1.

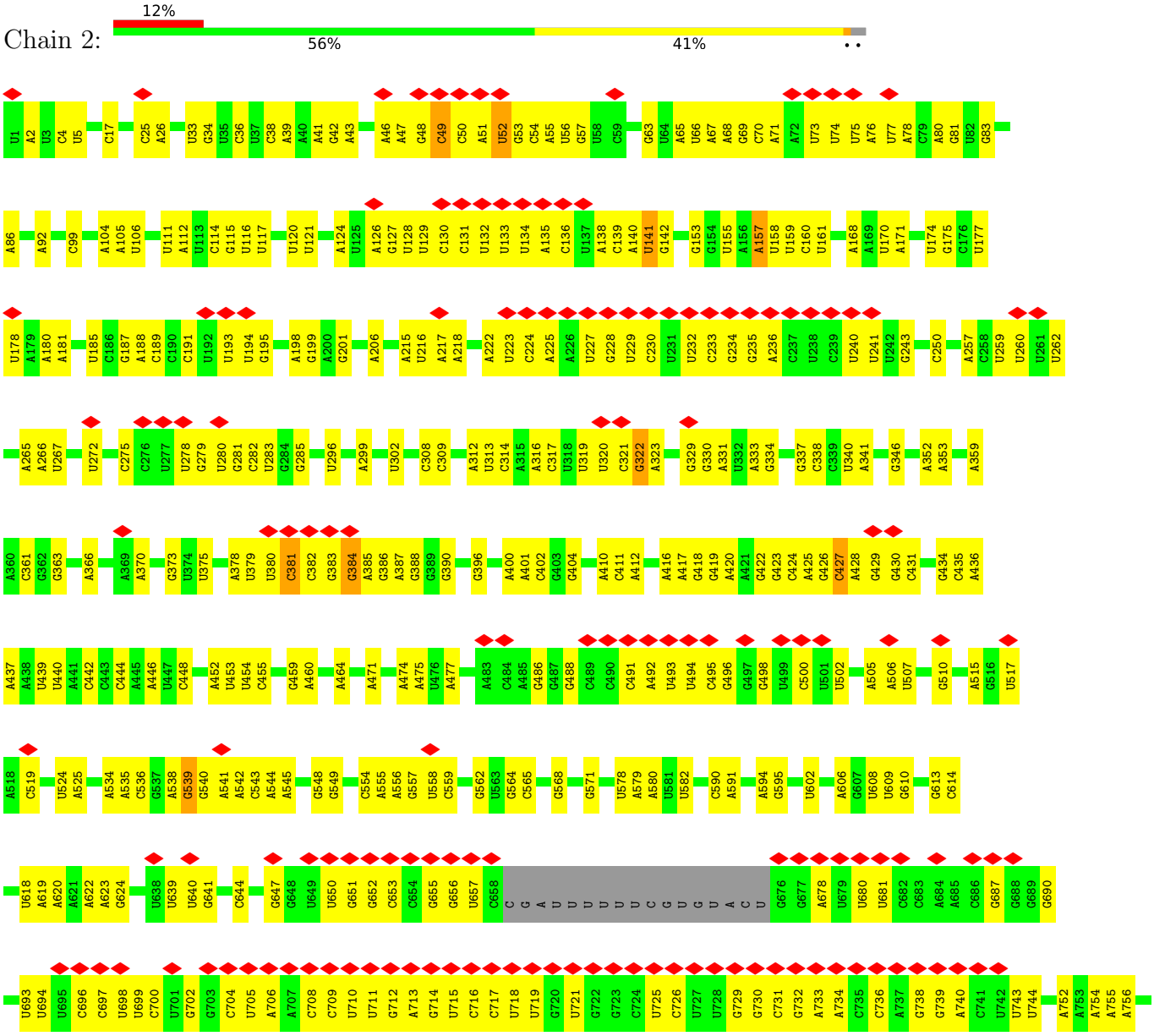
Mol	Chain	Residues	Atoms					AltConf	Trace
86	BT	154	Total	C	N	O	S	0	0
			1143	709	195	230	9		

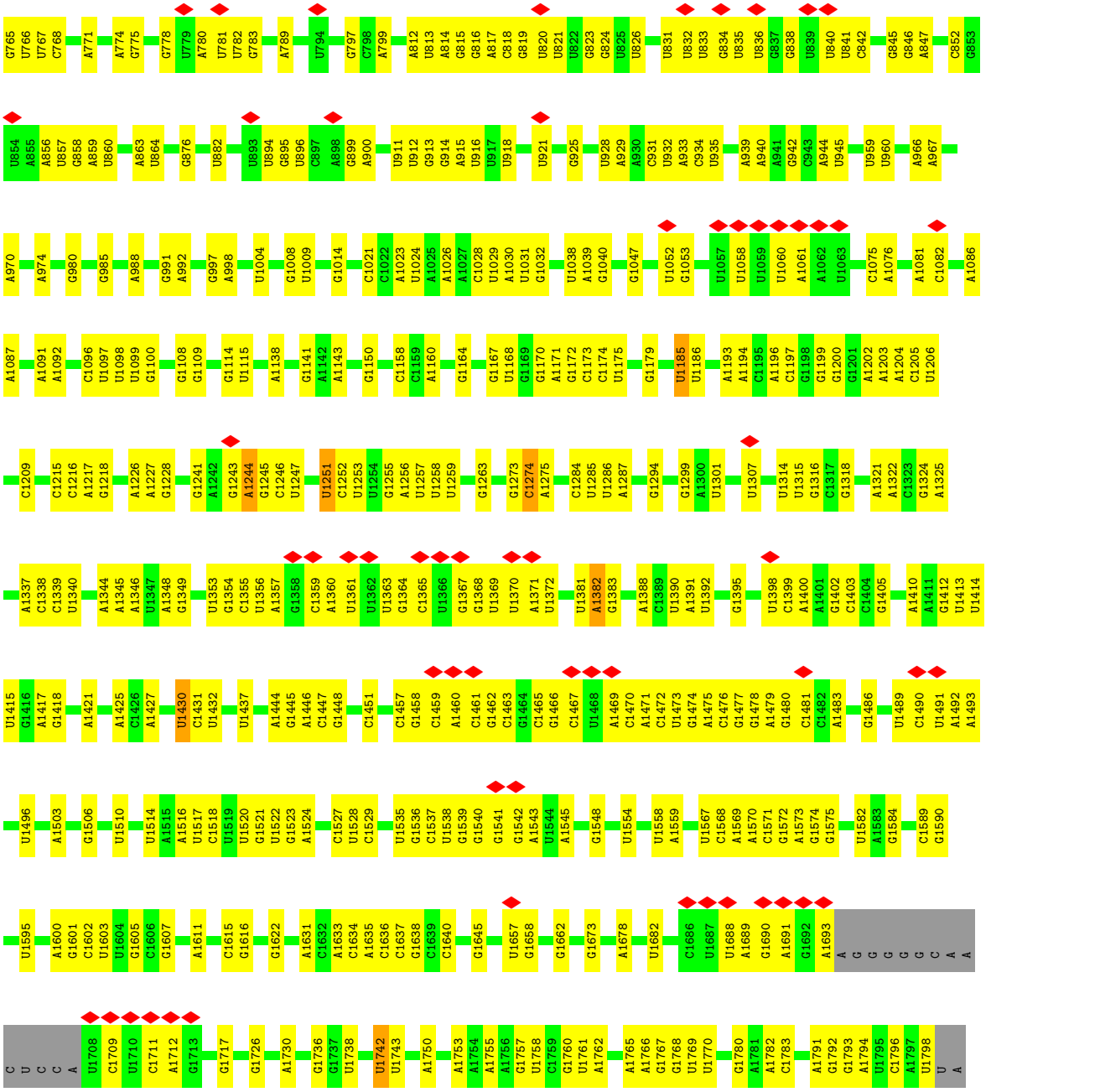
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 18S ribosomal RNA

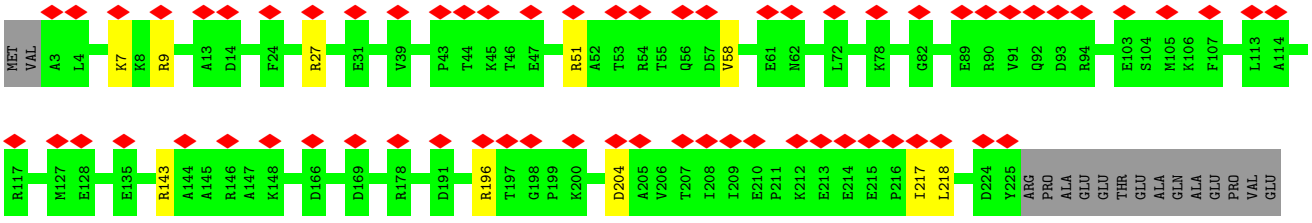
Chain 2:





• Molecule 2: 40S ribosomal protein S3

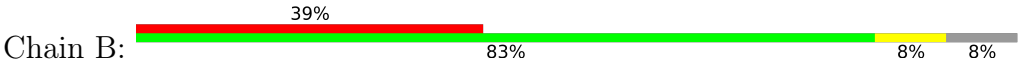
Chain A:

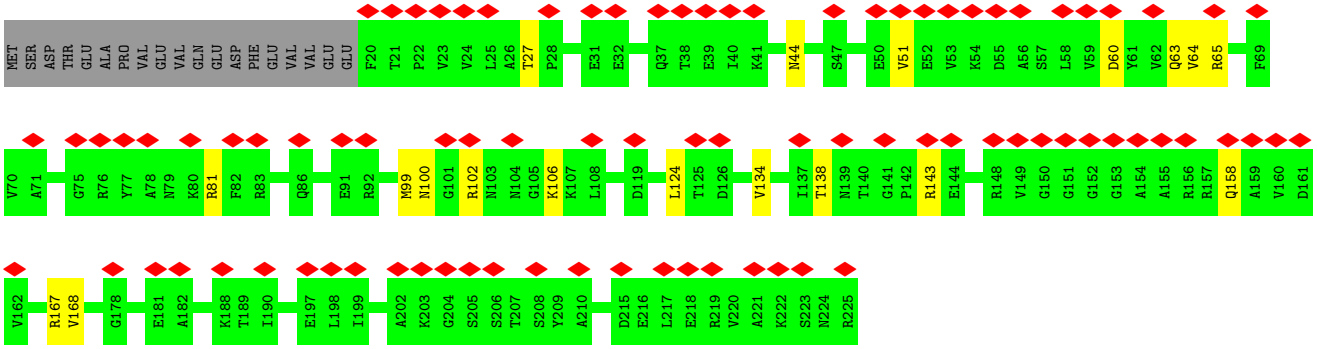


ALA

• Molecule 3: 40S ribosomal protein S5

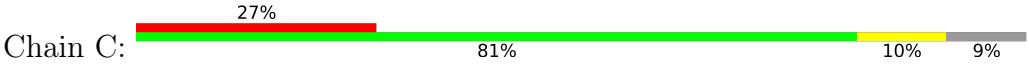
Chain B:

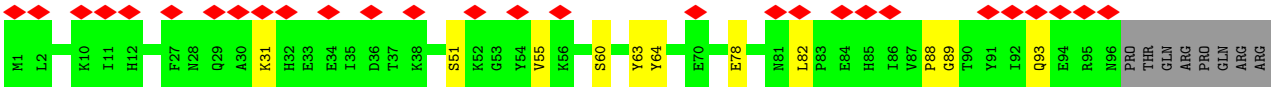




• Molecule 4: 40S ribosomal protein S10-A

Chain C:

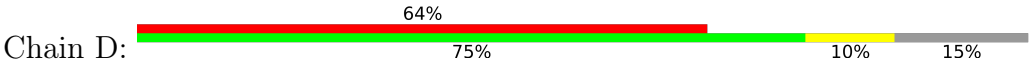


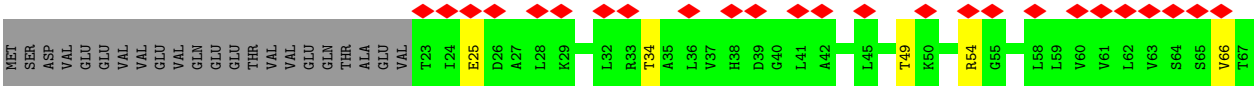


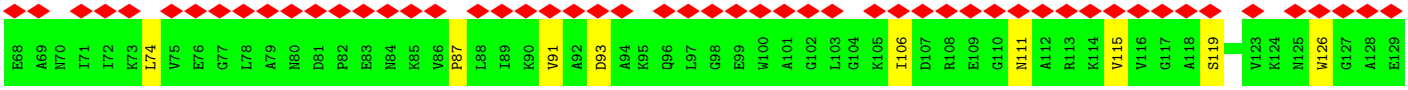
TYR

• Molecule 5: 40S ribosomal protein S12

Chain D:

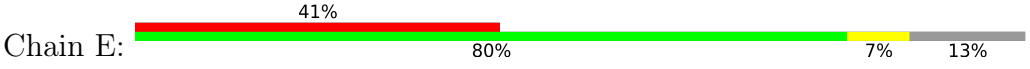


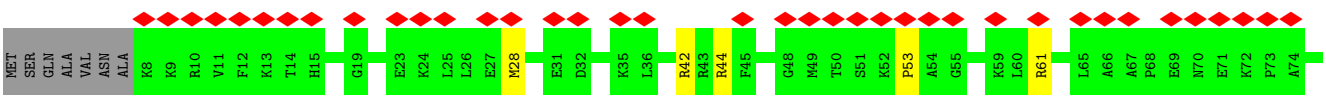


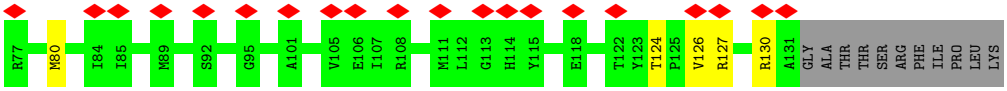


• Molecule 6: 40S ribosomal protein S15

Chain E:

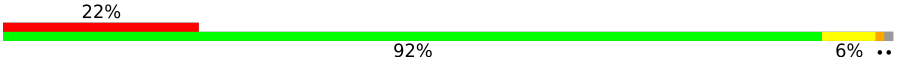


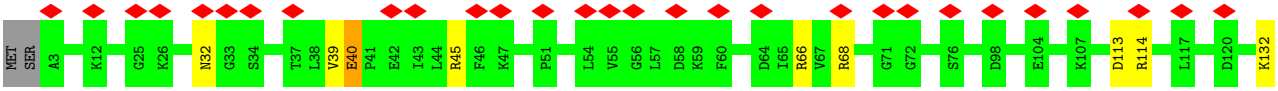




• Molecule 7: 40S ribosomal protein S16-A

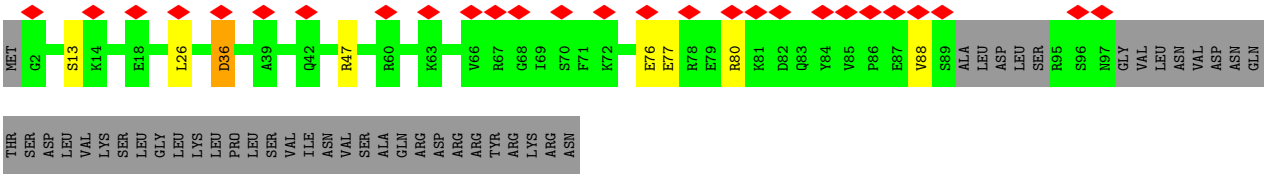
Chain F:





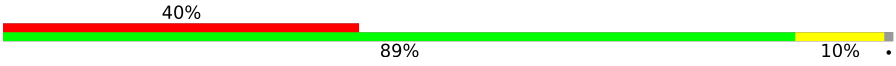
• Molecule 8: 40S ribosomal protein S17-B

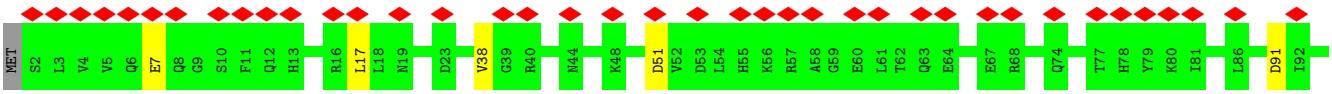
Chain G:

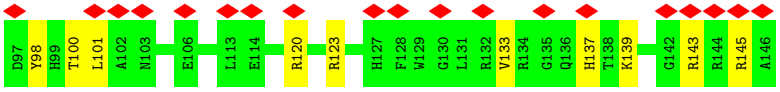


• Molecule 9: 40S ribosomal protein S18-A

Chain H:

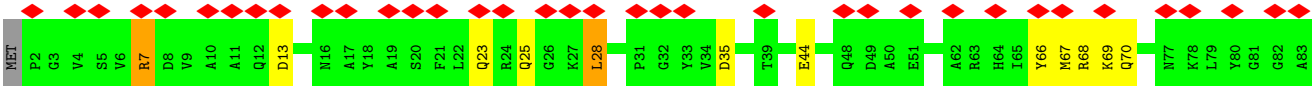


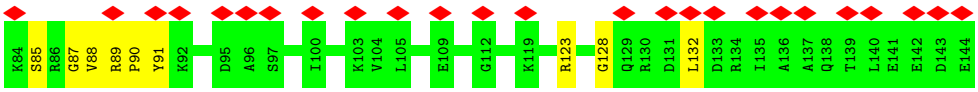




• Molecule 10: 40S ribosomal protein S19-A

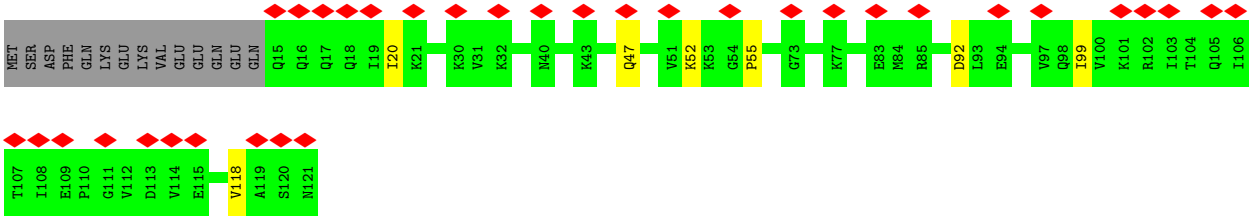
Chain I:



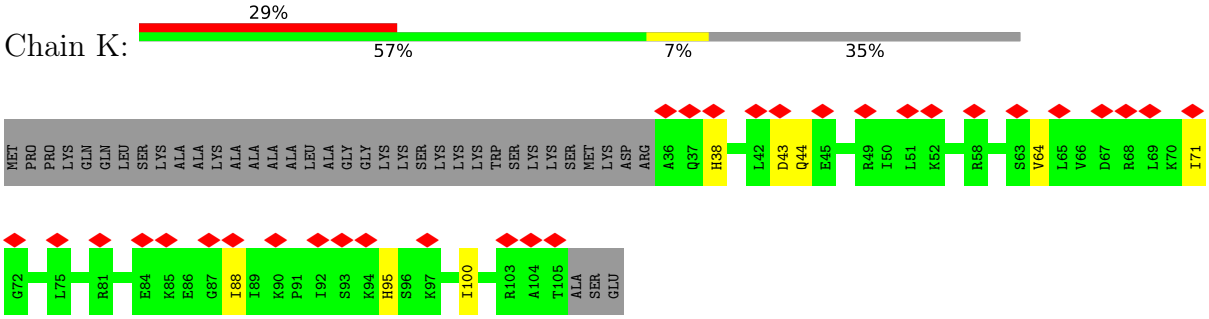


• Molecule 11: 40S ribosomal protein S20

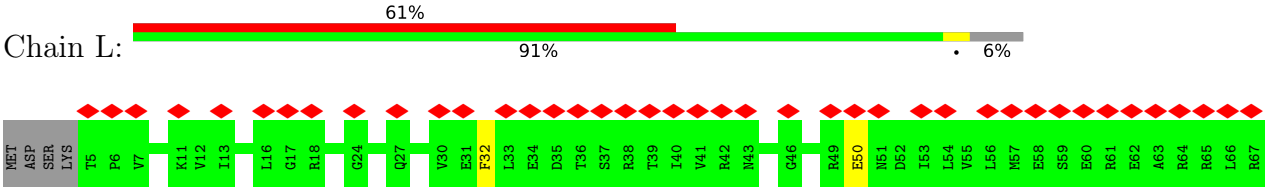
Chain J:



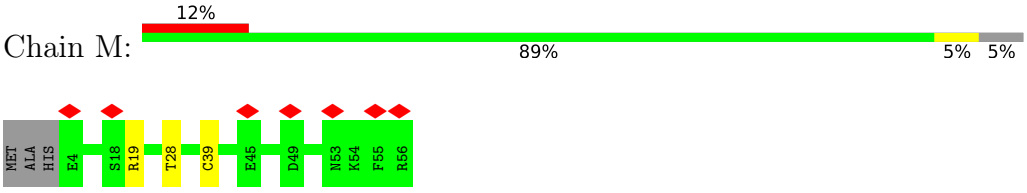
• Molecule 12: 40S ribosomal protein S25-A



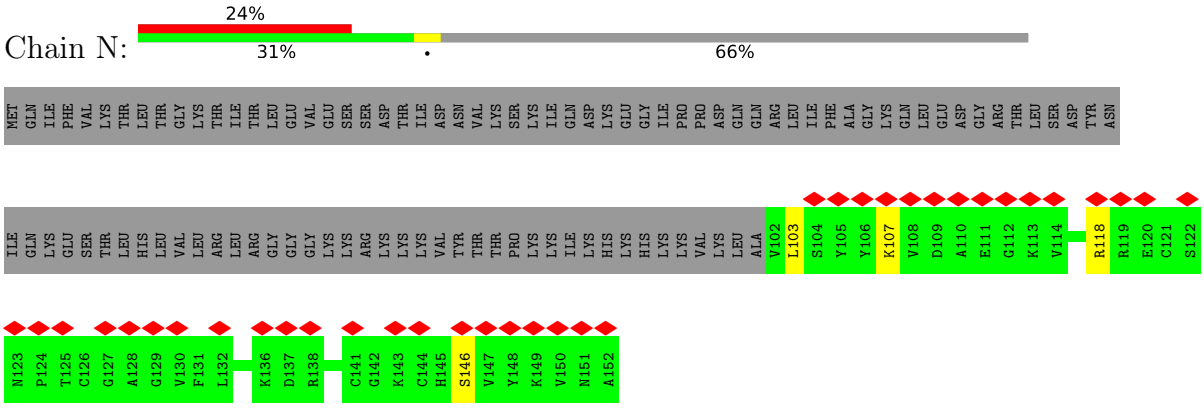
• Molecule 13: 40S ribosomal protein S28-B



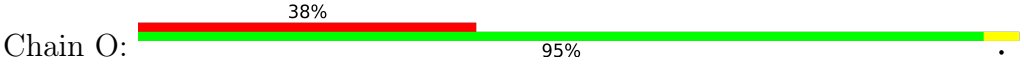
• Molecule 14: 40S ribosomal protein S29-A

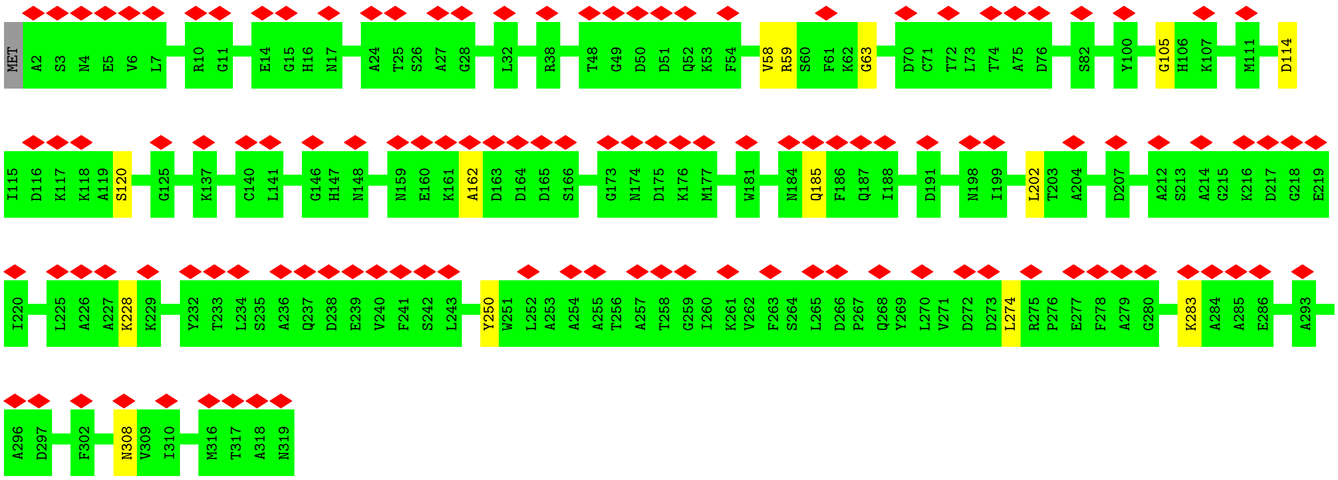


• Molecule 15: Ubiquitin-40S ribosomal protein S31



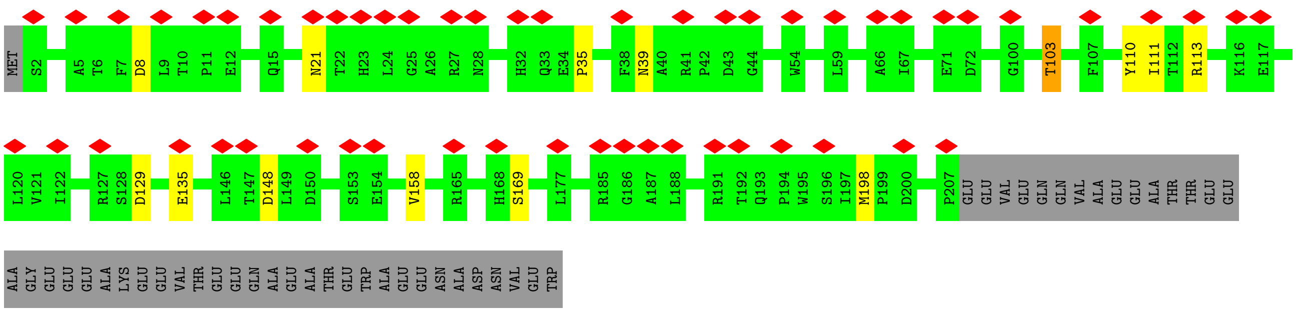
• Molecule 16: Guanine nucleotide-binding protein subunit beta-like protein





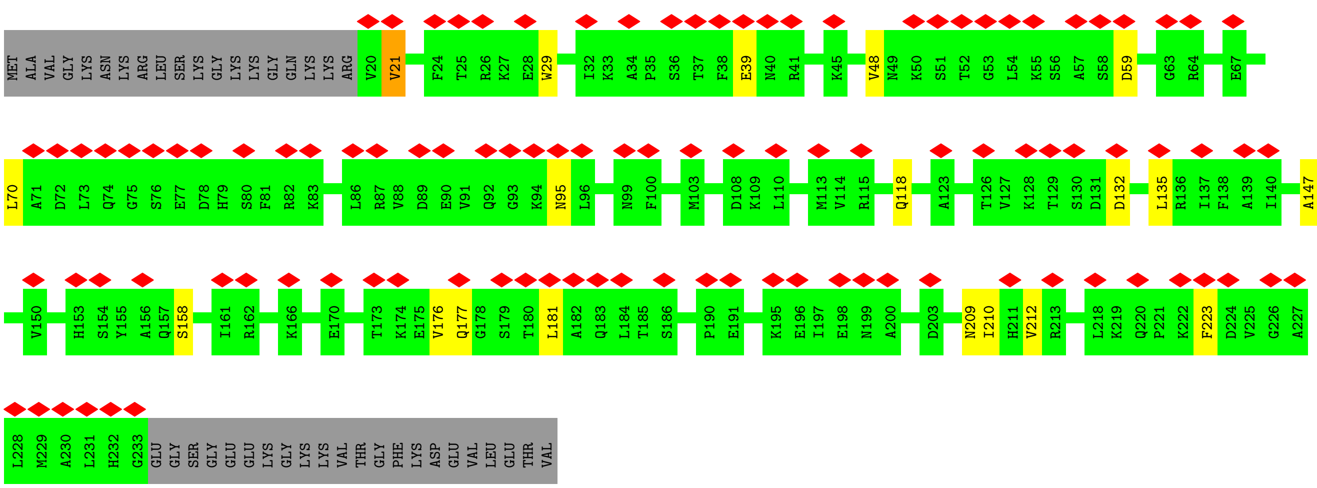
- Molecule 17: 40S ribosomal protein S0-A

Chain P:



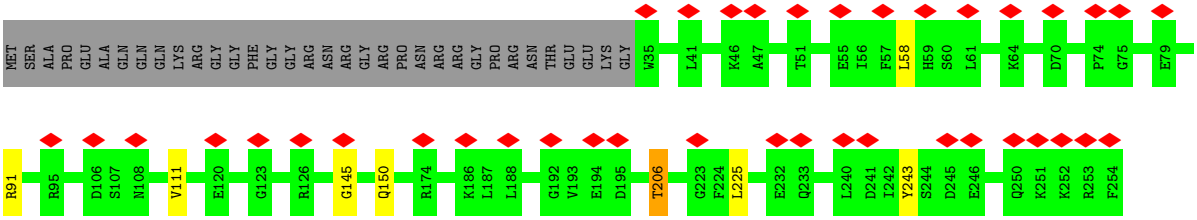
- Molecule 18: 40S ribosomal protein S1-A

Chain Q:



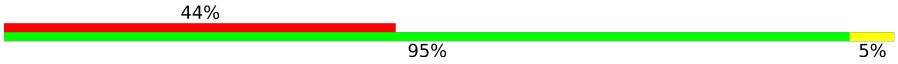
- Molecule 19: 40S ribosomal protein S2

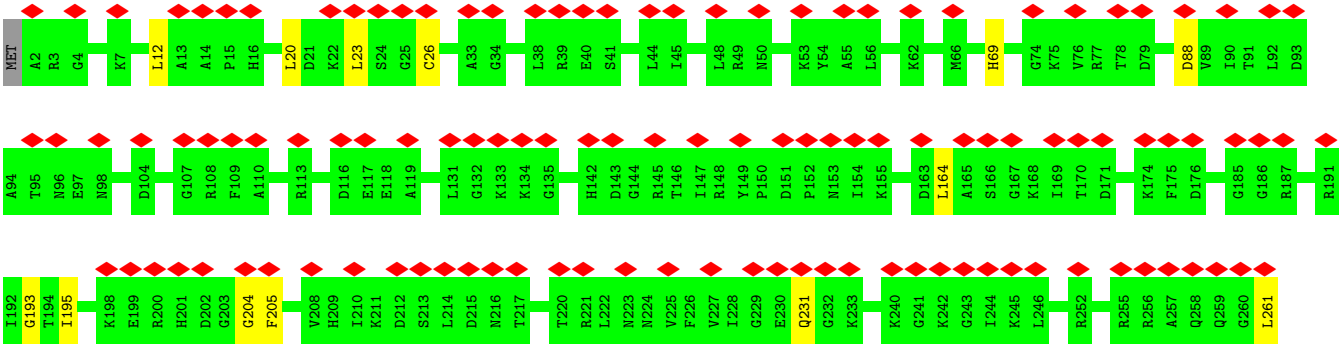
Chain R:



• Molecule 20: 40S ribosomal protein S4-A

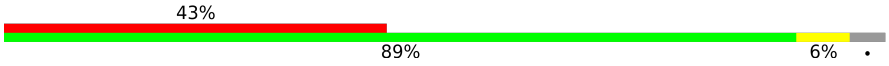
Chain S:

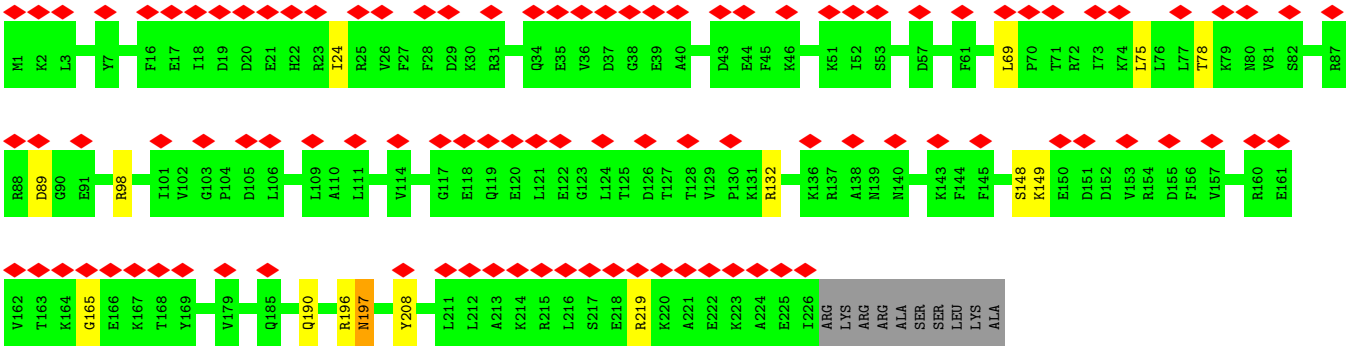




• Molecule 21: 40S ribosomal protein S6-A

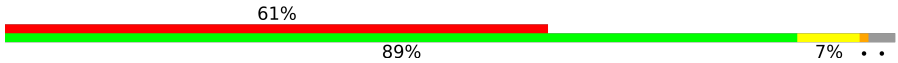
Chain T:

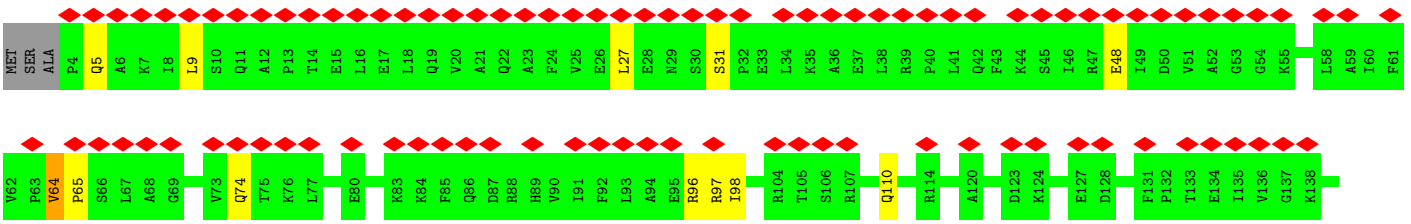


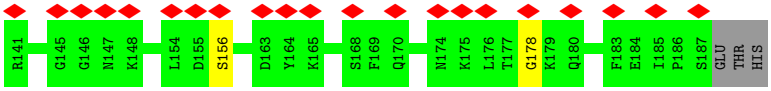


• Molecule 22: 40S ribosomal protein S7-A

Chain U:

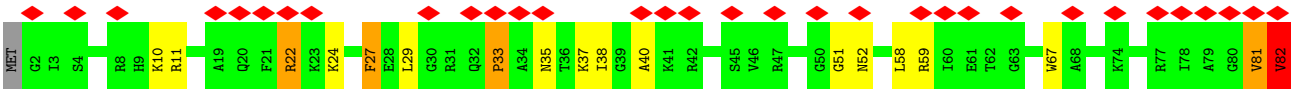


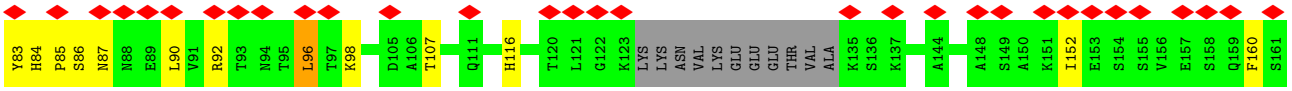


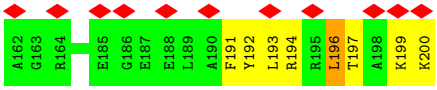


• Molecule 23: 40S ribosomal protein S8-A

Chain V:

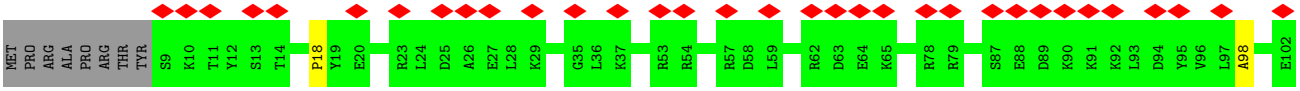


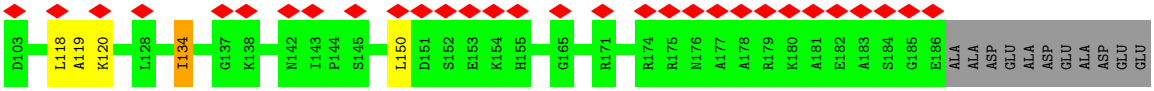




• Molecule 24: 40S ribosomal protein S9-A

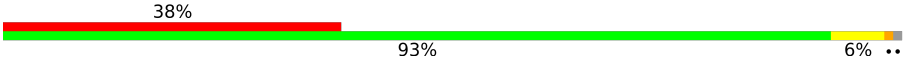
Chain W:

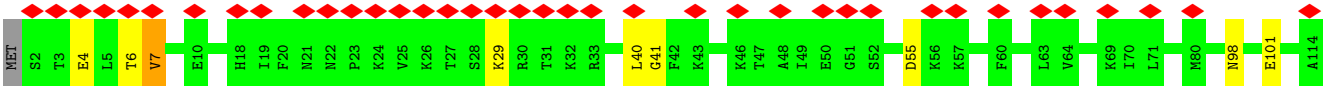


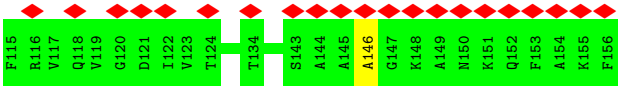


• Molecule 25: 40S ribosomal protein S11-A

Chain X:

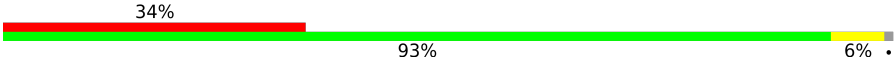


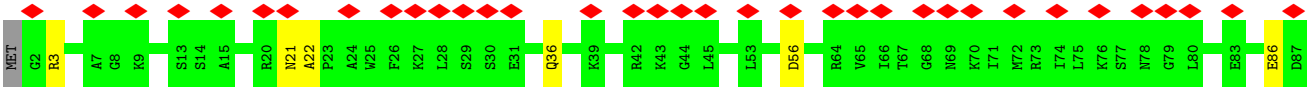


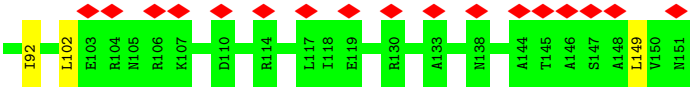


• Molecule 26: 40S ribosomal protein S13

Chain Y:

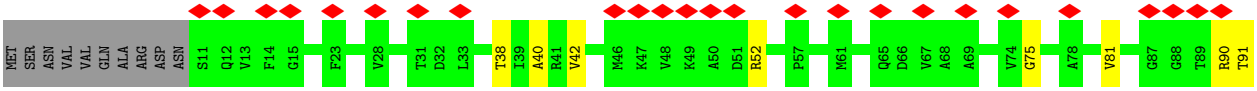


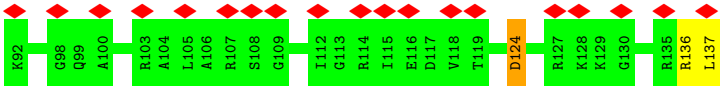




• Molecule 27: 40S ribosomal protein S14-A

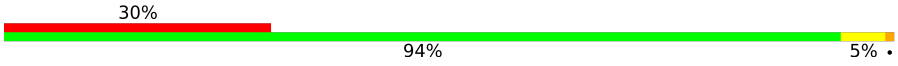
Chain Z:

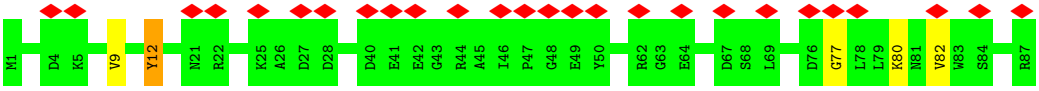




• Molecule 28: 40S ribosomal protein S21-A

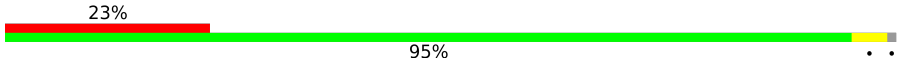
Chain a:

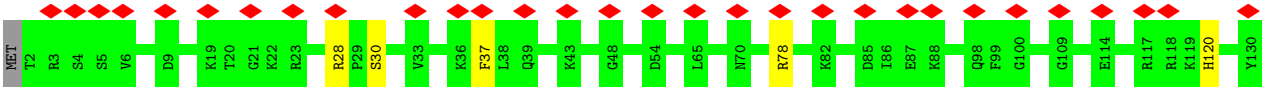




• Molecule 29: 40S ribosomal protein S22-A

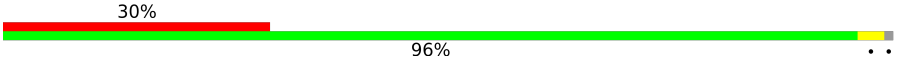
Chain b:

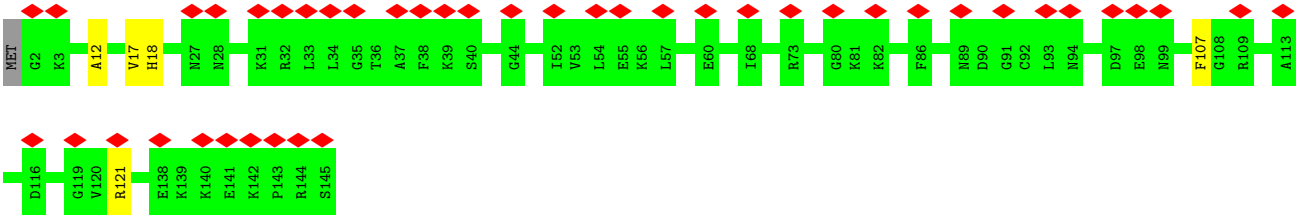




• Molecule 30: 40S ribosomal protein S23-A

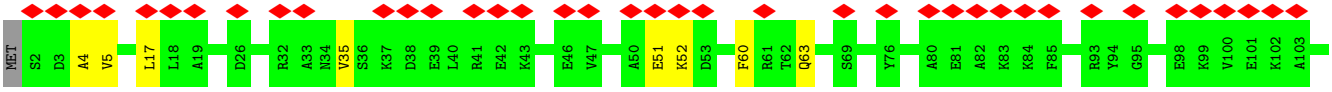
Chain c:

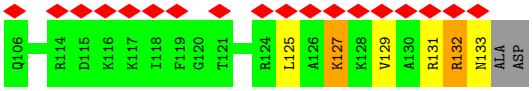




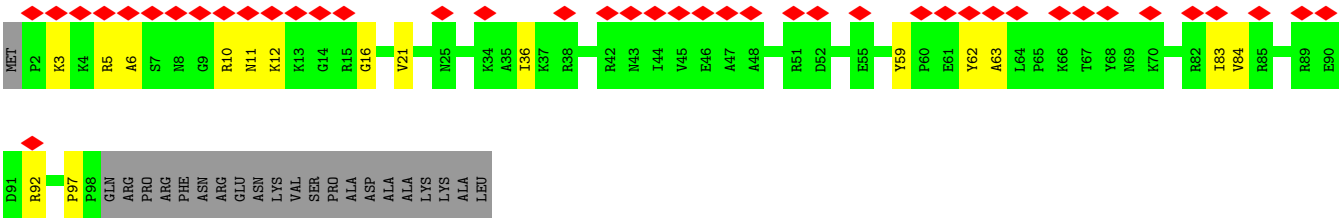
• Molecule 31: 40S ribosomal protein S24-A

Chain d:

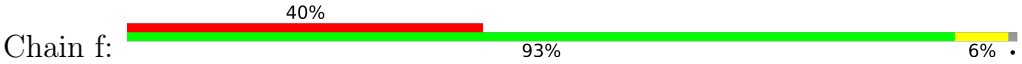


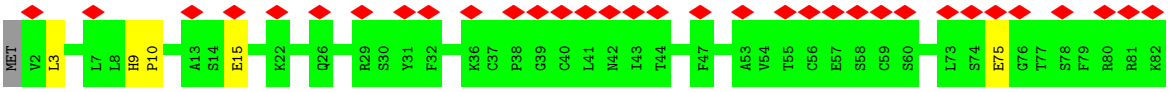


• Molecule 32: 40S ribosomal protein S26-A

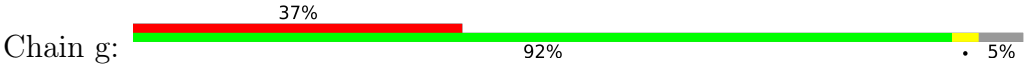


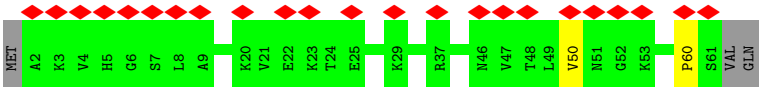
• Molecule 33: 40S ribosomal protein S27-A



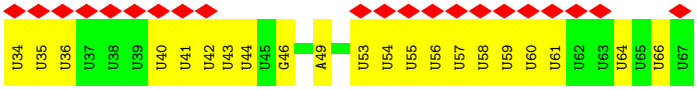


• Molecule 34: 40S ribosomal protein S30-A

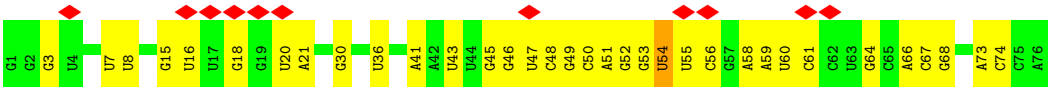




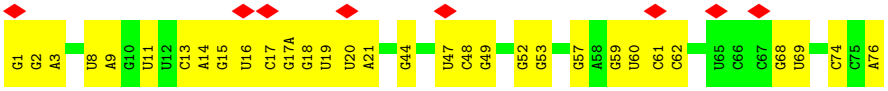
• Molecule 35: mRNA



• Molecule 36: A-site tRNA

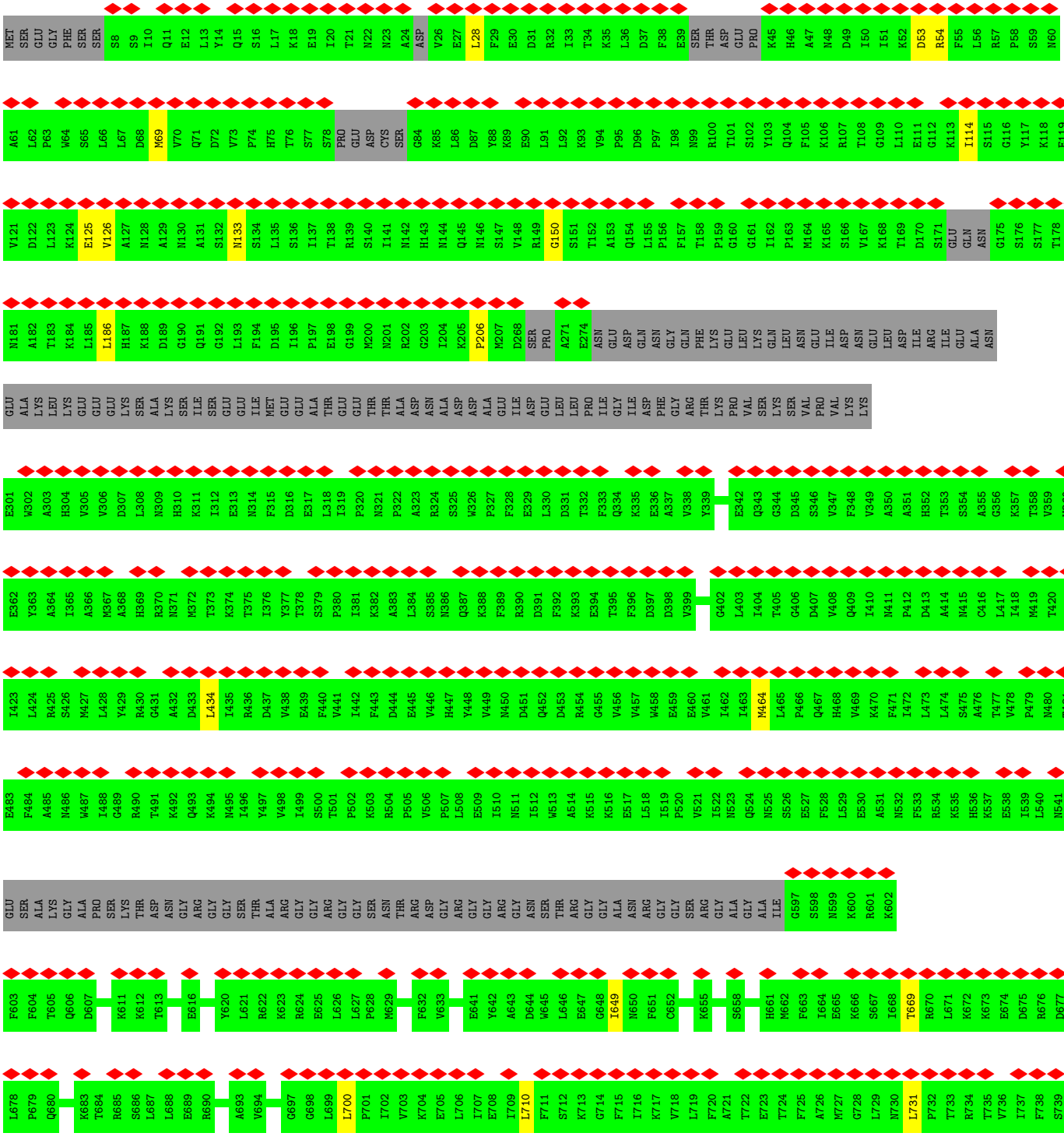


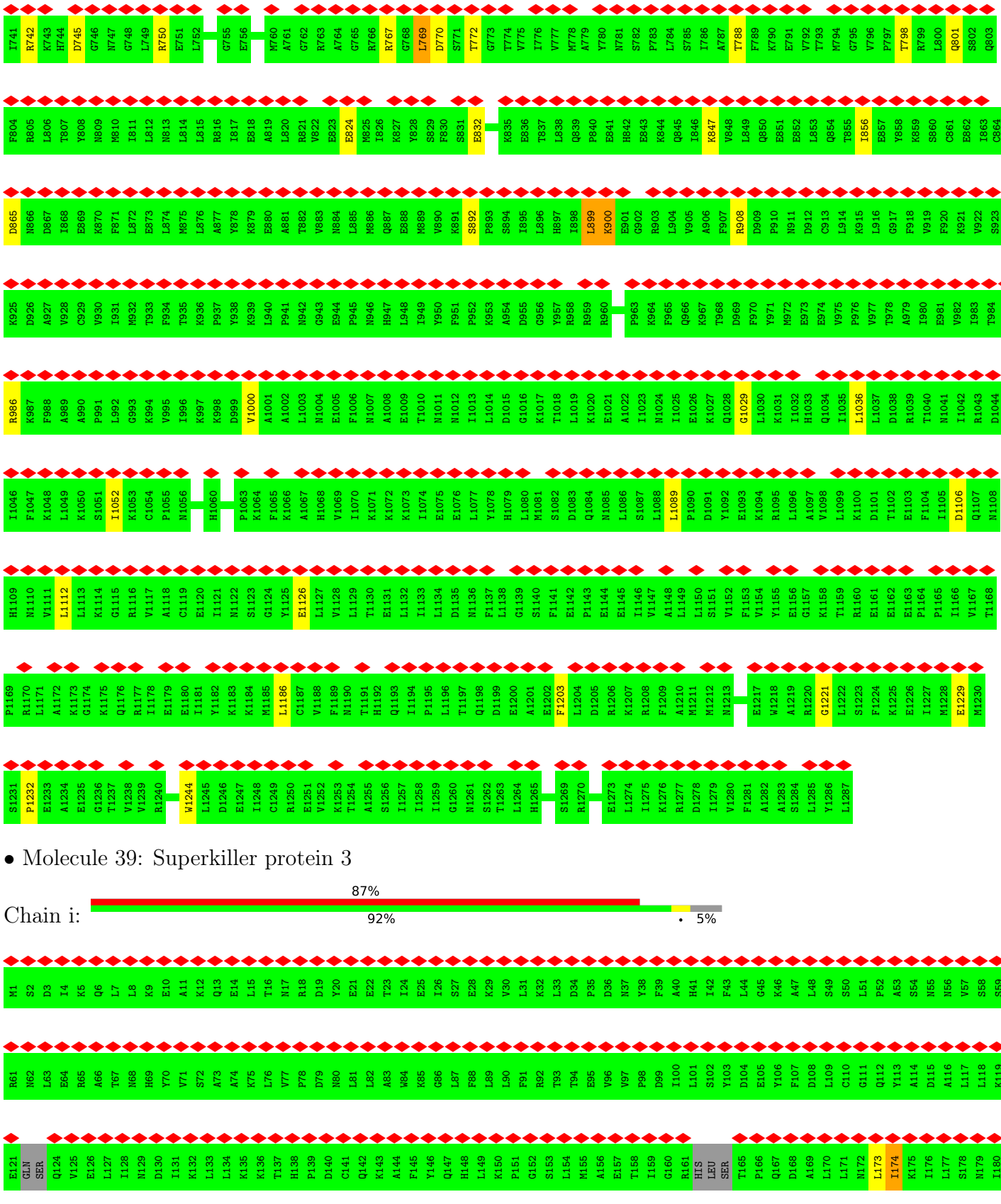
• Molecule 37: P-site tRNA



• Molecule 38: Antiviral helicase SKI2

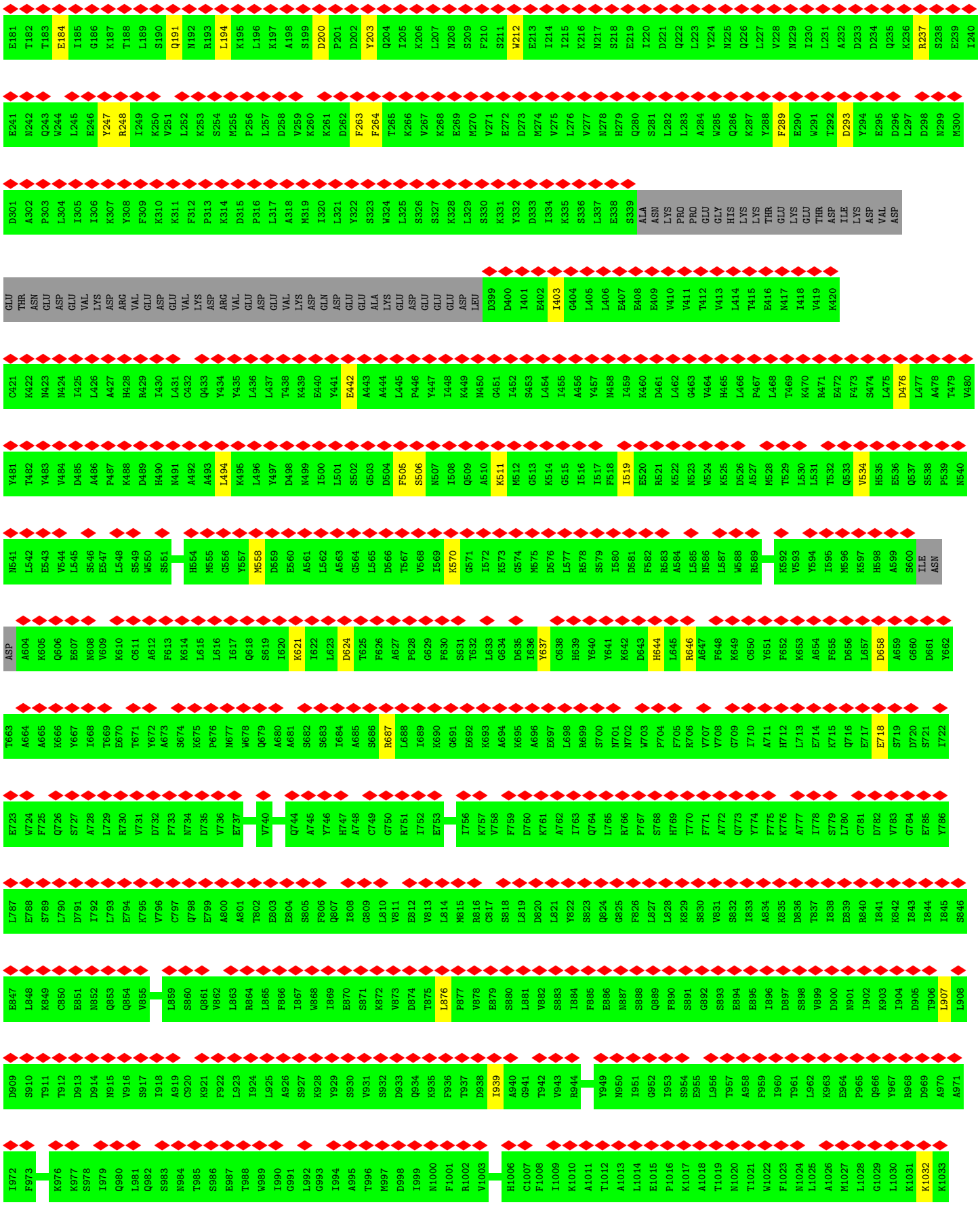
Chain h:

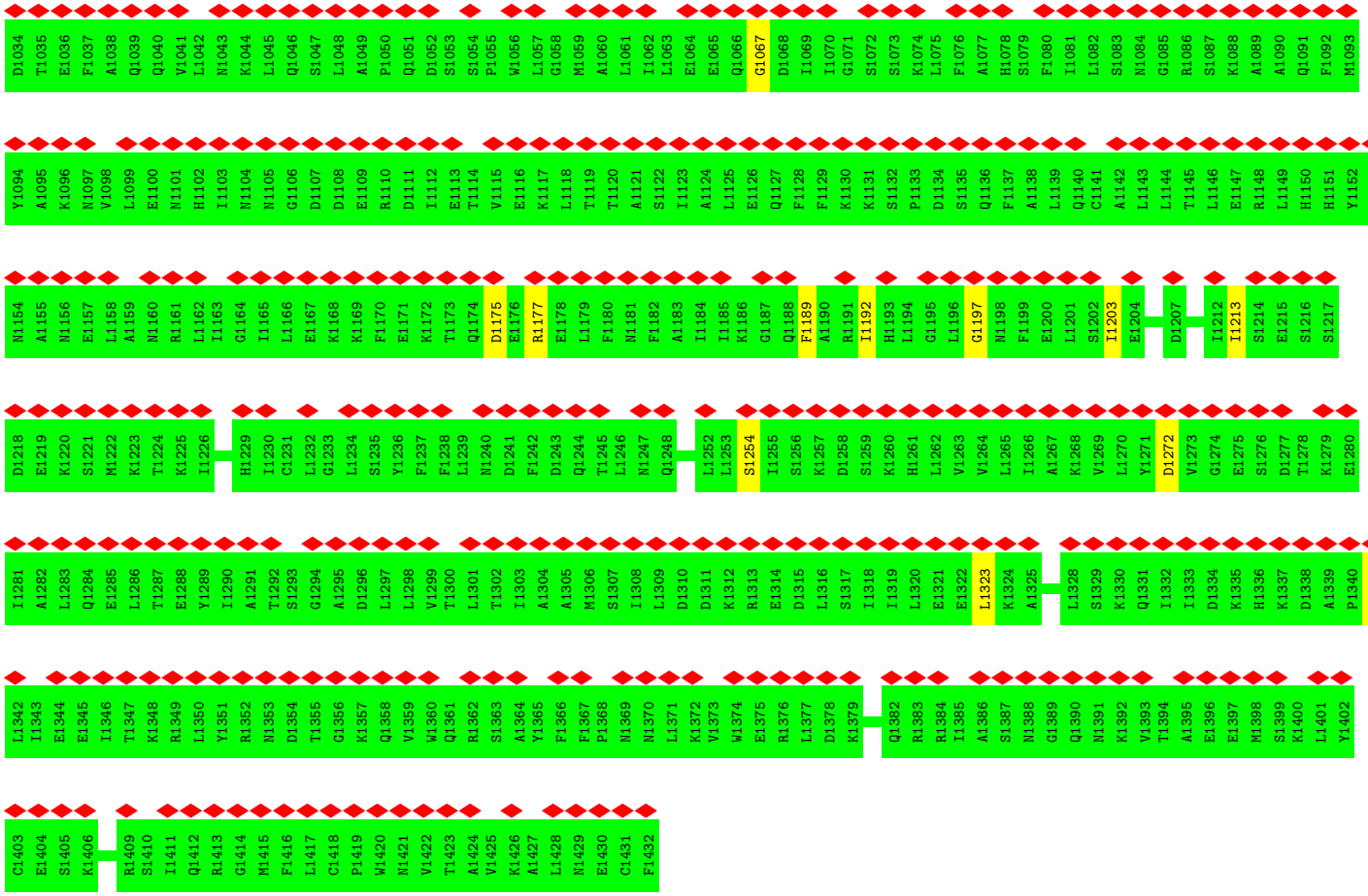




• Molecule 39: Superkiller protein 3

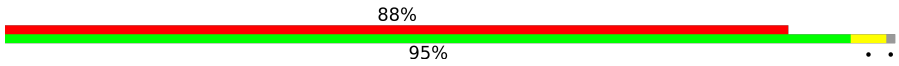
Chain i:

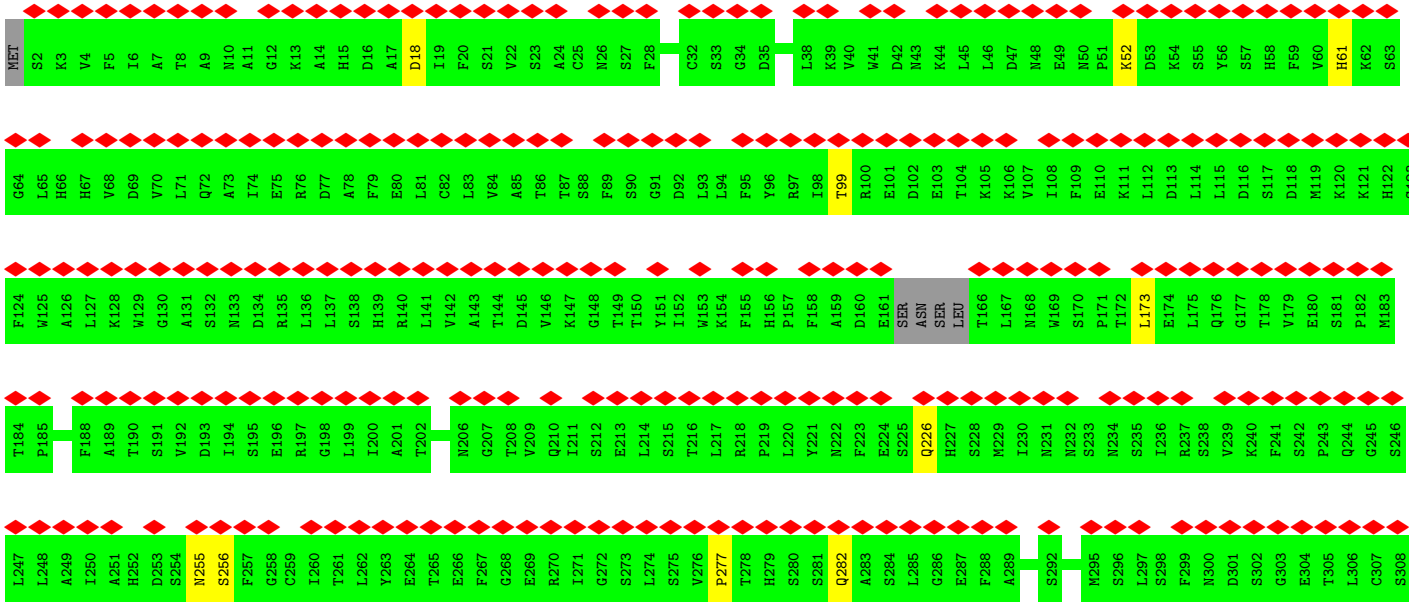

E181 T182 T183 E184 I185 G186 K187 T188 L189 S190 Q191 N192 R193 L194 K195 L196 K197 A198 S199 D200 P201 D202 Y203 Q204 I205 K206 L207 N208 S209 F210 S211 W212 E213 I214 I215 K216 N217 S218 E219 I220 D221 Q222 L223 Y224 N225 Q226 L227 V228 N229 I230 L231 A232 D233 D234 Q235 K236 R237 S238 E239 I240
E241 N242 Q243 W244 L245 E246 Y247 R248 T249 K250 V251 L252 K253 S254 M255 P256 L257 D258 V259 K260 K261 D262 F263 F264 T265 K266 V267 K268 E269 M270 V271 E272 D273 M274 V275 L276 V277 N278 H279 Q280 S281 L282 L283 A284 W285 Q286 K287 Y288 F289 E290 W291 T292 D293 Y294 E295 D296 L297 D298 N299 N300
D301 A302 P303 L304 I305 I306 K307 Y308 F309 K310 K311 F312 P313 K314 D315 P316 L317 A318 M319 I320 L321 Y322 S323 W324 L325 S326 S327 K328 L329 S330 K331 Y332 D333 I334 K335 S336 L337 E338 S339 ALA ASN LYS PRO PRO GLU GLY HIS LYS LYS THR GLU LYS GLU THR ASP ILE LYS ASP VAL ASP
GLU THR ASN GLU ASP GLU VAL LYS ASP ARG VAL GLU ASP GLU VAL LYS ASP ARG VAL GLU ASP GLU VAL LYS ASP GLU GLU ALA LYS GLU ASP GLU GLU GLU ASP LEU D399 D400 I401 E402 I403 G404 L405 L406 E407 E408 E409 V410 V411 T412 V413 L414 T415 E416 N417 I418 V419 K420
C421 K422 N423 N424 I425 L426 A427 H428 R429 I430 L431 C432 Q433 Y434 Y435 L436 L437 T438 K439 E440 Y441 E442 A443 A444 L445 P446 Y447 I448 K449 N450 G451 I452 S453 L454 I455 A456 Y457 N458 I459 K460 D461 L462 G463 V464 H465 L466 P467 L468 T469 K470 R471 E472 F473 S474 L475 D476 L477 A478 T479 V480
Y481 T482 Y483 V484 D485 A486 P487 K488 D489 H490 N491 A492 A493 L494 K495 L496 Y497 D498 N499 I500 L501 S502 G503 D504 F505 S506 N507 I508 Q509 A510 K511 M512 G513 K514 G515 I516 I517 F518 I519 E520 R521 K522 N523 W524 K525 D526 A527 M528 T529 L530 L531 T532 Q533 V534 H535 E536 Q537 S538 P539 N540
N541 L542 E543 V544 L545 S546 E547 L548 S549 W550 S551 H554 M555 G556 Y557 M558 D559 E560 A561 L562 A563 G564 L565 D566 T567 V568 I569 K570 G571 I572 K573 G574 M575 D576 L577 R578 S579 I580 D581 F582 R583 A584 L585 N586 L587 W588 R589 K592 V593 Y594 I595 M596 K597 H598 A599 S600 ILE ASN
ASP A604 K605 Q606 E607 N608 V609 K610 C611 A612 F613 K614 L615 L616 I617 Q618 S619 I620 K621 I622 L623 D624 T625 F626 A627 P628 G629 F630 S631 T632 L633 G634 D635 I636 Y637 C638 H639 Y640 Y641 K642 D643 H644 L645 R646 A647 F648 K649 C650 Y651 F652 K653 A654 F655 D656 L657 D658 A659 G660 D661 Y662
T663 A664 A665 K666 Y667 I668 T669 E670 T671 Y672 A673 S674 K675 P676 N677 W678 Q679 A680 A681 S682 S683 I684 A685 S686 R687 L688 I689 K690 G691 E692 K693 A694 K695 A696 E697 L698 R699 S700 N701 N702 W703 P704 F705 R706 V707 V708 G709 I710 A711 H712 L713 E714 K715 Q716 E717 E718 S719 D720 S721 I722
E723 W724 F725 Q726 S727 A728 L729 R730 V731 D732 P733 N734 D735 V736 E737 V740 Q744 A745 Y746 H747 A748 C749 G750 R751 I752 E753 I756 K757 V758 F759 D760 K761 A762 I763 Q764 L765 R766 P767 S768 H769 T770 F771 A772 Q773 Y774 F775 K776 A777 I778 S779 L780 C781 D782 V783 G784 E785 Y786
L787 E788 S789 L790 D791 I792 L793 E794 K795 V796 C797 Q798 E799 A800 A801 T802 E803 E804 S805 F806 Q807 I808 G809 L810 V811 E812 V813 L814 M815 R816 C817 S818 L819 D820 L821 Y822 S823 Q824 G825 F826 L827 L828 K829 S830 V831 S832 I833 A834 K835 D836 T837 I838 E839 R840 I841 K842 I843 I844 I845 S846
E847 L848 K849 C850 E851 N852 Q853 Q854 V855 L859 S860 Q861 V862 L863 R864 L865 F866 I867 W868 I869 E870 S871 K872 V873 D874 T875 L876 P877 V878 E879 S880 L881 V882 S883 I884 F885 E886 N887 S888 Q889 F890 S891 Q892 S893 E894 E895 I896 D897 S898 V899 D900 N901 I902 K903 I904 D905 T906 L907 L908
D909 S910 T911 T912 D913 D914 N915 V916 S917 I918 A919 C920 K921 F922 L923 I924 L925 A926 S927 K928 Y929 S930 V931 S932 D933 Q934 K935 F936 T937 D938 I939 A940 G941 T942 V943 R944 Y949 N950 I951 G952 I953 S954 E955 L956 T957 A958 F959 I960 T961 L962 K963 E964 P965 Q966 Y967 R968 D969 A970 A971
I972 F973 K976 K977 S978 I979 Q980 L981 Q982 S983 N984 T985 S986 E987 T988 W989 I990 G991 L992 G993 I994 A995 T996 M997 D998 I999 N1000 F1001 R1002 V1003 H1006 C1007 F1008 I1009 K1010 A1011 T1012 A1013 L1014 E1015 P1016 K1017 A1018 T1019 N1020 T1021 W1022 F1023 N1024 L1025 A1026 M1027 L1028 G1029 L1030 K1031 K1032 K1033

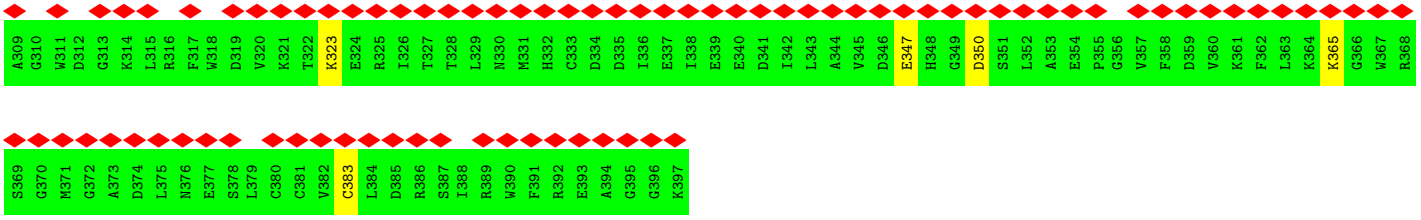


• Molecule 40: Antiviral protein SKI8

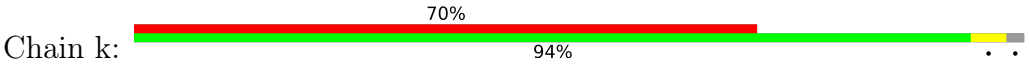
Chain j:

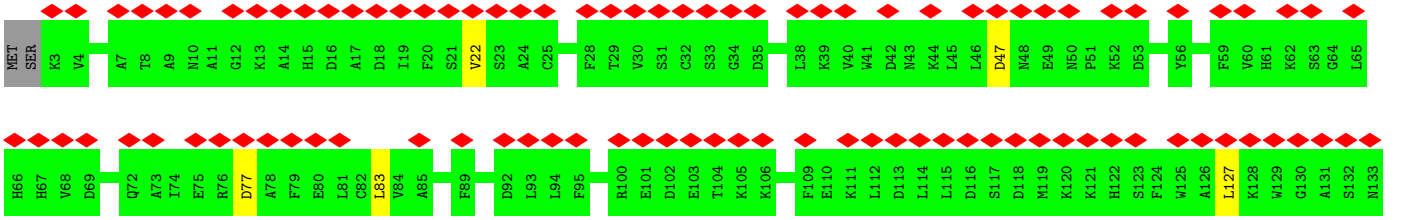


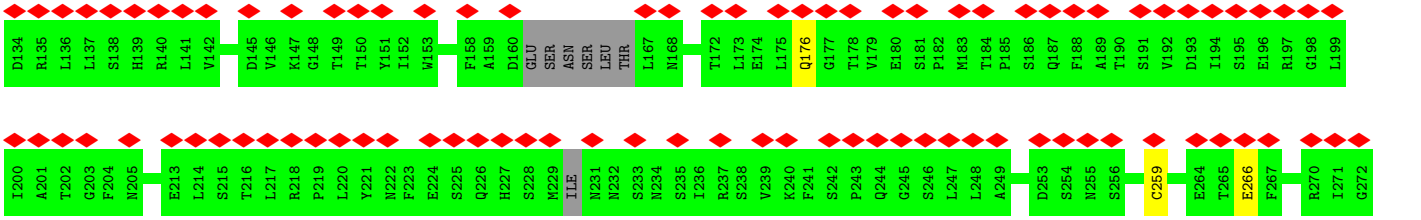


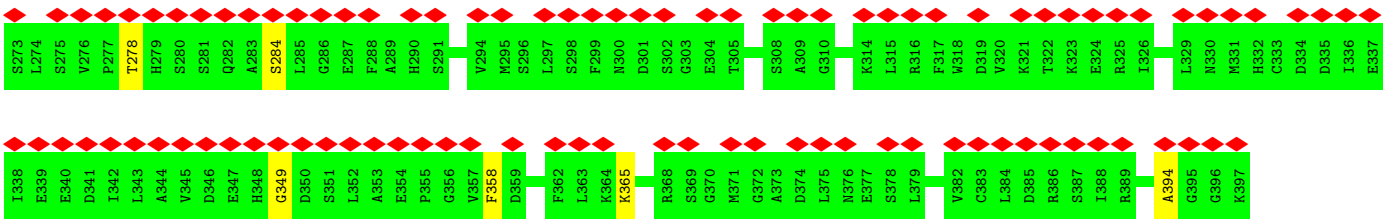


• Molecule 40: Antiviral protein SKI8

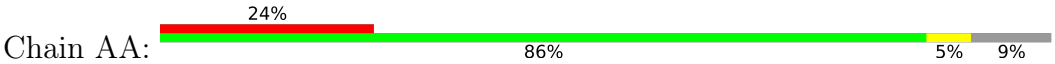


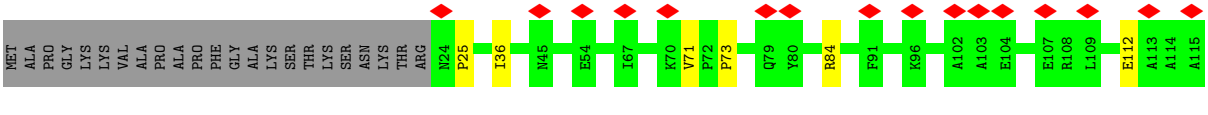


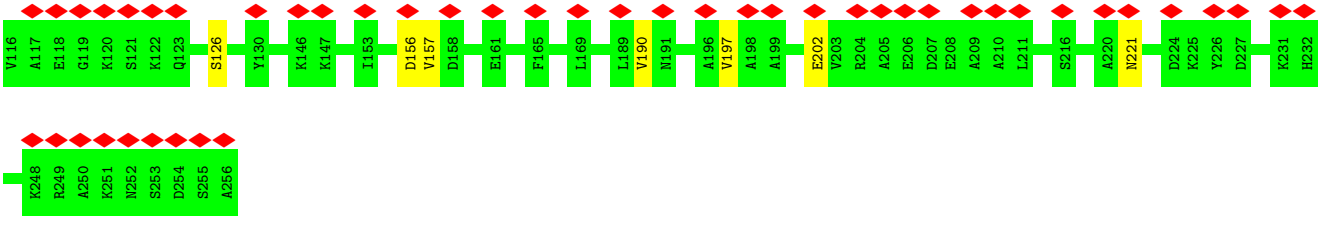




• Molecule 41: 60S ribosomal protein L8-A

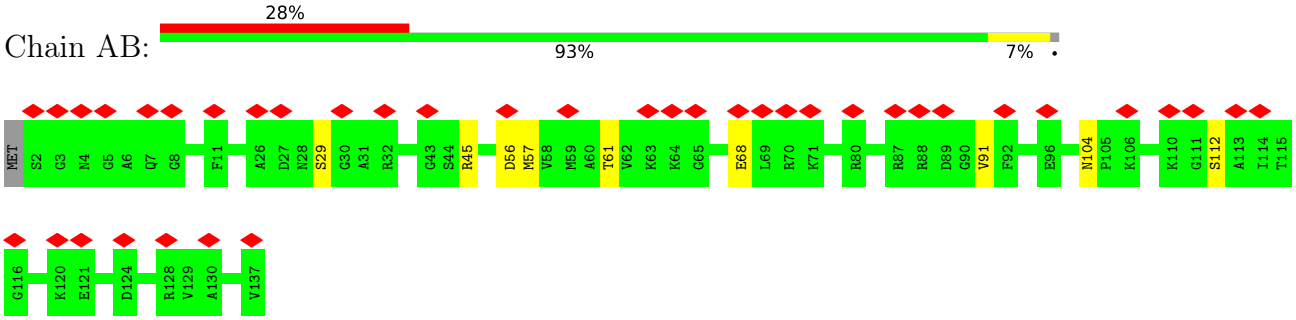






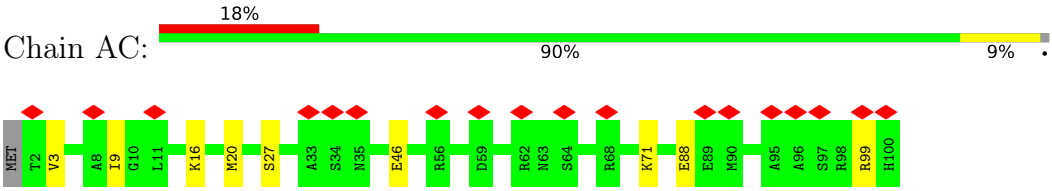
• Molecule 42: 60S ribosomal protein L23-A

Chain AB:



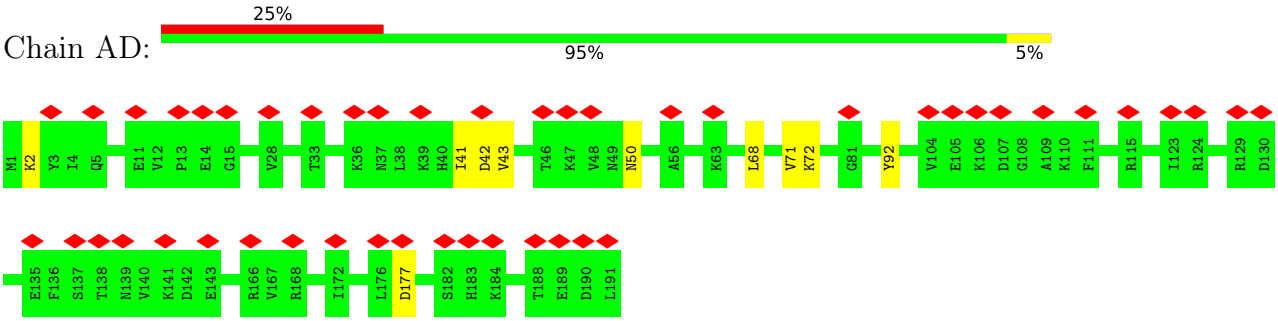
• Molecule 43: 60S ribosomal protein L36-A

Chain AC:



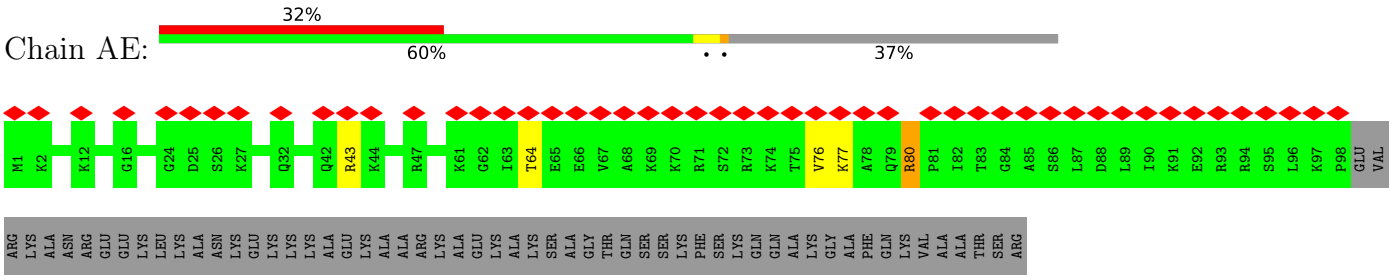
• Molecule 44: 60S ribosomal protein L9-A

Chain AD:



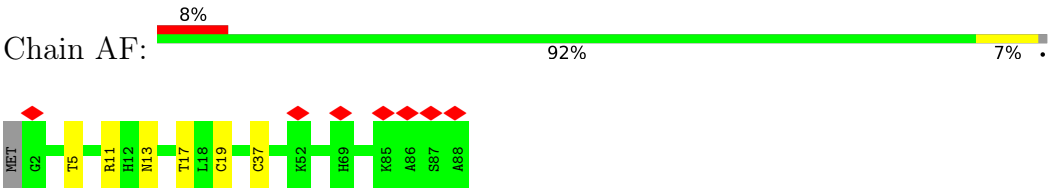
• Molecule 45: 60S ribosomal protein L24-A

Chain AE:



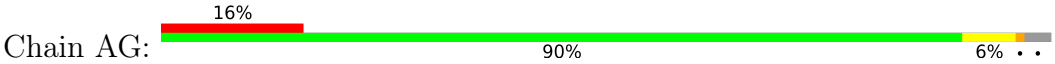
• Molecule 46: 60S ribosomal protein L37-A

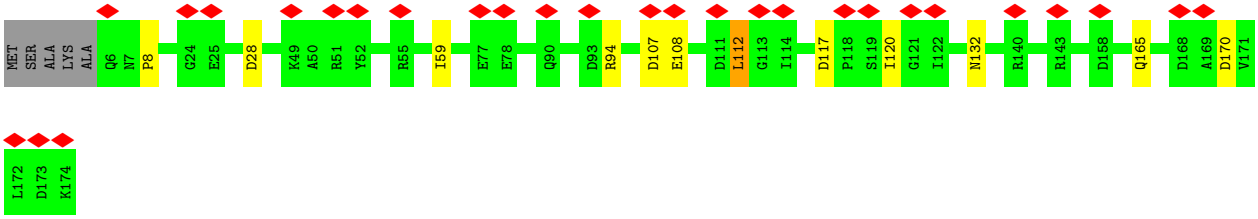
Chain AF:



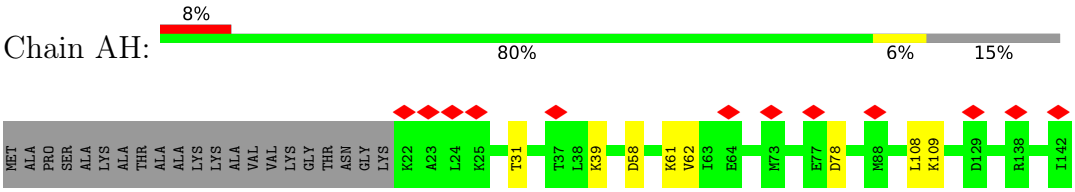
• Molecule 47: 60S ribosomal protein L11-A

Chain AG:

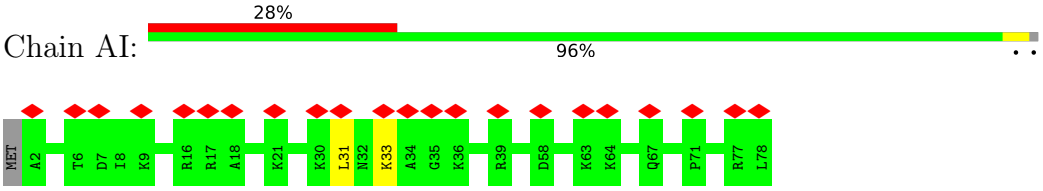




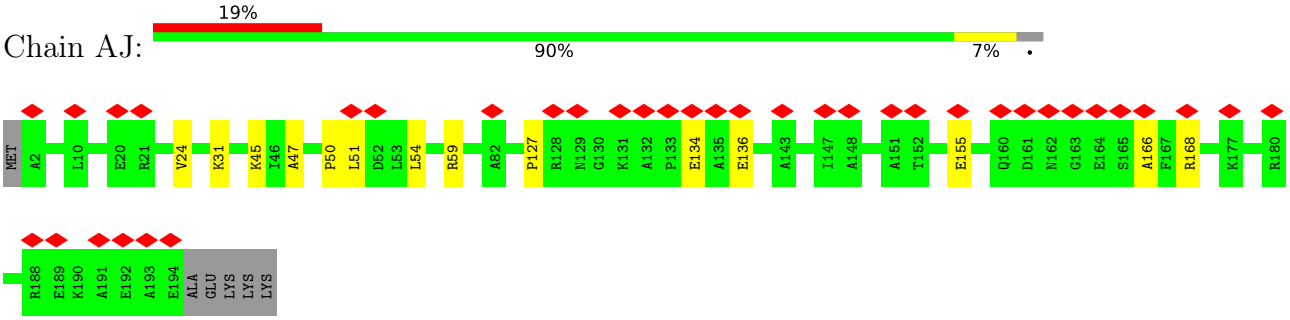
• Molecule 48: 60S ribosomal protein L25



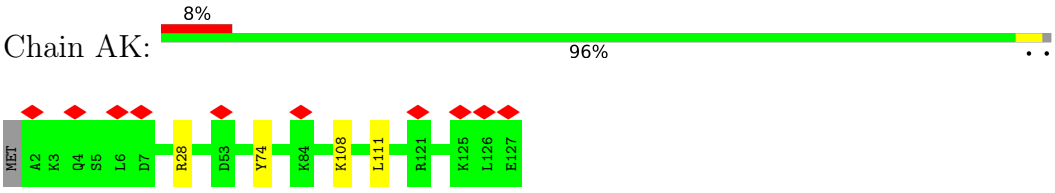
• Molecule 49: 60S ribosomal protein L38



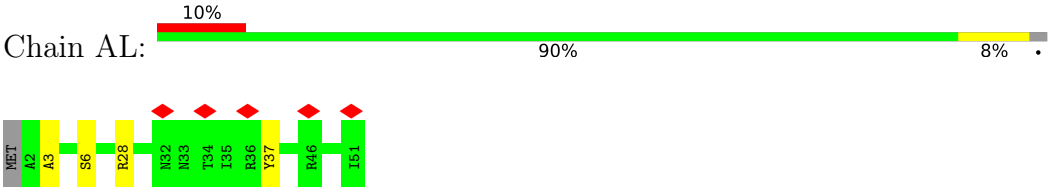
• Molecule 50: 60S ribosomal protein L13-A



• Molecule 51: 60S ribosomal protein L26-A

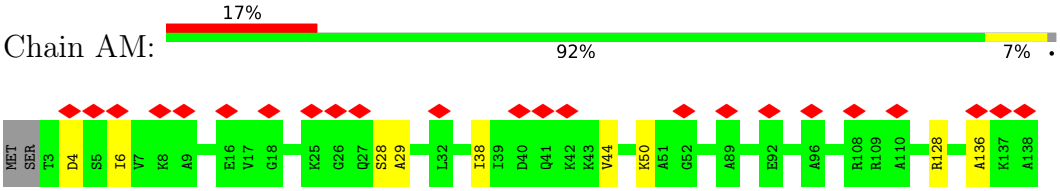


• Molecule 52: 60S ribosomal protein L39



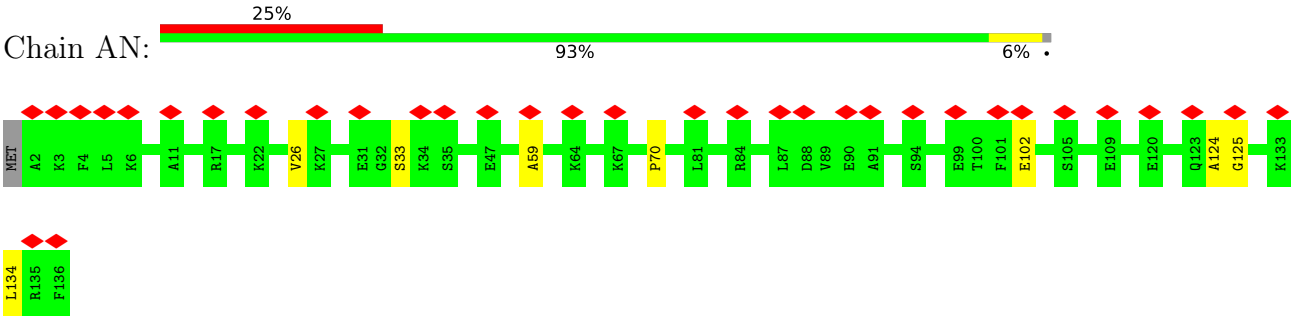
• Molecule 53: 60S ribosomal protein L14-A

Chain AM:



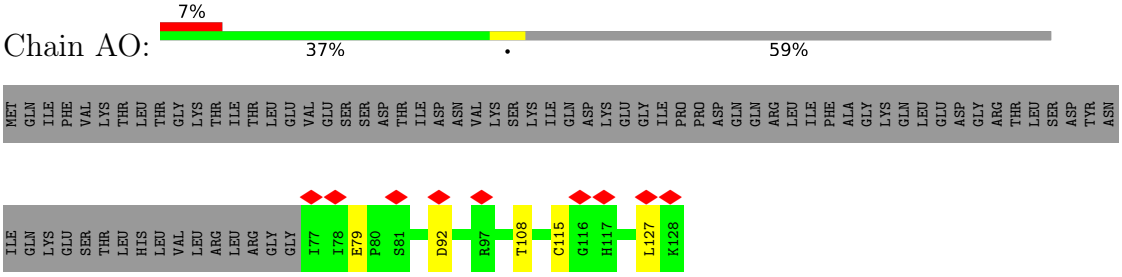
• Molecule 54: 60S ribosomal protein L27-A

Chain AN:



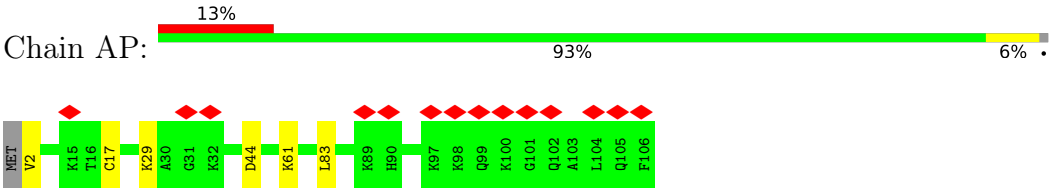
• Molecule 55: Ubiquitin-60S ribosomal protein L40

Chain AO:



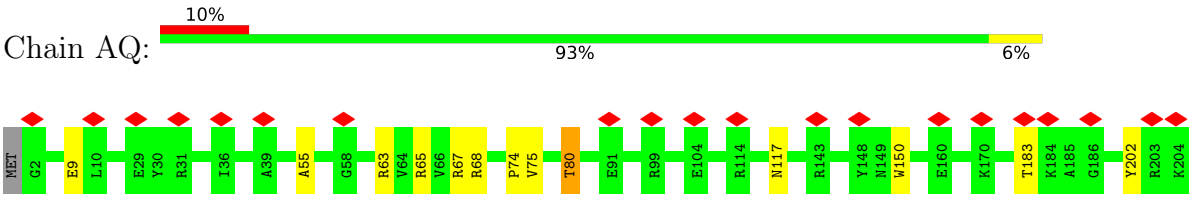
• Molecule 56: 60S ribosomal protein L42-A

Chain AP:



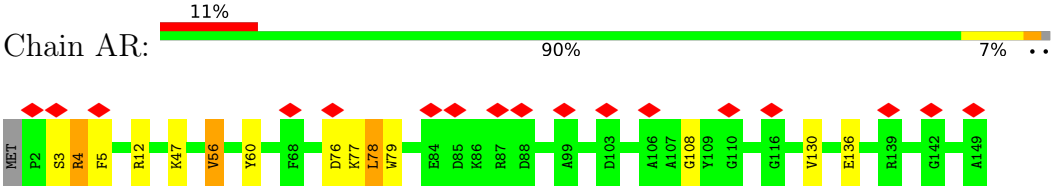
• Molecule 57: 60S ribosomal protein L15-A

Chain AQ:



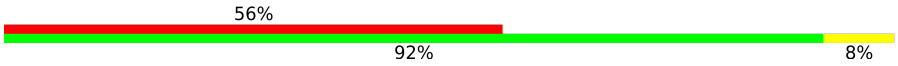
• Molecule 58: 60S ribosomal protein L28

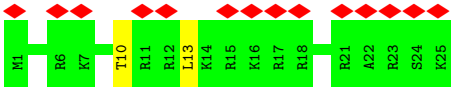
Chain AR:



• Molecule 59: 60S ribosomal protein L41-A

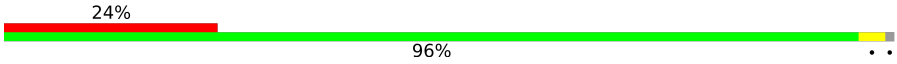
Chain AS:

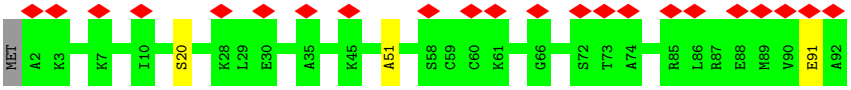




• Molecule 60: 60S ribosomal protein L43-A

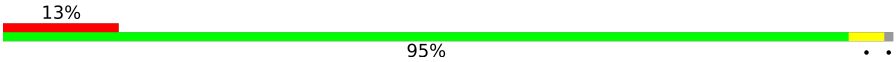
Chain AT:

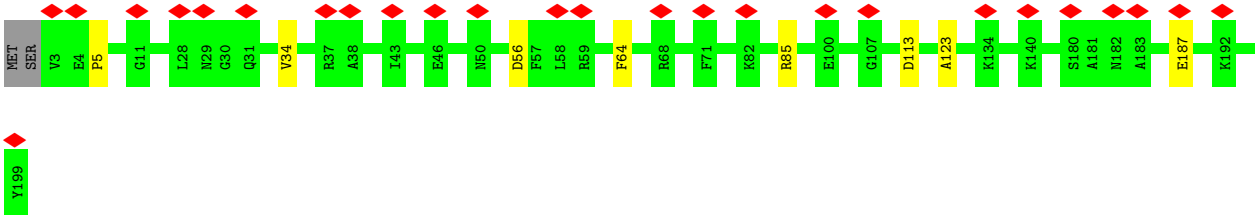




• Molecule 61: 60S ribosomal protein L16-A

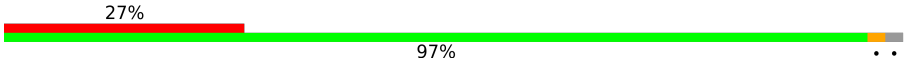
Chain AU:

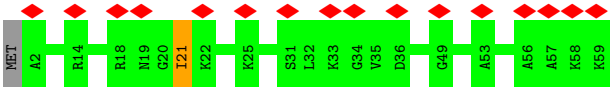




• Molecule 62: 60S ribosomal protein L29

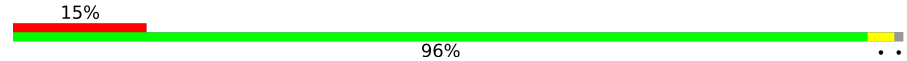
Chain AV:

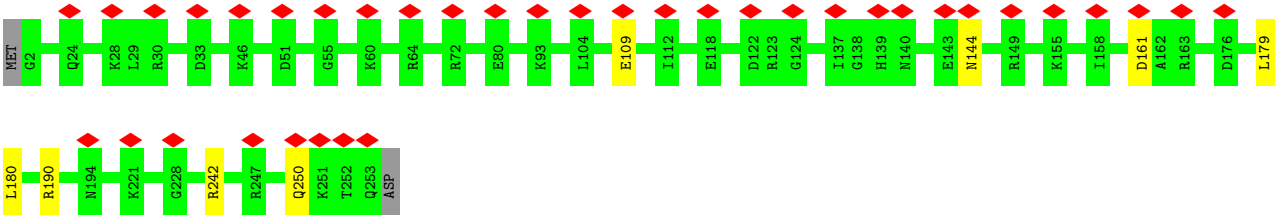




• Molecule 63: 60S ribosomal protein L2-A

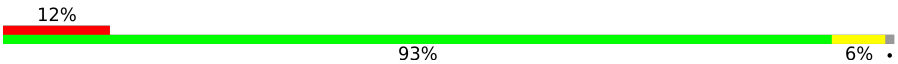
Chain AW:

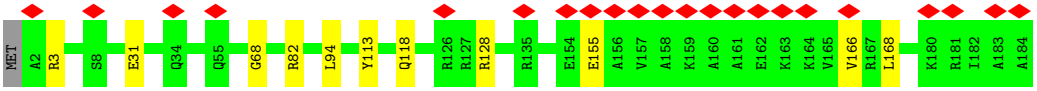




• Molecule 64: 60S ribosomal protein L17-A

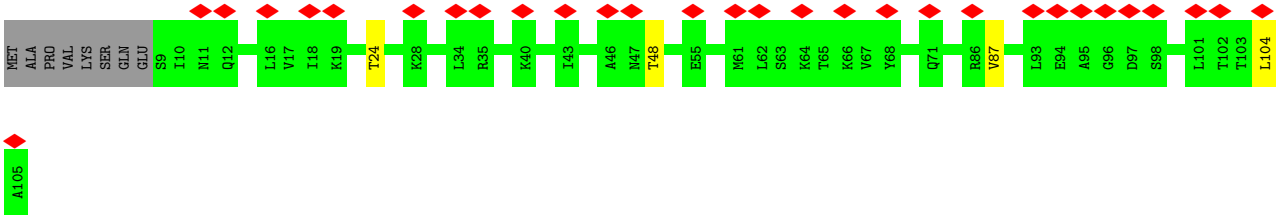
Chain AX:





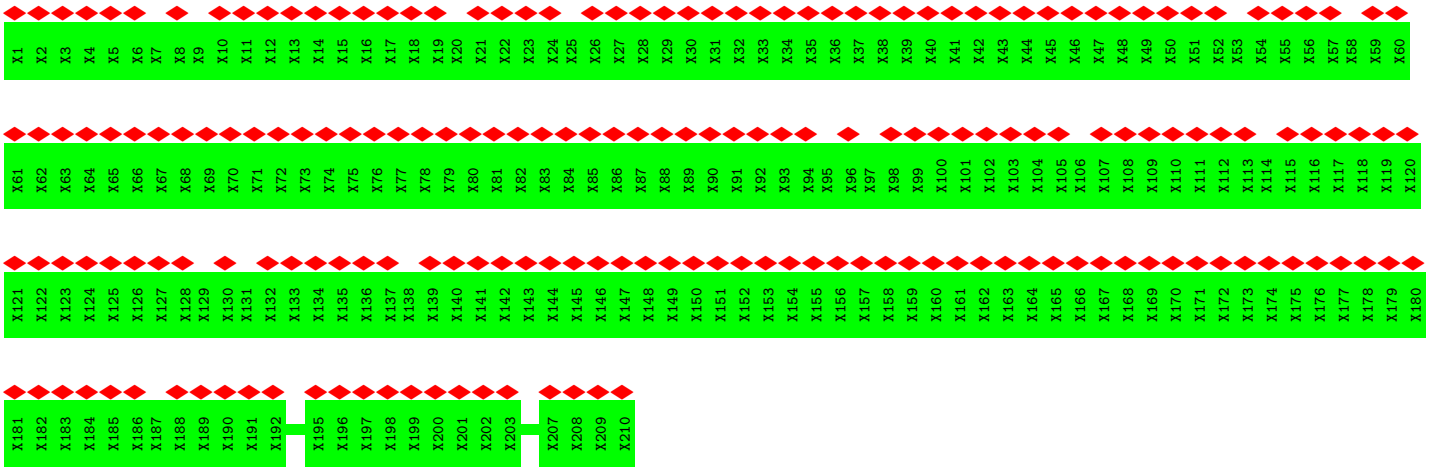
• Molecule 65: 60S ribosomal protein L30

Chain AY:



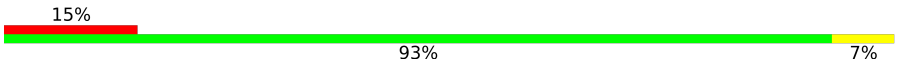
• Molecule 66: uL1

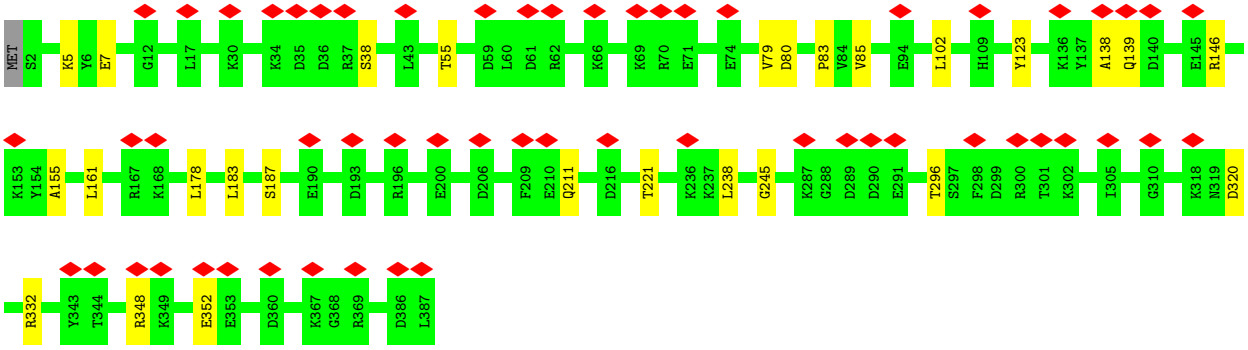
Chain AZ:



• Molecule 67: 60S ribosomal protein L3

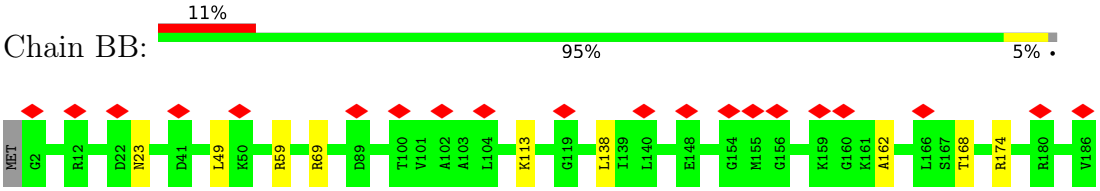
Chain BA:





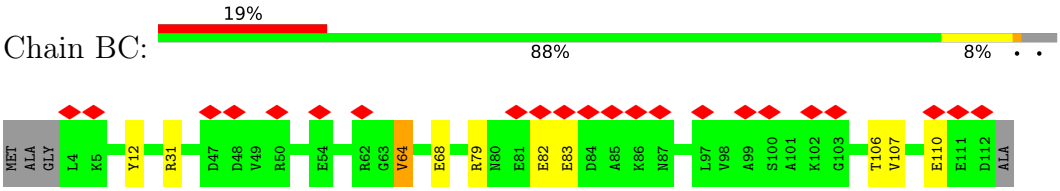
• Molecule 68: 60S ribosomal protein L18-A

Chain BB:



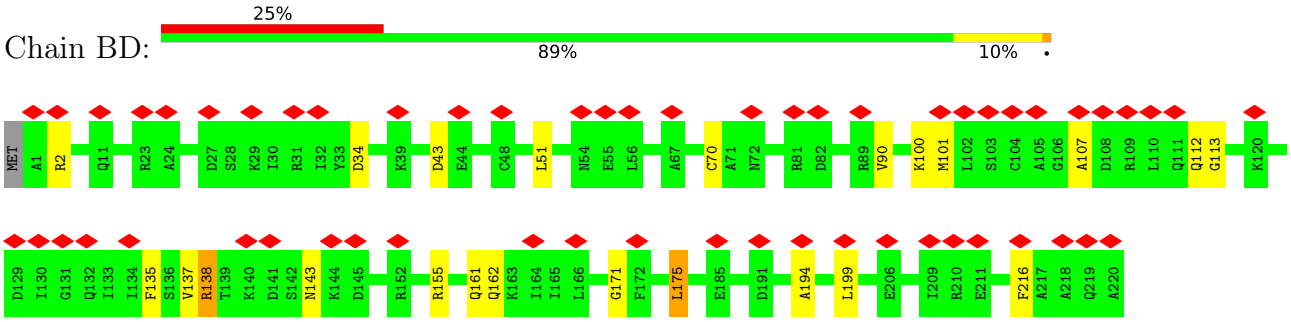
• Molecule 69: 60S ribosomal protein L31-A

Chain BC:



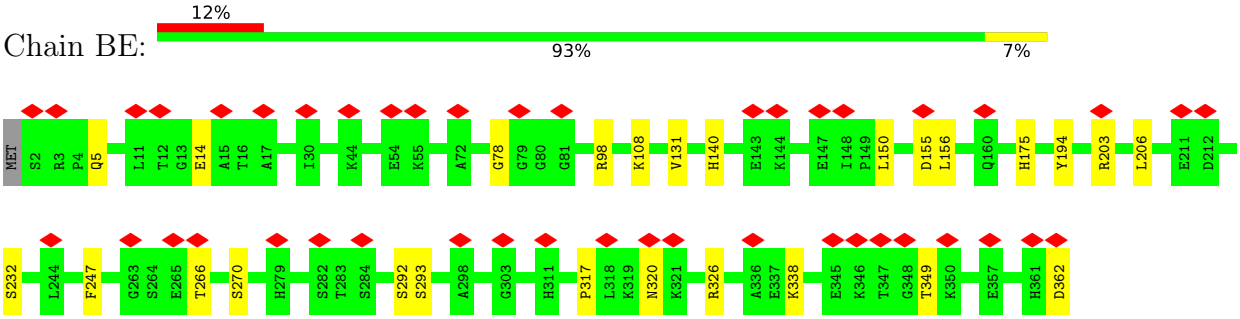
• Molecule 70: 60S ribosomal protein L10

Chain BD:



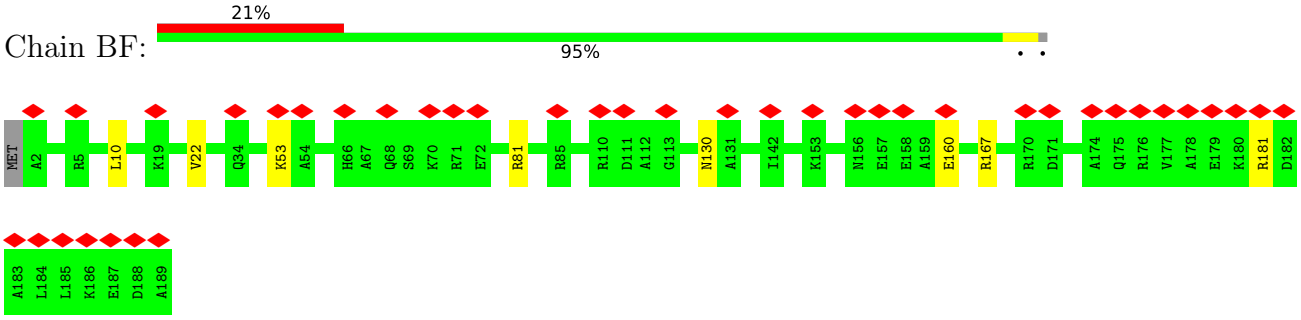
• Molecule 71: 60S ribosomal protein L4-A

Chain BE:



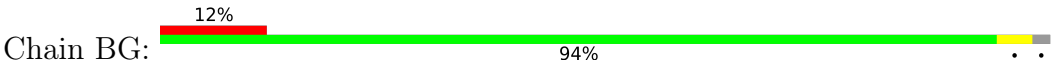
• Molecule 72: 60S ribosomal protein L19-A

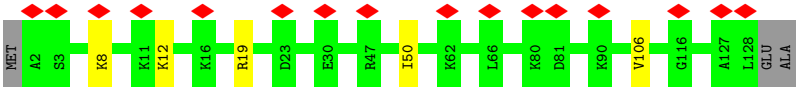
Chain BF:



• Molecule 73: 60S ribosomal protein L32

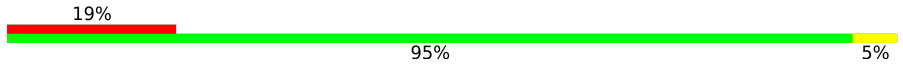
Chain BG:

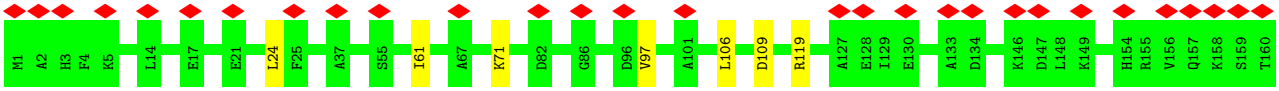


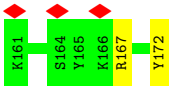


• Molecule 74: 60S ribosomal protein L20-A

Chain BH:

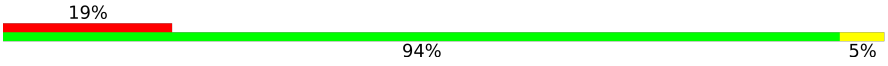


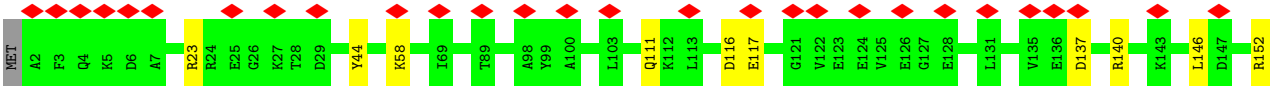


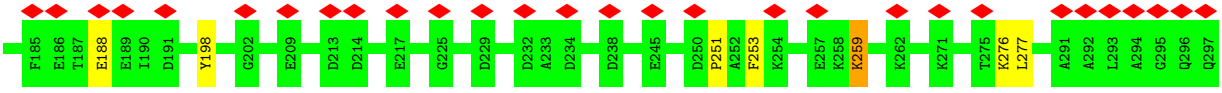


• Molecule 75: 60S ribosomal protein L5

Chain BI:

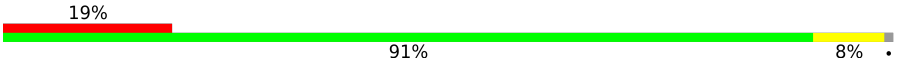


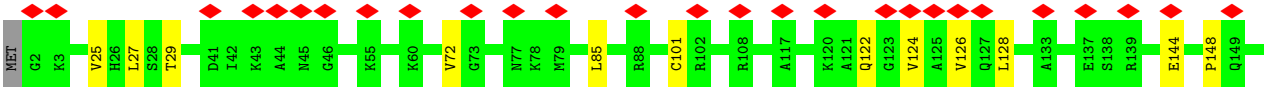


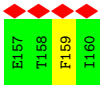


• Molecule 76: 60S ribosomal protein L21-A

Chain BJ:

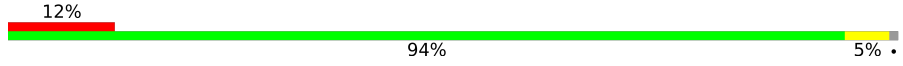


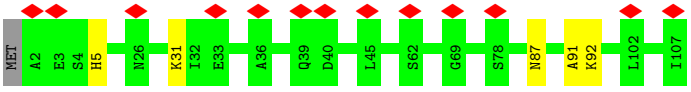




• Molecule 77: 60S ribosomal protein L33-A

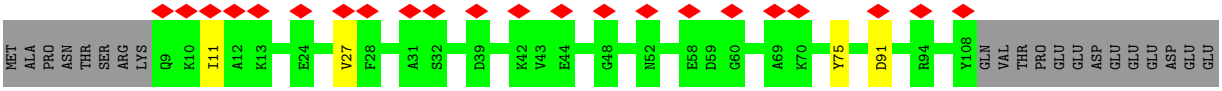
Chain BK:





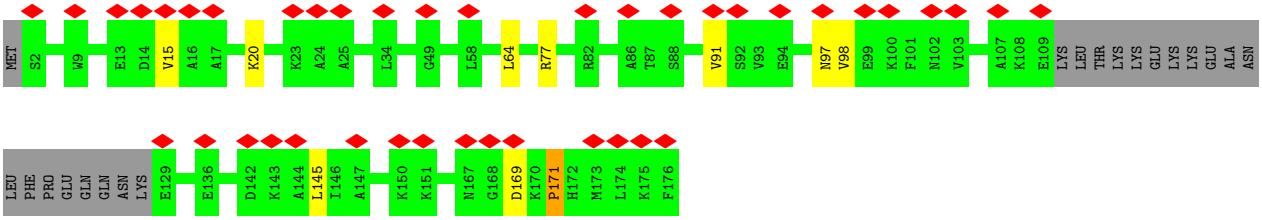
• Molecule 78: 60S ribosomal protein L22-A

Chain BL:



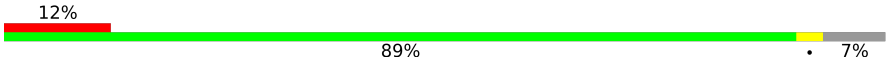
• Molecule 79: 60S ribosomal protein L6-A

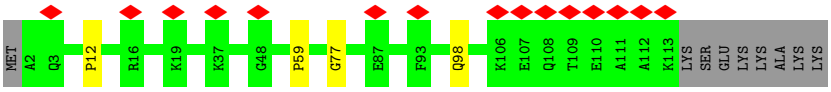
Chain BM:



• Molecule 80: 60S ribosomal protein L34-A

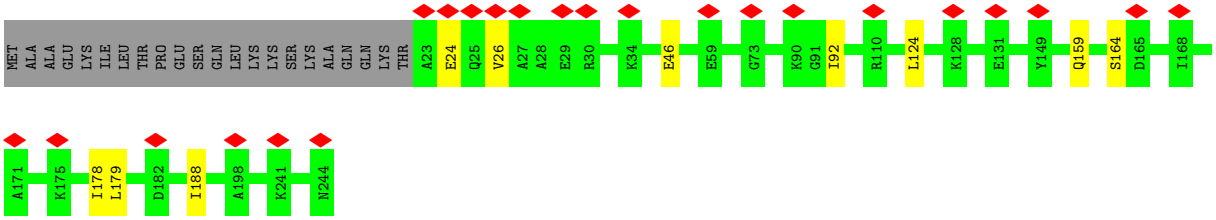
Chain BN:





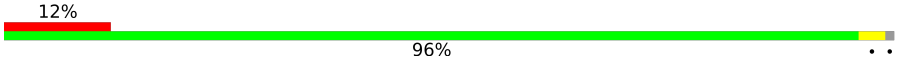
• Molecule 81: 60S ribosomal protein L7-A

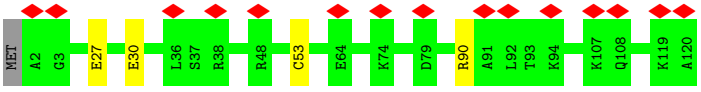
Chain BO:



• Molecule 82: 60S ribosomal protein L35-A

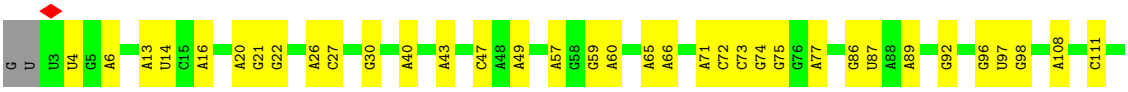
Chain BP:

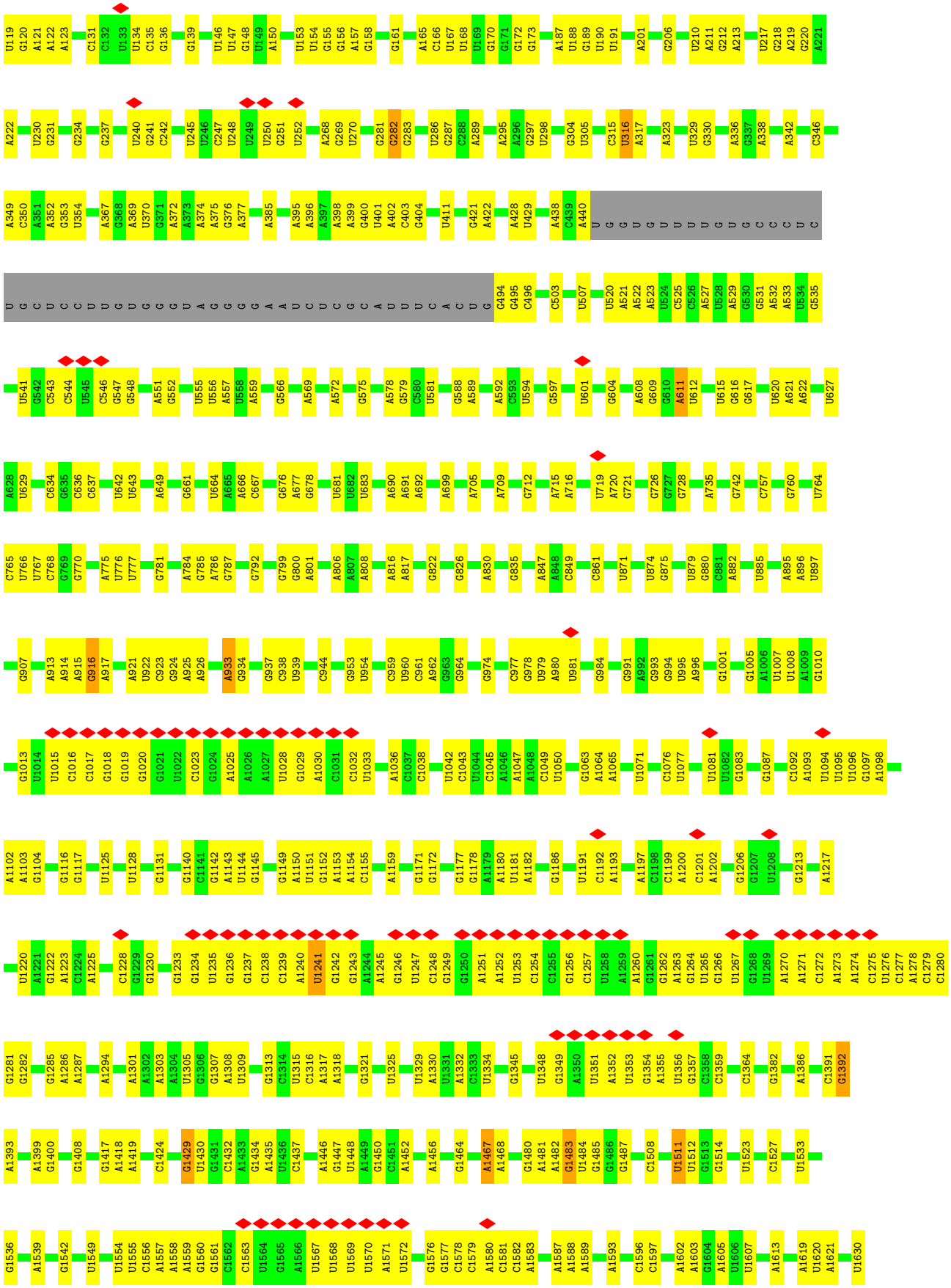


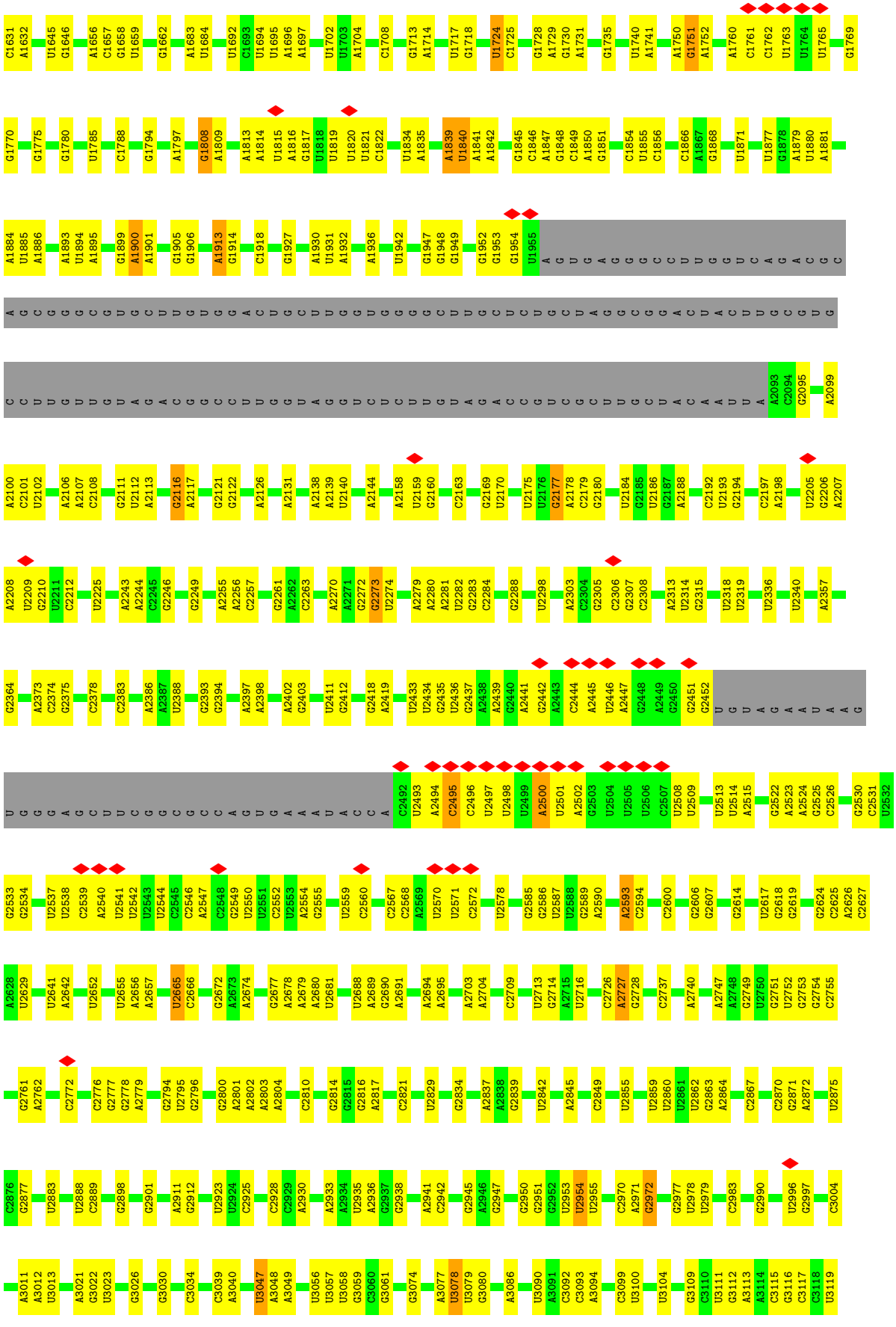


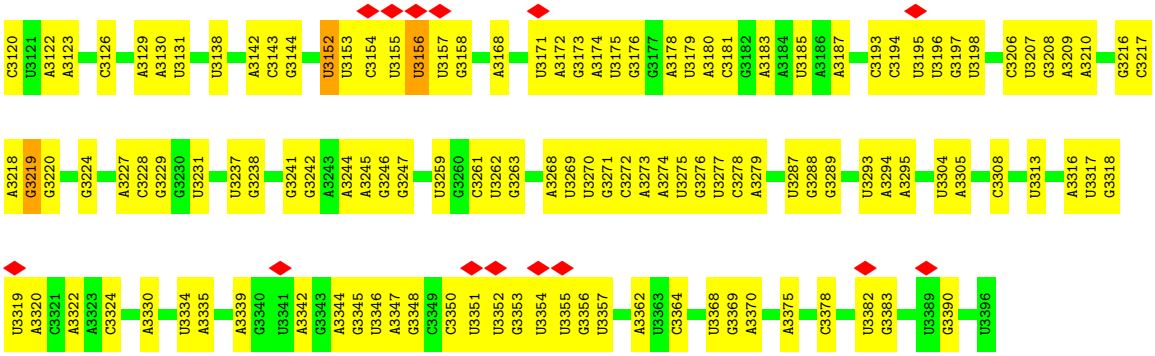
• Molecule 83: 25S ribosomal RNA

Chain BQ:







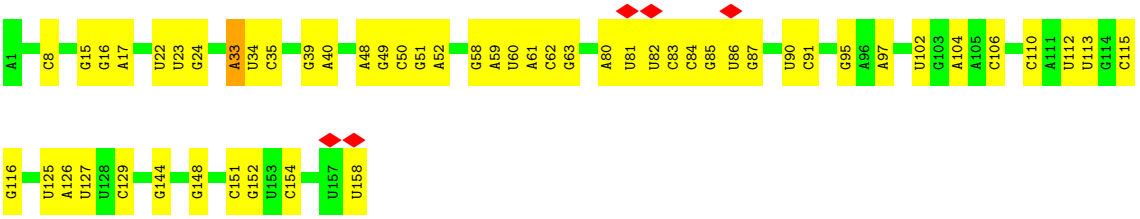


• Molecule 84: 5S ribosomal RNA

Chain BR:

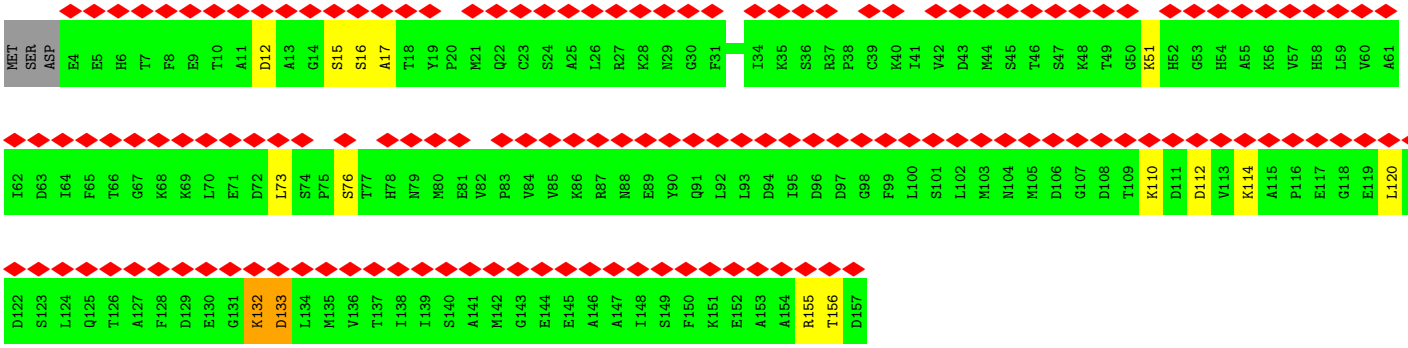
• Molecule 85: 5.8S ribosomal RNA

Chain BS:



• Molecule 86: Eukaryotic translation initiation factor 5A-1

Chain BT:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31503	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 ($e^-/Å^2$)	2.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.075	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	520.32, 520.32, 520.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5CT

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	2	0.33	2/42103 (0.0%)	0.73	20/65603 (0.0%)
2	A	0.37	0/1759	0.62	0/2368
3	B	0.39	0/1629	0.67	0/2202
4	C	0.39	0/833	0.59	0/1126
5	D	0.40	0/885	0.61	0/1202
6	E	0.40	0/998	0.64	0/1341
7	F	0.40	0/1125	0.69	1/1510 (0.1%)
8	G	0.49	2/754 (0.3%)	0.74	1/1005 (0.1%)
9	H	0.41	0/1211	0.75	0/1628
10	I	0.42	0/1130	0.68	0/1517
11	J	0.36	0/865	0.62	0/1169
12	K	0.40	0/571	0.65	0/768
13	L	0.37	0/499	0.69	0/670
14	M	0.38	0/452	0.63	0/600
15	N	0.39	0/404	0.61	0/542
16	O	0.35	0/2489	0.52	0/3389
17	P	0.39	0/1617	0.62	0/2215
18	Q	0.40	0/1735	0.62	0/2335
19	R	0.35	0/1702	0.57	0/2310
20	S	0.39	0/2109	0.61	0/2839
21	T	0.38	0/1823	0.62	0/2439
22	U	0.40	0/1506	0.57	0/2028
23	V	0.46	0/1514	0.78	1/2021 (0.0%)
24	W	0.40	0/1456	0.65	0/1949
25	X	0.42	2/1239 (0.2%)	0.56	0/1673
26	Y	0.39	0/1215	0.66	0/1638
27	Z	0.41	0/901	0.71	0/1217
28	a	0.38	0/693	0.64	0/935
29	b	0.35	0/1038	0.65	1/1395 (0.1%)
30	c	0.36	0/1139	0.61	0/1518
31	d	0.41	0/1074	0.70	2/1431 (0.1%)
32	e	0.61	0/782	0.80	0/1047

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	f	0.37	0/620	0.57	0/838
34	g	0.39	0/481	0.60	0/640
35	l	0.47	1/764 (0.1%)	0.79	0/1179
36	m	0.26	0/1799	0.72	1/2801 (0.0%)
37	n	0.36	1/1835 (0.1%)	0.71	0/2858
38	h	0.40	2/8985 (0.0%)	0.56	1/12155 (0.0%)
39	i	0.38	0/10027	0.54	0/13707
40	j	0.37	0/3001	0.52	0/4083
40	k	0.37	0/2988	0.54	0/4060
41	AA	0.42	0/1836	0.63	0/2481
42	AB	0.39	0/1018	0.66	0/1369
43	AC	0.43	0/778	0.73	0/1034
44	AD	0.41	0/1539	0.66	0/2073
45	AE	0.42	0/712	0.66	1/958 (0.1%)
46	AF	0.45	0/696	0.74	0/923
47	AG	0.43	0/1374	0.71	0/1842
48	AH	0.38	0/979	0.64	0/1321
49	AI	0.40	0/618	0.61	0/826
50	AJ	0.45	0/1568	0.74	0/2106
51	AK	0.39	0/1004	0.67	0/1341
52	AL	0.44	0/443	0.74	0/588
53	AM	0.40	0/1068	0.70	0/1438
54	AN	0.41	0/1118	0.65	0/1497
55	AO	0.42	0/423	0.69	0/562
56	AP	0.41	0/860	0.66	0/1136
57	AQ	0.44	0/1757	0.77	1/2354 (0.0%)
58	AR	0.42	0/1204	0.73	1/1612 (0.1%)
59	AS	0.50	0/234	0.86	0/300
60	AT	0.39	0/701	0.72	0/934
61	AU	0.41	0/1585	0.66	0/2128
62	AV	0.39	0/473	0.66	0/629
63	AW	0.39	0/1948	0.75	0/2617
64	AX	0.42	0/1443	0.73	0/1944
65	AY	0.41	0/750	0.63	0/1008
67	BA	0.41	0/3146	0.69	0/4228
68	BB	0.40	0/1465	0.73	0/1965
69	BC	0.39	0/890	0.67	0/1196
70	BD	0.43	0/1807	0.71	0/2425
71	BE	0.41	0/2800	0.68	0/3790
72	BF	0.43	0/1538	0.71	0/2050
73	BG	0.39	0/1041	0.64	0/1394
74	BH	0.41	0/1481	0.67	0/1990
75	BI	0.42	0/2425	0.66	0/3271

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	BJ	0.40	0/1300	0.68	0/1743
77	BK	0.41	0/868	0.69	0/1168
78	BL	0.44	0/812	0.60	0/1099
79	BM	0.40	0/1260	0.65	0/1694
80	BN	0.41	0/890	0.71	0/1189
81	BO	0.42	0/1821	0.67	0/2451
82	BP	0.39	0/978	0.69	0/1301
83	BQ	0.34	4/75774 (0.0%)	0.75	37/118137 (0.0%)
84	BR	0.31	0/2883	0.73	1/4491 (0.0%)
85	BS	0.32	0/3745	0.73	1/5829 (0.0%)
86	BT	0.32	0/1142	0.61	0/1537
All	All	0.37	14/243945 (0.0%)	0.70	70/355920 (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
9	H	0	1
10	I	0	2
21	T	0	2
22	U	0	1
23	V	0	3
32	e	0	2
57	AQ	0	1
58	AR	0	2
63	AW	0	1
69	BC	0	1
70	BD	0	1
86	BT	0	1
All	All	0	18

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	52	U	O3'-P	23.25	1.89	1.61
83	BQ	683	U	N1-C2	10.32	1.47	1.38
37	n	1	G	OP3-P	-10.19	1.49	1.61
35	l	34	U	OP3-P	-10.13	1.49	1.61
83	BQ	683	U	C4-C5	8.78	1.51	1.43
38	h	832	GLU	CD-OE2	7.78	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	BQ	683	U	N1-C6	7.31	1.44	1.38
1	2	1589	C	N1-C6	7.31	1.41	1.37
83	BQ	683	U	N3-C4	7.13	1.44	1.38
38	h	832	GLU	CD-OE1	6.90	1.33	1.25
8	G	36	ASP	CG-OD1	6.01	1.39	1.25
25	X	101	GLU	CD-OE2	5.35	1.31	1.25
25	X	101	GLU	CD-OE1	5.06	1.31	1.25
8	G	36	ASP	CG-OD2	5.01	1.36	1.25

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	52	U	P-O3'-C3'	-14.01	102.89	119.70
1	2	52	U	C5'-C4'-O4'	-13.02	93.47	109.10
83	BQ	2972	G	N9-C1'-C2'	-11.36	99.23	114.00
1	2	428	A	N9-C1'-C2'	-10.27	100.66	114.00
83	BQ	933	A	C2'-C3'-O3'	9.73	130.90	109.50
83	BQ	1808	G	C2'-C3'-O3'	9.26	129.86	109.50
83	BQ	282	G	C2'-C3'-O3'	8.92	129.12	109.50
1	2	157	A	N9-C1'-C2'	-8.65	102.48	112.00
83	BQ	2970	C	N1-C1'-C2'	-8.24	102.93	112.00
7	F	40	GLU	C-N-CD	-8.22	102.51	120.60
83	BQ	1429	G	C2'-C3'-O3'	8.03	127.17	109.50
83	BQ	1511	U	C2'-C3'-O3'	8.01	127.11	109.50
83	BQ	2116	G	C2'-C3'-O3'	7.71	126.45	109.50
83	BQ	316	U	C2'-C3'-O3'	7.15	125.23	109.50
83	BQ	2972	G	C4'-C3'-O3'	7.03	127.05	113.00
1	2	428	A	C4'-C3'-O3'	6.91	126.83	113.00
83	BQ	1913	A	C2'-C3'-O3'	6.88	124.71	113.70
83	BQ	1241	U	C4'-C3'-O3'	6.64	126.29	113.00
1	2	1185	U	C2'-C3'-O3'	6.45	124.02	113.70
83	BQ	2177	G	C2'-C3'-O3'	6.44	124.00	113.70
1	2	384	G	C4'-C3'-O3'	6.42	125.84	113.00
1	2	427	C	N1-C1'-C2'	-6.39	104.97	112.00
83	BQ	3047	U	O4'-C1'-N1	6.21	113.17	108.20
83	BQ	1467	A	C2'-C3'-O3'	6.06	123.39	113.70
1	2	1274	C	C2'-C3'-O3'	6.04	123.36	113.70
1	2	1430	U	C2'-C3'-O3'	6.00	123.30	113.70
83	BQ	1483	G	C2'-C3'-O3'	5.97	123.26	113.70
83	BQ	1840	U	N1-C1'-C2'	5.96	121.75	114.00
58	AR	4	ARG	N-CA-C	5.94	127.03	111.00
1	2	412	A	N9-C1'-C2'	-5.90	105.51	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	132	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	2	1742	U	C2'-C3'-O3'	5.84	123.05	113.70
29	b	28	ARG	C-N-CD	-5.83	107.77	120.60
83	BQ	611	A	C2'-C3'-O3'	5.74	122.89	113.70
1	2	49	C	C1'-C2'-O2'	-5.70	93.49	110.60
83	BQ	2593	A	C2'-C3'-O3'	5.68	122.80	113.70
23	V	200	LYS	N-CA-C	5.67	126.30	111.00
1	2	1251	U	C2'-C3'-O3'	5.63	122.71	113.70
83	BQ	2495	C	C2'-C3'-O3'	5.63	122.71	113.70
83	BQ	1839	A	C2'-C3'-O3'	5.62	122.69	113.70
83	BQ	683	U	N3-C4-C5	5.58	117.95	114.60
83	BQ	1751	G	C2'-C3'-O3'	5.57	122.61	113.70
83	BQ	916	G	C4'-C3'-O3'	5.53	124.06	113.00
83	BQ	2273	G	C2'-C3'-O3'	5.51	122.52	113.70
83	BQ	2954	U	C4'-C3'-O3'	-5.42	98.01	109.40
83	BQ	2727	A	C2'-C3'-O3'	5.41	122.36	113.70
83	BQ	3156	U	C2'-C3'-O3'	5.39	122.33	113.70
1	2	381	C	N1-C1'-C2'	5.37	120.99	114.00
83	BQ	1392	G	C2'-C3'-O3'	5.37	122.29	113.70
83	BQ	3078	U	C2'-C3'-O3'	5.35	122.26	113.70
83	BQ	3219	G	C2'-C3'-O3'	5.33	122.22	113.70
83	BQ	1724	U	C4'-C3'-O3'	5.30	123.60	113.00
45	AE	80	ARG	C-N-CA	5.27	144.12	122.00
83	BQ	2500	A	C2'-C3'-O3'	5.22	122.05	113.70
83	BQ	1900	A	C2'-C3'-O3'	5.21	122.04	113.70
83	BQ	3152	U	N1-C1'-C2'	5.21	120.77	114.00
1	2	1382	A	C2'-C3'-O3'	5.21	122.03	113.70
85	BS	33	A	C4'-C3'-O3'	5.20	123.40	113.00
1	2	322	G	C2'-C3'-O3'	5.20	122.02	113.70
8	G	36	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	2	141	U	C4'-C3'-O3'	5.16	123.32	113.00
38	h	899	LEU	CA-CB-CG	5.16	127.16	115.30
1	2	1244	A	C2'-C3'-O3'	5.14	121.93	113.70
83	BQ	2972	G	C1'-C2'-O2'	-5.13	95.22	110.60
1	2	539	G	C2'-C3'-O3'	5.09	121.85	113.70
83	BQ	2665	U	C4'-C3'-O3'	5.09	123.17	113.00
84	BR	77	G	C2'-C3'-O3'	5.07	121.81	113.70
36	m	54	U	C4'-C3'-O3'	5.05	123.11	113.00
31	d	132	ARG	NE-CZ-NH1	5.02	122.81	120.30
57	AQ	63	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
57	AQ	202	TYR	Peptide
58	AR	3	SER	Peptide
58	AR	5	PHE	Peptide
63	AW	250	GLN	Peptide
69	BC	12	TYR	Peptide
70	BD	171	GLY	Peptide
86	BT	76	SER	Peptide
9	H	143	ARG	Peptide
10	I	88	VAL	Peptide
10	I	89	ARG	Peptide
21	T	196	ARG	Peptide
21	T	197	ASN	Peptide
22	U	64	VAL	Peptide
23	V	33	PRO	Peptide
23	V	82	VAL	Peptide
23	V	84	HIS	Peptide
32	e	5	ARG	Peptide
32	e	6	ALA	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	221/240 (92%)	194 (88%)	24 (11%)	3 (1%)	11 46
3	B	204/225 (91%)	172 (84%)	24 (12%)	8 (4%)	3 28
4	C	94/105 (90%)	72 (77%)	16 (17%)	6 (6%)	1 20
5	D	119/143 (83%)	92 (77%)	17 (14%)	10 (8%)	1 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	E	122/142 (86%)	101 (83%)	18 (15%)	3 (2%)	5 36
7	F	139/143 (97%)	119 (86%)	15 (11%)	5 (4%)	3 30
8	G	87/136 (64%)	73 (84%)	11 (13%)	3 (3%)	3 31
9	H	143/146 (98%)	123 (86%)	17 (12%)	3 (2%)	7 40
10	I	141/144 (98%)	112 (79%)	21 (15%)	8 (6%)	1 21
11	J	105/121 (87%)	94 (90%)	10 (10%)	1 (1%)	15 52
12	K	68/108 (63%)	54 (79%)	9 (13%)	5 (7%)	1 16
13	L	61/67 (91%)	57 (93%)	4 (7%)	0	100 100
14	M	51/56 (91%)	41 (80%)	10 (20%)	0	100 100
15	N	49/152 (32%)	40 (82%)	6 (12%)	3 (6%)	1 20
16	O	316/319 (99%)	274 (87%)	37 (12%)	5 (2%)	9 44
17	P	204/252 (81%)	176 (86%)	20 (10%)	8 (4%)	3 28
18	Q	212/255 (83%)	170 (80%)	31 (15%)	11 (5%)	2 23
19	R	218/254 (86%)	184 (84%)	30 (14%)	4 (2%)	8 42
20	S	258/261 (99%)	213 (83%)	36 (14%)	9 (4%)	3 31
21	T	224/236 (95%)	188 (84%)	29 (13%)	7 (3%)	4 33
22	U	182/190 (96%)	142 (78%)	31 (17%)	9 (5%)	2 24
23	V	184/200 (92%)	128 (70%)	30 (16%)	26 (14%)	0 4
24	W	176/197 (89%)	149 (85%)	21 (12%)	6 (3%)	3 31
25	X	153/156 (98%)	129 (84%)	17 (11%)	7 (5%)	2 24
26	Y	148/151 (98%)	134 (90%)	11 (7%)	3 (2%)	7 41
27	Z	125/137 (91%)	103 (82%)	17 (14%)	5 (4%)	3 28
28	a	85/87 (98%)	67 (79%)	14 (16%)	4 (5%)	2 24
29	b	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	6 37
30	c	142/145 (98%)	120 (84%)	21 (15%)	1 (1%)	22 60
31	d	130/135 (96%)	109 (84%)	14 (11%)	7 (5%)	2 22
32	e	95/119 (80%)	70 (74%)	17 (18%)	8 (8%)	1 13
33	f	79/82 (96%)	61 (77%)	14 (18%)	4 (5%)	2 23
34	g	58/63 (92%)	48 (83%)	8 (14%)	2 (3%)	3 31
38	h	1107/1287 (86%)	965 (87%)	124 (11%)	18 (2%)	9 44
39	i	1355/1432 (95%)	1158 (86%)	172 (13%)	25 (2%)	8 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	j	388/397 (98%)	335 (86%)	46 (12%)	7 (2%)	8	42
40	k	382/397 (96%)	333 (87%)	40 (10%)	9 (2%)	6	37
41	AA	231/256 (90%)	194 (84%)	32 (14%)	5 (2%)	6	39
42	AB	134/137 (98%)	117 (87%)	14 (10%)	3 (2%)	6	39
43	AC	97/100 (97%)	80 (82%)	13 (13%)	4 (4%)	3	27
44	AD	189/191 (99%)	166 (88%)	19 (10%)	4 (2%)	7	40
45	AE	96/155 (62%)	73 (76%)	18 (19%)	5 (5%)	2	23
46	AF	85/88 (97%)	70 (82%)	14 (16%)	1 (1%)	13	50
47	AG	167/174 (96%)	143 (86%)	18 (11%)	6 (4%)	3	30
48	AH	119/142 (84%)	103 (87%)	14 (12%)	2 (2%)	9	43
49	AI	75/78 (96%)	66 (88%)	8 (11%)	1 (1%)	12	48
50	AJ	191/199 (96%)	158 (83%)	27 (14%)	6 (3%)	4	33
51	AK	124/127 (98%)	115 (93%)	9 (7%)	0	100	100
52	AL	48/51 (94%)	42 (88%)	5 (10%)	1 (2%)	7	40
53	AM	134/138 (97%)	119 (89%)	12 (9%)	3 (2%)	6	39
54	AN	133/136 (98%)	118 (89%)	10 (8%)	5 (4%)	3	29
55	AO	50/128 (39%)	45 (90%)	3 (6%)	2 (4%)	3	28
56	AP	103/106 (97%)	86 (84%)	16 (16%)	1 (1%)	15	52
57	AQ	201/204 (98%)	175 (87%)	21 (10%)	5 (2%)	5	36
58	AR	146/149 (98%)	118 (81%)	21 (14%)	7 (5%)	2	24
59	AS	23/25 (92%)	23 (100%)	0	0	100	100
60	AT	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	14	51
61	AU	195/199 (98%)	177 (91%)	15 (8%)	3 (2%)	10	46
62	AV	56/59 (95%)	50 (89%)	5 (9%)	1 (2%)	8	42
63	AW	250/254 (98%)	218 (87%)	31 (12%)	1 (0%)	34	70
64	AX	181/184 (98%)	158 (87%)	19 (10%)	4 (2%)	6	39
65	AY	95/105 (90%)	86 (90%)	8 (8%)	1 (1%)	14	51
67	BA	384/387 (99%)	332 (86%)	41 (11%)	11 (3%)	4	34
68	BB	183/186 (98%)	163 (89%)	17 (9%)	3 (2%)	9	44
69	BC	107/113 (95%)	94 (88%)	11 (10%)	2 (2%)	8	42
70	BD	218/221 (99%)	185 (85%)	24 (11%)	9 (4%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	BE	359/362 (99%)	306 (85%)	38 (11%)	15 (4%)	3	26
72	BF	186/189 (98%)	167 (90%)	16 (9%)	3 (2%)	9	44
73	BG	125/130 (96%)	110 (88%)	13 (10%)	2 (2%)	9	44
74	BH	170/172 (99%)	151 (89%)	16 (9%)	3 (2%)	8	42
75	BI	294/297 (99%)	263 (90%)	22 (8%)	9 (3%)	4	33
76	BJ	157/160 (98%)	133 (85%)	18 (12%)	6 (4%)	3	29
77	BK	104/107 (97%)	93 (89%)	9 (9%)	2 (2%)	8	42
78	BL	98/121 (81%)	79 (81%)	16 (16%)	3 (3%)	4	33
79	BM	152/176 (86%)	137 (90%)	11 (7%)	4 (3%)	5	36
80	BN	110/121 (91%)	104 (94%)	3 (3%)	3 (3%)	5	35
81	BO	220/244 (90%)	199 (90%)	16 (7%)	5 (2%)	6	38
82	BP	117/120 (98%)	106 (91%)	10 (8%)	1 (1%)	17	54
86	BT	151/157 (96%)	127 (84%)	14 (9%)	10 (7%)	1	19
All	All	14299/15550 (92%)	12246 (86%)	1644 (12%)	409 (3%)	7	34

All (409) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	196	ARG
3	B	100	ASN
5	D	115	VAL
5	D	126	TRP
7	F	32	ASN
7	F	40	GLU
7	F	45	ARG
7	F	113	ASP
10	I	69	LYS
17	P	110	TYR
18	Q	132	ASP
18	Q	176	VAL
20	S	12	LEU
20	S	69	HIS
20	S	231	GLN
23	V	11	ARG
23	V	27	PHE
23	V	33	PRO
23	V	35	ASN

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Mol	Chain	Res	Type
23	V	83	TYR
23	V	85	PRO
23	V	192	TYR
23	V	193	LEU
23	V	194	ARG
24	W	98	ALA
24	W	134	ILE
25	X	7	VAL
26	Y	22	ALA
27	Z	91	THR
27	Z	124	ASP
30	c	12	ALA
38	h	126	VAL
38	h	900	LYS
38	h	1203	PHE
39	i	203	TYR
39	i	1032	LYS
40	k	278	THR
40	k	365	LYS
42	AB	29	SER
44	AD	42	ASP
44	AD	50	ASN
45	AE	64	THR
47	AG	8	PRO
50	AJ	47	ALA
50	AJ	166	ALA
53	AM	136	ALA
57	AQ	75	VAL
58	AR	12	ARG
58	AR	78	LEU
62	AV	21	ILE
63	AW	144	ASN
67	BA	5	LYS
67	BA	138	ALA
69	BC	64	VAL
70	BD	135	PHE
70	BD	138	ARG
71	BE	292	SER
75	BI	116	ASP
76	BJ	25	VAL
76	BJ	124	VAL
76	BJ	144	GLU

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Mol	Chain	Res	Type
76	BJ	159	PHE
77	BK	92	LYS
79	BM	171	PRO
81	BO	164	SER
86	BT	110	LYS
86	BT	112	ASP
86	BT	133	ASP
2	A	217	ILE
2	A	218	LEU
3	B	44	ASN
3	B	60	ASP
4	C	60	SER
4	C	64	TYR
5	D	25	GLU
5	D	91	VAL
5	D	106	ILE
7	F	39	VAL
8	G	76	GLU
8	G	77	GLU
8	G	88	VAL
9	H	7	GLU
9	H	51	ASP
10	I	7	ARG
11	J	55	PRO
12	K	71	ILE
15	N	107	LYS
15	N	146	SER
17	P	21	ASN
17	P	39	ASN
17	P	169	SER
18	Q	158	SER
19	R	91	ARG
19	R	145	GLY
19	R	206	THR
20	S	23	LEU
21	T	148	SER
21	T	219	ARG
22	U	74	GLN
22	U	110	GLN
23	V	10	LYS
23	V	24	LYS
23	V	52	ASN

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Mol	Chain	Res	Type
23	V	86	SER
23	V	152	ILE
23	V	191	PHE
24	W	119	ALA
25	X	6	THR
27	Z	42	VAL
29	b	78	ARG
31	d	35	VAL
31	d	51	GLU
31	d	52	LYS
31	d	60	PHE
31	d	127	LYS
32	e	36	ILE
32	e	63	ALA
38	h	649	ILE
38	h	986	ARG
38	h	1052	ILE
39	i	200	ASP
39	i	264	PHE
39	i	624	ASP
40	j	255	ASN
40	j	323	LYS
40	k	266	GLU
41	AA	156	ASP
42	AB	45	ARG
43	AC	99	ARG
45	AE	77	LYS
48	AH	109	LYS
50	AJ	51	LEU
52	AL	3	ALA
57	AQ	55	ALA
58	AR	47	LYS
61	AU	123	ALA
61	AU	187	GLU
64	AX	68	GLY
64	AX	166	VAL
67	BA	38	SER
67	BA	332	ARG
67	BA	348	ARG
67	BA	352	GLU
70	BD	113	GLY
70	BD	194	ALA

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Mol	Chain	Res	Type
71	BE	131	VAL
71	BE	140	HIS
71	BE	293	SER
72	BF	130	ASN
73	BG	50	ILE
74	BH	24	LEU
74	BH	97	VAL
75	BI	276	LYS
82	BP	90	ARG
86	BT	15	SER
86	BT	132	LYS
86	BT	156	THR
3	B	81	ARG
4	C	93	GLN
5	D	87	PRO
9	H	139	LYS
10	I	28	LEU
10	I	67	MET
10	I	128	GLY
17	P	35	PRO
18	Q	177	GLN
18	Q	209	ASN
18	Q	223	PHE
20	S	20	LEU
20	S	205	PHE
22	U	97	ARG
22	U	156	SER
23	V	96	LEU
23	V	98	LYS
23	V	116	HIS
23	V	196	LEU
24	W	120	LYS
24	W	150	LEU
25	X	55	ASP
29	b	30	SER
31	d	4	ALA
32	e	83	ILE
33	f	3	LEU
33	f	10	PRO
38	h	28	LEU
38	h	53	ASP
38	h	769	LEU

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Mol	Chain	Res	Type
39	i	442	GLU
39	i	494	LEU
39	i	506	SER
39	i	621	LYS
39	i	658	ASP
39	i	1254	SER
40	j	365	LYS
40	k	77	ASP
42	AB	112	SER
43	AC	27	SER
47	AG	112	LEU
49	AI	33	LYS
54	AN	59	ALA
54	AN	102	GLU
54	AN	125	GLY
57	AQ	80	THR
58	AR	77	LYS
58	AR	108	GLY
61	AU	5	PRO
64	AX	155	GLU
67	BA	7	GLU
68	BB	23	ASN
70	BD	2	ARG
71	BE	232	SER
71	BE	338	LYS
72	BF	53	LYS
76	BJ	29	THR
77	BK	91	ALA
78	BL	91	ASP
79	BM	20	LYS
79	BM	97	ASN
81	BO	159	GLN
86	BT	16	SER
86	BT	17	ALA
86	BT	114	LYS
3	B	63	GLN
3	B	64	VAL
5	D	93	ASP
10	I	132	LEU
12	K	44	GLN
15	N	118	ARG
17	P	103	THR

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Mol	Chain	Res	Type
18	Q	39	GLU
18	Q	147	ALA
21	T	132	ARG
21	T	197	ASN
23	V	22	ARG
23	V	37	LYS
23	V	81	VAL
23	V	87	ASN
25	X	29	LYS
26	Y	3	ARG
27	Z	75	GLY
28	a	9	VAL
32	e	59	TYR
32	e	62	TYR
33	f	15	GLU
34	g	60	PRO
38	h	125	GLU
38	h	133	ASN
39	i	174	ILE
39	i	212	TRP
39	i	939	ILE
39	i	1175	ASP
40	j	282	GLN
40	k	47	ASP
40	k	284	SER
44	AD	2	LYS
44	AD	41	ILE
46	AF	11	ARG
48	AH	62	VAL
53	AM	29	ALA
55	AO	79	GLU
55	AO	92	ASP
56	AP	17	CYS
57	AQ	150	TRP
67	BA	187	SER
68	BB	162	ALA
70	BD	100	LYS
70	BD	107	ALA
71	BE	14	GLU
71	BE	266	THR
71	BE	270	SER
71	BE	320	ASN

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Mol	Chain	Res	Type
72	BF	81	ARG
75	BI	188	GLU
75	BI	259	LYS
79	BM	98	VAL
3	B	65	ARG
5	D	111	ASN
5	D	119	SER
6	E	28	MET
6	E	53	PRO
6	E	127	ARG
10	I	90	PRO
12	K	38	HIS
12	K	43	ASP
12	K	88	ILE
16	O	120	SER
16	O	162	ALA
16	O	283	LYS
17	P	111	ILE
18	Q	210	ILE
19	R	150	GLN
20	S	195	ILE
21	T	69	LEU
23	V	40	ALA
23	V	51	GLY
25	X	146	ALA
26	Y	21	ASN
27	Z	40	ALA
29	b	120	HIS
31	d	5	VAL
32	e	97	PRO
38	h	767	ARG
39	i	263	PHE
39	i	1177	ARG
40	j	256	SER
40	k	22	VAL
45	AE	43	ARG
47	AG	94	ARG
47	AG	108	GLU
50	AJ	155	GLU
54	AN	70	PRO
54	AN	124	ALA
58	AR	56	VAL

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Mol	Chain	Res	Type
58	AR	79	TRP
64	AX	3	ARG
67	BA	155	ALA
69	BC	83	GLU
70	BD	112	GLN
70	BD	175	LEU
71	BE	5	GLN
71	BE	155	ASP
71	BE	175	HIS
71	BE	317	PRO
73	BG	12	LYS
75	BI	44	TYR
75	BI	137	ASP
75	BI	253	PHE
75	BI	277	LEU
78	BL	11	ILE
80	BN	59	PRO
86	BT	12	ASP
4	C	51	SER
10	I	87	GLY
21	T	149	LYS
22	U	64	VAL
22	U	96	ARG
22	U	98	ILE
23	V	82	VAL
25	X	4	GLU
28	a	12	TYR
28	a	82	VAL
33	f	75	GLU
38	h	114	ILE
38	h	150	GLY
39	i	403	ILE
39	i	570	LYS
39	i	876	LEU
39	i	1067	GLY
39	i	1213	ILE
40	j	52	LYS
40	k	394	ALA
41	AA	25	PRO
41	AA	36	ILE
41	AA	157	VAL
43	AC	3	VAL

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Mol	Chain	Res	Type
45	AE	80	ARG
47	AG	120	ILE
50	AJ	50	PRO
60	AT	51	ALA
76	BJ	148	PRO
80	BN	77	GLY
81	BO	178	ILE
5	D	66	VAL
18	Q	21	VAL
22	U	178	GLY
32	e	16	GLY
34	g	50	VAL
38	h	1029	GLY
39	i	1197	GLY
39	i	1203	ILE
43	AC	9	ILE
47	AG	117	ASP
53	AM	6	ILE
67	BA	245	GLY
78	BL	27	VAL
81	BO	188	ILE
16	O	63	GLY
21	T	165	GLY
32	e	84	VAL
57	AQ	74	PRO
71	BE	78	GLY
75	BI	251	PRO
4	C	88	PRO
4	C	89	GLY
16	O	105	GLY
28	a	77	GLY
38	h	206	PRO
38	h	1232	PRO
40	k	349	GLY
65	AY	87	VAL
74	BH	167	ARG
81	BO	26	VAL
17	P	158	VAL
20	S	204	GLY
22	U	65	PRO
38	h	1221	GLY
41	AA	73	PRO

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Mol	Chain	Res	Type
50	AJ	127	PRO
68	BB	59	ARG
80	BN	12	PRO
3	B	51	VAL
18	Q	48	VAL
20	S	193	GLY
24	W	18	PRO
25	X	41	GLY
39	i	1192	ILE
40	j	277	PRO
45	AE	76	VAL
67	BA	83	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	182/195 (93%)	175 (96%)	7 (4%)	33	61
3	B	173/191 (91%)	162 (94%)	11 (6%)	17	48
4	C	88/98 (90%)	83 (94%)	5 (6%)	20	52
5	D	89/119 (75%)	85 (96%)	4 (4%)	27	57
6	E	101/118 (86%)	94 (93%)	7 (7%)	15	46
7	F	117/119 (98%)	113 (97%)	4 (3%)	37	64
8	G	80/124 (64%)	75 (94%)	5 (6%)	18	49
9	H	128/129 (99%)	117 (91%)	11 (9%)	10	40
10	I	115/116 (99%)	102 (89%)	13 (11%)	6	28
11	J	100/114 (88%)	94 (94%)	6 (6%)	19	50
12	K	61/89 (68%)	58 (95%)	3 (5%)	25	55
13	L	56/60 (93%)	54 (96%)	2 (4%)	35	63
14	M	47/49 (96%)	44 (94%)	3 (6%)	17	48
15	N	43/135 (32%)	42 (98%)	1 (2%)	50	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	O	259/262 (99%)	250 (96%)	9 (4%)	36	64
17	P	164/210 (78%)	157 (96%)	7 (4%)	29	58
18	Q	191/224 (85%)	182 (95%)	9 (5%)	26	56
19	R	180/205 (88%)	175 (97%)	5 (3%)	43	68
20	S	221/222 (100%)	217 (98%)	4 (2%)	59	77
21	T	188/201 (94%)	181 (96%)	7 (4%)	34	62
22	U	165/170 (97%)	160 (97%)	5 (3%)	41	66
23	V	150/161 (93%)	133 (89%)	17 (11%)	6	28
24	W	152/166 (92%)	150 (99%)	2 (1%)	69	82
25	X	129/137 (94%)	126 (98%)	3 (2%)	50	72
26	Y	127/128 (99%)	121 (95%)	6 (5%)	26	56
27	Z	81/105 (77%)	74 (91%)	7 (9%)	10	40
28	a	74/74 (100%)	72 (97%)	2 (3%)	44	69
29	b	110/111 (99%)	109 (99%)	1 (1%)	78	88
30	c	119/120 (99%)	115 (97%)	4 (3%)	37	64
31	d	111/113 (98%)	103 (93%)	8 (7%)	14	45
32	e	83/101 (82%)	77 (93%)	6 (7%)	14	45
33	f	70/71 (99%)	69 (99%)	1 (1%)	67	81
34	g	50/54 (93%)	50 (100%)	0	100	100
38	h	936/1139 (82%)	901 (96%)	35 (4%)	34	62
39	i	849/1279 (66%)	823 (97%)	26 (3%)	40	65
40	j	296/347 (85%)	288 (97%)	8 (3%)	44	69
40	k	295/347 (85%)	290 (98%)	5 (2%)	60	78
41	AA	187/208 (90%)	179 (96%)	8 (4%)	29	58
42	AB	104/105 (99%)	98 (94%)	6 (6%)	20	51
43	AC	81/82 (99%)	76 (94%)	5 (6%)	18	49
44	AD	171/171 (100%)	165 (96%)	6 (4%)	36	64
45	AE	57/129 (44%)	57 (100%)	0	100	100
46	AF	70/71 (99%)	65 (93%)	5 (7%)	14	45
47	AG	147/150 (98%)	140 (95%)	7 (5%)	25	56
48	AH	104/118 (88%)	98 (94%)	6 (6%)	20	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	AI	68/69 (99%)	67 (98%)	1 (2%)	65	81
50	AJ	154/159 (97%)	146 (95%)	8 (5%)	23	54
51	AK	109/110 (99%)	105 (96%)	4 (4%)	34	62
52	AL	45/46 (98%)	42 (93%)	3 (7%)	16	47
53	AM	107/109 (98%)	101 (94%)	6 (6%)	21	52
54	AN	115/116 (99%)	112 (97%)	3 (3%)	46	69
55	AO	47/116 (40%)	44 (94%)	3 (6%)	17	48
56	AP	90/91 (99%)	85 (94%)	5 (6%)	21	52
57	AQ	175/176 (99%)	168 (96%)	7 (4%)	31	59
58	AR	118/119 (99%)	111 (94%)	7 (6%)	19	51
59	AS	23/23 (100%)	21 (91%)	2 (9%)	10	38
60	AT	71/72 (99%)	69 (97%)	2 (3%)	43	68
61	AU	160/162 (99%)	155 (97%)	5 (3%)	40	65
62	AV	46/47 (98%)	45 (98%)	1 (2%)	52	72
63	AW	193/196 (98%)	187 (97%)	6 (3%)	40	65
64	AX	140/146 (96%)	133 (95%)	7 (5%)	24	55
65	AY	81/88 (92%)	78 (96%)	3 (4%)	34	62
67	BA	320/323 (99%)	304 (95%)	16 (5%)	24	55
68	BB	150/151 (99%)	144 (96%)	6 (4%)	31	59
69	BC	92/97 (95%)	84 (91%)	8 (9%)	10	38
70	BD	184/187 (98%)	169 (92%)	15 (8%)	11	40
71	BE	288/289 (100%)	277 (96%)	11 (4%)	33	61
72	BF	153/154 (99%)	148 (97%)	5 (3%)	38	65
73	BG	109/111 (98%)	106 (97%)	3 (3%)	43	68
74	BH	156/156 (100%)	150 (96%)	6 (4%)	33	61
75	BI	244/245 (100%)	235 (96%)	9 (4%)	34	62
76	BJ	136/137 (99%)	129 (95%)	7 (5%)	24	54
77	BK	90/91 (99%)	87 (97%)	3 (3%)	38	65
78	BL	87/107 (81%)	86 (99%)	1 (1%)	73	85
79	BM	134/153 (88%)	127 (95%)	7 (5%)	23	54
80	BN	95/103 (92%)	94 (99%)	1 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
81	BO	186/205 (91%)	181 (97%)	5 (3%)	44 69
82	BP	104/105 (99%)	101 (97%)	3 (3%)	42 67
86	BT	118/132 (89%)	113 (96%)	5 (4%)	30 58
All	All	11689/13228 (88%)	11203 (96%)	486 (4%)	33 58

All (486) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	7	LYS
2	A	9	ARG
2	A	27	ARG
2	A	51	ARG
2	A	58	VAL
2	A	143	ARG
2	A	204	ASP
3	B	27	THR
3	B	99	MET
3	B	102	ARG
3	B	106	LYS
3	B	124	LEU
3	B	134	VAL
3	B	138	THR
3	B	143	ARG
3	B	158	GLN
3	B	167	ARG
3	B	168	VAL
4	C	31	LYS
4	C	55	VAL
4	C	63	TYR
4	C	78	GLU
4	C	82	LEU
5	D	34	THR
5	D	49	THR
5	D	54	ARG
5	D	74	LEU
6	E	42	ARG
6	E	44	ARG
6	E	61	ARG
6	E	80	MET
6	E	124	THR
6	E	126	VAL

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Mol	Chain	Res	Type
6	E	130	ARG
7	F	66	ARG
7	F	68	ARG
7	F	114	ARG
7	F	132	LYS
8	G	13	SER
8	G	26	LEU
8	G	36	ASP
8	G	47	ARG
8	G	80	ARG
9	H	17	LEU
9	H	38	VAL
9	H	91	ASP
9	H	98	TYR
9	H	100	THR
9	H	101	LEU
9	H	120	ARG
9	H	123	ARG
9	H	133	VAL
9	H	137	HIS
9	H	145	ARG
10	I	7	ARG
10	I	13	ASP
10	I	23	GLN
10	I	25	GLN
10	I	28	LEU
10	I	35	ASP
10	I	44	GLU
10	I	66	TYR
10	I	68	ARG
10	I	70	GLN
10	I	85	SER
10	I	91	TYR
10	I	123	ARG
11	J	20	ILE
11	J	47	GLN
11	J	52	LYS
11	J	92	ASP
11	J	99	ILE
11	J	118	VAL
12	K	64	VAL
12	K	95	HIS

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Mol	Chain	Res	Type
12	K	100	ILE
13	L	32	PHE
13	L	50	GLU
14	M	19	ARG
14	M	28	THR
14	M	39	CYS
15	N	103	LEU
16	O	58	VAL
16	O	59	ARG
16	O	114	ASP
16	O	185	GLN
16	O	202	LEU
16	O	228	LYS
16	O	250	TYR
16	O	274	LEU
16	O	308	ASN
17	P	8	ASP
17	P	103	THR
17	P	113	ARG
17	P	129	ASP
17	P	135	GLU
17	P	148	ASP
17	P	198	MET
18	Q	21	VAL
18	Q	29	TRP
18	Q	59	ASP
18	Q	70	LEU
18	Q	95	ASN
18	Q	118	GLN
18	Q	135	LEU
18	Q	181	LEU
18	Q	212	VAL
19	R	58	LEU
19	R	111	VAL
19	R	206	THR
19	R	225	LEU
19	R	243	TYR
20	S	26	CYS
20	S	88	ASP
20	S	164	LEU
20	S	261	LEU
21	T	24	ILE

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Mol	Chain	Res	Type
21	T	75	LEU
21	T	78	THR
21	T	89	ASP
21	T	98	ARG
21	T	190	GLN
21	T	208	TYR
22	U	5	GLN
22	U	9	LEU
22	U	27	LEU
22	U	31	SER
22	U	48	GLU
23	V	22	ARG
23	V	27	PHE
23	V	29	LEU
23	V	38	ILE
23	V	58	LEU
23	V	59	ARG
23	V	67	TRP
23	V	81	VAL
23	V	82	VAL
23	V	90	LEU
23	V	92	ARG
23	V	96	LEU
23	V	107	THR
23	V	160	PHE
23	V	196	LEU
23	V	197	THR
23	V	199	LYS
24	W	118	LEU
24	W	134	ILE
25	X	7	VAL
25	X	40	LEU
25	X	98	ASN
26	Y	36	GLN
26	Y	56	ASP
26	Y	86	GLU
26	Y	92	ILE
26	Y	102	LEU
26	Y	149	LEU
27	Z	38	THR
27	Z	52	ARG
27	Z	81	VAL

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Mol	Chain	Res	Type
27	Z	90	ARG
27	Z	124	ASP
27	Z	136	ARG
27	Z	137	LEU
28	a	12	TYR
28	a	80	LYS
29	b	37	PHE
30	c	17	VAL
30	c	18	HIS
30	c	107	PHE
30	c	121	ARG
31	d	17	LEU
31	d	63	GLN
31	d	125	LEU
31	d	127	LYS
31	d	129	VAL
31	d	131	ARG
31	d	132	ARG
31	d	133	ASN
32	e	3	LYS
32	e	10	ARG
32	e	11	ASN
32	e	12	LYS
32	e	21	VAL
32	e	92	ARG
33	f	9	HIS
38	h	54	ARG
38	h	69	MET
38	h	186	LEU
38	h	434	LEU
38	h	464	MET
38	h	669	THR
38	h	700	LEU
38	h	710	LEU
38	h	731	LEU
38	h	742	ARG
38	h	745	ASP
38	h	750	ARG
38	h	769	LEU
38	h	770	ASP
38	h	772	THR
38	h	788	THR

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Mol	Chain	Res	Type
38	h	798	THR
38	h	801	GLN
38	h	824	GLU
38	h	847	LYS
38	h	856	ILE
38	h	865	ASP
38	h	892	SER
38	h	899	LEU
38	h	900	LYS
38	h	908	ARG
38	h	1000	VAL
38	h	1036	LEU
38	h	1089	LEU
38	h	1106	ASP
38	h	1112	LEU
38	h	1126	GLU
38	h	1186	LEU
38	h	1229	GLU
38	h	1244	TRP
39	i	173	LEU
39	i	174	ILE
39	i	184	GLU
39	i	191	GLN
39	i	194	LEU
39	i	237	ARG
39	i	247	TYR
39	i	248	ARG
39	i	289	PHE
39	i	293	ASP
39	i	476	ASP
39	i	505	PHE
39	i	511	LYS
39	i	519	ILE
39	i	534	VAL
39	i	558	MET
39	i	637	TYR
39	i	644	HIS
39	i	646	ARG
39	i	687	ARG
39	i	718	GLU
39	i	907	LEU
39	i	1189	PHE

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Mol	Chain	Res	Type
39	i	1272	ASP
39	i	1323	LEU
39	i	1341	TYR
40	j	18	ASP
40	j	61	HIS
40	j	99	THR
40	j	173	LEU
40	j	226	GLN
40	j	347	GLU
40	j	350	ASP
40	j	383	CYS
40	k	83	LEU
40	k	127	LEU
40	k	176	GLN
40	k	259	CYS
40	k	358	PHE
41	AA	71	VAL
41	AA	84	ARG
41	AA	112	GLU
41	AA	126	SER
41	AA	190	VAL
41	AA	197	VAL
41	AA	202	GLU
41	AA	221	ASN
42	AB	56	ASP
42	AB	57	MET
42	AB	61	THR
42	AB	68	GLU
42	AB	91	VAL
42	AB	104	ASN
43	AC	16	LYS
43	AC	20	MET
43	AC	46	GLU
43	AC	71	LYS
43	AC	88	GLU
44	AD	43	VAL
44	AD	68	LEU
44	AD	71	VAL
44	AD	72	LYS
44	AD	92	TYR
44	AD	177	ASP
46	AF	5	THR

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Mol	Chain	Res	Type
46	AF	13	ASN
46	AF	17	THR
46	AF	19	CYS
46	AF	37	CYS
47	AG	28	ASP
47	AG	59	ILE
47	AG	107	ASP
47	AG	112	LEU
47	AG	132	ASN
47	AG	165	GLN
47	AG	170	ASP
48	AH	31	THR
48	AH	39	LYS
48	AH	58	ASP
48	AH	61	LYS
48	AH	78	ASP
48	AH	108	LEU
49	AI	31	LEU
50	AJ	24	VAL
50	AJ	31	LYS
50	AJ	45	LYS
50	AJ	54	LEU
50	AJ	59	ARG
50	AJ	134	GLU
50	AJ	136	GLU
50	AJ	168	ARG
51	AK	28	ARG
51	AK	74	TYR
51	AK	108	LYS
51	AK	111	LEU
52	AL	6	SER
52	AL	28	ARG
52	AL	37	TYR
53	AM	4	ASP
53	AM	28	SER
53	AM	38	ILE
53	AM	44	VAL
53	AM	50	LYS
53	AM	128	ARG
54	AN	26	VAL
54	AN	33	SER
54	AN	134	LEU

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Mol	Chain	Res	Type
55	AO	108	THR
55	AO	115	CYS
55	AO	127	LEU
56	AP	2	VAL
56	AP	29	LYS
56	AP	44	ASP
56	AP	61	LYS
56	AP	83	LEU
57	AQ	9	GLU
57	AQ	65	ARG
57	AQ	67	ARG
57	AQ	68	ARG
57	AQ	80	THR
57	AQ	117	ASN
57	AQ	183	THR
58	AR	4	ARG
58	AR	56	VAL
58	AR	60	TYR
58	AR	76	ASP
58	AR	78	LEU
58	AR	130	VAL
58	AR	136	GLU
59	AS	10	THR
59	AS	13	LEU
60	AT	20	SER
60	AT	91	GLU
61	AU	34	VAL
61	AU	56	ASP
61	AU	64	PHE
61	AU	85	ARG
61	AU	113	ASP
62	AV	21	ILE
63	AW	109	GLU
63	AW	161	ASP
63	AW	179	LEU
63	AW	180	LEU
63	AW	190	ARG
63	AW	242	ARG
64	AX	31	GLU
64	AX	82	ARG
64	AX	94	LEU
64	AX	113	TYR

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Mol	Chain	Res	Type
64	AX	118	GLN
64	AX	128	ARG
64	AX	168	LEU
65	AY	24	THR
65	AY	48	THR
65	AY	104	LEU
67	BA	55	THR
67	BA	79	VAL
67	BA	80	ASP
67	BA	85	VAL
67	BA	102	LEU
67	BA	123	TYR
67	BA	139	GLN
67	BA	146	ARG
67	BA	161	LEU
67	BA	178	LEU
67	BA	183	LEU
67	BA	211	GLN
67	BA	221	THR
67	BA	238	LEU
67	BA	296	THR
67	BA	320	ASP
68	BB	49	LEU
68	BB	69	ARG
68	BB	113	LYS
68	BB	138	LEU
68	BB	168	THR
68	BB	174	ARG
69	BC	31	ARG
69	BC	64	VAL
69	BC	68	GLU
69	BC	79	ARG
69	BC	82	GLU
69	BC	106	THR
69	BC	107	VAL
69	BC	110	GLU
70	BD	34	ASP
70	BD	43	ASP
70	BD	51	LEU
70	BD	70	CYS
70	BD	90	VAL
70	BD	101	MET

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Mol	Chain	Res	Type
70	BD	137	VAL
70	BD	138	ARG
70	BD	143	ASN
70	BD	155	ARG
70	BD	161	GLN
70	BD	162	GLN
70	BD	175	LEU
70	BD	199	LEU
70	BD	216	PHE
71	BE	98	ARG
71	BE	108	LYS
71	BE	150	LEU
71	BE	156	LEU
71	BE	194	TYR
71	BE	203	ARG
71	BE	206	LEU
71	BE	247	PHE
71	BE	326	ARG
71	BE	349	THR
71	BE	362	ASP
72	BF	10	LEU
72	BF	22	VAL
72	BF	160	GLU
72	BF	167	ARG
72	BF	181	ARG
73	BG	8	LYS
73	BG	19	ARG
73	BG	106	VAL
74	BH	61	ILE
74	BH	71	LYS
74	BH	106	LEU
74	BH	109	ASP
74	BH	119	ARG
74	BH	172	TYR
75	BI	23	ARG
75	BI	58	LYS
75	BI	111	GLN
75	BI	117	GLU
75	BI	140	ARG
75	BI	146	LEU
75	BI	152	ARG
75	BI	198	TYR

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Mol	Chain	Res	Type
75	BI	259	LYS
76	BJ	27	LEU
76	BJ	72	VAL
76	BJ	85	LEU
76	BJ	101	CYS
76	BJ	122	GLN
76	BJ	126	VAL
76	BJ	128	LEU
77	BK	5	HIS
77	BK	31	LYS
77	BK	87	ASN
78	BL	75	TYR
79	BM	15	VAL
79	BM	64	LEU
79	BM	77	ARG
79	BM	91	VAL
79	BM	145	LEU
79	BM	169	ASP
79	BM	171	PRO
80	BN	98	GLN
81	BO	24	GLU
81	BO	46	GLU
81	BO	92	ILE
81	BO	124	LEU
81	BO	179	LEU
82	BP	27	GLU
82	BP	30	GLU
82	BP	53	CYS
86	BT	73	LEU
86	BT	120	LEU
86	BT	132	LYS
86	BT	133	ASP
86	BT	155	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	74	GLN
2	A	101	GLN
3	B	104	ASN
3	B	139	ASN
7	F	83	GLN

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Mol	Chain	Res	Type
8	G	42	GLN
9	H	44	ASN
9	H	90	ASN
9	H	122	HIS
10	I	25	GLN
11	J	17	GLN
14	M	53	ASN
15	N	123	ASN
16	O	185	GLN
16	O	198	ASN
18	Q	49	ASN
18	Q	74	GLN
18	Q	99	ASN
18	Q	146	GLN
18	Q	183	GLN
18	Q	211	HIS
19	R	89	GLN
20	S	96	ASN
20	S	98	ASN
21	T	176	GLN
22	U	29	ASN
23	V	88	ASN
23	V	119	GLN
26	Y	36	GLN
29	b	15	ASN
31	d	63	GLN
34	g	51	ASN
38	h	680	GLN
38	h	1261	ASN
39	i	69	HIS
39	i	172	ASN
39	i	191	GLN
39	i	507	ASN
39	i	701	ASN
39	i	773	GLN
39	i	853	GLN
39	i	982	GLN
39	i	1066	GLN
39	i	1228	ASN
39	i	1250	GLN
40	j	187	GLN
40	k	176	GLN

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Mol	Chain	Res	Type
41	AA	240	ASN
44	AD	37	ASN
44	AD	157	ASN
47	AG	132	ASN
50	AJ	37	ASN
52	AL	32	ASN
52	AL	33	ASN
52	AL	50	ASN
53	AM	56	GLN
53	AM	62	GLN
56	AP	27	GLN
58	AR	44	ASN
58	AR	65	GLN
61	AU	14	HIS
61	AU	26	GLN
63	AW	19	HIS
63	AW	47	GLN
63	AW	194	ASN
63	AW	209	HIS
63	AW	211	HIS
63	AW	217	GLN
64	AX	97	ASN
65	AY	11	ASN
65	AY	47	ASN
65	AY	71	GLN
70	BD	161	GLN
70	BD	207	ASN
71	BE	48	GLN
71	BE	59	GLN
71	BE	114	ASN
71	BE	116	ASN
71	BE	260	GLN
72	BF	144	GLN
72	BF	166	ASN
75	BI	63	GLN
76	BJ	98	HIS
76	BJ	122	GLN
77	BK	87	ASN
79	BM	167	ASN
81	BO	157	ASN
82	BP	16	GLN
82	BP	20	GLN

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Mol	Chain	Res	Type
82	BP	99	GLN
86	BT	88	ASN
86	BT	125	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1764/1800 (98%)	729 (41%)	100 (5%)
35	l	33/34 (97%)	20 (60%)	0
36	m	75/76 (98%)	34 (45%)	0
37	n	76/77 (98%)	30 (39%)	0
83	BQ	3162/3396 (93%)	1066 (33%)	177 (5%)
84	BR	120/121 (99%)	35 (29%)	7 (5%)
85	BS	157/158 (99%)	50 (31%)	10 (6%)
All	All	5387/5662 (95%)	1964 (36%)	294 (5%)

All (1964) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	5	U
1	2	17	C
1	2	25	C
1	2	26	A
1	2	33	U
1	2	34	G
1	2	36	C
1	2	38	C
1	2	39	A
1	2	41	A
1	2	42	G
1	2	43	A
1	2	46	A
1	2	47	A
1	2	48	G
1	2	49	C
1	2	50	C
1	2	51	A
1	2	52	U
1	2	53	G

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Mol	Chain	Res	Type
1	2	54	C
1	2	55	A
1	2	56	U
1	2	57	G
1	2	63	G
1	2	65	A
1	2	66	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	70	C
1	2	71	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	78	A
1	2	80	A
1	2	81	G
1	2	83	G
1	2	86	A
1	2	92	A
1	2	99	C
1	2	104	A
1	2	105	A
1	2	106	U
1	2	111	U
1	2	112	A
1	2	114	C
1	2	115	G
1	2	116	U
1	2	117	U
1	2	120	U
1	2	121	U
1	2	124	A
1	2	127	G
1	2	129	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U

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Mol	Chain	Res	Type
1	2	135	A
1	2	136	C
1	2	138	A
1	2	139	C
1	2	140	A
1	2	141	U
1	2	142	G
1	2	153	G
1	2	155	U
1	2	157	A
1	2	158	U
1	2	159	U
1	2	160	C
1	2	161	U
1	2	168	A
1	2	170	U
1	2	171	A
1	2	174	U
1	2	175	G
1	2	177	U
1	2	178	U
1	2	180	A
1	2	181	A
1	2	185	U
1	2	187	G
1	2	188	A
1	2	189	C
1	2	191	C
1	2	193	U
1	2	194	U
1	2	195	G
1	2	198	A
1	2	199	G
1	2	201	G
1	2	206	A
1	2	215	A
1	2	216	U
1	2	217	A
1	2	218	A
1	2	222	A
1	2	223	U
1	2	224	C

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Mol	Chain	Res	Type
1	2	225	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	230	C
1	2	232	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	236	A
1	2	240	U
1	2	241	U
1	2	243	G
1	2	250	C
1	2	257	A
1	2	259	U
1	2	260	U
1	2	262	U
1	2	265	A
1	2	266	A
1	2	267	U
1	2	272	U
1	2	275	C
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	282	C
1	2	283	U
1	2	285	G
1	2	296	U
1	2	299	A
1	2	302	U
1	2	308	C
1	2	309	C
1	2	312	A
1	2	313	U
1	2	314	C
1	2	316	A
1	2	317	C
1	2	319	U
1	2	320	U

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Mol	Chain	Res	Type
1	2	321	C
1	2	322	G
1	2	323	A
1	2	329	G
1	2	330	G
1	2	331	A
1	2	333	A
1	2	334	G
1	2	337	G
1	2	338	C
1	2	340	U
1	2	341	A
1	2	346	G
1	2	352	A
1	2	353	A
1	2	359	A
1	2	361	C
1	2	363	G
1	2	366	A
1	2	370	A
1	2	373	G
1	2	375	U
1	2	378	A
1	2	380	U
1	2	381	C
1	2	382	C
1	2	383	G
1	2	384	G
1	2	385	A
1	2	386	G
1	2	387	A
1	2	388	G
1	2	390	G
1	2	396	G
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	411	C
1	2	416	A
1	2	417	A
1	2	418	G

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Mol	Chain	Res	Type
1	2	419	G
1	2	420	A
1	2	422	G
1	2	423	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	427	C
1	2	429	G
1	2	430	G
1	2	431	C
1	2	434	G
1	2	435	C
1	2	436	A
1	2	437	A
1	2	439	U
1	2	440	U
1	2	442	C
1	2	444	C
1	2	446	A
1	2	448	C
1	2	452	A
1	2	453	U
1	2	454	U
1	2	455	C
1	2	459	G
1	2	460	A
1	2	464	A
1	2	471	A
1	2	474	A
1	2	475	A
1	2	477	A
1	2	486	G
1	2	488	G
1	2	491	C
1	2	492	A
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	498	G
1	2	500	C

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Mol	Chain	Res	Type
1	2	502	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	510	G
1	2	515	A
1	2	517	U
1	2	519	C
1	2	524	U
1	2	525	A
1	2	534	A
1	2	535	A
1	2	536	C
1	2	538	A
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	545	A
1	2	548	G
1	2	549	G
1	2	554	C
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	562	G
1	2	564	G
1	2	565	C
1	2	568	G
1	2	571	G
1	2	578	U
1	2	579	A
1	2	580	A
1	2	582	U
1	2	590	C
1	2	591	A
1	2	594	A
1	2	595	G
1	2	602	U

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Mol	Chain	Res	Type
1	2	606	A
1	2	608	U
1	2	610	G
1	2	614	C
1	2	618	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	639	U
1	2	640	U
1	2	641	G
1	2	644	C
1	2	647	G
1	2	650	U
1	2	651	G
1	2	652	G
1	2	653	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	678	A
1	2	680	U
1	2	681	U
1	2	687	G
1	2	690	G
1	2	693	U
1	2	694	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	699	U
1	2	700	C
1	2	702	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	711	U

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Mol	Chain	Res	Type
1	2	712	G
1	2	713	A
1	2	714	G
1	2	715	U
1	2	716	C
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	725	U
1	2	726	C
1	2	729	G
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	738	G
1	2	739	G
1	2	740	A
1	2	743	U
1	2	744	U
1	2	752	A
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	767	U
1	2	768	C
1	2	771	A
1	2	774	A
1	2	775	G
1	2	778	G
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	789	A
1	2	797	G
1	2	799	A

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Mol	Chain	Res	Type
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	816	G
1	2	817	A
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	824	G
1	2	826	U
1	2	831	U
1	2	832	U
1	2	833	U
1	2	834	G
1	2	835	U
1	2	836	U
1	2	838	G
1	2	840	U
1	2	841	U
1	2	842	C
1	2	845	G
1	2	846	G
1	2	847	A
1	2	852	C
1	2	856	A
1	2	857	U
1	2	858	G
1	2	859	A
1	2	860	U
1	2	863	A
1	2	864	U
1	2	876	G
1	2	882	U
1	2	894	U
1	2	895	G
1	2	896	U
1	2	899	G
1	2	900	A
1	2	911	U

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Mol	Chain	Res	Type
1	2	912	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	916	U
1	2	918	U
1	2	921	U
1	2	925	G
1	2	929	A
1	2	931	C
1	2	932	U
1	2	933	A
1	2	934	C
1	2	935	U
1	2	939	A
1	2	940	A
1	2	942	G
1	2	944	A
1	2	945	U
1	2	959	U
1	2	960	U
1	2	966	A
1	2	967	A
1	2	970	A
1	2	974	A
1	2	980	G
1	2	985	G
1	2	988	A
1	2	991	G
1	2	992	A
1	2	997	G
1	2	998	A
1	2	1004	U
1	2	1008	G
1	2	1009	U
1	2	1014	G
1	2	1021	C
1	2	1023	A
1	2	1024	U
1	2	1026	A
1	2	1028	C
1	2	1029	U

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Mol	Chain	Res	Type
1	2	1030	A
1	2	1031	U
1	2	1032	G
1	2	1038	U
1	2	1039	A
1	2	1040	G
1	2	1047	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1060	U
1	2	1061	A
1	2	1075	C
1	2	1076	A
1	2	1081	A
1	2	1082	C
1	2	1086	A
1	2	1087	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1098	U
1	2	1099	U
1	2	1100	G
1	2	1108	G
1	2	1109	G
1	2	1114	G
1	2	1115	U
1	2	1138	A
1	2	1141	G
1	2	1143	A
1	2	1150	G
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1168	U
1	2	1170	G
1	2	1171	A
1	2	1172	G
1	2	1173	C

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Mol	Chain	Res	Type
1	2	1174	C
1	2	1175	U
1	2	1179	G
1	2	1185	U
1	2	1186	U
1	2	1193	A
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1203	A
1	2	1204	A
1	2	1205	C
1	2	1206	U
1	2	1209	C
1	2	1215	C
1	2	1216	C
1	2	1217	A
1	2	1218	G
1	2	1227	A
1	2	1228	G
1	2	1241	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1247	U
1	2	1251	U
1	2	1252	C
1	2	1253	U
1	2	1255	G
1	2	1256	A
1	2	1257	U
1	2	1258	U
1	2	1259	U
1	2	1263	G
1	2	1273	G
1	2	1274	C
1	2	1275	A
1	2	1284	C

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Mol	Chain	Res	Type
1	2	1285	U
1	2	1286	U
1	2	1287	A
1	2	1294	G
1	2	1299	G
1	2	1301	U
1	2	1307	U
1	2	1314	U
1	2	1315	U
1	2	1316	G
1	2	1318	G
1	2	1321	A
1	2	1322	A
1	2	1324	G
1	2	1325	A
1	2	1337	A
1	2	1338	C
1	2	1339	C
1	2	1340	U
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1348	A
1	2	1349	G
1	2	1353	U
1	2	1354	G
1	2	1355	C
1	2	1356	U
1	2	1359	C
1	2	1360	A
1	2	1361	U
1	2	1363	U
1	2	1364	G
1	2	1365	C
1	2	1367	G
1	2	1368	G
1	2	1369	U
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1381	U
1	2	1382	A

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Mol	Chain	Res	Type
1	2	1383	G
1	2	1388	A
1	2	1390	U
1	2	1391	A
1	2	1392	U
1	2	1395	G
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1402	G
1	2	1403	C
1	2	1405	G
1	2	1410	A
1	2	1413	U
1	2	1414	U
1	2	1415	U
1	2	1417	A
1	2	1418	G
1	2	1421	A
1	2	1425	A
1	2	1427	A
1	2	1431	C
1	2	1432	U
1	2	1437	U
1	2	1444	A
1	2	1445	G
1	2	1446	A
1	2	1447	C
1	2	1448	G
1	2	1451	C
1	2	1458	G
1	2	1459	C
1	2	1460	A
1	2	1461	C
1	2	1462	G
1	2	1463	C
1	2	1465	C
1	2	1466	G
1	2	1467	C
1	2	1469	A
1	2	1470	C
1	2	1471	A

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Mol	Chain	Res	Type
1	2	1472	C
1	2	1473	U
1	2	1474	G
1	2	1475	A
1	2	1476	C
1	2	1477	G
1	2	1478	G
1	2	1479	A
1	2	1480	G
1	2	1481	C
1	2	1483	A
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1496	U
1	2	1503	A
1	2	1506	G
1	2	1510	U
1	2	1514	U
1	2	1516	A
1	2	1517	U
1	2	1518	C
1	2	1520	U
1	2	1521	G
1	2	1522	U
1	2	1523	G
1	2	1524	A
1	2	1527	C
1	2	1528	U
1	2	1529	C
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1540	G
1	2	1541	G
1	2	1542	G
1	2	1543	A
1	2	1545	A

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Mol	Chain	Res	Type
1	2	1548	G
1	2	1554	U
1	2	1558	U
1	2	1559	A
1	2	1567	U
1	2	1568	C
1	2	1569	A
1	2	1570	A
1	2	1571	C
1	2	1572	G
1	2	1573	A
1	2	1574	G
1	2	1575	G
1	2	1582	U
1	2	1584	G
1	2	1590	G
1	2	1595	U
1	2	1600	A
1	2	1601	G
1	2	1602	C
1	2	1603	U
1	2	1605	G
1	2	1607	G
1	2	1611	A
1	2	1616	G
1	2	1622	G
1	2	1631	A
1	2	1633	A
1	2	1634	C
1	2	1635	A
1	2	1636	C
1	2	1637	C
1	2	1638	G
1	2	1640	C
1	2	1645	G
1	2	1657	U
1	2	1658	G
1	2	1662	G
1	2	1673	G
1	2	1678	A
1	2	1682	U
1	2	1688	U

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Mol	Chain	Res	Type
1	2	1689	A
1	2	1690	G
1	2	1691	A
1	2	1693	A
1	2	1709	C
1	2	1711	C
1	2	1712	A
1	2	1717	G
1	2	1726	G
1	2	1730	A
1	2	1736	G
1	2	1738	U
1	2	1742	U
1	2	1743	U
1	2	1750	A
1	2	1753	A
1	2	1755	A
1	2	1757	G
1	2	1758	U
1	2	1760	G
1	2	1762	A
1	2	1765	A
1	2	1766	A
1	2	1767	G
1	2	1768	G
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1796	C
1	2	1798	U
35	l	35	U
35	l	36	U
35	l	40	U
35	l	41	U
35	l	42	U
35	l	43	U
35	l	44	U

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Mol	Chain	Res	Type
35	l	46	G
35	l	49	A
35	l	53	U
35	l	54	U
35	l	55	U
35	l	56	U
35	l	57	U
35	l	58	U
35	l	59	U
35	l	60	U
35	l	61	U
35	l	64	U
35	l	66	U
36	m	3	G
36	m	7	U
36	m	8	U
36	m	15	G
36	m	16	U
36	m	18	G
36	m	20	U
36	m	21	A
36	m	30	G
36	m	36	U
36	m	41	A
36	m	43	U
36	m	45	G
36	m	46	G
36	m	47	U
36	m	48	C
36	m	49	G
36	m	50	C
36	m	51	A
36	m	52	G
36	m	53	G
36	m	54	U
36	m	55	U
36	m	56	C
36	m	58	A
36	m	59	A
36	m	60	U
36	m	61	C
36	m	64	G

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Mol	Chain	Res	Type
36	m	66	A
36	m	67	C
36	m	68	G
36	m	73	A
36	m	74	C
37	n	2	G
37	n	3	A
37	n	8	U
37	n	9	A
37	n	11	U
37	n	13	C
37	n	14	A
37	n	15	G
37	n	16	U
37	n	17	C
37	n	17(A)	G
37	n	18	G
37	n	19	U
37	n	20	U
37	n	21	A
37	n	44	G
37	n	47	U
37	n	48	C
37	n	49	G
37	n	52	G
37	n	53	G
37	n	57	G
37	n	59	G
37	n	60	U
37	n	61	C
37	n	62	C
37	n	68	G
37	n	69	U
37	n	74	C
37	n	76	A
83	BQ	4	U
83	BQ	6	A
83	BQ	13	A
83	BQ	14	U
83	BQ	16	A
83	BQ	20	A
83	BQ	21	G

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Mol	Chain	Res	Type
83	BQ	22	G
83	BQ	26	A
83	BQ	27	C
83	BQ	30	G
83	BQ	40	A
83	BQ	43	A
83	BQ	47	C
83	BQ	49	A
83	BQ	57	A
83	BQ	59	G
83	BQ	60	A
83	BQ	65	A
83	BQ	66	A
83	BQ	71	A
83	BQ	72	C
83	BQ	73	C
83	BQ	74	G
83	BQ	75	G
83	BQ	77	A
83	BQ	86	G
83	BQ	87	U
83	BQ	89	A
83	BQ	92	G
83	BQ	96	G
83	BQ	97	U
83	BQ	98	G
83	BQ	108	A
83	BQ	111	C
83	BQ	119	U
83	BQ	120	G
83	BQ	121	A
83	BQ	122	A
83	BQ	123	A
83	BQ	131	C
83	BQ	134	U
83	BQ	135	C
83	BQ	136	G
83	BQ	139	G
83	BQ	146	U
83	BQ	147	U
83	BQ	148	G
83	BQ	150	A

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Mol	Chain	Res	Type
83	BQ	153	U
83	BQ	154	U
83	BQ	155	G
83	BQ	156	G
83	BQ	157	A
83	BQ	158	G
83	BQ	161	G
83	BQ	165	A
83	BQ	166	C
83	BQ	167	U
83	BQ	168	U
83	BQ	170	G
83	BQ	172	G
83	BQ	173	G
83	BQ	187	A
83	BQ	188	U
83	BQ	189	G
83	BQ	190	U
83	BQ	191	U
83	BQ	201	A
83	BQ	206	G
83	BQ	210	U
83	BQ	211	A
83	BQ	212	G
83	BQ	213	A
83	BQ	217	U
83	BQ	218	G
83	BQ	219	A
83	BQ	220	G
83	BQ	222	A
83	BQ	230	U
83	BQ	231	G
83	BQ	234	G
83	BQ	237	G
83	BQ	240	U
83	BQ	241	G
83	BQ	242	C
83	BQ	245	U
83	BQ	247	C
83	BQ	248	U
83	BQ	250	U
83	BQ	251	G

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Mol	Chain	Res	Type
83	BQ	252	U
83	BQ	268	A
83	BQ	269	G
83	BQ	270	U
83	BQ	281	G
83	BQ	282	G
83	BQ	283	G
83	BQ	286	U
83	BQ	287	G
83	BQ	289	A
83	BQ	295	A
83	BQ	297	G
83	BQ	298	U
83	BQ	304	G
83	BQ	305	U
83	BQ	315	C
83	BQ	317	A
83	BQ	323	A
83	BQ	329	U
83	BQ	330	G
83	BQ	336	A
83	BQ	338	A
83	BQ	342	A
83	BQ	346	C
83	BQ	349	A
83	BQ	350	C
83	BQ	353	G
83	BQ	354	U
83	BQ	367	A
83	BQ	370	U
83	BQ	372	A
83	BQ	375	A
83	BQ	376	G
83	BQ	377	A
83	BQ	385	A
83	BQ	395	A
83	BQ	396	A
83	BQ	398	A
83	BQ	399	A
83	BQ	400	G
83	BQ	401	U
83	BQ	402	A

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Mol	Chain	Res	Type
83	BQ	403	C
83	BQ	404	G
83	BQ	421	G
83	BQ	422	A
83	BQ	428	A
83	BQ	429	U
83	BQ	438	A
83	BQ	440	A
83	BQ	495	G
83	BQ	496	C
83	BQ	503	C
83	BQ	507	U
83	BQ	520	U
83	BQ	521	A
83	BQ	522	A
83	BQ	523	A
83	BQ	525	C
83	BQ	527	A
83	BQ	529	A
83	BQ	531	G
83	BQ	532	A
83	BQ	533	A
83	BQ	535	G
83	BQ	541	U
83	BQ	543	C
83	BQ	544	C
83	BQ	546	C
83	BQ	547	G
83	BQ	548	G
83	BQ	551	A
83	BQ	552	G
83	BQ	555	U
83	BQ	557	A
83	BQ	559	A
83	BQ	566	G
83	BQ	569	A
83	BQ	572	A
83	BQ	575	G
83	BQ	578	A
83	BQ	579	G
83	BQ	581	U
83	BQ	588	G

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Mol	Chain	Res	Type
83	BQ	589	A
83	BQ	592	A
83	BQ	594	U
83	BQ	597	G
83	BQ	601	U
83	BQ	604	G
83	BQ	608	A
83	BQ	609	G
83	BQ	611	A
83	BQ	612	U
83	BQ	615	U
83	BQ	616	G
83	BQ	617	G
83	BQ	620	U
83	BQ	621	A
83	BQ	622	A
83	BQ	627	U
83	BQ	629	U
83	BQ	634	C
83	BQ	636	C
83	BQ	637	C
83	BQ	642	U
83	BQ	643	U
83	BQ	649	A
83	BQ	661	G
83	BQ	664	U
83	BQ	666	A
83	BQ	667	C
83	BQ	676	G
83	BQ	677	A
83	BQ	678	G
83	BQ	681	U
83	BQ	690	A
83	BQ	691	A
83	BQ	692	A
83	BQ	699	A
83	BQ	705	A
83	BQ	709	A
83	BQ	712	G
83	BQ	715	A
83	BQ	716	A
83	BQ	719	U

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Mol	Chain	Res	Type
83	BQ	720	A
83	BQ	721	G
83	BQ	726	G
83	BQ	728	G
83	BQ	735	A
83	BQ	742	G
83	BQ	757	C
83	BQ	760	G
83	BQ	764	U
83	BQ	765	C
83	BQ	766	U
83	BQ	767	U
83	BQ	768	C
83	BQ	770	G
83	BQ	776	U
83	BQ	777	U
83	BQ	781	G
83	BQ	784	A
83	BQ	785	G
83	BQ	787	G
83	BQ	792	G
83	BQ	799	G
83	BQ	800	G
83	BQ	801	A
83	BQ	806	A
83	BQ	808	A
83	BQ	816	A
83	BQ	817	A
83	BQ	826	G
83	BQ	830	A
83	BQ	835	G
83	BQ	847	A
83	BQ	849	C
83	BQ	861	C
83	BQ	871	U
83	BQ	874	U
83	BQ	875	G
83	BQ	879	U
83	BQ	880	G
83	BQ	882	A
83	BQ	885	U
83	BQ	895	A

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Mol	Chain	Res	Type
83	BQ	896	A
83	BQ	897	U
83	BQ	907	G
83	BQ	913	A
83	BQ	914	A
83	BQ	915	A
83	BQ	916	G
83	BQ	917	A
83	BQ	921	A
83	BQ	922	U
83	BQ	923	C
83	BQ	924	G
83	BQ	925	A
83	BQ	926	A
83	BQ	933	A
83	BQ	934	G
83	BQ	937	G
83	BQ	938	C
83	BQ	939	U
83	BQ	944	C
83	BQ	953	G
83	BQ	954	U
83	BQ	959	C
83	BQ	960	U
83	BQ	961	C
83	BQ	962	A
83	BQ	964	G
83	BQ	974	G
83	BQ	977	C
83	BQ	979	U
83	BQ	980	A
83	BQ	981	U
83	BQ	984	G
83	BQ	991	G
83	BQ	993	G
83	BQ	994	G
83	BQ	995	U
83	BQ	996	A
83	BQ	1001	G
83	BQ	1005	G
83	BQ	1007	U
83	BQ	1008	U

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Mol	Chain	Res	Type
83	BQ	1010	G
83	BQ	1013	G
83	BQ	1015	U
83	BQ	1016	C
83	BQ	1017	C
83	BQ	1018	G
83	BQ	1019	G
83	BQ	1020	G
83	BQ	1023	C
83	BQ	1025	A
83	BQ	1028	U
83	BQ	1029	G
83	BQ	1030	A
83	BQ	1032	C
83	BQ	1033	U
83	BQ	1036	A
83	BQ	1038	C
83	BQ	1042	U
83	BQ	1043	C
83	BQ	1045	C
83	BQ	1047	A
83	BQ	1049	C
83	BQ	1050	U
83	BQ	1063	G
83	BQ	1065	A
83	BQ	1071	U
83	BQ	1076	C
83	BQ	1077	U
83	BQ	1081	U
83	BQ	1083	G
83	BQ	1087	G
83	BQ	1092	C
83	BQ	1093	A
83	BQ	1094	U
83	BQ	1095	U
83	BQ	1096	U
83	BQ	1097	G
83	BQ	1098	A
83	BQ	1102	A
83	BQ	1103	A
83	BQ	1104	G
83	BQ	1117	G

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Mol	Chain	Res	Type
83	BQ	1125	U
83	BQ	1128	U
83	BQ	1131	G
83	BQ	1140	G
83	BQ	1142	G
83	BQ	1143	A
83	BQ	1144	U
83	BQ	1145	G
83	BQ	1149	G
83	BQ	1150	A
83	BQ	1151	U
83	BQ	1153	A
83	BQ	1154	A
83	BQ	1155	C
83	BQ	1159	A
83	BQ	1171	G
83	BQ	1172	G
83	BQ	1177	G
83	BQ	1178	G
83	BQ	1180	A
83	BQ	1181	U
83	BQ	1182	A
83	BQ	1186	G
83	BQ	1191	U
83	BQ	1192	C
83	BQ	1193	A
83	BQ	1197	A
83	BQ	1199	C
83	BQ	1200	A
83	BQ	1201	C
83	BQ	1202	A
83	BQ	1206	G
83	BQ	1213	G
83	BQ	1217	A
83	BQ	1220	U
83	BQ	1222	G
83	BQ	1223	A
83	BQ	1225	A
83	BQ	1228	C
83	BQ	1230	G
83	BQ	1233	G
83	BQ	1234	G

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Mol	Chain	Res	Type
83	BQ	1235	U
83	BQ	1236	G
83	BQ	1237	G
83	BQ	1238	C
83	BQ	1239	C
83	BQ	1240	A
83	BQ	1241	U
83	BQ	1242	G
83	BQ	1243	G
83	BQ	1245	A
83	BQ	1246	G
83	BQ	1247	U
83	BQ	1248	C
83	BQ	1249	G
83	BQ	1251	A
83	BQ	1252	A
83	BQ	1253	U
83	BQ	1254	C
83	BQ	1256	G
83	BQ	1257	C
83	BQ	1260	A
83	BQ	1262	G
83	BQ	1263	A
83	BQ	1264	G
83	BQ	1265	U
83	BQ	1266	G
83	BQ	1267	U
83	BQ	1270	A
83	BQ	1271	A
83	BQ	1272	C
83	BQ	1273	A
83	BQ	1274	A
83	BQ	1275	C
83	BQ	1276	U
83	BQ	1277	C
83	BQ	1278	A
83	BQ	1279	C
83	BQ	1280	C
83	BQ	1281	G
83	BQ	1282	G
83	BQ	1285	G
83	BQ	1286	A

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Mol	Chain	Res	Type
83	BQ	1287	A
83	BQ	1294	A
83	BQ	1301	A
83	BQ	1303	A
83	BQ	1305	U
83	BQ	1308	A
83	BQ	1309	U
83	BQ	1313	G
83	BQ	1315	U
83	BQ	1316	C
83	BQ	1317	A
83	BQ	1318	A
83	BQ	1321	G
83	BQ	1325	U
83	BQ	1329	U
83	BQ	1330	A
83	BQ	1332	A
83	BQ	1334	U
83	BQ	1345	G
83	BQ	1348	U
83	BQ	1349	G
83	BQ	1351	U
83	BQ	1353	U
83	BQ	1354	G
83	BQ	1355	A
83	BQ	1356	U
83	BQ	1357	G
83	BQ	1359	C
83	BQ	1364	C
83	BQ	1382	G
83	BQ	1386	A
83	BQ	1391	C
83	BQ	1392	G
83	BQ	1393	A
83	BQ	1399	A
83	BQ	1400	G
83	BQ	1408	G
83	BQ	1418	A
83	BQ	1419	A
83	BQ	1424	C
83	BQ	1429	G
83	BQ	1430	U

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Mol	Chain	Res	Type
83	BQ	1432	C
83	BQ	1434	G
83	BQ	1435	A
83	BQ	1437	C
83	BQ	1446	A
83	BQ	1447	G
83	BQ	1448	U
83	BQ	1450	G
83	BQ	1452	A
83	BQ	1456	A
83	BQ	1464	G
83	BQ	1468	A
83	BQ	1480	G
83	BQ	1481	A
83	BQ	1482	A
83	BQ	1483	G
83	BQ	1484	U
83	BQ	1485	G
83	BQ	1487	G
83	BQ	1508	C
83	BQ	1512	U
83	BQ	1514	G
83	BQ	1523	U
83	BQ	1527	C
83	BQ	1533	U
83	BQ	1536	G
83	BQ	1539	A
83	BQ	1542	G
83	BQ	1549	U
83	BQ	1554	U
83	BQ	1555	U
83	BQ	1556	C
83	BQ	1557	A
83	BQ	1558	A
83	BQ	1559	A
83	BQ	1560	G
83	BQ	1561	G
83	BQ	1563	C
83	BQ	1567	U
83	BQ	1568	U
83	BQ	1569	U
83	BQ	1570	U

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Mol	Chain	Res	Type
83	BQ	1571	A
83	BQ	1572	U
83	BQ	1576	G
83	BQ	1577	G
83	BQ	1578	C
83	BQ	1579	C
83	BQ	1580	A
83	BQ	1581	C
83	BQ	1582	C
83	BQ	1583	A
83	BQ	1587	A
83	BQ	1588	A
83	BQ	1589	A
83	BQ	1593	A
83	BQ	1596	C
83	BQ	1597	C
83	BQ	1602	A
83	BQ	1603	A
83	BQ	1605	A
83	BQ	1613	A
83	BQ	1619	A
83	BQ	1620	U
83	BQ	1621	A
83	BQ	1630	U
83	BQ	1631	C
83	BQ	1632	A
83	BQ	1645	U
83	BQ	1646	G
83	BQ	1656	A
83	BQ	1657	C
83	BQ	1658	G
83	BQ	1659	U
83	BQ	1662	G
83	BQ	1683	A
83	BQ	1684	U
83	BQ	1692	U
83	BQ	1694	U
83	BQ	1696	A
83	BQ	1697	A
83	BQ	1702	U
83	BQ	1704	A
83	BQ	1708	C

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Mol	Chain	Res	Type
83	BQ	1713	G
83	BQ	1714	A
83	BQ	1717	U
83	BQ	1718	G
83	BQ	1724	U
83	BQ	1725	C
83	BQ	1728	G
83	BQ	1729	A
83	BQ	1730	G
83	BQ	1731	A
83	BQ	1735	G
83	BQ	1740	U
83	BQ	1741	A
83	BQ	1750	A
83	BQ	1751	G
83	BQ	1752	A
83	BQ	1760	A
83	BQ	1761	C
83	BQ	1762	C
83	BQ	1763	U
83	BQ	1765	U
83	BQ	1769	G
83	BQ	1770	G
83	BQ	1775	G
83	BQ	1780	G
83	BQ	1785	U
83	BQ	1788	C
83	BQ	1794	G
83	BQ	1797	A
83	BQ	1809	A
83	BQ	1813	A
83	BQ	1814	A
83	BQ	1815	U
83	BQ	1816	A
83	BQ	1817	G
83	BQ	1819	U
83	BQ	1820	U
83	BQ	1821	U
83	BQ	1822	C
83	BQ	1834	U
83	BQ	1835	A
83	BQ	1839	A

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Mol	Chain	Res	Type
83	BQ	1840	U
83	BQ	1841	A
83	BQ	1842	A
83	BQ	1845	G
83	BQ	1846	C
83	BQ	1847	A
83	BQ	1848	G
83	BQ	1849	C
83	BQ	1851	G
83	BQ	1854	C
83	BQ	1855	U
83	BQ	1856	C
83	BQ	1866	C
83	BQ	1868	G
83	BQ	1871	U
83	BQ	1877	U
83	BQ	1879	A
83	BQ	1880	U
83	BQ	1881	A
83	BQ	1884	A
83	BQ	1885	U
83	BQ	1886	A
83	BQ	1893	A
83	BQ	1894	U
83	BQ	1895	A
83	BQ	1899	G
83	BQ	1900	A
83	BQ	1901	A
83	BQ	1905	G
83	BQ	1906	G
83	BQ	1914	G
83	BQ	1918	C
83	BQ	1927	G
83	BQ	1930	A
83	BQ	1931	U
83	BQ	1932	A
83	BQ	1936	A
83	BQ	1942	U
83	BQ	1947	G
83	BQ	1948	G
83	BQ	1949	G
83	BQ	1952	G

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Mol	Chain	Res	Type
83	BQ	1953	G
83	BQ	1954	G
83	BQ	2095	G
83	BQ	2099	A
83	BQ	2100	A
83	BQ	2101	C
83	BQ	2102	U
83	BQ	2106	A
83	BQ	2107	A
83	BQ	2108	C
83	BQ	2111	G
83	BQ	2112	U
83	BQ	2113	A
83	BQ	2116	G
83	BQ	2117	A
83	BQ	2121	G
83	BQ	2122	G
83	BQ	2126	A
83	BQ	2131	A
83	BQ	2138	A
83	BQ	2139	A
83	BQ	2140	U
83	BQ	2158	A
83	BQ	2159	U
83	BQ	2160	G
83	BQ	2163	C
83	BQ	2169	G
83	BQ	2170	U
83	BQ	2175	U
83	BQ	2178	A
83	BQ	2179	C
83	BQ	2180	G
83	BQ	2184	U
83	BQ	2186	U
83	BQ	2188	A
83	BQ	2192	C
83	BQ	2193	U
83	BQ	2194	G
83	BQ	2197	C
83	BQ	2198	A
83	BQ	2205	U
83	BQ	2206	G

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Mol	Chain	Res	Type
83	BQ	2207	A
83	BQ	2208	A
83	BQ	2209	U
83	BQ	2210	G
83	BQ	2212	C
83	BQ	2225	U
83	BQ	2243	A
83	BQ	2244	A
83	BQ	2246	G
83	BQ	2249	G
83	BQ	2255	A
83	BQ	2256	A
83	BQ	2257	C
83	BQ	2261	G
83	BQ	2263	C
83	BQ	2270	A
83	BQ	2272	G
83	BQ	2274	U
83	BQ	2279	A
83	BQ	2280	A
83	BQ	2281	A
83	BQ	2282	U
83	BQ	2283	G
83	BQ	2284	C
83	BQ	2288	G
83	BQ	2298	U
83	BQ	2303	A
83	BQ	2306	C
83	BQ	2307	G
83	BQ	2308	C
83	BQ	2313	A
83	BQ	2314	U
83	BQ	2315	G
83	BQ	2318	U
83	BQ	2319	U
83	BQ	2336	U
83	BQ	2340	U
83	BQ	2357	A
83	BQ	2364	G
83	BQ	2373	A
83	BQ	2374	C
83	BQ	2375	G

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Mol	Chain	Res	Type
83	BQ	2378	C
83	BQ	2383	C
83	BQ	2386	A
83	BQ	2388	U
83	BQ	2393	G
83	BQ	2394	G
83	BQ	2397	A
83	BQ	2398	A
83	BQ	2402	A
83	BQ	2403	G
83	BQ	2411	U
83	BQ	2412	G
83	BQ	2418	G
83	BQ	2419	A
83	BQ	2433	U
83	BQ	2435	G
83	BQ	2436	U
83	BQ	2437	G
83	BQ	2439	A
83	BQ	2441	A
83	BQ	2442	G
83	BQ	2444	C
83	BQ	2445	A
83	BQ	2446	U
83	BQ	2447	A
83	BQ	2451	G
83	BQ	2452	G
83	BQ	2493	U
83	BQ	2494	A
83	BQ	2496	C
83	BQ	2497	U
83	BQ	2498	U
83	BQ	2501	U
83	BQ	2502	A
83	BQ	2508	U
83	BQ	2509	U
83	BQ	2514	U
83	BQ	2515	A
83	BQ	2522	G
83	BQ	2523	A
83	BQ	2524	A
83	BQ	2526	C

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Mol	Chain	Res	Type
83	BQ	2530	G
83	BQ	2531	C
83	BQ	2533	G
83	BQ	2534	G
83	BQ	2537	U
83	BQ	2538	U
83	BQ	2539	C
83	BQ	2540	A
83	BQ	2541	U
83	BQ	2542	U
83	BQ	2544	U
83	BQ	2546	C
83	BQ	2547	A
83	BQ	2550	U
83	BQ	2552	C
83	BQ	2554	A
83	BQ	2555	G
83	BQ	2559	U
83	BQ	2560	C
83	BQ	2567	C
83	BQ	2568	C
83	BQ	2570	U
83	BQ	2571	U
83	BQ	2572	C
83	BQ	2578	U
83	BQ	2585	G
83	BQ	2587	U
83	BQ	2589	G
83	BQ	2590	A
83	BQ	2593	A
83	BQ	2594	C
83	BQ	2600	C
83	BQ	2606	G
83	BQ	2607	G
83	BQ	2614	G
83	BQ	2618	G
83	BQ	2619	G
83	BQ	2624	G
83	BQ	2626	A
83	BQ	2627	C
83	BQ	2629	U
83	BQ	2641	U

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Mol	Chain	Res	Type
83	BQ	2642	A
83	BQ	2652	U
83	BQ	2655	U
83	BQ	2656	A
83	BQ	2657	A
83	BQ	2666	C
83	BQ	2672	G
83	BQ	2674	A
83	BQ	2678	A
83	BQ	2679	A
83	BQ	2681	U
83	BQ	2688	U
83	BQ	2689	A
83	BQ	2690	G
83	BQ	2691	A
83	BQ	2694	A
83	BQ	2695	A
83	BQ	2703	A
83	BQ	2704	A
83	BQ	2709	C
83	BQ	2713	U
83	BQ	2714	G
83	BQ	2716	U
83	BQ	2726	C
83	BQ	2727	A
83	BQ	2728	G
83	BQ	2737	C
83	BQ	2740	A
83	BQ	2747	A
83	BQ	2749	G
83	BQ	2751	G
83	BQ	2752	U
83	BQ	2753	G
83	BQ	2754	G
83	BQ	2755	C
83	BQ	2761	G
83	BQ	2762	A
83	BQ	2772	C
83	BQ	2776	C
83	BQ	2777	G
83	BQ	2778	G
83	BQ	2779	A

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Mol	Chain	Res	Type
83	BQ	2795	U
83	BQ	2796	G
83	BQ	2800	G
83	BQ	2801	A
83	BQ	2802	A
83	BQ	2803	A
83	BQ	2804	A
83	BQ	2810	C
83	BQ	2814	G
83	BQ	2816	G
83	BQ	2817	A
83	BQ	2821	C
83	BQ	2829	U
83	BQ	2834	G
83	BQ	2837	A
83	BQ	2839	G
83	BQ	2842	U
83	BQ	2845	A
83	BQ	2849	C
83	BQ	2855	U
83	BQ	2859	U
83	BQ	2860	U
83	BQ	2862	U
83	BQ	2863	G
83	BQ	2864	A
83	BQ	2867	C
83	BQ	2870	C
83	BQ	2871	G
83	BQ	2872	A
83	BQ	2875	U
83	BQ	2877	G
83	BQ	2883	U
83	BQ	2888	U
83	BQ	2889	C
83	BQ	2898	G
83	BQ	2901	G
83	BQ	2911	A
83	BQ	2912	G
83	BQ	2923	U
83	BQ	2925	C
83	BQ	2928	C
83	BQ	2930	A

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Mol	Chain	Res	Type
83	BQ	2933	A
83	BQ	2935	U
83	BQ	2936	A
83	BQ	2938	G
83	BQ	2941	A
83	BQ	2942	C
83	BQ	2945	G
83	BQ	2947	G
83	BQ	2950	G
83	BQ	2951	G
83	BQ	2953	U
83	BQ	2954	U
83	BQ	2955	U
83	BQ	2971	A
83	BQ	2972	G
83	BQ	2977	G
83	BQ	2978	U
83	BQ	2979	U
83	BQ	2983	C
83	BQ	2990	G
83	BQ	2996	U
83	BQ	2997	G
83	BQ	3004	C
83	BQ	3012	A
83	BQ	3013	U
83	BQ	3022	G
83	BQ	3023	U
83	BQ	3026	G
83	BQ	3030	G
83	BQ	3034	C
83	BQ	3039	C
83	BQ	3040	A
83	BQ	3047	U
83	BQ	3048	A
83	BQ	3049	A
83	BQ	3056	U
83	BQ	3057	U
83	BQ	3058	U
83	BQ	3059	G
83	BQ	3061	G
83	BQ	3074	G
83	BQ	3077	A

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Mol	Chain	Res	Type
83	BQ	3078	U
83	BQ	3079	U
83	BQ	3080	G
83	BQ	3086	A
83	BQ	3090	U
83	BQ	3092	C
83	BQ	3094	A
83	BQ	3099	C
83	BQ	3100	U
83	BQ	3104	U
83	BQ	3109	G
83	BQ	3111	U
83	BQ	3112	G
83	BQ	3113	A
83	BQ	3115	C
83	BQ	3116	G
83	BQ	3117	C
83	BQ	3119	U
83	BQ	3120	C
83	BQ	3122	A
83	BQ	3123	A
83	BQ	3126	C
83	BQ	3129	A
83	BQ	3130	A
83	BQ	3131	U
83	BQ	3138	U
83	BQ	3142	A
83	BQ	3143	C
83	BQ	3144	G
83	BQ	3152	U
83	BQ	3153	U
83	BQ	3154	C
83	BQ	3155	U
83	BQ	3156	U
83	BQ	3157	U
83	BQ	3158	G
83	BQ	3168	A
83	BQ	3171	U
83	BQ	3172	A
83	BQ	3173	G
83	BQ	3174	A
83	BQ	3175	U

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Mol	Chain	Res	Type
83	BQ	3176	G
83	BQ	3178	A
83	BQ	3179	U
83	BQ	3180	A
83	BQ	3181	C
83	BQ	3183	A
83	BQ	3185	U
83	BQ	3187	A
83	BQ	3193	C
83	BQ	3194	C
83	BQ	3195	U
83	BQ	3197	G
83	BQ	3198	U
83	BQ	3206	C
83	BQ	3207	U
83	BQ	3208	G
83	BQ	3209	A
83	BQ	3210	A
83	BQ	3216	G
83	BQ	3217	C
83	BQ	3218	A
83	BQ	3220	G
83	BQ	3224	G
83	BQ	3227	A
83	BQ	3228	C
83	BQ	3229	G
83	BQ	3231	U
83	BQ	3237	U
83	BQ	3238	G
83	BQ	3241	G
83	BQ	3242	G
83	BQ	3244	A
83	BQ	3245	A
83	BQ	3246	G
83	BQ	3247	G
83	BQ	3259	U
83	BQ	3261	C
83	BQ	3262	U
83	BQ	3263	G
83	BQ	3268	A
83	BQ	3269	U
83	BQ	3270	U

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Mol	Chain	Res	Type
83	BQ	3271	G
83	BQ	3272	C
83	BQ	3273	A
83	BQ	3274	A
83	BQ	3275	U
83	BQ	3276	G
83	BQ	3277	U
83	BQ	3278	C
83	BQ	3279	A
83	BQ	3287	U
83	BQ	3288	G
83	BQ	3289	G
83	BQ	3294	A
83	BQ	3295	A
83	BQ	3304	U
83	BQ	3305	A
83	BQ	3308	C
83	BQ	3313	U
83	BQ	3316	A
83	BQ	3317	U
83	BQ	3318	G
83	BQ	3319	U
83	BQ	3320	A
83	BQ	3322	A
83	BQ	3324	C
83	BQ	3330	A
83	BQ	3334	U
83	BQ	3335	A
83	BQ	3339	A
83	BQ	3342	A
83	BQ	3345	G
83	BQ	3346	U
83	BQ	3347	A
83	BQ	3348	G
83	BQ	3351	U
83	BQ	3352	U
83	BQ	3353	G
83	BQ	3354	U
83	BQ	3355	U
83	BQ	3356	G
83	BQ	3357	U
83	BQ	3362	A

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Mol	Chain	Res	Type
83	BQ	3364	C
83	BQ	3368	U
83	BQ	3369	G
83	BQ	3370	A
83	BQ	3375	A
83	BQ	3378	C
83	BQ	3382	U
83	BQ	3383	G
83	BQ	3390	G
84	BR	10	C
84	BR	11	A
84	BR	13	A
84	BR	14	U
84	BR	19	C
84	BR	20	A
84	BR	22	A
84	BR	23	A
84	BR	26	C
84	BR	29	C
84	BR	32	U
84	BR	33	U
84	BR	41	G
84	BR	42	A
84	BR	49	G
84	BR	53	U
84	BR	54	U
84	BR	55	A
84	BR	56	A
84	BR	65	G
84	BR	71	G
84	BR	73	C
84	BR	74	C
84	BR	77	G
84	BR	78	U
84	BR	79	A
84	BR	87	G
84	BR	91	G
84	BR	99	G
84	BR	101	G
84	BR	102	A
84	BR	103	A
84	BR	111	U

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Mol	Chain	Res	Type
84	BR	112	G
84	BR	121	U
85	BS	8	C
85	BS	15	G
85	BS	16	G
85	BS	17	A
85	BS	22	U
85	BS	23	U
85	BS	24	G
85	BS	34	U
85	BS	35	C
85	BS	39	G
85	BS	40	A
85	BS	49	G
85	BS	50	C
85	BS	51	G
85	BS	52	A
85	BS	59	A
85	BS	60	U
85	BS	61	A
85	BS	62	C
85	BS	63	G
85	BS	80	A
85	BS	81	U
85	BS	82	U
85	BS	83	C
85	BS	84	C
85	BS	85	G
85	BS	86	U
85	BS	87	G
85	BS	90	U
85	BS	91	C
85	BS	95	G
85	BS	97	A
85	BS	102	U
85	BS	104	A
85	BS	106	C
85	BS	110	C
85	BS	112	U
85	BS	113	U
85	BS	115	C
85	BS	116	G

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Mol	Chain	Res	Type
85	BS	125	U
85	BS	126	A
85	BS	127	U
85	BS	129	C
85	BS	144	G
85	BS	148	G
85	BS	151	C
85	BS	152	G
85	BS	154	C
85	BS	158	U

All (294) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	42	G
1	2	51	A
1	2	52	U
1	2	53	G
1	2	54	C
1	2	55	A
1	2	66	U
1	2	68	A
1	2	77	U
1	2	104	A
1	2	114	C
1	2	115	G
1	2	126	A
1	2	128	U
1	2	132	U
1	2	139	C
1	2	141	U
1	2	158	U
1	2	159	U
1	2	174	U
1	2	224	C
1	2	266	A
1	2	278	U
1	2	280	U
1	2	312	A
1	2	313	U
1	2	322	G
1	2	352	A

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Mol	Chain	Res	Type
1	2	379	U
1	2	380	U
1	2	381	C
1	2	385	A
1	2	387	A
1	2	400	A
1	2	410	A
1	2	411	C
1	2	425	A
1	2	429	G
1	2	430	G
1	2	439	U
1	2	454	U
1	2	539	G
1	2	541	A
1	2	555	A
1	2	578	U
1	2	609	U
1	2	613	G
1	2	619	A
1	2	639	U
1	2	696	C
1	2	699	U
1	2	705	U
1	2	711	U
1	2	754	A
1	2	765	G
1	2	766	U
1	2	782	U
1	2	819	G
1	2	913	G
1	2	928	U
1	2	944	A
1	2	1023	A
1	2	1081	A
1	2	1092	A
1	2	1108	G
1	2	1114	G
1	2	1173	C
1	2	1185	U
1	2	1193	A
1	2	1226	A

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Mol	Chain	Res	Type
1	2	1244	A
1	2	1245	G
1	2	1251	U
1	2	1256	A
1	2	1273	G
1	2	1274	C
1	2	1314	U
1	2	1344	A
1	2	1357	A
1	2	1369	U
1	2	1370	U
1	2	1382	A
1	2	1399	C
1	2	1412	G
1	2	1430	U
1	2	1457	C
1	2	1472	C
1	2	1481	C
1	2	1520	U
1	2	1539	G
1	2	1570	A
1	2	1573	A
1	2	1601	G
1	2	1615	C
1	2	1633	A
1	2	1636	C
1	2	1742	U
1	2	1761	U
1	2	1767	G
1	2	1791	A
83	BQ	13	A
83	BQ	21	G
83	BQ	40	A
83	BQ	43	A
83	BQ	66	A
83	BQ	71	A
83	BQ	86	G
83	BQ	97	U
83	BQ	154	U
83	BQ	155	G
83	BQ	189	G
83	BQ	211	A

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Mol	Chain	Res	Type
83	BQ	269	G
83	BQ	282	G
83	BQ	316	U
83	BQ	349	A
83	BQ	352	A
83	BQ	353	G
83	BQ	369	A
83	BQ	374	A
83	BQ	376	G
83	BQ	400	G
83	BQ	411	U
83	BQ	494	G
83	BQ	547	G
83	BQ	556	U
83	BQ	588	G
83	BQ	611	A
83	BQ	621	A
83	BQ	677	A
83	BQ	715	A
83	BQ	764	U
83	BQ	767	U
83	BQ	775	A
83	BQ	786	A
83	BQ	806	A
83	BQ	816	A
83	BQ	822	G
83	BQ	895	A
83	BQ	896	A
83	BQ	916	G
83	BQ	921	A
83	BQ	923	C
83	BQ	924	G
83	BQ	933	A
83	BQ	961	C
83	BQ	978	G
83	BQ	979	U
83	BQ	980	A
83	BQ	993	G
83	BQ	1064	A
83	BQ	1095	U
83	BQ	1096	U
83	BQ	1103	A

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Mol	Chain	Res	Type
83	BQ	1116	G
83	BQ	1144	U
83	BQ	1152	G
83	BQ	1154	A
83	BQ	1177	G
83	BQ	1222	G
83	BQ	1241	U
83	BQ	1253	U
83	BQ	1307	G
83	BQ	1352	A
83	BQ	1355	A
83	BQ	1392	G
83	BQ	1417	G
83	BQ	1418	A
83	BQ	1429	G
83	BQ	1467	A
83	BQ	1481	A
83	BQ	1482	A
83	BQ	1483	G
83	BQ	1511	U
83	BQ	1554	U
83	BQ	1568	U
83	BQ	1580	A
83	BQ	1607	U
83	BQ	1695	U
83	BQ	1724	U
83	BQ	1729	A
83	BQ	1730	G
83	BQ	1751	G
83	BQ	1808	G
83	BQ	1815	U
83	BQ	1816	A
83	BQ	1820	U
83	BQ	1839	A
83	BQ	1840	U
83	BQ	1846	C
83	BQ	1847	A
83	BQ	1849	C
83	BQ	1850	A
83	BQ	1885	U
83	BQ	1900	A
83	BQ	1913	A

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Mol	Chain	Res	Type
83	BQ	2101	C
83	BQ	2112	U
83	BQ	2116	G
83	BQ	2138	A
83	BQ	2144	A
83	BQ	2159	U
83	BQ	2177	G
83	BQ	2178	A
83	BQ	2198	A
83	BQ	2208	A
83	BQ	2256	A
83	BQ	2273	G
83	BQ	2279	A
83	BQ	2281	A
83	BQ	2282	U
83	BQ	2283	G
83	BQ	2305	G
83	BQ	2313	A
83	BQ	2433	U
83	BQ	2434	U
83	BQ	2445	A
83	BQ	2493	U
83	BQ	2495	C
83	BQ	2500	A
83	BQ	2501	U
83	BQ	2513	U
83	BQ	2514	U
83	BQ	2525	G
83	BQ	2539	C
83	BQ	2541	U
83	BQ	2549	G
83	BQ	2554	A
83	BQ	2586	G
83	BQ	2593	A
83	BQ	2617	U
83	BQ	2625	C
83	BQ	2665	U
83	BQ	2677	G
83	BQ	2680	A
83	BQ	2689	A
83	BQ	2703	A
83	BQ	2727	A

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Mol	Chain	Res	Type
83	BQ	2754	G
83	BQ	2794	G
83	BQ	2801	A
83	BQ	2803	A
83	BQ	2816	G
83	BQ	2898	G
83	BQ	2911	A
83	BQ	2941	A
83	BQ	2950	G
83	BQ	2953	U
83	BQ	2954	U
83	BQ	2971	A
83	BQ	3011	A
83	BQ	3021	A
83	BQ	3022	G
83	BQ	3047	U
83	BQ	3048	A
83	BQ	3057	U
83	BQ	3078	U
83	BQ	3093	C
83	BQ	3143	C
83	BQ	3156	U
83	BQ	3172	A
83	BQ	3175	U
83	BQ	3179	U
83	BQ	3196	U
83	BQ	3216	G
83	BQ	3219	G
83	BQ	3241	G
83	BQ	3269	U
83	BQ	3272	C
83	BQ	3274	A
83	BQ	3293	U
83	BQ	3317	U
83	BQ	3344	A
83	BQ	3345	G
83	BQ	3350	C
83	BQ	3353	G
83	BQ	3382	U
84	BR	12	U
84	BR	32	U
84	BR	41	G

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Mol	Chain	Res	Type
84	BR	54	U
84	BR	77	G
84	BR	86	U
84	BR	111	U
85	BS	22	U
85	BS	23	U
85	BS	33	A
85	BS	34	U
85	BS	39	G
85	BS	48	A
85	BS	58	G
85	BS	85	G
85	BS	112	U
85	BS	125	U

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

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	$\#\|Z\| > 2$
86	5CT	BT	51	86	13,14,15	0.34	0	9,15,17	1.20	2 (22%)

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
86	5CT	BT	51	86	-	5/13/14/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	BT	51	5CT	C1-NZ-CE	-2.30	108.27	113.42
86	BT	51	5CT	C4-C3-C2	-2.03	109.19	113.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	BT	51	5CT	O-C-CA-CB
86	BT	51	5CT	C2-C3-C4-N1
86	BT	51	5CT	CG-CD-CE-NZ
86	BT	51	5CT	C2-C1-NZ-CE
86	BT	51	5CT	CD-CE-NZ-C1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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
1	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	52:U	O3'	53:G	P	1.89

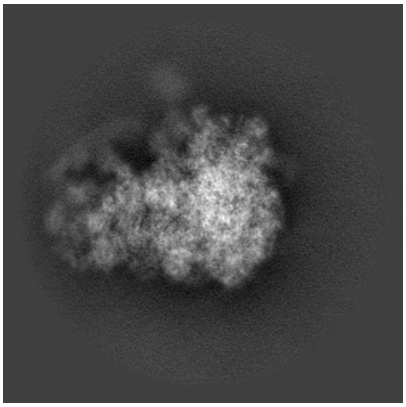
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3461. These allow visual inspection of the internal detail of the map and identification of artifacts.

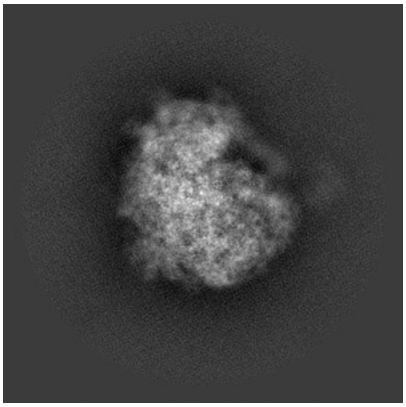
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

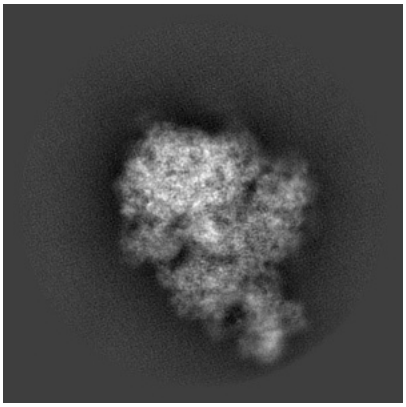
6.1.1 Primary map



X



Y

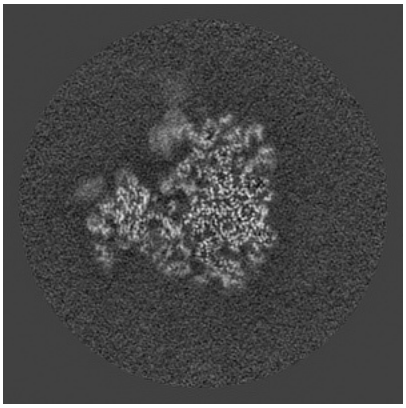


Z

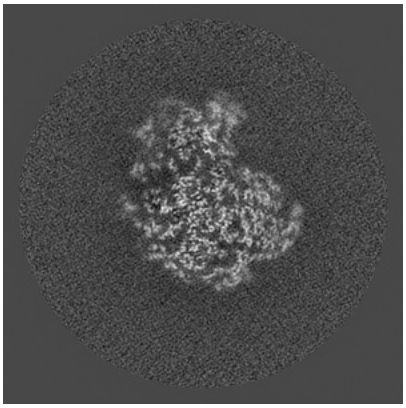
The images above show the map projected in three orthogonal directions.

6.2 Central slices

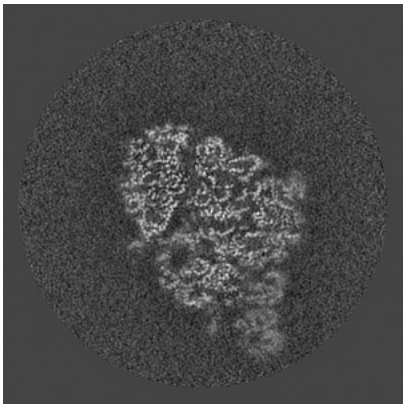
6.2.1 Primary map



X Index: 240



Y Index: 240

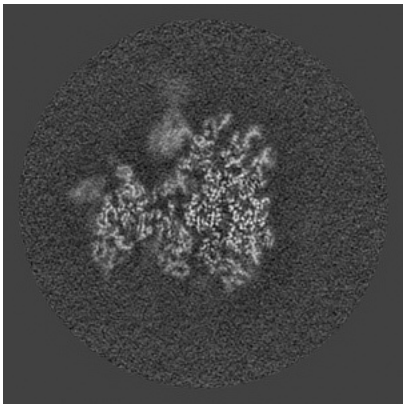


Z Index: 240

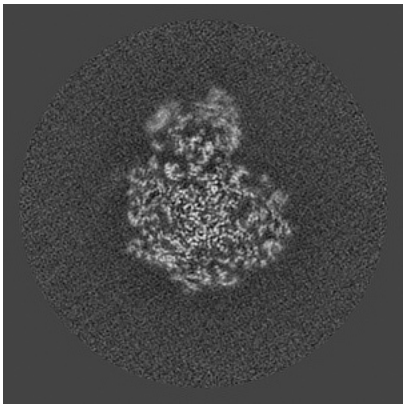
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

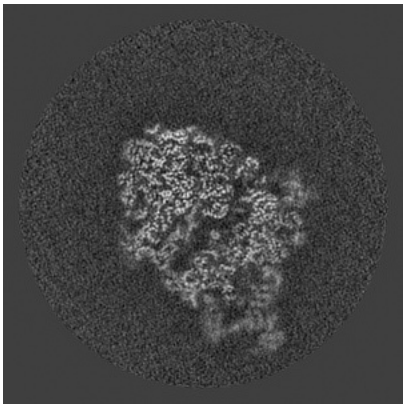
6.3.1 Primary map



X Index: 245



Y Index: 253

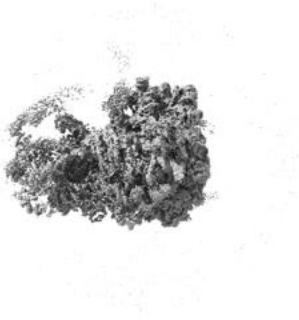


Z Index: 247

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

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

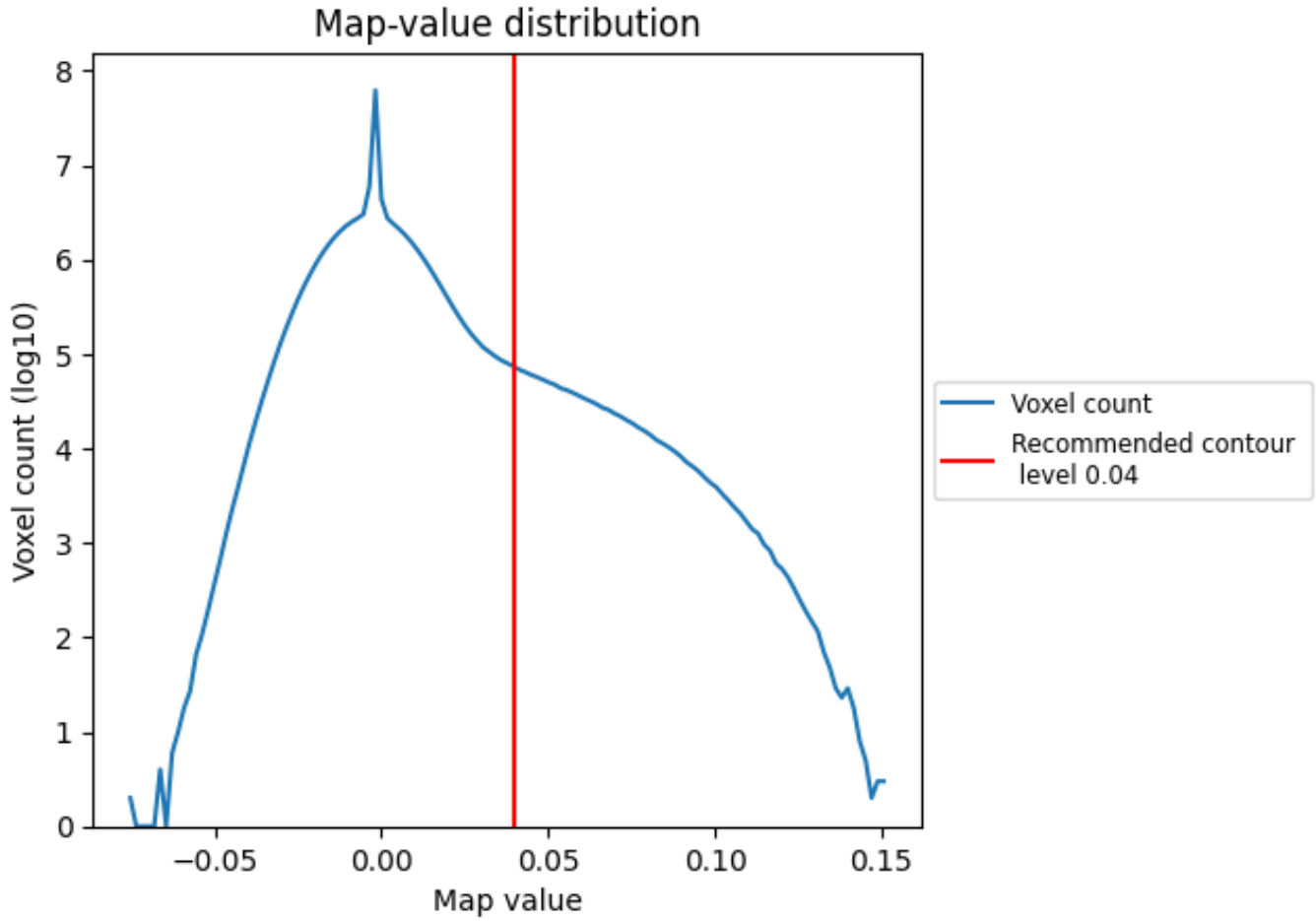
6.5 Mask visualisation (i)

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

7 Map analysis

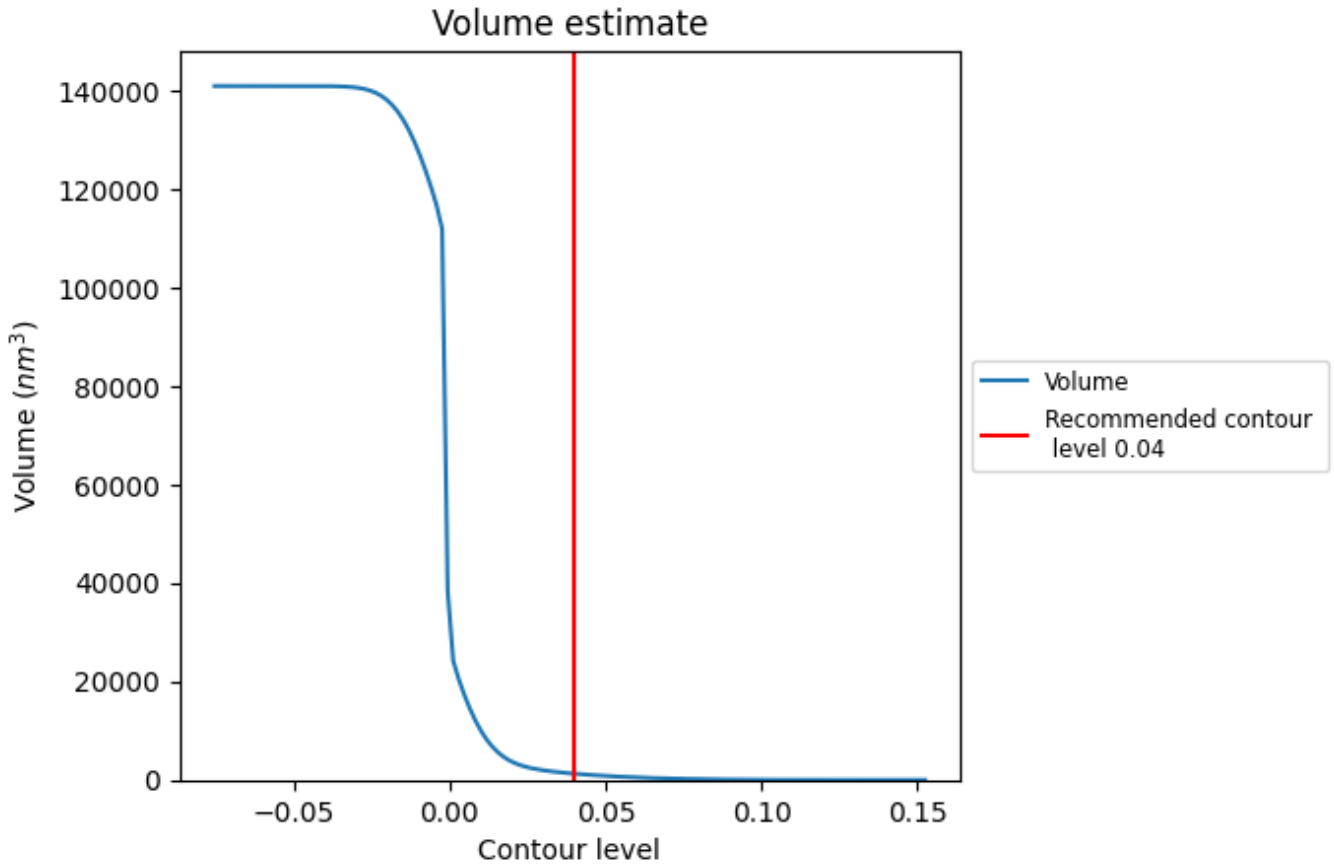
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

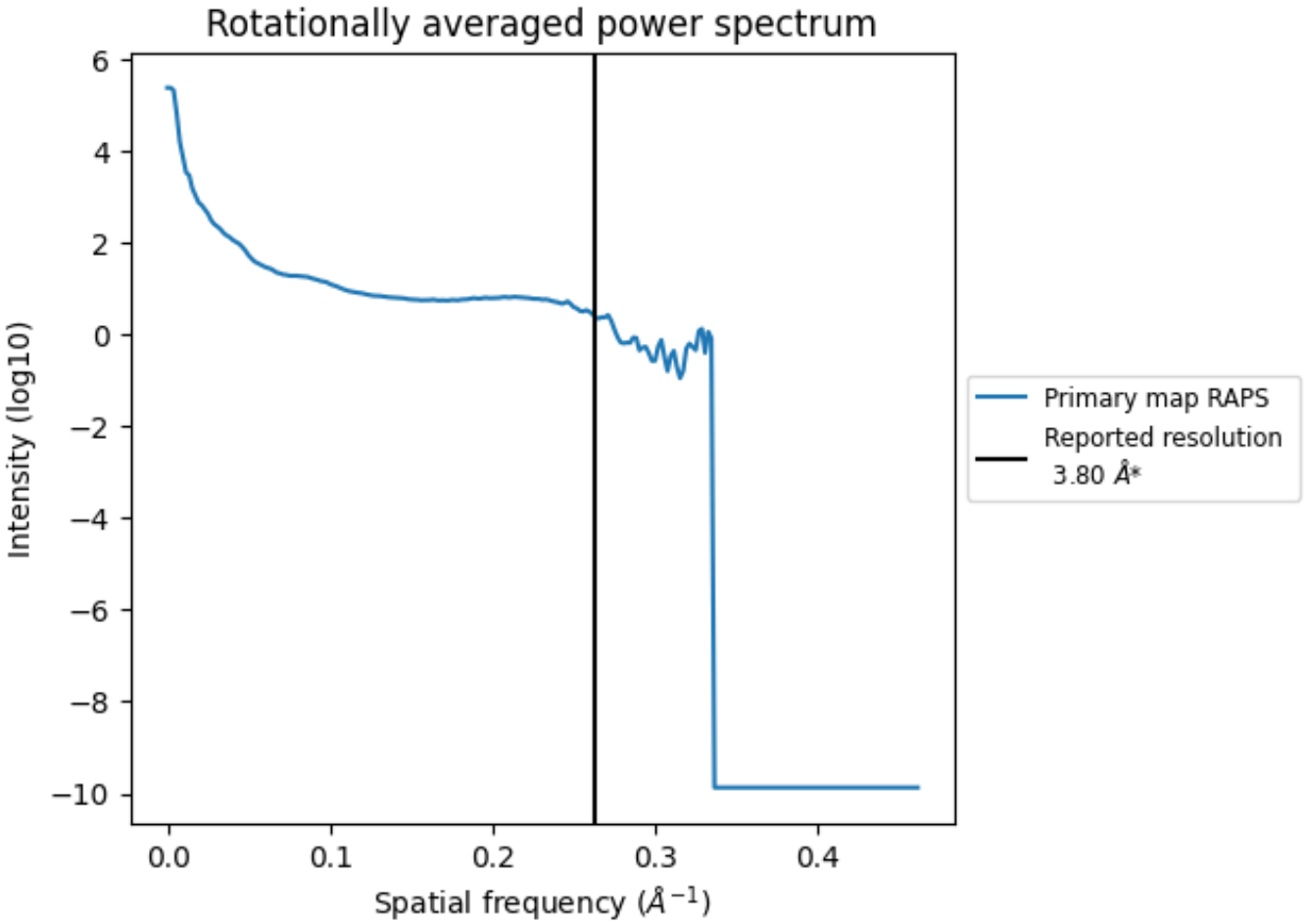
7.2 Volume estimate



The volume at the recommended contour level is 1270 nm^3; this corresponds to an approximate mass of 1147 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

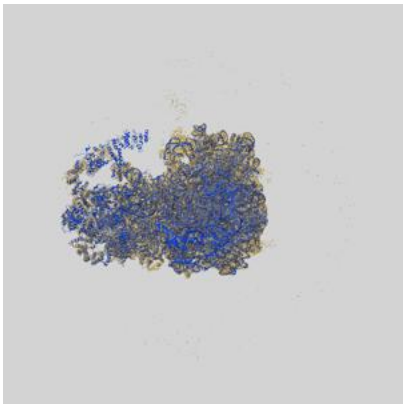
8 Fourier-Shell correlation (i)

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

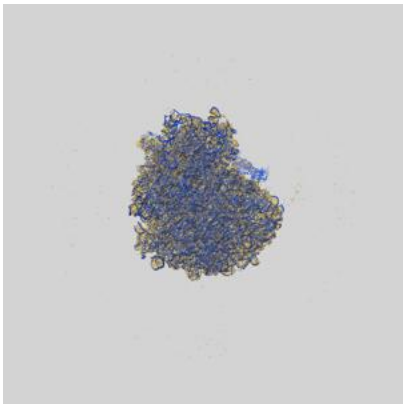
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3461 and PDB model 5MC6. Per-residue inclusion information can be found in section 3 on page 20.

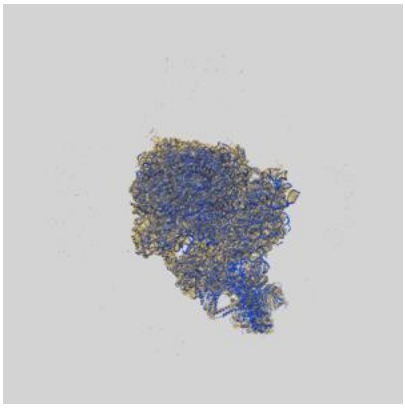
9.1 Map-model overlay



X



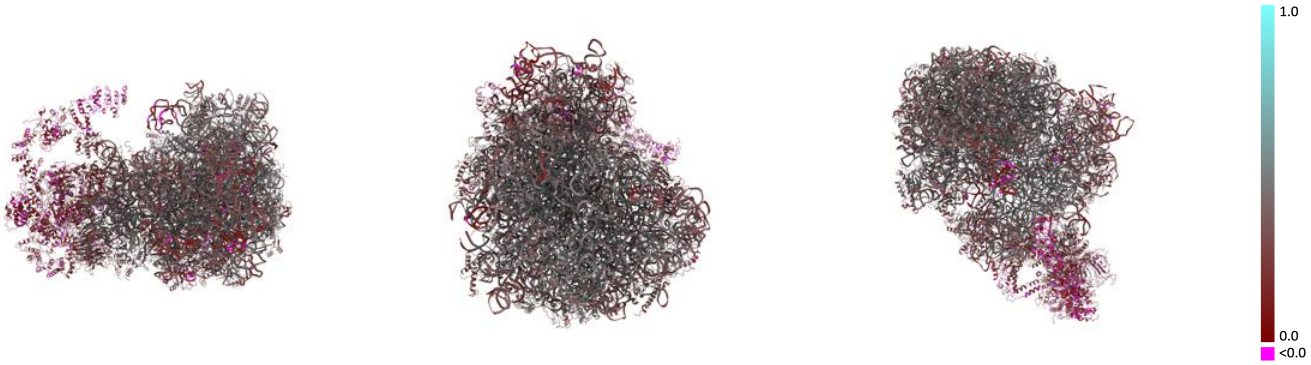
Y



Z

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.

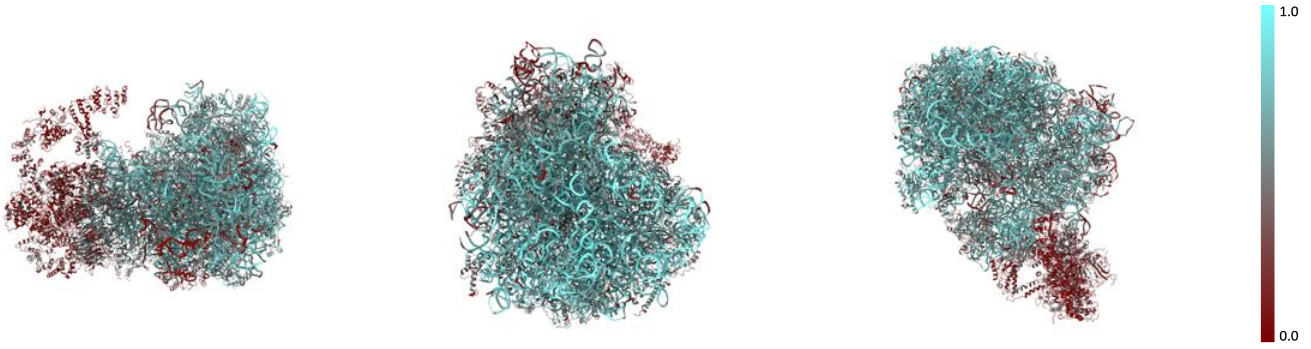
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

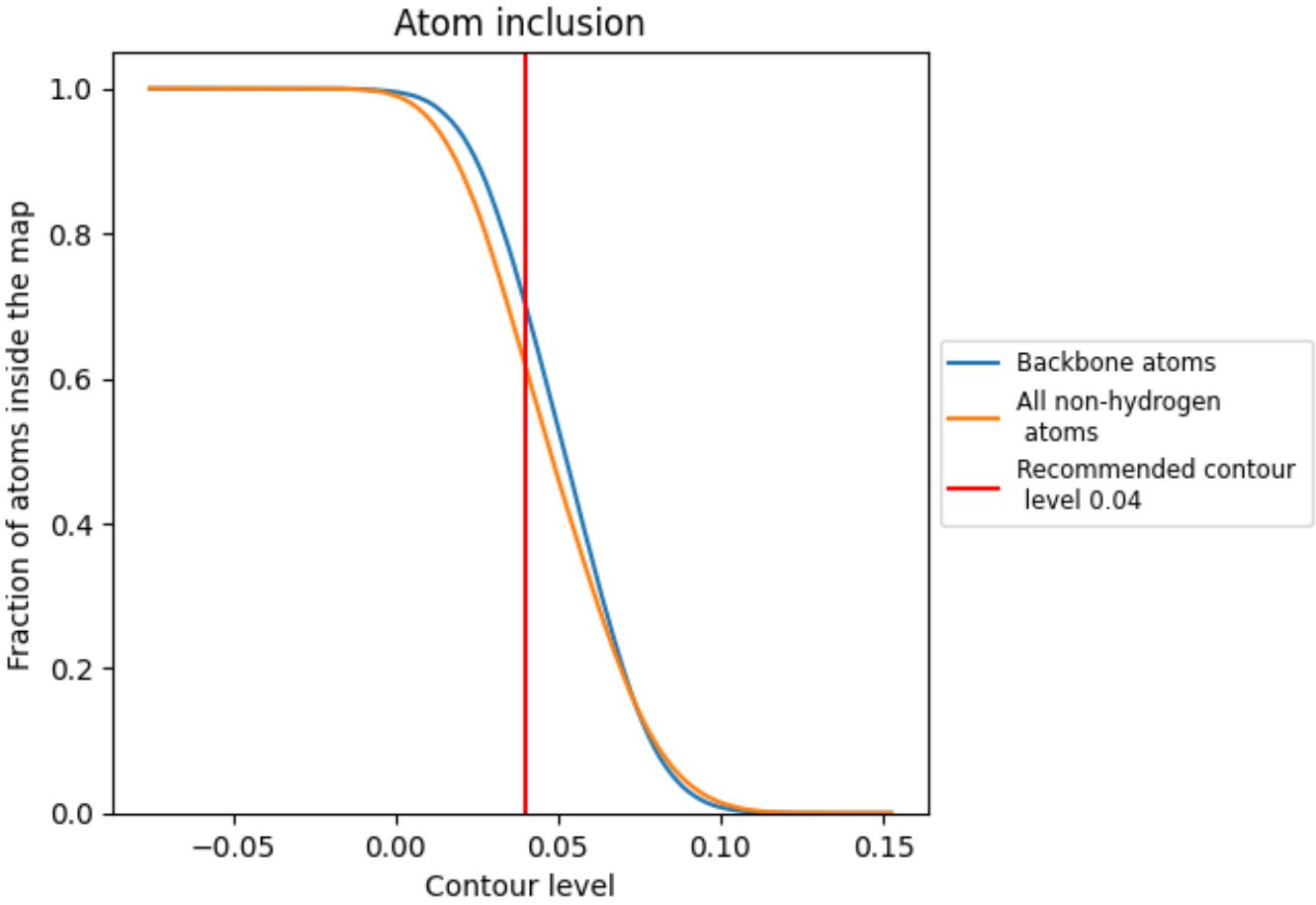
9.3 Atom inclusion mapped to coordinate model



X Y Z

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, 70% of all backbone atoms, 62% 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	0.6174	0.3620
2	0.7276	0.3590
A	0.4944	0.3910
AA	0.5147	0.3680
AB	0.5169	0.4220
AC	0.5584	0.3700
AD	0.5208	0.3780
AE	0.4085	0.3450
AF	0.6687	0.4610
AG	0.5802	0.3740
AH	0.6242	0.4290
AI	0.5159	0.3720
AJ	0.5992	0.3970
AK	0.6429	0.4260
AL	0.6241	0.4640
AM	0.5595	0.3630
AN	0.5397	0.3760
AO	0.5856	0.4030
AP	0.5882	0.4350
AQ	0.6359	0.4330
AR	0.6322	0.4220
AS	0.4009	0.3980
AT	0.5590	0.4280
AU	0.5951	0.4140
AV	0.5686	0.3950
AW	0.5982	0.4500
AX	0.6265	0.4410
AY	0.5164	0.3840
AZ	0.1600	0.3360
B	0.4322	0.3190
BA	0.6074	0.4230
BB	0.6194	0.4260
BC	0.5776	0.4330
BD	0.5236	0.3950
BE	0.6266	0.4240

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Chain	Atom inclusion	Q-score
BF	0.5682	0.3980
BG	0.6016	0.4350
BH	0.5735	0.4020
BI	0.5982	0.3630
BJ	0.5685	0.4280
BK	0.6127	0.4340
BL	0.5358	0.3630
BM	0.5598	0.3760
BN	0.5852	0.4230
BO	0.6062	0.3950
BP	0.6193	0.3980
BQ	0.8208	0.4040
BR	0.8841	0.4050
BS	0.8616	0.4220
BT	0.1121	0.2900
C	0.4711	0.3480
D	0.2722	0.2450
E	0.4299	0.2960
F	0.5134	0.3470
G	0.4917	0.3700
H	0.4705	0.3120
I	0.4422	0.2390
J	0.4857	0.3610
K	0.4516	0.2770
L	0.3312	0.3320
M	0.6288	0.4270
N	0.2972	0.1920
O	0.4575	0.3280
P	0.5107	0.3600
Q	0.4163	0.3170
R	0.5481	0.4150
S	0.4374	0.3460
T	0.4164	0.3090
U	0.3127	0.2740
V	0.4666	0.2950
W	0.5198	0.3250
X	0.4484	0.3800
Y	0.4978	0.3600
Z	0.4838	0.3360
a	0.5000	0.3860
b	0.5381	0.4090
c	0.4945	0.4090

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Chain	Atom inclusion	Q-score
d	0.4222	0.2950
e	0.4357	0.3140
f	0.4359	0.3540
g	0.4420	0.3550
h	0.1761	0.2120
i	0.1487	0.1490
j	0.1567	0.1890
k	0.2925	0.2970
l	0.3367	0.3130
m	0.6034	0.3260
n	0.6442	0.3490