Full wwPDB EM Validation Report

Dec 12, 2022 – 07:10 am GMT

PDB ID	:	6XYW
EMDB ID	:	EMD-10654
Title	:	Structure of the plant mitochondrial ribosome
Authors	:	Soufari, H.; Waltz, F.; Bochler, A.; Giege, P.; Hashem, Y.
Deposited on	:	2020-01-31
Resolution	:	3.86 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:

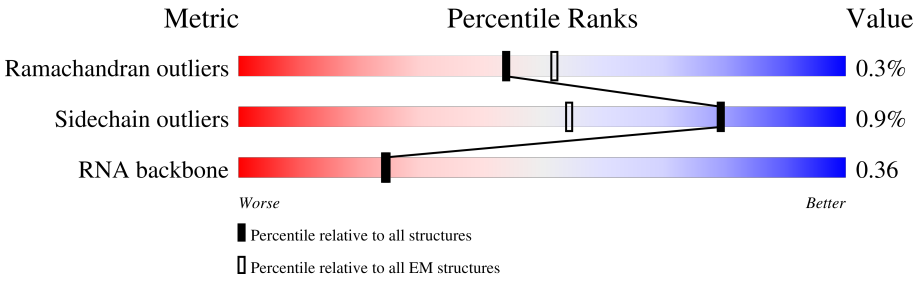
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.86 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	Aa	349	27% 72%
2	Ab	214	72% 28%
3	Ac	324	67% 33%
4	AD	173	35% 65%
5	Ad	300	69% 30%
6	Ae	185	11% 77% 22%
7	Af	102	55% 98%
8	Ag	221	23% 77%

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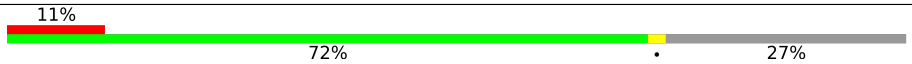
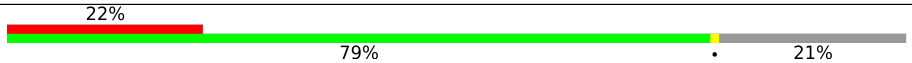
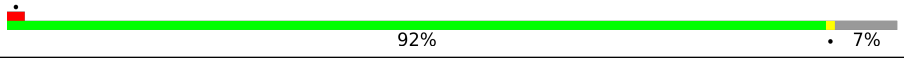
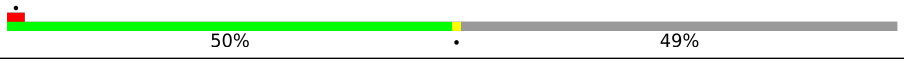
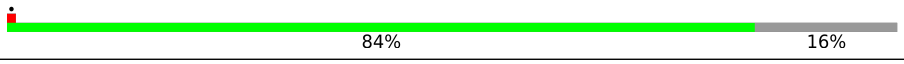
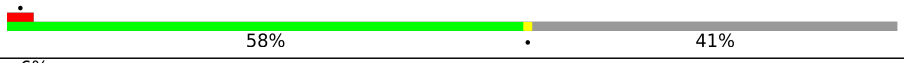
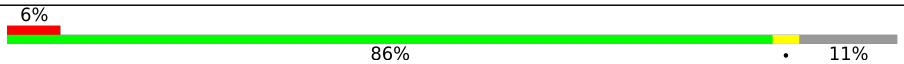
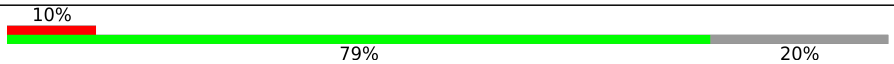
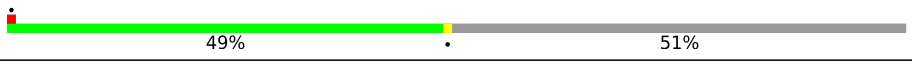
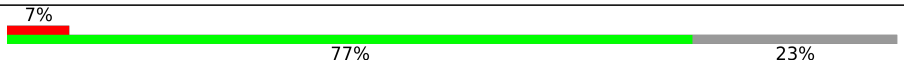
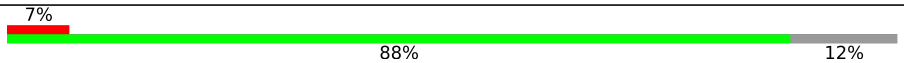
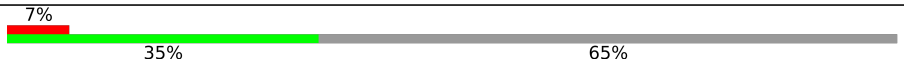
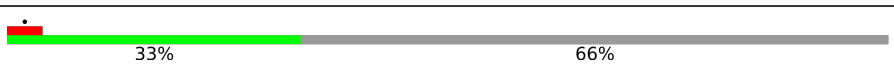
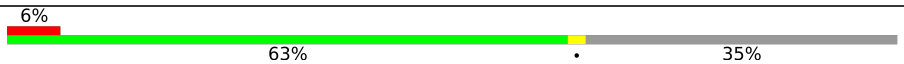
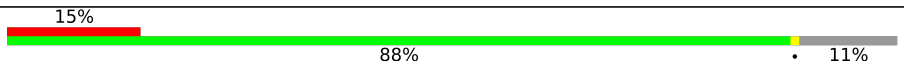
Mol	Chain	Length	Quality of chain
9	Ai	155	
10	Aj	205	
11	Ak	173	
12	Al	281	
13	Am	179	
14	An	160	
15	Ao	114	
16	Ap	222	
17	Aq	126	
18	Ar	270	
19	As	269	
20	At	178	
21	Au	159	
22	Av	249	
23	Aw	154	
24	Ax	212	
25	Ay	144	
26	AA	76	
27	AB	134	
28	AC	58	
29	AE	103	
30	AF	250	
31	AG	94	
32	AH	146	
33	AI	233	

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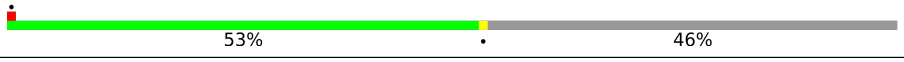
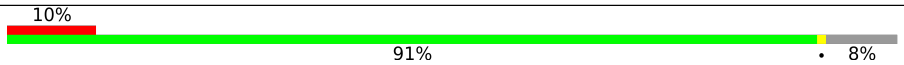
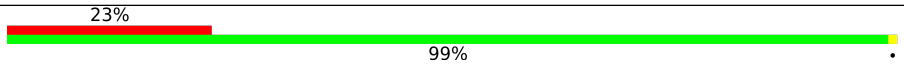
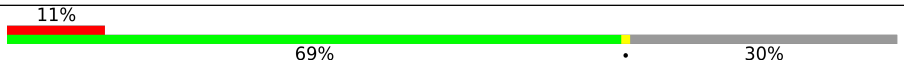
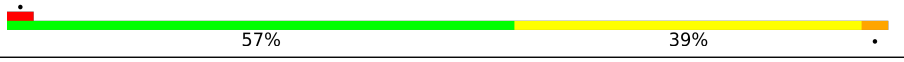
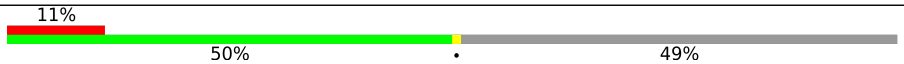
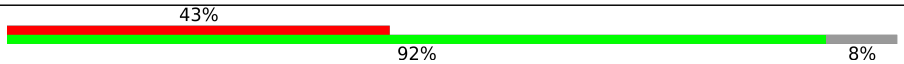
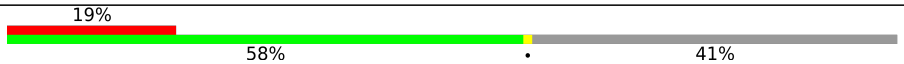
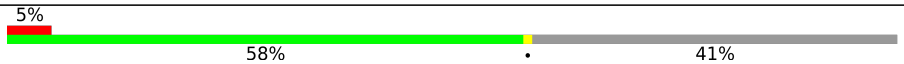
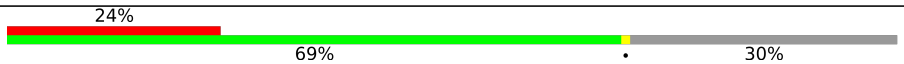
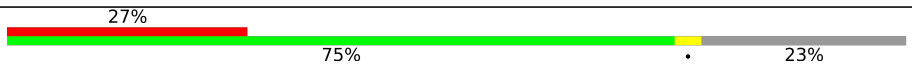
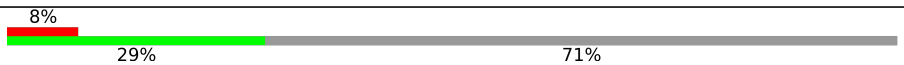
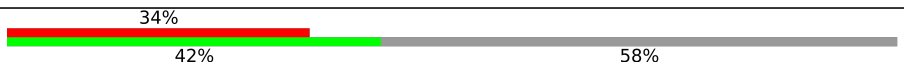
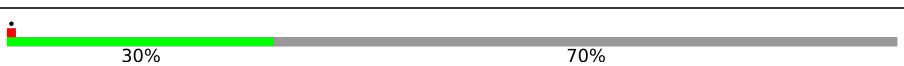
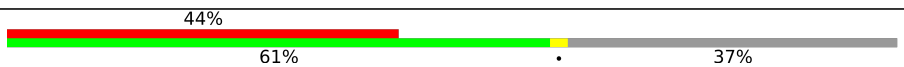
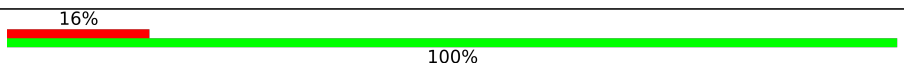
Mol	Chain	Length	Quality of chain
34	AJ	127	
35	AK	130	
36	AL	81	
37	AM	151	
38	AN	188	
39	AO	491	
40	AP	669	
41	AQ	521	
42	AR	29	
43	1	2842	
44	3	118	
45	Bb	556	
46	Bf	148	
47	Bh	430	
48	Bi	241	
49	Bl	154	
50	Bm	164	
51	Br	212	
52	Bw	480	
53	Bx	102	
54	Bz	419	
55	BA	91	
56	Bt	98	
57	BG	576	
58	BP	91	

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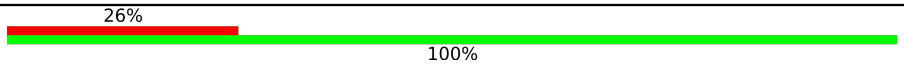
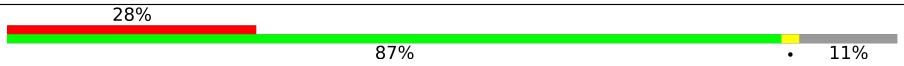
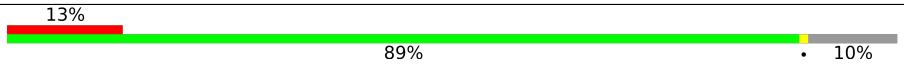
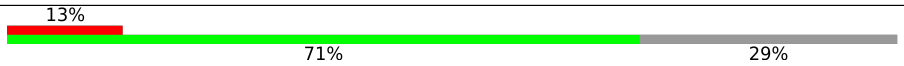
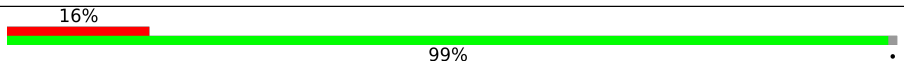
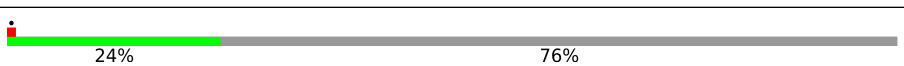
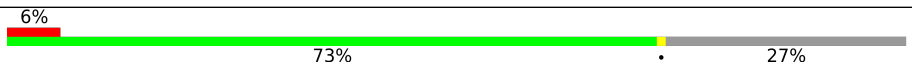
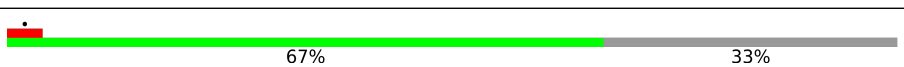
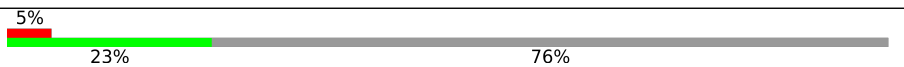
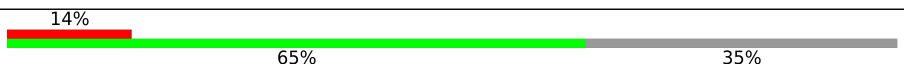
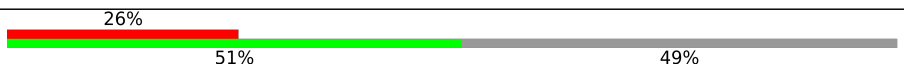
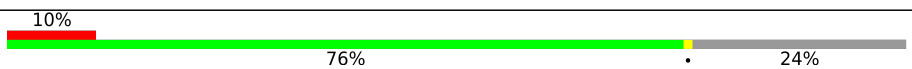
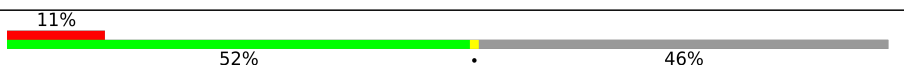
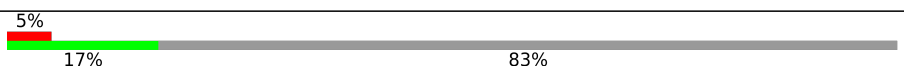
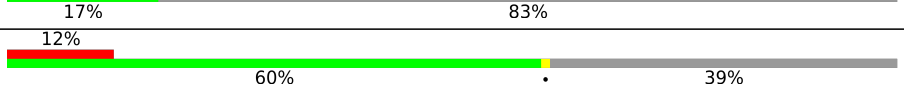
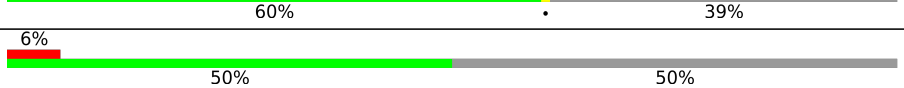
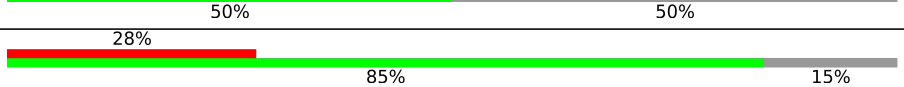
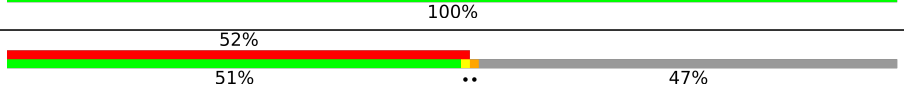
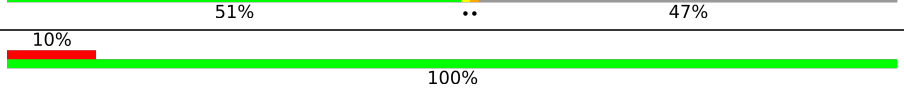
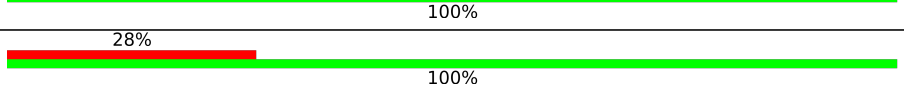
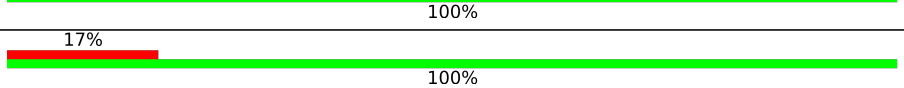
Mol	Chain	Length	Quality of chain
59	BF	123	
60	Ba	219	
61	Bc	362	
62	Bd	515	
63	Be	139	
64	Bg	129	
65	Bj	314	
66	Bn	419	
67	Bo	135	
68	Bp	116	
69	Bq	261	
70	Bs	101	
71	Bu	195	
72	Bv	195	
73	By	142	
74	BB	137	
75	BC	112	
76	BD	420	
77	BE	409	
78	BI	266	
79	BJ	349	
80	BH	390	
81	BN	69	
82	BM	79	
83	BO	30	

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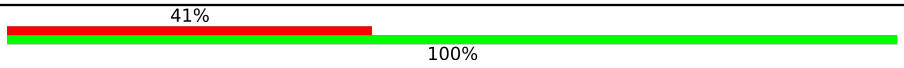
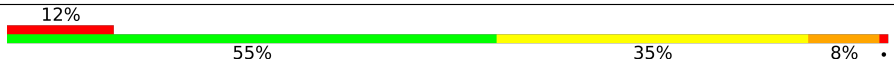
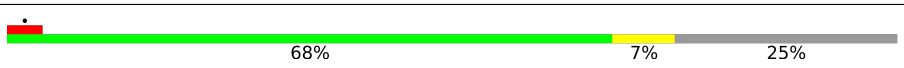
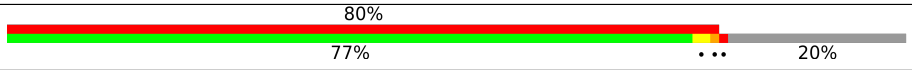
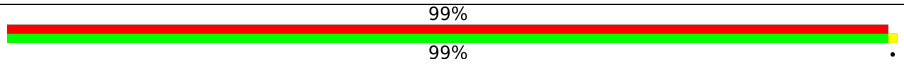
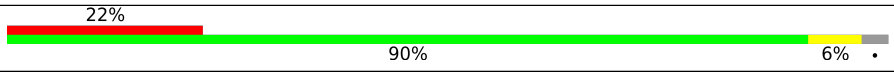
Mol	Chain	Length	Quality of chain
84	BL	64	
85	2	1743	
86	Az	109	
87	Ah	171	
88	BK	316	
89	Bk	125	

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 189336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	96	Total	C	N	O	S	0	0
			753	465	152	133	3		

- Molecule 2 is a protein called Expressed protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	155	Total	C	N	O	S	0	0
			1144	709	224	200	11		

- Molecule 3 is a protein called 50S ribosomal protein L3-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ac	218	Total	C	N	O	S	0	0
			1674	1058	318	288	10		

- Molecule 4 is a protein called Ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	60	Total	C	N	O	S	0	0
			506	327	102	76	1		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ad	209	Total	C	N	O	S	0	0
			1649	1043	311	288	7		

- Molecule 6 is a protein called 60S ribosomal protein L5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ae	144	Total	C	N	O	S	0	0
			1171	760	191	212	8		

- Molecule 7 is a protein called Putative ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Af	100	Total	C	N	O	S	0	0
			797	517	141	134	5		

- Molecule 8 is a protein called Ribosomal protein L9/RNase H1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ag	51	Total	C	N	O	S	0	0
			406	265	70	70	1		

- Molecule 9 is a protein called At4g35490.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ai	138	Total	C	N	O	S	0	0
			1056	677	182	190	7		

- Molecule 10 is a protein called At1g01640.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Aj	155	Total	C	N	O	S	0	0
			1267	800	244	217	6		

- Molecule 11 is a protein called 50S ribosomal protein HLP, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ak	127	Total	C	N	O	S	0	0
			962	605	183	169	5		

- Molecule 12 is a protein called Ribosomal protein L18e/L15 superfamily protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Al	180	Total	C	N	O	S	0	0
			1407	897	274	234	2		

- Molecule 13 is a protein called 60S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Am	142	Total	C	N	O	S	0	0
			1111	702	219	182	8		

- Molecule 14 is a protein called At5g09770.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	An	141	Total	C	N	O	S	0	0
			1139	708	228	198	5		

- Molecule 15 is a protein called At5g27820.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ao	106	Total	C	N	O	S	0	0
			835	532	152	146	5		

- Molecule 16 is a protein called At1g24240/F3I6_17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ap	114	Total	C	N	O	S	0	0
			935	600	178	155	2		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Aq	106	Total	C	N	O	S	0	0
			888	557	178	148	5		

- Molecule 18 is a protein called 50S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ar	137	Total	C	N	O	S	0	0
			1106	707	196	201	2		

- Molecule 19 is a protein called AT1G52370 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	As	121	Total	C	N	O	S	0	0
			937	587	184	163	3		

- Molecule 20 is a protein called At4g39880.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	At	105	Total	C	N	O	S	0	0
			840	545	148	145	2		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Au	142	Total	C	N	O	S	0	0
			1112	702	210	196	4		

- Molecule 22 is a protein called Ribosomal protein L25/Gln-tRNA synthetase, anti-codon-binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Av	198	Total	C	N	O	S	0	0
			1523	968	270	281	4		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Aw	76	Total	C	N	O	0	0
			606	387	117	102		

- Molecule 24 is a protein called AT4g31460/F3L17_30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ax	99	Total	C	N	O	S	0	0
			809	511	151	143	4		

- Molecule 25 is a protein called At1g07830/F24B9_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ay	111	Total	C	N	O	S	0	0
			943	592	175	168	8		

- Molecule 26 is a protein called Ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AA	37	Total	C	N	O	S	0	0
			299	187	57	54	1		

- Molecule 27 is a protein called At1g26740/T24P13_11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AB	41	Total	C	N	O	S	0	0
			319	203	67	45	4		

- Molecule 28 is a protein called At3g06320.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AC	51	Total	C	N	O	S	0	0
			432	283	77	70	2		

- Molecule 29 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AE	36	Total	C	N	O	S	0	0
			297	183	63	47	4		

- Molecule 30 is a protein called At4g05400.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AF	84	Total	C	N	O	S	0	0
			663	419	115	127	2		

- Molecule 31 is a protein called At5g40080.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AG	61	Total	C	N	O	S	0	0
			485	316	84	83	2		

- Molecule 32 is a protein called Mitochondrial ribosomal protein L51/S25/CI-B8 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AH	110	Total	C	N	O	S	0	0
			879	553	168	154	4		

- Molecule 33 is a protein called At1g14620/T5E21_15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AI	207	Total	C	N	O	S	0	0
			1714	1118	282	306	8		

- Molecule 34 is a protein called 39S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AJ	81	Total	C	N	O	S	0	0
			632	392	115	121	4		

- Molecule 35 is a protein called At4g22000.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AK	87	Total	C	N	O	S	0	0
			732	456	143	125	8		

- Molecule 36 is a protein called Uncharacterized protein At1g27435/F17L21.30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AL	52	Total	C	N	O	S	0	0
			400	246	82	71	1		

- Molecule 37 is a protein called At1g73940/F2P9_19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AM	82	Total	C	N	O	S	0	0
			651	425	114	108	4		

- Molecule 38 is a protein called At3g51010.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	AN	80	Total	C	N	O	S	0	0
			664	406	141	115	2		

- Molecule 39 is a protein called Pentatricopeptide repeat-containing protein At1g60770.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AO	452	Total	C	N	O	S	0	0
			3595	2276	615	682	22		

- Molecule 40 is a protein called rPPR*.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	AP	669	Total	C	N	O	0	0
			3345	2007	669	669		

- Molecule 41 is a protein called Pentatricopeptide repeat-containing protein PNM1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AQ	366	Total	C	N	O	S	0	0
			2900	1835	501	537	27		

- Molecule 42 is a protein called UNK-6.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	AR	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 43 is a RNA chain called RNA (2842-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1	2842	Total	C	N	O	P	6	0
			60842	27171	11068	19760	2843		

- Molecule 44 is a RNA chain called RNA (118-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3	118	Total	C	N	O	P	0	0
			2513	1124	453	819	117		

- Molecule 45 is a protein called Ribosomal protein S3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bb	281	Total	C	N	O	S	0	0
			2293	1489	413	383	8		

- Molecule 46 is a protein called Ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bf	136	Total	C	N	O	S	0	0
			1106	699	216	187	4		

- Molecule 47 is a protein called 30S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Bh	123	Total	C	N	O	S	0	0
			975	616	187	168	4		

- Molecule 48 is a protein called 40S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bi	101	Total	C	N	O	S	0	0
			857	556	161	135	5		

- Molecule 49 is a protein called Small ribosomal subunit protein S13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bl	91	Total	C	N	O	S	0	0
			729	442	153	132	2		

- Molecule 50 is a protein called At2g34520.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bm	96	Total	C	N	O	S	0	0
			794	495	165	130	4		

- Molecule 51 is a protein called 40S ribosomal protein S19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Br	83	Total	C	N	O	S	0	0
			685	439	130	112	4		

- Molecule 52 is a protein called Mitochondrial 28S ribosomal protein S29-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bw	337	Total	C	N	O	S	0	0
			2722	1752	469	488	13		

- Molecule 53 is a protein called 37S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Bx	79	Total	C	N	O	S	0	0
			641	402	125	112	2		

- Molecule 54 is a protein called AT3G18240 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bz	123	Total	C	N	O	S	0	0
			1010	634	198	175	3		

- Molecule 55 is a protein called CX9C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BA	38	Total	C	N	O	S	0	0
			293	181	50	54	8		

- Molecule 56 is a protein called 30S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bt	29	Total	C	N	O	S	0	0
			239	149	50	39	1		

- Molecule 57 is a protein called Pentatricopeptide repeat-containing protein At3g02650, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	BG	364	Total	C	N	O	0	0
			1795	1067	364	364		

- Molecule 58 is a protein called UNK-5.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	BP	91	Total	C	N	O	0	0
			455	273	91	91		

- Molecule 59 is a protein called mS31/mS46.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	BF	123	Total	C	N	O	0	0
			615	369	123	123		

- Molecule 60 is a protein called Ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Ba	195	Total	C	N	O	S	0	0
			1563	1003	276	273	11		

- Molecule 61 is a protein called Ribosomal protein S4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bc	327	Total	C	N	O	S	0	0
			2772	1781	526	454	11		

- Molecule 62 is a protein called At1g64880.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bd	216	Total	C	N	O	S	0	0
			1730	1097	310	317	6		

- Molecule 63 is a protein called Translation elongation factor EF1B/ribosomal protein S6 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Be	99	Total	C	N	O	S	0	0
			819	529	147	137	6		

- Molecule 64 is a protein called 40S ribosomal protein S15a-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bg	128	Total	C	N	O	S	0	0
			1042	657	194	188	3		

- Molecule 65 is a protein called Probable ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Bj	123	Total	C	N	O	S	0	0
			955	590	188	172	5		

- Molecule 66 is a protein called At1g15810/F7H2_23.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bn	100	Total	C	N	O	S	0	0
			814	509	150	149	6		

- Molecule 67 is a protein called 30S ribosomal protein S16-2, chloroplastic/mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bo	99	Total	C	N	O	S	0	0
			780	496	152	127	5		

- Molecule 68 is a protein called Nucleic acid-binding, OB-fold-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bp	78	Total	C	N	O	S	0	0
			636	405	120	108	3		

- Molecule 69 is a protein called F10K1.8 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bq	62	Total	C	N	O	S	0	0
			492	313	91	87	1		

- Molecule 70 is a protein called Ribosomal protein S21 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bs	66	Total	C	N	O	S	0	0
			539	337	106	94	2		

- Molecule 71 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bu	100	Total	C	N	O	S	0	0
			800	508	147	140	5		

- Molecule 72 is a protein called AT5g49210/K21P3_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bv	149	Total	C	N	O	S	0	0
			1278	800	237	237	4		

- Molecule 73 is a protein called 28S ribosomal S34 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	By	76	Total	C	N	O	S	0	0
			619	404	115	98	2		

- Molecule 74 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	BB	23	Total	C	N	O	S	0	0
			203	129	46	27	1		

- Molecule 75 is a protein called At5g26800.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	BC	68	Total	C	N	O	S	0	0
			544	356	99	88	1		

- Molecule 76 is a protein called Gb|AAC32909.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	BD	210	Total	C	N	O	S	0	0
			1768	1113	317	328	10		

- Molecule 77 is a protein called 3-hydroxyisobutyryl-CoA hydrolase-like protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	BE	348	Total	C	N	O	S	0	0
			2697	1716	446	517	18		

- Molecule 78 is a protein called rPPR*.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	BI	266	Total	C	N	O	0	0
			1330	798	266	266		

- Molecule 79 is a protein called rPPR*.

Mol	Chain	Residues	Atoms				AltConf	Trace
79	BJ	349	Total	C	N	O	0	0
			1745	1047	349	349		

- Molecule 80 is a protein called Adenylyl cyclase.

Mol	Chain	Residues	Atoms				AltConf	Trace
80	BH	206	Total	C	N	O	0	0
			1023	611	206	206		

- Molecule 81 is a protein called UNK-3.

Mol	Chain	Residues	Atoms				AltConf	Trace
81	BN	69	Total	C	N	O	0	0
			345	207	69	69		

- Molecule 82 is a protein called UNK-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	BM	79	Total	C	N	O	0	0
			395	237	79	79		

- Molecule 83 is a protein called UNK-4.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	BO	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 84 is a protein called UNK-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
84	BL	64	Total	C	N	O	0	0
			320	192	64	64		

- Molecule 85 is a RNA chain called RNA (1743-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
85	2	1743	Total	C	N	O	P	0	0
			37379	16678	6858	12100	1743		

- Molecule 86 is a protein called At5g55140.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Az	82	Total	C	N	O	S	0	0
			660	406	135	114	5		

- Molecule 87 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Ah	137	Total	C	N	O	S	0	0
			1098	706	187	200	5		

- Molecule 88 is a protein called rPPR*.

Mol	Chain	Residues	Atoms				AltConf	Trace
88	BK	316	Total	C	N	O	0	0
			1580	948	316	316		

- Molecule 89 is a protein called Ribosomal protein S12, mitochondrial.

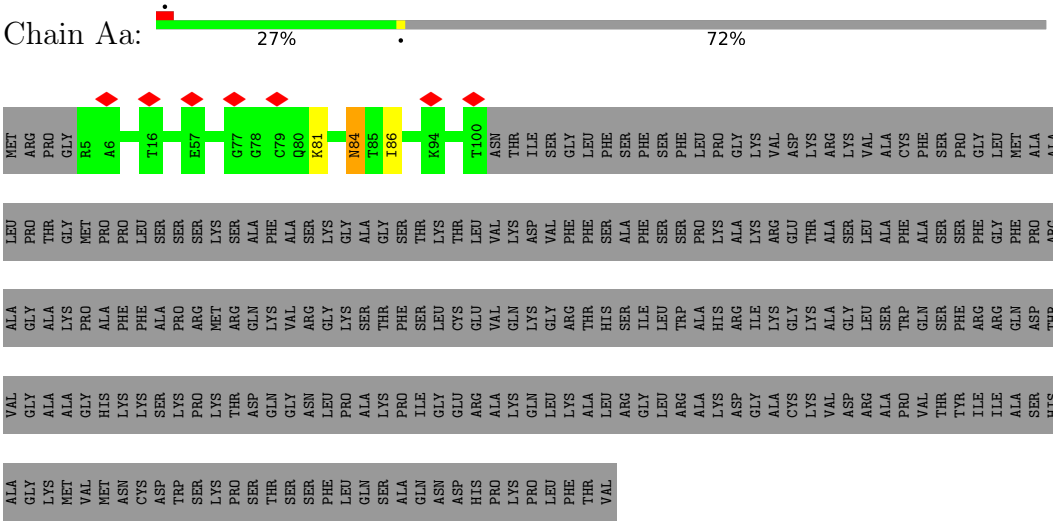
Mol	Chain	Residues	Atoms					AltConf	Trace
89	Bk	121	Total	C	N	O	S	0	0
			968	598	204	162	4		

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.

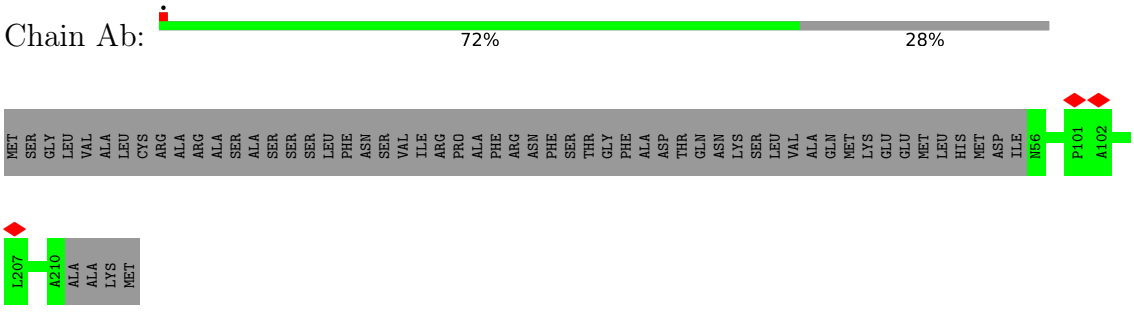
• Molecule 1: 60S ribosomal protein L2, mitochondrial

Chain Aa:



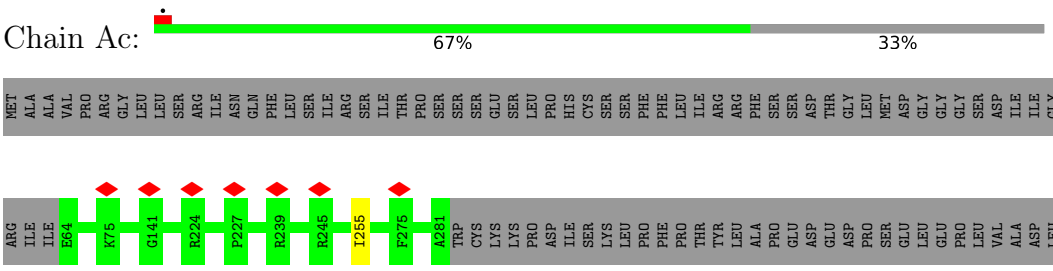
• Molecule 2: Expressed protein

Chain Ab:



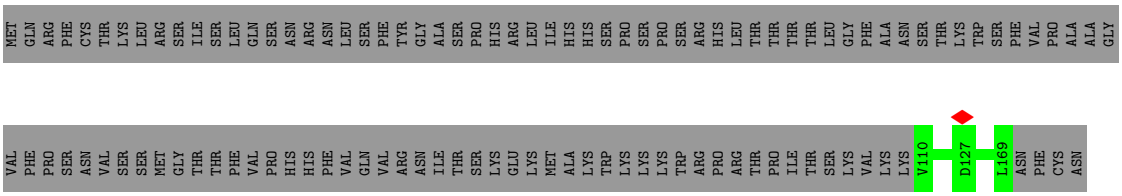
• Molecule 3: 50S ribosomal protein L3-2, mitochondrial

Chain Ac:



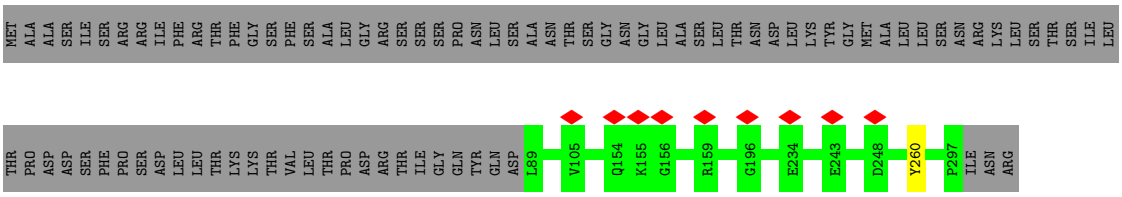
• Molecule 4: Ribosomal protein L35

Chain AD:



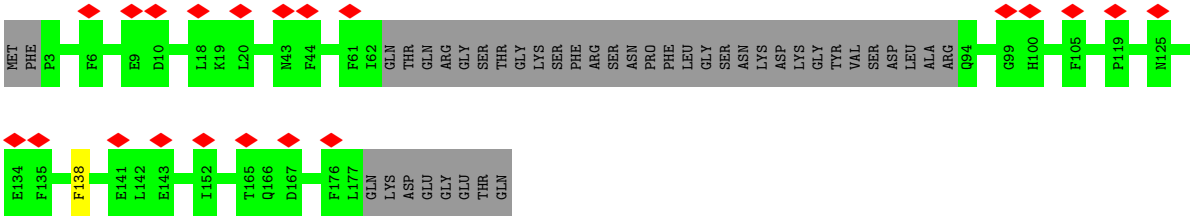
• Molecule 5: 50S ribosomal protein L4

Chain Ad:



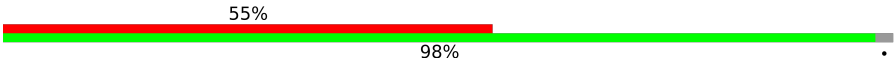
• Molecule 6: 60S ribosomal protein L5, mitochondrial

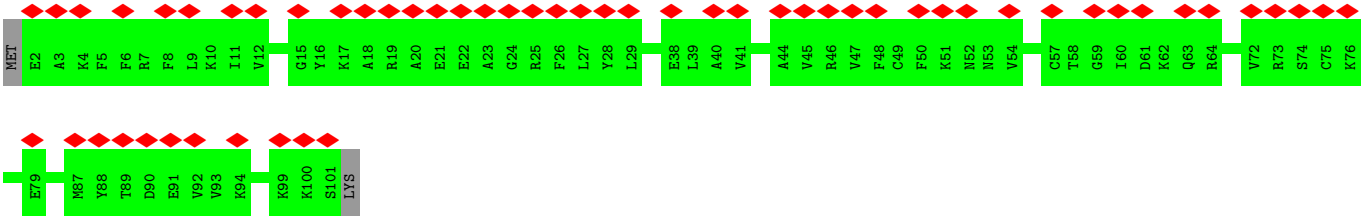
Chain Ae:



• Molecule 7: Putative ribosomal protein L6

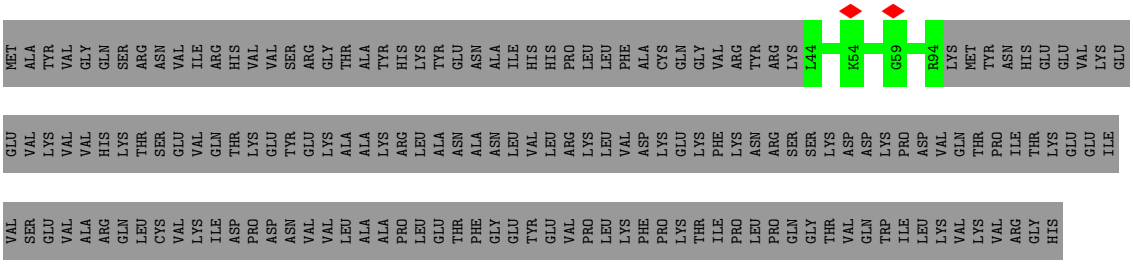
Chain Af:





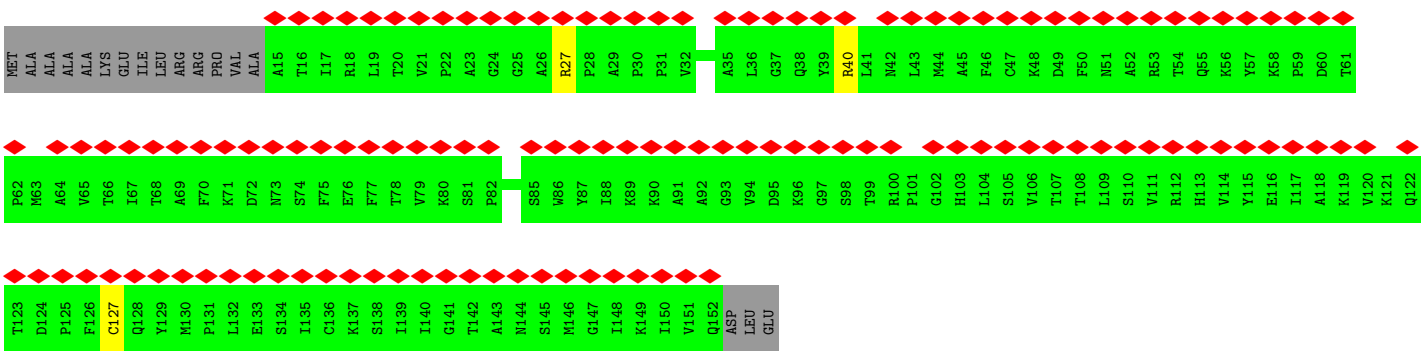
• Molecule 8: Ribosomal protein L9/RNase H1

Chain Ag:



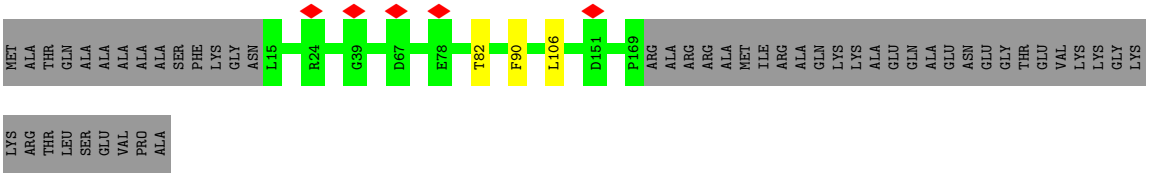
• Molecule 9: At4g35490

Chain Ai:



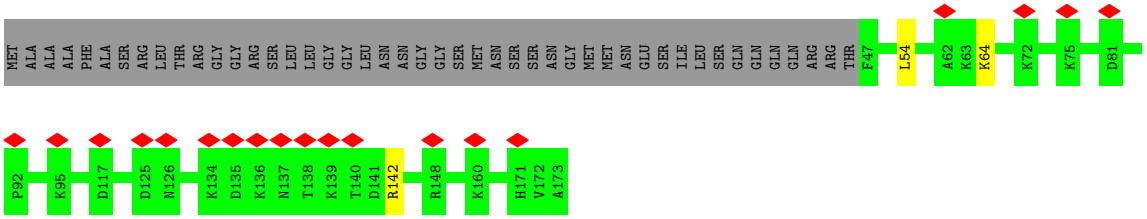
• Molecule 10: At1g01640

Chain Aj:



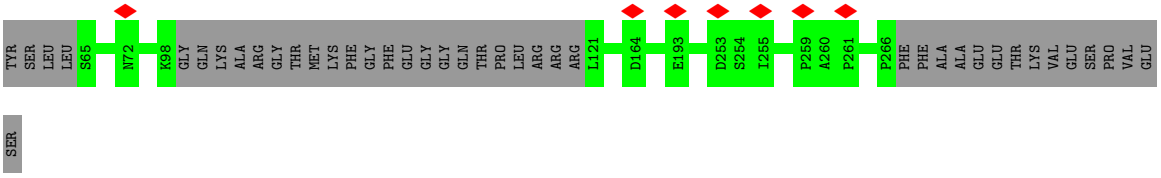
• Molecule 11: 50S ribosomal protein HLP, mitochondrial

Chain Ak:

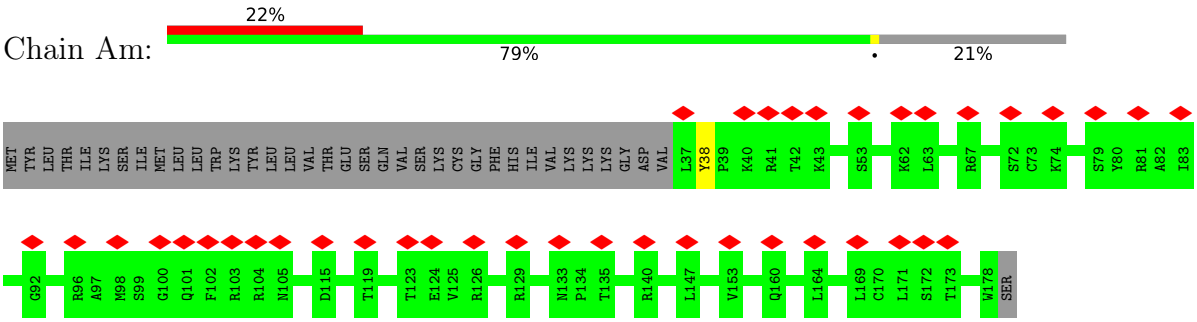


• Molecule 12: Ribosomal protein L18e/L15 superfamily protein

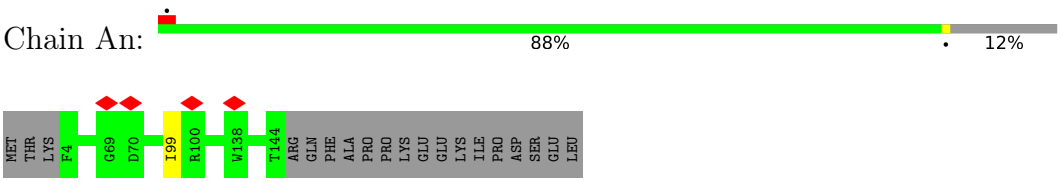
Chain Al:



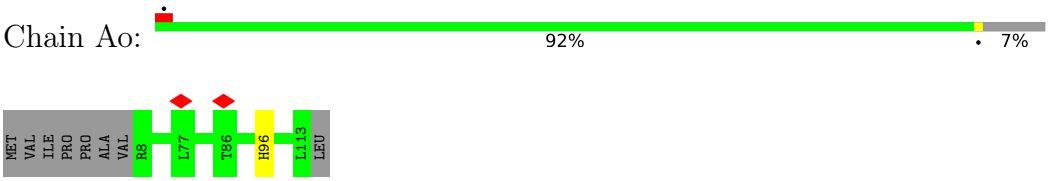
• Molecule 13: 60S ribosomal protein L16, mitochondrial



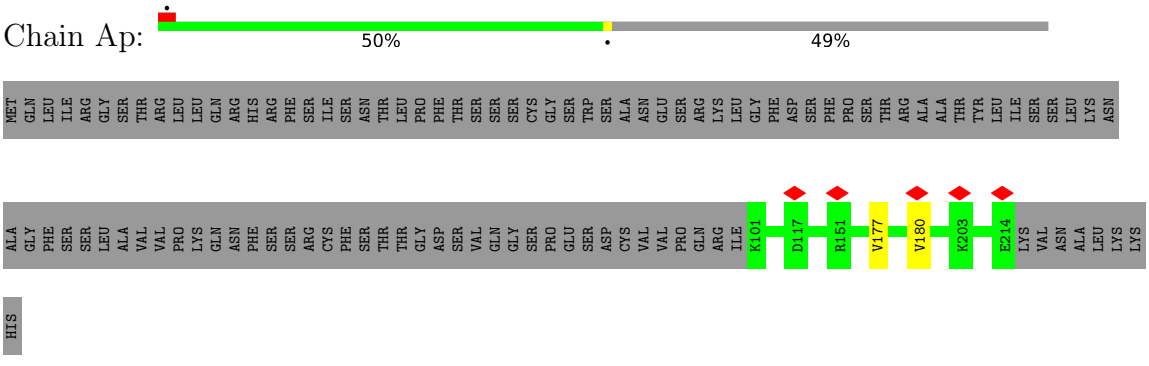
• Molecule 14: At5g09770



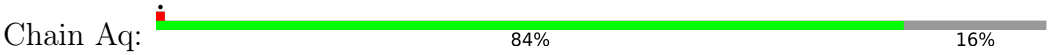
• Molecule 15: At5g27820

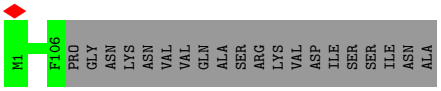


• Molecule 16: At1g24240/F3I6_17



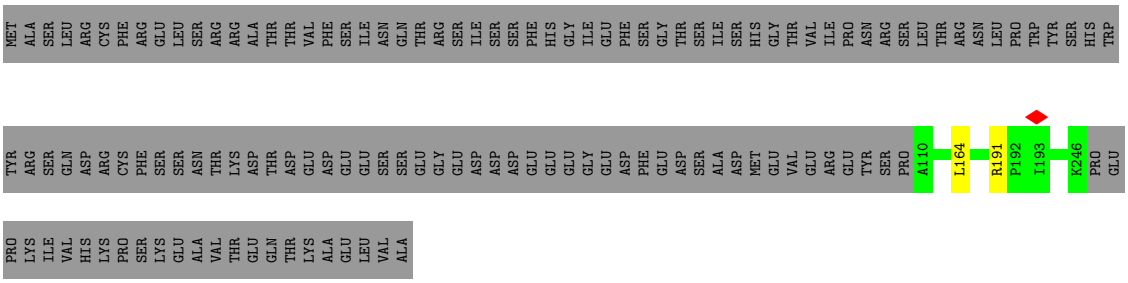
• Molecule 17: 50S ribosomal protein L20





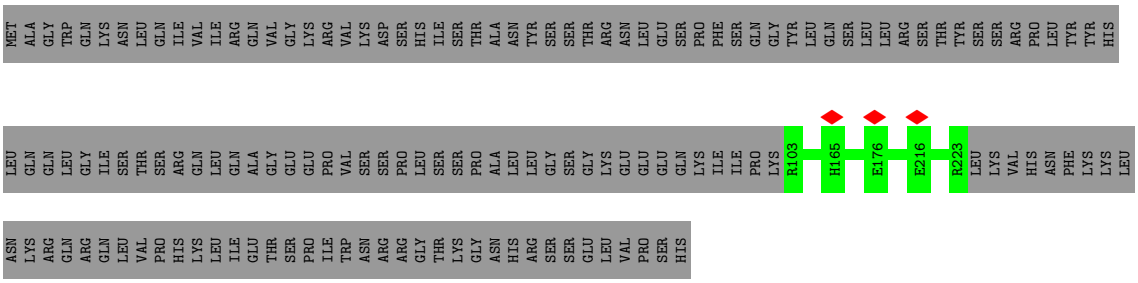
• Molecule 18: 50S ribosomal protein L21, mitochondrial

Chain Ar:



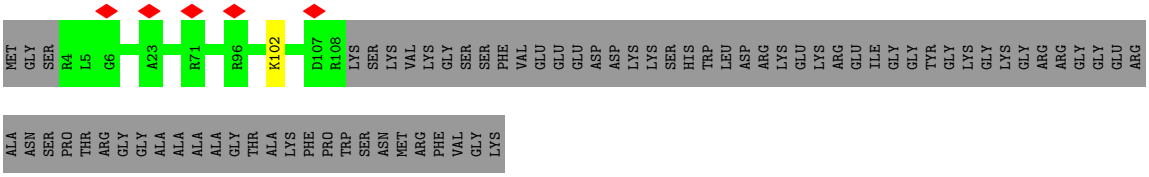
• Molecule 19: AT1G52370 protein

Chain As:



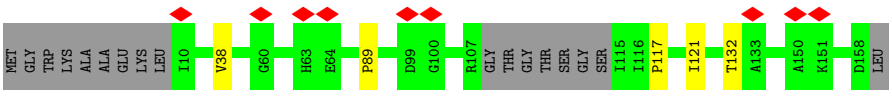
• Molecule 20: At4g39880

Chain At:



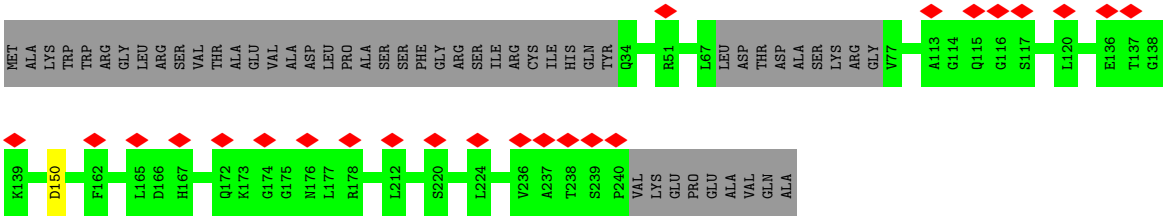
• Molecule 21: 50S ribosomal protein L24

Chain Au:



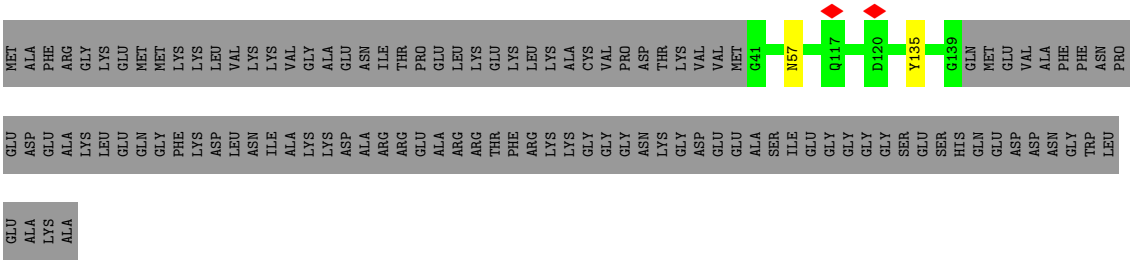
• Molecule 22: Ribosomal protein L25/Gln-tRNA synthetase, anti-codon-binding domain-containing protein

Chain Av:

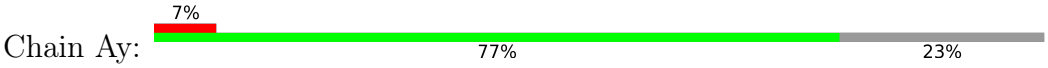


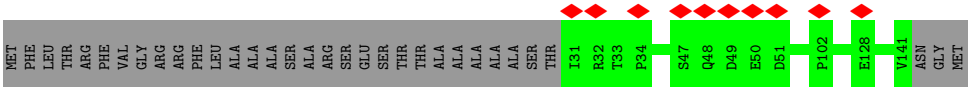
• Molecule 23: 50S ribosomal protein L27

• Molecule 24: AT4g31460/F3L17_30



• Molecule 25: At1g07830/F24B9_7



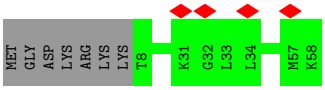


• Molecule 26: Ribosomal protein L31

• Molecule 27: At1g26740/T24P13_11

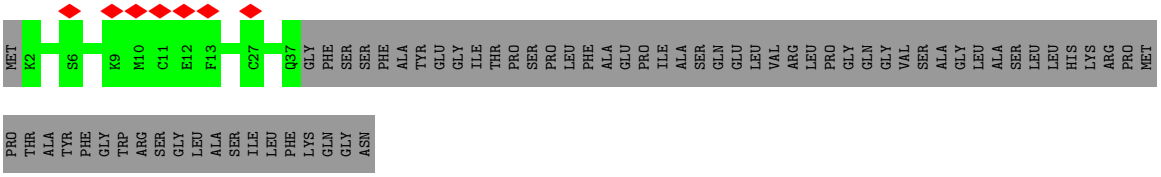
• Molecule 28: At3g06320

Chain AC:



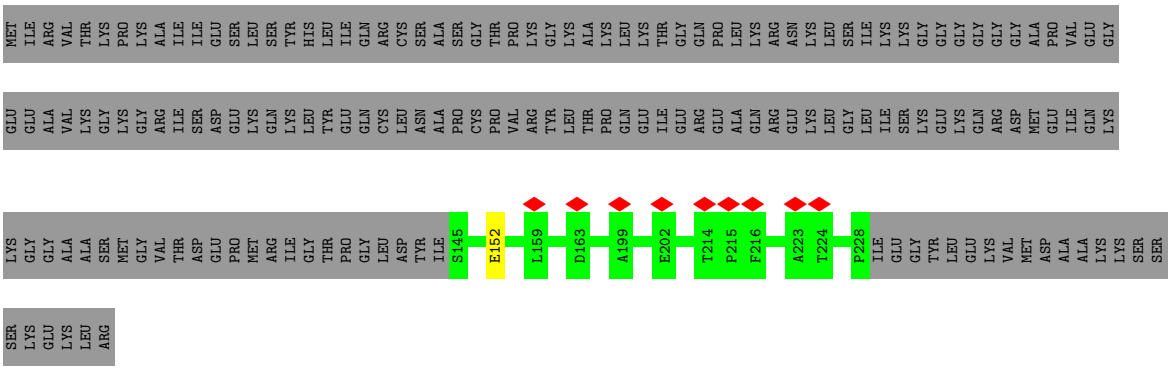
• Molecule 29: Ribosomal protein

Chain AE:



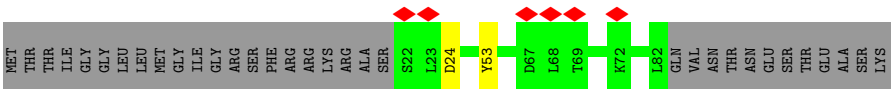
• Molecule 30: At4g05400

Chain AF:



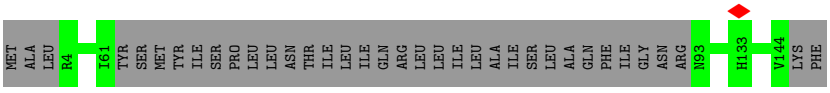
• Molecule 31: At5g40080

Chain AG:



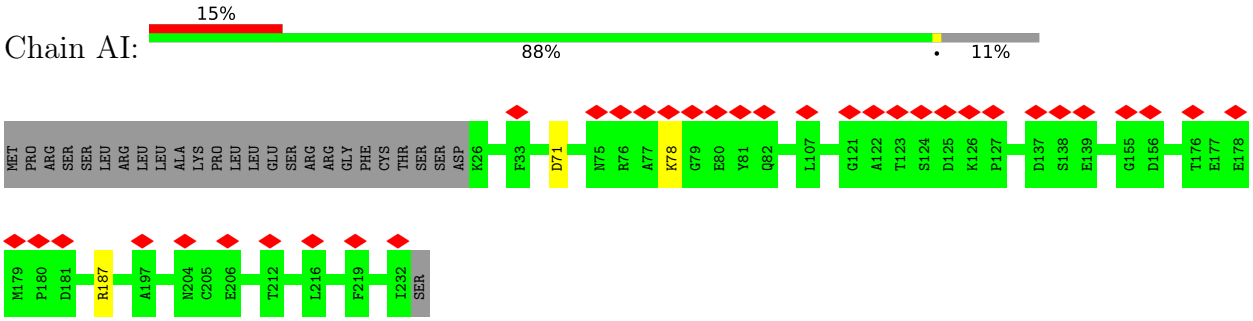
• Molecule 32: Mitochondrial ribosomal protein L51/S25/CI-B8 family protein

Chain AH:



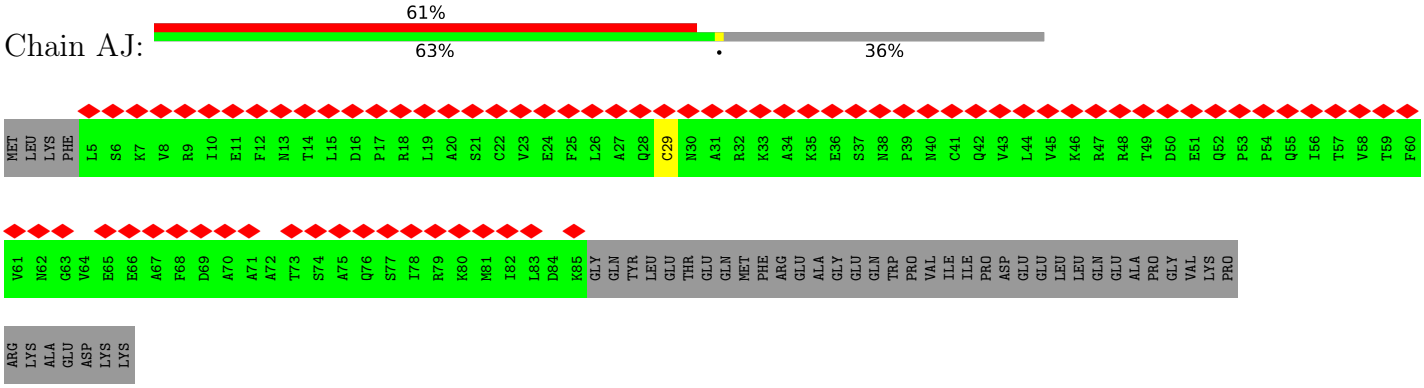
• Molecule 33: At1g14620/T5E21_15

Chain AI:



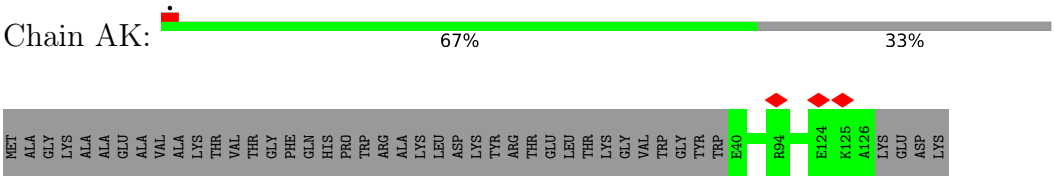
• Molecule 34: 39S ribosomal protein

Chain AJ:



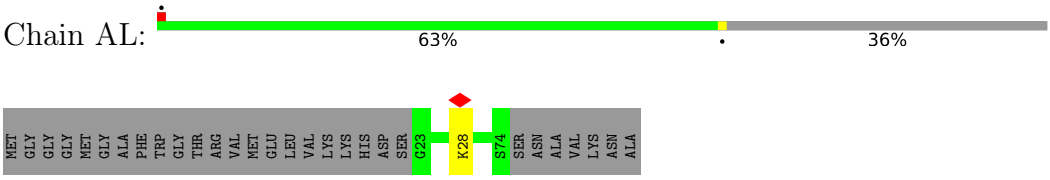
• Molecule 35: At4g22000

Chain AK:



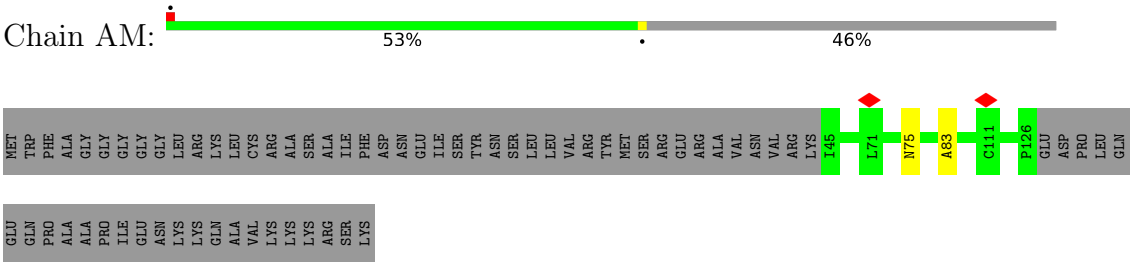
• Molecule 36: Uncharacterized protein At1g27435/F17L21.30

Chain AL:



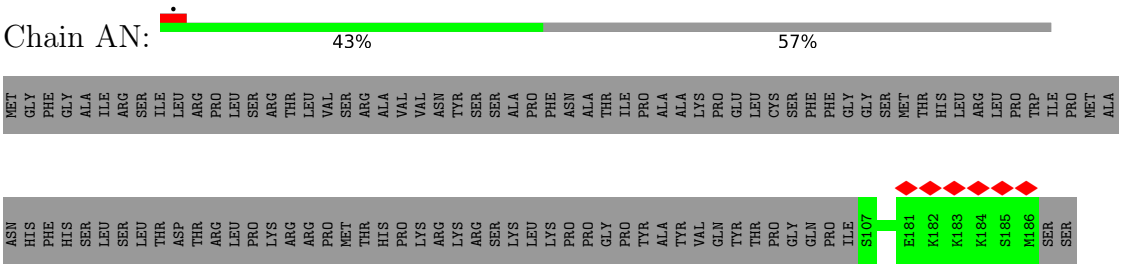
• Molecule 37: At1g73940/F2P9_19

Chain AM:



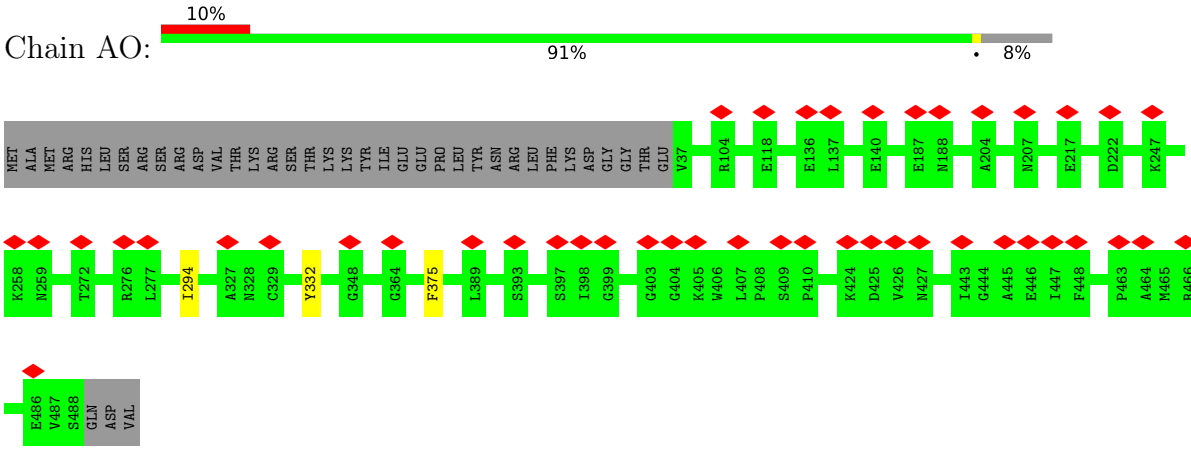
• Molecule 38: At3g51010

Chain AN:



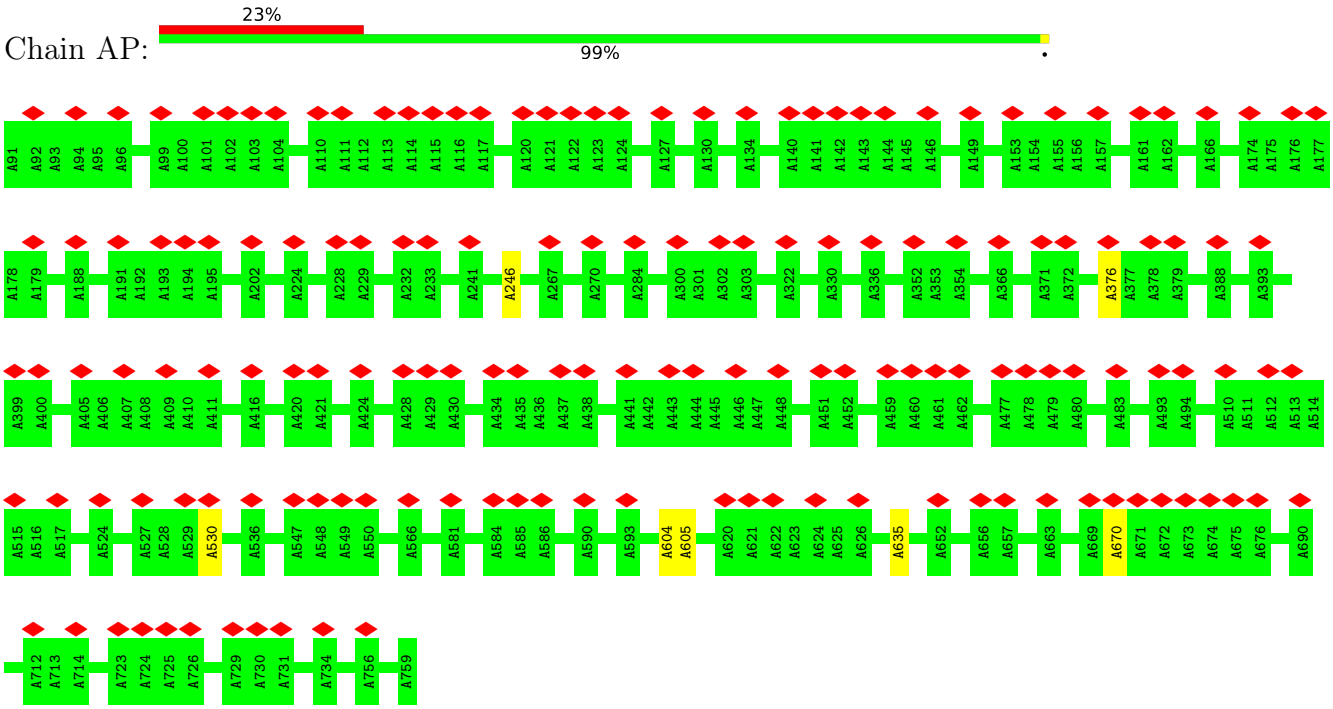
• Molecule 39: Pentatricopeptide repeat-containing protein At1g60770

Chain AO:



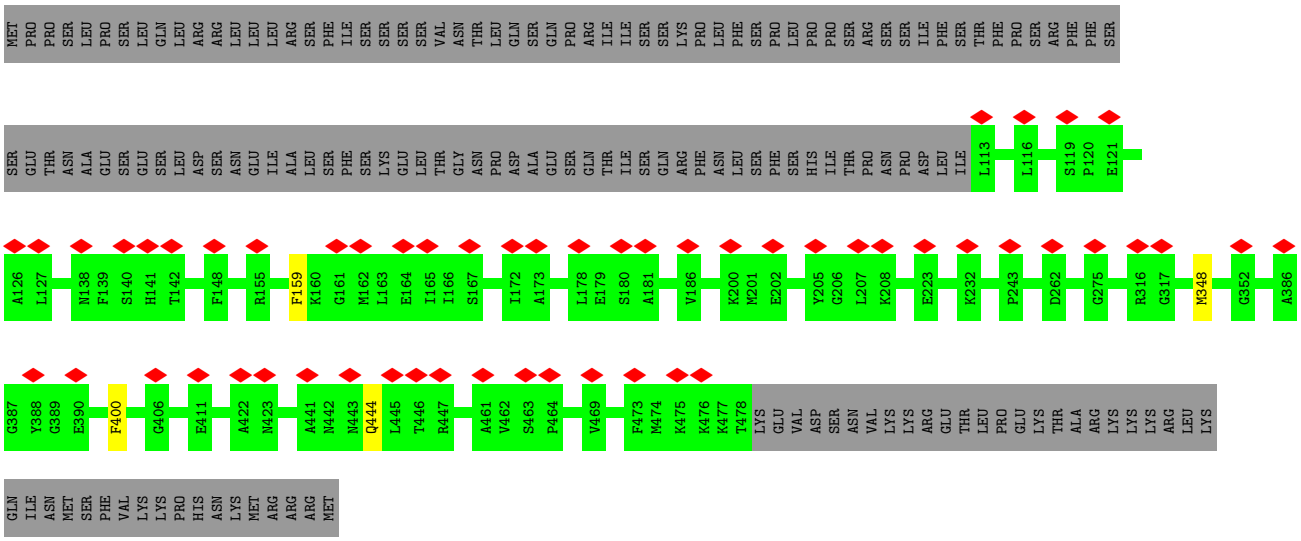
• Molecule 40: rPPR*

Chain AP:

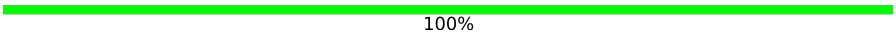


• Molecule 41: Pentatricopeptide repeat-containing protein PNM1, mitochondrial

Chain AQ:



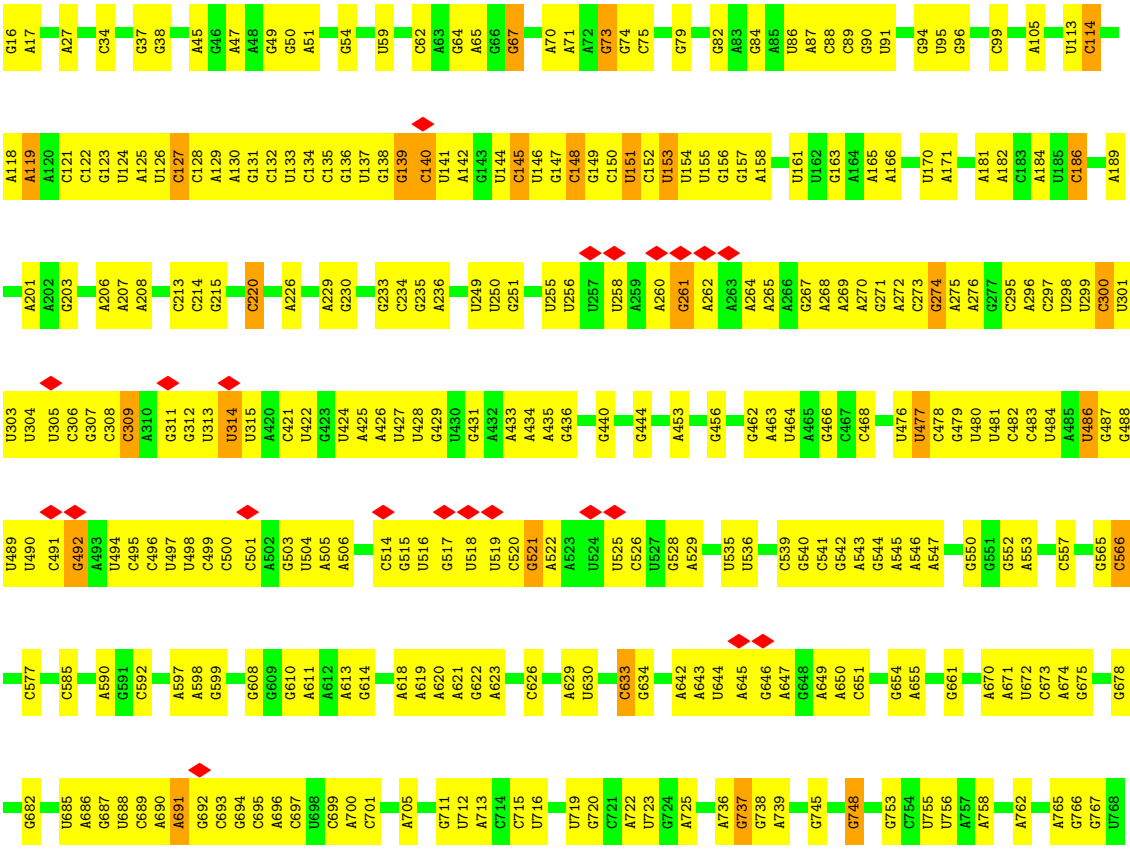
• Molecule 42: UNK-6

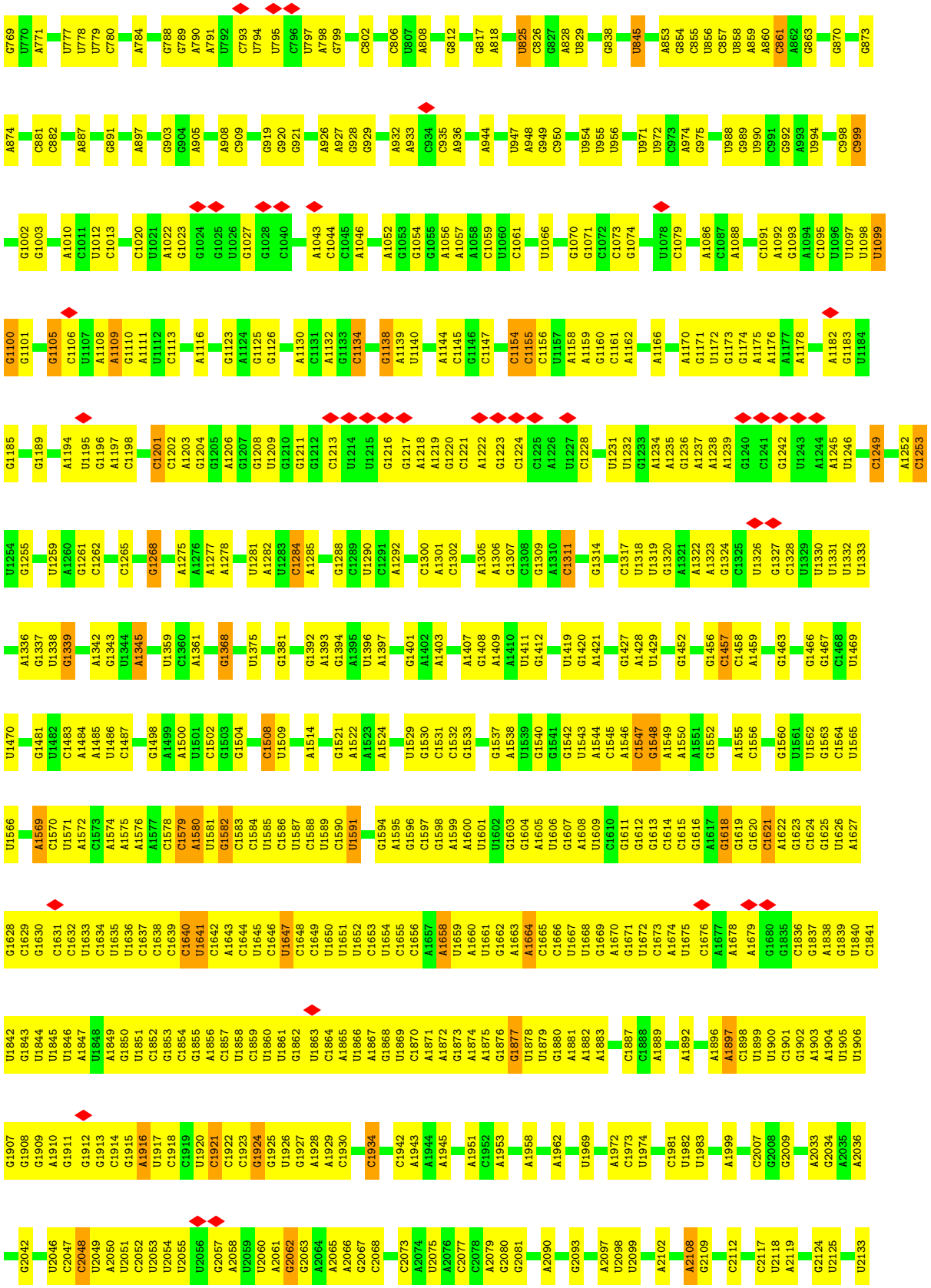
Chain AR: 

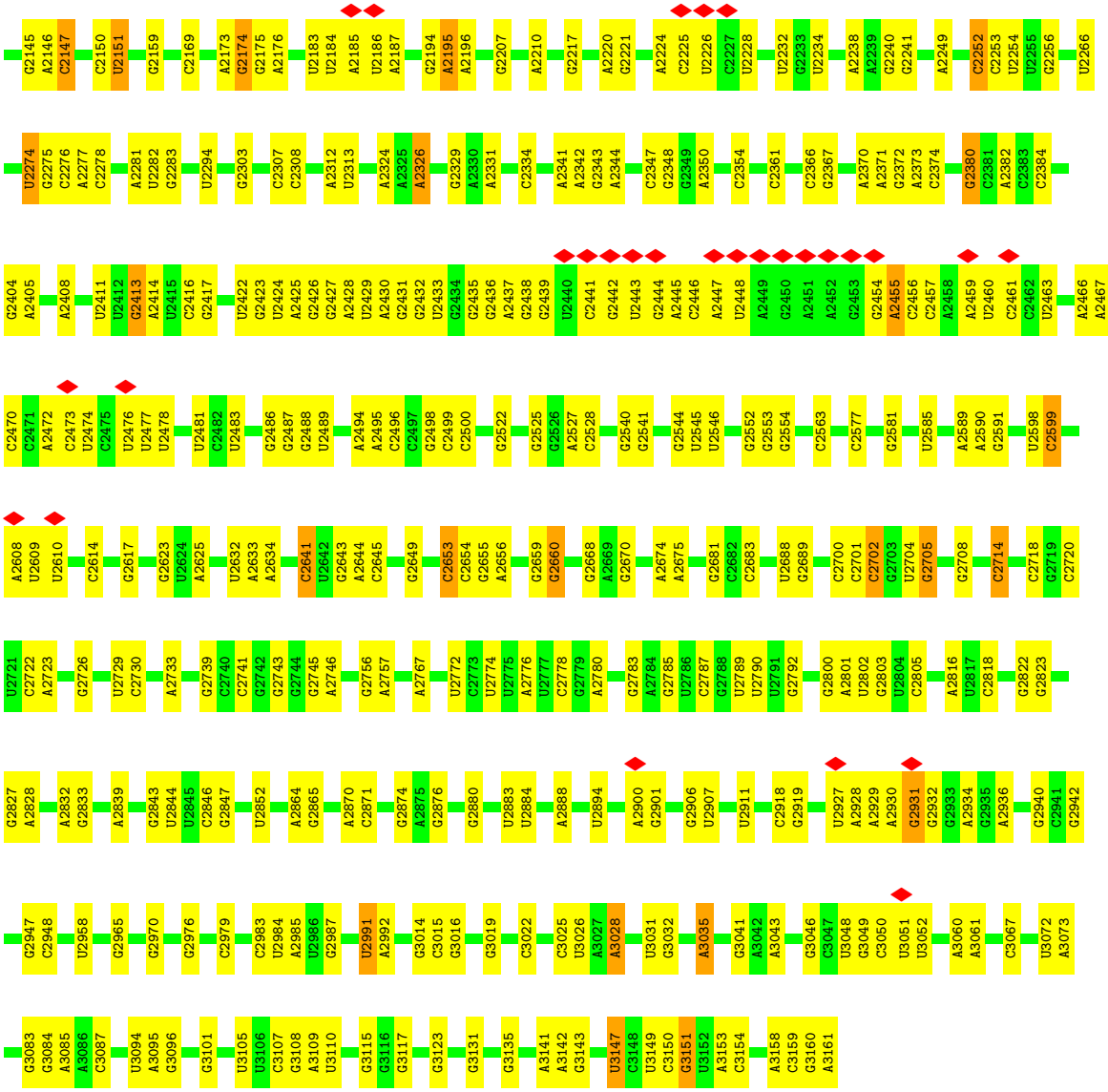
There are no outlier residues recorded for this chain.

• Molecule 43: RNA (2842-MER)

Chain 1: 

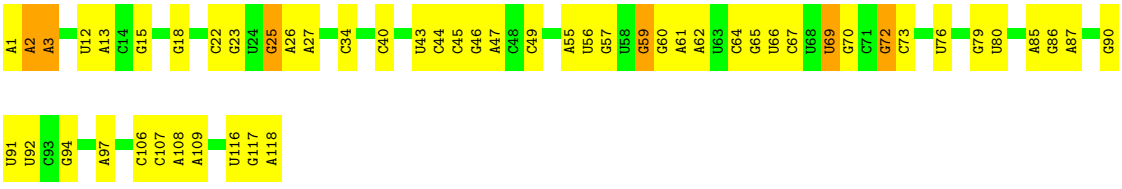






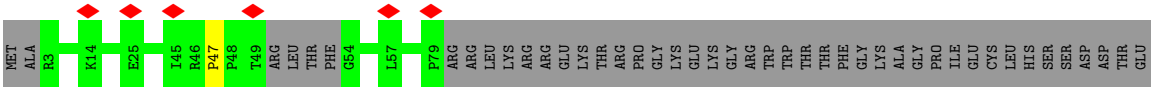
• Molecule 44: RNA (118-MER)

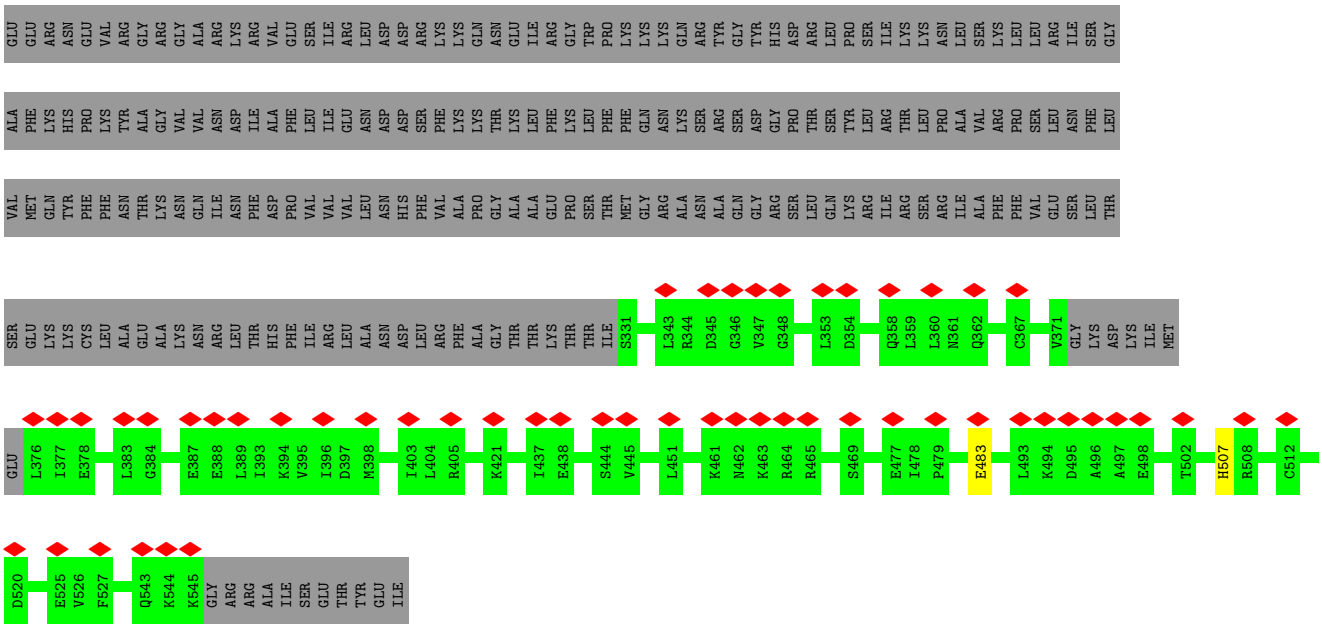
Chain 3:



• Molecule 45: Ribosomal protein S3, mitochondrial

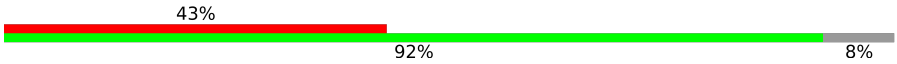
Chain Bb:

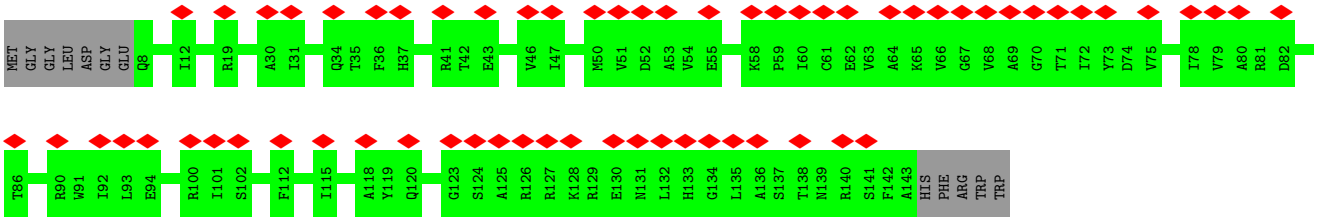




• Molecule 46: Ribosomal protein S7, mitochondrial

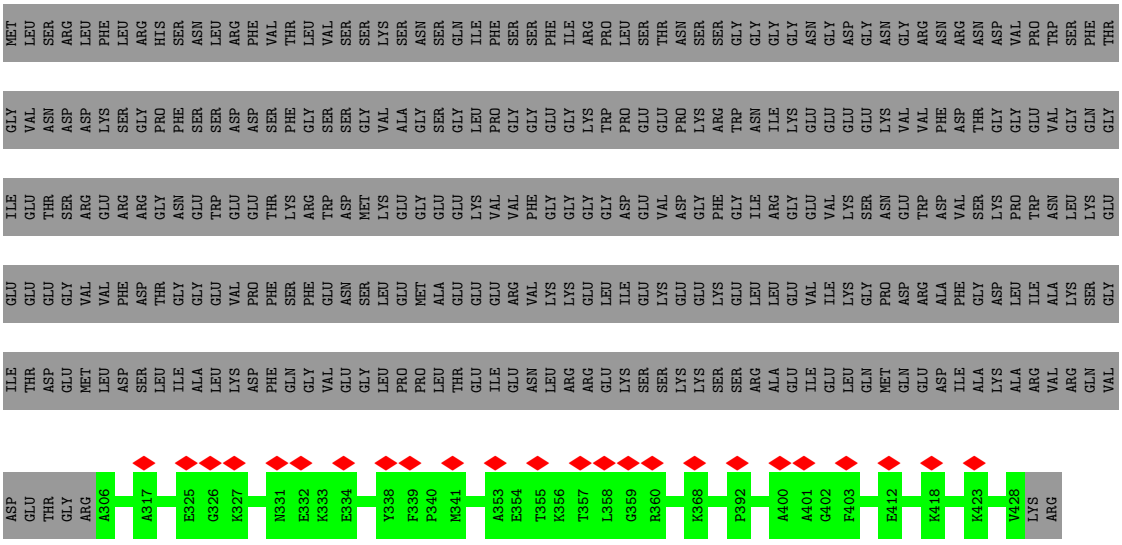
Chain Bf:





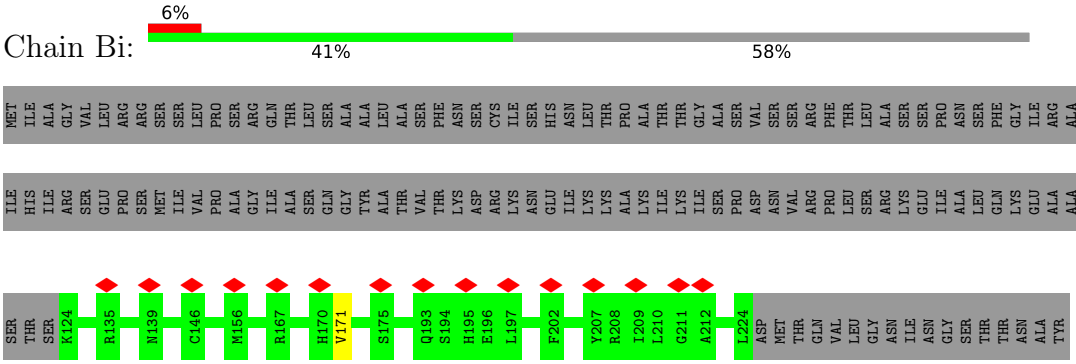
• Molecule 47: 30S ribosomal protein S9, mitochondrial

Chain Bh:



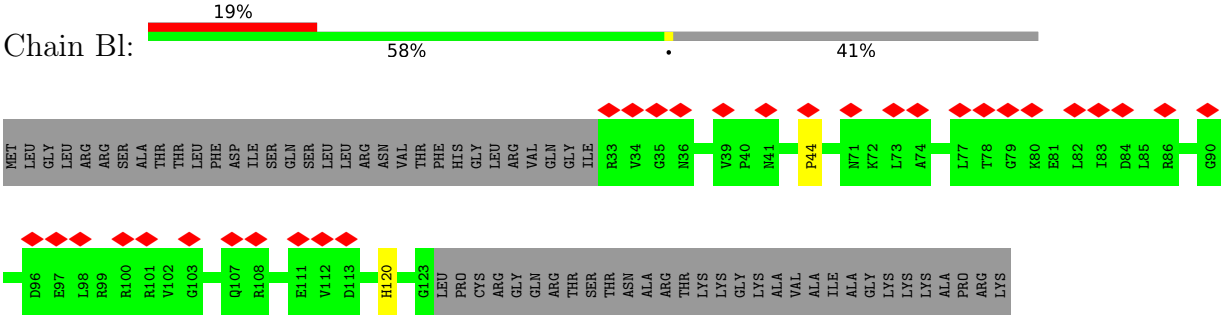
• Molecule 48: 40S ribosomal protein S10, mitochondrial

Chain Bi:



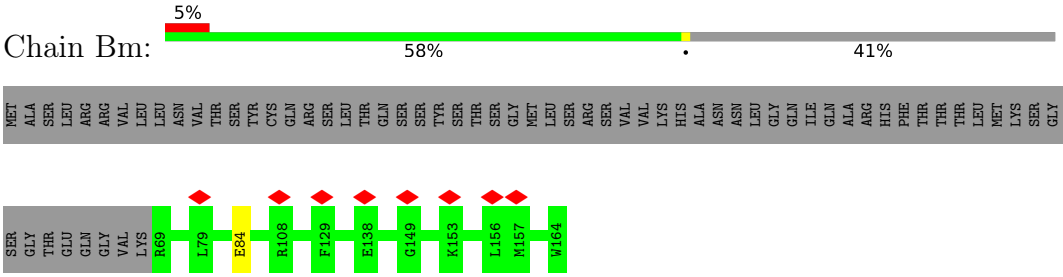
• Molecule 49: Small ribosomal subunit protein S13, mitochondrial

Chain Bl:



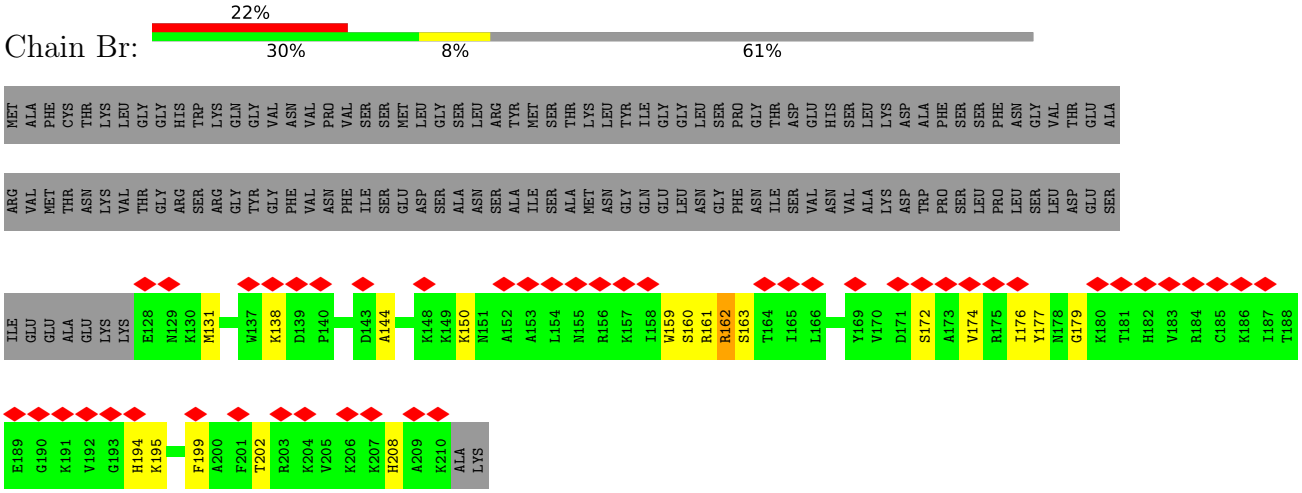
• Molecule 50: At2g34520

Chain Bm:



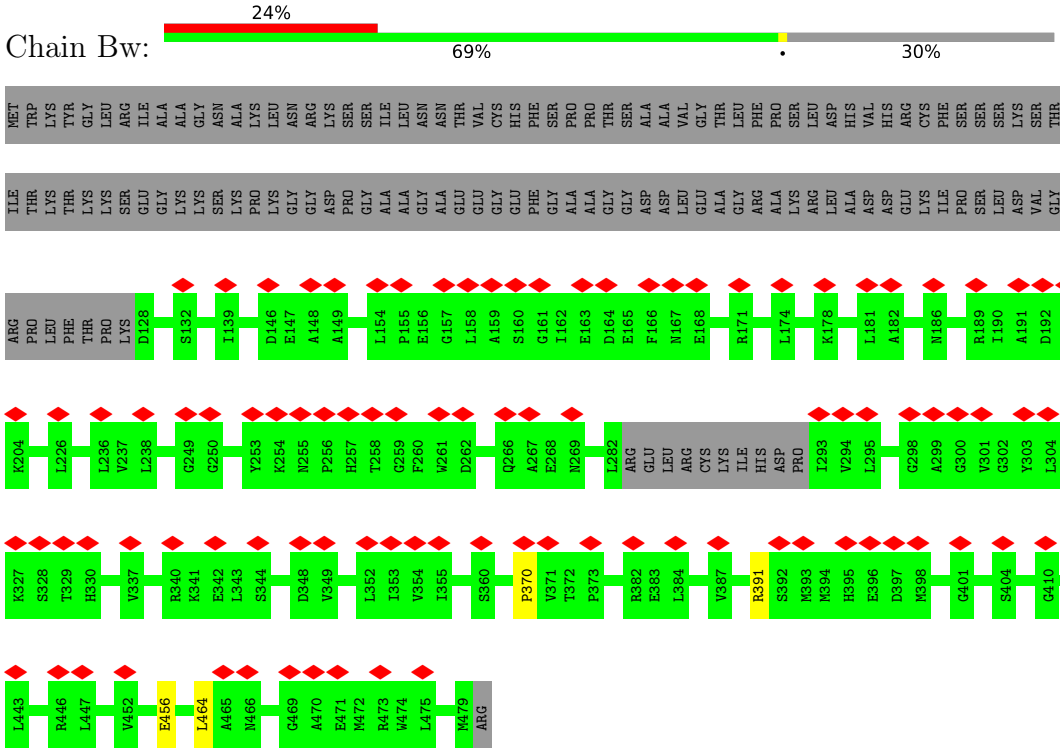
• Molecule 51: 40S ribosomal protein S19, mitochondrial

Chain Br:



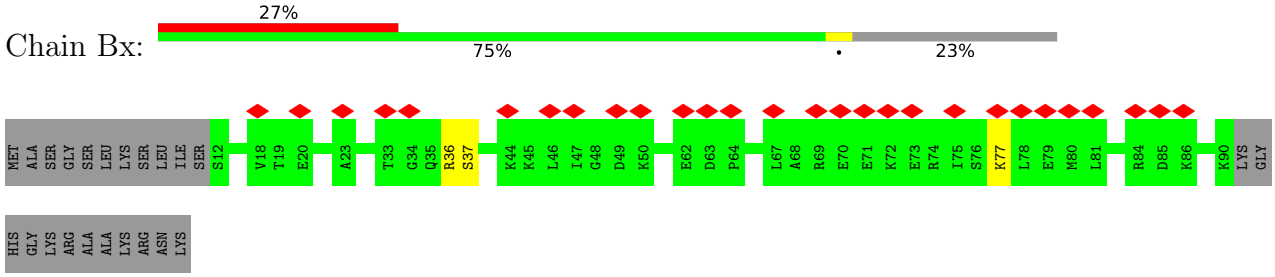
• Molecule 52: Mitochondrial 28S ribosomal protein S29-like protein

Chain Bw:



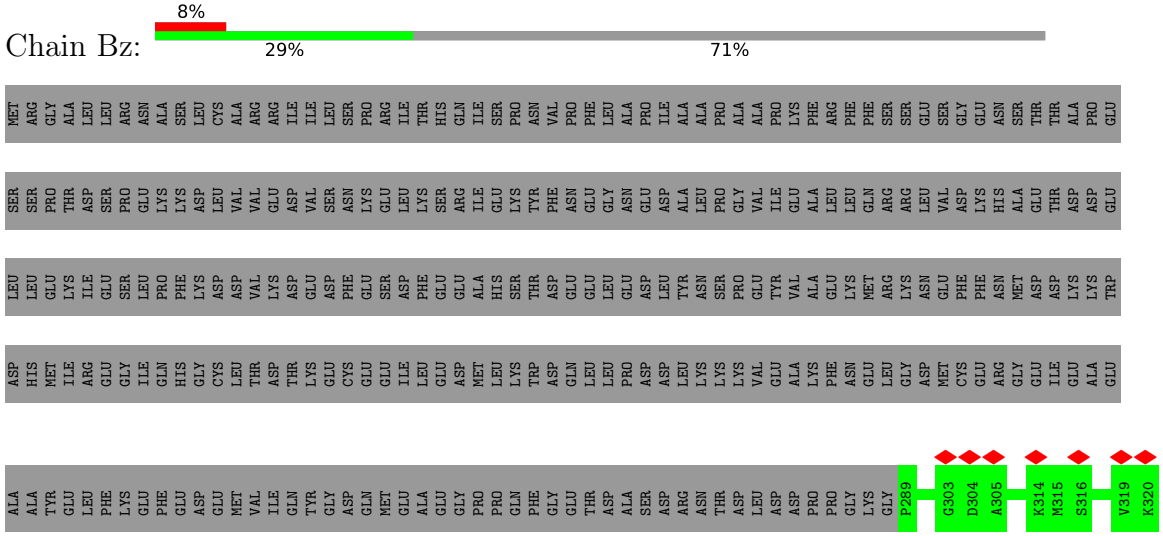
• Molecule 53: 37S ribosomal protein S27

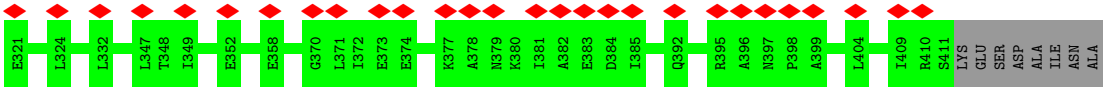
Chain Bx:



• Molecule 54: AT3G18240 protein

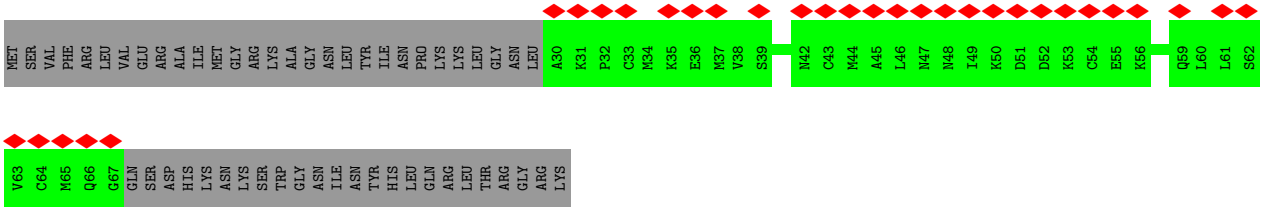
Chain Bz:





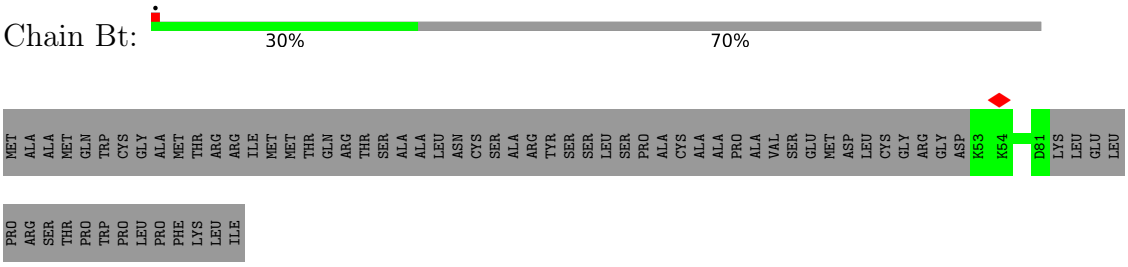
• Molecule 55: CX9C domain-containing protein

Chain BA:



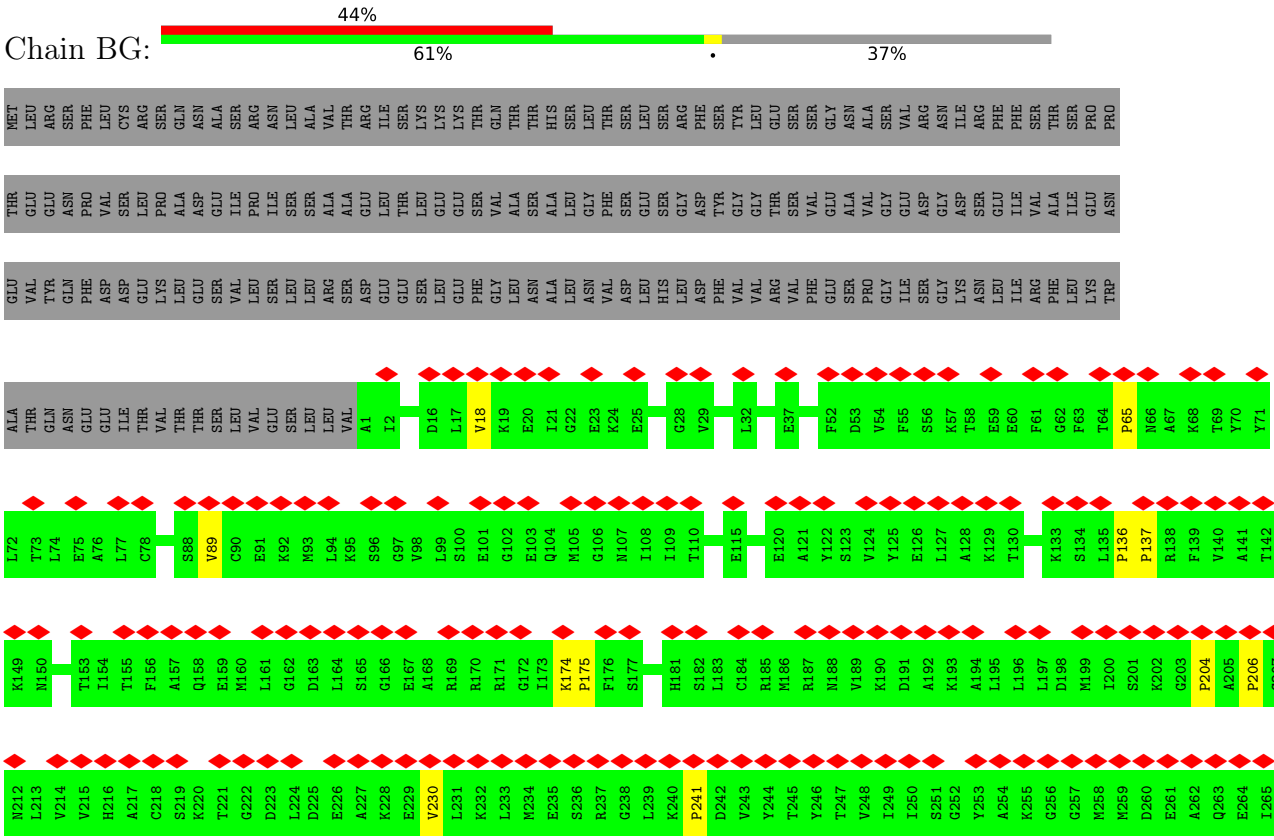
• Molecule 56: 30S ribosomal protein S31, mitochondrial

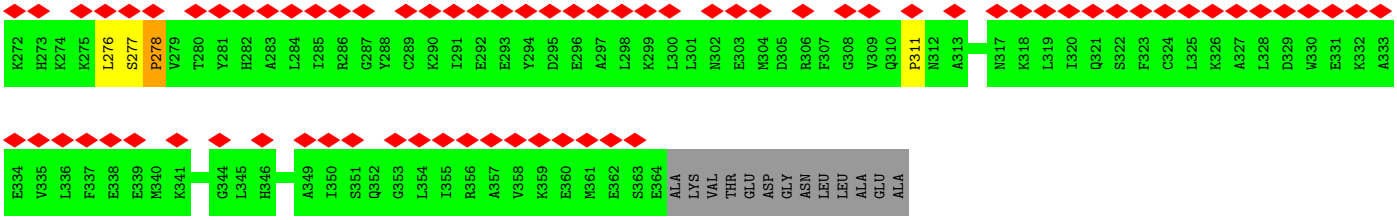
Chain Bt:



• Molecule 57: Pentatricopeptide repeat-containing protein At3g02650, mitochondrial

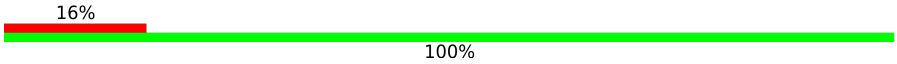
Chain BG:

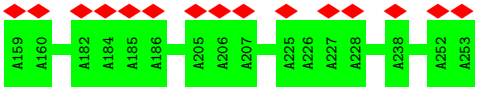




• Molecule 58: UNK-5

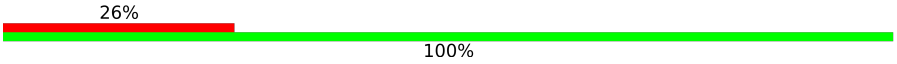
Chain BP:

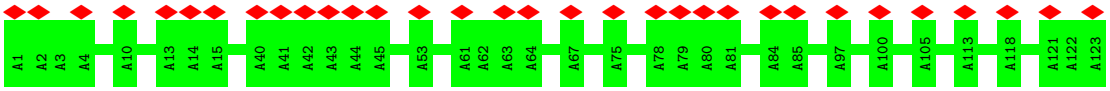




• Molecule 59: mS31/mS46

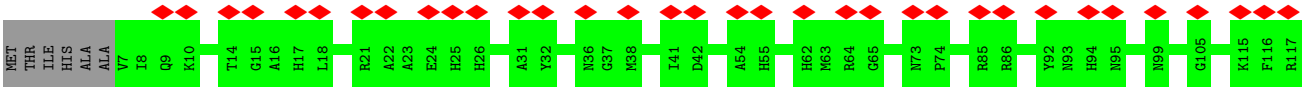
Chain BF:

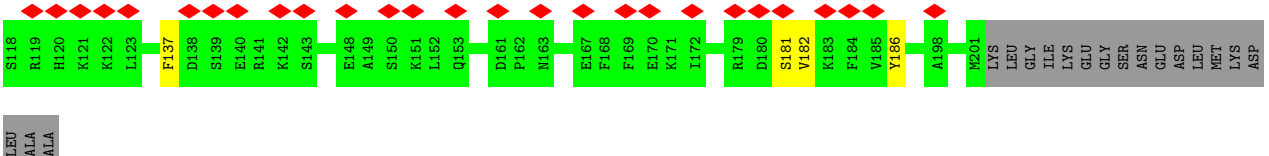




• Molecule 60: Ribosomal protein S2, mitochondrial

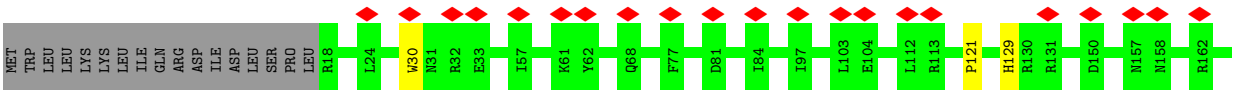
Chain Ba:

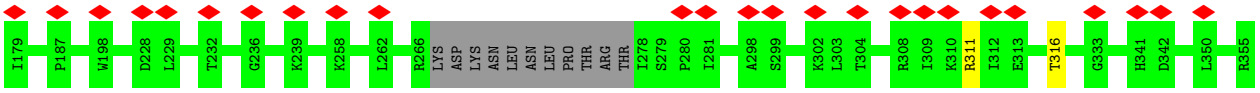




• Molecule 61: Ribosomal protein S4, mitochondrial

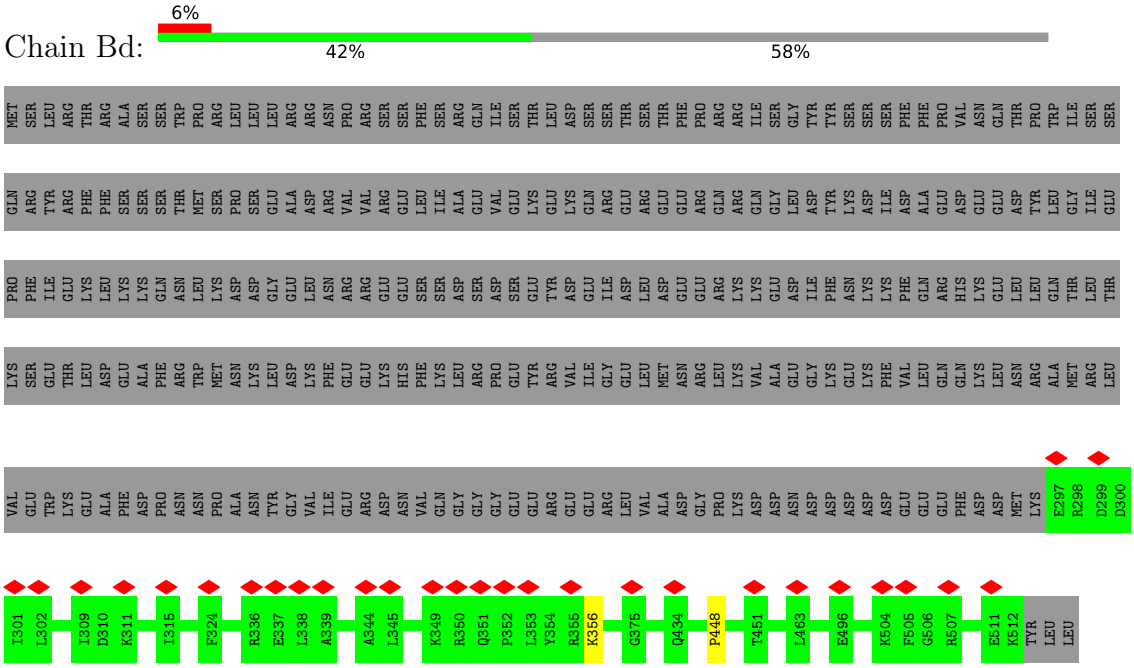
Chain Bc:





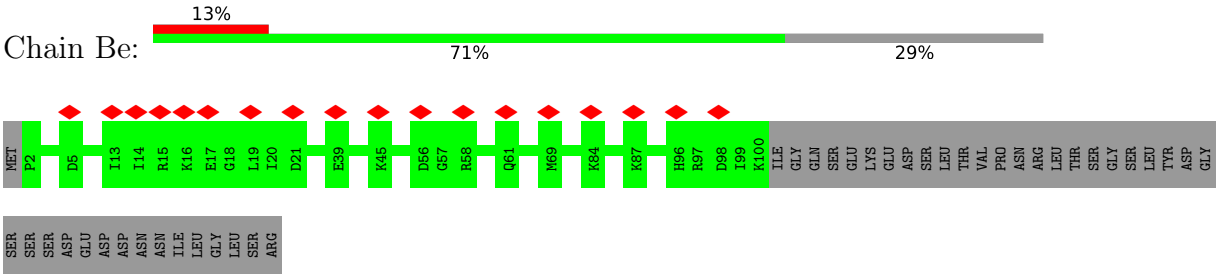
• Molecule 62: At1g64880

Chain Bd:



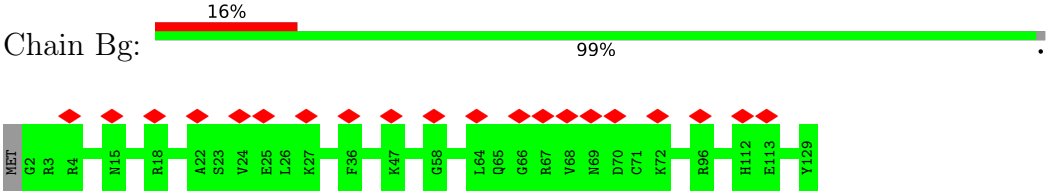
• Molecule 63: Translation elongation factor EF1B/ribosomal protein S6 family protein

Chain Be:



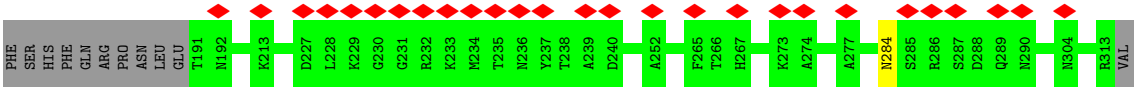
• Molecule 64: 40S ribosomal protein S15a-5

Chain Bg:



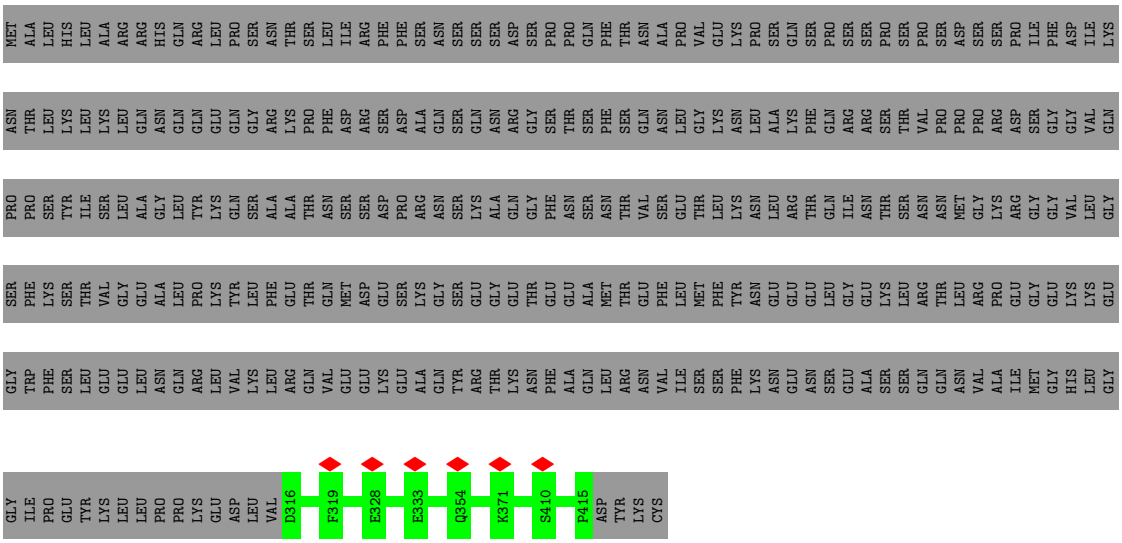
• Molecule 65: Probable ribosomal protein S11, mitochondrial

Chain Bj:



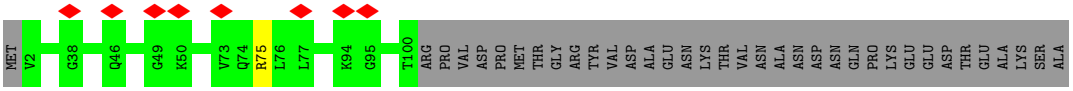
• Molecule 66: At1g15810/F7H2_23

Chain Bn:



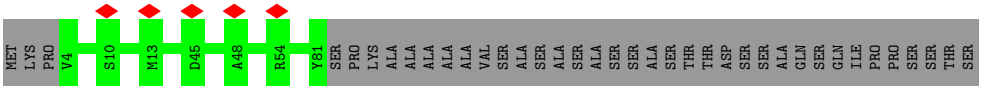
• Molecule 67: 30S ribosomal protein S16-2, chloroplastic/mitochondrial

Chain Bo:



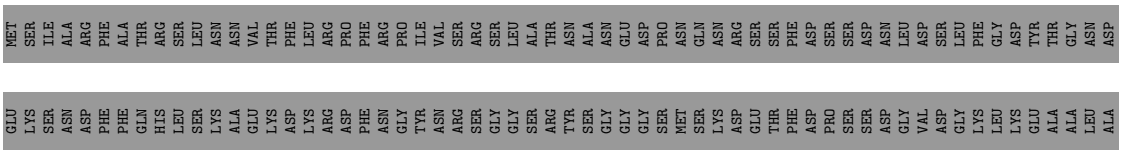
• Molecule 68: Nucleic acid-binding, OB-fold-like protein

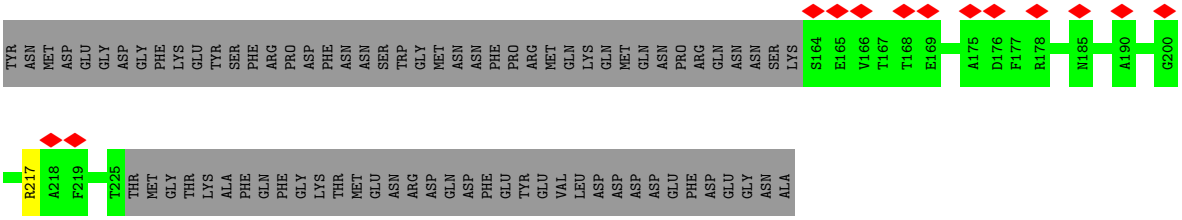
Chain Bp:



• Molecule 69: F10K1.8 protein

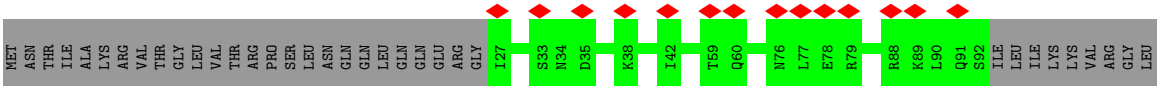
Chain Bq:





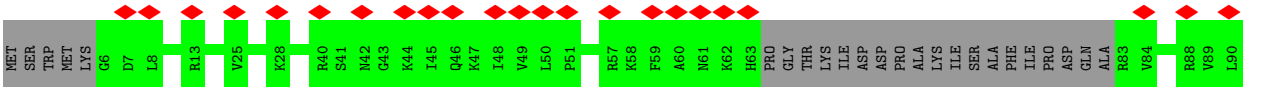
• Molecule 70: Ribosomal protein S21 family protein

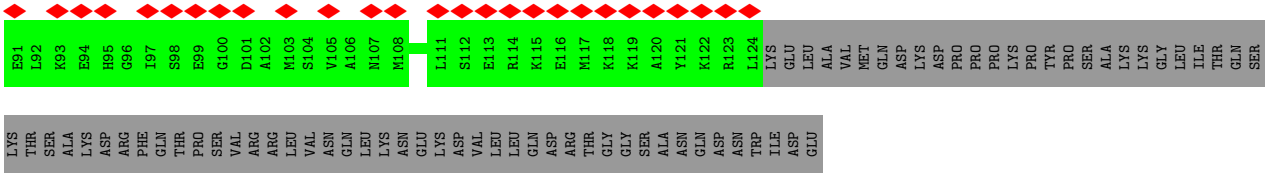
Chain Bs:



• Molecule 71: Uncharacterized protein

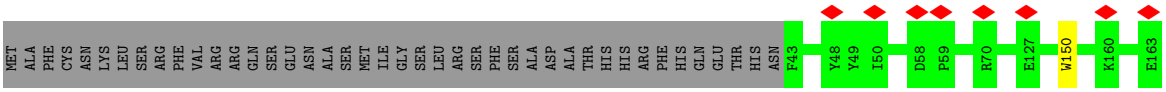
Chain Bu:

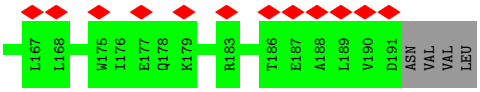




• Molecule 72: AT5g49210/K21P3_8

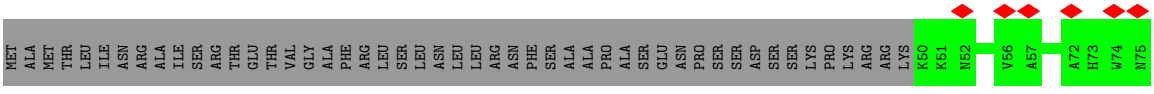
Chain Bv:

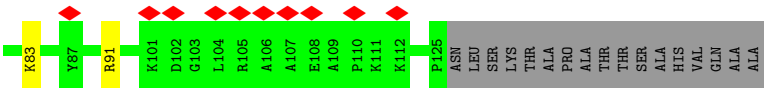




• Molecule 73: 28S ribosomal S34 protein

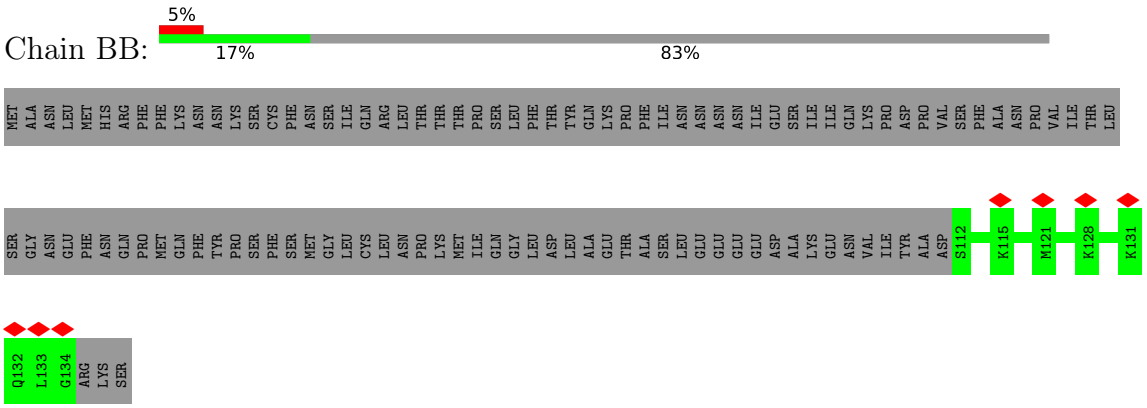
Chain By:





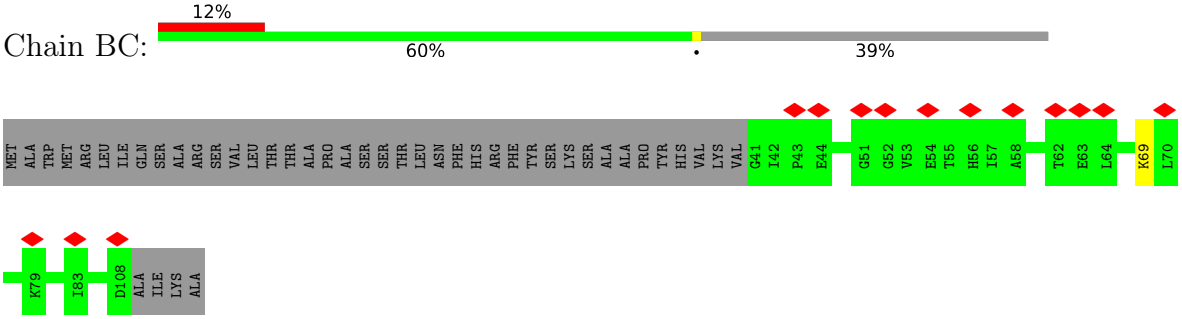
• Molecule 74: mS38

Chain BB:



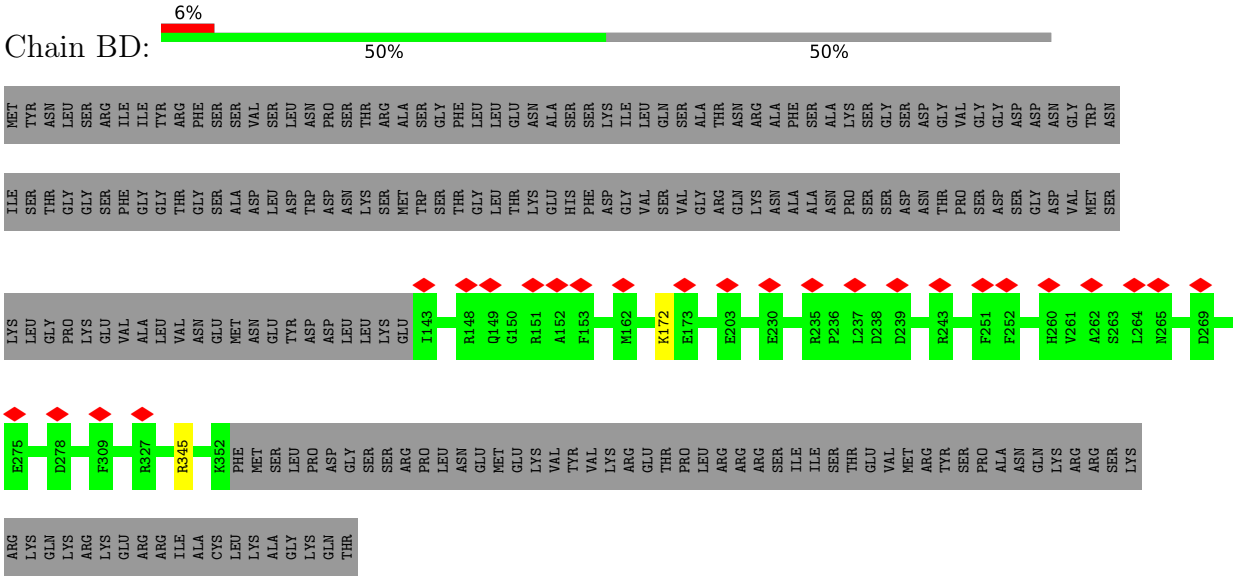
• Molecule 75: At5g26800

Chain BC:



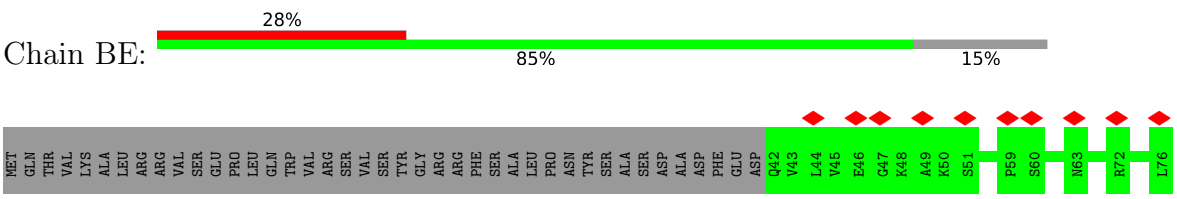
• Molecule 76: Gb|AAC32909.1

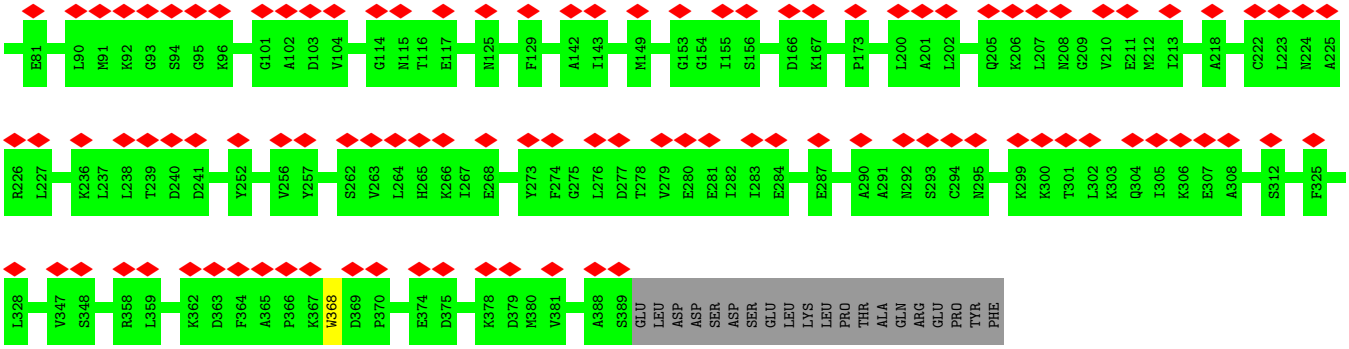
Chain BD:



• Molecule 77: 3-hydroxyisobutyryl-CoA hydrolase-like protein 2, mitochondrial

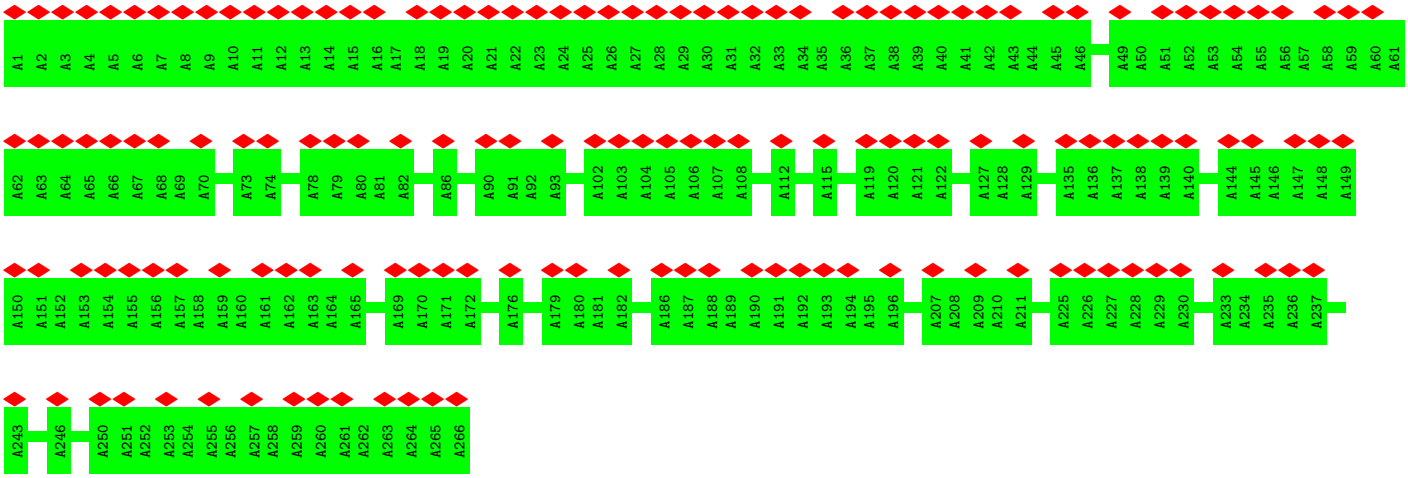
Chain BE:





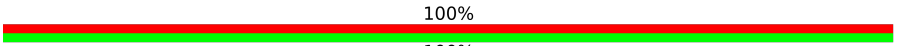
• Molecule 78: rPPR*

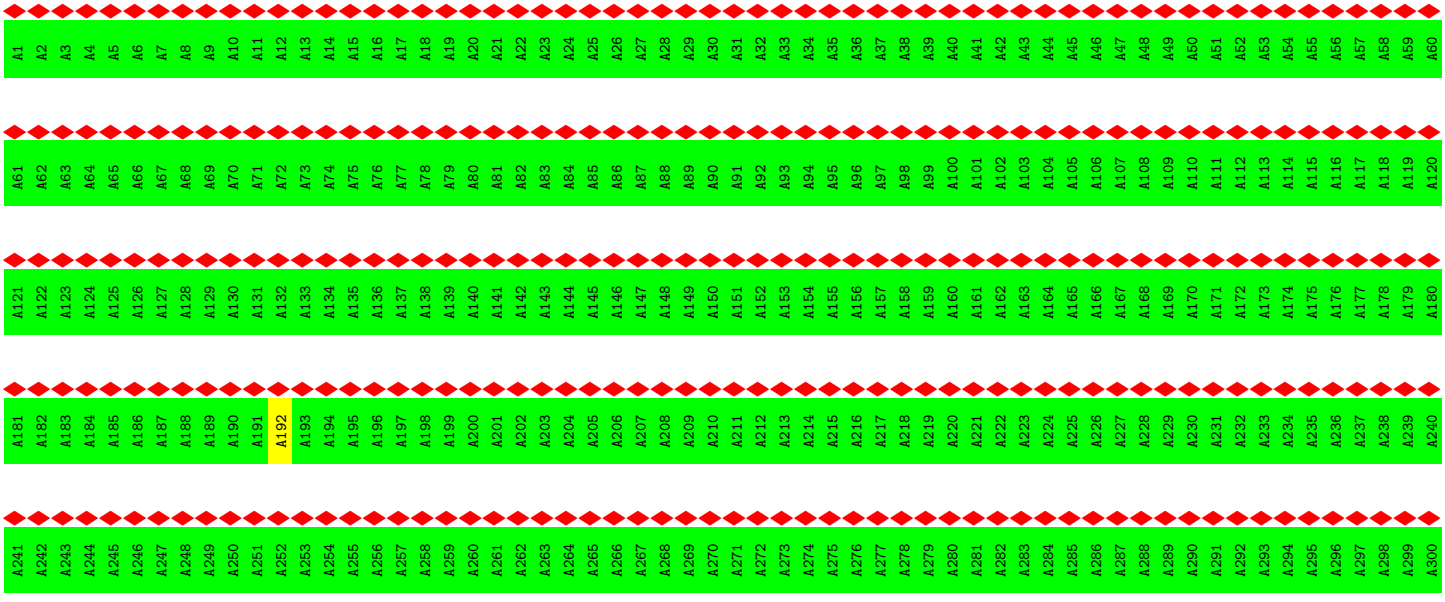
Chain BI:

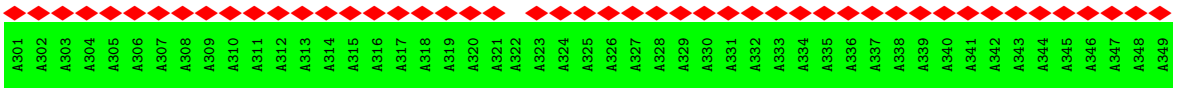


• Molecule 79: rPPR*

Chain BJ:

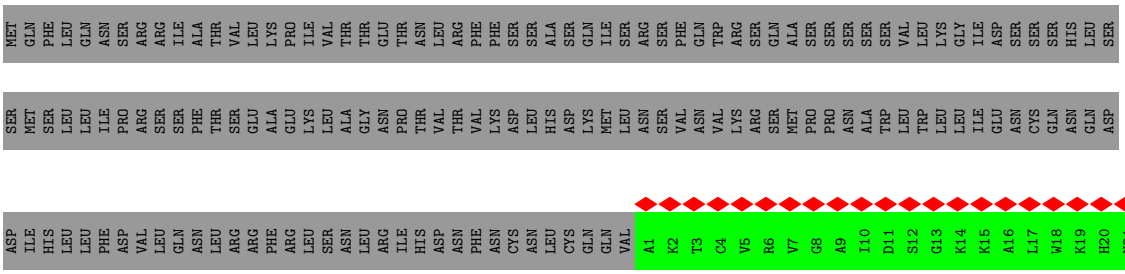






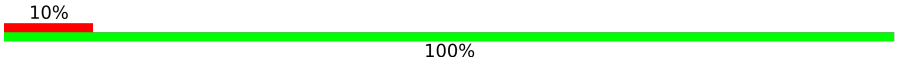
• Molecule 80: Adenylyl cyclase

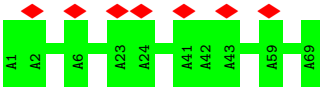
Chain BH:



• Molecule 81: UNK-3

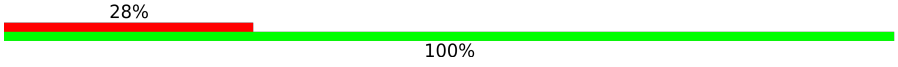
Chain BN:

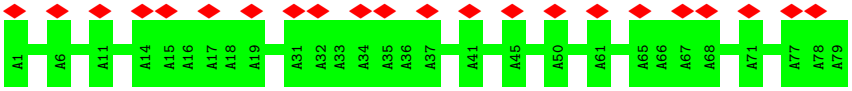




• Molecule 82: UNK-2

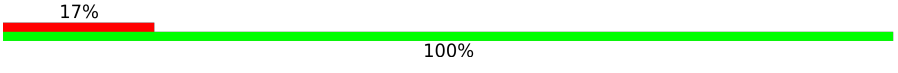
Chain BM:

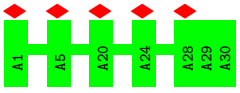




• Molecule 83: UNK-4

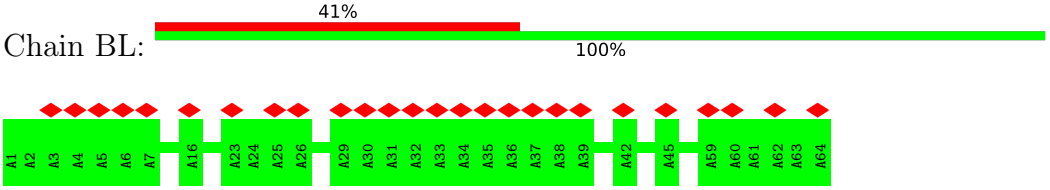
Chain BO:





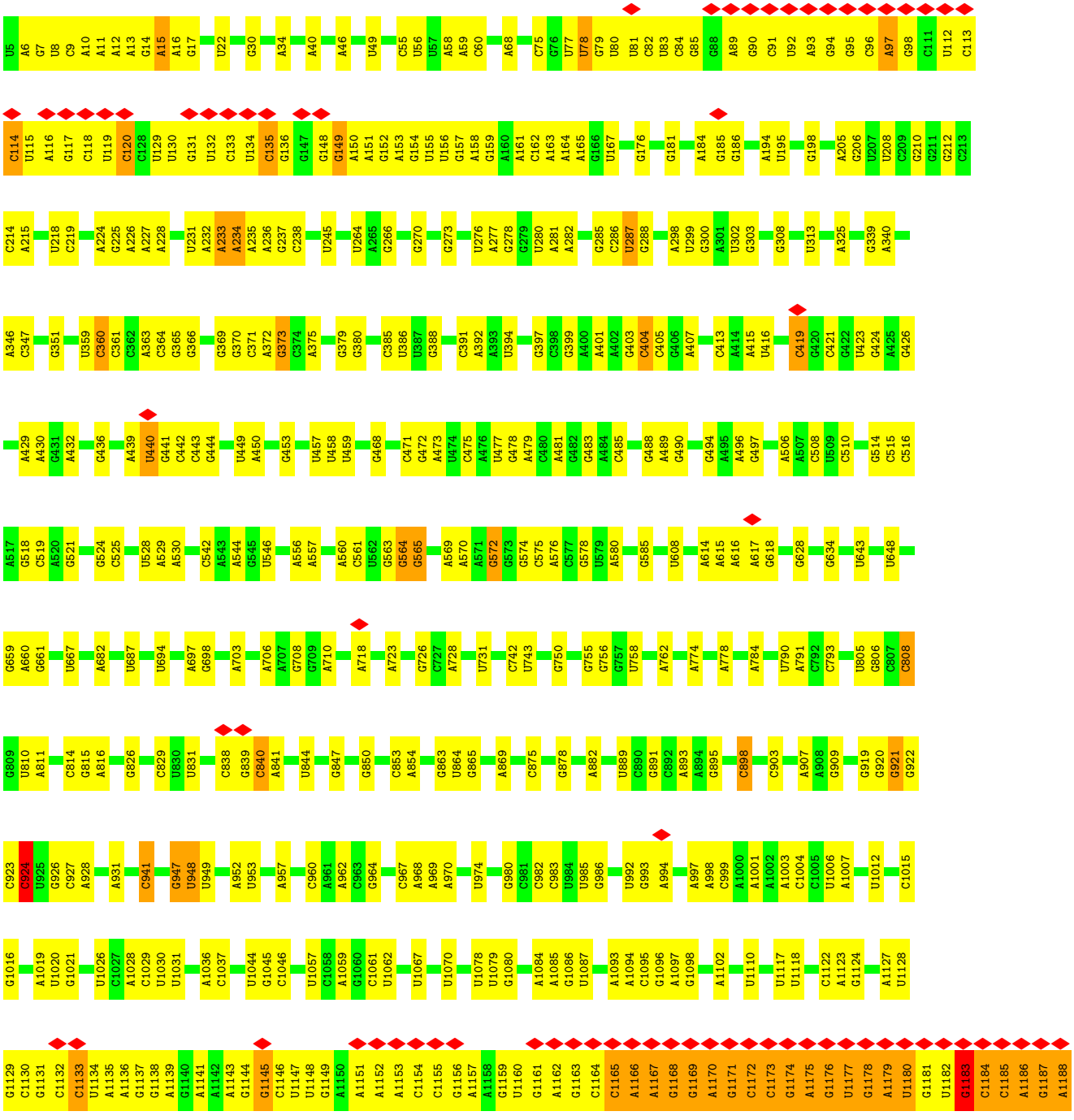
• Molecule 84: UNK-1

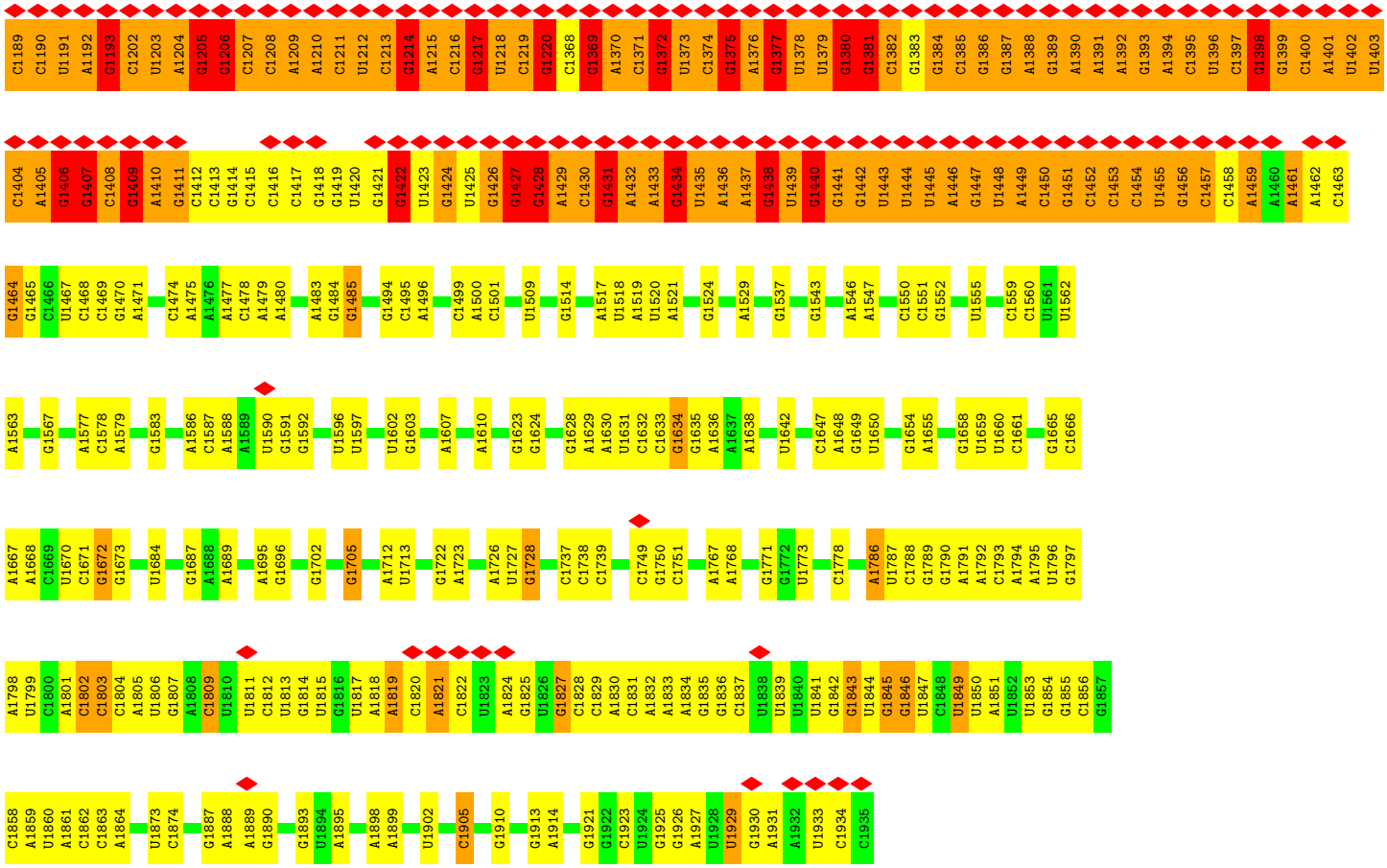
Chain BL:



• Molecule 85: RNA (1743-MER)

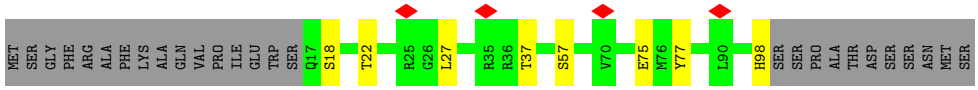
Chain 2:





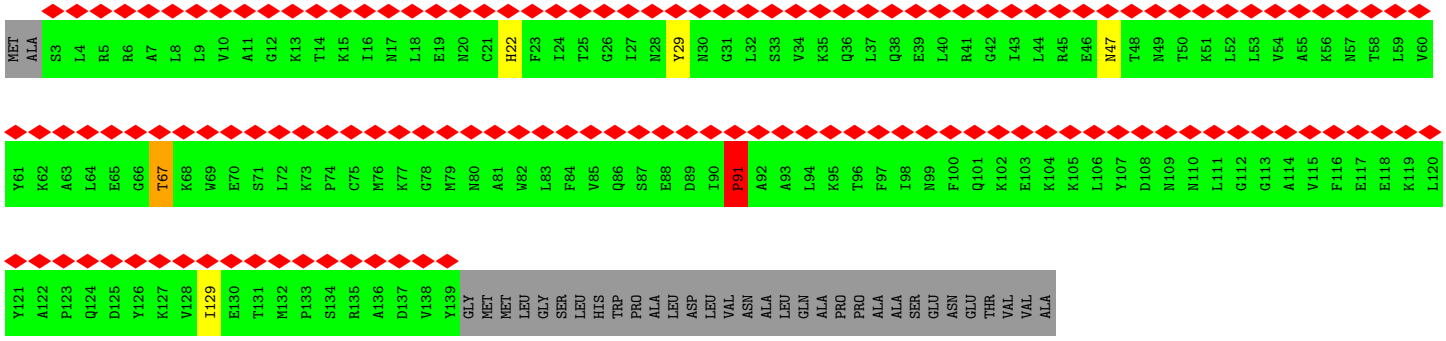
• Molecule 86: At5g55140

Chain Az:



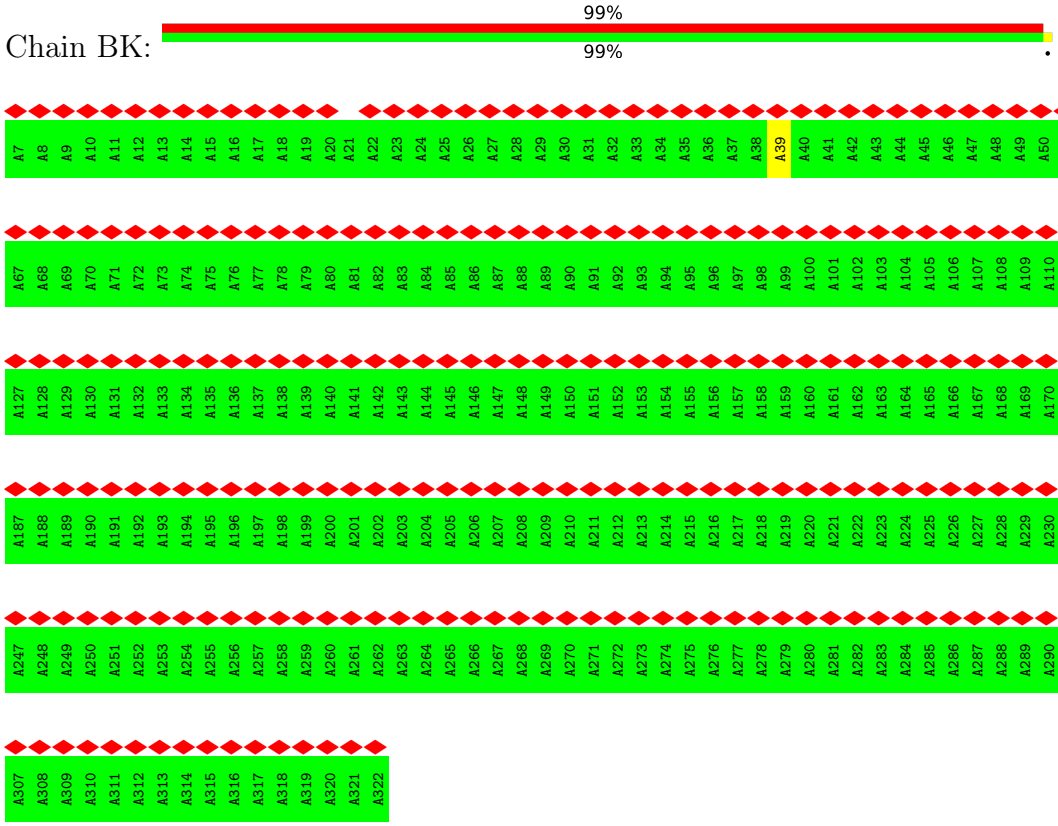
• Molecule 87: 50S ribosomal protein L10

Chain Ah:



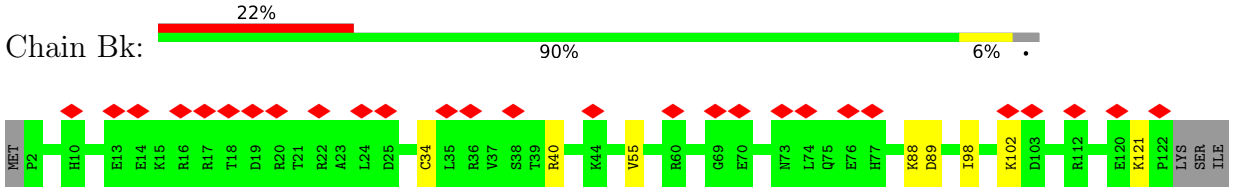
• Molecule 88: rPPR*

Chain BK:



• Molecule 89: Ribosomal protein S12, mitochondrial

Chain Bk:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65280	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.196	Depositor
Minimum map value	-0.082	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	484.0, 484.0, 484.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.21, 1.21, 1.21	Depositor

5 Model quality

5.1 Standard geometry

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	Aa	0.49	0/764	0.66	1/1020 (0.1%)
2	Ab	0.46	0/1165	0.57	0/1554
3	Ac	0.48	0/1710	0.63	1/2294 (0.0%)
4	AD	0.47	0/518	0.57	0/686
5	Ad	0.47	0/1680	0.59	0/2267
6	Ae	0.39	0/1198	0.62	1/1620 (0.1%)
7	Af	0.36	0/815	0.54	0/1091
8	Ag	0.39	0/413	0.59	0/557
9	Ai	0.33	0/1081	0.53	0/1467
10	Aj	0.45	0/1294	0.55	0/1738
11	Ak	0.46	0/972	0.56	0/1300
12	Al	0.44	0/1433	0.59	0/1914
13	Am	0.40	0/1135	0.60	0/1518
14	An	0.50	0/1159	0.63	0/1556
15	Ao	0.41	0/849	0.55	0/1141
16	Ap	0.48	0/947	0.61	0/1268
17	Aq	0.48	0/902	0.57	0/1195
18	Ar	0.45	0/1124	0.61	0/1508
19	As	0.51	0/947	0.62	0/1273
20	At	0.49	0/854	0.60	0/1145
21	Au	0.47	0/1133	0.68	0/1527
22	Av	0.40	0/1546	0.60	0/2091
23	Aw	0.49	0/620	0.55	0/829
24	Ax	0.50	0/826	0.54	0/1105
25	Ay	0.49	0/962	0.65	0/1290
26	AA	0.44	0/303	0.70	0/400
27	AB	0.53	0/326	0.68	1/433 (0.2%)
28	AC	0.51	0/441	0.56	0/584
29	AE	0.39	0/300	0.49	0/394
30	AF	0.40	0/674	0.59	0/908
31	AG	0.55	0/500	0.65	0/677
32	AH	0.42	0/894	0.59	0/1205
33	AI	0.39	0/1765	0.54	0/2388
34	AJ	0.34	0/639	0.58	0/862

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	AK	0.40	0/744	0.56	0/984
36	AL	0.40	0/407	0.57	0/549
37	AM	0.39	0/667	0.56	0/899
38	AN	0.37	0/667	0.48	0/877
39	AO	0.38	0/3654	0.56	0/4927
40	AP	0.30	0/3344	0.50	1/4680 (0.0%)
41	AQ	0.36	0/2947	0.56	0/3942
42	AR	0.26	0/144	0.44	0/200
43	1	1.01	19/68131 (0.0%)	1.17	290/106225 (0.3%)
44	3	0.79	0/2810	1.13	8/4378 (0.2%)
45	Bb	0.40	0/2346	0.54	0/3146
46	Bf	0.32	0/1121	0.53	0/1501
47	Bh	0.34	0/995	0.54	0/1336
48	Bi	0.37	0/878	0.61	0/1175
49	Bl	0.34	0/738	0.63	0/987
50	Bm	0.36	0/807	0.54	0/1072
51	Br	0.65	1/700 (0.1%)	1.16	7/932 (0.8%)
52	Bw	0.33	0/2793	0.58	0/3785
53	Bx	0.36	0/653	0.54	0/873
54	Bz	0.35	0/1027	0.50	0/1371
55	BA	0.33	0/294	0.52	0/388
56	Bt	0.35	0/240	0.52	0/307
57	BG	0.27	0/1794	0.58	9/2495 (0.4%)
58	BP	0.25	0/451	0.33	0/625
59	BF	0.28	0/614	0.47	0/858
60	Ba	0.42	0/1600	0.65	4/2162 (0.2%)
61	Bc	0.36	0/2831	0.56	0/3795
62	Bd	0.46	0/1755	0.59	0/2351
63	Be	0.37	0/834	0.59	0/1115
64	Bg	0.43	0/1059	0.58	0/1424
65	Bj	0.35	0/967	0.54	0/1293
66	Bn	0.38	0/826	0.53	0/1099
67	Bo	0.40	0/800	0.62	0/1074
68	Bp	0.40	0/647	0.57	0/868
69	Bq	0.39	0/497	0.54	0/664
70	Bs	0.32	0/542	0.49	0/716
71	Bu	0.33	0/815	0.53	0/1091
72	Bv	0.35	0/1294	0.51	0/1721
73	By	0.36	0/639	0.55	0/860
74	BB	0.39	0/204	0.41	0/260
75	BC	0.32	0/556	0.53	0/745
76	BD	0.38	0/1805	0.55	0/2409
77	BE	0.36	0/2751	0.55	0/3723

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
78	BI	0.28	0/1329	0.44	0/1859
79	BJ	0.28	0/1744	0.43	0/2440
80	BH	0.26	0/1022	0.57	6/1425 (0.4%)
81	BN	0.27	0/344	0.43	0/480
82	BM	0.27	0/394	0.39	0/550
83	BO	0.24	0/149	0.33	0/207
84	BL	0.27	0/319	0.43	0/445
85	2	1.38	186/41845 (0.4%)	1.37	337/65247 (0.5%)
86	Az	0.72	0/669	0.95	1/898 (0.1%)
87	Ah	0.71	0/1117	0.97	2/1505 (0.1%)
88	BK	0.70	0/1579	0.81	0/2209
89	Bk	0.59	0/985	0.78	0/1315
All	All	0.91	206/202773 (0.1%)	1.03	669/297267 (0.2%)

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
18	Ar	0	2
20	At	0	1
21	Au	0	1
24	Ax	0	1
26	AA	0	1
27	AB	0	1
33	AI	0	1
37	AM	0	2
39	AO	0	2
40	AP	0	3
41	AQ	0	1
48	Bi	0	1
49	Bl	0	1
51	Br	0	2
52	Bw	0	1
61	Bc	0	1
62	Bd	0	2
65	Bj	0	1
79	BJ	0	1
85	2	5	30
87	Ah	0	2
All	All	5	58

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	2	1391	A	O3'-P	-54.84	0.95	1.61
85	2	1402	U	O3'-P	-47.11	1.04	1.61
85	2	1450	C	O3'-P	46.76	2.17	1.61
85	2	1385	C	O3'-P	-44.51	1.07	1.61
85	2	1379	U	O3'-P	-44.30	1.07	1.61
85	2	1403	U	P-O5'	-43.17	1.16	1.59
85	2	1428	G	O3'-P	-36.99	1.16	1.61
85	2	1451	G	O3'-P	35.27	2.03	1.61
85	2	1445	U	O3'-P	-35.05	1.19	1.61
85	2	1404	C	O3'-P	-33.10	1.21	1.61
85	2	1166	A	O3'-P	-33.09	1.21	1.61
85	2	1390	A	O3'-P	31.52	1.99	1.61
85	2	1167	A	O3'-P	-30.50	1.24	1.61
85	2	1179	A	O3'-P	-28.26	1.27	1.61
85	2	1206	G	O3'-P	-27.52	1.28	1.61
85	2	1381	G	O3'-P	-26.89	1.28	1.61
85	2	1406	G	O3'-P	-25.60	1.30	1.61
85	2	1169	G	P-O5'	23.96	1.83	1.59
85	2	1438	G	O3'-P	-22.58	1.34	1.61
85	2	1207	C	O3'-P	-21.31	1.35	1.61
85	2	1169	G	O3'-P	20.83	1.86	1.61
85	2	1381	G	C5'-C4'	-20.38	1.26	1.51
85	2	1431	G	O3'-P	-20.37	1.36	1.61
85	2	1408	C	O3'-P	-20.05	1.37	1.61
85	2	1430	C	O3'-P	-20.04	1.37	1.61
85	2	1429	A	C3'-O3'	-19.44	1.15	1.42
85	2	1205	G	P-O5'	-19.23	1.40	1.59
85	2	1191	U	O3'-P	-18.63	1.38	1.61
85	2	1202	C	O3'-P	18.52	1.83	1.61
85	2	1378	U	O3'-P	-18.23	1.39	1.61
85	2	1187	G	O3'-P	17.70	1.82	1.61
85	2	1177	U	O3'-P	-17.00	1.40	1.61
85	2	1403	U	O3'-P	-16.98	1.40	1.61
85	2	1437	A	O3'-P	16.78	1.81	1.61
85	2	1439	U	O3'-P	-16.00	1.42	1.61
85	2	1186	A	O3'-P	-14.77	1.43	1.61
85	2	1392	A	O3'-P	-14.48	1.43	1.61
85	2	1447	G	O3'-P	-14.46	1.43	1.61
85	2	1400	C	O3'-P	-14.43	1.43	1.61
85	2	1455	U	O3'-P	-14.43	1.43	1.61
85	2	1217	G	O3'-P	-14.41	1.43	1.61
85	2	1401	A	O3'-P	-14.39	1.43	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	2	1219	C	O3'-P	-14.39	1.43	1.61
85	2	1448	U	O3'-P	-14.39	1.43	1.61
85	2	1443	U	O3'-P	-14.37	1.44	1.61
85	2	1212	U	O3'-P	-14.37	1.44	1.61
85	2	1398	G	O3'-P	-14.36	1.44	1.61
85	2	1210	A	O3'-P	-14.36	1.44	1.61
85	2	1213	C	O3'-P	-14.36	1.44	1.61
85	2	1452	C	O3'-P	-14.36	1.44	1.61
85	2	1218	U	O3'-P	-14.35	1.44	1.61
85	2	1395	C	O3'-P	-14.34	1.44	1.61
85	2	1446	A	O3'-P	-14.33	1.44	1.61
85	2	1397	C	O3'-P	-14.33	1.44	1.61
85	2	1384	G	O3'-P	-14.33	1.44	1.61
85	2	1209	A	O3'-P	-14.32	1.44	1.61
85	2	1214	G	O3'-P	-14.32	1.44	1.61
85	2	1444	U	O3'-P	-14.31	1.44	1.61
85	2	1396	U	O3'-P	-14.30	1.44	1.61
85	2	1216	C	O3'-P	-14.29	1.44	1.61
85	2	1453	C	O3'-P	-14.29	1.44	1.61
85	2	1388	A	O3'-P	-14.28	1.44	1.61
85	2	1215	A	O3'-P	-14.27	1.44	1.61
85	2	1389	G	O3'-P	-14.27	1.44	1.61
85	2	1394	A	O3'-P	-14.27	1.44	1.61
85	2	1211	C	O3'-P	-14.23	1.44	1.61
85	2	1170	A	O3'-P	14.10	1.78	1.61
85	2	1427	G	O3'-P	-14.03	1.44	1.61
85	2	1165	C	O3'-P	13.22	1.77	1.61
85	2	1433	A	O3'-P	-12.74	1.45	1.61
85	2	1456	G	O3'-P	-12.62	1.46	1.61
85	2	1168	G	O3'-P	-12.59	1.46	1.61
85	2	1407	G	O3'-P	-12.18	1.46	1.61
85	2	1386	G	O3'-P	-12.06	1.46	1.61
85	2	1409	G	C2'-O2'	11.42	1.56	1.41
85	2	1443	U	O5'-C5'	-10.07	1.26	1.42
85	2	1383	G	O3'-P	-9.86	1.49	1.61
85	2	1457	C	O3'-P	-9.57	1.49	1.61
85	2	1184	C	O3'-P	-8.88	1.50	1.61
85	2	1368	C	O3'-P	-8.88	1.50	1.61
85	2	1175	A	O3'-P	-8.87	1.50	1.61
85	2	1377	G	O3'-P	-8.85	1.50	1.61
85	2	1171	G	O3'-P	-8.83	1.50	1.61
85	2	1173	C	O3'-P	-8.82	1.50	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	2	1371	C	O3'-P	-8.81	1.50	1.61
85	2	1185	C	O3'-P	-8.81	1.50	1.61
85	2	1374	C	O3'-P	-8.80	1.50	1.61
85	2	1180	U	O3'-P	-8.80	1.50	1.61
85	2	1372	G	O3'-P	-8.79	1.50	1.61
85	2	1172	C	O3'-P	-8.79	1.50	1.61
85	2	1435	U	O3'-P	-8.79	1.50	1.61
85	2	1426	G	O3'-P	-8.78	1.50	1.61
85	2	1174	G	O3'-P	-8.78	1.50	1.61
85	2	1432	A	O3'-P	-8.78	1.50	1.61
85	2	1373	U	O3'-P	-8.78	1.50	1.61
85	2	1375	G	O3'-P	-8.77	1.50	1.61
85	2	1370	A	O3'-P	-8.77	1.50	1.61
85	2	1192	A	O3'-P	-8.77	1.50	1.61
85	2	1178	G	O3'-P	-8.76	1.50	1.61
85	2	1189	C	O3'-P	-8.76	1.50	1.61
85	2	1190	C	O3'-P	-8.76	1.50	1.61
85	2	1376	A	O3'-P	-8.74	1.50	1.61
85	2	1183	G	O3'-P	-8.74	1.50	1.61
85	2	1176	G	O3'-P	-8.71	1.50	1.61
85	2	1182	U	O3'-P	-8.71	1.50	1.61
85	2	1369	G	O3'-P	-8.71	1.50	1.61
85	2	1436	A	O3'-P	-8.71	1.50	1.61
85	2	1434	G	O3'-P	-8.71	1.50	1.61
85	2	1424	G	O3'-P	-8.69	1.50	1.61
85	2	1403	U	C3'-O3'	-8.56	1.30	1.42
85	2	1454	C	O3'-P	-8.45	1.51	1.61
85	2	1405	A	O3'-P	-8.42	1.51	1.61
85	2	1400	C	C1'-N1	8.22	1.61	1.48
85	2	1379	U	C5'-C4'	-8.19	1.41	1.51
85	2	1212	U	C1'-N1	8.19	1.61	1.48
85	2	1395	C	C1'-N1	8.18	1.61	1.48
85	2	1218	U	C1'-N1	8.17	1.61	1.48
85	2	1383	G	C1'-N9	8.15	1.60	1.48
85	2	1404	C	C1'-N1	8.14	1.60	1.48
85	2	1443	U	C1'-N1	8.14	1.60	1.48
85	2	1203	U	C1'-N1	8.13	1.60	1.48
85	2	1405	A	C1'-N9	8.11	1.60	1.48
85	2	1447	G	C1'-N9	8.10	1.60	1.48
85	2	1444	U	C1'-N1	8.10	1.60	1.48
85	2	1448	U	C1'-N1	8.09	1.60	1.48
85	2	1403	U	C1'-N1	8.06	1.60	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	2	1391	A	C1'-N9	8.06	1.60	1.48
85	2	1177	U	C1'-N1	-7.95	1.35	1.46
85	2	1380	G	C1'-N9	-7.93	1.35	1.46
85	2	1431	G	C1'-N9	-7.93	1.35	1.46
85	2	1169	G	C1'-N9	-7.92	1.35	1.46
85	2	1377	G	C1'-N9	-7.92	1.35	1.46
85	2	1435	U	C1'-N1	-7.89	1.35	1.46
85	2	1369	G	C1'-N9	-7.89	1.35	1.46
85	2	1193	G	C1'-N9	-7.88	1.35	1.46
85	2	1422	G	C1'-N9	-7.88	1.35	1.46
85	2	1407	G	C1'-N9	-7.88	1.35	1.46
85	2	1427	G	C1'-N9	-7.88	1.35	1.46
85	2	1406	G	C1'-N9	-7.87	1.35	1.46
85	2	1434	G	C1'-N9	-7.85	1.35	1.46
85	2	1424	G	C1'-N9	-7.85	1.35	1.46
85	2	1381	G	C1'-N9	-7.84	1.35	1.46
85	2	1440	G	C1'-N9	-7.84	1.35	1.46
85	2	1179	A	C1'-N9	-7.83	1.35	1.46
85	2	1428	G	C1'-N9	-7.83	1.35	1.46
85	2	1183	G	C1'-N9	-7.83	1.35	1.46
85	2	1438	G	C1'-N9	-7.83	1.35	1.46
85	2	1426	G	C1'-N9	-7.82	1.35	1.46
85	2	1459	A	C3'-O3'	-7.82	1.31	1.42
85	2	1442	G	C1'-N9	-7.82	1.35	1.46
85	2	1441	G	C1'-N9	-7.81	1.35	1.46
85	2	1187	G	C1'-N9	-7.80	1.35	1.46
85	2	1172	C	C1'-N1	-7.80	1.35	1.46
85	2	1175	A	C1'-N9	-7.79	1.35	1.46
85	2	1372	G	C1'-N9	-7.79	1.35	1.46
85	2	1375	G	C1'-N9	-7.79	1.35	1.46
85	2	1382	C	O3'-P	7.67	1.70	1.61
85	2	1188	A	O3'-P	7.61	1.70	1.61
85	2	921	G	C3'-O3'	7.08	1.52	1.42
43	1	1664	A	N9-C4	-7.00	1.33	1.37
85	2	1410	A	P-OP2	6.98	1.60	1.49
85	2	1380	G	O3'-P	6.94	1.69	1.61
85	2	1205	G	O3'-P	-6.81	1.52	1.61
43	1	2380	G	N9-C4	-6.78	1.32	1.38
85	2	1169	G	C5'-C4'	-6.62	1.43	1.51
43	1	3028	A	N9-C4	-6.49	1.33	1.37
43	1	2380	G	C2-N3	-6.29	1.27	1.32
85	2	1393	G	O3'-P	-6.24	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1	2380	G	N3-C4	-6.13	1.31	1.35
43	1	654	G	N9-C4	-6.09	1.33	1.38
85	2	1409	G	C3'-C2'	5.97	1.59	1.52
85	2	1404	C	C3'-O3'	5.83	1.50	1.42
85	2	1409	G	O3'-P	-5.71	1.54	1.61
43	1	2326	A	N7-C5	-5.68	1.35	1.39
85	2	1208	C	P-O5'	-5.67	1.54	1.59
43	1	932	A	N9-C4	-5.57	1.34	1.37
43	1	944	A	N9-C4	-5.53	1.34	1.37
43	1	236	A	N9-C4	-5.50	1.34	1.37
85	2	1167	A	C1'-N9	-5.50	1.39	1.46
85	2	1176	G	C1'-N9	-5.49	1.39	1.46
85	2	1186	A	C1'-N9	-5.47	1.39	1.46
85	2	1171	G	C1'-N9	-5.46	1.39	1.46
85	2	1432	A	C1'-N9	-5.45	1.39	1.46
85	2	1437	A	C1'-N9	-5.45	1.39	1.46
43	1	105	A	N9-C4	-5.44	1.34	1.37
43	1	905	A	N9-C4	-5.43	1.34	1.37
85	2	1376	A	C1'-N9	-5.42	1.39	1.46
85	2	1166	A	C1'-N9	-5.42	1.39	1.46
85	2	1188	A	C1'-N9	-5.42	1.39	1.46
85	2	1192	A	C1'-N9	-5.41	1.39	1.46
85	2	1433	A	C1'-N9	-5.41	1.39	1.46
85	2	1168	G	C1'-N9	-5.40	1.39	1.46
85	2	1436	A	C1'-N9	-5.39	1.39	1.46
85	2	1429	A	C1'-N9	-5.38	1.39	1.46
51	Br	161	ARG	CZ-NH2	-5.37	1.26	1.33
85	2	1203	U	O3'-P	5.37	1.67	1.61
43	1	2741	C	C2-O2	-5.34	1.19	1.24
85	2	1370	A	C1'-N9	-5.34	1.39	1.46
85	2	1180	U	C1'-N1	-5.33	1.39	1.46
43	1	1658	A	N9-C4	-5.28	1.34	1.37
43	1	654	G	N3-C4	-5.27	1.31	1.35
43	1	613	A	N9-C4	-5.24	1.34	1.37
43	1	2888	A	N9-C4	-5.21	1.34	1.37
43	1	903	G	N3-C4	-5.04	1.31	1.35
43	1	2108	A	N9-C4	-5.04	1.34	1.37
85	2	1411	G	O5'-C5'	5.03	1.52	1.44

All (669) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	2	1428	G	P-O3'-C3'	39.63	167.26	119.70
85	2	1404	C	P-O3'-C3'	35.06	161.77	119.70
85	2	1454	C	P-O3'-C3'	34.74	161.39	119.70
85	2	1457	C	P-O3'-C3'	32.50	158.70	119.70
85	2	1391	A	P-O3'-C3'	32.21	158.35	119.70
85	2	1445	U	O3'-P-O5'	-31.99	43.22	104.00
85	2	1166	A	P-O3'-C3'	29.96	155.66	119.70
85	2	1380	G	P-O3'-C3'	-28.59	85.40	119.70
85	2	234	A	OP1-P-OP2	-28.35	77.08	119.60
85	2	1165	C	P-O3'-C3'	-27.35	86.88	119.70
85	2	234	A	O5'-P-OP2	-26.21	79.25	110.70
85	2	1381	G	P-O5'-C5'	25.45	161.61	120.90
85	2	1169	G	P-O3'-C3'	24.60	149.22	119.70
85	2	1378	U	P-O3'-C3'	24.12	148.64	119.70
85	2	1205	G	P-O5'-C5'	23.72	158.86	120.90
85	2	1433	A	P-O3'-C3'	23.64	148.07	119.70
85	2	1207	C	P-O3'-C3'	23.58	148.00	119.70
85	2	1451	G	O3'-P-O5'	23.41	148.48	104.00
85	2	1379	U	O5'-C5'-C4'	22.73	154.89	111.70
85	2	1382	C	P-O3'-C3'	-22.66	92.50	119.70
85	2	1382	C	P-O5'-C5'	21.56	155.40	120.90
85	2	1187	G	P-O3'-C3'	-21.45	93.96	119.70
85	2	1393	G	OP1-P-O3'	21.16	151.75	105.20
85	2	1445	U	OP1-P-O3'	20.98	151.36	105.20
85	2	1409	G	C4'-C3'-O3'	20.55	154.09	113.00
85	2	1407	G	P-O5'-C5'	19.77	152.53	120.90
85	2	1451	G	OP1-P-O3'	-19.41	62.50	105.20
85	2	1178	G	O5'-C5'-C4'	19.39	148.54	111.70
85	2	1379	U	P-O3'-C3'	19.36	142.94	119.70
85	2	1169	G	O5'-C5'-C4'	19.32	148.42	111.70
85	2	1178	G	P-O5'-C5'	19.07	151.41	120.90
85	2	1400	C	P-O3'-C3'	19.07	142.58	119.70
85	2	1202	C	P-O3'-C3'	19.00	142.50	119.70
85	2	1388	A	P-O3'-C3'	-18.95	96.96	119.70
85	2	1445	U	P-O3'-C3'	-18.95	96.96	119.70
85	2	1443	U	P-O5'-C5'	18.86	151.08	120.90
85	2	1409	G	C2'-C3'-O3'	-18.19	69.48	109.50
85	2	1391	A	OP1-P-O3'	17.87	144.51	105.20
85	2	234	A	O5'-P-OP1	17.66	131.90	110.70
85	2	1188	A	O5'-C5'-C4'	17.17	144.32	111.70
85	2	1186	A	P-O3'-C3'	-16.62	99.76	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	2	1457	C	OP1-P-O3'	16.34	141.14	105.20
85	2	1187	G	OP2-P-O3'	16.23	140.89	105.20
85	2	1165	C	C5'-C4'-O4'	15.74	127.99	109.10
85	2	1422	G	O3'-P-O5'	15.70	133.83	104.00
85	2	1207	C	O5'-C5'-C4'	15.32	140.81	111.70
51	Br	161	ARG	NE-CZ-NH1	15.23	127.92	120.30
85	2	1403	U	P-O5'-C5'	15.01	144.92	120.90
85	2	1403	U	O5'-P-OP1	14.81	128.47	110.70
85	2	1455	U	P-O5'-C5'	14.66	144.35	120.90
85	2	1205	G	P-O3'-C3'	-14.21	102.65	119.70
85	2	1440	G	O3'-P-O5'	-14.20	77.03	104.00
85	2	1168	G	P-O3'-C3'	14.07	136.58	119.70
85	2	1390	A	P-O3'-C3'	-14.04	102.85	119.70
85	2	1382	C	OP1-P-O3'	13.91	135.80	105.20
85	2	1186	A	OP2-P-O3'	13.65	135.24	105.20
85	2	1206	G	OP1-P-O3'	13.62	135.16	105.20
85	2	1391	A	OP2-P-O3'	-13.52	75.47	105.20
85	2	1169	G	O3'-P-O5'	13.35	129.37	104.00
85	2	1206	G	P-O3'-C3'	13.29	135.65	119.70
85	2	1402	U	P-O3'-C3'	13.09	135.41	119.70
85	2	1445	U	OP2-P-O3'	-13.06	76.47	105.20
43	1	2380	G	N3-C4-N9	-13.04	118.18	126.00
85	2	1206	G	O3'-P-O5'	-12.68	79.91	104.00
85	2	1381	G	O3'-P-O5'	12.40	127.56	104.00
85	2	1439	U	OP2-P-O3'	12.24	132.14	105.20
85	2	1378	U	OP1-P-O3'	12.21	132.07	105.20
85	2	1409	G	O4'-C4'-C3'	12.15	116.15	104.00
85	2	1393	G	OP2-P-O3'	-12.07	78.64	105.20
85	2	1189	C	O5'-C5'-C4'	12.06	134.62	111.70
85	2	1203	U	P-O3'-C3'	11.99	134.09	119.70
85	2	1442	G	P-O3'-C3'	-11.98	105.32	119.70
85	2	233	A	OP2-P-O3'	11.97	131.53	105.20
85	2	1440	G	P-O3'-C3'	11.90	133.98	119.70
85	2	1406	G	O3'-P-O5'	-11.83	81.53	104.00
85	2	1187	G	OP1-P-O3'	-11.77	79.31	105.20
85	2	1404	C	C4'-C3'-O3'	11.74	136.49	113.00
85	2	1382	C	O3'-P-O5'	-11.73	81.71	104.00
85	2	1409	G	N9-C1'-C2'	11.63	129.12	114.00
85	2	1457	C	OP2-P-O3'	-11.60	79.68	105.20
85	2	1407	G	P-O3'-C3'	-11.53	105.86	119.70
85	2	1167	A	P-O3'-C3'	11.50	133.50	119.70
85	2	1409	G	C5'-C4'-O4'	11.45	122.84	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	2	1437	A	O3'-P-O5'	-11.45	82.24	104.00
85	2	1205	G	OP2-P-O3'	11.35	130.17	105.20
85	2	1403	U	P-O3'-C3'	11.30	133.26	119.70
85	2	1178	G	P-O3'-C3'	11.25	133.20	119.70
85	2	1437	A	P-O3'-C3'	-10.97	106.53	119.70
85	2	1439	U	P-O3'-C3'	10.92	132.81	119.70
85	2	1204	A	P-O5'-C5'	10.83	138.22	120.90
85	2	1206	G	C2'-C3'-O3'	10.83	133.32	109.50
85	2	1188	A	P-O3'-C3'	10.80	132.66	119.70
85	2	233	A	OP1-P-O3'	-10.80	81.45	105.20
85	2	1410	A	C4-N9-C1'	-10.76	106.93	126.30
85	2	1393	G	O3'-P-O5'	-10.70	83.67	104.00
85	2	1437	A	OP1-P-O3'	10.66	128.66	105.20
85	2	1430	C	OP1-P-O3'	10.57	128.47	105.20
85	2	233	A	O3'-P-O5'	-10.56	83.94	104.00
85	2	1449	A	O3'-P-O5'	10.54	124.02	104.00
85	2	1410	A	C8-N9-C1'	10.44	146.50	127.70
85	2	1205	G	O5'-P-OP1	10.23	122.97	110.70
85	2	1440	G	OP1-P-O3'	10.09	127.39	105.20
85	2	1450	C	O3'-P-O5'	10.06	123.12	104.00
85	2	1378	U	OP2-P-O3'	-9.88	83.46	105.20
85	2	1439	U	O3'-P-O5'	-9.81	85.36	104.00
85	2	1410	A	C4'-C3'-O3'	9.70	132.40	113.00
85	2	1431	G	P-O3'-C3'	9.70	131.34	119.70
85	2	1204	A	O5'-C5'-C4'	9.63	129.99	111.70
85	2	1177	U	OP2-P-O3'	9.62	126.37	105.20
85	2	1177	U	O4'-C1'-N1	9.62	115.89	108.20
85	2	1205	G	O5'-C5'-C4'	-9.62	93.43	111.70
85	2	1206	G	P-O5'-C5'	9.58	136.22	120.90
85	2	924	C	N1-C1'-C2'	-9.55	101.50	112.00
85	2	1377	G	O4'-C1'-N9	9.54	115.83	108.20
85	2	1169	G	OP2-P-O3'	-9.51	84.27	105.20
85	2	1203	U	O5'-C5'-C4'	9.51	129.78	111.70
85	2	1434	G	O4'-C1'-N9	9.51	115.81	108.20
85	2	1407	G	O4'-C1'-N9	9.49	115.79	108.20
85	2	1427	G	O4'-C1'-N9	9.49	115.79	108.20
85	2	1424	G	O4'-C1'-N9	9.48	115.78	108.20
85	2	1422	G	O4'-C1'-N9	9.48	115.78	108.20
43	1	881	C	N3-C2-O2	-9.45	115.29	121.90
85	2	1187	G	O4'-C1'-N9	9.45	115.76	108.20
85	2	1369	G	O4'-C1'-N9	9.44	115.75	108.20
85	2	1175	A	O4'-C1'-N9	9.44	115.75	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	2	1431	G	O4'-C1'-N9	9.44	115.75	108.20
85	2	1193	G	O4'-C1'-N9	9.43	115.75	108.20
85	2	1428	G	O4'-C1'-N9	9.43	115.74	108.20
85	2	1440	G	O4'-C1'-N9	9.43	115.74	108.20
85	2	1438	G	O4'-C1'-N9	9.42	115.73	108.20
85	2	1380	G	O4'-C1'-N9	9.41	115.73	108.20
85	2	1442	G	O4'-C1'-N9	9.41	115.73	108.20
85	2	1169	G	O4'-C1'-N9	9.40	115.72	108.20
85	2	1179	A	O4'-C1'-N9	9.40	115.72	108.20
85	2	1381	G	O4'-C1'-N9	9.39	115.72	108.20
85	2	1406	G	O4'-C1'-N9	9.39	115.71	108.20
85	2	1375	G	O4'-C1'-N9	9.38	115.71	108.20
85	2	1172	C	O4'-C1'-N1	9.38	115.71	108.20
85	2	1183	G	O4'-C1'-N9	9.38	115.70	108.20
85	2	1186	A	O3'-P-O5'	-9.37	86.19	104.00
85	2	1435	U	O4'-C1'-N1	9.37	115.70	108.20
85	2	1426	G	O4'-C1'-N9	9.37	115.69	108.20
85	2	1372	G	O4'-C1'-N9	9.36	115.69	108.20
85	2	1441	G	O4'-C1'-N9	9.28	115.62	108.20
43	1	1209	U	N3-C4-O4	9.23	125.86	119.40
85	2	808	C	C2-N1-C1'	9.20	128.92	118.80
43	1	2380	G	C5-C6-O6	9.20	134.12	128.60
85	2	1170	A	O3'-P-O5'	9.20	121.47	104.00
43	1	633	C	N1-C2-O2	9.16	124.40	118.90
85	2	1406	G	OP2-P-O3'	9.03	125.07	105.20
85	2	1165	C	OP2-P-O3'	9.03	125.06	105.20
85	2	1380	G	O5'-C5'-C4'	9.02	128.84	111.70
43	1	2380	G	N9-C4-C5	9.01	109.00	105.40
85	2	1404	C	OP2-P-O3'	8.94	124.86	105.20
43	1	999	C	C2-N3-C4	-8.93	115.43	119.90
85	2	1454	C	O3'-P-O5'	-8.88	87.12	104.00
43	1	1100	G	O4'-C1'-N9	8.86	115.28	108.20
85	2	78	U	C2-N1-C1'	-8.85	107.08	117.70
85	2	1459	A	C2'-C3'-O3'	8.84	128.95	109.50
85	2	1400	C	OP1-P-O3'	8.81	124.59	105.20
85	2	1438	G	P-O3'-C3'	8.77	130.23	119.70
43	1	998	C	N3-C2-O2	-8.75	115.78	121.90
85	2	1429	A	O3'-P-O5'	8.57	120.28	104.00
85	2	1399	G	O3'-P-O5'	8.54	120.22	104.00
43	1	633	C	C2-N1-C1'	8.51	128.16	118.80
85	2	1404	C	OP1-P-O3'	-8.50	86.50	105.20
43	1	1877	G	C4-C5-N7	8.49	114.20	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	2380	G	N3-C4-C5	8.43	132.81	128.60
85	2	898	C	N3-C2-O2	-8.41	116.02	121.90
85	2	1408	C	O3'-P-O5'	-8.40	88.04	104.00
43	1	1921	C	C2-N1-C1'	8.35	127.98	118.80
85	2	1205	G	OP1-P-O3'	-8.34	86.86	105.20
85	2	1433	A	OP1-P-O3'	8.34	123.54	105.20
43	1	139	G	N3-C4-N9	-8.33	121.00	126.00
43	1	2380	G	C8-N9-C1'	8.31	137.80	127.00
43	1	1236	G	N3-C4-N9	-8.26	121.05	126.00
60	Ba	181	SER	N-CA-C	8.26	133.29	111.00
85	2	1214	G	O4'-C1'-N9	8.24	114.79	108.20
85	2	1385	C	O4'-C1'-N1	8.23	114.78	108.20
85	2	1217	G	O4'-C1'-N9	8.23	114.78	108.20
85	2	1384	G	O4'-C1'-N9	8.21	114.76	108.20
85	2	1397	C	O4'-C1'-N1	8.21	114.77	108.20
85	2	1206	G	O4'-C1'-N9	8.20	114.76	108.20
85	2	1398	G	O4'-C1'-N9	8.20	114.76	108.20
85	2	1220	G	O4'-C1'-N9	8.19	114.75	108.20
85	2	1450	C	O4'-C1'-N1	8.17	114.73	108.20
85	2	1205	G	O4'-C1'-N9	8.15	114.72	108.20
85	2	1409	G	O5'-P-OP1	8.15	120.48	110.70
85	2	1204	A	OP2-P-O3'	-8.11	87.36	105.20
85	2	440	U	C2-N1-C1'	8.10	127.42	117.70
85	2	1179	A	O3'-P-O5'	8.10	119.40	104.00
43	1	1100	G	N3-C4-N9	-8.01	121.19	126.00
43	1	1879	U	C2-N1-C1'	7.92	127.20	117.70
43	1	1100	G	C4-N9-C1'	-7.85	116.29	126.50
43	1	1877	G	N9-C4-C5	-7.79	102.28	105.40
85	2	808	C	C6-N1-C2	-7.77	117.19	120.30
85	2	1843	G	N3-C4-N9	-7.76	121.35	126.00
43	1	1591	U	O4'-C1'-N1	7.74	114.39	108.20
43	1	1664	A	C8-N9-C4	7.71	108.89	105.80
43	1	1641	U	C2-N1-C1'	7.70	126.94	117.70
85	2	1145	G	C4-N9-C1'	-7.69	116.50	126.50
85	2	1454	C	OP2-P-O3'	7.69	122.11	105.20
85	2	1387	G	P-O3'-C3'	7.65	128.88	119.70
43	1	1059	C	N1-C2-O2	7.61	123.47	118.90
40	AP	670	ALA	CB-CA-C	-7.60	98.70	110.10
85	2	1208	C	P-O5'-C5'	7.60	133.06	120.90
85	2	1177	U	OP1-P-O3'	-7.57	88.54	105.20
85	2	1387	G	OP1-P-O3'	7.55	121.80	105.20
43	1	2931	G	P-O3'-C3'	7.54	128.74	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	1201	C	N1-C2-O2	7.52	123.41	118.90
43	1	1134	C	C2-N1-C1'	7.51	127.07	118.80
85	2	1430	C	O3'-P-O5'	-7.51	89.73	104.00
43	1	1921	C	N1-C2-O2	7.48	123.39	118.90
85	2	1205	G	O5'-P-OP2	-7.48	98.97	105.70
85	2	1379	U	C5'-C4'-C3'	7.46	127.94	116.00
85	2	1407	G	O3'-P-O5'	-7.45	89.84	104.00
85	2	1422	G	OP2-P-O3'	-7.45	88.81	105.20
43	1	2741	C	N3-C2-O2	-7.39	116.73	121.90
85	2	440	U	N1-C2-O2	7.38	127.97	122.80
43	1	2702	C	C2-N3-C4	-7.38	116.21	119.90
85	2	78	U	C6-N1-C1'	7.35	131.50	121.20
43	1	2380	G	C4-N9-C1'	-7.35	116.95	126.50
43	1	1921	C	C6-N1-C1'	-7.34	111.99	120.80
43	1	1209	U	C5-C4-O4	-7.30	121.52	125.90
43	1	2380	G	N1-C6-O6	-7.29	115.52	119.90
85	2	1409	G	C8-N9-C1'	-7.28	117.53	127.00
43	1	2641	C	N1-C2-O2	7.24	123.25	118.90
43	1	882	C	C2-N3-C4	-7.24	116.28	119.90
85	2	1410	A	C3'-C2'-C1'	7.23	107.29	101.50
43	1	633	C	C6-N1-C1'	-7.23	112.12	120.80
43	1	2741	C	C6-N1-C2	-7.20	117.42	120.30
85	2	404	C	N1-C2-O2	7.15	123.19	118.90
43	1	2326	A	N1-C6-N6	7.10	122.86	118.60
43	1	654	G	N3-C4-N9	-7.09	121.75	126.00
43	1	1100	G	C8-N9-C1'	7.06	136.17	127.00
43	1	1071	G	C2-N3-C4	-7.05	108.38	111.90
43	1	1877	G	N3-C2-N2	7.04	124.83	119.90
85	2	1145	G	C8-N9-C1'	7.04	136.16	127.00
85	2	1831	C	N1-C2-O2	7.03	123.12	118.90
85	2	1438	G	O5'-C5'-C4'	-7.03	98.35	111.70
43	1	1470	U	C2-N1-C1'	7.03	126.13	117.70
85	2	1165	C	O3'-P-O5'	-7.01	90.68	104.00
43	1	2326	A	C6-C5-N7	-7.00	127.40	132.30
43	1	1236	G	C4-N9-C1'	-7.00	117.41	126.50
43	1	1934	C	C6-N1-C2	-6.98	117.51	120.30
43	1	999	C	C2-N1-C1'	-6.96	111.14	118.80
43	1	2380	G	C2-N3-C4	-6.94	108.43	111.90
85	2	1167	A	O3'-P-O5'	6.92	117.16	104.00
85	2	1843	G	C8-N9-C1'	6.92	135.99	127.00
43	1	2741	C	N1-C2-N3	6.90	124.03	119.20
85	2	1403	U	O5'-P-OP2	-6.90	99.49	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	2	898	C	N1-C2-O2	6.90	123.04	118.90
43	1	954	U	N3-C4-O4	-6.85	114.61	119.40
85	2	15	A	N1-C6-N6	6.83	122.70	118.60
85	2	1168	G	OP2-P-O3'	6.83	120.22	105.20
85	2	1177	U	P-O3'-C3'	6.82	127.88	119.70
85	2	1408	C	P-O3'-C3'	6.81	127.87	119.70
85	2	1409	G	C3'-C2'-O2'	-6.80	93.58	113.30
43	1	1100	G	N3-C4-C5	6.77	131.98	128.60
43	1	1871	A	N9-C4-C5	-6.77	103.09	105.80
43	1	1236	G	C8-N9-C1'	6.76	135.79	127.00
85	2	1827	G	C5-C6-O6	-6.75	124.55	128.60
85	2	1461	A	C2'-C3'-O3'	6.75	124.49	113.70
43	1	882	C	N1-C2-N3	6.74	123.92	119.20
85	2	1672	G	N7-C8-N9	6.73	116.47	113.10
85	2	1802	C	C2-N1-C1'	-6.73	111.40	118.80
43	1	1307	G	C8-N9-C1'	-6.69	118.30	127.00
85	2	808	C	N1-C2-O2	6.68	122.91	118.90
43	1	1618	G	C4-N9-C1'	-6.65	117.85	126.50
85	2	1403	U	O3'-P-O5'	-6.64	91.38	104.00
43	1	1934	C	N3-C2-O2	-6.64	117.25	121.90
85	2	1819	A	N1-C2-N3	6.63	132.61	129.30
43	1	2660	G	N3-C4-N9	-6.62	122.03	126.00
43	1	2374	C	C6-N1-C2	-6.62	117.65	120.30
43	1	2252	C	N1-C2-O2	6.59	122.86	118.90
85	2	1862	C	N3-C2-O2	-6.59	117.29	121.90
85	2	1428	G	OP1-P-O3'	-6.55	90.78	105.20
43	1	2274	U	N3-C2-O2	-6.55	117.61	122.20
85	2	1176	G	O3'-P-O5'	6.55	116.44	104.00
43	1	2380	G	C6-C5-N7	6.54	134.33	130.40
43	1	1236	G	N3-C4-C5	6.53	131.87	128.60
43	1	2654	C	C2-N1-C1'	-6.53	111.62	118.80
43	1	1457	C	C2-N1-C1'	6.52	125.97	118.80
6	Ae	138	PHE	C-N-CA	6.52	137.99	121.70
85	2	1176	G	OP2-P-O3'	-6.50	90.90	105.20
43	1	1109	A	N7-C8-N9	-6.50	110.55	113.80
43	1	1134	C	N1-C2-O2	6.50	122.80	118.90
43	1	825	U	C2-N1-C1'	6.47	125.47	117.70
43	1	1647	U	P-O3'-C3'	6.47	127.47	119.70
85	2	397	G	N1-C6-O6	-6.47	116.02	119.90
43	1	1307	G	N3-C4-N9	6.47	129.88	126.00
57	BG	278	PRO	N-CA-CB	6.47	111.06	103.30
85	2	1410	A	O4'-C4'-C3'	6.47	111.27	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	139	G	C8-N9-C1'	6.46	135.40	127.00
43	1	999	C	N1-C2-N3	6.46	123.72	119.20
43	1	1249	C	N3-C2-O2	-6.46	117.38	121.90
43	1	633	C	N3-C2-O2	-6.44	117.39	121.90
43	1	1879	U	C6-N1-C1'	-6.43	112.20	121.20
43	1	274	G	O4'-C1'-N9	6.42	113.34	108.20
85	2	1843	G	C4-N9-C1'	-6.40	118.19	126.50
43	1	1099	U	O4'-C1'-N1	6.39	113.31	108.20
43	1	1368	G	O4'-C1'-N9	6.38	113.31	108.20
85	2	1831	C	N3-C2-O2	-6.38	117.44	121.90
85	2	1208	C	O3'-P-O5'	-6.38	91.89	104.00
43	1	1231	U	C5-C6-N1	6.37	125.89	122.70
43	1	2174	G	O4'-C1'-N9	6.37	113.30	108.20
85	2	440	U	N3-C2-O2	-6.36	117.75	122.20
85	2	924	C	O4'-C1'-N1	6.36	113.29	108.20
43	1	1307	G	C4-N9-C1'	6.36	134.76	126.50
85	2	114	C	C2-N1-C1'	-6.35	111.81	118.80
85	2	1887	G	N3-C4-N9	-6.35	122.19	126.00
43	1	2252	C	C2-N1-C1'	6.31	125.74	118.80
43	1	881	C	C6-N1-C2	-6.30	117.78	120.30
43	1	2382	A	C4-C5-C6	6.30	120.15	117.00
43	1	2931	G	OP2-P-O3'	6.29	119.04	105.20
85	2	1728	G	C4-N9-C1'	-6.28	118.33	126.50
85	2	1166	A	OP2-P-O3'	-6.28	91.39	105.20
85	2	1393	G	P-O3'-C3'	-6.27	112.17	119.70
43	1	1154	C	C2-N1-C1'	6.27	125.69	118.80
85	2	1438	G	OP2-P-O3'	-6.26	91.42	105.20
85	2	1166	A	O3'-P-O5'	6.26	115.90	104.00
43	1	477	U	C5-C6-N1	6.26	125.83	122.70
1	Aa	84	ASN	CB-CA-C	-6.25	97.89	110.40
43	1	114	C	C2-N1-C1'	6.25	125.67	118.80
85	2	1387	G	OP2-P-O3'	-6.25	91.46	105.20
43	1	654	G	C2-N3-C4	-6.24	108.78	111.90
85	2	808	C	C5-C6-N1	6.24	124.12	121.00
43	1	654	G	N3-C4-C5	6.23	131.71	128.60
85	2	808	C	N3-C2-O2	-6.21	117.55	121.90
85	2	924	C	C1'-C2'-O2'	-6.21	91.97	110.60
43	1	3067	C	N3-C2-O2	-6.21	117.55	121.90
44	3	2	A	C1'-C2'-O2'	6.20	129.20	110.60
85	2	1145	G	N3-C4-N9	-6.18	122.29	126.00
43	1	1155	C	C6-N1-C2	-6.18	117.83	120.30
43	1	1457	C	N1-C2-O2	6.18	122.61	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	2	1456	G	P-O3'-C3'	6.18	127.12	119.70
43	1	1268	G	N3-C2-N2	-6.17	115.58	119.90
85	2	875	C	N3-C2-O2	-6.17	117.58	121.90
43	1	139	G	C4-N9-C1'	-6.16	118.50	126.50
43	1	140	C	P-O3'-C3'	6.14	127.07	119.70
43	1	999	C	C6-N1-C1'	6.14	128.17	120.80
85	2	1827	G	N1-C6-O6	6.14	123.59	119.90
43	1	2413	G	O4'-C1'-N9	6.14	113.11	108.20
43	1	1579	C	C2-N1-C1'	-6.13	112.06	118.80
43	1	434	A	O4'-C1'-N9	6.12	113.10	108.20
43	1	1202	C	N3-C2-O2	-6.12	117.61	121.90
85	2	1165	C	C5'-C4'-C3'	6.11	125.78	116.00
43	1	954	U	C2-N1-C1'	-6.11	110.37	117.70
85	2	1431	G	O3'-P-O5'	6.11	115.61	104.00
85	2	1819	A	O4'-C1'-N9	-6.11	103.31	108.20
43	1	1059	C	N3-C2-O2	-6.11	117.63	121.90
43	1	2455	A	C8-N9-C4	-6.10	103.36	105.80
85	2	1845	G	N9-C4-C5	-6.09	102.96	105.40
43	1	2660	G	C5-C6-O6	6.08	132.25	128.60
43	1	1109	A	C8-N9-C4	6.06	108.22	105.80
43	1	826	C	C6-N1-C2	-6.06	117.88	120.30
43	1	992	G	N3-C4-C5	6.06	131.63	128.60
43	1	1569	A	C2-N3-C4	-6.06	107.57	110.60
43	1	486	U	O4'-C1'-N1	6.06	113.05	108.20
85	2	1923	C	N3-C2-O2	-6.06	117.66	121.90
85	2	1803	C	C5-C6-N1	6.03	124.01	121.00
43	1	2093	G	C4-N9-C1'	6.02	134.33	126.50
80	BH	184	PRO	N-CA-CB	6.02	110.53	103.30
85	2	1845	G	C4-C5-N7	6.02	113.21	110.80
43	1	1579	C	O4'-C1'-N1	6.01	113.01	108.20
85	2	1843	G	N9-C4-C5	6.00	107.80	105.40
43	1	1134	C	N3-C2-O2	-5.99	117.71	121.90
43	1	1621	C	P-O3'-C3'	5.99	126.89	119.70
43	1	2500	C	C6-N1-C1'	5.99	127.99	120.80
43	1	139	G	N9-C4-C5	5.99	107.80	105.40
57	BG	175	PRO	N-CA-CB	5.98	110.48	103.30
43	1	314	U	O4'-C1'-N1	-5.98	103.42	108.20
43	1	1201	C	C2-N1-C1'	5.98	125.38	118.80
87	Ah	91	PRO	CA-N-CD	-5.97	103.14	111.50
43	1	861	C	C5-C6-N1	5.96	123.98	121.00
85	2	808	C	C6-N1-C1'	-5.96	113.65	120.80
43	1	2062	G	N3-C4-N9	5.96	129.57	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	Br	179	GLY	N-CA-C	-5.95	98.23	113.10
43	1	2544	G	C6-C5-N7	-5.94	126.84	130.40
43	1	309	C	N1-C2-O2	5.93	122.46	118.90
43	1	999	C	N1-C2-O2	-5.93	115.34	118.90
43	1	119	A	O5'-P-OP2	-5.91	100.38	105.70
44	3	3	A	N9-C1'-C2'	-5.90	105.51	112.00
43	1	1345	A	C8-N9-C4	-5.90	103.44	105.80
85	2	287	U	C2-N1-C1'	-5.90	110.62	117.70
57	BG	241	PRO	N-CA-CB	5.90	110.38	103.30
43	1	1547	C	O4'-C1'-N1	5.89	112.92	108.20
43	1	1640	C	N1-C2-O2	5.89	122.44	118.90
43	1	716	U	N1-C2-O2	-5.89	118.68	122.80
43	1	3151	G	C4-C5-N7	5.88	113.15	110.80
43	1	903	G	C6-N1-C2	-5.87	121.58	125.10
80	BH	165	PRO	N-CA-CB	5.87	110.34	103.30
85	2	1399	G	OP2-P-O3'	-5.87	92.29	105.20
43	1	1618	G	C8-N9-C1'	5.87	134.62	127.00
43	1	2326	A	C4-C5-C6	5.86	119.93	117.00
43	1	2641	C	N3-C2-O2	-5.85	117.81	121.90
85	2	149	G	C4-N9-C1'	-5.84	118.91	126.50
43	1	1401	G	C8-N9-C4	-5.83	104.07	106.40
85	2	1862	C	N1-C2-O2	5.83	122.40	118.90
85	2	1438	G	O3'-P-O5'	5.82	115.06	104.00
43	1	2546	U	C2-N1-C1'	5.82	124.69	117.70
43	1	2500	C	C2-N1-C1'	-5.82	112.40	118.80
43	1	2705	G	C4-N9-C1'	5.82	134.06	126.50
85	2	1433	A	OP2-P-O3'	-5.82	92.40	105.20
43	1	521	G	N3-C4-N9	5.81	129.49	126.00
57	BG	311	PRO	N-CA-CB	5.81	110.28	103.30
43	1	2787	C	N1-C2-O2	5.81	122.39	118.90
43	1	2048	C	N3-C2-O2	-5.81	117.83	121.90
43	1	127	C	C6-N1-C1'	-5.81	113.83	120.80
85	2	1410	A	O4'-C1'-N9	-5.81	103.55	108.20
85	2	1202	C	O3'-P-O5'	5.81	115.03	104.00
43	1	2577	C	C6-N1-C2	-5.79	117.98	120.30
43	1	1339	G	C6-C5-N7	-5.79	126.93	130.40
43	1	1223	G	N9-C4-C5	5.79	107.71	105.40
43	1	1236	G	C6-C5-N7	5.78	133.87	130.40
85	2	397	G	C5-C6-O6	5.78	132.07	128.60
85	2	1485	G	N3-C4-C5	5.78	131.49	128.60
57	BG	204	PRO	N-CA-CB	5.77	110.22	103.30
85	2	1464	G	OP1-P-O3'	5.77	117.89	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	2	440	U	C6-N1-C1'	-5.77	113.13	121.20
85	2	1849	U	OP1-P-O3'	5.77	117.89	105.20
85	2	97	A	O4'-C1'-N9	5.76	112.81	108.20
43	1	1221	C	C6-N1-C2	-5.75	118.00	120.30
43	1	2942	G	N3-C4-N9	-5.75	122.55	126.00
85	2	1887	G	N3-C4-C5	5.75	131.47	128.60
57	BG	206	PRO	N-CA-CB	5.75	110.20	103.30
85	2	1402	U	O3'-P-O5'	-5.74	93.09	104.00
85	2	1827	G	N9-C4-C5	-5.74	103.10	105.40
85	2	1405	A	P-O3'-C3'	5.74	126.58	119.70
85	2	1845	G	N3-C4-N9	5.73	129.44	126.00
51	Br	195	LYS	CB-CA-C	5.72	121.84	110.40
43	1	114	C	N1-C2-O2	5.72	122.33	118.90
43	1	2544	G	C4-N9-C1'	5.72	133.93	126.50
43	1	691	A	O4'-C1'-N9	5.71	112.77	108.20
43	1	2741	C	C5-C4-N4	5.71	124.19	120.20
43	1	2991	U	C2-N1-C1'	5.70	124.54	117.70
85	2	891	G	C6-C5-N7	-5.70	126.98	130.40
80	BH	64	PRO	N-CA-CB	5.69	110.13	103.30
43	1	1871	A	N1-C6-N6	5.68	122.01	118.60
43	1	2252	C	N3-C2-O2	-5.68	117.92	121.90
85	2	1145	G	C6-C5-N7	5.66	133.80	130.40
43	1	2382	A	C8-N9-C4	-5.65	103.54	105.80
57	BG	137	PRO	N-CA-CB	5.65	110.08	103.30
43	1	3067	C	N1-C2-O2	5.65	122.29	118.90
85	2	1202	C	OP2-P-O3'	-5.65	92.78	105.20
44	3	59	G	C6-C5-N7	-5.64	127.02	130.40
85	2	564	G	C4-N9-C1'	5.64	133.83	126.50
85	2	369	G	N3-C4-N9	-5.63	122.62	126.00
43	1	1508	C	N1-C2-N3	5.63	123.14	119.20
43	1	3028	A	C2-N3-C4	-5.63	107.79	110.60
80	BH	27	PRO	N-CA-CB	5.63	110.05	103.30
85	2	1383	G	OP1-P-O3'	5.62	117.57	105.20
43	1	1231	U	C2-N3-C4	5.62	130.37	127.00
43	1	220	C	C6-N1-C2	-5.62	118.05	120.30
43	1	229	A	C8-N9-C4	5.62	108.05	105.80
43	1	2062	G	C6-C5-N7	-5.61	127.03	130.40
43	1	1134	C	C6-N1-C1'	-5.61	114.07	120.80
85	2	1728	G	C8-N9-C1'	5.59	134.27	127.00
43	1	2546	U	C5-C6-N1	5.59	125.50	122.70
43	1	1105	G	N1-C6-O6	-5.59	116.55	119.90
43	1	1877	G	C6-C5-N7	-5.59	127.05	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	2880	G	C8-N9-C4	-5.58	104.17	106.40
57	BG	136	PRO	N-CA-CB	5.58	110.00	103.30
85	2	1802	C	C6-N1-C1'	5.58	127.49	120.80
43	1	1871	A	C5-C6-N6	-5.57	119.25	123.70
85	2	149	G	C8-N9-C1'	5.57	134.24	127.00
43	1	220	C	C2-N1-C1'	5.56	124.92	118.80
51	Br	194	HIS	CB-CA-C	5.56	121.52	110.40
85	2	1634	G	N3-C4-C5	5.54	131.37	128.60
57	BG	65	PRO	N-CA-CB	5.54	109.95	103.30
85	2	1410	A	C2'-C3'-O3'	-5.54	97.32	109.50
44	3	72	G	N3-C4-C5	5.53	131.37	128.60
43	1	1547	C	N3-C4-N4	-5.53	114.13	118.00
43	1	1877	G	N1-C2-N2	-5.53	111.22	116.20
43	1	2093	G	C8-N9-C1'	-5.52	119.82	127.00
85	2	1846	G	O4'-C1'-N9	5.50	112.60	108.20
80	BH	150	PRO	N-CA-CB	5.50	109.90	103.30
43	1	2435	G	N3-C4-N9	5.49	129.29	126.00
43	1	1070	G	C6-N1-C2	-5.47	121.81	125.10
43	1	34	C	N3-C4-N4	-5.47	114.17	118.00
43	1	992	G	N3-C4-N9	-5.47	122.72	126.00
85	2	1386	G	O3'-P-O5'	-5.47	93.60	104.00
43	1	2382	A	C4-N9-C1'	5.47	136.14	126.30
43	1	2714	C	N3-C2-O2	-5.47	118.07	121.90
43	1	3147	U	C2-N1-C1'	5.47	124.26	117.70
85	2	924	C	C2'-C3'-O3'	-5.47	97.48	109.50
43	1	2660	G	N1-C6-O6	-5.46	116.62	119.90
44	3	25	G	OP2-P-O3'	5.46	117.22	105.20
43	1	1138	G	O4'-C1'-N9	-5.46	103.83	108.20
43	1	1249	C	N1-C2-O2	5.46	122.17	118.90
43	1	998	C	N1-C2-N3	5.45	123.02	119.20
60	Ba	182	VAL	N-CA-C	-5.45	96.28	111.00
27	AB	114	CYS	CA-CB-SG	5.45	123.81	114.00
43	1	2326	A	N7-C8-N9	5.45	116.53	113.80
43	1	151	U	C5-C6-N1	5.45	125.42	122.70
43	1	1311	C	C2-N1-C1'	5.45	124.79	118.80
43	1	2435	G	C8-N9-C1'	-5.44	119.93	127.00
85	2	1827	G	C4-C5-N7	5.44	112.98	110.80
85	2	1464	G	P-O3'-C3'	5.44	126.22	119.70
43	1	1185	G	N3-C2-N2	-5.44	116.09	119.90
43	1	863	G	C6-C5-N7	-5.43	127.14	130.40
51	Br	161	ARG	NH1-CZ-NH2	-5.43	113.42	119.40
85	2	1385	C	OP2-P-O3'	5.43	117.15	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	1548	G	O4'-C1'-N9	5.43	112.54	108.20
43	1	492	G	C4-N9-C1'	5.43	133.56	126.50
43	1	2435	G	C4-N9-C1'	5.42	133.55	126.50
85	2	1186	A	OP1-P-O3'	-5.42	93.28	105.20
43	1	769	G	N3-C4-C5	5.42	131.31	128.60
85	2	643	U	N3-C2-O2	-5.41	118.41	122.20
43	1	1470	U	C6-N1-C1'	-5.40	113.64	121.20
85	2	941	C	C2-N1-C1'	5.40	124.74	118.80
43	1	858	U	C2-N1-C1'	5.40	124.18	117.70
43	1	999	C	C5-C6-N1	-5.39	118.30	121.00
43	1	2151	U	C2-N1-C1'	5.39	124.17	117.70
43	1	2591	G	N3-C4-N9	5.39	129.24	126.00
43	1	858	U	N1-C2-O2	5.39	126.58	122.80
43	1	2256	G	C6-C5-N7	-5.39	127.16	130.40
43	1	261	G	O4'-C1'-N9	5.38	112.51	108.20
43	1	73	G	C6-C5-N7	-5.38	127.17	130.40
43	1	812	G	C4-N9-C1'	5.38	133.50	126.50
43	1	1253	C	N1-C2-O2	5.38	122.13	118.90
87	Ah	91	PRO	CB-CA-C	5.38	125.44	112.00
85	2	1220	G	N9-C1'-C2'	-5.37	106.09	112.00
43	1	148	C	C2-N1-C1'	5.36	124.70	118.80
43	1	748	G	C8-N9-C1'	-5.36	120.03	127.00
80	BH	61	PRO	N-CA-CB	5.35	109.72	103.30
43	1	3035	A	O4'-C1'-N9	5.35	112.48	108.20
85	2	572	G	N3-C4-C5	5.35	131.27	128.60
43	1	139	G	C5-C6-O6	5.34	131.81	128.60
85	2	1634	G	C4-N9-C1'	-5.34	119.56	126.50
85	2	360	C	C6-N1-C2	5.34	122.44	120.30
43	1	1481	G	N3-C4-N9	-5.34	122.80	126.00
85	2	1845	G	C8-N9-C1'	-5.33	120.07	127.00
3	Ac	255	ILE	C-N-CA	-5.33	108.38	121.70
85	2	1398	G	N9-C1'-C2'	-5.33	106.14	112.00
85	2	1385	C	N1-C1'-C2'	-5.32	106.14	112.00
43	1	2195	A	C8-N9-C4	-5.32	103.67	105.80
43	1	882	C	N1-C2-O2	-5.32	115.71	118.90
43	1	1470	U	N3-C2-O2	-5.32	118.48	122.20
85	2	1809	C	N1-C2-O2	5.31	122.09	118.90
43	1	1579	C	C6-N1-C1'	5.31	127.17	120.80
85	2	1384	G	N9-C1'-C2'	-5.31	106.16	112.00
43	1	2417	G	C5-C6-O6	-5.31	125.42	128.60
85	2	1205	G	N9-C1'-C2'	-5.30	106.17	112.00
85	2	1214	G	N9-C1'-C2'	-5.30	106.17	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	2	1450	C	N1-C1'-C2'	-5.30	106.17	112.00
43	1	2599	C	C2-N1-C1'	5.30	124.63	118.80
85	2	1929	U	P-O3'-C3'	5.30	126.06	119.70
43	1	59	U	O4'-C1'-N1	-5.30	103.96	108.20
43	1	1284	C	C2-N1-C1'	5.29	124.62	118.80
43	1	3028	A	O4'-C1'-N9	-5.29	103.97	108.20
44	3	72	G	N3-C4-N9	-5.29	122.82	126.00
43	1	2062	G	N9-C4-C5	-5.29	103.28	105.40
85	2	840	C	O4'-C1'-N1	5.29	112.43	108.20
43	1	1070	G	N1-C2-N3	5.29	127.07	123.90
43	1	2714	C	N1-C2-O2	5.28	122.07	118.90
85	2	1803	C	C6-N1-C2	-5.28	118.19	120.30
43	1	1580	A	O4'-C1'-N9	-5.28	103.97	108.20
85	2	1397	C	N1-C1'-C2'	-5.28	106.19	112.00
43	1	2062	G	C8-N9-C1'	-5.28	120.14	127.00
85	2	1206	G	N9-C1'-C2'	-5.28	106.19	112.00
43	1	153	U	O4'-C1'-N1	-5.28	103.98	108.20
43	1	932	A	C8-N9-C4	5.27	107.91	105.80
43	1	3025	C	N3-C2-O2	-5.27	118.21	121.90
85	2	1802	C	N1-C2-O2	-5.27	115.74	118.90
43	1	825	U	C6-N1-C1'	-5.26	113.83	121.20
43	1	2741	C	C6-N1-C1'	5.26	127.11	120.80
85	2	1217	G	N9-C1'-C2'	-5.26	106.22	112.00
43	1	492	G	N3-C4-C5	-5.26	125.97	128.60
43	1	300	C	N1-C2-O2	5.25	122.05	118.90
43	1	2093	G	C6-C5-N7	-5.25	127.25	130.40
43	1	1641	U	C6-N1-C1'	-5.25	113.86	121.20
43	1	1871	A	N3-C4-N9	5.24	131.59	127.40
43	1	1155	C	C2-N1-C1'	5.24	124.56	118.80
85	2	1905	C	N3-C2-O2	-5.23	118.24	121.90
85	2	1133	C	N1-C2-O2	5.23	122.04	118.90
43	1	2062	G	C4-C5-N7	5.22	112.89	110.80
44	3	73	C	C5-C6-N1	5.22	123.61	121.00
43	1	1664	A	N7-C8-N9	-5.22	111.19	113.80
85	2	135	C	C2-N1-C1'	-5.21	113.07	118.80
85	2	1428	G	OP2-P-O3'	5.21	116.67	105.20
85	2	1672	G	C6-C5-N7	-5.21	127.27	130.40
60	Ba	181	SER	CB-CA-C	-5.21	100.20	110.10
43	1	1562	U	C2-N1-C1'	5.20	123.94	117.70
85	2	1449	A	OP1-P-O3'	-5.20	93.76	105.20
43	1	139	G	N3-C4-C5	5.20	131.20	128.60
85	2	1634	G	N3-C4-N9	-5.20	122.88	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	2	1407	G	O5'-C5'-C4'	5.19	121.57	111.70
43	1	1502	C	C2-N1-C1'	5.18	124.50	118.80
43	1	2653	C	N3-C2-O2	-5.18	118.27	121.90
43	1	812	G	C6-C5-N7	-5.18	127.29	130.40
43	1	1302	C	C6-N1-C2	-5.18	118.23	120.30
85	2	373	G	C4-N9-C1'	5.17	133.23	126.50
86	Az	57	SER	N-CA-C	-5.17	97.04	111.00
43	1	998	C	C6-N1-C1'	5.17	127.00	120.80
43	1	1111	A	C8-N9-C4	-5.17	103.73	105.80
85	2	114	C	C6-N1-C1'	5.17	127.00	120.80
85	2	1786	A	O4'-C1'-N9	5.17	112.33	108.20
43	1	858	U	N3-C2-O2	-5.17	118.58	122.20
43	1	2348	G	C4-N9-C1'	5.17	133.21	126.50
43	1	145	C	C2-N1-C1'	-5.16	113.12	118.80
43	1	1916	A	P-O3'-C3'	5.16	125.90	119.70
43	1	2062	G	C4-N9-C1'	5.16	133.21	126.50
43	1	806	C	C6-N1-C2	-5.16	118.24	120.30
43	1	2382	A	C6-C5-N7	-5.16	128.69	132.30
85	2	15	A	C4-C5-N7	5.16	113.28	110.70
43	1	1582	G	O4'-C1'-N9	5.16	112.33	108.20
43	1	1664	A	C4-N9-C1'	-5.15	117.03	126.30
43	1	2361	C	O4'-C1'-N1	-5.15	104.08	108.20
51	Br	161	ARG	CG-CD-NE	5.15	122.62	111.80
43	1	2839	A	N9-C4-C5	5.15	107.86	105.80
43	1	887	A	C6-N1-C2	-5.14	115.51	118.60
85	2	485	C	N3-C2-O2	-5.14	118.30	121.90
43	1	2563	C	C6-N1-C2	-5.13	118.25	120.30
85	2	1379	U	C5'-C4'-O4'	-5.13	102.94	109.10
85	2	1406	G	O5'-C5'-C4'	5.13	121.44	111.70
43	1	566	C	N1-C2-O2	5.12	121.97	118.90
85	2	948	U	OP1-P-O3'	5.12	116.47	105.20
85	2	1887	G	C4-N9-C1'	-5.12	119.84	126.50
43	1	1100	G	C6-C5-N7	5.12	133.47	130.40
43	1	3151	G	N9-C4-C5	-5.12	103.35	105.40
43	1	67	G	C4-N9-C1'	5.12	133.15	126.50
43	1	2705	G	C8-N9-C1'	-5.12	120.35	127.00
43	1	1457	C	C6-N1-C1'	-5.11	114.67	120.80
43	1	1879	U	N1-C2-O2	5.10	126.37	122.80
43	1	127	C	C2-N1-C1'	5.10	124.41	118.80
85	2	565	G	C4-N9-C1'	5.10	133.13	126.50
43	1	2042	G	N3-C4-N9	5.09	129.06	126.00
43	1	1170	A	C4-N9-C1'	5.09	135.46	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	1924	G	O4'-C1'-N9	5.09	112.27	108.20
85	2	1485	G	O4'-C1'-N9	5.09	112.27	108.20
43	1	1962	A	N9-C4-C5	-5.08	103.77	105.80
43	1	2500	C	N1-C2-O2	-5.08	115.85	118.90
85	2	1405	A	O3'-P-O5'	-5.08	94.35	104.00
43	1	1221	C	C5-C6-N1	5.08	123.54	121.00
85	2	1845	G	C6-C5-N7	-5.08	127.35	130.40
85	2	1427	G	P-O3'-C3'	5.08	125.79	119.70
43	1	845	U	C2-N1-C1'	5.07	123.78	117.70
43	1	2112	C	C6-N1-C2	-5.06	118.27	120.30
43	1	1170	A	C8-N9-C1'	-5.06	118.59	127.70
43	1	2654	C	C6-N1-C1'	5.06	126.87	120.80
85	2	1381	G	OP1-P-O3'	-5.06	94.08	105.20
43	1	1201	C	N3-C2-O2	-5.05	118.36	121.90
51	Br	162	ARG	CB-CA-C	5.05	120.50	110.40
85	2	1821	A	O4'-C1'-N9	-5.05	104.16	108.20
43	1	2147	C	C2-N1-C1'	5.05	124.35	118.80
85	2	1405	A	O5'-C5'-C4'	5.05	121.29	111.70
43	1	2384	C	C6-N1-C2	-5.05	118.28	120.30
43	1	2660	G	N9-C4-C5	5.05	107.42	105.40
85	2	947	G	C8-N9-C1'	-5.05	120.44	127.00
43	1	73	G	C4-C5-N7	5.04	112.82	110.80
43	1	2326	A	C4-N9-C1'	5.04	135.38	126.30
60	Ba	182	VAL	N-CA-CB	5.04	122.60	111.50
43	1	186	C	N3-C2-O2	-5.04	118.37	121.90
85	2	1567	G	N3-C4-N9	-5.04	122.98	126.00
43	1	2546	U	C5-C4-O4	-5.04	122.88	125.90
85	2	419	C	O4'-C1'-N1	5.04	112.23	108.20
85	2	15	A	C6-C5-N7	-5.03	128.78	132.30
43	1	1154	C	C6-N1-C1'	-5.03	114.76	120.80
85	2	898	C	C6-N1-C2	-5.03	118.29	120.30
85	2	1705	G	C4-N9-C1'	5.03	133.04	126.50
85	2	120	C	C6-N1-C1'	5.03	126.83	120.80
43	1	2256	G	C4-N9-C1'	5.02	133.03	126.50
43	1	737	G	N3-C4-N9	-5.02	122.99	126.00
43	1	1897	A	C4-C5-N7	5.01	113.21	110.70
43	1	1228	C	N3-C2-O2	-5.01	118.39	121.90
85	2	1705	G	C8-N9-C1'	-5.01	120.49	127.00
43	1	529	A	N1-C6-N6	5.00	121.60	118.60
44	3	69	U	N3-C2-O2	-5.00	118.70	122.20

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
85	2	1165	C	C4’
85	2	1206	G	C3’
85	2	1404	C	C3’
85	2	1409	G	C4’
85	2	1410	A	C2’

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
85	2	1183	G	Sidechain
85	2	1187	G	Sidechain
85	2	1193	G	Sidechain
85	2	1205	G	Sidechain
85	2	1206	G	Sidechain
85	2	1214	G	Sidechain
85	2	1217	G	Sidechain
85	2	1220	G	Sidechain
85	2	1369	G	Sidechain
85	2	1372	G	Sidechain
85	2	1375	G	Sidechain
85	2	1377	G	Sidechain
85	2	1380	G	Sidechain
85	2	1381	G	Sidechain
85	2	1398	G	Sidechain
85	2	1406	G	Sidechain
85	2	1407	G	Sidechain
85	2	1409	G	Sidechain
85	2	1422	G	Sidechain
85	2	1424	G	Sidechain
85	2	1426	G	Sidechain
85	2	1427	G	Sidechain
85	2	1428	G	Sidechain
85	2	1431	G	Sidechain
85	2	1434	G	Sidechain
85	2	1438	G	Sidechain
85	2	1440	G	Sidechain
85	2	1441	G	Sidechain
85	2	1442	G	Sidechain
85	2	924	C	Sidechain
26	AA	57	ARG	Peptide
27	AB	124	CYS	Peptide
33	AI	78	LYS	Peptide
37	AM	75	ASN	Peptide

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Mol	Chain	Res	Type	Group
37	AM	83	ALA	Peptide
39	AO	294	ILE	Peptide
39	AO	332	TYR	Peptide
40	AP	246	ALA	Peptide
40	AP	605	ALA	Peptide
40	AP	635	ALA	Peptide
41	AQ	444	GLN	Peptide
87	Ah	22	HIS	Sidechain
87	Ah	29	TYR	Sidechain
18	Ar	164	LEU	Peptide
18	Ar	191	ARG	Peptide
20	At	102	LYS	Peptide
21	Au	132	THR	Peptide
24	Ax	57	ASN	Peptide
79	BJ	192	ALA	Peptide
61	Bc	316	THR	Peptide
62	Bd	356	LYS	Peptide
62	Bd	448	PRO	Peptide
48	Bi	171	VAL	Peptide
65	Bj	284	ASN	Peptide
49	Bl	120	HIS	Peptide
51	Br	144	ALA	Mainchain
51	Br	174	VAL	Mainchain
52	Bw	464	LEU	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Aa	94/349 (27%)	78 (83%)	14 (15%)	2 (2%)	7 38
2	Ab	153/214 (72%)	129 (84%)	24 (16%)	0	100 100
3	Ac	216/324 (67%)	167 (77%)	49 (23%)	0	100 100
4	AD	58/173 (34%)	49 (84%)	9 (16%)	0	100 100
5	Ad	207/300 (69%)	186 (90%)	21 (10%)	0	100 100
6	Ae	142/185 (77%)	114 (80%)	28 (20%)	0	100 100
7	Af	98/102 (96%)	80 (82%)	18 (18%)	0	100 100
8	Ag	49/221 (22%)	43 (88%)	6 (12%)	0	100 100
9	Ai	136/155 (88%)	120 (88%)	16 (12%)	0	100 100
10	Aj	153/205 (75%)	119 (78%)	34 (22%)	0	100 100
11	Ak	125/173 (72%)	102 (82%)	23 (18%)	0	100 100
12	Al	176/281 (63%)	145 (82%)	31 (18%)	0	100 100
13	Am	140/179 (78%)	122 (87%)	18 (13%)	0	100 100
14	An	139/160 (87%)	114 (82%)	24 (17%)	1 (1%)	22 59
15	Ao	104/114 (91%)	83 (80%)	21 (20%)	0	100 100
16	Ap	112/222 (50%)	91 (81%)	21 (19%)	0	100 100
17	Aq	104/126 (82%)	92 (88%)	12 (12%)	0	100 100
18	Ar	135/270 (50%)	101 (75%)	34 (25%)	0	100 100
19	As	119/269 (44%)	106 (89%)	13 (11%)	0	100 100
20	At	103/178 (58%)	80 (78%)	23 (22%)	0	100 100
21	Au	138/159 (87%)	97 (70%)	39 (28%)	2 (1%)	11 45
22	Av	194/249 (78%)	166 (86%)	28 (14%)	0	100 100
23	Aw	74/154 (48%)	63 (85%)	11 (15%)	0	100 100
24	Ax	97/212 (46%)	85 (88%)	12 (12%)	0	100 100
25	Ay	109/144 (76%)	87 (80%)	22 (20%)	0	100 100
26	AA	35/76 (46%)	27 (77%)	8 (23%)	0	100 100
27	AB	39/134 (29%)	27 (69%)	12 (31%)	0	100 100
28	AC	49/58 (84%)	43 (88%)	6 (12%)	0	100 100
29	AE	34/103 (33%)	29 (85%)	5 (15%)	0	100 100
30	AF	82/250 (33%)	74 (90%)	8 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	AG	59/94 (63%)	40 (68%)	18 (30%)	1 (2%)	9 42
32	AH	106/146 (73%)	90 (85%)	16 (15%)	0	100 100
33	AI	205/233 (88%)	161 (78%)	44 (22%)	0	100 100
34	AJ	79/127 (62%)	59 (75%)	20 (25%)	0	100 100
35	AK	85/130 (65%)	74 (87%)	11 (13%)	0	100 100
36	AL	50/81 (62%)	39 (78%)	11 (22%)	0	100 100
37	AM	80/151 (53%)	71 (89%)	9 (11%)	0	100 100
38	AN	78/188 (42%)	70 (90%)	8 (10%)	0	100 100
39	AO	450/491 (92%)	387 (86%)	63 (14%)	0	100 100
40	AP	667/669 (100%)	531 (80%)	133 (20%)	3 (0%)	34 70
41	AQ	364/521 (70%)	312 (86%)	51 (14%)	1 (0%)	41 74
42	AR	27/29 (93%)	21 (78%)	6 (22%)	0	100 100
45	Bb	271/556 (49%)	218 (80%)	52 (19%)	1 (0%)	34 70
46	Bf	134/148 (90%)	122 (91%)	12 (9%)	0	100 100
47	Bh	121/430 (28%)	100 (83%)	21 (17%)	0	100 100
48	Bi	99/241 (41%)	76 (77%)	23 (23%)	0	100 100
49	Bl	89/154 (58%)	53 (60%)	35 (39%)	1 (1%)	14 50
50	Bm	94/164 (57%)	63 (67%)	30 (32%)	1 (1%)	14 50
51	Br	81/212 (38%)	64 (79%)	12 (15%)	5 (6%)	1 19
52	Bw	331/480 (69%)	234 (71%)	94 (28%)	3 (1%)	17 53
53	Bx	77/102 (76%)	61 (79%)	16 (21%)	0	100 100
54	Bz	121/419 (29%)	110 (91%)	11 (9%)	0	100 100
55	BA	36/91 (40%)	28 (78%)	8 (22%)	0	100 100
56	Bt	27/98 (28%)	22 (82%)	5 (18%)	0	100 100
57	BG	362/576 (63%)	309 (85%)	46 (13%)	7 (2%)	8 40
58	BP	83/91 (91%)	81 (98%)	2 (2%)	0	100 100
59	BF	121/123 (98%)	98 (81%)	23 (19%)	0	100 100
60	Ba	193/219 (88%)	146 (76%)	47 (24%)	0	100 100
61	Bc	323/362 (89%)	255 (79%)	66 (20%)	2 (1%)	25 62
62	Bd	214/515 (42%)	170 (79%)	44 (21%)	0	100 100
63	Be	97/139 (70%)	72 (74%)	25 (26%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	Bg	126/129 (98%)	101 (80%)	25 (20%)	0	100	100
65	Bj	121/314 (38%)	97 (80%)	24 (20%)	0	100	100
66	Bn	98/419 (23%)	86 (88%)	12 (12%)	0	100	100
67	Bo	97/135 (72%)	75 (77%)	22 (23%)	0	100	100
68	Bp	76/116 (66%)	59 (78%)	17 (22%)	0	100	100
69	Bq	60/261 (23%)	51 (85%)	9 (15%)	0	100	100
70	Bs	64/101 (63%)	53 (83%)	11 (17%)	0	100	100
71	Bu	96/195 (49%)	78 (81%)	18 (19%)	0	100	100
72	Bv	147/195 (75%)	119 (81%)	28 (19%)	0	100	100
73	By	74/142 (52%)	62 (84%)	12 (16%)	0	100	100
74	BB	21/137 (15%)	20 (95%)	1 (5%)	0	100	100
75	BC	66/112 (59%)	53 (80%)	13 (20%)	0	100	100
76	BD	208/420 (50%)	164 (79%)	43 (21%)	1 (0%)	29	66
77	BE	346/409 (85%)	277 (80%)	69 (20%)	0	100	100
78	BI	264/266 (99%)	227 (86%)	37 (14%)	0	100	100
79	BJ	347/349 (99%)	301 (87%)	46 (13%)	0	100	100
80	BH	204/390 (52%)	176 (86%)	24 (12%)	4 (2%)	7	39
81	BN	67/69 (97%)	57 (85%)	10 (15%)	0	100	100
82	BM	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
83	BO	28/30 (93%)	28 (100%)	0	0	100	100
84	BL	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
86	Az	80/109 (73%)	73 (91%)	6 (8%)	1 (1%)	12	46
87	Ah	135/171 (79%)	126 (93%)	7 (5%)	2 (2%)	10	44
88	BK	314/316 (99%)	289 (92%)	23 (7%)	2 (1%)	25	62
89	Bk	119/125 (95%)	114 (96%)	4 (3%)	1 (1%)	19	56
All	All	11835/18772 (63%)	9765 (82%)	2029 (17%)	41 (0%)	44	74

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	BG	89	VAL
57	BG	277	SER
57	BG	278	PRO

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Mol	Chain	Res	Type
87	Ah	91	PRO
1	Aa	81	LYS
51	Br	162	ARG
57	BG	18	VAL
88	BK	39	ALA
88	BK	303	ALA
1	Aa	84	ASN
40	AP	604	ALA
50	Bm	84	GLU
57	BG	276	LEU
80	BH	165	PRO
40	AP	376	ALA
40	AP	530	ALA
45	Bb	47	PRO
51	Br	150	LYS
51	Br	176	ILE
57	BG	230	VAL
61	Bc	30	TRP
87	Ah	67	THR
89	Bk	102	LYS
21	Au	117	PRO
51	Br	138	LYS
51	Br	208	HIS
76	BD	345	ARG
31	AG	24	ASP
41	AQ	348	MET
49	Bl	44	PRO
52	Bw	456	GLU
80	BH	61	PRO
80	BH	149	LYS
21	Au	89	PRO
52	Bw	420	PRO
57	BG	174	LYS
86	Az	27	LEU
61	Bc	121	PRO
80	BH	150	PRO
14	An	99	ILE
52	Bw	370	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
1	Aa	82/284 (29%)	81 (99%)	1 (1%)	71 83
2	Ab	121/169 (72%)	121 (100%)	0	100 100
3	Ac	174/267 (65%)	174 (100%)	0	100 100
4	AD	54/158 (34%)	54 (100%)	0	100 100
5	Ad	181/260 (70%)	180 (99%)	1 (1%)	86 91
6	Ae	133/168 (79%)	133 (100%)	0	100 100
7	Af	84/86 (98%)	84 (100%)	0	100 100
8	Ag	43/196 (22%)	43 (100%)	0	100 100
9	Ai	116/128 (91%)	113 (97%)	3 (3%)	46 68
10	Aj	135/170 (79%)	132 (98%)	3 (2%)	52 71
11	Ak	103/138 (75%)	100 (97%)	3 (3%)	42 65
12	Al	147/236 (62%)	147 (100%)	0	100 100
13	Am	111/146 (76%)	110 (99%)	1 (1%)	78 88
14	An	119/137 (87%)	119 (100%)	0	100 100
15	Ao	91/98 (93%)	90 (99%)	1 (1%)	73 84
16	Ap	103/199 (52%)	101 (98%)	2 (2%)	57 75
17	Aq	93/110 (84%)	93 (100%)	0	100 100
18	Ar	122/244 (50%)	122 (100%)	0	100 100
19	As	98/233 (42%)	98 (100%)	0	100 100
20	At	92/146 (63%)	92 (100%)	0	100 100
21	Au	121/132 (92%)	119 (98%)	2 (2%)	60 77
22	Av	175/216 (81%)	174 (99%)	1 (1%)	86 91
23	Aw	64/126 (51%)	63 (98%)	1 (2%)	62 79
24	Ax	83/173 (48%)	82 (99%)	1 (1%)	71 83
25	Ay	105/127 (83%)	105 (100%)	0	100 100
26	AA	28/65 (43%)	28 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	AB	36/116 (31%)	36 (100%)	0	100 100
28	AC	46/52 (88%)	46 (100%)	0	100 100
29	AE	35/87 (40%)	35 (100%)	0	100 100
30	AF	70/206 (34%)	69 (99%)	1 (1%)	67 81
31	AG	55/82 (67%)	54 (98%)	1 (2%)	59 77
32	AH	98/130 (75%)	98 (100%)	0	100 100
33	AI	185/209 (88%)	183 (99%)	2 (1%)	73 84
34	AJ	71/111 (64%)	70 (99%)	1 (1%)	67 81
35	AK	76/109 (70%)	76 (100%)	0	100 100
36	AL	42/63 (67%)	41 (98%)	1 (2%)	49 69
37	AM	73/130 (56%)	73 (100%)	0	100 100
38	AN	69/163 (42%)	69 (100%)	0	100 100
39	AO	388/424 (92%)	387 (100%)	1 (0%)	92 95
41	AQ	311/461 (68%)	309 (99%)	2 (1%)	86 91
45	Bb	243/495 (49%)	241 (99%)	2 (1%)	81 89
46	Bf	116/125 (93%)	116 (100%)	0	100 100
47	Bh	99/360 (28%)	99 (100%)	0	100 100
48	Bi	94/211 (44%)	94 (100%)	0	100 100
49	Bl	78/129 (60%)	78 (100%)	0	100 100
50	Bm	84/144 (58%)	84 (100%)	0	100 100
51	Br	73/180 (41%)	65 (89%)	8 (11%)	6 28
52	Bw	289/404 (72%)	288 (100%)	1 (0%)	92 95
53	Bx	68/85 (80%)	65 (96%)	3 (4%)	28 56
54	Bz	107/368 (29%)	107 (100%)	0	100 100
55	BA	35/81 (43%)	35 (100%)	0	100 100
56	Bt	25/81 (31%)	25 (100%)	0	100 100
60	Ba	173/191 (91%)	171 (99%)	2 (1%)	71 83
61	Bc	310/343 (90%)	308 (99%)	2 (1%)	86 91
62	Bd	185/463 (40%)	185 (100%)	0	100 100
63	Be	90/126 (71%)	90 (100%)	0	100 100
64	Bg	112/113 (99%)	112 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	Bj	103/264 (39%)	103 (100%)	0	100	100
66	Bn	94/378 (25%)	94 (100%)	0	100	100
67	Bo	82/113 (73%)	81 (99%)	1 (1%)	71	83
68	Bp	71/99 (72%)	71 (100%)	0	100	100
69	Bq	51/224 (23%)	50 (98%)	1 (2%)	55	74
70	Bs	61/92 (66%)	61 (100%)	0	100	100
71	Bu	86/170 (51%)	86 (100%)	0	100	100
72	Bv	132/173 (76%)	131 (99%)	1 (1%)	81	89
73	By	61/115 (53%)	59 (97%)	2 (3%)	38	63
74	BB	22/127 (17%)	22 (100%)	0	100	100
75	BC	58/94 (62%)	57 (98%)	1 (2%)	60	77
76	BD	188/368 (51%)	187 (100%)	1 (0%)	88	93
77	BE	296/351 (84%)	295 (100%)	1 (0%)	92	95
86	Az	73/96 (76%)	67 (92%)	6 (8%)	11	40
87	Ah	119/144 (83%)	115 (97%)	4 (3%)	37	62
89	Bk	104/108 (96%)	97 (93%)	7 (7%)	16	46
All	All	8115/13570 (60%)	8043 (99%)	72 (1%)	79	88

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	86	ILE
5	Ad	260	TYR
9	Ai	27	ARG
9	Ai	40	ARG
9	Ai	127	CYS
10	Aj	82	THR
10	Aj	90	PHE
10	Aj	106	LEU
11	Ak	54	LEU
11	Ak	64	LYS
11	Ak	142	ARG
13	Am	38	TYR
15	Ao	96	HIS
16	Ap	177	VAL
16	Ap	180	VAL

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Mol	Chain	Res	Type
21	Au	38	VAL
21	Au	121	ILE
22	Av	150	ASP
23	Aw	103	THR
24	Ax	135	TYR
30	AF	152	GLU
31	AG	53	TYR
33	AI	71	ASP
33	AI	187	ARG
34	AJ	29	CYS
36	AL	28	LYS
39	AO	375	PHE
41	AQ	159	PHE
41	AQ	400	PHE
45	Bb	483	GLU
45	Bb	507	HIS
51	Br	131	MET
51	Br	159	TRP
51	Br	160	SER
51	Br	163	SER
51	Br	172	SER
51	Br	177	TYR
51	Br	199	PHE
51	Br	202	THR
52	Bw	391	ARG
53	Bx	36	ARG
53	Bx	37	SER
53	Bx	77	LYS
60	Ba	137	PHE
60	Ba	186	TYR
61	Bc	129	HIS
61	Bc	311	ARG
67	Bo	75	ARG
69	Bq	217	ARG
72	Bv	150	TRP
73	By	83	LYS
73	By	91	ARG
75	BC	69	LYS
76	BD	172	LYS
77	BE	368	TRP
86	Az	18	SER
86	Az	22	THR

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Mol	Chain	Res	Type
86	Az	37	THR
86	Az	75	GLU
86	Az	77	TYR
86	Az	98	HIS
87	Ah	47	ASN
87	Ah	67	THR
87	Ah	91	PRO
87	Ah	129	ILE
89	Bk	34	CYS
89	Bk	40	ARG
89	Bk	55	VAL
89	Bk	88	LYS
89	Bk	89	ASP
89	Bk	98	ILE
89	Bk	121	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	64	ASN
1	Aa	84	ASN
2	Ab	160	ASN
3	Ac	124	GLN
3	Ac	134	HIS
3	Ac	175	HIS
3	Ac	194	GLN
3	Ac	209	HIS
3	Ac	223	GLN
3	Ac	267	GLN
4	AD	154	GLN
5	Ad	162	HIS
5	Ad	225	ASN
5	Ad	231	ASN
5	Ad	259	HIS
5	Ad	277	HIS
6	Ae	24	ASN
6	Ae	59	GLN
6	Ae	151	HIS
7	Af	67	GLN
8	Ag	71	ASN
9	Ai	55	GLN
9	Ai	128	GLN

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Mol	Chain	Res	Type
9	Ai	144	ASN
9	Ai	152	GLN
10	Aj	26	ASN
10	Aj	48	GLN
11	Ak	49	GLN
11	Ak	126	ASN
11	Ak	162	HIS
11	Ak	171	HIS
12	Al	248	GLN
13	Am	145	GLN
14	An	82	HIS
15	Ao	36	HIS
17	Aq	60	GLN
17	Aq	61	HIS
17	Aq	64	ASN
17	Aq	67	ASN
18	Ar	149	HIS
18	Ar	170	ASN
18	Ar	222	ASN
19	As	164	ASN
19	As	191	HIS
20	At	11	HIS
21	Au	75	HIS
22	Av	37	GLN
22	Av	110	GLN
22	Av	132	HIS
24	Ax	65	ASN
24	Ax	74	ASN
24	Ax	96	HIS
25	Ay	48	GLN
25	Ay	85	ASN
25	Ay	90	GLN
25	Ay	100	GLN
25	Ay	103	ASN
26	AA	37	HIS
26	AA	59	ASN
27	AB	91	HIS
29	AE	35	GLN
29	AE	37	GLN
33	AI	59	GLN
33	AI	159	HIS
33	AI	223	GLN

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Mol	Chain	Res	Type
34	AJ	30	ASN
36	AL	39	ASN
36	AL	70	ASN
37	AM	93	HIS
38	AN	177	GLN
39	AO	87	ASN
39	AO	147	ASN
39	AO	153	ASN
39	AO	162	ASN
39	AO	246	GLN
39	AO	259	ASN
39	AO	261	GLN
39	AO	299	ASN
39	AO	304	ASN
39	AO	307	GLN
39	AO	313	ASN
39	AO	462	HIS
41	AQ	130	ASN
41	AQ	193	GLN
41	AQ	226	HIS
41	AQ	354	GLN
41	AQ	412	HIS
41	AQ	423	ASN
41	AQ	442	ASN
45	Bb	15	ASN
45	Bb	507	HIS
46	Bf	120	GLN
47	Bh	426	GLN
49	Bl	36	ASN
49	Bl	71	ASN
49	Bl	107	GLN
50	Bm	125	ASN
52	Bw	136	HIS
52	Bw	186	ASN
52	Bw	248	HIS
52	Bw	255	ASN
52	Bw	330	HIS
52	Bw	405	HIS
54	Bz	294	GLN
54	Bz	356	HIS
54	Bz	360	ASN
55	BA	47	ASN

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Mol	Chain	Res	Type
55	BA	57	GLN
60	Ba	17	HIS
60	Ba	25	HIS
60	Ba	26	HIS
60	Ba	88	GLN
61	Bc	31	ASN
61	Bc	47	ASN
61	Bc	122	GLN
61	Bc	135	ASN
61	Bc	148	HIS
61	Bc	185	HIS
61	Bc	186	GLN
61	Bc	219	GLN
61	Bc	322	ASN
61	Bc	338	HIS
62	Bd	351	GLN
62	Bd	361	HIS
62	Bd	470	ASN
63	Be	59	HIS
63	Be	66	GLN
63	Be	80	HIS
64	Bg	15	ASN
64	Bg	69	ASN
64	Bg	123	GLN
65	Bj	304	ASN
66	Bn	357	GLN
66	Bn	364	HIS
67	Bo	33	HIS
68	Bp	14	GLN
68	Bp	26	HIS
68	Bp	31	ASN
69	Bq	174	ASN
70	Bs	48	GLN
70	Bs	62	HIS
72	Bv	137	GLN
72	Bv	171	GLN
73	By	68	HIS
75	BC	56	HIS
76	BD	147	ASN
76	BD	310	ASN
77	BE	109	HIS
77	BE	112	ASN

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Mol	Chain	Res	Type
77	BE	251	GLN
77	BE	265	HIS
86	Az	34	HIS
87	Ah	28	ASN
89	Bk	5	ASN
89	Bk	61	HIS
89	Bk	96	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
43	1	2836/2842 (99%)	1125 (39%)	66 (2%)
44	3	118/118 (100%)	49 (41%)	7 (5%)
85	2	1733/1743 (99%)	757 (43%)	66 (3%)
All	All	4687/4703 (99%)	1931 (41%)	139 (2%)

All (1931) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
43	1	17	A
43	1	27	A
43	1	37	G
43	1	38	G
43	1	45	A
43	1	47	A
43	1	49	G
43	1	50	G
43	1	51	A
43	1	54	G
43	1	62	C
43	1	64	G
43	1	65	A
43	1	67	G
43	1	70	A
43	1	71	A
43	1	73	G
43	1	74	G
43	1	75	C
43	1	79	G
43	1	82	G
43	1	84	G

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Mol	Chain	Res	Type
43	1	86	U
43	1	87	A
43	1	88	C
43	1	89	C
43	1	90	G
43	1	91	U
43	1	94	G
43	1	95	U
43	1	96	G
43	1	99	C
43	1	113	U
43	1	114	C
43	1	118	A
43	1	119	A
43	1	121	C
43	1	122	C
43	1	123	G
43	1	124	U
43	1	125	A
43	1	126	U
43	1	127	C
43	1	128	C
43	1	129	A
43	1	130	A
43	1	131	G
43	1	132	C
43	1	133	U
43	1	134	C
43	1	135	C
43	1	136	G
43	1	137	U
43	1	138	G
43	1	139	G
43	1	140	C
43	1	141	U
43	1	142	A
43	1	144	U
43	1	145	C
43	1	146	U
43	1	147	G
43	1	148	C
43	1	149	G

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Mol	Chain	Res	Type
43	1	150	C
43	1	151	U
43	1	152	C
43	1	153	U
43	1	154	U
43	1	155	U
43	1	156	G
43	1	157	G
43	1	158	A
43	1	161	U
43	1	163	G
43	1	165	A
43	1	166	A
43	1	170	U
43	1	171	A
43	1	181	A
43	1	182	A
43	1	184	A
43	1	186	C
43	1	189	A
43	1	201	A
43	1	203	G
43	1	206	A
43	1	207	A
43	1	208	A
43	1	213	C
43	1	214	C
43	1	215	G
43	1	220	C
43	1	226	A
43	1	230	G
43	1	233	G
43	1	234	C
43	1	235	G
43	1	249	U
43	1	250	U
43	1	251	G
43	1	255	U
43	1	256	U
43	1	258	U
43	1	260	A
43	1	261	G

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Mol	Chain	Res	Type
43	1	262	A
43	1	264	A
43	1	265	A
43	1	267	G
43	1	268	A
43	1	269	A
43	1	270	A
43	1	271	G
43	1	272	A
43	1	273	C
43	1	274	G
43	1	275	A
43	1	276	A
43	1	296	A
43	1	297	C
43	1	298	U
43	1	299	U
43	1	300	C
43	1	301	U
43	1	302	U
43	1	303	U
43	1	304	U
43	1	305	U
43	1	306	C
43	1	307	G
43	1	308	C
43	1	309	C
43	1	311	G
43	1	312	G
43	1	313	U
43	1	314	U
43	1	315	U
43	1	421	C
43	1	422	U
43	1	424	U
43	1	425	A
43	1	426	A
43	1	428	U
43	1	429	G
43	1	431	G
43	1	433	A
43	1	435	A

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Mol	Chain	Res	Type
43	1	436	G
43	1	440	G
43	1	444	G
43	1	453	A
43	1	456	G
43	1	462	G
43	1	463	A
43	1	464	U
43	1	466	G
43	1	468	C
43	1	477	U
43	1	478	C
43	1	479	G
43	1	480	U
43	1	481	U
43	1	482	C
43	1	483	C
43	1	484	U
43	1	486	U
43	1	487	G
43	1	488	G
43	1	489	U
43	1	490	U
43	1	491	C
43	1	492	G
43	1	494	U
43	1	495	C
43	1	496	C
43	1	498	U
43	1	499	C
43	1	500	C
43	1	501	C
43	1	503	G
43	1	504	U
43	1	505	A
43	1	506	A
43	1	514	C
43	1	515	G
43	1	516	U
43	1	517	G
43	1	518	U
43	1	519	U

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Mol	Chain	Res	Type
43	1	520	C
43	1	521	G
43	1	522	A
43	1	525	U
43	1	526	C
43	1	528	G
43	1	535	U
43	1	536	U
43	1	539	C
43	1	540	G
43	1	541	C
43	1	542	G
43	1	543	A
43	1	544	G
43	1	545	A
43	1	546	A
43	1	547	A
43	1	550	G
43	1	552	G
43	1	553	A
43	1	557	C
43	1	565	G
43	1	566	C
43	1	572	U
43	1	577	C
43	1	585	C
43	1	590	A
43	1	592	C
43	1	597	A
43	1	598	A
43	1	599	G
43	1	608	G
43	1	610	G
43	1	611	A
43	1	614	G
43	1	619	A
43	1	621	A
43	1	622	G
43	1	623	A
43	1	626	C
43	1	629	A
43	1	630	U

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Mol	Chain	Res	Type
43	1	633	C
43	1	634	G
43	1	642	A
43	1	643	A
43	1	644	U
43	1	645	A
43	1	646	G
43	1	647	A
43	1	649	A
43	1	650	A
43	1	651	C
43	1	655	A
43	1	661	G
43	1	670	A
43	1	671	A
43	1	672	U
43	1	673	C
43	1	674	A
43	1	675	G
43	1	678	G
43	1	682	G
43	1	685	U
43	1	686	A
43	1	687	G
43	1	688	U
43	1	689	C
43	1	690	A
43	1	691	A
43	1	692	G
43	1	693	C
43	1	694	G
43	1	695	C
43	1	696	A
43	1	697	C
43	1	699	C
43	1	700	A
43	1	701	C
43	1	705	A
43	1	711	G
43	1	712	U
43	1	713	A
43	1	715	C

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Mol	Chain	Res	Type
43	1	719	U
43	1	720	G
43	1	722	A
43	1	723	U
43	1	725	A
43	1	736	A
43	1	737	G
43	1	738	G
43	1	739	A
43	1	745	G
43	1	748	G
43	1	753	G
43	1	755	U
43	1	756	U
43	1	758	A
43	1	762	A
43	1	765	A
43	1	766	G
43	1	767	G
43	1	771	A
43	1	777	U
43	1	778	U
43	1	779	U
43	1	780	C
43	1	784	A
43	1	788	G
43	1	789	G
43	1	790	A
43	1	791	A
43	1	793	C
43	1	794	U
43	1	795	U
43	1	797	U
43	1	798	A
43	1	799	G
43	1	802	C
43	1	808	A
43	1	817	G
43	1	818	A
43	1	825	U
43	1	828	A
43	1	829	U

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Mol	Chain	Res	Type
43	1	838	G
43	1	845	U
43	1	853	A
43	1	854	G
43	1	855	C
43	1	856	U
43	1	857	C
43	1	859	A
43	1	860	A
43	1	861	C
43	1	870	G
43	1	873	G
43	1	874	A
43	1	891	G
43	1	897	A
43	1	908	A
43	1	909	C
43	1	919	G
43	1	920	G
43	1	921	G
43	1	926	A
43	1	927	A
43	1	928	G
43	1	929	G
43	1	933	A
43	1	935	C
43	1	936	A
43	1	947	U
43	1	948	A
43	1	949	G
43	1	950	C
43	1	955	U
43	1	956	U
43	1	971	U
43	1	972	U
43	1	974	A
43	1	975	G
43	1	988	U
43	1	989	G
43	1	990	U
43	1	994	U
43	1	999	C

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Mol	Chain	Res	Type
43	1	1002	G
43	1	1003	G
43	1	1010	A
43	1	1012	U
43	1	1013	C
43	1	1020	C
43	1	1022	A
43	1	1023	G
43	1	1027	G
43	1	1043	A
43	1	1044	C
43	1	1046	A
43	1	1052	A
43	1	1054	G
43	1	1056	A
43	1	1057	A
43	1	1061	C
43	1	1066	U
43	1	1073	C
43	1	1074	G
43	1	1079	C
43	1	1086	A
43	1	1088	A
43	1	1092	A
43	1	1093	G
43	1	1095	C
43	1	1097	U
43	1	1098	U
43	1	1099	U
43	1	1100	G
43	1	1101	G
43	1	1105	G
43	1	1106	C
43	1	1108	A
43	1	1109	A
43	1	1110	G
43	1	1113	C
43	1	1116	A
43	1	1123	G
43	1	1125	G
43	1	1126	G
43	1	1130	A

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Mol	Chain	Res	Type
43	1	1132	A
43	1	1134	C
43	1	1138	G
43	1	1139	A
43	1	1140	U
43	1	1144	A
43	1	1145	C
43	1	1147	C
43	1	1154	C
43	1	1155	C
43	1	1156	C
43	1	1158	A
43	1	1159	A
43	1	1160	G
43	1	1161	C
43	1	1162	A
43	1	1166	A
43	1	1171	G
43	1	1172	U
43	1	1173	G
43	1	1174	G
43	1	1175	A
43	1	1176	A
43	1	1178	A
43	1	1182	A
43	1	1183	G
43	1	1189	G
43	1	1194	A
43	1	1195	U
43	1	1196	G
43	1	1197	A
43	1	1198	C
43	1	1201	C
43	1	1203	A
43	1	1204	G
43	1	1206	A
43	1	1208	G
43	1	1211	G
43	1	1213	C
43	1	1216	G
43	1	1217	G
43	1	1218	A

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Mol	Chain	Res	Type
43	1	1219	A
43	1	1220	G
43	1	1222	A
43	1	1224	C
43	1	1232	U
43	1	1234	A
43	1	1235	A
43	1	1237	A
43	1	1238	A
43	1	1239	A
43	1	1242	G
43	1	1245	A
43	1	1246	U
43	1	1249	C
43	1	1252	A
43	1	1253	C
43	1	1255	G
43	1	1259	U
43	1	1261	G
43	1	1262	C
43	1	1265	C
43	1	1268	G
43	1	1275	A
43	1	1277	A
43	1	1278	A
43	1	1281	U
43	1	1282	A
43	1	1284	C
43	1	1285	A
43	1	1288	G
43	1	1290	U
43	1	1292	A
43	1	1300	C
43	1	1301	A
43	1	1305	A
43	1	1306	A
43	1	1309	G
43	1	1311	C
43	1	1314	G
43	1	1318	U
43	1	1319	U
43	1	1320	G

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Mol	Chain	Res	Type
43	1	1322	A
43	1	1324	G
43	1	1326	U
43	1	1327	G
43	1	1328	C
43	1	1330	U
43	1	1331	U
43	1	1332	U
43	1	1333	U
43	1	1336	A
43	1	1337	G
43	1	1338	U
43	1	1339	G
43	1	1342	A
43	1	1343	G
43	1	1345	A
43	1	1359	U
43	1	1361	A
43	1	1368	G
43	1	1375	U
43	1	1381	G
43	1	1392	G
43	1	1393	A
43	1	1394	G
43	1	1397	A
43	1	1403	A
43	1	1407	A
43	1	1408	G
43	1	1409	A
43	1	1411	U
43	1	1412	G
43	1	1419	U
43	1	1420	G
43	1	1421	A
43	1	1427	G
43	1	1428	A
43	1	1429	U
43	1	1452	G
43	1	1456	G
43	1	1457	C
43	1	1458	C
43	1	1459	A

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Mol	Chain	Res	Type
43	1	1463	G
43	1	1466	G
43	1	1467	G
43	1	1469	U
43	1	1483	C
43	1	1484	A
43	1	1485	A
43	1	1486	U
43	1	1487	C
43	1	1498	G
43	1	1500	A
43	1	1504	G
43	1	1508	C
43	1	1509	U
43	1	1514	A
43	1	1521	G
43	1	1522	A
43	1	1524	A
43	1	1529	U
43	1	1530	G
43	1	1531	C
43	1	1532	C
43	1	1533	G
43	1	1537	G
43	1	1538	A
43	1	1540	G
43	1	1542	G
43	1	1543	U
43	1	1544	A
43	1	1545	C
43	1	1546	A
43	1	1547	C
43	1	1548	G
43	1	1549	A
43	1	1550	A
43	1	1552	G
43	1	1555	A
43	1	1556	C
43	1	1560	G
43	1	1563	G
43	1	1564	C
43	1	1565	U

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Mol	Chain	Res	Type
43	1	1566	U
43	1	1569	A
43	1	1570	C
43	1	1571	U
43	1	1572	A
43	1	1574	A
43	1	1575	A
43	1	1576	A
43	1	1578	C
43	1	1579	C
43	1	1580	A
43	1	1581	U
43	1	1582	G
43	1	1583	C
43	1	1584	C
43	1	1585	U
43	1	1586	C
43	1	1587	U
43	1	1588	C
43	1	1589	U
43	1	1590	C
43	1	1591	U
43	1	1594	G
43	1	1595	A
43	1	1596	G
43	1	1597	C
43	1	1598	G
43	1	1599	A
43	1	1600	A
43	1	1601	U
43	1	1603	G
43	1	1604	G
43	1	1605	A
43	1	1606	U
43	1	1607	G
43	1	1608	A
43	1	1609	U
43	1	1611	G
43	1	1612	G
43	1	1613	G
43	1	1614	C
43	1	1615	C

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Mol	Chain	Res	Type
43	1	1616	G
43	1	1618	G
43	1	1619	G
43	1	1620	G
43	1	1621	C
43	1	1622	A
43	1	1623	G
43	1	1624	C
43	1	1625	G
43	1	1626	U
43	1	1627	A
43	1	1628	G
43	1	1629	C
43	1	1630	G
43	1	1631	C
43	1	1632	C
43	1	1633	U
43	1	1634	C
43	1	1635	U
43	1	1636	U
43	1	1637	C
43	1	1638	C
43	1	1639	C
43	1	1640	C
43	1	1641	U
43	1	1642	C
43	1	1643	A
43	1	1644	C
43	1	1645	U
43	1	1646	C
43	1	1647	U
43	1	1648	C
43	1	1649	C
43	1	1650	U
43	1	1651	U
43	1	1652	U
43	1	1653	C
43	1	1654	U
43	1	1655	C
43	1	1656	C
43	1	1658	A
43	1	1659	U

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Mol	Chain	Res	Type
43	1	1660	A
43	1	1661	U
43	1	1662	G
43	1	1663	A
43	1	1664	A
43	1	1665	C
43	1	1666	C
43	1	1667	U
43	1	1668	U
43	1	1669	G
43	1	1670	A
43	1	1671	G
43	1	1672	U
43	1	1673	C
43	1	1674	A
43	1	1675	U
43	1	1676	C
43	1	1678	A
43	1	1679	A
43	1	1836	C
43	1	1837	G
43	1	1838	A
43	1	1839	G
43	1	1840	U
43	1	1841	C
43	1	1842	U
43	1	1843	G
43	1	1844	U
43	1	1845	U
43	1	1846	U
43	1	1847	A
43	1	1849	A
43	1	1850	G
43	1	1851	U
43	1	1852	C
43	1	1853	G
43	1	1854	C
43	1	1855	G
43	1	1856	A
43	1	1857	C
43	1	1858	U
43	1	1859	C

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Mol	Chain	Res	Type
43	1	1860	U
43	1	1861	U
43	1	1862	G
43	1	1863	U
43	1	1864	C
43	1	1865	A
43	1	1866	U
43	1	1867	A
43	1	1868	G
43	1	1869	U
43	1	1870	C
43	1	1872	A
43	1	1873	G
43	1	1874	A
43	1	1875	A
43	1	1876	G
43	1	1877	G
43	1	1878	U
43	1	1880	G
43	1	1881	A
43	1	1882	A
43	1	1883	A
43	1	1887	C
43	1	1889	A
43	1	1892	A
43	1	1896	A
43	1	1897	A
43	1	1898	C
43	1	1899	U
43	1	1900	U
43	1	1901	C
43	1	1902	G
43	1	1903	A
43	1	1904	A
43	1	1905	U
43	1	1906	U
43	1	1907	G
43	1	1908	G
43	1	1909	G
43	1	1910	A
43	1	1911	G
43	1	1912	G

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Mol	Chain	Res	Type
43	1	1913	G
43	1	1914	C
43	1	1915	G
43	1	1916	A
43	1	1917	U
43	1	1918	C
43	1	1920	U
43	1	1921	C
43	1	1922	C
43	1	1923	C
43	1	1924	G
43	1	1925	G
43	1	1926	U
43	1	1927	G
43	1	1929	A
43	1	1930	C
43	1	1934	C
43	1	1942	C
43	1	1943	A
43	1	1945	A
43	1	1951	A
43	1	1953	A
43	1	1958	A
43	1	1969	U
43	1	1972	A
43	1	1973	C
43	1	1974	U
43	1	1981	C
43	1	1982	U
43	1	1983	U
43	1	1999	A
43	1	2007	C
43	1	2009	G
43	1	2033	A
43	1	2034	G
43	1	2036	A
43	1	2046	U
43	1	2047	C
43	1	2048	C
43	1	2049	U
43	1	2050	A
43	1	2051	U

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Mol	Chain	Res	Type
43	1	2052	C
43	1	2053	U
43	1	2054	U
43	1	2055	U
43	1	2057	G
43	1	2058	A
43	1	2060	U
43	1	2061	A
43	1	2062	G
43	1	2063	G
43	1	2065	A
43	1	2066	A
43	1	2067	G
43	1	2068	C
43	1	2073	C
43	1	2075	U
43	1	2077	C
43	1	2079	A
43	1	2080	G
43	1	2081	G
43	1	2090	A
43	1	2097	A
43	1	2098	U
43	1	2099	U
43	1	2102	A
43	1	2108	A
43	1	2109	G
43	1	2117	C
43	1	2118	U
43	1	2119	A
43	1	2124	G
43	1	2125	U
43	1	2133	U
43	1	2145	G
43	1	2146	A
43	1	2147	C
43	1	2150	C
43	1	2151	U
43	1	2159	G
43	1	2169	C
43	1	2173	A
43	1	2174	G

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Mol	Chain	Res	Type
43	1	2175	G
43	1	2176	A
43	1	2183	U
43	1	2184	U
43	1	2185	A
43	1	2186	U
43	1	2187	A
43	1	2194	G
43	1	2195	A
43	1	2196	A
43	1	2207	G
43	1	2210	A
43	1	2217	G
43	1	2220	A
43	1	2221	G
43	1	2224	A
43	1	2225	C
43	1	2226	U
43	1	2228	U
43	1	2232	U
43	1	2234	U
43	1	2238	A
43	1	2240	G
43	1	2241	G
43	1	2249	A
43	1	2252	C
43	1	2253	C
43	1	2254	U
43	1	2266	U
43	1	2274	U
43	1	2275	G
43	1	2276	C
43	1	2277	A
43	1	2278	C
43	1	2281	A
43	1	2282	U
43	1	2283	G
43	1	2294	U
43	1	2303	G
43	1	2307	C
43	1	2308	C
43	1	2312	A

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Mol	Chain	Res	Type
43	1	2313	U
43	1	2324	A
43	1	2326	A
43	1	2329	G
43	1	2331	A
43	1	2334	C
43	1	2341	A
43	1	2342	A
43	1	2343	G
43	1	2344	A
43	1	2347	C
43	1	2350	A
43	1	2354	C
43	1	2366	C
43	1	2367	G
43	1	2370	A
43	1	2371	A
43	1	2372	G
43	1	2373	A
43	1	2380	G
43	1	2404	G
43	1	2405	A
43	1	2408	A
43	1	2411	U
43	1	2413	G
43	1	2414	A
43	1	2416	C
43	1	2422	U
43	1	2423	G
43	1	2424	U
43	1	2425	A
43	1	2426	G
43	1	2427	G
43	1	2428	A
43	1	2429	U
43	1	2430	A
43	1	2431	G
43	1	2432	G
43	1	2433	U
43	1	2436	G
43	1	2437	A
43	1	2438	G

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Mol	Chain	Res	Type
43	1	2439	G
43	1	2441	C
43	1	2442	G
43	1	2443	U
43	1	2444	G
43	1	2445	A
43	1	2446	C
43	1	2447	A
43	1	2448	U
43	1	2454	G
43	1	2455	A
43	1	2456	C
43	1	2457	C
43	1	2459	A
43	1	2460	U
43	1	2461	C
43	1	2463	U
43	1	2466	A
43	1	2467	A
43	1	2468	G
43	1	2469	A
43	1	2470	C
43	1	2472	A
43	1	2473	C
43	1	2474	U
43	1	2476	U
43	1	2477	U
43	1	2478	U
43	1	2481	U
43	1	2483	U
43	1	2486	G
43	1	2487	G
43	1	2488	G
43	1	2489	U
43	1	2494	A
43	1	2495	A
43	1	2496	C
43	1	2499	C
43	1	2522	G
43	1	2525	G
43	1	2527	A
43	1	2528	C

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Mol	Chain	Res	Type
43	1	2540	G
43	1	2541	G
43	1	2545	U
43	1	2552	G
43	1	2553	G
43	1	2554	G
43	1	2581	G
43	1	2585	U
43	1	2589	A
43	1	2590	A
43	1	2599	C
43	1	2608	A
43	1	2609	U
43	1	2610	U
43	1	2614	C
43	1	2617	G
43	1	2623	G
43	1	2625	A
43	1	2632	U
43	1	2633	A
43	1	2634	A
43	1	2641	C
43	1	2643	G
43	1	2644	A
43	1	2645	C
43	1	2649	G
43	1	2653	C
43	1	2655	G
43	1	2656	A
43	1	2659	G
43	1	2660	G
43	1	2668	G
43	1	2670	G
43	1	2674	A
43	1	2675	A
43	1	2681	G
43	1	2683	C
43	1	2688	U
43	1	2689	G
43	1	2700	C
43	1	2701	C
43	1	2702	C

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Mol	Chain	Res	Type
43	1	2704	U
43	1	2705	G
43	1	2708	G
43	1	2714	C
43	1	2718	C
43	1	2720	C
43	1	2722	C
43	1	2723	A
43	1	2726	G
43	1	2729	U
43	1	2730	C
43	1	2733	A
43	1	2739	G
43	1	2743	G
43	1	2745	G
43	1	2746	A
43	1	2756	G
43	1	2757	A
43	1	2767	A
43	1	2772	U
43	1	2774	U
43	1	2776	A
43	1	2778	C
43	1	2780	A
43	1	2783	G
43	1	2785	G
43	1	2789	U
43	1	2790	U
43	1	2792	G
43	1	2800	G
43	1	2801	A
43	1	2802	U
43	1	2803	G
43	1	2805	C
43	1	2816	A
43	1	2818	C
43	1	2822	G
43	1	2823	G
43	1	2827	G
43	1	2828	A
43	1	2832	A
43	1	2833	G

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Mol	Chain	Res	Type
43	1	2843	G
43	1	2844	U
43	1	2846	C
43	1	2847	G
43	1	2852	U
43	1	2864	A
43	1	2865	G
43	1	2870	A
43	1	2871	C
43	1	2874	G
43	1	2876	G
43	1	2883	U
43	1	2884	U
43	1	2894	U
43	1	2900	A
43	1	2901	G
43	1	2906	G
43	1	2907	U
43	1	2911	U
43	1	2918	C
43	1	2919	G
43	1	2927	U
43	1	2928	A
43	1	2929	A
43	1	2930	A
43	1	2931	G
43	1	2932	G
43	1	2934	A
43	1	2936	A
43	1	2940	G
43	1	2947	G
43	1	2948	C
43	1	2958	U
43	1	2965	G
43	1	2970	G
43	1	2976	G
43	1	2979	C
43	1	2983	C
43	1	2984	U
43	1	2985	A
43	1	2987	G
43	1	2991	U

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Mol	Chain	Res	Type
43	1	2992	A
43	1	3014	G
43	1	3015	C
43	1	3016	G
43	1	3019	G
43	1	3022	C
43	1	3026	U
43	1	3028	A
43	1	3031	U
43	1	3032	G
43	1	3035	A
43	1	3041	G
43	1	3043	A
43	1	3046	G
43	1	3048	U
43	1	3050	C
43	1	3051	U
43	1	3052	U
43	1	3060	A
43	1	3061	A
43	1	3072	U
43	1	3073	A
43	1	3083	G
43	1	3084	G
43	1	3085	A
43	1	3087	C
43	1	3094	U
43	1	3095	A
43	1	3096	G
43	1	3101	G
43	1	3105	U
43	1	3107	C
43	1	3108	G
43	1	3109	A
43	1	3110	U
43	1	3115	G
43	1	3117	G
43	1	3123	G
43	1	3131	G
43	1	3135	G
43	1	3141	A
43	1	3142	A

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Mol	Chain	Res	Type
43	1	3143	G
43	1	3147	U
43	1	3149	U
43	1	3150	C
43	1	3151	G
43	1	3153	A
43	1	3154	C
43	1	3158[A]	A
43	1	3159[A]	C
43	1	3160[A]	G
43	1	3161[A]	A
44	3	2	A
44	3	3	A
44	3	13	A
44	3	15	G
44	3	18	G
44	3	22	C
44	3	23	G
44	3	25	G
44	3	26	A
44	3	27	A
44	3	34	C
44	3	40	C
44	3	43	U
44	3	44	C
44	3	45	C
44	3	46	G
44	3	47	A
44	3	49	C
44	3	55	A
44	3	56	U
44	3	57	G
44	3	59	G
44	3	60	G
44	3	61	A
44	3	62	A
44	3	65	G
44	3	66	U
44	3	67	C
44	3	69	U
44	3	70	G
44	3	72	G

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Mol	Chain	Res	Type
44	3	76	U
44	3	79	G
44	3	80	U
44	3	85	A
44	3	86	G
44	3	87	A
44	3	90	G
44	3	91	U
44	3	92	U
44	3	94	G
44	3	97	A
44	3	106	C
44	3	107	C
44	3	108	A
44	3	109	A
44	3	116	U
44	3	117	G
44	3	118	A
85	2	6	A
85	2	7	G
85	2	8	U
85	2	9	C
85	2	10	A
85	2	11	A
85	2	12	A
85	2	13	A
85	2	14	G
85	2	15	A
85	2	16	A
85	2	17	G
85	2	22	U
85	2	30	G
85	2	34	A
85	2	40	A
85	2	46	A
85	2	49	U
85	2	55	C
85	2	56	U
85	2	58	A
85	2	59	A
85	2	60	C
85	2	68	A

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Mol	Chain	Res	Type
85	2	75	C
85	2	77	U
85	2	78	U
85	2	79	G
85	2	80	U
85	2	81	U
85	2	82	C
85	2	83	U
85	2	84	C
85	2	85	G
85	2	89	A
85	2	90	G
85	2	91	C
85	2	92	U
85	2	93	A
85	2	94	G
85	2	95	G
85	2	96	C
85	2	97	A
85	2	98	G
85	2	112	U
85	2	113	C
85	2	114	C
85	2	115	U
85	2	116	A
85	2	117	G
85	2	118	C
85	2	119	U
85	2	120	C
85	2	129	U
85	2	130	U
85	2	131	G
85	2	132	U
85	2	133	C
85	2	134	U
85	2	135	C
85	2	136	G
85	2	148	G
85	2	149	G
85	2	150	A
85	2	151	A
85	2	152	G

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Mol	Chain	Res	Type
85	2	153	A
85	2	154	G
85	2	155	U
85	2	156	U
85	2	157	G
85	2	158	A
85	2	159	G
85	2	161	A
85	2	162	C
85	2	163	A
85	2	164	A
85	2	165	A
85	2	167	U
85	2	176	G
85	2	181	G
85	2	184	A
85	2	185	G
85	2	186	G
85	2	194	A
85	2	195	U
85	2	198	G
85	2	205	A
85	2	206	G
85	2	208	U
85	2	210	G
85	2	212	G
85	2	214	C
85	2	215	A
85	2	218	U
85	2	219	C
85	2	224	A
85	2	225	G
85	2	226	A
85	2	227	A
85	2	228	A
85	2	231	U
85	2	232	A
85	2	233	A
85	2	234	A
85	2	235	A
85	2	236	A
85	2	237	G

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Mol	Chain	Res	Type
85	2	238	C
85	2	245	U
85	2	264	U
85	2	266	G
85	2	270	G
85	2	273	G
85	2	276	U
85	2	277	A
85	2	278	G
85	2	280	U
85	2	281	A
85	2	282	A
85	2	285	G
85	2	286	C
85	2	287	U
85	2	288	G
85	2	298	A
85	2	299	U
85	2	300	G
85	2	302	U
85	2	303	G
85	2	308	G
85	2	313	U
85	2	325	A
85	2	339	G
85	2	340	A
85	2	346	A
85	2	347	C
85	2	351	G
85	2	359	U
85	2	360	C
85	2	361	C
85	2	363	A
85	2	364	C
85	2	365	G
85	2	366	G
85	2	370	G
85	2	371	C
85	2	372	A
85	2	373	G
85	2	375	A
85	2	379	G

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Mol	Chain	Res	Type
85	2	380	G
85	2	385	C
85	2	386	U
85	2	388	G
85	2	391	C
85	2	392	A
85	2	394	U
85	2	399	G
85	2	401	A
85	2	403	G
85	2	404	C
85	2	405	C
85	2	407	A
85	2	413	C
85	2	415	A
85	2	416	U
85	2	419	C
85	2	421	C
85	2	423	U
85	2	424	G
85	2	426	G
85	2	429	A
85	2	430	A
85	2	432	A
85	2	436	G
85	2	439	A
85	2	440	U
85	2	441	G
85	2	442	C
85	2	443	C
85	2	444	G
85	2	449	U
85	2	450	A
85	2	453	G
85	2	457	U
85	2	459	U
85	2	468	G
85	2	471	C
85	2	473	A
85	2	475	C
85	2	478	G
85	2	479	A

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Mol	Chain	Res	Type
85	2	481	A
85	2	483	G
85	2	488	G
85	2	489	A
85	2	490	G
85	2	494	G
85	2	497	G
85	2	506	A
85	2	508	C
85	2	510	C
85	2	514	G
85	2	515	C
85	2	516	C
85	2	518	G
85	2	519	C
85	2	521	G
85	2	524	G
85	2	525	C
85	2	528	U
85	2	529	A
85	2	530	A
85	2	542	C
85	2	544	A
85	2	546	U
85	2	556	A
85	2	557	A
85	2	560	A
85	2	561	C
85	2	563	G
85	2	564	G
85	2	565	G
85	2	569	A
85	2	570	A
85	2	572	G
85	2	574	G
85	2	575	C
85	2	576	A
85	2	578	G
85	2	580	A
85	2	585	G
85	2	608	U
85	2	614	A

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Mol	Chain	Res	Type
85	2	615	A
85	2	616	A
85	2	617	A
85	2	618	G
85	2	628	G
85	2	634	G
85	2	648	U
85	2	659	G
85	2	660	A
85	2	661	G
85	2	667	U
85	2	682	A
85	2	687	U
85	2	694	U
85	2	697	A
85	2	698	G
85	2	703	A
85	2	706	A
85	2	708	G
85	2	710	A
85	2	718	A
85	2	723	A
85	2	726	G
85	2	728	A
85	2	731	U
85	2	742	C
85	2	743	U
85	2	750	G
85	2	755	G
85	2	756	G
85	2	758	U
85	2	762	A
85	2	774	A
85	2	778	A
85	2	784	A
85	2	790	U
85	2	791	A
85	2	793	C
85	2	805	U
85	2	806	G
85	2	808	C
85	2	810	U

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Mol	Chain	Res	Type
85	2	811	A
85	2	814	C
85	2	815	G
85	2	816	A
85	2	826	G
85	2	829	C
85	2	831	U
85	2	838	C
85	2	839	G
85	2	840	C
85	2	841	A
85	2	844	U
85	2	847	G
85	2	850	G
85	2	853	C
85	2	854	A
85	2	863	G
85	2	864	U
85	2	865	G
85	2	869	A
85	2	878	G
85	2	882	A
85	2	889	U
85	2	893	A
85	2	895	G
85	2	898	C
85	2	903	C
85	2	907	A
85	2	909	G
85	2	919	G
85	2	920	G
85	2	921	G
85	2	922	G
85	2	923	C
85	2	924	C
85	2	926	G
85	2	927	C
85	2	928	A
85	2	931	A
85	2	941	C
85	2	947	G
85	2	948	U

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Mol	Chain	Res	Type
85	2	949	U
85	2	952	A
85	2	953	U
85	2	957	A
85	2	960	C
85	2	962	A
85	2	964	G
85	2	967	C
85	2	968	A
85	2	969	A
85	2	970	A
85	2	974	U
85	2	980	G
85	2	982	C
85	2	983	C
85	2	985	U
85	2	986	G
85	2	992	U
85	2	993	G
85	2	994	A
85	2	997	A
85	2	998	A
85	2	999	C
85	2	1001	A
85	2	1003	A
85	2	1004	C
85	2	1006	U
85	2	1007	A
85	2	1012	U
85	2	1015	C
85	2	1016	G
85	2	1019	A
85	2	1020	U
85	2	1021	G
85	2	1026	U
85	2	1028	A
85	2	1029	C
85	2	1030	U
85	2	1031	U
85	2	1036	A
85	2	1037	C
85	2	1044	U

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Mol	Chain	Res	Type
85	2	1045	G
85	2	1046	C
85	2	1057	U
85	2	1059	A
85	2	1061	C
85	2	1062	U
85	2	1067	U
85	2	1070	U
85	2	1078	U
85	2	1079	U
85	2	1080	G
85	2	1084	A
85	2	1085	A
85	2	1086	G
85	2	1087	U
85	2	1093	A
85	2	1094	A
85	2	1095	C
85	2	1096	G
85	2	1097	A
85	2	1098	G
85	2	1102	A
85	2	1110	U
85	2	1117	U
85	2	1118	U
85	2	1122	C
85	2	1123	A
85	2	1124	G
85	2	1127	A
85	2	1128	U
85	2	1129	G
85	2	1130	C
85	2	1131	G
85	2	1132	C
85	2	1133	C
85	2	1134	U
85	2	1135	A
85	2	1136	A
85	2	1137	G
85	2	1138	G
85	2	1139	A
85	2	1141	A

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Mol	Chain	Res	Type
85	2	1143	A
85	2	1144	G
85	2	1145	G
85	2	1146	C
85	2	1147	U
85	2	1148	U
85	2	1149	G
85	2	1151	A
85	2	1152	A
85	2	1153	A
85	2	1154	C
85	2	1155	C
85	2	1156	G
85	2	1157	A
85	2	1159	G
85	2	1160	U
85	2	1161	G
85	2	1162	A
85	2	1163	G
85	2	1164	C
85	2	1165	C
85	2	1166	A
85	2	1167	A
85	2	1168	G
85	2	1169	G
85	2	1170	A
85	2	1171	G
85	2	1172	C
85	2	1173	C
85	2	1174	G
85	2	1175	A
85	2	1176	G
85	2	1177	U
85	2	1178	G
85	2	1179	A
85	2	1180	U
85	2	1181	G
85	2	1183	G
85	2	1184	C
85	2	1185	C
85	2	1186	A
85	2	1188	A

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Mol	Chain	Res	Type
85	2	1189	C
85	2	1190	C
85	2	1191	U
85	2	1192	A
85	2	1193	G
85	2	1203	U
85	2	1204	A
85	2	1205	G
85	2	1206	G
85	2	1207	C
85	2	1208	C
85	2	1209	A
85	2	1210	A
85	2	1211	C
85	2	1212	U
85	2	1213	C
85	2	1214	G
85	2	1215	A
85	2	1216	C
85	2	1217	G
85	2	1218	U
85	2	1219	C
85	2	1220	G
85	2	1369	G
85	2	1370	A
85	2	1371	C
85	2	1372	G
85	2	1373	U
85	2	1374	C
85	2	1375	G
85	2	1376	A
85	2	1377	G
85	2	1378	U
85	2	1379	U
85	2	1380	G
85	2	1381	G
85	2	1382	C
85	2	1384	G
85	2	1385	C
85	2	1386	G
85	2	1387	G
85	2	1388	A

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Mol	Chain	Res	Type
85	2	1389	G
85	2	1390	A
85	2	1391	A
85	2	1392	A
85	2	1393	G
85	2	1394	A
85	2	1395	C
85	2	1396	U
85	2	1397	C
85	2	1398	G
85	2	1399	G
85	2	1400	C
85	2	1401	A
85	2	1402	U
85	2	1403	U
85	2	1404	C
85	2	1405	A
85	2	1406	G
85	2	1407	G
85	2	1408	C
85	2	1409	G
85	2	1410	A
85	2	1411	G
85	2	1412	C
85	2	1413	C
85	2	1414	G
85	2	1415	C
85	2	1416	C
85	2	1417	C
85	2	1418	G
85	2	1419	G
85	2	1420	U
85	2	1421	G
85	2	1422	G
85	2	1423	U
85	2	1425	U
85	2	1427	G
85	2	1428	G
85	2	1429	A
85	2	1430	C
85	2	1431	G
85	2	1432	A

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Mol	Chain	Res	Type
85	2	1433	A
85	2	1434	G
85	2	1435	U
85	2	1436	A
85	2	1437	A
85	2	1438	G
85	2	1439	U
85	2	1440	G
85	2	1443	U
85	2	1444	U
85	2	1445	U
85	2	1446	A
85	2	1447	G
85	2	1448	U
85	2	1449	A
85	2	1450	C
85	2	1451	G
85	2	1452	C
85	2	1453	C
85	2	1454	C
85	2	1455	U
85	2	1456	G
85	2	1457	C
85	2	1458	C
85	2	1459	A
85	2	1461	A
85	2	1462	A
85	2	1463	C
85	2	1464	G
85	2	1465	G
85	2	1467	U
85	2	1468	C
85	2	1469	C
85	2	1470	G
85	2	1471	A
85	2	1474	C
85	2	1475	A
85	2	1477	A
85	2	1478	C
85	2	1479	A
85	2	1480	A
85	2	1483	A

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Mol	Chain	Res	Type
85	2	1485	G
85	2	1494	G
85	2	1495	C
85	2	1496	A
85	2	1499	C
85	2	1500	A
85	2	1501	C
85	2	1509	U
85	2	1514	G
85	2	1517	A
85	2	1518	U
85	2	1519	A
85	2	1520	U
85	2	1521	A
85	2	1524	G
85	2	1529	A
85	2	1537	G
85	2	1543	G
85	2	1546	A
85	2	1547	A
85	2	1550	C
85	2	1551	C
85	2	1552	G
85	2	1555	U
85	2	1559	C
85	2	1560	C
85	2	1562	U
85	2	1563	A
85	2	1577	A
85	2	1578	C
85	2	1579	A
85	2	1583	G
85	2	1586	A
85	2	1587	C
85	2	1588	A
85	2	1590	U
85	2	1591	G
85	2	1592	G
85	2	1596	U
85	2	1597	U
85	2	1602	U
85	2	1603	G

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Mol	Chain	Res	Type
85	2	1607	A
85	2	1610	A
85	2	1623	G
85	2	1624	G
85	2	1628	G
85	2	1630	A
85	2	1631	U
85	2	1632	C
85	2	1633	C
85	2	1634	G
85	2	1635	G
85	2	1636	A
85	2	1638	A
85	2	1642	U
85	2	1647	C
85	2	1648	A
85	2	1649	G
85	2	1650	U
85	2	1654	G
85	2	1655	A
85	2	1658	G
85	2	1659	U
85	2	1660	U
85	2	1661	C
85	2	1665	G
85	2	1666	C
85	2	1667	A
85	2	1668	A
85	2	1670	U
85	2	1671	C
85	2	1672	G
85	2	1673	G
85	2	1684	U
85	2	1687	G
85	2	1689	A
85	2	1695	A
85	2	1696	G
85	2	1702	G
85	2	1705	G
85	2	1712	A
85	2	1713	U
85	2	1722	G

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Mol	Chain	Res	Type
85	2	1723	A
85	2	1726	A
85	2	1727	U
85	2	1728	G
85	2	1737	C
85	2	1738	C
85	2	1739	C
85	2	1749	C
85	2	1750	G
85	2	1751	C
85	2	1767	A
85	2	1768	A
85	2	1771	G
85	2	1773	U
85	2	1778	C
85	2	1786	A
85	2	1787	U
85	2	1788	C
85	2	1789	G
85	2	1790	G
85	2	1791	A
85	2	1792	A
85	2	1793	C
85	2	1794	A
85	2	1795	A
85	2	1796	U
85	2	1797	G
85	2	1798	A
85	2	1799	U
85	2	1801	A
85	2	1802	C
85	2	1803	C
85	2	1804	C
85	2	1805	A
85	2	1806	U
85	2	1807	G
85	2	1809	C
85	2	1811	U
85	2	1812	C
85	2	1813	U
85	2	1814	G
85	2	1815	U

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Mol	Chain	Res	Type
85	2	1817	U
85	2	1818	A
85	2	1819	A
85	2	1820	C
85	2	1821	A
85	2	1822	C
85	2	1824	A
85	2	1825	G
85	2	1827	G
85	2	1828	C
85	2	1829	C
85	2	1830	A
85	2	1832	A
85	2	1833	A
85	2	1834	A
85	2	1835	G
85	2	1836	G
85	2	1837	C
85	2	1839	U
85	2	1841	U
85	2	1842	G
85	2	1843	G
85	2	1844	U
85	2	1845	G
85	2	1846	G
85	2	1847	U
85	2	1849	U
85	2	1850	U
85	2	1851	A
85	2	1853	U
85	2	1854	G
85	2	1855	G
85	2	1856	C
85	2	1858	C
85	2	1859	A
85	2	1860	U
85	2	1861	A
85	2	1864	A
85	2	1873	U
85	2	1874	C
85	2	1888	A
85	2	1889	A

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Mol	Chain	Res	Type
85	2	1890	G
85	2	1893	G
85	2	1895	A
85	2	1898	A
85	2	1899	A
85	2	1902	U
85	2	1905	C
85	2	1910	G
85	2	1913	G
85	2	1914	A
85	2	1921	G
85	2	1925	G
85	2	1926	G
85	2	1927	A
85	2	1929	U
85	2	1930	G
85	2	1931	A
85	2	1933	U
85	2	1934	C

All (139) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
43	1	16	G
43	1	49	G
43	1	118	A
43	1	130	A
43	1	140	C
43	1	249	U
43	1	295	C
43	1	297	C
43	1	427	U
43	1	428	U
43	1	476	U
43	1	487	G
43	1	497	U
43	1	618	A
43	1	620	A
43	1	633	C
43	1	643	A
43	1	645	A
43	1	671	A

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Mol	Chain	Res	Type
43	1	687	G
43	1	766	G
43	1	778	U
43	1	856	U
43	1	928	G
43	1	1091	C
43	1	1317	C
43	1	1323	A
43	1	1332	U
43	1	1396	U
43	1	1419	U
43	1	1532	C
43	1	1543	U
43	1	1555	A
43	1	1618	G
43	1	1621	C
43	1	1628	G
43	1	1641	U
43	1	1647	U
43	1	1665	C
43	1	1842	U
43	1	1851	U
43	1	1861	U
43	1	1910	A
43	1	1913	G
43	1	1915	G
43	1	1916	A
43	1	1928	A
43	1	2050	A
43	1	2051	U
43	1	2057	G
43	1	2186	U
43	1	2413	G
43	1	2436	G
43	1	2438	G
43	1	2454	G
43	1	2466	A
43	1	2487	G
43	1	2498	G
43	1	2598	U
43	1	2928	A
43	1	2931	G

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Mol	Chain	Res	Type
43	1	2991	U
43	1	3014	G
43	1	3049	G
43	1	3050	C
43	1	3095	A
44	3	1	A
44	3	2	A
44	3	12	U
44	3	25	G
44	3	60	G
44	3	61	A
44	3	64	C
85	2	6	A
85	2	83	U
85	2	84	C
85	2	225	G
85	2	231	U
85	2	232	A
85	2	233	A
85	2	235	A
85	2	285	G
85	2	415	A
85	2	449	U
85	2	458	U
85	2	472	G
85	2	477	U
85	2	496	A
85	2	564	G
85	2	615	A
85	2	839	G
85	2	853	C
85	2	920	G
85	2	921	G
85	2	922	G
85	2	923	C
85	2	948	U
85	2	997	A
85	2	1117	U
85	2	1154	C
85	2	1163	G
85	2	1164	C
85	2	1165	C

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Mol	Chain	Res	Type
85	2	1166	A
85	2	1169	G
85	2	1202	C
85	2	1203	U
85	2	1206	G
85	2	1379	U
85	2	1385	C
85	2	1402	U
85	2	1403	U
85	2	1404	C
85	2	1408	C
85	2	1425	U
85	2	1428	G
85	2	1459	A
85	2	1461	A
85	2	1464	G
85	2	1478	C
85	2	1484	G
85	2	1494	G
85	2	1495	C
85	2	1551	C
85	2	1629	A
85	2	1634	G
85	2	1667	A
85	2	1670	U
85	2	1738	C
85	2	1792	A
85	2	1795	A
85	2	1796	U
85	2	1797	G
85	2	1798	A
85	2	1799	U
85	2	1814	G
85	2	1849	U
85	2	1863	C
85	2	1929	U

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

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

5.5 Carbohydrates (i)

There are no 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
85	2	39
43	1	5
58	BP	3
45	Bb	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	120:C	O3'	128:C	P	28.73
1	BP	204:ALA	C	205:ALA	N	21.29
1	2	1193:G	O3'	1202:C	P	17.46
1	2	1220:G	O3'	1368:C	P	17.36
1	2	98:G	O3'	111:C	P	17.08
1	2	85:G	O3'	88:G	P	13.31
1	1	2502:C	O3'	2521:G	P	12.95
1	2	136:G	O3'	147:G	P	11.30
1	BP	182:ALA	C	184:ALA	N	10.41
1	1	1028:G	O3'	1040:C	P	10.02
1	Bb	389:LEU	C	393:ILE	N	7.49
1	1	315:U	O3'	420:A	P	7.35
1	BP	229:ALA	C	233:ALA	N	6.94
1	1	277:G	O3'	295:C	P	5.91
1	1	1680:G	O3'	1835:G	P	5.74
1	2	1181:G	O3'	1182:U	P	3.49
1	2	1441:G	O3'	1442:G	P	2.51

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1425:U	O3'	1426:G	P	2.36
1	2	1423:U	O3'	1424:G	P	2.20
1	2	1450:C	O3'	1451:G	P	2.17
1	2	1451:G	O3'	1452:C	P	2.03
1	2	1390:A	O3'	1391:A	P	1.99
1	2	1169:G	O3'	1170:A	P	1.86
1	2	1202:C	O3'	1203:U	P	1.83
1	2	1187:G	O3'	1188:A	P	1.82
1	2	1437:A	O3'	1438:G	P	1.81
1	2	1170:A	O3'	1171:G	P	1.78
1	2	1165:C	O3'	1166:A	P	1.77
1	2	1378:U	O3'	1379:U	P	1.39
1	2	1191:U	O3'	1192:A	P	1.38
1	2	1408:C	O3'	1409:G	P	1.37
1	2	1430:C	O3'	1431:G	P	1.37
1	2	1431:G	O3'	1432:A	P	1.36
1	2	1207:C	O3'	1208:C	P	1.35
1	2	1438:G	O3'	1439:U	P	1.34
1	2	1406:G	O3'	1407:G	P	1.30
1	2	1206:G	O3'	1207:C	P	1.28
1	2	1381:G	O3'	1382:C	P	1.28
1	2	1179:A	O3'	1180:U	P	1.27
1	2	1167:A	O3'	1168:G	P	1.24
1	2	1166:A	O3'	1167:A	P	1.21
1	2	1404:C	O3'	1405:A	P	1.21
1	2	1445:U	O3'	1446:A	P	1.19
1	2	1428:G	O3'	1429:A	P	1.16
1	2	1379:U	O3'	1380:G	P	1.08
1	2	1385:C	O3'	1386:G	P	1.07
1	2	1402:U	O3'	1403:U	P	1.04
1	2	1391:A	O3'	1392:A	P	0.95

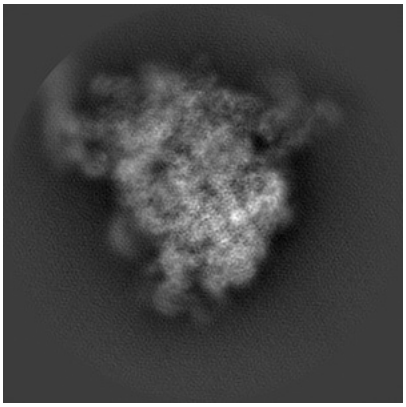
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10654. These allow visual inspection of the internal detail of the map and identification of artifacts.

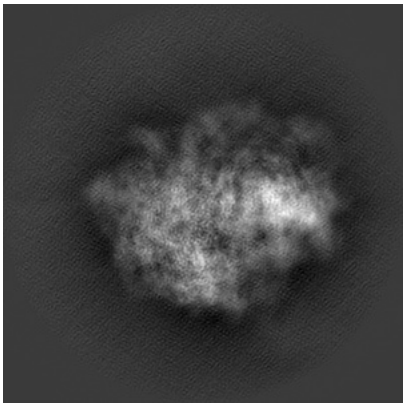
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

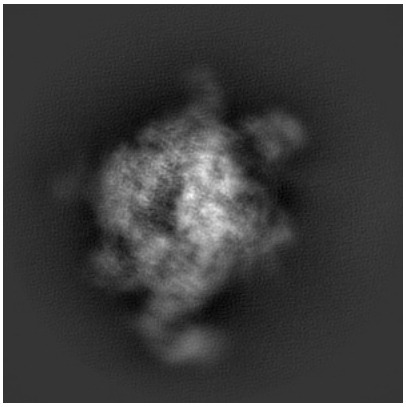
6.1.1 Primary map



X



Y

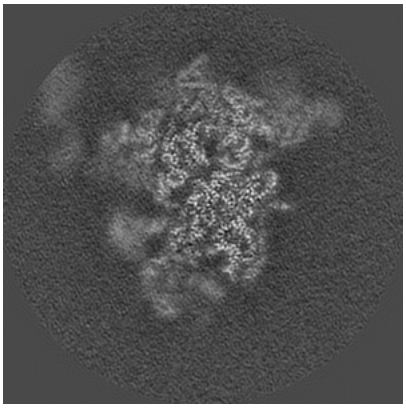


Z

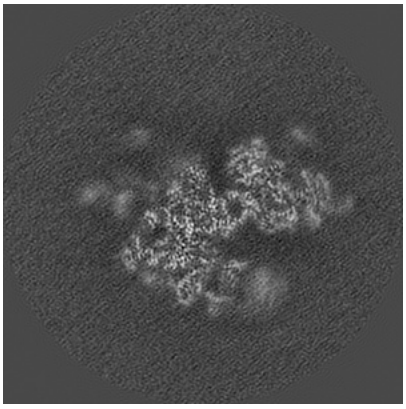
The images above show the map projected in three orthogonal directions.

6.2 Central slices

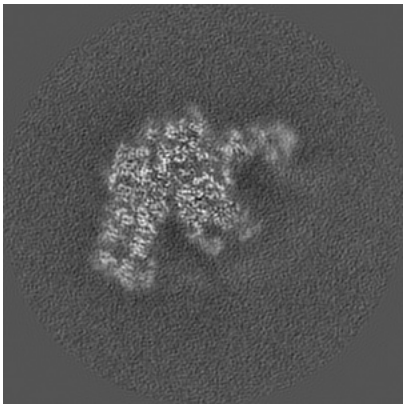
6.2.1 Primary map



X Index: 200



Y Index: 200

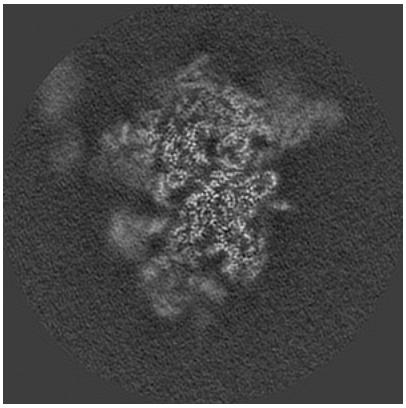


Z Index: 200

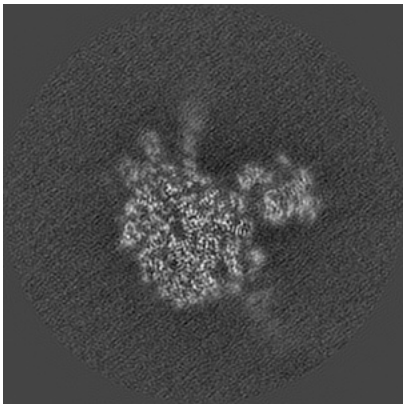
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

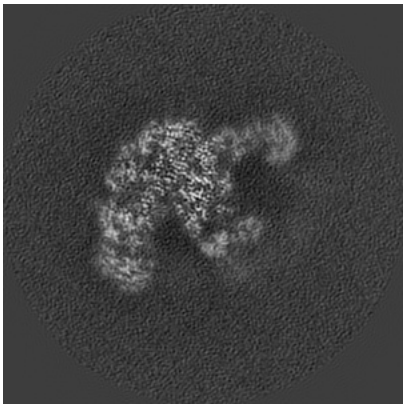
6.3.1 Primary map



X Index: 201



Y Index: 229



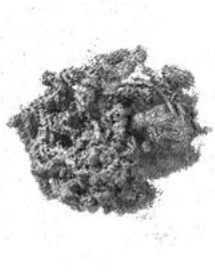
Z Index: 205

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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

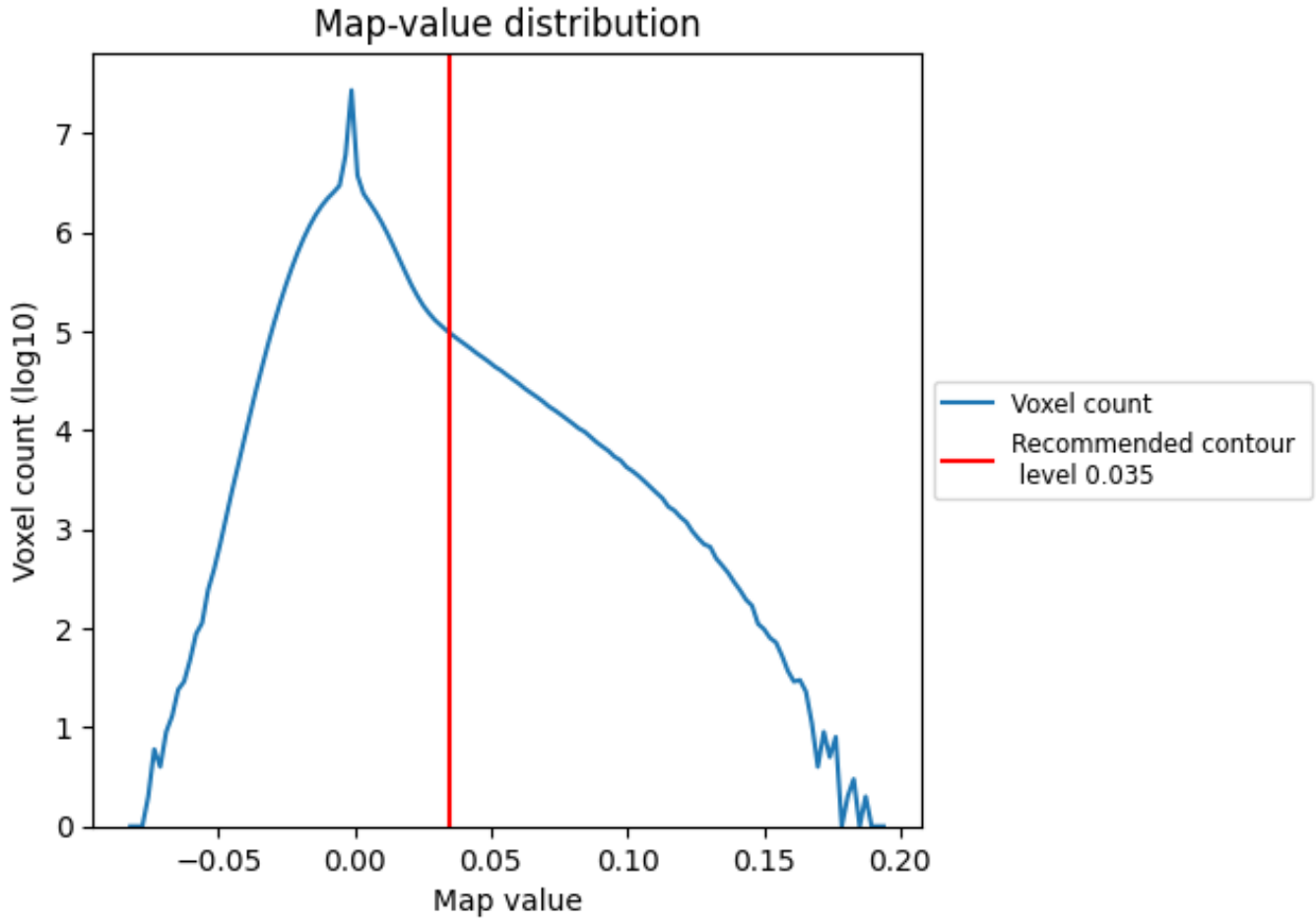
6.5 Mask visualisation (i)

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

7 Map analysis

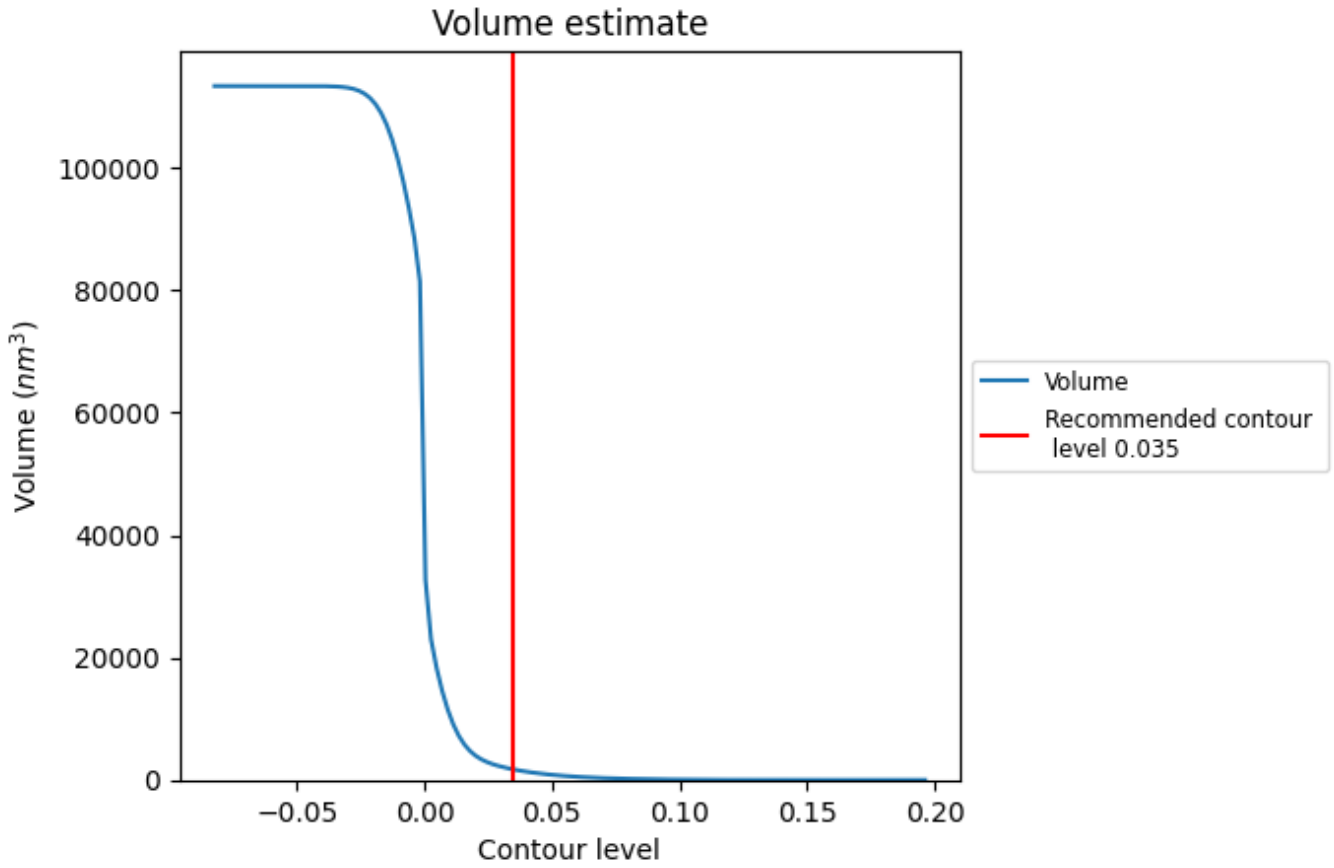
This section contains the results of statistical analysis of the map.

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.

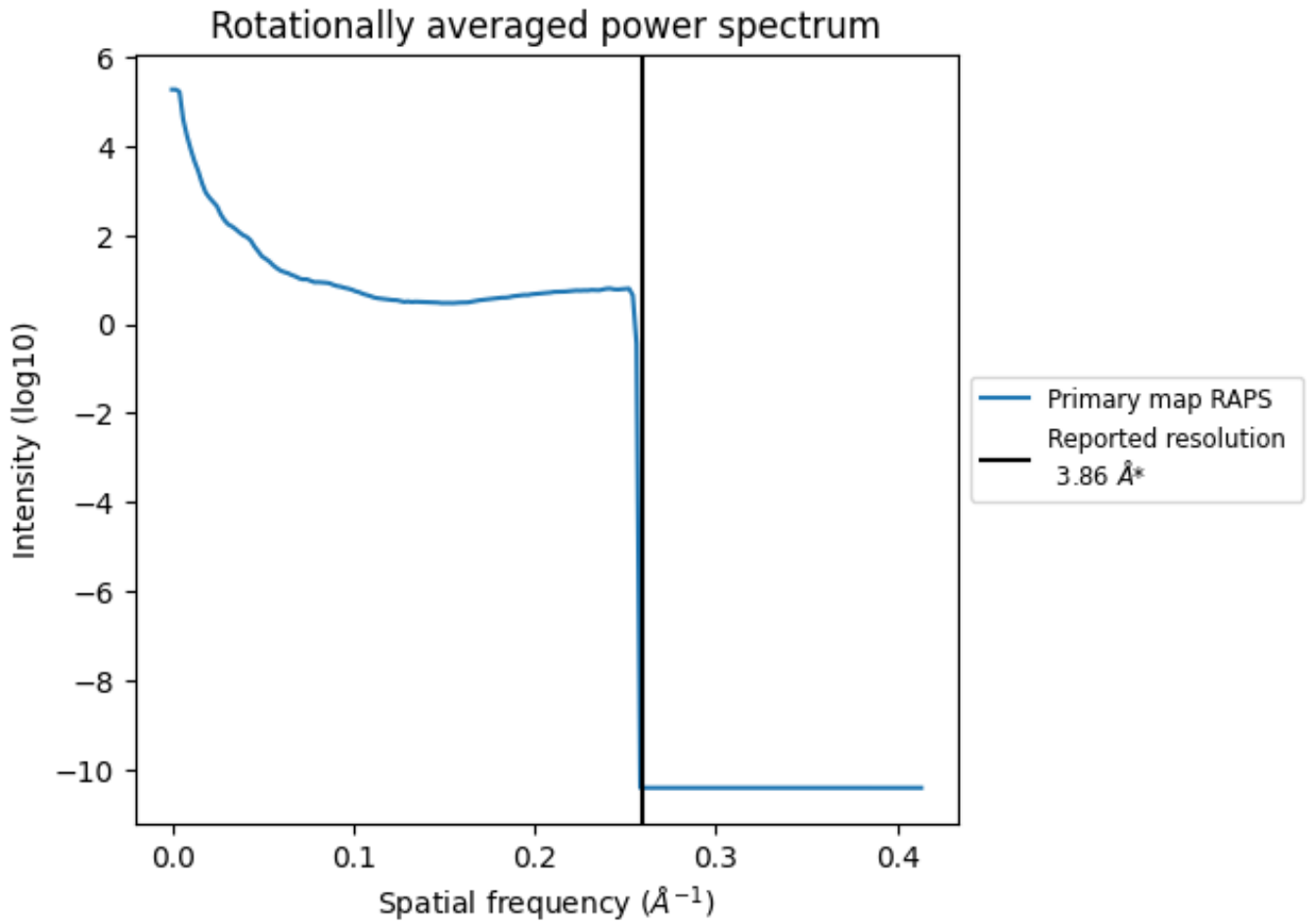
7.2 Volume estimate



The volume at the recommended contour level is 1711 nm^3; this corresponds to an approximate mass of 1546 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 0.259 Å^{-1}

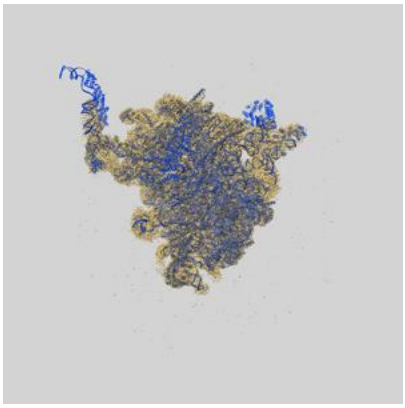
8 Fourier-Shell correlation

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

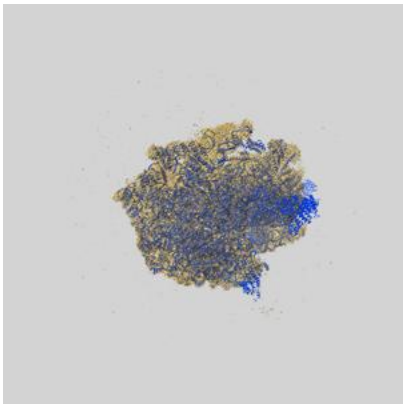
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10654 and PDB model 6XYW. Per-residue inclusion information can be found in section 3 on page 20.

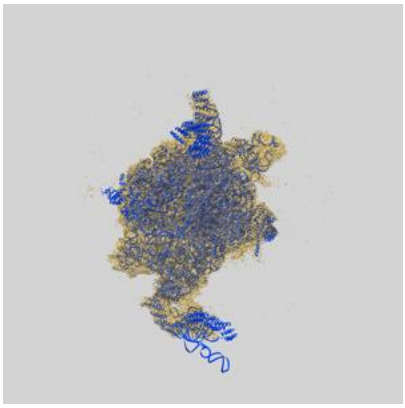
9.1 Map-model overlay



X



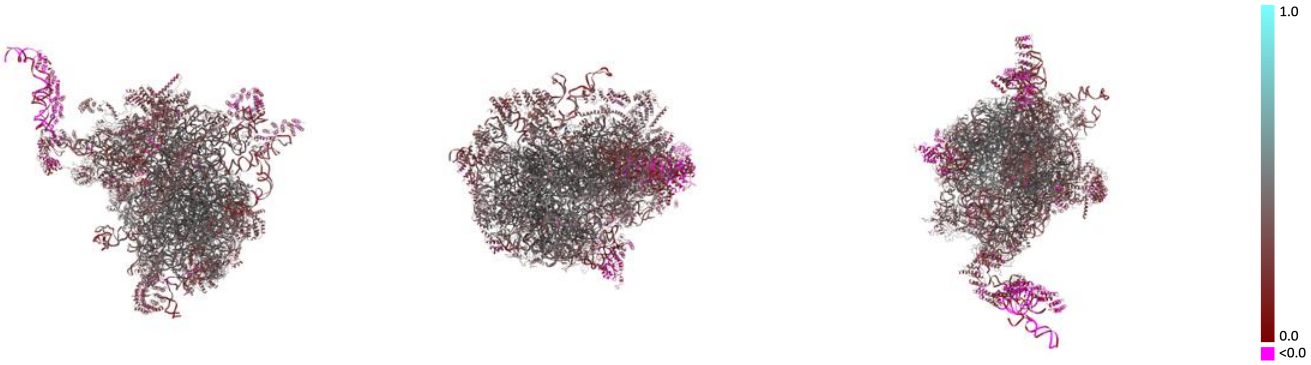
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

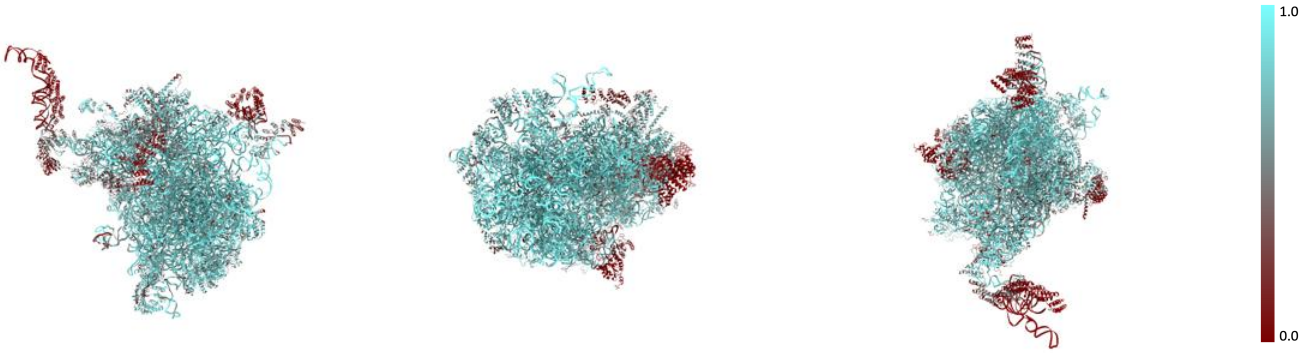
9.2 Q-score mapped to coordinate model (i)



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.

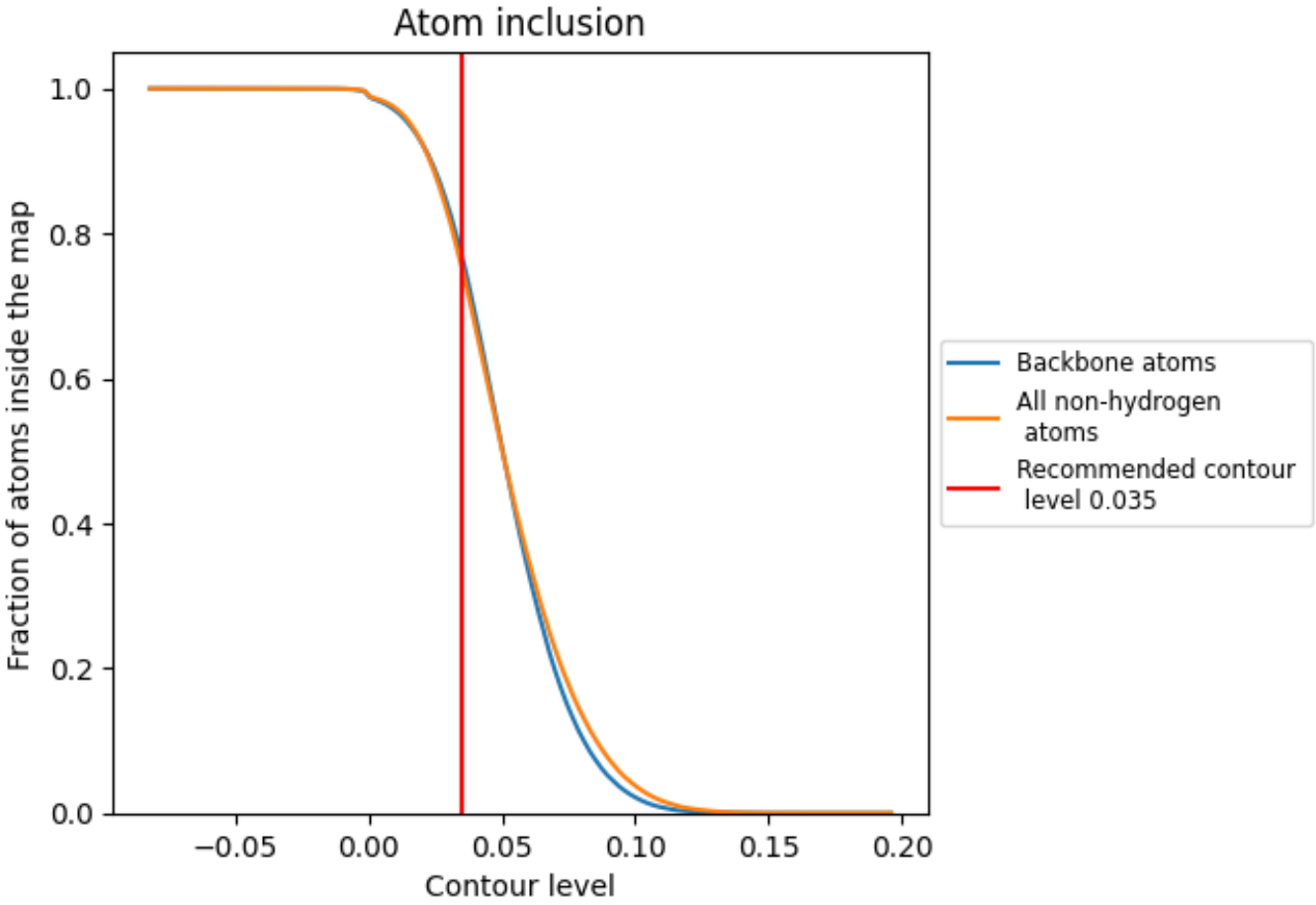
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 75% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7508	0.3590
1	0.8947	0.3950
2	0.8175	0.3350
3	0.9542	0.3880
AA	0.7603	0.3460
AB	0.8155	0.4640
AC	0.8333	0.4390
AD	0.8078	0.4600
AE	0.6678	0.4590
AF	0.7149	0.3070
AG	0.7705	0.4460
AH	0.8197	0.4400
AI	0.6968	0.3330
AJ	0.0548	0.1150
AK	0.7830	0.4140
AL	0.8420	0.4380
AM	0.7885	0.4290
AN	0.7230	0.4140
AO	0.7123	0.3420
AP	0.6909	0.2700
AQ	0.6644	0.3290
AR	0.9034	0.3810
Aa	0.7228	0.4570
Ab	0.7975	0.4760
Ac	0.8153	0.4450
Ad	0.7901	0.4370
Ae	0.6476	0.3570
Af	0.3756	0.3710
Ag	0.7506	0.4030
Ah	0.0083	-0.0030
Ai	0.1069	0.1780
Aj	0.8209	0.4370
Ak	0.6508	0.4550
Al	0.7710	0.4360
Am	0.5369	0.4340

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Chain	Atom inclusion	Q-score
An	0.8234	0.4470
Ao	0.8350	0.4090
Ap	0.7597	0.4430
Aq	0.8175	0.4250
Ar	0.8074	0.4250
As	0.7925	0.4550
At	0.7482	0.4530
Au	0.7814	0.3890
Av	0.6893	0.3670
Aw	0.8373	0.4560
Ax	0.7877	0.4540
Ay	0.7522	0.3860
Az	0.7421	0.3300
BA	0.2150	0.2410
BB	0.5102	0.4510
BC	0.6497	0.3240
BD	0.6816	0.3430
BE	0.5398	0.3120
BF	0.6715	0.3470
BG	0.3521	0.2080
BH	0.0538	0.2250
BI	0.4173	0.2170
BJ	0.0160	0.1570
BK	0.0234	0.0260
BL	0.5844	0.2630
BM	0.6557	0.3030
BN	0.7942	0.3430
BO	0.7867	0.3040
BP	0.7626	0.2640
Ba	0.5294	0.3400
Bb	0.6206	0.3850
Bc	0.6583	0.3540
Bd	0.6631	0.4100
Be	0.6496	0.3760
Bf	0.4272	0.3190
Bg	0.6425	0.4110
Bh	0.6490	0.3370
Bi	0.6695	0.3420
Bj	0.6294	0.3770
Bk	0.5828	0.3110
Bl	0.5263	0.3330
Bm	0.7073	0.4040

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Chain	Atom inclusion	Q-score
Bn	0.7274	0.3950
Bo	0.7430	0.4110
Bp	0.7435	0.4300
Bq	0.6125	0.3900
Br	0.3838	0.0570
Bs	0.5446	0.3960
Bt	0.7586	0.4240
Bu	0.4106	0.3400
Bv	0.6364	0.3060
Bw	0.5525	0.3120
Bx	0.5355	0.3790
By	0.6645	0.3250
Bz	0.5722	0.3380