



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 12:48 am BST

PDB ID : 4V7T
Title : Crystal structure of the E. coli ribosome bound to chloramphenicol.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-14
Resolution : 3.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

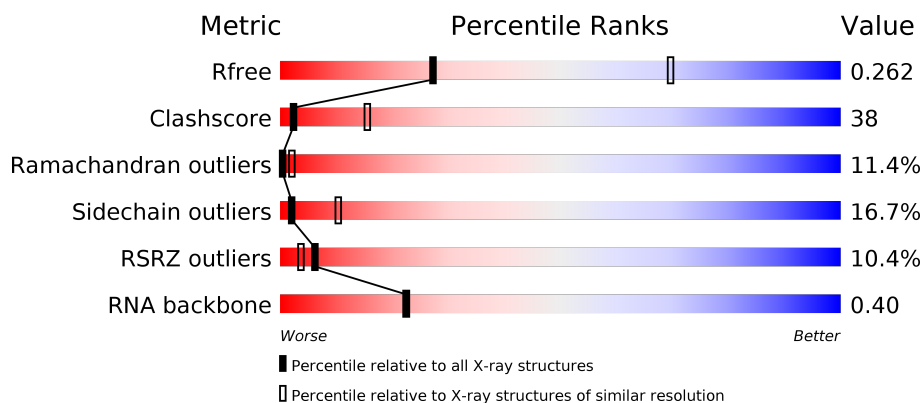
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	AA	1533	<div> <div>24%</div> <div>44%</div> <div>16%</div> <div>17%</div> </div>
2	AB	218	<div> <div>32%</div> <div>25%</div> <div>54%</div> <div>18%</div> </div>
2	CB	218	<div> <div>19%</div> <div>30%</div> <div>54%</div> <div>14%</div> </div>
3	AC	206	<div> <div>6%</div> <div>36%</div> <div>52%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
14	AN	100	
14	CN	100	
15	AO	88	
15	CO	88	
16	AP	82	
17	AQ	80	

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Mol	Chain	Length	Quality of chain
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
23	BB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	

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Mol	Chain	Length	Quality of chain
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	

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Mol	Chain	Length	Quality of chain
44	BW	79	
44	DW	79	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	
53	CA	1530	
54	CG	150	
55	CM	113	
56	CP	80	
57	DA	2904	
58	DB	117	
59	DF	178	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	3007	-	-	-	X
60	MG	DA	3019	-	-	-	X
60	MG	DA	3025	-	-	-	X
60	MG	DA	3061	-	-	-	X
60	MG	DA	3062	-	-	-	X
60	MG	DA	3063	-	-	-	X
60	MG	DA	3073	-	-	-	X
60	MG	DA	3075	-	-	-	X
60	MG	DA	3077	-	-	-	X
60	MG	DA	3107	-	-	-	X
60	MG	DA	3124	-	-	-	X
60	MG	DA	3127	-	-	-	X
60	MG	DA	3130	-	-	-	X
60	MG	DJ	201	-	-	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 284499 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
4	CD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	CH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	CI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	CK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
12	CL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	CN	95	Total	C	N	O	S	0	0	0
			769	480	159	127	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	S	0	0	0
			456	288	86	82				
18	CR	55	Total	C	N	O	S	0	0	0
			456	288	86	82				

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	CS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
20	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
25	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
26	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
28	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
30	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
31	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
33	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
34	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BO	116	Total	C	N	O	0	0	0
			892	552	178	162			
36	DO	116	Total	C	N	O	0	0	0
			892	552	178	162			

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
37	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BQ	117	Total	C	N	O	0	0	0
			947	604	192	151			
38	DQ	117	Total	C	N	O	0	0	0
			947	604	192	151			

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
40	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	102	Total	C	N	O		0	0	0
			780	492	146	142				
42	DU	102	Total	C	N	O		0	0	0
			780	492	146	142				

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
43	DV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
44	DW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
45	DX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
46	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
47	DZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
48	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

- Molecule 50 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
50	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
51	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
52	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 53 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 54 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	CG	150	Total	C	N	O	S	0	0	0
			1175	730	226	215	4			

- Molecule 55 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	CM	113	Total	C	N	O	S	0	0	0
			877	541	177	156	3			

- Molecule 56 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	CP	80	Total	C	N	O	S	0	0	0
			639	400	126	112	1			

- Molecule 57 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 58 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 59 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

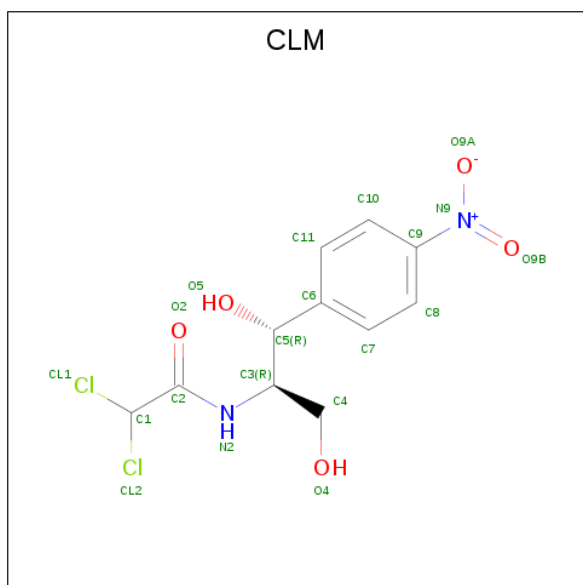
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BB	4	Total	Mg	0	0
			4	4		
60	DE	1	Total	Mg	0	0
			1	1		
60	BA	135	Total	Mg	0	0
			135	135		
60	CA	42	Total	Mg	0	0
			42	42		
60	DJ	1	Total	Mg	0	0
			1	1		
60	BL	1	Total	Mg	0	0
			1	1		
60	DA	133	Total	Mg	0	0
			133	133		
60	AA	42	Total	Mg	0	0
			42	42		
60	AN	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DC	1	Total	Mg	0	0
			1	1		
60	DB	1	Total	Mg	0	0
			1	1		

- Molecule 61 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	BA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	B4	1	Total	Zn	0	0
			1	1		
62	D4	1	Total	Zn	0	0
			1	1		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AA	197	Total	O	0	0
			197	197		
63	AL	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AN	6	Total 6	O 6	0	0
63	AT	2	Total 2	O 2	0	0
63	AU	1	Total 1	O 1	0	0
63	BA	608	Total 608	O 608	0	0
63	BB	19	Total 19	O 19	0	0
63	BC	8	Total 8	O 8	0	0
63	BD	2	Total 2	O 2	0	0
63	BE	1	Total 1	O 1	0	0
63	BL	4	Total 4	O 4	0	0
63	BN	2	Total 2	O 2	0	0
63	BQ	1	Total 1	O 1	0	0
63	BT	2	Total 2	O 2	0	0
63	BV	1	Total 1	O 1	0	0
63	B2	2	Total 2	O 2	0	0
63	B3	2	Total 2	O 2	0	0
63	B4	2	Total 2	O 2	0	0
63	CA	195	Total 195	O 195	0	0
63	CE	3	Total 3	O 3	0	0
63	CI	1	Total 1	O 1	0	0
63	CL	1	Total 1	O 1	0	0
63	CN	3	Total 3	O 3	0	0

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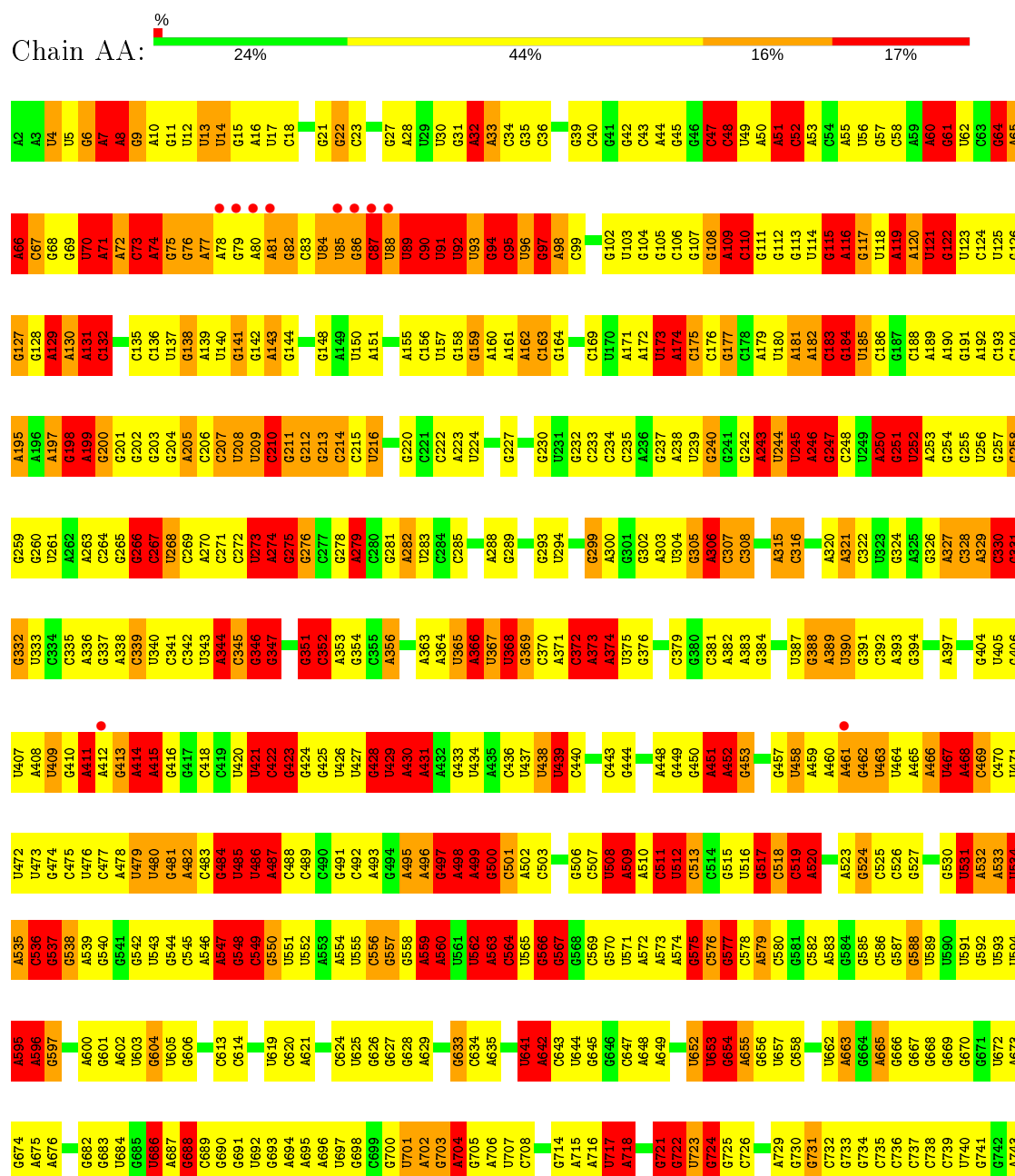
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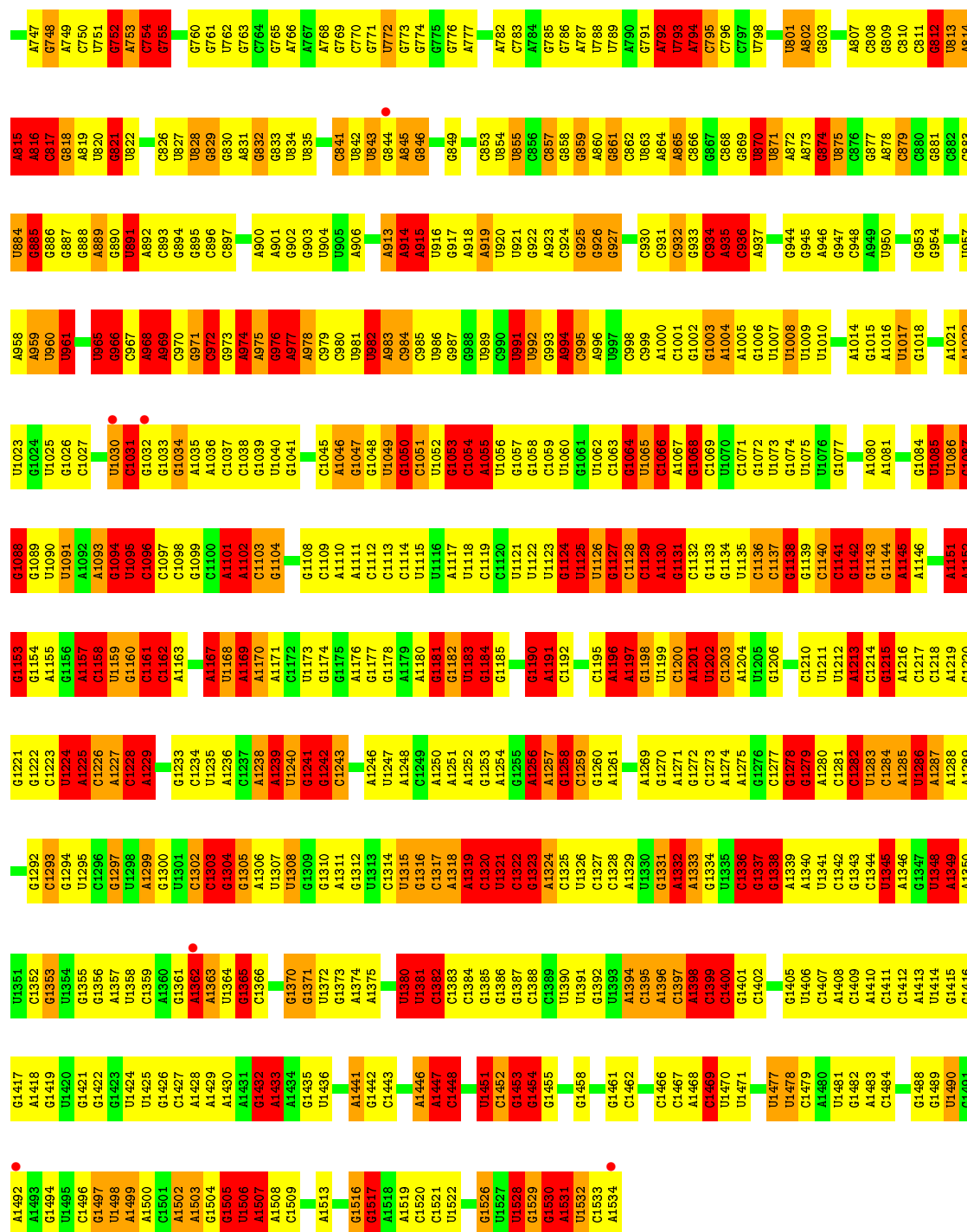
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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63	CU	2	Total O 2 2	0	0
63	DA	603	Total O 603 603	0	0
63	DB	4	Total O 4 4	0	0
63	DC	10	Total O 10 10	0	0
63	DD	1	Total O 1 1	0	0
63	DE	3	Total O 3 3	0	0
63	DJ	4	Total O 4 4	0	0
63	DL	5	Total O 5 5	0	0
63	DN	2	Total O 2 2	0	0
63	DT	2	Total O 2 2	0	0
63	DU	2	Total O 2 2	0	0
63	DV	1	Total O 1 1	0	0
63	D2	1	Total O 1 1	0	0
63	D3	1	Total O 1 1	0	0
63	D4	4	Total O 4 4	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

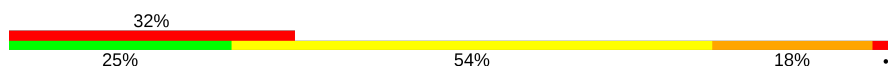
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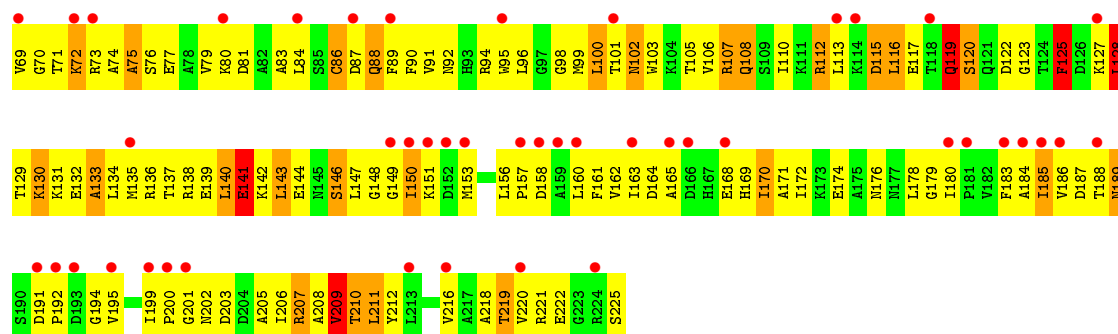




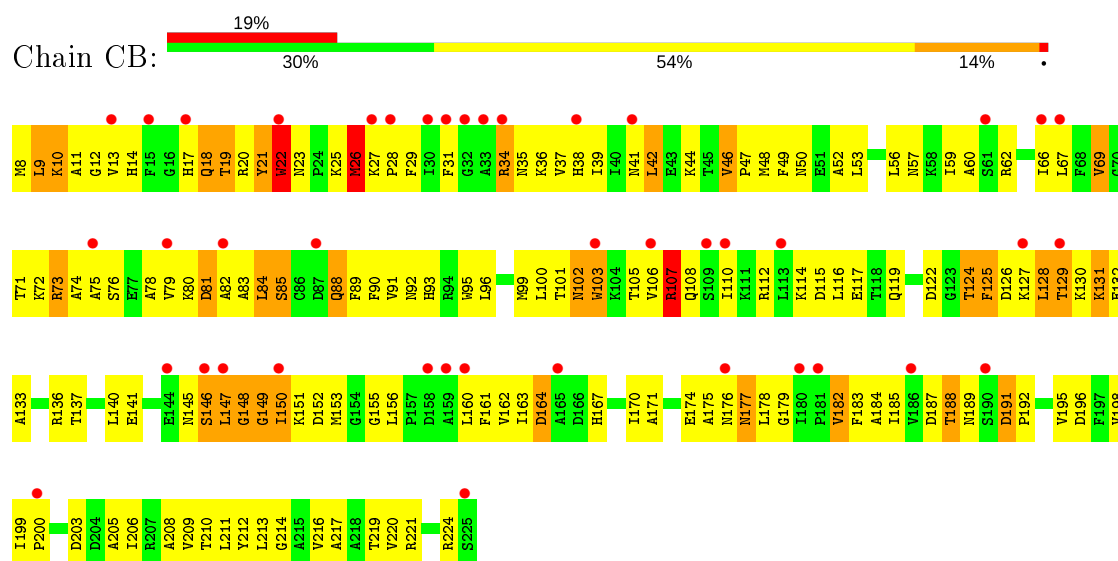
• Molecule 2: 30S ribosomal protein S2

Chain AB:

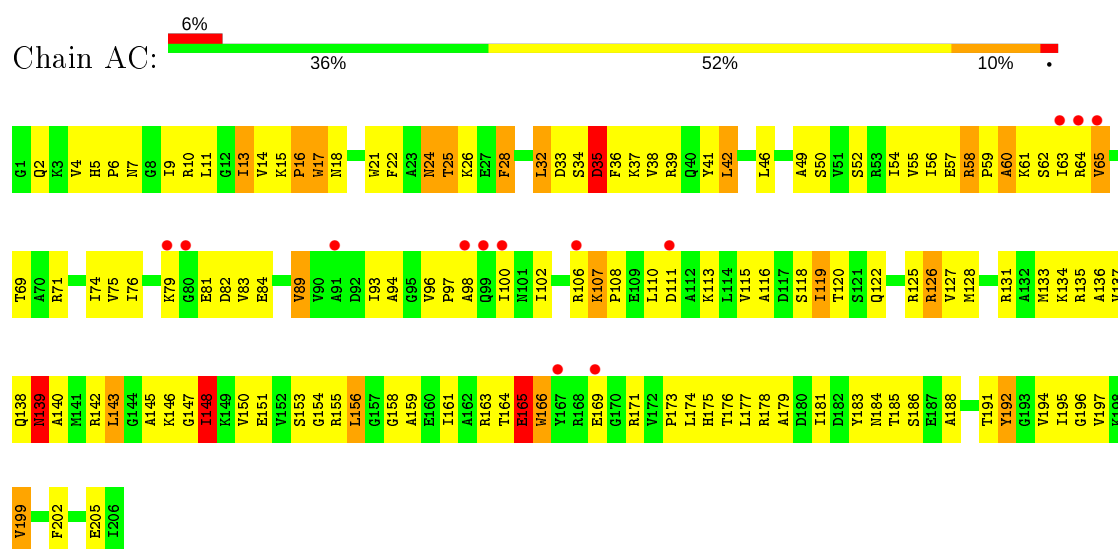




• Molecule 2: 30S ribosomal protein S2

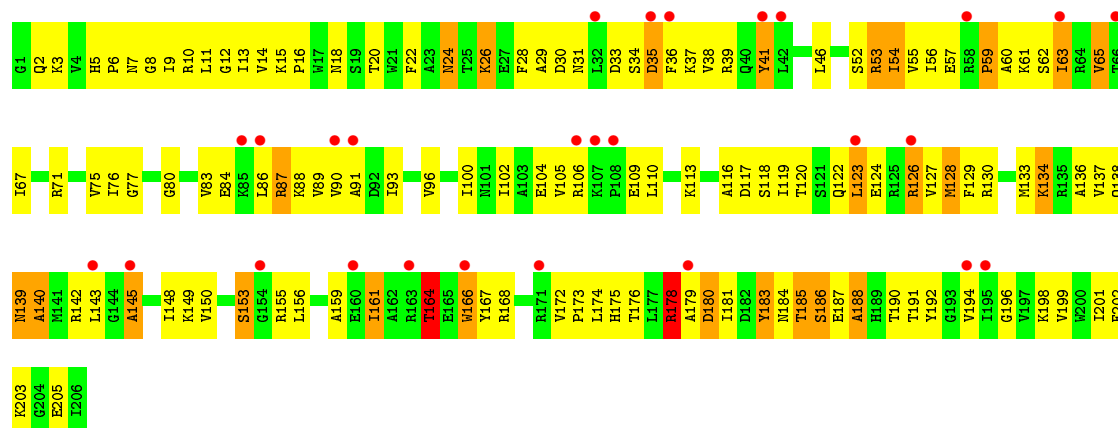


• Molecule 3: 30S ribosomal protein S3

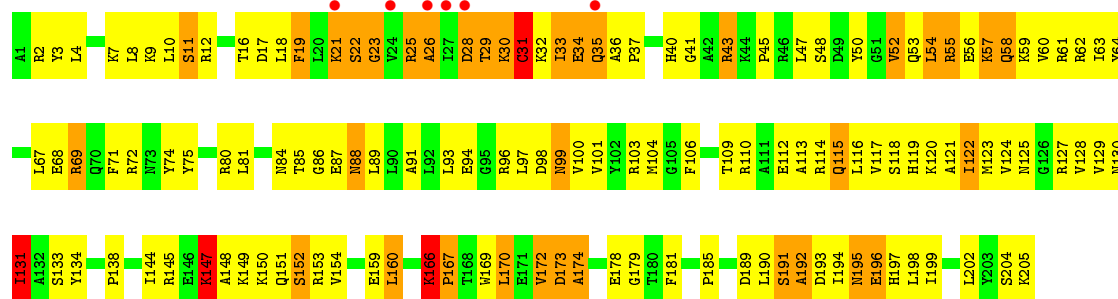


• Molecule 3: 30S ribosomal protein S3

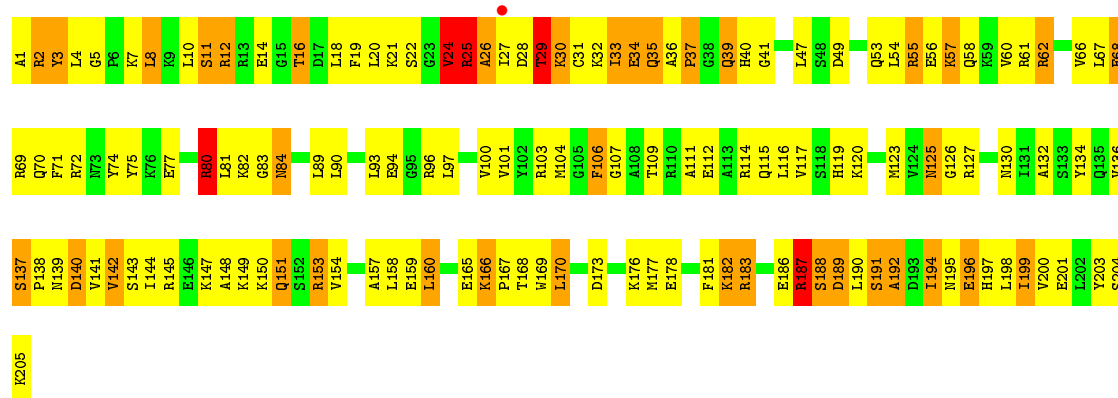
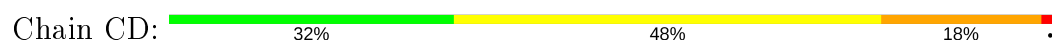




• Molecule 4: 30S ribosomal protein S4

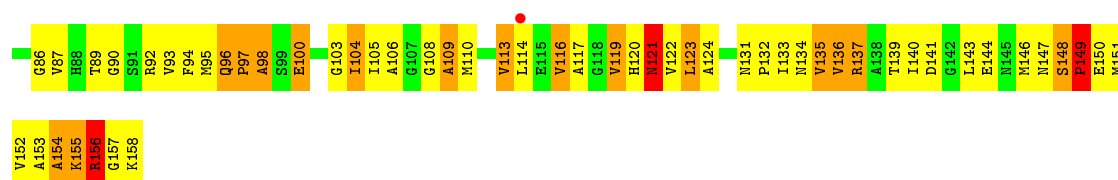


• Molecule 4: 30S ribosomal protein S4

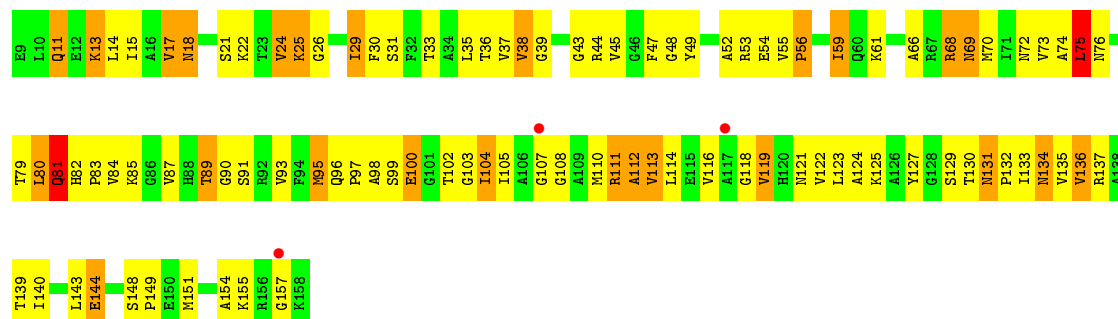


• Molecule 5: 30S ribosomal protein S5

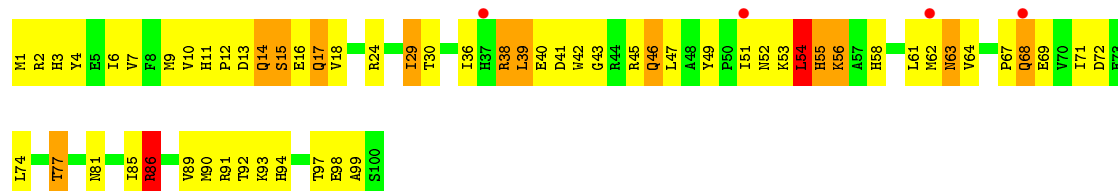




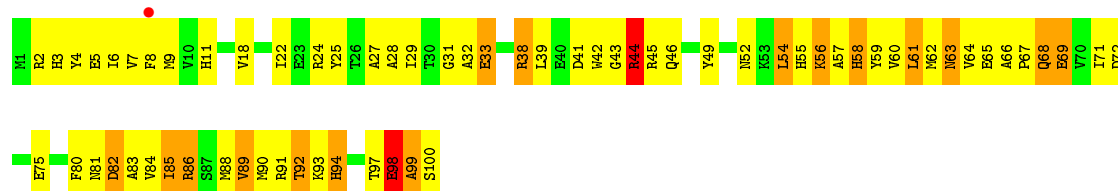
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

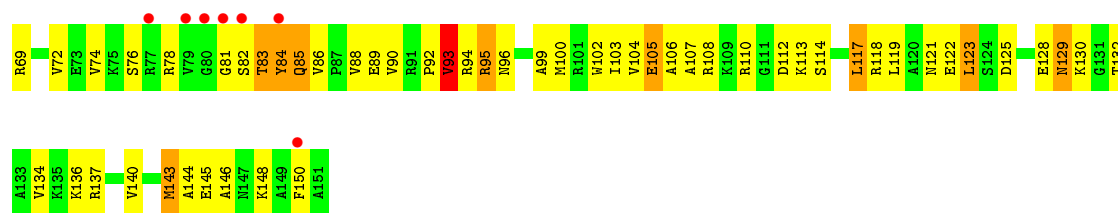


• Molecule 6: 30S ribosomal protein S6

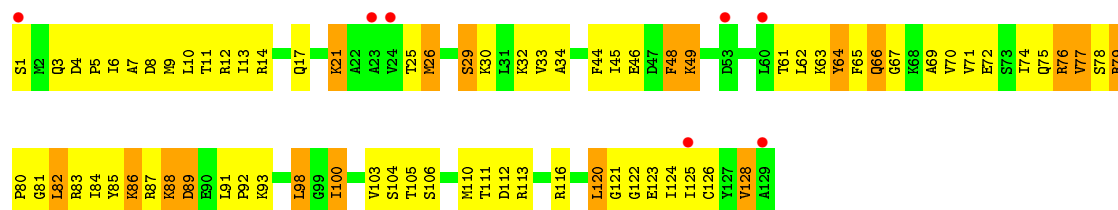
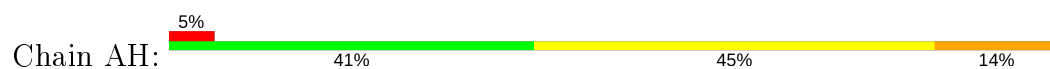


• Molecule 7: 30S ribosomal protein S7

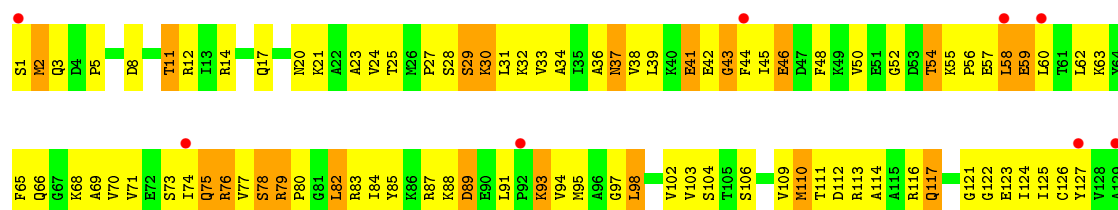




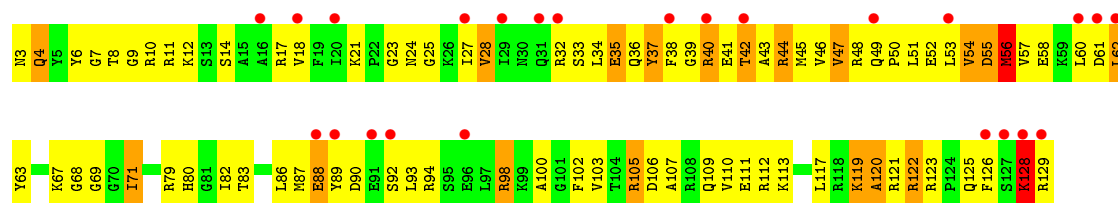
• Molecule 8: 30S ribosomal protein S8



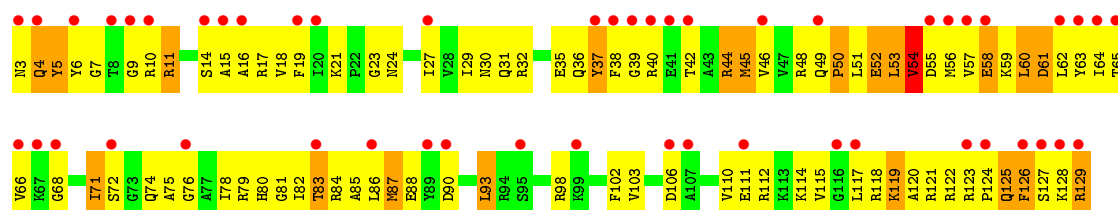
• Molecule 8: 30S ribosomal protein S8



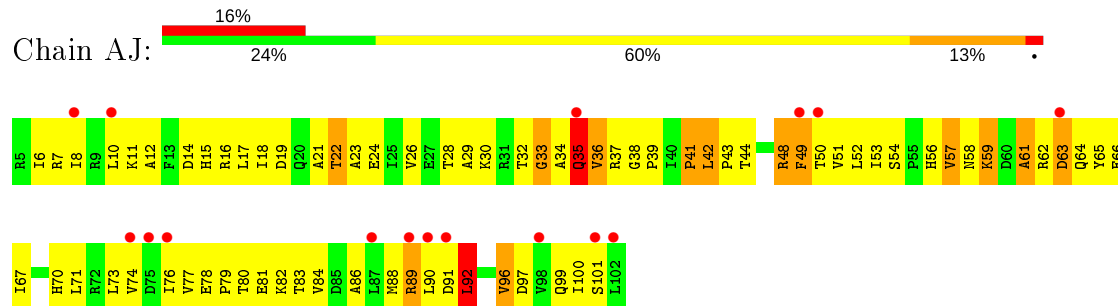
• Molecule 9: 30S ribosomal protein S9



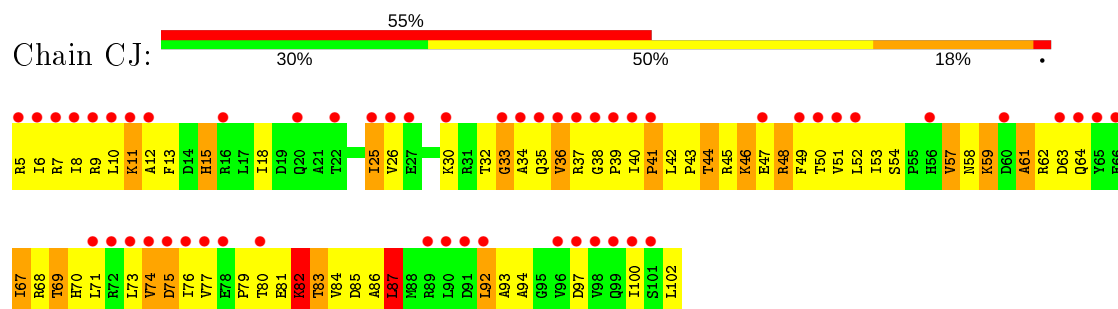
• Molecule 9: 30S ribosomal protein S9



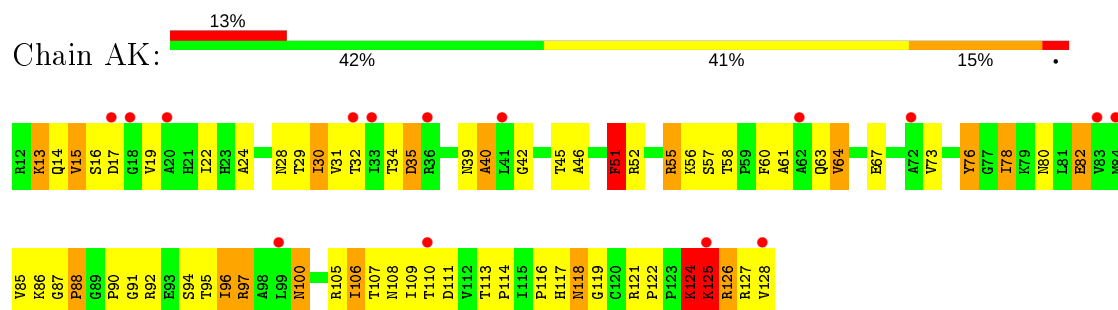
- Molecule 10: 30S ribosomal protein S10



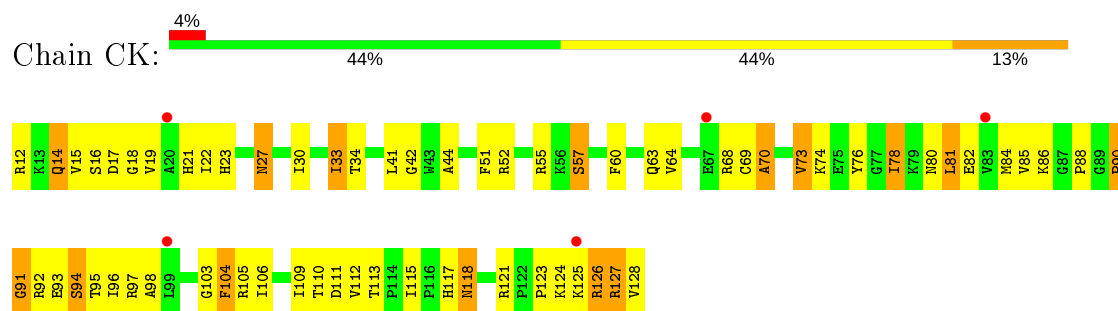
- Molecule 10: 30S ribosomal protein S10



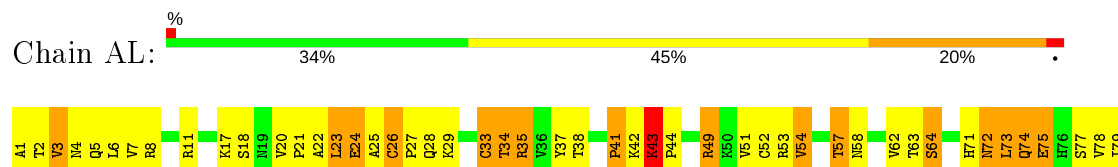
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

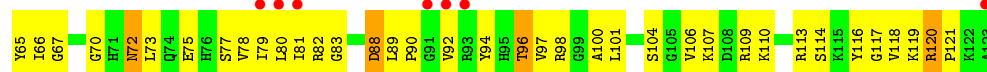


- Molecule 12: 30S ribosomal protein S12

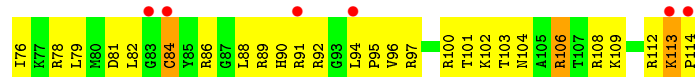
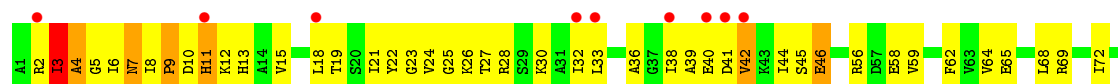




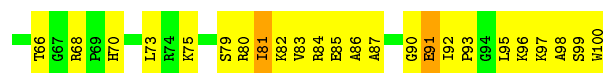
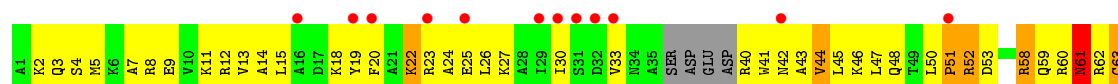
• Molecule 12: 30S ribosomal protein S12



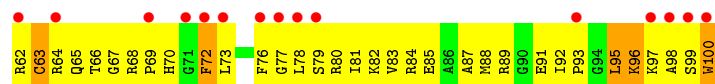
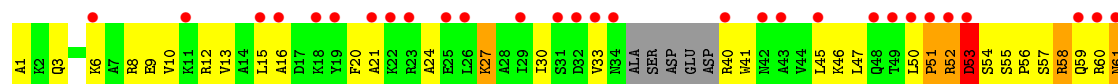
• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14

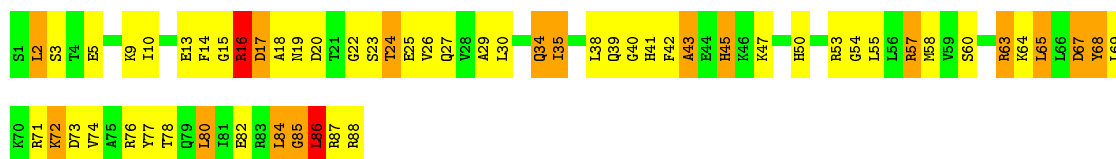


• Molecule 14: 30S ribosomal protein S14



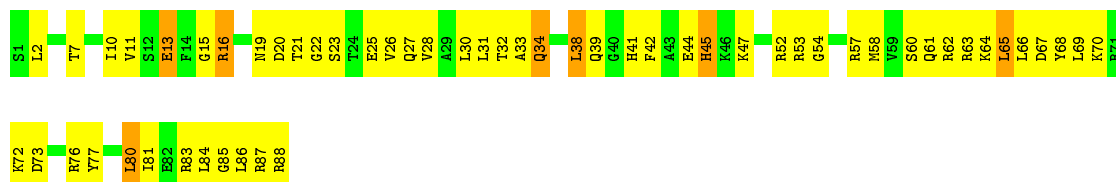
• Molecule 15: 30S ribosomal protein S15





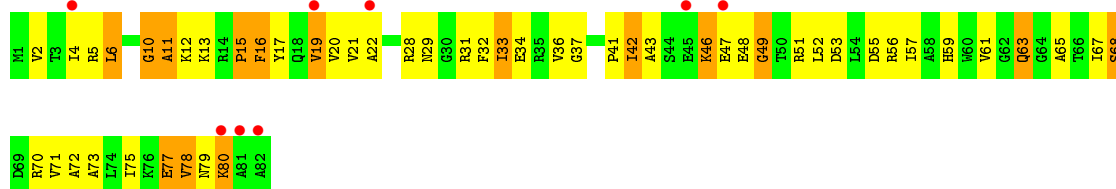
- Molecule 15: 30S ribosomal protein S15

Chain CO: 36% 56% 8%



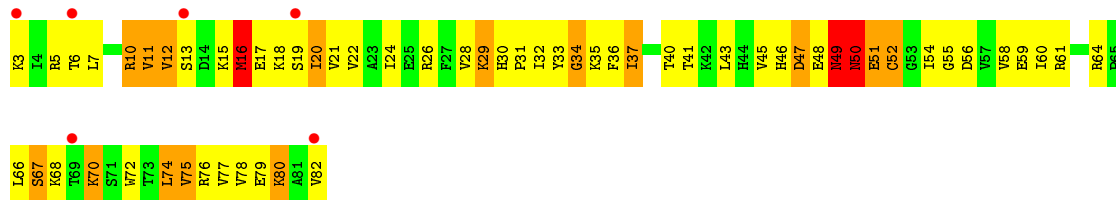
- Molecule 16: 30S ribosomal protein S16

Chain AP: 10% 38% 44% 18%



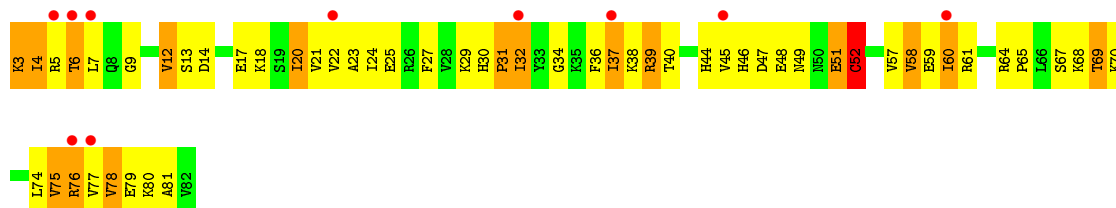
- Molecule 17: 30S ribosomal protein S17

Chain AQ: 8% 25% 53% 19%

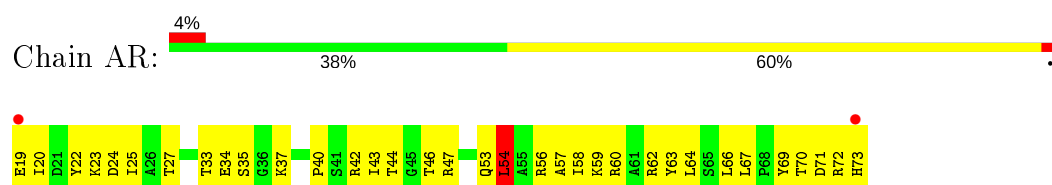


- Molecule 18: 30S ribosomal protein S18

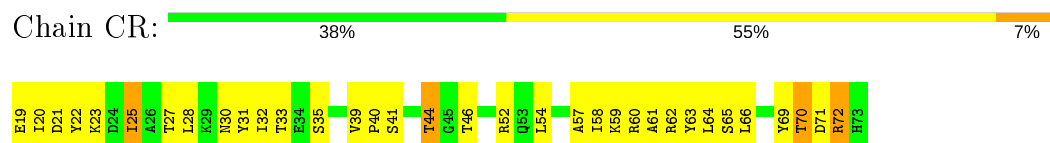
Chain CQ: 13% 31% 48% 20%



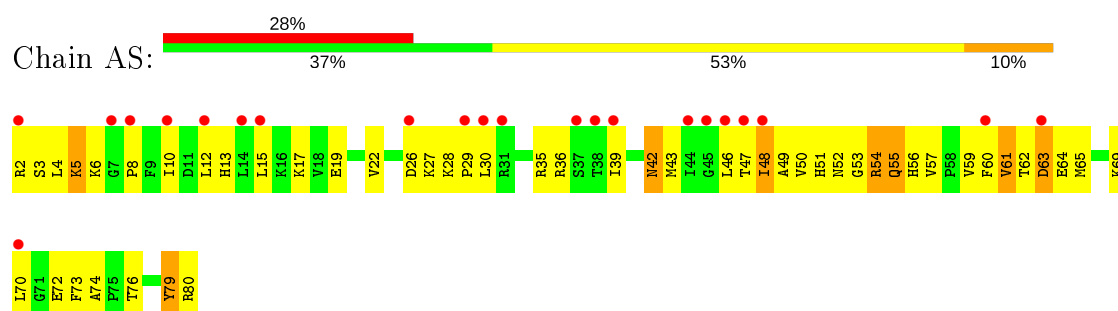
- Molecule 19: 30S ribosomal protein S19



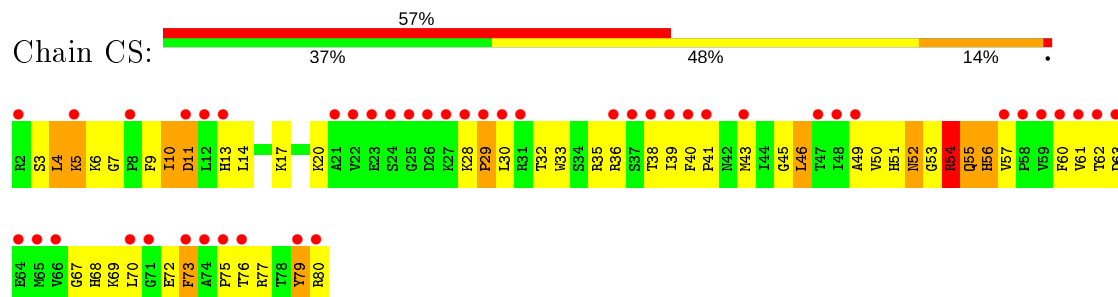
• Molecule 18: 30S ribosomal protein S18



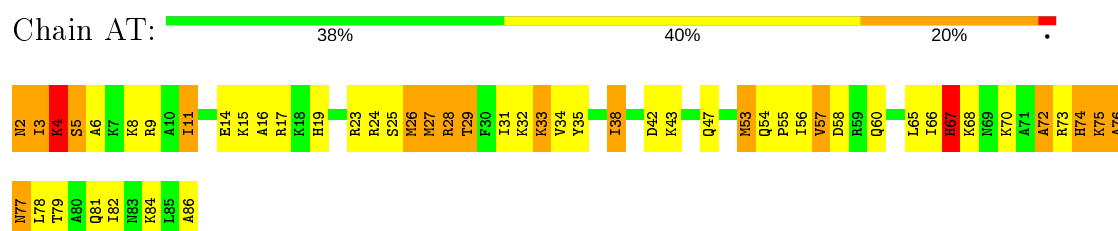
• Molecule 19: 30S ribosomal protein S19



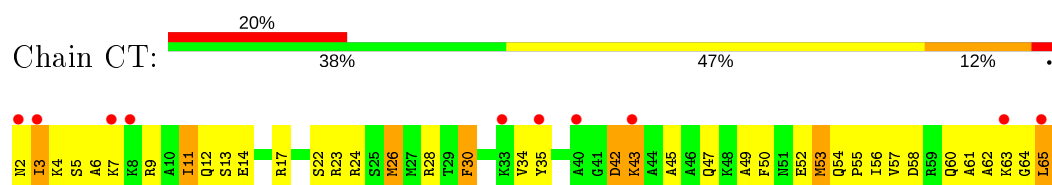
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20

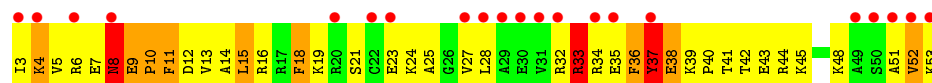


• Molecule 20: 30S ribosomal protein S20

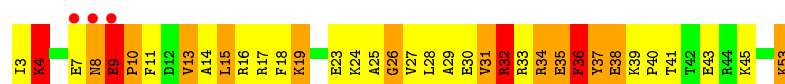




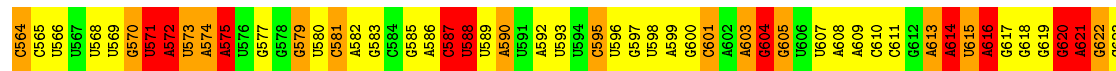
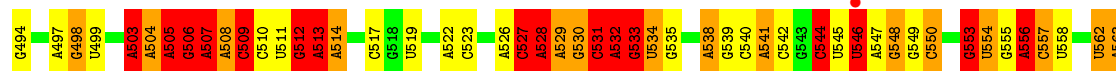
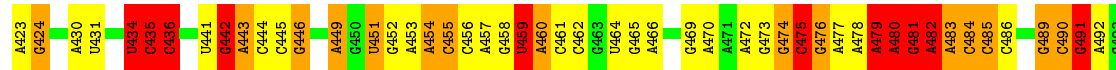
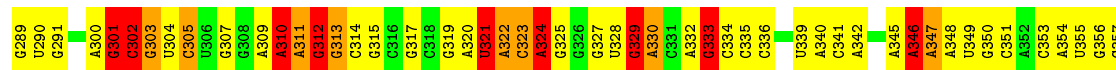
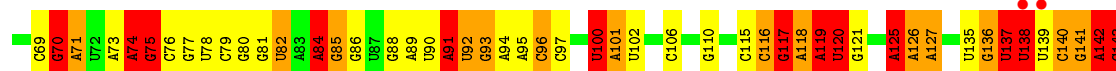
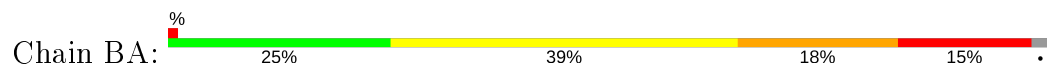
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

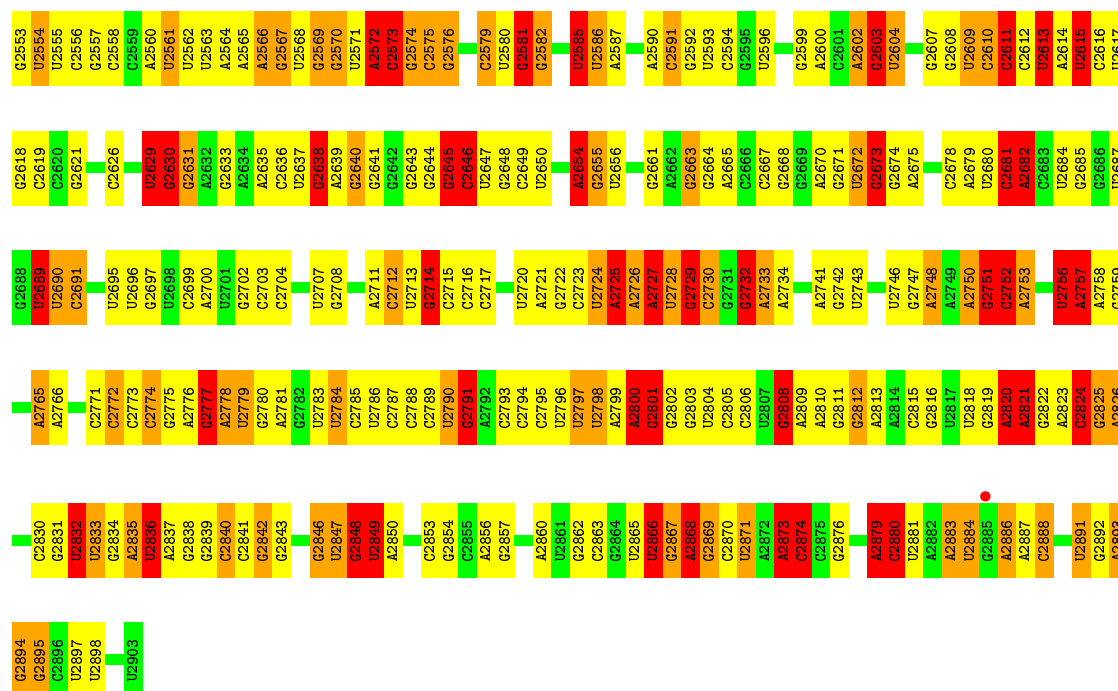


- Molecule 22: 23S rRNA



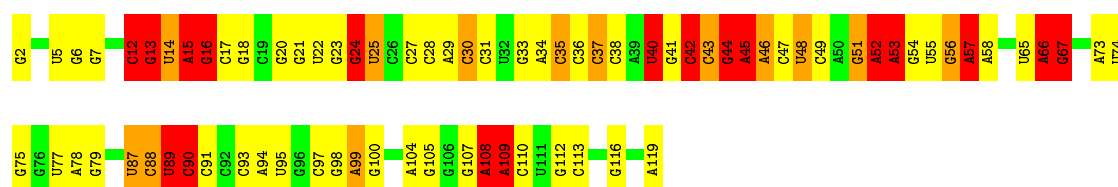


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U2489	C2424	U2356	U2291	G2223	G2157	U2092	U2027	G1958	U1886	U1817	G1749	A1616
G2490	G2357	G2223	U2292	G2223	A	U2092	U2028	G1959	U1887	U1818	G1750	C1617
U2491	A2358	A2358	U2293	G2224	G	G2093	G2029	U1960	A1889	U1819	A1754	A1618
U2492	C2427	C2359	G2294	A2225	C	A2094	A2030	C1961	U1890	U1820	A1755	G1619
U2493	G2428	G2360	C2295	G2226	C	G2094	A2031	U1962	U1891	A1821	G1756	G1622
G2494	G2429	G2361	U2296	A2227	G	G2102	G2032	U1963	U1892	C1822	A1757	G1623
G2495	A2430	G2362	G2297	G2228	A	C2103	A2033	U1964	A1899	G1823	U1758	G1624
C2496	U2431	G2363	U2298	G2229	C	C2104	U2034	C1965	A1900	U1824	A1689	U1625
C2498	A2434	G2364	U2299	G2230	C	U2105	G2035	A1966	A1901	U1825	C1760	C1626
C2499	A2435	G2365	U2300	G2231	U	U2106	C2036	U1967	C1902	G1826	C1761	A1627
U2500	G2436	G2366	U2301	C2232	U	G2107	A2037	U1968	G1905	U1827	A1762	G1628
C2501	U2437	G2367	U2302	U2233	G	A2108	G2038	A1969	G1906	G1828	G1763	G1629
A2503	G2438	G2368	G2303	G2234	A	U2109	U2039	A1970	G1907	A1829	U1764	U1630
A2504	U2439	G2369	U2304	G2235	U	U2110	G2040	U1971	A1908	G1830	U1765	G1631
G2505	C2440	G2370	U2305	G2236	A	U	A2042	G1972	C1908	G1832	G1766	G1632
U2506	U2441	G2371	U2306	G2237	U	G	C2043	U1976	G1909	C1833	U1769	A1634
C2507	G2442	G2372	U2307	G2238	A	U	C2044	U1977	G1910	U1834	G1770	A1635
G2508	G2443	G2373	U2308	U2243	A	U	G2045	G1978	U1911	G1835	G1771	U1636
A2512	U2444	G2374	U2309	U2244	C	A	C2046	G1979	G1912	C1836	C1772	U1637
A2513	G2445	G2375	U2310	U2245	C	G	G2047	G1980	A1913	U1837	C1773	C1638
U2514	G2446	G2376	U2311	U2246	A	G	C2048	U1981	A1914	C1838	C1774	G1639
C2515	G2447	G2377	U2312	U2247	C	A	G2049	U1982	U1915	G1839	U1775	A1640
C2516	U2448	G2378	U2313	U2248	U	U	C2050	G1983	A1916	G1840	G1776	A1641
C2517	A2449	G2379	U2314	U2249	G	A	C2051	U1984	U1917	U1841	U1777	U1712
A2518	G2450	G2380	U2315	U2250	U	G	A2052	C1985	A1918	G1842	U1778	G1642
U2519	U2451	G2381	U2316	G2251	C	U	G2053	U1986	C1920	C1844	U1779	A1713
C2520	G2452	G2382	U2317	G2252	U	G	A2054	G1989	G1921	U1847	U1780	G1643
U2521	U2453	G2383	U2318	G2253	U	G	C2055	U1990	U1922	A1848	U1781	C1644
G2524	G2454	G2384	U2319	U2254	C	U	G2056	U1991	G1923	U1849	U1782	G1645
G2525	U2455	G2385	U2320	U2255	U	A	C2057	U1992	U1924	U1850	A1783	U1646
G2526	U2456	G2386	U2321	U2256	U	G	A2058	U1993	C1925	G1851	U1784	U1647
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G2529	A2459	G2389	U2324	U2259	U	U	G2061	A1998	A1928	U1854	A1787	A1651
A2530	U2460	G2390	U2325	U2260	U	U	C2062	C1999	G1929	A1855	A1788	A1652
A2531	G2461	G2391	U2326	U2261	G	G2133	C2063	C2000	U1930	U1856	A1789	G1653
G2532	C2462	G2392	U2327	U2262	A	A2134	C2064	C2001	U1931	G1857	C1790	A1654
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C2538	C2464	G2394	U2329	U2264	U	U	C2066	A2005	G1933	G1859	G1727	G1656
C2539	U2465	G2395	U2330	U2265	U	G2136	C2067	C2006	C1934	U1859	C1728	U1657
G2540	G2466	G2396	U2331	U2266	U	A2137	U2068	U2007	G1935	U1860	U1729	C1658
A2541	U2467	G2397	U2332	U2267	C	U2138	G2069	C2008	A1936	G1861	U1736	G1659
A2542	G2468	G2398	U2333	U2268	U	U2139	A2070	C2009	A1937	U1862	G1731	G1660
G2543	U2469	G2399	U2334	U2269	U	G2140	A2071	U2011	A1938	G1863	C1732	A1664
A2544	A2470	G2400	U2335	U2270	U	A2141	C2072	G2012	G1941	U1864	G1733	A1665
A2545	G2471	G2401	U2336	U2271	U	C2142	U2075	A2013	C1942	U1865	G1734	G1666
C2546	U2472	G2402	U2337	U2272	U	G2143	U2076	A2014	U1943	A1866	A1735	G1667
A2547	G2473	G2403	U2338	U2273	U	C2144	A2077	A2015	U1944	G1867	A1801	A1668
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G2553	U2479	G2409	U2344	U2279	U	C2150	C2082	C2021	A1953	G1873	G1811	G1674
A2554	A2480	G2410	U2345	U2280	U	U2151	G2083	U2022	U1954	C1874	U1812	A1675
A2555	G2481	G2411	U2346	U2281	U	C2152	U2084	G2023	A1955	A1875	G1813	A1676
G2556	U2482	G2412	U2347	U2282	U	U2153	G2085	U2024	U1956	A1876	U1746	A1677
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G2558	U2484	G2414	U2349	U2284	U	C2155	U2087	G2026				
C2559	G2485	G2415	U2350	U2285	U	U2156	U2088	G2027				
U2560	A2486	G2416	U2351	U2286	U	C2157	U2089	G2028				
A2561	G2487	G2417	U2352	U2287	U	U2158	U2090	G2029				
G2562	U2488	G2418	U2353	U2288	U	C2159	U2091	G2030				
A2563	G2489	G2419	U2354	U2289	U	U2160	U2092	G2031				
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U2566	A2492	G2422	U2357	U2292	U	C2163	U2095	G2034				
A2567	G2493	G2423	U2358	U2293	U	U2164	U2096	G2035				
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A2576	A2502	U2432	U2367	U2302	U	U2173	U2105	G2044				
U2577	U2503	G2433	U2368	U2303	U	C2174	U2106	G2045				
G2578	A2504	G2434	U2369	U2304	U	U2175	U2107	G2046				
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A2589	A2514	G2445	U2380	U2315	U	U2186	U2118	G2057				
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A2591	A2516	G2447	U2382	U2317	U	C2188	U2120	G2059				
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C2594	U2519	G2450	U2385	U2320	U	C2191	U2123	G2062				
A2595	A2520	U2451	U2386	U2321	U	U2192	U2124	G2063				
U2596	C2521	G2452	U2387	U2322	U	U2193	U2125	G2064				
G2597	U2522	U2453	U2388	U2323	U	C2194	U2126	G2065				
A2598	A2523	G2454	U2389	U2324	U	U2195	U2127	G2066				
C2599	U2524	U2455	U2390	U2325	U	U2196	U2128	G2067				
U2600	G2525	G2456	U2391	U2326	U	C2197	U2129	G2068				
A2601	A2526	U2457	U2392	U2327	U	U2198	U2130	G2069				
C2602	U2527	G2458	U2393	U2328	U	U2199	U2131	G2070				
U2603	A2528	U2459	U2394	U2329	U	C2200	U2132	G2071				
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G2605	U											



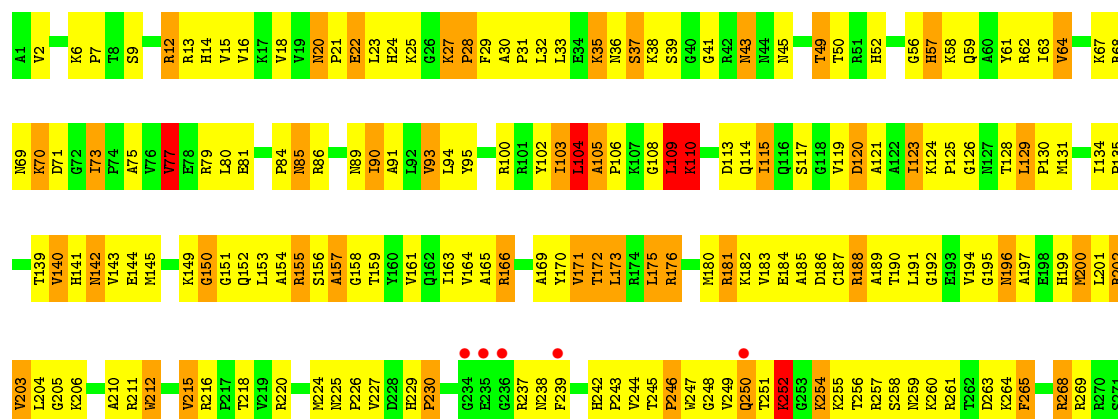
• Molecule 23: 5S rRNA

Chain BB: 35% 39% 11% 15%

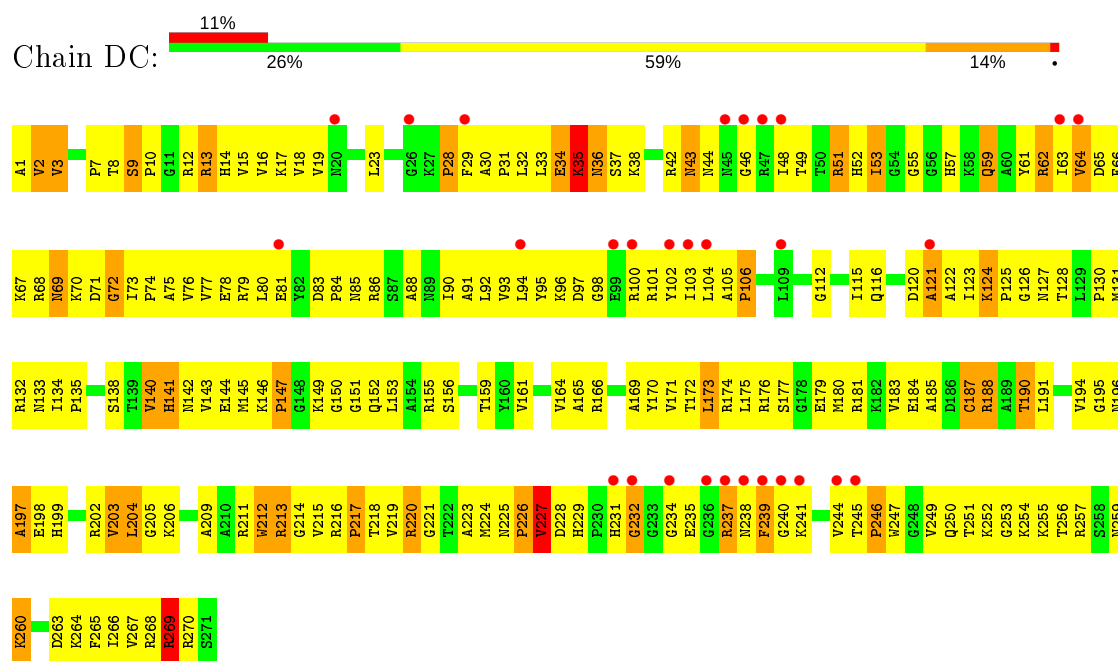


• Molecule 24: 50S ribosomal protein L2

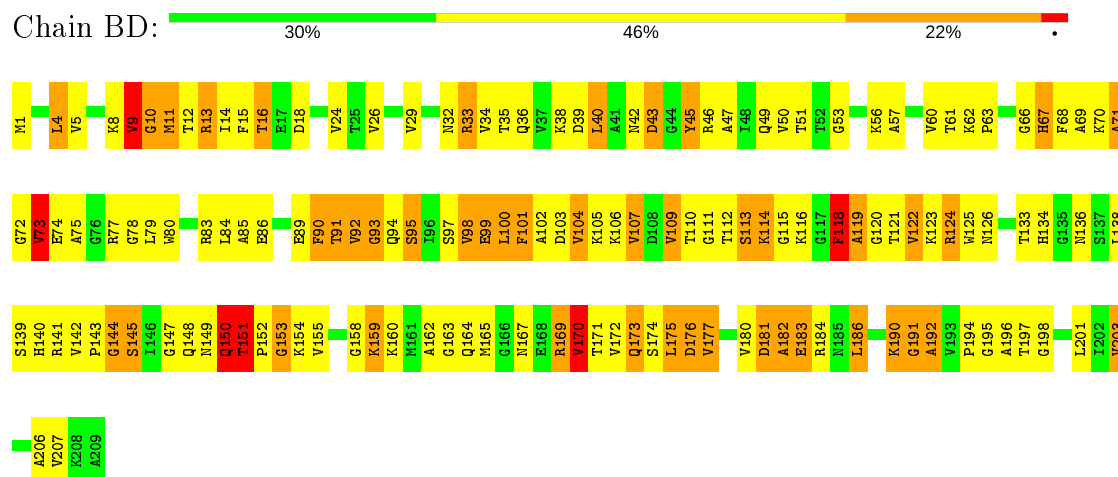
Chain BC: 2% 32% 48% 17%



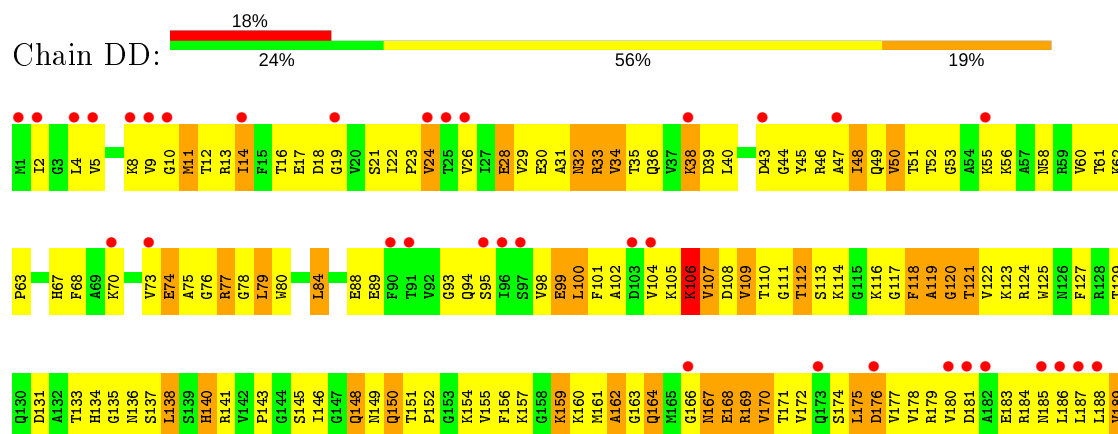
• Molecule 24: 50S ribosomal protein L2

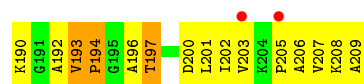


- Molecule 25: 50S ribosomal protein L3

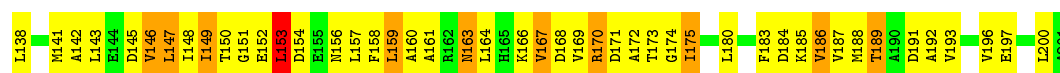


- Molecule 25: 50S ribosomal protein L3

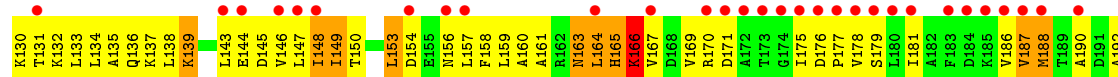
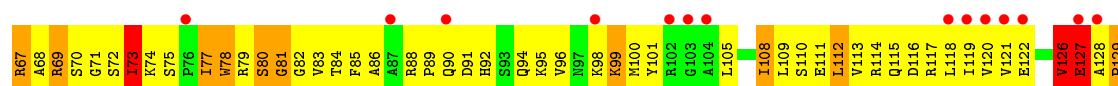
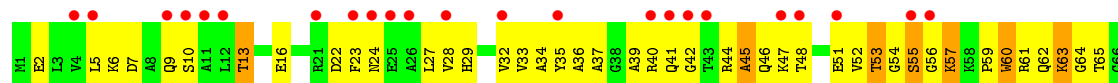




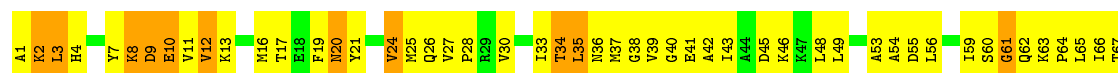
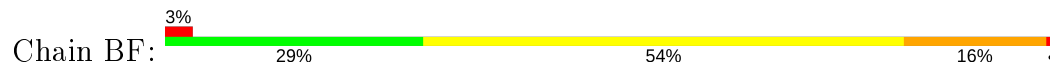
- Molecule 26: 50S ribosomal protein L4



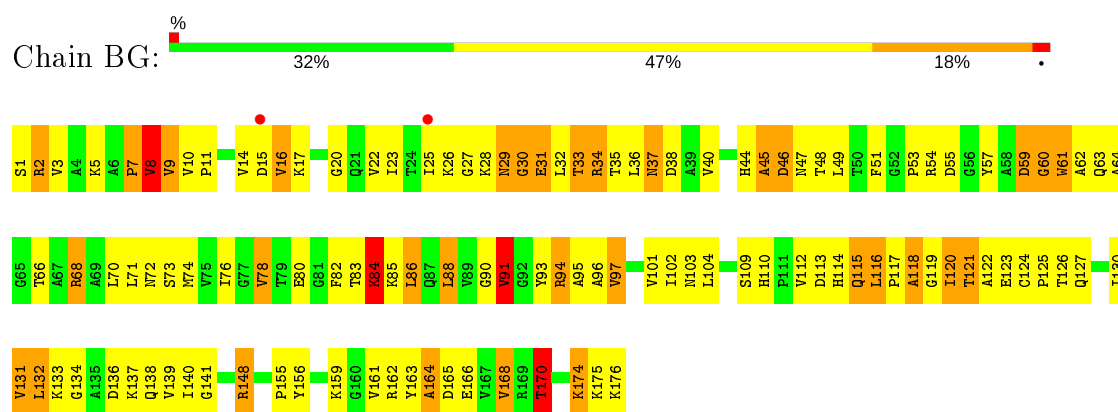
- Molecule 26: 50S ribosomal protein L4



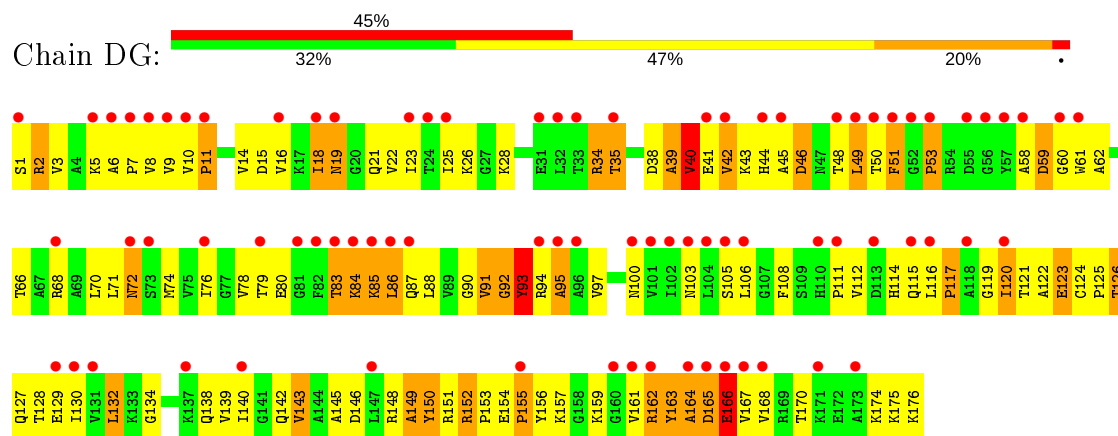
- Molecule 27: 50S ribosomal protein L5



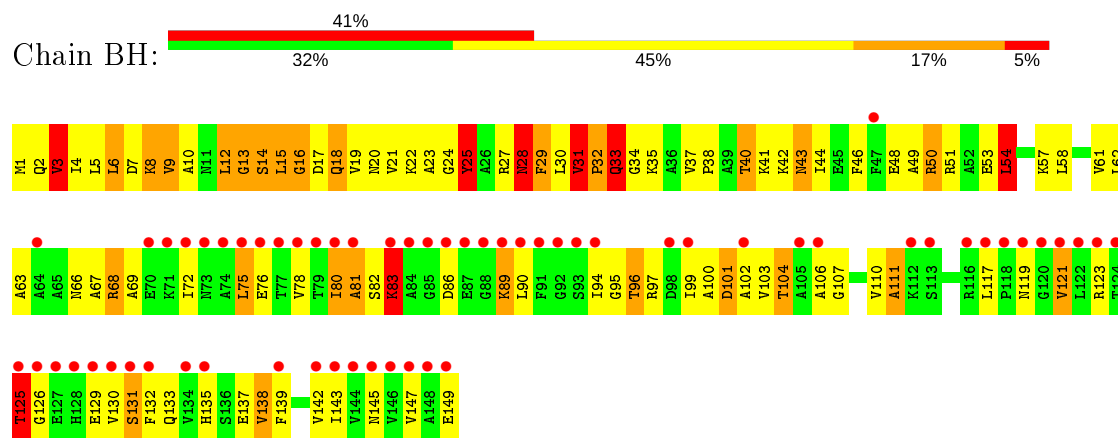
- Molecule 28: 50S ribosomal protein L6



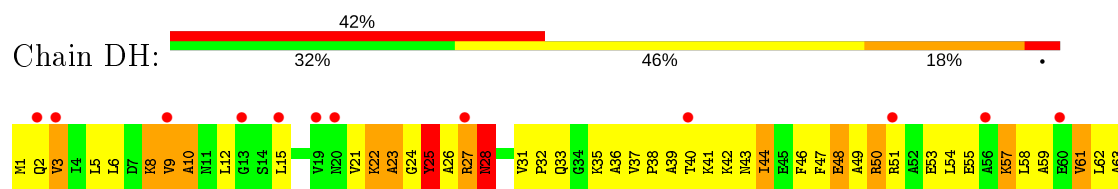
• Molecule 28: 50S ribosomal protein L6

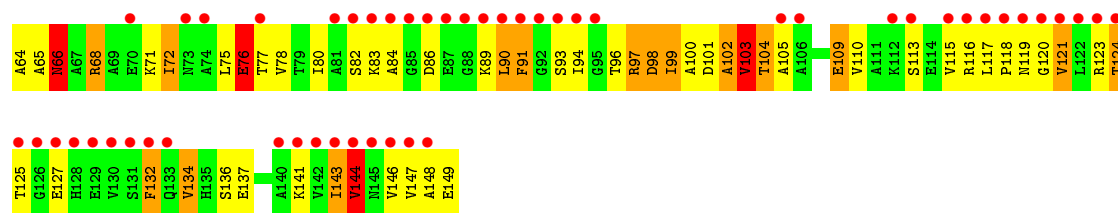


• Molecule 29: 50S ribosomal protein L9

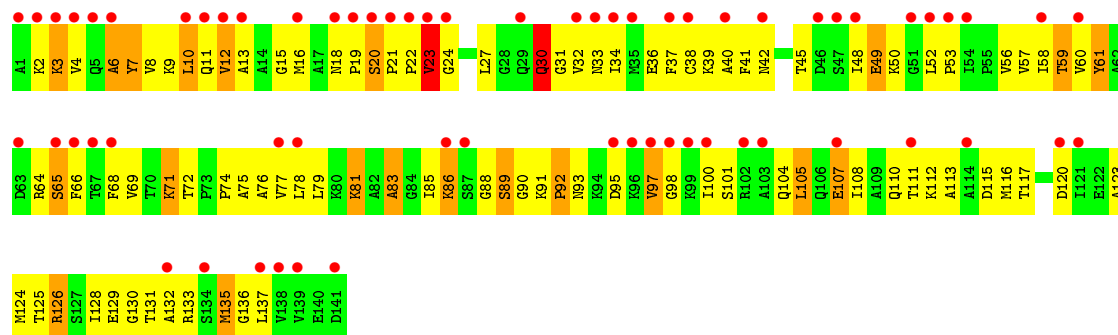


• Molecule 29: 50S ribosomal protein L9

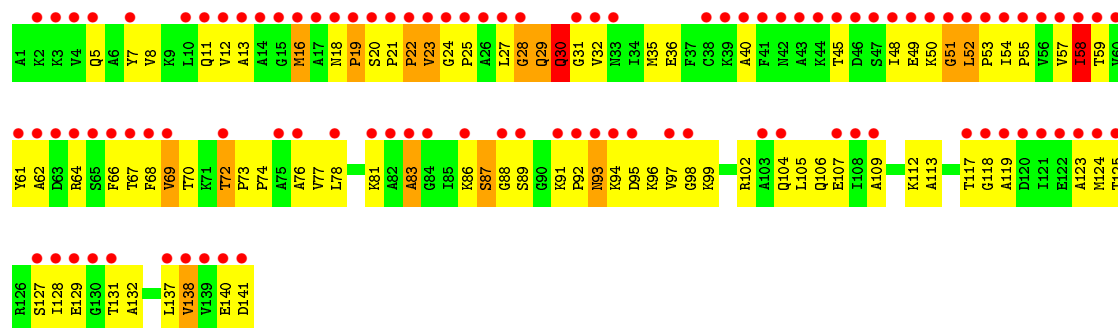
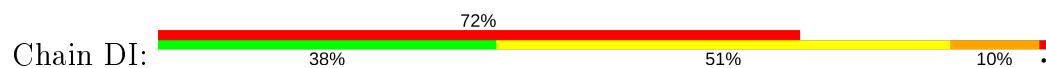




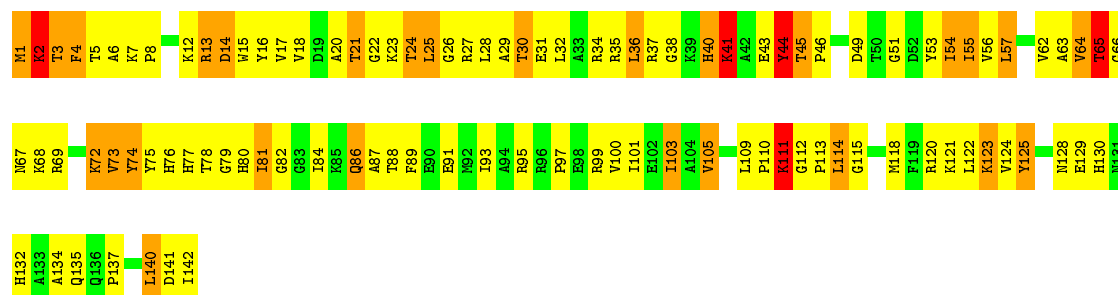
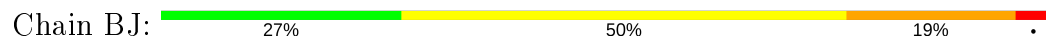
• Molecule 30: 50S ribosomal protein L11



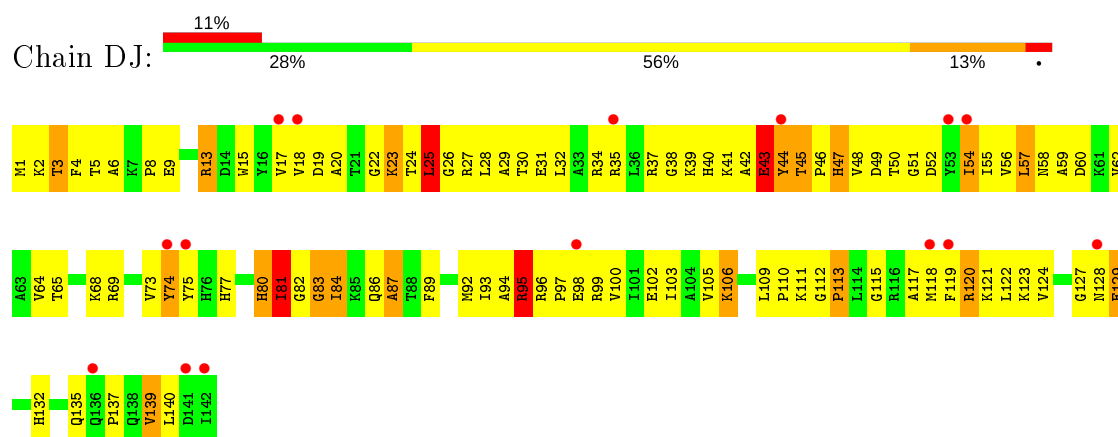
• Molecule 30: 50S ribosomal protein L11



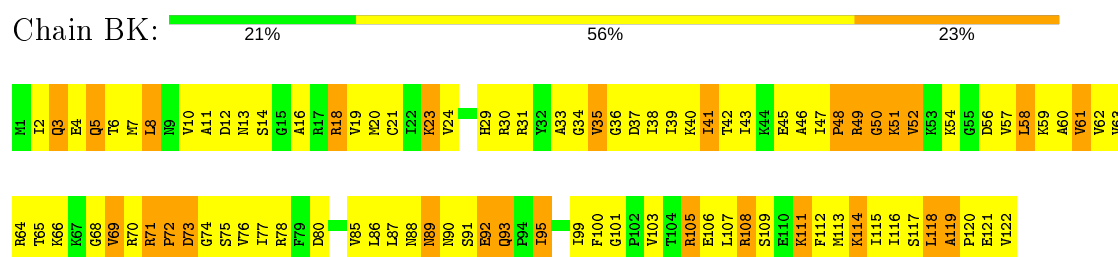
• Molecule 31: 50S ribosomal protein L13



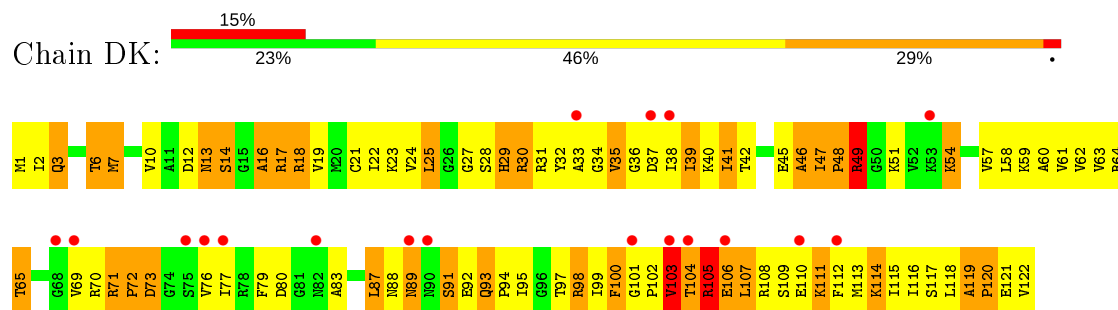
• Molecule 31: 50S ribosomal protein L13



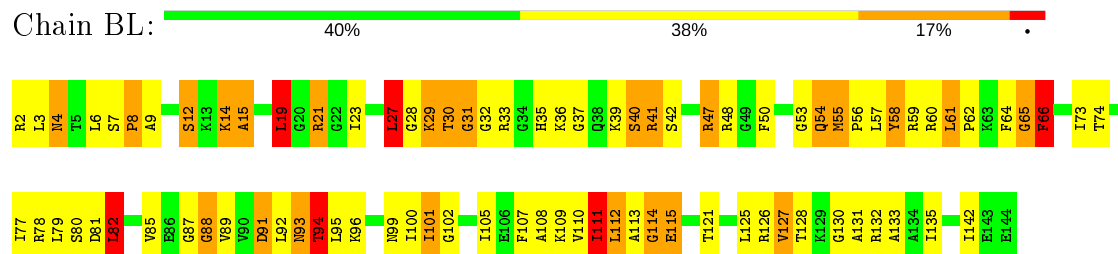
- Molecule 32: 50S ribosomal protein L14



- Molecule 32: 50S ribosomal protein L14

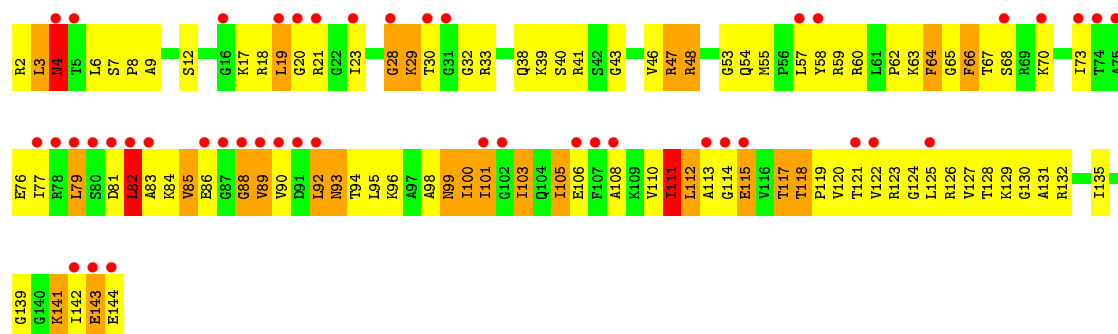


- Molecule 33: 50S ribosomal protein L15



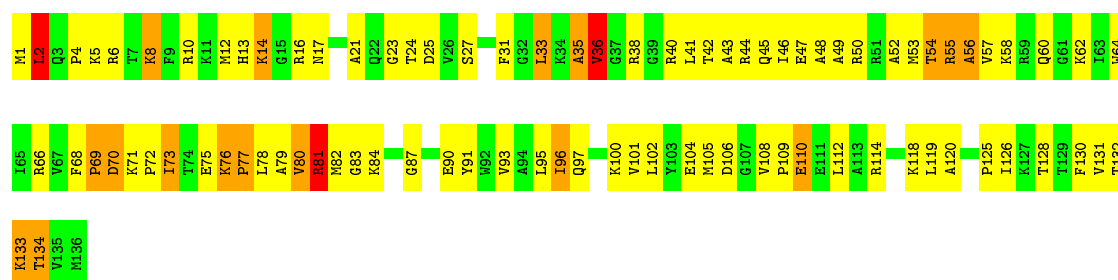
- Molecule 33: 50S ribosomal protein L15





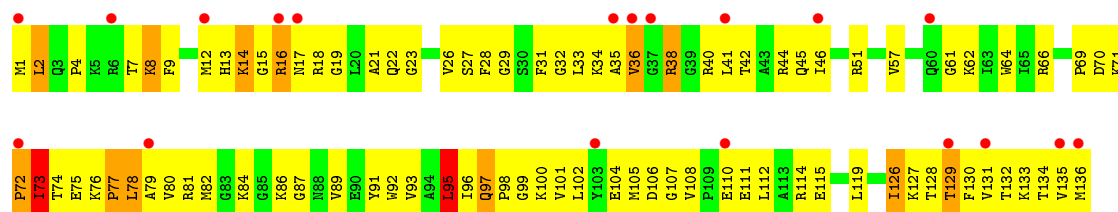
- Molecule 34: 50S ribosomal protein L16

Chain BM: 35% 51% 13%



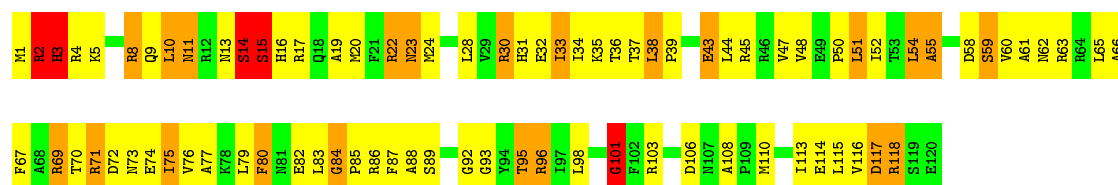
- Molecule 34: 50S ribosomal protein L16

Chain DM: 14% 33% 57% 9%



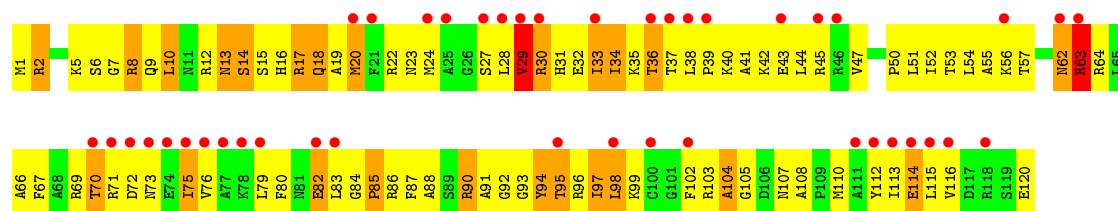
- Molecule 35: 50S ribosomal protein L17

Chain BN: 30% 48% 18%



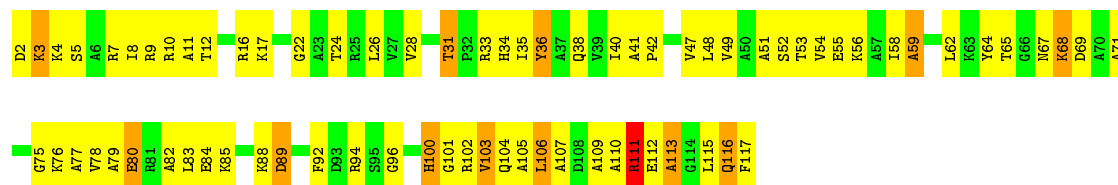
- Molecule 35: 50S ribosomal protein L17

Chain DN: 35% 23% 55% 20%



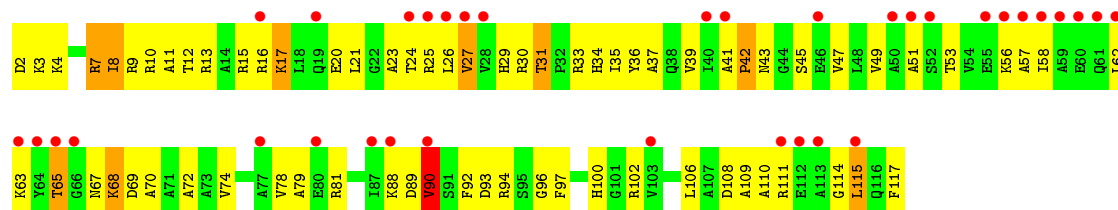
• Molecule 36: 50S ribosomal protein L18

Chain BO: 36% 53% 10% .



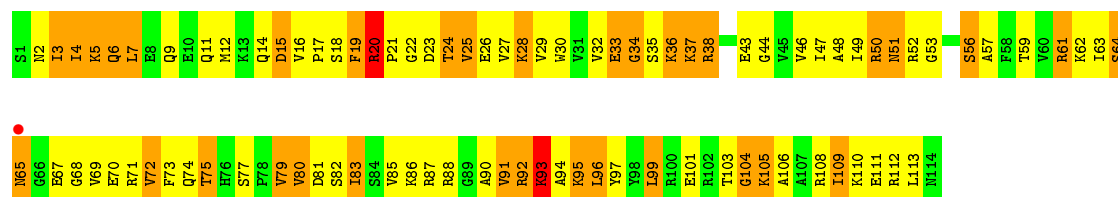
• Molecule 36: 50S ribosomal protein L18

Chain DO: 30% 40% 52% 8% .



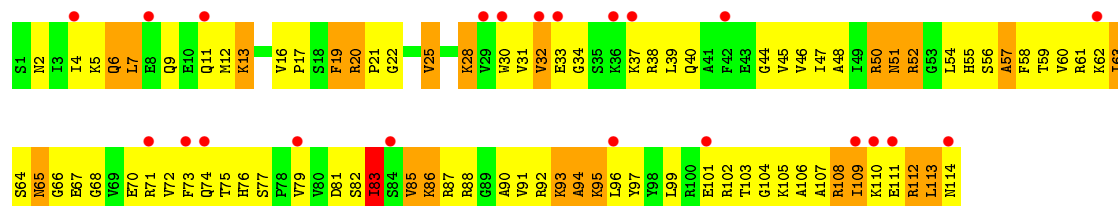
• Molecule 37: 50S ribosomal protein L19

Chain BP: % 21% 47% 30% .



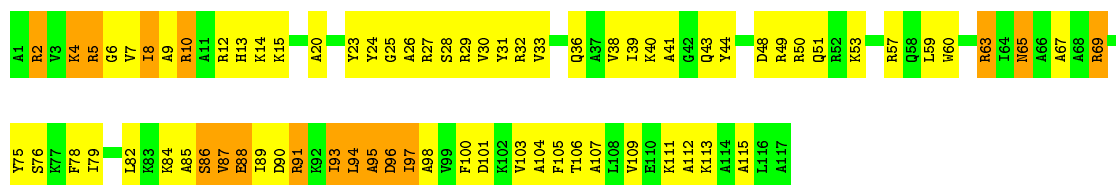
• Molecule 37: 50S ribosomal protein L19

Chain DP: 19% 23% 56% 20% .



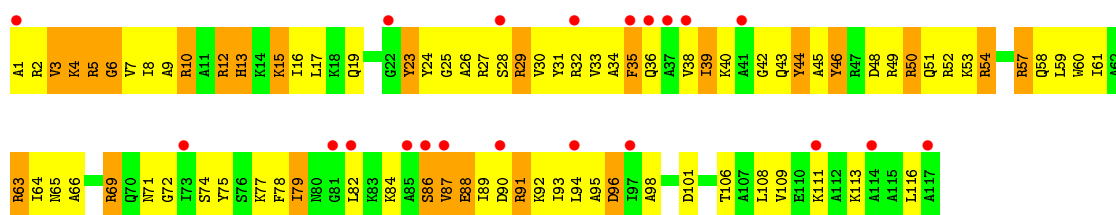
- Molecule 38: 50S ribosomal protein L20

Chain BQ: 



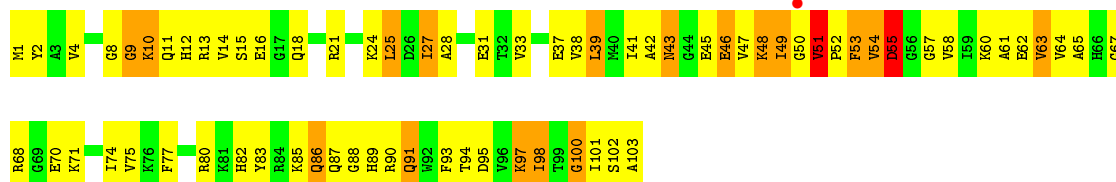
- Molecule 38: 50S ribosomal protein L20

Chain DQ: 



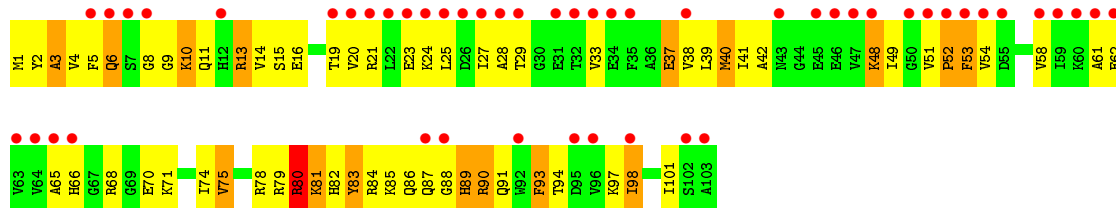
- Molecule 39: 50S ribosomal protein L21

Chain BR: 



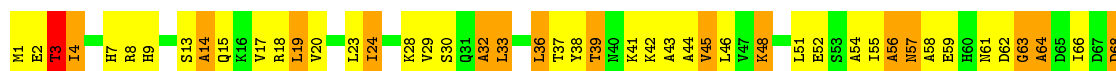
- Molecule 39: 50S ribosomal protein L21

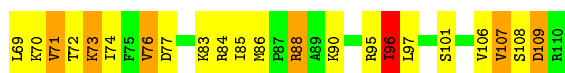
Chain DR: 



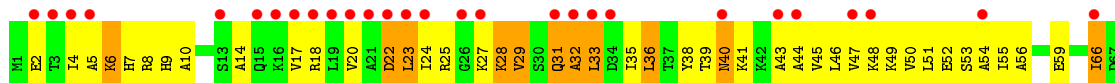
- Molecule 40: 50S ribosomal protein L22

Chain BS: 

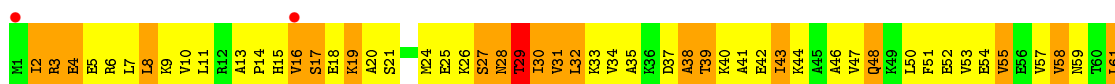
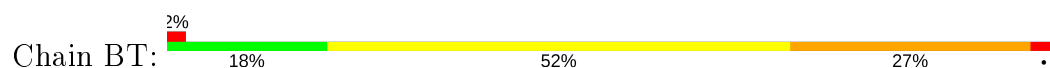




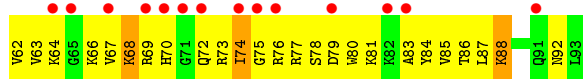
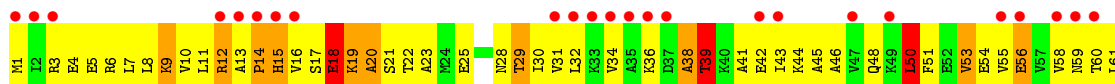
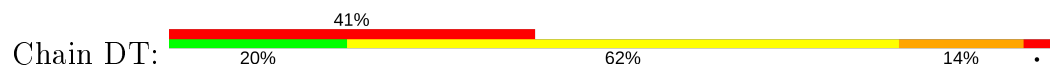
- Molecule 40: 50S ribosomal protein L22



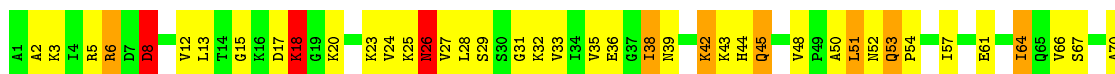
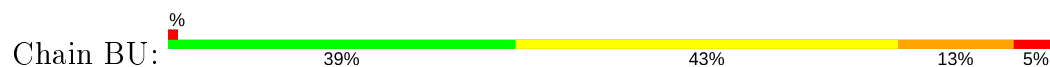
- Molecule 41: 50S ribosomal protein L23



- Molecule 41: 50S ribosomal protein L23

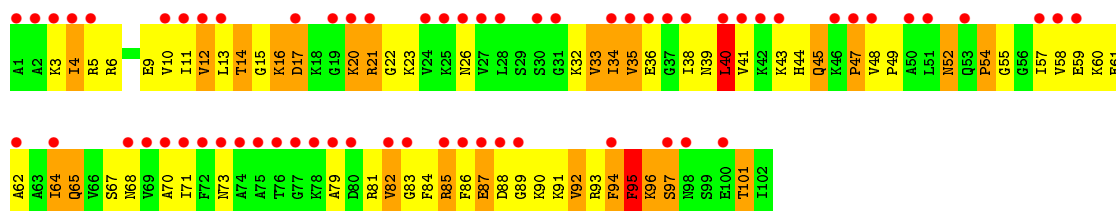


- Molecule 42: 50S ribosomal protein L24

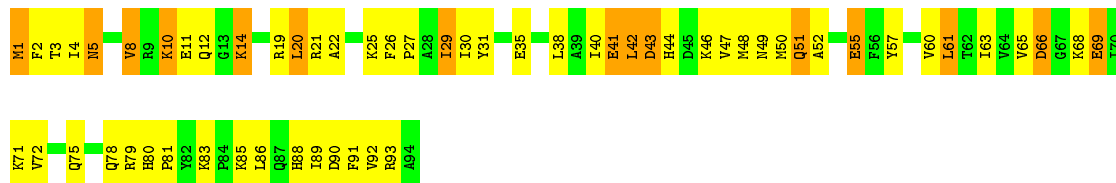


- Molecule 42: 50S ribosomal protein L24

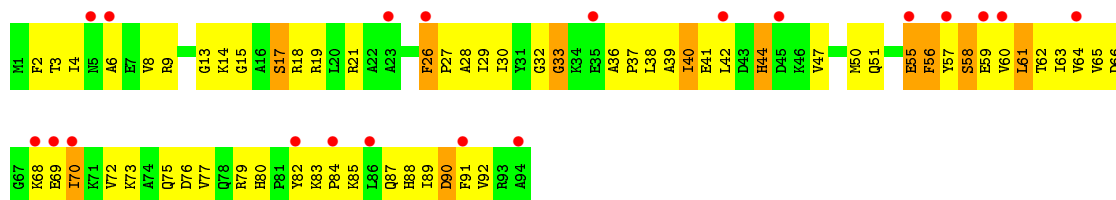




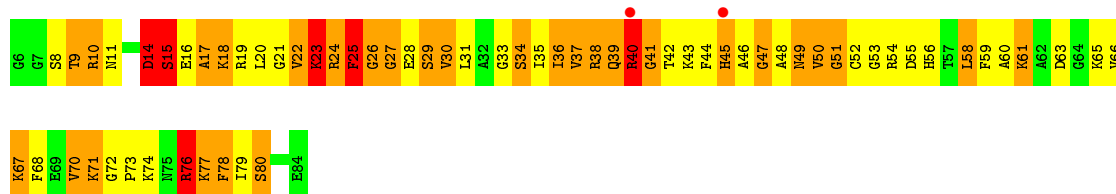
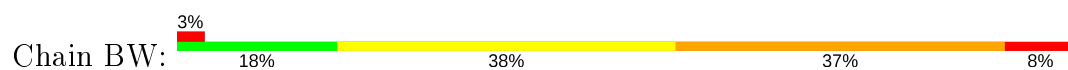
• Molecule 43: 50S ribosomal protein L25



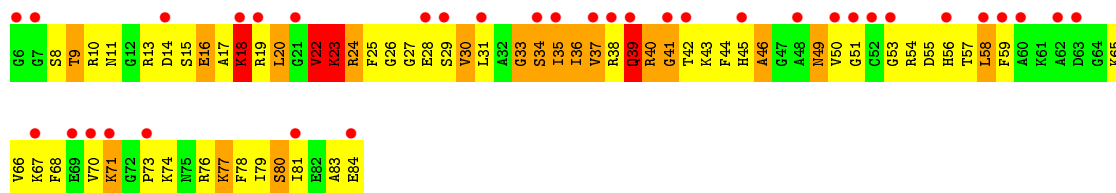
• Molecule 43: 50S ribosomal protein L25



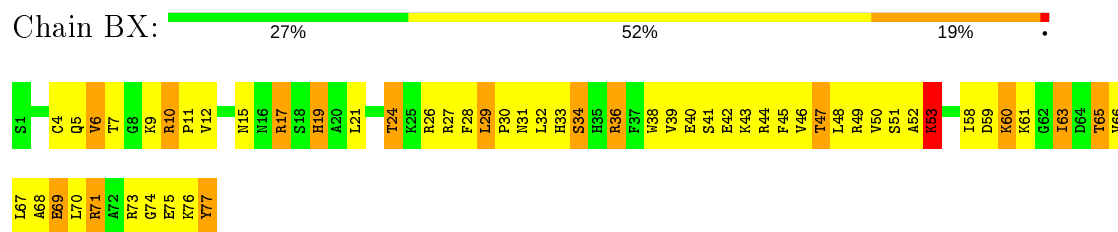
• Molecule 44: 50S ribosomal protein L27



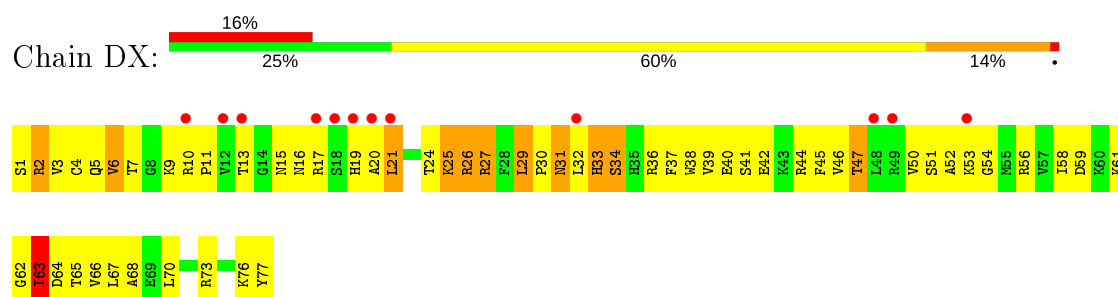
• Molecule 44: 50S ribosomal protein L27



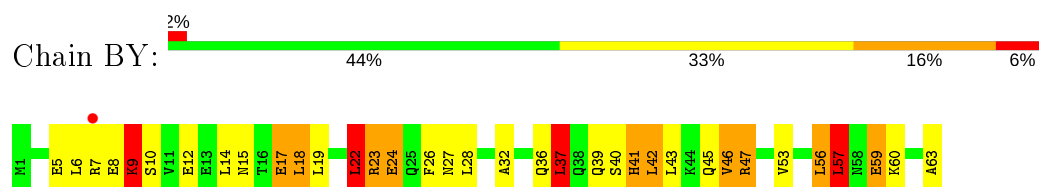
• Molecule 45: 50S ribosomal protein L28



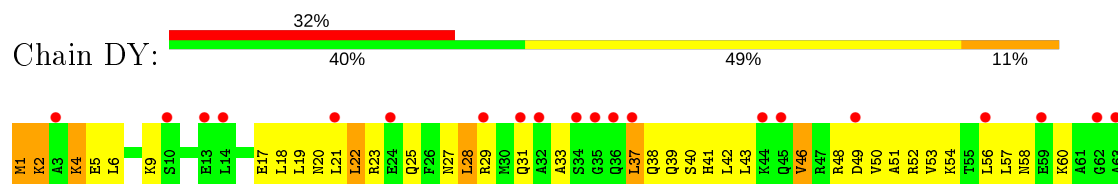
- Molecule 45: 50S ribosomal protein L28



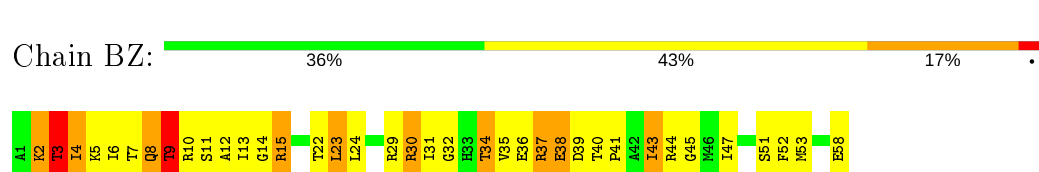
- Molecule 46: 50S ribosomal protein L29



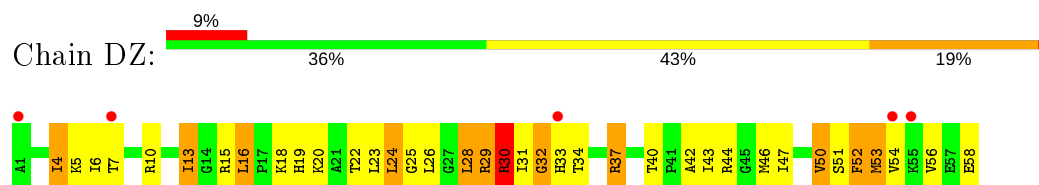
- Molecule 46: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30



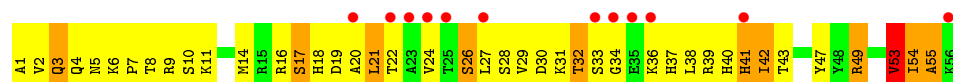
- Molecule 48: 50S ribosomal protein L32

Chain B0: 



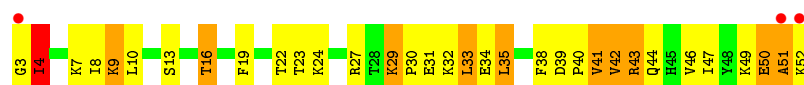
- Molecule 48: 50S ribosomal protein L32

Chain D0: 



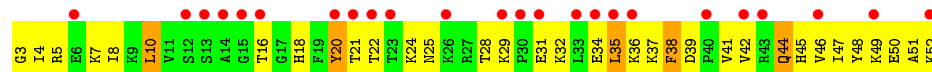
- Molecule 49: 50S ribosomal protein L33

Chain B1: 



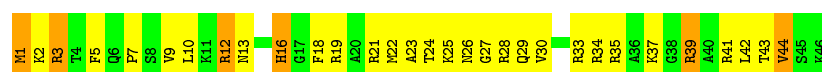
- Molecule 49: 50S ribosomal protein L33

Chain D1: 



- Molecule 50: 50S ribosomal protein L34

Chain B2: 



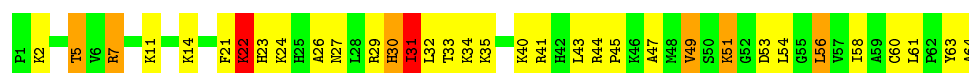
- Molecule 50: 50S ribosomal protein L34

Chain D2: 

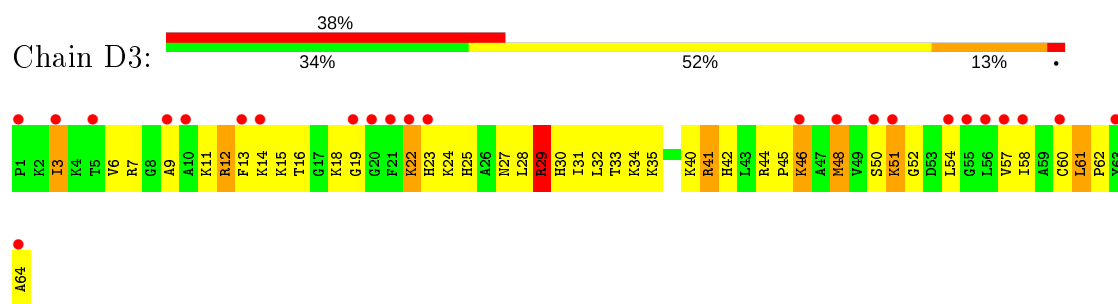


- Molecule 51: 50S ribosomal protein L35

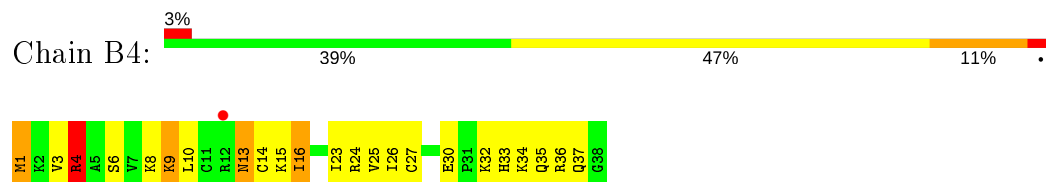
Chain B3: 



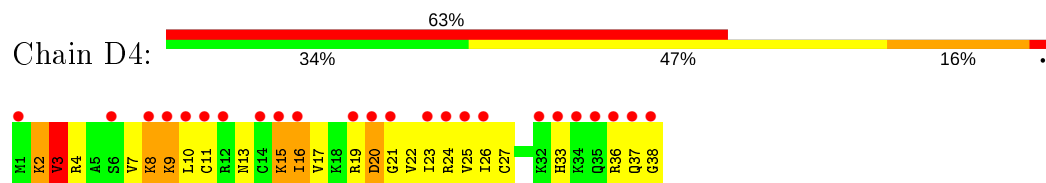
- Molecule 51: 50S ribosomal protein L35



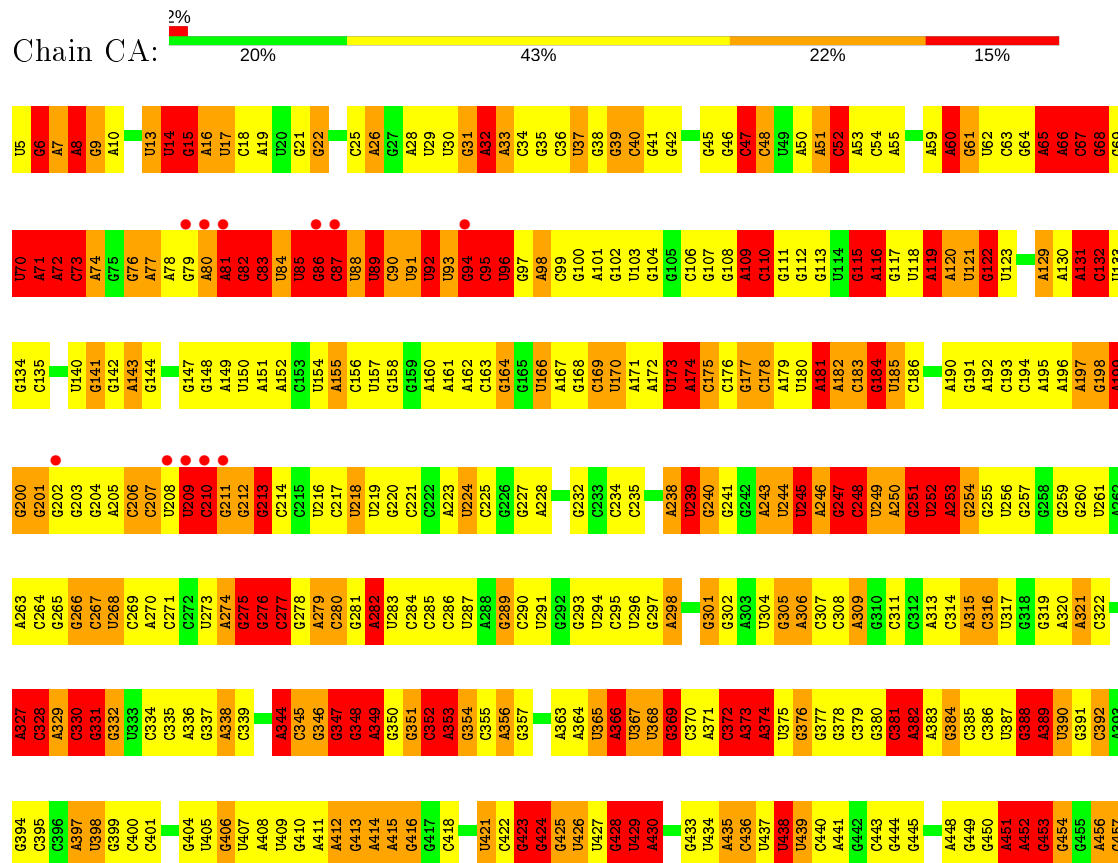
- Molecule 52: 50S ribosomal protein L36



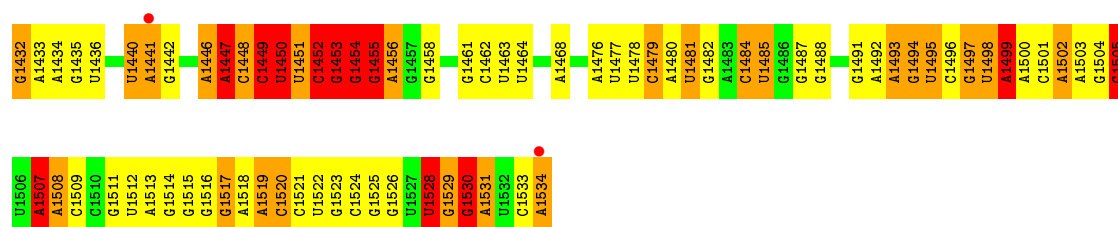
- Molecule 52: 50S ribosomal protein L36



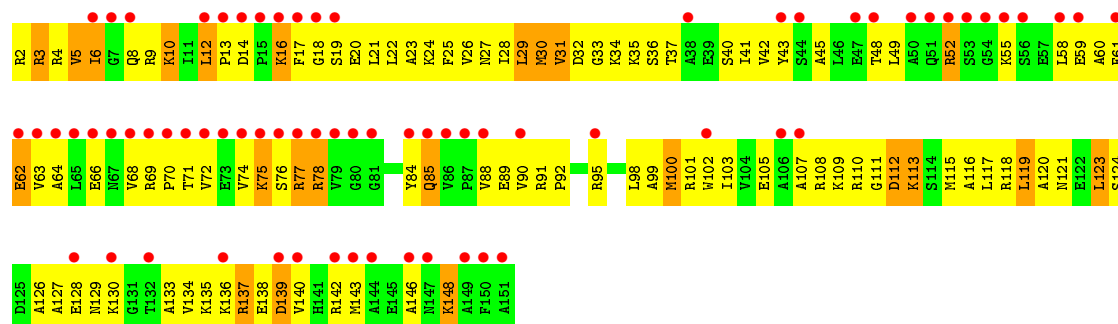
- Molecule 53: 16S rRNA



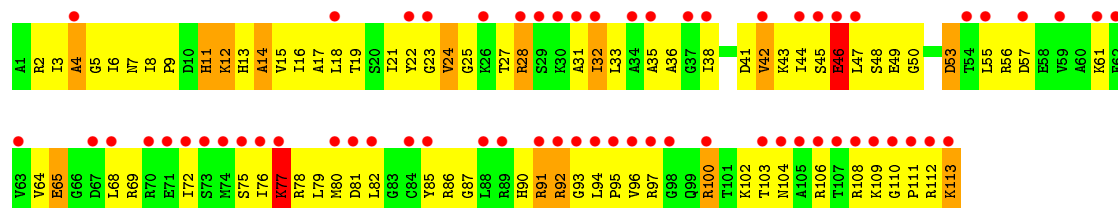
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U1364	A1299	A1238	A1176	C1112	C1051	G988	C924	C853	A784	C719	C654	C580	A520	A489
G1365	G1300	A1239	G1177	U1105	U1052	U989	G925	U854	G785	C720	A655	G581	G521	A461
C1366	U1301	U1240	G1178	C1114	G1053	C990	G926	G855	G721	G722	C658	C582	A523	G462
A1367	C1302	G1241	A1179	U991	C1054	U992	G927	G858	A790	U723	C659	G583	G524	U463
C1368	C1303	G1242	A1180	A1117	A1055	G993	C931	G859	A792	G724	C660	C587	C525	U464
C1369	G1304	C1243	G1181	U1118	U1056	A994	C932	A860	A793	G725	C661	G587	C526	A465
G1370	G1305	G1244	G1182	C1119	G1057	A994	C933	G861	U794	G726	C662	U589	C527	A466
U1371	U1308	C1245	U1183	U1123	G1058	C995	G934	C862	A795	G727	C663	C588	C528	U467
G1372	A1246	U1247	G1184	U1124	C1059	A996	A935	C863	C795	G728	C664	C589	C529	A468
G1373	G1309	G1248	G1185	G1123	U1060	U997	A936	U863	C796	A729	A665	A595	G530	C469
A1374	G1310	A1249	G1186	U1125	G1061	C998	C936	A864	U801	G730	C665	A596	U531	C470
A1375	A1311	C1249	G1187	U1126	U1062	C999	A937	A865	A802	G731	C667	G597	A532	U471
U1376	G1312	A1250	A1188	G1227	C1063	A1000	A938	C866	G803	G732	C668	U598	U533	U472
G1378	U1313	U1189	U1189	C1128	G1064	G1001	G939	G867	U804	G733	C669	C599	U534	U473
G1379	C1314	A1251	G1190	C1129	U1065	G1002	C940	C868	G734	G735	C670	A600	G535	G474
U1380	U1315	G1253	A1191	A1130	C1066	G1003	G941	C869	A807	G736	C671	G604	C536	C475
G1381	G1316	A1254	C1192	G1131	A1067	A1004	G942	U870	C808	U672	C672	U605	G537	U476
C1382	C1317	G1255	G1193	C1132	G1068	A1005	G945	U871	G809	A673	C673	U606	G538	C477
C1383	A1318	A1256	U1194	G1133	C1069	G1006	G946	A872	G810	C674	C674	C606	A539	A478
C1384	A1319	A1257	C1195	G1134	U1070	U1007	A947	A873	C817	C738	A675	A607	G540	U479
G1385	G1320	A1258	A1196	U1135	C1071	U1008	G947	U874	C811	C739	A676	A608	G541	U480
G1386	U1321	C1259	A1197	C1136	G1072	U1009	C948	U875	G812	U740	A677	C609	G542	G481
G1387	G1386	G1260	G1198	C1137	U1073	U1010	U950	C876	U813	G741	U677	U610	U543	A482
C1388	C1322	A1261	U1199	G1138	G1074	C1011	U951	G877	A814	G745	C679	C611	G544	C483
U1389	G1323	C1262	G1200	G1339	U1075	A1012	G951	A878	A815	A746	C680	C612	C545	G484
A1324	A1324	C1263	A1201	C1140	U1076	G1013	U952	C879	A816	A747	C681	C613	U552	U485
C1325	C1325	U1202	U1202	C1141	G1077	A1014	G953	C880	C817	G748	C682	C614	A547	U486
U1326	U1326	C1264	C1203	G1142	U1078	G1015	U955	C881	G818	A749	C683	C615	G548	A487
C1327	C1327	G1265	G1193	G1143	G1079	A1016	U955	C882	A819	C750	C684	C616	C549	C488
G1328	G1328	C1266	U1199	G1144	U1080	U1017	U955	C883	U820	G751	C685	C617	G550	C489
C1329	A1329	C1267	G1206	A1145	A1081	G1018	A958	U884	G821	G752	C686	C618	U551	C490
U1330	U1330	G1268	G1207	A1146	A1082	A1019	A959	G885	U822	G753	C687	C619	U552	G491
G1331	G1331	C1269	C1208	A1147	U1083	G1020	U960	C886	C823	A754	C688	C620	A553	C492
A1332	A1332	A1270	G1209	C1148	G1084	A1021	U961	C887	C824	G755	C689	C621	A554	A493
C1333	C1333	G1271	C1210	U1148	U1085	A1022	C962	C888	A825	G756	C690	C622	U555	G494
G1334	G1334	C1272	U1211	C1149	U1086	U1023	G963	C889	C826	U757	C691	C623	C556	A495
U1335	U1335	G1273	U1212	A1150	U1087	G1024	A964	C890	U827	U757	U692	C630	C557	A496
C1336	C1336	A1274	C1214	A1151	G1087	U1025	U965	C891	U828	C758	C693	C631	G557	G497
G1337	G1337	C1275	G1215	A1152	U1088	G1026	U966	A892	G829	A759	C694	C632	A558	A498
G1338	G1338	A1276	A1216	G1153	G1089	U1026	C967	C893	A830	G760	A695	C633	A559	A499
A1339	A1339	C1277	G1217	G1154	U1090	U1029	A968	C899	G832	U761	A696	C634	U561	G500
U1340	U1340	G1278	C1218	A1155	U1091	U1030	A969	C900	G833	U762	C695	C635	U562	C501
C1341	C1341	A1280	A1219	G1156	A1092	G1031	C970	A901	U834	C763	C696	C636	A563	A502
G1342	G1342	C1281	G1220	C1158	U1093	G1032	G971	A906	U835	G765	C700	C637	C564	C503
A1343	A1343	U1282	G1221	U1159	U1095	A1035	C972	A907	G836	A766	A701	C638	C565	G504
C1344	C1344	U1283	G1222	G1160	C1096	A1036	G973	A909	C840	A767	A702	C639	U565	G505
A1345	A1345	C1284	C1223	A1161	C1097	G1037	A974	C910	C841	A768	A703	C640	U566	U508
G1346	G1346	A1285	U1224	C1162	U1098	G1038	G975	A913	U842	G769	A705	C641	G567	A509
U1347	U1347	U1286	C1225	U1165	G1100	G1039	A977	A914	U843	C770	C706	C642	C568	C569
C1348	C1348	A1287	C1226	G1166	A1101	U1040	A978	A915	U844	G774	C643	C644	C570	A510
A1349	A1349	U1288	A1227	A1167	C1102	G1041	C979	C980	G844	G775	C645	C646	U571	C511
A1350	A1350	A1289	C1228	U1168	C1103	A1042	C980	A915	C846	G776	A712	C647	A572	U512
G1356	G1356	G1292	G1230	A1169	G1104	G1043	U981	A918	G847	A777	G713	C648	A573	C513
U1357	U1357	C1293	G1231	A1170	A1105	U982	U981	A919	C848	G778	A714	C649	A574	C514
A1358	A1358	G1294	U1232	A1171	G1106	A1046	A983	A919	C849	G779	A715	C650	G575	G515
C1359	C1359	U1295	U1172	A1172	C1107	G1047	C984	U920	G849	A780	A716	C651	C576	U516
A1360	A1360	C1296	U1173	U1173	G1108	G1048	C985	U921	U850	A781	C651	C652	G577	C517
G1361	G1361	A1297	U1235	G1174	C1109	U1049	U986	G922	G851	A782	U717	C652	C578	C518



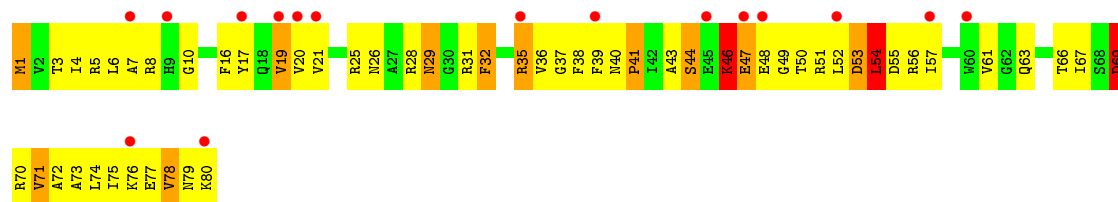
• Molecule 54: 30S ribosomal protein S7



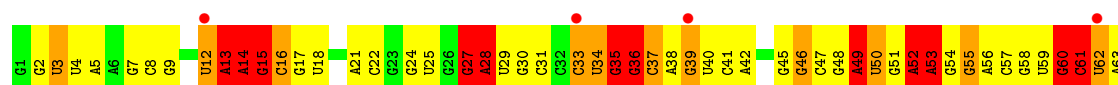
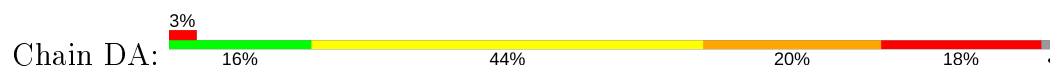
• Molecule 55: 30S ribosomal protein S13



• Molecule 56: 30S ribosomal protein S16



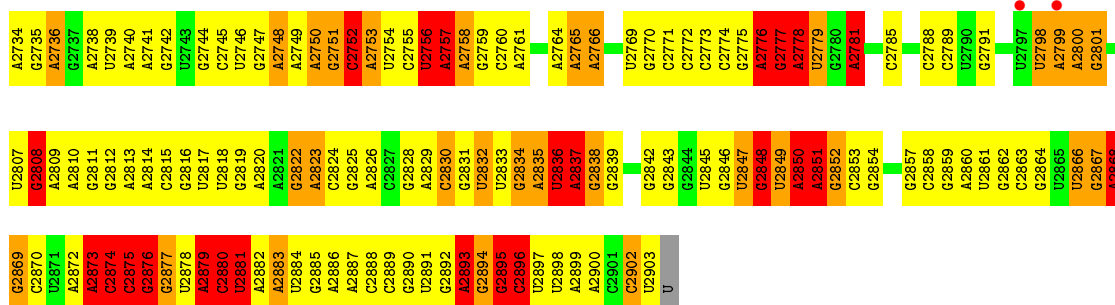
• Molecule 57: 23S rRNA



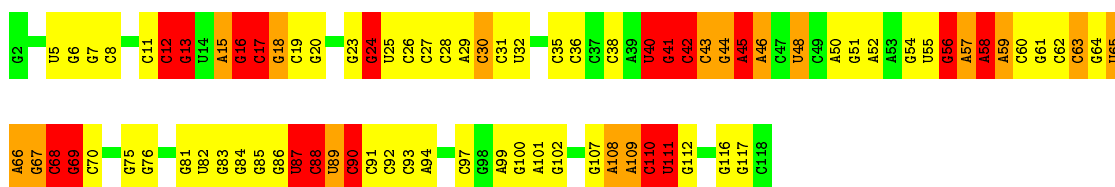
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G	A820	A756	G630	G570	G498	G438	G377	C316	G248	G186	A126	U65
G	A821	G757	A831	U571	U499	A439	G378	C317	C249	G187	A127	G66
G	A822	A632	A632	A572	A502	C440	C379	C318	C250	G188	C128	U67
U	C823	U762	C633	U573	A503	U441	G380	G319	A251	G189	C129	G68
C	C824	G763	C634	A574	A504	G442	G381	G320	C130	A190	C130	C69
A	A825	A764	C635	A575	A504	A443	A382	U821	A320	A191	A131	G70
U	U826	C765	C636	U576	A505	C444	C383	U822	A355	A192	A132	A71
C	U827	U766	A637	G577	G506	C445	A384	C323	A256	U193	U133	U72
C	U828	G767	G638	G578	A507	G446	C385	G324	G260	G194	G134	A73
C	A829	A705	U639	G579	A508	A447	G386	G325	A262	A195	U135	A74
G	G830	A706	C640	U580	C509	U448	U387	G326	A263	A196	U136	G75
G	G831	G771	U641	C581	G510	A449	G388	G327	C264	A197	U137	G76
C	U832	C772	U642	A582	U511	G450	G389	U328	C265	C198	U138	G77
U	A833	U773	A643	G583	U512	U451	U390	G329	A266	A199	U139	U78
U	G834	G774	A644	C584	A513	G452	A391	G330	G266	U200	C140	C79
A	C835	G775	C645	G585	A514	A453	U392	C331	G141	C201	G142	G80
C	G836	G776	G711	A586	A515	A454	G393	A332	A270	U202	A143	G81
C	G837	G777	G712	C587	C516	C455	U395	G333	G271	C203	C143	U82
C	C838	G778	G713	U588	C517	C456	G396	C334	A272	A204	A144	A83
U	U839	U779	A715	U589	G518	A457	U397	C335	G273	G205	C145	A84
C	C840	A716	A716	A590	U519	G458	C398	C336	C274	U206	C146	G85
C		C717	G651	U591		U459	U399	C337	C275	A207	A147	G86
C	G843	A718	U652	A592	G524	A460	G400	C338	U276	C208	U148	U87
C	A844	A783	U653	U593	U525	C461	A401	U339	G277	C209	U149	G88
C	A845	G784	A854	U594	A526	A462	A402	A340	U150	C210	U150	A89
C	U846	G785	A655	C595	C527	G463	U403	C341	C151	C211	C151	U90
C	U847	G786	G656	U596	A528	U464	A404	U280	A152	G212	A152	A91
C	C848	C787	U657	G597	A529	G465	U405	C343	U153	G154	U154	U92
C	U849	U724	U658	U598	G530	A466	G406	A344	A216	G215	A155	G93
C	U850	A789	G659	A599	C531	G467	G407	A345	A217	A218	A156	A94
C	C851	U790	C660	G600	A532	G468	G408	A346	G285	G219	A157	A95
C	U852	G791	A661	C601	G533	G469	G409	A347	U286	G159	C157	C96
C	U853	A792	G662	A602	U534	A470	G410	U348	U287	U160	U158	C97
C	C854	A793	G663	G604	G535	A471	G411	U349	U288	G161	A161	U99
C	G855	A794	G664	G605	G536	G472	A412	G350	G289	U162	U162	U100
C	G856	C795	U665	G606	G537	G473	C413	C351	U290	C163	C163	A103
C	C857	C796	A666	U606	A538	C474	C414	A352	U291	C164	C164	A104
C	G858	G797	U667	U607	G544	C475	A415	C353	U293	C225	U166	C105
C	G859	G798	A668	A608	U545	G476	U416	A354	A294	A226	G167	C106
C	U860	G799	G669	A609	U546	A477	C417	U355	G295	C228	G168	G108
C	A861	A800	C736	C610	A547	A478	C418	G356	U296	G229	C169	C109
C	G862	G801	C737	C611	G548	A479	U419	C357	G297	C230	U170	C110
C	A863	A802	C672	C612	C549	A480	C420	U358	G298	A231	U171	G110
C	G864	U803	C673	A613	C550	G481	C421	G361	A299	G232	A172	A111
C	C865	A804	G674	A614	G551	A482	A422	A362	A300	A233	U173	U112
C	A866	G805	A675	U615	U552	A483	A423	G363	G301	U234	C179	U120
C	C867	C806	A676	A616	G553	C484	G424	C302	C302	U235	A181	G121
C	U868	U807	A677	G617	U554	C485	G425	G303	G297	A174	A182	G122
C	G869	G808	C678	G618	G555	C486	C426	U304	C236	G175	C183	G123
C	U870	G809	C679	G619	U558	C487	U427	C366	C237	G176	C184	G124
C	U871	U810	G682	U620	G562	G488	A428	G367	C238	C177		
C	U872	U747	G683	A621	U562	G489	A429	A368	C239	G178		
C	C873	C812	U883	G622	A563	C490	A430	G369	C240	C179		
C	G874	A749	G684	C623	A564	C491	U431	G370	A241	C190		
C	A875	C814	A685	C624	C564	A492	A432	A371	G242	A181		
C	C876	C815	U686	G625	C565	G493	C433	G372	U243	A182		
C	A877	C816	C687	A626	U566	G494	U434	U373	A244	C183		
C	U878	C817	U688	U567	C435	G495	C435	A374	G245	G123		
G		G818	A689	U568	U568	G496	C436	G375	C314	G246		

U1769	G1706	U1636	C1575	U1513	C1451	A1385	U1325	A1265	A1204	A1142	A1077	C1013	G949
A1773	G1707	C1637	U1576	G1514	C1451	C1386	U1326	G1266	A1205	A1143	U1078	A1014	G950
C1774	C1708	C1638	C1577	A1515	A1452	A1387	G1452	G1267	G1206	A1144	C1079	G1016	G951
U1775	U1709	A1639	U1578	G1516	A1453	A1388	A1327	A1268	C1207	C1145	U1081	G952	G952
G1776	G1710	A1640	A1579	G1517	G1455	G1389	C1329	A1269	C1208	C1146	U1082	U1019	G953
U1777	G1711		G1581	C1518	G1456	U1391	U1331	G1270	U1209	A1147	U1083		G956
U1778	U1712		C1582	G1520	A1457	A1392	G1332	G1271	G1210	U1084	A1020	A1020	G957
U1779	A1713	C1647	U1583	A1521	U1458	A1393	G1333	A1272	C1212	U1085	A1021	A1021	G958
U1780	U1714	U1648	U1584	A1522	G1459	U1394	G1334	A1274	A1213	A1086	G1022	G1022	G959
U1781	G1715	G1649	U1585	A1523	U1460	A1395	G1335	A1275	A1214	U1087	U1023	U1023	A960
U1782	U1716	A1650	A1586	G1524	G1461	U1396	A1336	A1276	G1215	A1088	G1025	G1025	G961
A1783	A1717	G1651	G1587	U1525	C1462	U1397	G1337	G1277	G1216	A1089	G1026	G1026	G962
A1784	G1718	A1652	G1588	C1526		C1398	G1338	G1278	U1217	A1090	A1027	A1027	G963
A1785		G1653	U1589	G1527	G1466	C1399	G1339	G1279	G1218	G1091	G964	G964	G964
A1786		A1654	A1590	A1528	U1466	U1400	U1340	G1280	U1219	C1092	A1028	A1028	G965
A1787	A1722	A1655	A1591	G1529	U1467	G1401	G1341	G1281	G1220	G1093			G966
G1788	G1723	C1656	C1592	G1530	U1468	U1402	A1342	U1282	C1221	A1032			
A1789	G1724	A1593	C1593	C1531	A1469	A1403	G1343	G1283	U1222	U1033			
C1790		U1594	U1594	A1532	A1470	C1404	U1344	A1284	U1223	U1034			
A1791	C1728	C1595	C1595	C1532	G1471	U1405	C1345	A1285		U1035			
G1792	U1729	A1596	A1596	A1534	G1472	U1406	G1346	A1286		U1036			
C1793	C1730	A1685	A1597	A1535	G1473	G1407	A1347	A1287		G1037			
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C1795	G1732	G1667	U1599	G1537	G1475	U1409	C1349	G1289	C1229	C1102			
U1796	G1733	A1688	C1600	G1538	U1476	G1410	C1350	C1290	A1230	A1103			
G1797		A1689	G1601	U1539	A1477	U1411	C1351	C1291	U1231				
U1798	A1735	C1670	U1602	G1540	G1478	U1412	U1352	G1292	G1232	U1107			
G1799	U1736	A1671	A1603	C1541	G1479	A1413	A1353	C1293	C1233	U1108			
C1800	G1737	A1672	C1604		A1480	A1414	A1354	U1294	U1234	C1110			
A1801	G1738	G1673	C1605	A1544	U1481	U1415	G1355	C1295	G1235	A1111			
A1802	A1739	C1674	C1606	A1545	G1482	G1416	G1356	G1296	G1236	G1112			
A1803	G1740	C1675	C1607	G1546	G1483	C1417	C1357	C1297	A1237	U1113			
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A1808	A1745	G1681	C1552	A1552	A1490	G1422	C1362	A1302	U1242	C1054			
A1809	A1746	G1682	A1553	A1553	G1491		G1363	G1303	G1243	G1055			
C1810	U1747	U1683	U1554	U1554	G1492		G1364	A1304	A1244	G1056			
G1811		G1684	G1555	G1555	C1493		A1365	C1305	G1245	A1057			
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G1814	C1752	G1687	A1617	C1558	A1496	U1429	G1368	A1308	U1248	U1060			
A1815	G1753	U1688	G1619	U1559	U1497	G1430	G1369	G1309	A1126	G1061			
C1816	A1754	A1689	G1620	G1560	C1498	A1431	C1370	G1310	G1250	G1062			
G1817	A1755	A1690	U1621	C1561	C1499	G1432	G1371	A1189	G1251	G1063			
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A1819	U1757	U1692	G1623	U1563	G1501	A1434	A1373	U1313	A1253	U1065			
U1820	G1758	U1693	U1624	C1564	A1502	G1435	G1374	C1314	A1254	U1066			
A1821	A1759	C1694	C1625	C1565	A1503	G1436	U1375	C1315	U1255	A1067			
C1822	C1760	G1695	A1626	A1566	A1504	C1437	C1376	G1316	G1256	G1068			
G1823	C1761	G1696	G1627	G1567	A1505	U1438	G1377	G1317	G1257	U1069			
G1824	A1762	G1697	G1628	G1568	U1506	A1439	A1378	U1318	U1258	C1070			
U1825	G1763	A1698	U1629	A1569	C1507	U1440	U1379	C1319	G1259	G1071			
G1826	C1764	G1699	A1630	A1570	A1508	G1441	G1380	C1320	U1260	C1072			
U1827	U1765	A1700		A1571	A1509	U1442	G1381	A1321	G1261	A1073			
G1828	G1766	A1701	G1633	A1572	G1510		G1382	A1322	A1262	G1074			
A1829	G1767	A1634	U1573	G1573	C1512		A1383	C1323	U1263	G1075			
C1830	G1768	G1703	A1635	C1574		G1447	G1384	G1324	A1264	C1076			

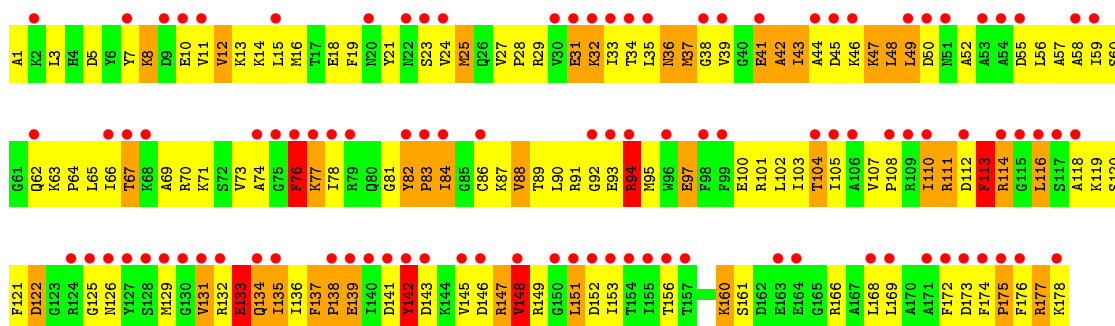
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C1831	C1832	C1833	U1834	C1838	G1839	U1840	G1841	G1842	C1843	C1844	C1845	A1846	A1847	A1848	A1849	G1850	A1853	A1854	U1855	U1856	G1857	G1862	U1865	A1866	G1867	G1868	G1869	G1870	A1871	A1872	G1873	G1874	G1875	A1876	A1877	G1878	C1879	U1880	G1881	U1882	G1883	G1884	A1885	U1886	G1887	G1888	A1889	U1890	G1893	U1898	A1899	A1900	A1901																												
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• Molecule 58: 5S rRNA



• Molecule 59: 50S ribosomal protein L5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.46Å 434.08Å 621.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.15 – 3.19 82.15 – 3.19	Depositor EDS
% Data completeness (in resolution range)	75.8 (82.15-3.19) 75.8 (82.15-3.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.19Å)	Xtriage
Refinement program	PHENIX ?, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.191 , 0.252 0.203 , 0.262	Depositor DCC
R_{free} test set	15290 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 85.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284499	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLM, ZN, MG

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	0.50	6/36834 (0.0%)	1.27	532/57462 (0.9%)
2	AB	0.40	2/1736 (0.1%)	0.57	4/2338 (0.2%)
2	CB	0.37	2/1736 (0.1%)	0.54	4/2338 (0.2%)
3	AC	0.26	0/1652	0.50	0/2225
3	CC	0.23	0/1652	0.44	0/2225
4	AD	0.29	0/1665	0.52	0/2227
4	CD	0.34	0/1665	0.57	0/2227
5	AE	0.37	1/1119 (0.1%)	0.59	0/1504
5	CE	0.31	0/1119	0.55	0/1504
6	AF	0.28	0/836	0.49	0/1128
6	CF	0.27	0/836	0.50	0/1128
7	AG	0.23	0/1196	0.46	0/1602
8	AH	0.29	0/989	0.54	0/1326
8	CH	0.26	0/989	0.49	0/1326
9	AI	0.23	0/1034	0.47	0/1375
9	CI	0.22	0/1034	0.42	0/1375
10	AJ	0.24	0/797	0.49	0/1077
10	CJ	0.22	0/797	0.47	0/1077
11	AK	0.27	0/893	0.52	0/1205
11	CK	0.25	0/893	0.51	0/1205
12	AL	0.36	0/969	0.67	0/1300
12	CL	0.40	1/969 (0.1%)	0.56	0/1300
13	AM	0.22	0/893	0.47	0/1193
14	AN	0.25	0/785	0.49	0/1043
14	CN	0.21	0/780	0.39	0/1036
15	AO	0.27	0/722	0.47	0/964
15	CO	0.25	0/722	0.45	0/964
16	AP	0.28	0/659	0.49	0/884
17	AQ	0.35	0/658	0.56	0/881
17	CQ	0.27	0/658	0.51	0/881
18	AR	0.28	0/463	0.50	0/621
18	CR	0.28	0/463	0.46	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	AS	0.23	0/653	0.47	0/877
19	CS	0.21	0/653	0.42	0/877
20	AT	0.30	0/671	0.57	0/888
20	CT	0.25	0/671	0.50	0/888
21	AU	0.28	0/431	0.49	0/570
21	CU	0.31	0/431	0.60	0/570
22	BA	0.71	8/68626 (0.0%)	1.50	1274/107056 (1.2%)
23	BB	0.64	0/2828	1.43	38/4410 (0.9%)
24	BC	0.41	0/2122	0.69	1/2852 (0.0%)
24	DC	0.29	0/2122	0.53	0/2852
25	BD	0.48	0/1586	0.76	2/2134 (0.1%)
25	DD	0.28	0/1586	0.57	0/2134
26	BE	0.40	0/1571	0.66	1/2113 (0.0%)
26	DE	0.25	0/1571	0.47	0/2113
27	BF	0.31	0/1435	0.54	0/1926
28	BG	0.33	0/1343	0.60	0/1816
28	DG	0.22	0/1343	0.46	0/1816
29	BH	0.30	0/1122	0.50	0/1515
29	DH	0.34	1/1122 (0.1%)	0.50	0/1515
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.21	0/1046	0.43	0/1410
31	BJ	0.51	0/1152	0.75	0/1551
31	DJ	0.26	0/1152	0.57	1/1551 (0.1%)
32	BK	0.46	0/948	0.78	0/1268
32	DK	0.29	0/948	0.55	0/1268
33	BL	0.42	0/1054	0.75	1/1403 (0.1%)
33	DL	0.24	0/1054	0.51	0/1403
34	BM	0.44	0/1093	0.67	0/1460
34	DM	0.27	0/1093	0.48	0/1460
35	BN	0.45	0/974	0.70	1/1301 (0.1%)
35	DN	0.27	0/974	0.51	0/1301
36	BO	0.38	0/902	0.60	0/1209
36	DO	0.22	0/902	0.42	0/1209
37	BP	0.43	0/929	0.71	0/1242
37	DP	0.28	0/929	0.49	0/1242
38	BQ	0.52	0/960	0.76	0/1278
38	DQ	0.26	0/960	0.44	0/1278
39	BR	0.54	0/829	0.77	1/1107 (0.1%)
39	DR	0.25	0/829	0.48	0/1107
40	BS	0.50	0/864	0.73	0/1156
40	DS	0.27	0/864	0.51	0/1156
41	BT	0.43	0/745	0.71	0/994
41	DT	0.22	0/745	0.48	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
42	BU	0.39	0/788	0.70	0/1051
42	DU	0.23	0/788	0.46	0/1051
43	BV	0.39	0/766	0.61	0/1025
43	DV	0.23	0/766	0.43	0/1025
44	BW	0.53	0/603	0.82	0/797
44	DW	0.25	0/603	0.49	0/797
45	BX	0.37	0/635	0.66	0/848
45	DX	0.27	0/635	0.56	0/848
46	BY	0.33	0/510	0.62	0/677
46	DY	0.21	0/510	0.43	0/677
47	BZ	0.45	0/453	0.80	0/605
47	DZ	0.25	0/453	0.50	0/605
48	B0	0.43	0/450	0.71	0/599
48	D0	0.26	0/450	0.50	0/599
49	B1	0.31	0/417	0.57	0/554
49	D1	0.24	0/417	0.45	0/554
50	B2	0.41	0/380	0.71	0/498
50	D2	0.26	0/380	0.51	0/498
51	B3	0.43	0/513	0.66	0/676
51	D3	0.27	0/513	0.52	0/676
52	B4	0.39	0/303	0.69	0/397
52	D4	0.43	0/303	0.54	0/397
53	CA	0.47	6/36762 (0.0%)	1.24	525/57350 (0.9%)
54	CG	0.22	0/1188	0.44	0/1591
55	CM	0.19	0/885	0.41	0/1181
56	CP	0.28	0/649	0.52	0/870
57	DA	0.46	0/68314	1.28	1097/106569 (1.0%)
58	DB	0.51	1/2803 (0.0%)	1.21	38/4371 (0.9%)
59	DF	0.23	0/1444	0.48	0/1937
All	All	0.50	28/306773 (0.0%)	1.19	3520/458565 (0.8%)

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
2	CB	0	1
25	BD	0	1
35	BN	0	1
All	All	0	3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	DB	69	G	O3'-P	-16.79	1.41	1.61
1	AA	1047	G	O3'-P	-14.49	1.43	1.61
2	AB	107	ARG	C-N	11.33	1.60	1.34
53	CA	1396	A	O3'-P	-11.26	1.47	1.61
2	CB	146	SER	C-N	10.14	1.57	1.34

The worst 5 of 3520 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	CA	1396	A	P-O3'-C3'	16.36	139.33	119.70
57	DA	2586	U	N1-C1'-C2'	-15.75	93.52	114.00
22	BA	2283	C	N1-C1'-C2'	-15.29	94.12	114.00
57	DA	1997	C	N1-C1'-C2'	-14.86	94.69	114.00
23	BB	90	C	N1-C1'-C2'	-14.66	94.94	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	BD	9	VAL	Peptide
35	BN	101	GLY	Peptide
2	CB	107	ARG	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32895	0	16553	1473	0
2	AB	1705	0	1732	195	0
2	CB	1705	0	1732	176	0
3	AC	1625	0	1699	121	0
3	CC	1625	0	1699	127	0
4	AD	1643	0	1710	166	0
4	CD	1643	0	1710	177	0
5	AE	1106	0	1147	146	0
5	CE	1106	0	1148	123	0
6	AF	818	0	808	76	0
6	CF	818	0	808	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AG	1182	0	1240	89	0
8	AH	979	0	1034	102	0
8	CH	979	0	1034	115	0
9	AI	1022	0	1070	91	0
9	CI	1022	0	1070	108	0
10	AJ	787	0	828	83	0
10	CJ	787	0	828	93	0
11	AK	877	0	887	91	0
11	CK	877	0	887	79	0
12	AL	955	0	1019	92	0
12	CL	955	0	1019	100	0
13	AM	884	0	944	70	0
14	AN	774	0	827	81	0
14	CN	769	0	822	85	0
15	AO	714	0	737	59	0
15	CO	714	0	737	58	0
16	AP	649	0	666	62	0
17	AQ	649	0	691	81	0
17	CQ	649	0	691	70	0
18	AR	456	0	478	31	0
18	CR	456	0	478	47	0
19	AS	638	0	665	47	0
19	CS	638	0	665	64	0
20	AT	665	0	714	65	0
20	CT	665	0	714	61	0
21	AU	426	0	449	79	0
21	CU	426	0	449	80	0
22	BA	61274	0	30819	2356	0
23	BB	2529	0	1281	83	0
24	BC	2083	0	2157	223	0
24	DC	2083	0	2157	262	0
25	BD	1565	0	1616	223	0
25	DD	1565	0	1616	197	0
26	BE	1552	0	1619	152	0
26	DE	1552	0	1619	179	0
27	BF	1411	0	1447	140	0
28	BG	1323	0	1374	147	0
28	DG	1323	0	1374	131	0
29	BH	1111	0	1148	107	0
29	DH	1111	0	1148	115	0
30	BI	1032	0	1088	109	0
30	DI	1032	0	1088	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BJ	1129	0	1162	171	0
31	DJ	1129	0	1162	133	0
32	BK	939	0	1012	113	0
32	DK	939	0	1012	128	0
33	BL	1045	0	1117	122	0
33	DL	1045	0	1117	117	0
34	BM	1074	0	1157	99	0
34	DM	1074	0	1157	107	0
35	BN	961	0	1000	96	0
35	DN	961	0	1000	134	0
36	BO	892	0	923	75	0
36	DO	892	0	923	71	0
37	BP	917	0	965	139	0
37	DP	917	0	965	130	0
38	BQ	947	0	1022	153	0
38	DQ	947	0	1022	124	0
39	BR	816	0	839	116	0
39	DR	816	0	839	87	0
40	BS	857	0	922	81	0
40	DS	857	0	922	78	0
41	BT	739	0	807	112	0
41	DT	739	0	807	108	0
42	BU	780	0	834	52	0
42	DU	780	0	834	92	0
43	BV	753	0	780	70	0
43	DV	753	0	780	71	0
44	BW	596	0	610	201	0
44	DW	596	0	610	117	0
45	BX	625	0	655	67	0
45	DX	625	0	655	85	0
46	BY	509	0	543	44	0
46	DY	509	0	543	63	0
47	BZ	449	0	491	39	0
47	DZ	449	0	491	42	0
48	B0	444	0	461	33	0
48	D0	444	0	461	64	0
49	B1	410	0	440	38	0
49	D1	410	0	440	38	0
50	B2	377	0	418	37	0
50	D2	377	0	418	31	0
51	B3	504	0	574	46	0
51	D3	504	0	574	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	B4	302	0	340	39	0
52	D4	302	0	343	36	0
53	CA	32831	0	16521	1811	0
54	CG	1175	0	1230	125	0
55	CM	877	0	937	97	0
56	CP	639	0	656	71	0
57	DA	60995	0	30679	3815	0
58	DB	2507	0	1270	168	0
59	DF	1420	0	1460	194	0
60	AA	42	0	0	0	0
60	AN	1	0	0	0	0
60	BA	135	0	0	0	0
60	BB	4	0	0	0	0
60	BL	1	0	0	0	0
60	CA	42	0	0	0	0
60	DA	133	0	0	0	0
60	DB	1	0	0	0	0
60	DC	1	0	0	0	0
60	DE	1	0	0	0	0
60	DJ	1	0	0	0	0
61	BA	20	0	11	1	0
62	B4	1	0	0	0	0
62	D4	1	0	0	0	0
63	AA	197	0	0	11	0
63	AL	2	0	0	0	0
63	AN	6	0	0	1	0
63	AT	2	0	0	0	0
63	AU	1	0	0	0	0
63	B2	2	0	0	0	0
63	B3	2	0	0	0	0
63	B4	2	0	0	0	0
63	BA	608	0	0	43	0
63	BB	19	0	0	0	0
63	BC	8	0	0	0	0
63	BD	2	0	0	3	0
63	BE	1	0	0	0	0
63	BL	4	0	0	1	0
63	BN	2	0	0	0	0
63	BQ	1	0	0	0	0
63	BT	2	0	0	1	0
63	BV	1	0	0	1	0
63	CA	195	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	CE	3	0	0	1	0
63	CI	1	0	0	0	0
63	CL	1	0	0	0	0
63	CN	3	0	0	0	0
63	CT	2	0	0	0	0
63	CU	2	0	0	0	0
63	D2	1	0	0	1	0
63	D3	1	0	0	0	0
63	D4	4	0	0	0	0
63	DA	603	0	0	19	0
63	DB	4	0	0	0	0
63	DC	10	0	0	0	0
63	DD	1	0	0	0	0
63	DE	3	0	0	0	0
63	DJ	4	0	0	0	0
63	DL	5	0	0	0	0
63	DN	2	0	0	0	0
63	DT	2	0	0	0	0
63	DU	2	0	0	0	0
63	DV	1	0	0	0	0
All	All	284499	0	190851	17927	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

The worst 5 of 17927 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:DA:2092:U:H1'	57:DA:2093:G:C8	1.52	1.43
38:BQ:63:ARG:NH1	38:BQ:96:ASP:HA	1.44	1.29
57:DA:2092:U:O2'	57:DA:2093:G:H5"	1.08	1.24
38:BQ:63:ARG:HH12	38:BQ:96:ASP:CA	1.55	1.20
28:BG:83:THR:HA	28:BG:84:LYS:NZ	1.57	1.19

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	132 (61%)	55 (26%)	29 (13%)	0	1
2	CB	216/218 (99%)	149 (69%)	49 (23%)	18 (8%)	1	5
3	AC	204/206 (99%)	153 (75%)	34 (17%)	17 (8%)	1	5
3	CC	204/206 (99%)	145 (71%)	39 (19%)	20 (10%)	0	3
4	AD	203/205 (99%)	133 (66%)	43 (21%)	27 (13%)	0	1
4	CD	203/205 (99%)	138 (68%)	42 (21%)	23 (11%)	0	2
5	AE	148/150 (99%)	103 (70%)	28 (19%)	17 (12%)	0	2
5	CE	148/150 (99%)	106 (72%)	24 (16%)	18 (12%)	0	2
6	AF	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	1	8
6	CF	98/100 (98%)	68 (69%)	19 (19%)	11 (11%)	0	2
7	AG	149/151 (99%)	108 (72%)	35 (24%)	6 (4%)	3	21
8	AH	127/129 (98%)	94 (74%)	27 (21%)	6 (5%)	2	17
8	CH	127/129 (98%)	89 (70%)	29 (23%)	9 (7%)	1	8
9	AI	125/127 (98%)	84 (67%)	30 (24%)	11 (9%)	1	4
9	CI	125/127 (98%)	90 (72%)	23 (18%)	12 (10%)	0	3
10	AJ	96/98 (98%)	70 (73%)	16 (17%)	10 (10%)	0	3
10	CJ	96/98 (98%)	55 (57%)	26 (27%)	15 (16%)	0	1
11	AK	115/117 (98%)	86 (75%)	20 (17%)	9 (8%)	1	6
11	CK	115/117 (98%)	86 (75%)	20 (17%)	9 (8%)	1	6
12	AL	121/123 (98%)	88 (73%)	16 (13%)	17 (14%)	0	1
12	CL	121/123 (98%)	83 (69%)	30 (25%)	8 (7%)	1	9
13	AM	112/114 (98%)	84 (75%)	19 (17%)	9 (8%)	1	6
14	AN	92/100 (92%)	58 (63%)	22 (24%)	12 (13%)	0	1
14	CN	91/100 (91%)	60 (66%)	26 (29%)	5 (6%)	2	14
15	AO	86/88 (98%)	62 (72%)	13 (15%)	11 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	3	24
16	AP	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	0	2
17	AQ	78/80 (98%)	55 (70%)	11 (14%)	12 (15%)	0	1
17	CQ	78/80 (98%)	61 (78%)	8 (10%)	9 (12%)	0	2
18	AR	53/55 (96%)	41 (77%)	10 (19%)	2 (4%)	3	22
18	CR	53/55 (96%)	42 (79%)	10 (19%)	1 (2%)	8	39
19	AS	77/79 (98%)	59 (77%)	12 (16%)	6 (8%)	1	6
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	3
20	AT	83/85 (98%)	65 (78%)	10 (12%)	8 (10%)	0	3
20	CT	83/85 (98%)	61 (74%)	13 (16%)	9 (11%)	0	2
21	AU	49/51 (96%)	26 (53%)	15 (31%)	8 (16%)	0	0
21	CU	49/51 (96%)	21 (43%)	12 (24%)	16 (33%)	0	0
24	BC	269/271 (99%)	180 (67%)	61 (23%)	28 (10%)	0	3
24	DC	269/271 (99%)	164 (61%)	72 (27%)	33 (12%)	0	2
25	BD	207/209 (99%)	141 (68%)	37 (18%)	29 (14%)	0	1
25	DD	207/209 (99%)	134 (65%)	41 (20%)	32 (16%)	0	1
26	BE	199/201 (99%)	148 (74%)	31 (16%)	20 (10%)	0	3
26	DE	199/201 (99%)	120 (60%)	54 (27%)	25 (13%)	0	1
27	BF	175/177 (99%)	127 (73%)	29 (17%)	19 (11%)	0	2
28	BG	174/176 (99%)	116 (67%)	34 (20%)	24 (14%)	0	1
28	DG	174/176 (99%)	104 (60%)	39 (22%)	31 (18%)	0	0
29	BH	147/149 (99%)	63 (43%)	52 (35%)	32 (22%)	0	0
29	DH	147/149 (99%)	73 (50%)	53 (36%)	21 (14%)	0	1
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	0	3
30	DI	139/141 (99%)	83 (60%)	38 (27%)	18 (13%)	0	1
31	BJ	140/142 (99%)	106 (76%)	20 (14%)	14 (10%)	0	3
31	DJ	140/142 (99%)	92 (66%)	30 (21%)	18 (13%)	0	1
32	BK	120/122 (98%)	83 (69%)	20 (17%)	17 (14%)	0	1
32	DK	120/122 (98%)	77 (64%)	21 (18%)	22 (18%)	0	0
33	BL	141/143 (99%)	95 (67%)	30 (21%)	16 (11%)	0	2
33	DL	141/143 (99%)	78 (55%)	42 (30%)	21 (15%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BM	134/136 (98%)	96 (72%)	24 (18%)	14 (10%)	0	3
34	DM	134/136 (98%)	94 (70%)	25 (19%)	15 (11%)	0	2
35	BN	118/120 (98%)	88 (75%)	20 (17%)	10 (8%)	1	4
35	DN	118/120 (98%)	67 (57%)	35 (30%)	16 (14%)	0	1
36	BO	114/116 (98%)	88 (77%)	17 (15%)	9 (8%)	1	6
36	DO	114/116 (98%)	79 (69%)	27 (24%)	8 (7%)	1	8
37	BP	112/114 (98%)	74 (66%)	23 (20%)	15 (13%)	0	1
37	DP	112/114 (98%)	66 (59%)	28 (25%)	18 (16%)	0	0
38	BQ	115/117 (98%)	99 (86%)	9 (8%)	7 (6%)	1	12
38	DQ	115/117 (98%)	78 (68%)	24 (21%)	13 (11%)	0	2
39	BR	101/103 (98%)	82 (81%)	11 (11%)	8 (8%)	1	6
39	DR	101/103 (98%)	70 (69%)	21 (21%)	10 (10%)	0	3
40	BS	108/110 (98%)	83 (77%)	16 (15%)	9 (8%)	1	5
40	DS	108/110 (98%)	76 (70%)	24 (22%)	8 (7%)	1	7
41	BT	91/93 (98%)	58 (64%)	20 (22%)	13 (14%)	0	1
41	DT	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	0
42	BU	100/102 (98%)	70 (70%)	16 (16%)	14 (14%)	0	1
42	DU	100/102 (98%)	51 (51%)	27 (27%)	22 (22%)	0	0
43	BV	92/94 (98%)	77 (84%)	14 (15%)	1 (1%)	14	51
43	DV	92/94 (98%)	65 (71%)	22 (24%)	5 (5%)	2	14
44	BW	77/79 (98%)	31 (40%)	18 (23%)	28 (36%)	0	0
44	DW	77/79 (98%)	32 (42%)	26 (34%)	19 (25%)	0	0
45	BX	75/77 (97%)	58 (77%)	13 (17%)	4 (5%)	2	15
45	DX	75/77 (97%)	48 (64%)	19 (25%)	8 (11%)	0	2
46	BY	61/63 (97%)	40 (66%)	13 (21%)	8 (13%)	0	1
46	DY	61/63 (97%)	43 (70%)	13 (21%)	5 (8%)	1	5
47	BZ	56/58 (97%)	43 (77%)	10 (18%)	3 (5%)	2	14
47	DZ	56/58 (97%)	34 (61%)	16 (29%)	6 (11%)	0	2
48	B0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	0	3
48	D0	54/56 (96%)	40 (74%)	7 (13%)	7 (13%)	0	1
49	B1	48/50 (96%)	35 (73%)	10 (21%)	3 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	D1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	0	3
50	B2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	6	34
50	D2	44/46 (96%)	30 (68%)	7 (16%)	7 (16%)	0	0
51	B3	62/64 (97%)	51 (82%)	8 (13%)	3 (5%)	2	17
51	D3	62/64 (97%)	40 (64%)	17 (27%)	5 (8%)	1	5
52	B4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	1	5
52	D4	36/38 (95%)	22 (61%)	9 (25%)	5 (14%)	0	1
54	CG	148/150 (99%)	98 (66%)	42 (28%)	8 (5%)	2	14
55	CM	111/113 (98%)	63 (57%)	36 (32%)	12 (11%)	0	2
56	CP	78/80 (98%)	49 (63%)	19 (24%)	10 (13%)	0	1
59	DF	176/178 (99%)	98 (56%)	44 (25%)	34 (19%)	0	0
All	All	11238/11447 (98%)	7571 (67%)	2387 (21%)	1280 (11%)	0	2

5 of 1280 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	20	ARG
2	AB	40	ILE
2	AB	72	LYS
2	AB	75	ALA
2	AB	119	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	142 (79%)	38 (21%)	1	6
2	CB	180/180 (100%)	156 (87%)	24 (13%)	4	18
3	AC	170/170 (100%)	142 (84%)	28 (16%)	2	10
3	CC	170/170 (100%)	152 (89%)	18 (11%)	6	27
4	AD	172/172 (100%)	146 (85%)	26 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	172/172 (100%)	140 (81%)	32 (19%)	1	8
5	AE	113/113 (100%)	90 (80%)	23 (20%)	1	6
5	CE	113/113 (100%)	94 (83%)	19 (17%)	2	10
6	AF	87/87 (100%)	75 (86%)	12 (14%)	3	16
6	CF	87/87 (100%)	75 (86%)	12 (14%)	3	16
7	AG	124/124 (100%)	108 (87%)	16 (13%)	4	19
8	AH	104/104 (100%)	87 (84%)	17 (16%)	2	11
8	CH	104/104 (100%)	87 (84%)	17 (16%)	2	11
9	AI	105/105 (100%)	84 (80%)	21 (20%)	1	6
9	CI	105/105 (100%)	89 (85%)	16 (15%)	3	13
10	AJ	86/86 (100%)	72 (84%)	14 (16%)	2	11
10	CJ	86/86 (100%)	77 (90%)	9 (10%)	7	28
11	AK	90/90 (100%)	73 (81%)	17 (19%)	1	8
11	CK	90/90 (100%)	77 (86%)	13 (14%)	3	15
12	AL	103/103 (100%)	82 (80%)	21 (20%)	1	6
12	CL	103/103 (100%)	86 (84%)	17 (16%)	2	10
13	AM	92/92 (100%)	87 (95%)	5 (5%)	22	58
14	AN	79/83 (95%)	72 (91%)	7 (9%)	9	35
14	CN	79/83 (95%)	67 (85%)	12 (15%)	3	13
15	AO	76/76 (100%)	67 (88%)	9 (12%)	5	23
15	CO	76/76 (100%)	69 (91%)	7 (9%)	9	33
16	AP	65/65 (100%)	57 (88%)	8 (12%)	4	21
17	AQ	74/74 (100%)	58 (78%)	16 (22%)	1	5
17	CQ	74/74 (100%)	61 (82%)	13 (18%)	2	9
18	AR	48/48 (100%)	46 (96%)	2 (4%)	30	65
18	CR	48/48 (100%)	44 (92%)	4 (8%)	11	40
19	AS	70/70 (100%)	61 (87%)	9 (13%)	4	19
19	CS	70/70 (100%)	62 (89%)	8 (11%)	5	24
20	AT	65/65 (100%)	49 (75%)	16 (25%)	0	2
20	CT	65/65 (100%)	53 (82%)	12 (18%)	1	8
21	AU	44/44 (100%)	33 (75%)	11 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	44/44 (100%)	33 (75%)	11 (25%)	0	2
24	BC	216/216 (100%)	169 (78%)	47 (22%)	1	5
24	DC	216/216 (100%)	189 (88%)	27 (12%)	4	21
25	BD	164/164 (100%)	131 (80%)	33 (20%)	1	6
25	DD	164/164 (100%)	141 (86%)	23 (14%)	3	16
26	BE	165/165 (100%)	123 (74%)	42 (26%)	0	2
26	DE	165/165 (100%)	147 (89%)	18 (11%)	6	26
27	BF	148/148 (100%)	127 (86%)	21 (14%)	3	15
28	BG	137/137 (100%)	108 (79%)	29 (21%)	1	5
28	DG	137/137 (100%)	118 (86%)	19 (14%)	3	16
29	BH	114/114 (100%)	96 (84%)	18 (16%)	2	12
29	DH	114/114 (100%)	94 (82%)	20 (18%)	2	9
30	BI	109/109 (100%)	91 (84%)	18 (16%)	2	10
30	DI	109/109 (100%)	102 (94%)	7 (6%)	17	52
31	BJ	116/116 (100%)	87 (75%)	29 (25%)	0	2
31	DJ	116/116 (100%)	102 (88%)	14 (12%)	5	22
32	BK	103/103 (100%)	86 (84%)	17 (16%)	2	10
32	DK	103/103 (100%)	81 (79%)	22 (21%)	1	5
33	BL	102/102 (100%)	77 (76%)	25 (24%)	0	2
33	DL	102/102 (100%)	87 (85%)	15 (15%)	3	14
34	BM	109/109 (100%)	85 (78%)	24 (22%)	1	5
34	DM	109/109 (100%)	97 (89%)	12 (11%)	6	26
35	BN	100/100 (100%)	77 (77%)	23 (23%)	1	3
35	DN	100/100 (100%)	82 (82%)	18 (18%)	1	9
36	BO	86/86 (100%)	69 (80%)	17 (20%)	1	7
36	DO	86/86 (100%)	79 (92%)	7 (8%)	11	42
37	BP	99/99 (100%)	69 (70%)	30 (30%)	0	0
37	DP	99/99 (100%)	88 (89%)	11 (11%)	6	25
38	BQ	89/89 (100%)	75 (84%)	14 (16%)	2	12
38	DQ	89/89 (100%)	75 (84%)	14 (16%)	2	12
39	BR	84/84 (100%)	68 (81%)	16 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DR	84/84 (100%)	71 (84%)	13 (16%)	2	12
40	BS	93/93 (100%)	71 (76%)	22 (24%)	1	3
40	DS	93/93 (100%)	77 (83%)	16 (17%)	2	10
41	BT	80/80 (100%)	59 (74%)	21 (26%)	0	2
41	DT	80/80 (100%)	74 (92%)	6 (8%)	13	45
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	6
42	DU	83/83 (100%)	72 (87%)	11 (13%)	4	18
43	BV	78/78 (100%)	59 (76%)	19 (24%)	0	2
43	DV	78/78 (100%)	67 (86%)	11 (14%)	3	16
44	BW	59/59 (100%)	42 (71%)	17 (29%)	0	1
44	DW	59/59 (100%)	46 (78%)	13 (22%)	1	5
45	BX	67/67 (100%)	51 (76%)	16 (24%)	0	3
45	DX	67/67 (100%)	58 (87%)	9 (13%)	4	18
46	BY	55/55 (100%)	42 (76%)	13 (24%)	1	3
46	DY	55/55 (100%)	52 (94%)	3 (6%)	21	57
47	BZ	48/48 (100%)	34 (71%)	14 (29%)	0	1
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	2	10
48	B0	47/47 (100%)	38 (81%)	9 (19%)	1	8
48	D0	47/47 (100%)	40 (85%)	7 (15%)	3	14
49	B1	45/45 (100%)	36 (80%)	9 (20%)	1	6
49	D1	45/45 (100%)	41 (91%)	4 (9%)	9	35
50	B2	38/38 (100%)	31 (82%)	7 (18%)	1	8
50	D2	38/38 (100%)	34 (90%)	4 (10%)	7	28
51	B3	51/51 (100%)	44 (86%)	7 (14%)	3	17
51	D3	51/51 (100%)	42 (82%)	9 (18%)	2	9
52	B4	34/34 (100%)	29 (85%)	5 (15%)	3	14
52	D4	34/34 (100%)	27 (79%)	7 (21%)	1	6
54	CG	123/123 (100%)	101 (82%)	22 (18%)	2	9
55	CM	91/91 (100%)	80 (88%)	11 (12%)	5	22
56	CP	65/65 (100%)	52 (80%)	13 (20%)	1	6
59	DF	149/149 (100%)	123 (83%)	26 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9331/9339 (100%)	7772 (83%)	1559 (17%)	2 10

5 of 1559 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	BR	25	LEU
49	B1	35	LEU
39	DR	13	ARG
40	BS	33	LEU
43	BV	43	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 333 such sidechains are listed below:

Mol	Chain	Res	Type
41	BT	72	GLN
3	CC	7	ASN
41	DT	48	GLN
43	BV	5	ASN
50	B2	6	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	478 (31%)	237 (15%)
22	BA	2850/2903 (98%)	829 (29%)	411 (14%)
23	BB	117/118 (99%)	31 (26%)	17 (14%)
53	CA	1529/1530 (99%)	540 (35%)	242 (15%)
57	DA	2838/2904 (97%)	1042 (36%)	504 (17%)
58	DB	116/117 (99%)	37 (31%)	17 (14%)
All	All	8982/9105 (98%)	2957 (32%)	1428 (15%)

5 of 2957 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A
1	AA	9	G

5 of 1428 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2880	C
53	CA	816	A
57	DA	2289	G
23	BB	109	A
53	CA	331	G

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 365 ligands modelled in this entry, 364 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	CLM	BA	3136	-	19,20,20	2.56	4 (21%)	23,27,27	2.08	7 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	CLM	BA	3136	-	-	2/20/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BA	3136	CLM	O9B-N9	7.70	1.35	1.22
61	BA	3136	CLM	C11-C6	5.42	1.47	1.39
61	BA	3136	CLM	C2-N2	4.05	1.42	1.34
61	BA	3136	CLM	C8-C9	2.51	1.43	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	BA	3136	CLM	C3-N2-C2	-5.07	114.11	123.07
61	BA	3136	CLM	C6-C5-C3	4.57	119.68	111.64
61	BA	3136	CLM	C4-C3-N2	3.04	114.10	109.27
61	BA	3136	CLM	O4-C4-C3	3.00	118.37	111.09
61	BA	3136	CLM	O5-C5-C3	2.64	115.05	107.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

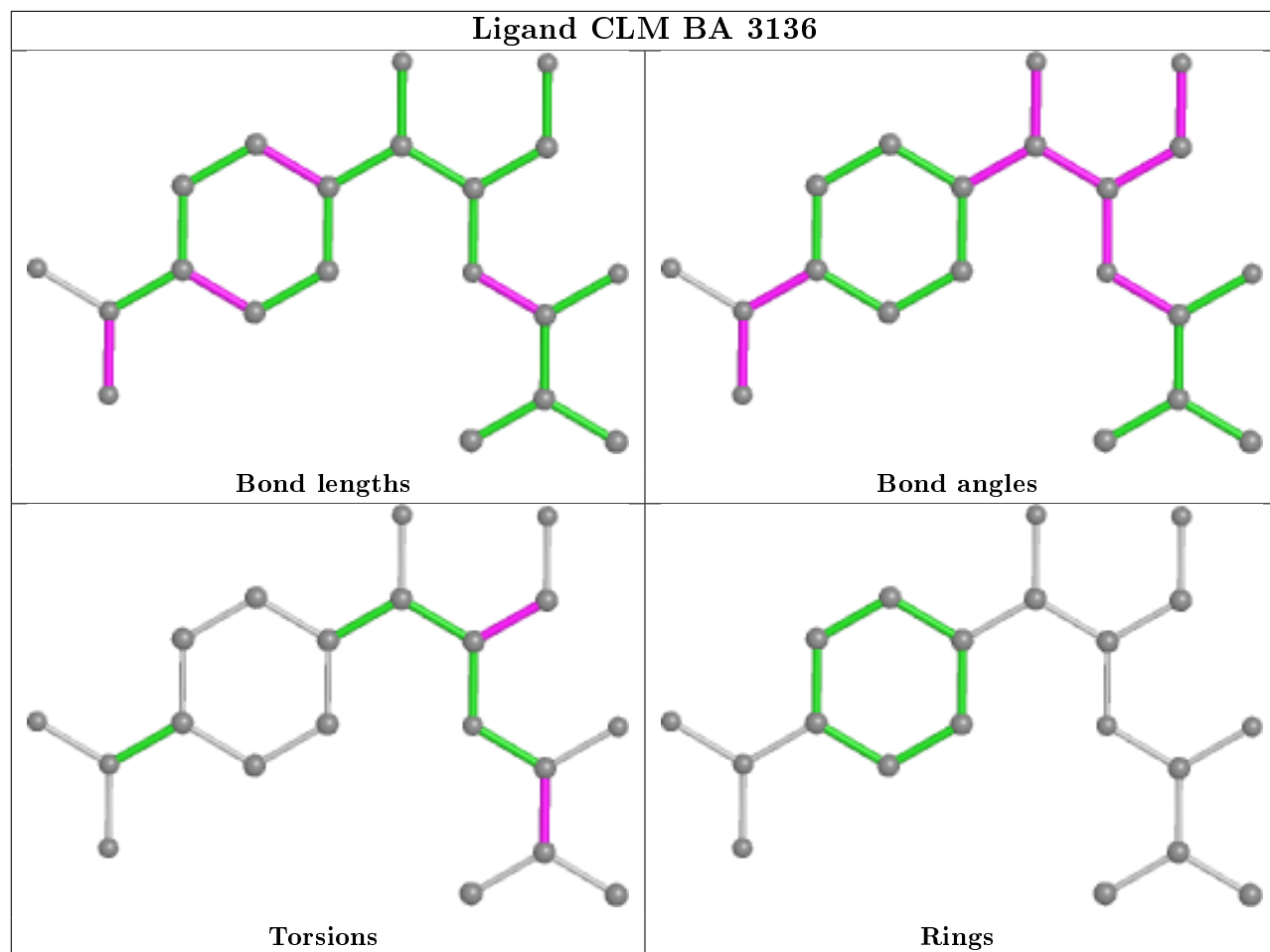
Mol	Chain	Res	Type	Atoms
61	BA	3136	CLM	N2-C3-C4-O4
61	BA	3136	CLM	CL2-C1-C2-N2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	BA	3136	CLM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1533/1533 (100%)	-0.64	16 (1%) 82 72	28, 82, 201, 415	0
2	AB	218/218 (100%)	1.62	69 (31%) 0 0	117, 160, 233, 278	0
2	CB	218/218 (100%)	1.15	42 (19%) 1 1	121, 173, 237, 292	0
3	AC	206/206 (100%)	0.48	13 (6%) 20 11	64, 107, 164, 196	0
3	CC	206/206 (100%)	1.04	27 (13%) 3 2	79, 158, 229, 303	0
4	AD	205/205 (100%)	-0.08	6 (2%) 51 36	45, 89, 164, 275	0
4	CD	205/205 (100%)	-0.30	1 (0%) 91 86	39, 61, 122, 254	0
5	AE	150/150 (100%)	-0.17	1 (0%) 87 81	57, 81, 142, 210	0
5	CE	150/150 (100%)	0.33	3 (2%) 65 51	67, 99, 157, 252	0
6	AF	100/100 (100%)	0.08	4 (4%) 38 25	55, 103, 161, 189	0
6	CF	100/100 (100%)	-0.05	1 (1%) 82 72	72, 116, 176, 217	0
7	AG	151/151 (100%)	0.46	13 (8%) 10 5	88, 150, 218, 247	0
8	AH	129/129 (100%)	0.14	7 (5%) 25 14	44, 82, 127, 184	0
8	CH	129/129 (100%)	0.60	8 (6%) 20 11	68, 113, 170, 246	0
9	AI	127/127 (100%)	0.99	24 (18%) 1 1	72, 154, 248, 287	0
9	CI	127/127 (100%)	1.95	50 (39%) 0 0	116, 201, 289, 319	0
10	AJ	98/98 (100%)	0.73	16 (16%) 1 1	78, 127, 203, 244	0
10	CJ	98/98 (100%)	2.74	54 (55%) 0 0	114, 204, 278, 301	0
11	AK	117/117 (100%)	0.81	15 (12%) 3 2	47, 117, 196, 238	0
11	CK	117/117 (100%)	0.22	5 (4%) 35 22	68, 117, 175, 239	0
12	AL	123/123 (100%)	-0.18	1 (0%) 86 78	24, 57, 121, 180	0
12	CL	123/123 (100%)	0.44	7 (5%) 23 13	44, 89, 144, 226	0
13	AM	114/114 (100%)	0.63	15 (13%) 3 2	90, 158, 240, 281	0
14	AN	96/100 (96%)	0.44	12 (12%) 3 2	76, 122, 214, 271	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	CN	95/100 (95%)	2.51	44 (46%) 0 0	123, 239, 369, 399	0
15	AO	88/88 (100%)	-0.42	0 100 100	40, 81, 123, 187	0
15	CO	88/88 (100%)	-0.00	0 100 100	76, 122, 190, 265	0
16	AP	82/82 (100%)	0.47	8 (9%) 7 4	46, 79, 155, 228	0
17	AQ	80/80 (100%)	0.38	6 (7%) 14 8	36, 79, 146, 244	0
17	CQ	80/80 (100%)	0.96	10 (12%) 3 2	61, 112, 163, 194	0
18	AR	55/55 (100%)	0.20	2 (3%) 42 27	60, 92, 174, 242	0
18	CR	55/55 (100%)	-0.01	0 100 100	48, 91, 159, 236	0
19	AS	79/79 (100%)	1.23	22 (27%) 0 0	95, 156, 236, 256	0
19	CS	79/79 (100%)	2.85	45 (56%) 0 0	206, 416, 490, 515	0
20	AT	85/85 (100%)	-0.26	0 100 100	46, 83, 124, 174	0
20	CT	85/85 (100%)	1.06	17 (20%) 1 1	76, 142, 200, 234	0
21	AU	51/51 (100%)	1.82	21 (41%) 0 0	91, 152, 216, 243	0
21	CU	51/51 (100%)	0.50	3 (5%) 22 13	82, 115, 208, 290	0
22	BA	2854/2903 (98%)	-0.56	38 (1%) 77 65	7, 31, 162, 401	0
23	BB	118/118 (100%)	-0.70	0 100 100	20, 45, 78, 115	0
24	BC	271/271 (100%)	-0.37	5 (1%) 68 55	13, 41, 96, 201	0
24	DC	271/271 (100%)	0.61	29 (10%) 6 3	45, 101, 160, 200	0
25	BD	209/209 (100%)	-0.48	0 100 100	7, 29, 80, 144	0
25	DD	209/209 (100%)	0.92	37 (17%) 1 1	60, 123, 193, 270	0
26	BE	201/201 (100%)	-0.37	0 100 100	7, 42, 105, 189	0
26	DE	201/201 (100%)	1.85	72 (35%) 0 0	68, 254, 429, 475	0
27	BF	177/177 (100%)	0.03	5 (2%) 53 37	33, 78, 142, 205	0
28	BG	176/176 (100%)	-0.12	2 (1%) 80 69	23, 62, 124, 215	0
28	DG	176/176 (100%)	2.07	80 (45%) 0 0	79, 207, 297, 363	0
29	BH	149/149 (100%)	3.00	61 (40%) 0 0	41, 178, 274, 301	0
29	DH	149/149 (100%)	2.64	63 (42%) 0 0	93, 182, 270, 305	0
30	BI	141/141 (100%)	2.33	64 (45%) 0 0	171, 257, 316, 355	0
30	DI	141/141 (100%)	3.92	101 (71%) 0 0	227, 344, 382, 400	0
31	BJ	142/142 (100%)	-0.55	0 100 100	9, 23, 68, 127	0
31	DJ	142/142 (100%)	0.62	15 (10%) 6 3	63, 122, 184, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
32	BK	122/122 (100%)	-0.51	0 100 100	14, 31, 84, 254	0
32	DK	122/122 (100%)	0.78	18 (14%) 2 1	57, 106, 172, 204	0
33	BL	143/143 (100%)	-0.53	0 100 100	9, 37, 80, 126	0
33	DL	143/143 (100%)	1.53	45 (31%) 0 0	68, 176, 296, 329	0
34	BM	136/136 (100%)	-0.56	0 100 100	9, 29, 71, 133	0
34	DM	136/136 (100%)	0.84	19 (13%) 2 1	47, 126, 187, 223	0
35	BN	120/120 (100%)	-0.55	0 100 100	10, 25, 48, 123	0
35	DN	120/120 (100%)	1.56	42 (35%) 0 0	90, 149, 231, 305	0
36	BO	116/116 (100%)	-0.33	0 100 100	28, 49, 93, 126	0
36	DO	116/116 (100%)	1.51	35 (30%) 0 0	132, 176, 238, 280	0
37	BP	114/114 (100%)	-0.37	1 (0%) 84 75	17, 39, 95, 184	0
37	DP	114/114 (100%)	1.07	22 (19%) 1 1	63, 122, 187, 204	0
38	BQ	117/117 (100%)	-0.64	0 100 100	7, 20, 46, 100	0
38	DQ	117/117 (100%)	0.99	21 (17%) 1 1	78, 127, 221, 298	0
39	BR	103/103 (100%)	-0.51	1 (0%) 82 72	7, 34, 78, 139	0
39	DR	103/103 (100%)	2.41	50 (48%) 0 0	80, 157, 275, 306	0
40	BS	110/110 (100%)	-0.58	0 100 100	8, 23, 56, 172	0
40	DS	110/110 (100%)	1.70	40 (36%) 0 0	69, 142, 254, 323	0
41	BT	93/93 (100%)	-0.12	2 (2%) 62 48	22, 53, 135, 194	0
41	DT	93/93 (100%)	2.14	38 (40%) 0 0	125, 241, 359, 398	0
42	BU	102/102 (100%)	-0.11	1 (0%) 82 72	22, 54, 111, 237	0
42	DU	102/102 (100%)	3.84	64 (62%) 0 0	135, 334, 460, 561	0
43	BV	94/94 (100%)	-0.30	0 100 100	18, 47, 89, 149	0
43	DV	94/94 (100%)	1.09	20 (21%) 0 1	109, 156, 208, 233	0
44	BW	79/79 (100%)	-0.19	2 (2%) 57 43	13, 36, 90, 194	0
44	DW	79/79 (100%)	2.00	35 (44%) 0 0	99, 166, 250, 315	0
45	BX	77/77 (100%)	-0.43	0 100 100	17, 42, 87, 113	0
45	DX	77/77 (100%)	0.78	12 (15%) 2 1	72, 122, 190, 222	0
46	BY	63/63 (100%)	-0.18	1 (1%) 72 59	34, 73, 121, 155	0
46	DY	63/63 (100%)	1.65	20 (31%) 0 0	159, 374, 464, 494	0
47	BZ	58/58 (100%)	-0.55	0 100 100	7, 26, 61, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	DZ	58/58 (100%)	0.60	5 (8%) 10 5	80, 142, 228, 257	0
48	B0	56/56 (100%)	-0.71	0 100 100	6, 26, 80, 127	0
48	D0	56/56 (100%)	1.28	12 (21%) 0 1	75, 148, 244, 284	0
49	B1	50/50 (100%)	0.72	3 (6%) 21 12	42, 66, 121, 173	0
49	D1	50/50 (100%)	2.09	24 (48%) 0 0	114, 179, 216, 264	0
50	B2	46/46 (100%)	-0.60	0 100 100	11, 27, 56, 164	0
50	D2	46/46 (100%)	1.27	9 (19%) 1 1	79, 130, 179, 205	0
51	B3	64/64 (100%)	-0.59	0 100 100	11, 29, 53, 81	0
51	D3	64/64 (100%)	1.69	24 (37%) 0 0	85, 145, 232, 281	0
52	B4	38/38 (100%)	0.17	1 (2%) 56 40	29, 53, 95, 103	0
52	D4	38/38 (100%)	2.60	24 (63%) 0 0	87, 165, 229, 248	0
53	CA	1530/1530 (100%)	-0.10	38 (2%) 57 43	43, 110, 301, 420	0
54	CG	150/150 (100%)	2.22	70 (46%) 0 0	101, 233, 303, 344	0
55	CM	113/113 (100%)	2.49	63 (55%) 0 0	226, 447, 522, 562	0
56	CP	80/80 (100%)	0.92	16 (20%) 1 1	49, 105, 165, 226	0
57	DA	2841/2904 (97%)	0.17	82 (2%) 51 36	51, 132, 279, 491	0
58	DB	117/117 (100%)	-0.23	0 100 100	107, 180, 240, 264	0
59	DF	178/178 (100%)	2.38	101 (56%) 0 0	175, 239, 286, 345	0
All	All	20431/20552 (99%)	0.31	2121 (10%) 6 4	6, 103, 285, 562	0

The worst 5 of 2121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	DH	92	GLY	21.7
14	CN	33	VAL	20.2
29	DH	124	THR	20.0
30	DI	51	GLY	19.6
29	DH	91	PHE	17.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	DA	3124	1/1	0.10	0.50	211,211,211,211	0
60	MG	DA	3025	1/1	0.12	1.43	253,253,253,253	0
60	MG	DA	3063	1/1	0.26	0.97	305,305,305,305	0
60	MG	DA	3062	1/1	0.27	2.37	262,262,262,262	0
60	MG	DA	3130	1/1	0.41	1.45	305,305,305,305	0
60	MG	DA	3019	1/1	0.48	0.89	252,252,252,252	0
60	MG	DA	3061	1/1	0.49	0.61	210,210,210,210	0
60	MG	DA	3037	1/1	0.50	0.18	203,203,203,203	0
60	MG	CA	1602	1/1	0.54	0.17	131,131,131,131	0
60	MG	DA	3105	1/1	0.54	0.23	305,305,305,305	0
60	MG	DA	3083	1/1	0.55	0.10	176,176,176,176	0
60	MG	DA	3127	1/1	0.56	1.91	274,274,274,274	0
60	MG	DE	301	1/1	0.58	0.31	191,191,191,191	0
60	MG	DA	3117	1/1	0.61	0.12	99,99,99,99	0
60	MG	DA	3085	1/1	0.62	0.16	127,127,127,127	0
60	MG	DA	3026	1/1	0.62	0.20	139,139,139,139	0
60	MG	DA	3011	1/1	0.63	0.27	215,215,215,215	0
60	MG	DA	3048	1/1	0.63	0.16	243,243,243,243	0
60	MG	DA	3075	1/1	0.63	0.51	229,229,229,229	0
60	MG	DJ	201	1/1	0.65	1.44	331,331,331,331	0
60	MG	DA	3044	1/1	0.66	0.13	230,230,230,230	0
60	MG	DA	3002	1/1	0.67	0.39	229,229,229,229	0
60	MG	CA	1630	1/1	0.69	0.12	176,176,176,176	0
60	MG	DA	3090	1/1	0.70	0.20	209,209,209,209	0
60	MG	DA	3077	1/1	0.71	0.79	259,259,259,259	0
60	MG	BA	3054	1/1	0.72	0.21	214,214,214,214	0
60	MG	DA	3030	1/1	0.72	0.20	66,66,66,66	0
60	MG	DA	3122	1/1	0.72	0.11	155,155,155,155	0
60	MG	DA	3008	1/1	0.72	0.23	153,153,153,153	0
60	MG	DA	3072	1/1	0.73	0.12	193,193,193,193	0
60	MG	DA	3107	1/1	0.73	0.60	201,201,201,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3068	1/1	0.73	0.11	174,174,174,174	0
60	MG	DA	3007	1/1	0.74	0.50	188,188,188,188	0
60	MG	DA	3073	1/1	0.74	1.21	276,276,276,276	0
60	MG	DA	3133	1/1	0.74	0.26	241,241,241,241	0
60	MG	DA	3108	1/1	0.74	0.31	123,123,123,123	0
60	MG	DA	3132	1/1	0.75	0.24	225,225,225,225	0
60	MG	DA	3017	1/1	0.76	0.23	147,147,147,147	0
60	MG	DA	3006	1/1	0.76	0.12	149,149,149,149	0
60	MG	DA	3110	1/1	0.76	0.24	174,174,174,174	0
60	MG	CA	1629	1/1	0.76	0.20	214,214,214,214	0
60	MG	AN	201	1/1	0.77	0.20	219,219,219,219	0
60	MG	DA	3109	1/1	0.77	0.33	169,169,169,169	0
60	MG	DA	3041	1/1	0.77	0.20	133,133,133,133	0
60	MG	CA	1622	1/1	0.77	0.12	196,196,196,196	0
60	MG	CA	1615	1/1	0.78	0.18	243,243,243,243	0
60	MG	DA	3023	1/1	0.78	0.18	90,90,90,90	0
60	MG	CA	1618	1/1	0.78	0.17	141,141,141,141	0
60	MG	DA	3013	1/1	0.78	0.36	209,209,209,209	0
60	MG	DA	3082	1/1	0.79	0.11	214,214,214,214	0
60	MG	AA	1610	1/1	0.79	0.08	200,200,200,200	0
60	MG	BA	3135	1/1	0.79	0.38	204,204,204,204	0
60	MG	CA	1623	1/1	0.80	0.12	79,79,79,79	0
60	MG	CA	1617	1/1	0.80	0.14	205,205,205,205	0
60	MG	DA	3027	1/1	0.80	0.54	277,277,277,277	0
60	MG	CA	1628	1/1	0.81	0.34	259,259,259,259	0
60	MG	BB	201	1/1	0.81	0.22	246,246,246,246	0
60	MG	DA	3024	1/1	0.81	0.14	147,147,147,147	0
60	MG	DA	3005	1/1	0.82	0.43	280,280,280,280	0
60	MG	CA	1601	1/1	0.82	0.08	123,123,123,123	0
60	MG	BA	3024	1/1	0.82	0.35	206,206,206,206	0
60	MG	CA	1616	1/1	0.82	0.35	279,279,279,279	0
60	MG	DA	3098	1/1	0.83	0.22	218,218,218,218	0
60	MG	BA	3058	1/1	0.83	0.18	106,106,106,106	0
60	MG	DA	3125	1/1	0.83	0.10	132,132,132,132	0
60	MG	BA	3086	1/1	0.83	0.20	144,144,144,144	0
60	MG	CA	1610	1/1	0.84	0.09	220,220,220,220	0
60	MG	DA	3056	1/1	0.84	0.37	243,243,243,243	0
60	MG	DA	3032	1/1	0.84	0.19	193,193,193,193	0
60	MG	DA	3050	1/1	0.84	0.17	89,89,89,89	0
60	MG	DA	3028	1/1	0.84	0.39	195,195,195,195	0
60	MG	DA	3046	1/1	0.84	0.17	152,152,152,152	0
60	MG	AA	1618	1/1	0.85	0.68	217,217,217,217	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	CA	1612	1/1	0.85	0.26	133,133,133,133	0
60	MG	BA	3097	1/1	0.85	0.15	182,182,182,182	0
60	MG	DA	3070	1/1	0.85	0.20	61,61,61,61	0
60	MG	DA	3040	1/1	0.86	0.21	120,120,120,120	0
60	MG	DA	3001	1/1	0.86	0.12	149,149,149,149	0
60	MG	BA	3092	1/1	0.86	0.07	30,30,30,30	0
60	MG	DA	3126	1/1	0.86	0.17	129,129,129,129	0
60	MG	DA	3068	1/1	0.87	0.28	225,225,225,225	0
60	MG	DA	3091	1/1	0.87	0.16	167,167,167,167	0
60	MG	DA	3103	1/1	0.87	0.16	36,36,36,36	0
60	MG	DA	3074	1/1	0.87	0.45	239,239,239,239	0
60	MG	DA	3003	1/1	0.87	0.97	253,253,253,253	0
60	MG	DA	3057	1/1	0.88	0.39	257,257,257,257	0
60	MG	CA	1642	1/1	0.88	0.07	121,121,121,121	0
60	MG	CA	1606	1/1	0.88	0.14	77,77,77,77	0
60	MG	DA	3045	1/1	0.88	0.14	76,76,76,76	0
60	MG	DA	3087	1/1	0.88	0.15	178,178,178,178	0
60	MG	CA	1632	1/1	0.88	0.17	143,143,143,143	0
60	MG	DA	3004	1/1	0.89	0.16	86,86,86,86	0
60	MG	BA	3044	1/1	0.89	0.16	56,56,56,56	0
60	MG	DA	3010	1/1	0.89	0.65	261,261,261,261	0
60	MG	DA	3101	1/1	0.89	0.11	73,73,73,73	0
60	MG	AA	1603	1/1	0.89	0.10	131,131,131,131	0
60	MG	CA	1640	1/1	0.89	0.29	171,171,171,171	0
60	MG	CA	1608	1/1	0.89	0.22	82,82,82,82	0
60	MG	DA	3119	1/1	0.89	0.22	84,84,84,84	0
60	MG	DA	3079	1/1	0.89	0.13	149,149,149,149	0
60	MG	DA	3012	1/1	0.89	0.12	57,57,57,57	0
60	MG	BA	3069	1/1	0.89	0.19	223,223,223,223	0
60	MG	DA	3112	1/1	0.89	0.08	114,114,114,114	0
60	MG	CA	1614	1/1	0.89	0.65	271,271,271,271	0
60	MG	AA	1617	1/1	0.90	0.13	111,111,111,111	0
60	MG	BA	3117	1/1	0.90	0.09	79,79,79,79	0
60	MG	DA	3029	1/1	0.90	0.17	135,135,135,135	0
60	MG	DB	201	1/1	0.90	0.12	109,109,109,109	0
60	MG	DA	3014	1/1	0.90	0.40	177,177,177,177	0
60	MG	DA	3071	1/1	0.90	0.09	136,136,136,136	0
60	MG	AA	1614	1/1	0.90	0.54	201,201,201,201	0
60	MG	CA	1634	1/1	0.90	0.16	200,200,200,200	0
60	MG	DA	3069	1/1	0.90	0.12	93,93,93,93	0
60	MG	BA	3132	1/1	0.90	0.40	145,145,145,145	0
60	MG	BA	3004	1/1	0.90	0.13	150,150,150,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3022	1/1	0.90	0.17	118,118,118,118	0
60	MG	BA	3103	1/1	0.90	0.20	8,8,8,8	0
60	MG	DA	3094	1/1	0.91	0.21	98,98,98,98	0
60	MG	DA	3043	1/1	0.91	0.22	112,112,112,112	0
60	MG	DA	3129	1/1	0.91	0.62	271,271,271,271	0
60	MG	DA	3095	1/1	0.91	0.15	110,110,110,110	0
60	MG	CA	1607	1/1	0.91	0.21	222,222,222,222	0
60	MG	DA	3042	1/1	0.91	0.14	166,166,166,166	0
60	MG	DA	3086	1/1	0.91	0.10	185,185,185,185	0
60	MG	DA	3031	1/1	0.91	0.10	121,121,121,121	0
60	MG	DC	301	1/1	0.91	0.15	134,134,134,134	0
60	MG	CA	1611	1/1	0.91	0.18	116,116,116,116	0
60	MG	DA	3058	1/1	0.91	0.10	204,204,204,204	0
60	MG	DA	3096	1/1	0.91	0.29	180,180,180,180	0
60	MG	BA	3022	1/1	0.91	0.11	20,20,20,20	0
60	MG	CA	1624	1/1	0.91	0.31	123,123,123,123	0
60	MG	DA	3121	1/1	0.91	0.15	114,114,114,114	0
60	MG	DA	3084	1/1	0.91	0.26	157,157,157,157	0
60	MG	BA	3089	1/1	0.91	0.08	39,39,39,39	0
60	MG	AA	1627	1/1	0.91	0.17	165,165,165,165	0
60	MG	DA	3078	1/1	0.92	0.11	95,95,95,95	0
60	MG	DA	3097	1/1	0.92	0.20	143,143,143,143	0
60	MG	DA	3049	1/1	0.92	0.14	150,150,150,150	0
60	MG	BA	3047	1/1	0.92	0.13	112,112,112,112	0
60	MG	AA	1620	1/1	0.92	0.08	120,120,120,120	0
62	ZN	D4	101	1/1	0.92	0.09	197,197,197,197	0
60	MG	BA	3094	1/1	0.92	0.07	42,42,42,42	0
60	MG	AA	1639	1/1	0.92	0.06	92,92,92,92	0
60	MG	AA	1638	1/1	0.92	0.11	139,139,139,139	0
60	MG	CA	1631	1/1	0.92	0.20	111,111,111,111	0
60	MG	CA	1637	1/1	0.92	0.19	140,140,140,140	0
60	MG	DA	3100	1/1	0.92	0.24	149,149,149,149	0
60	MG	BB	202	1/1	0.93	0.09	54,54,54,54	0
60	MG	DA	3131	1/1	0.93	0.10	104,104,104,104	0
60	MG	BA	3087	1/1	0.93	0.12	182,182,182,182	0
60	MG	AA	1623	1/1	0.93	0.07	104,104,104,104	0
60	MG	DA	3060	1/1	0.93	0.07	144,144,144,144	0
60	MG	DA	3053	1/1	0.93	0.10	78,78,78,78	0
60	MG	DA	3067	1/1	0.93	0.11	95,95,95,95	0
60	MG	CA	1627	1/1	0.93	0.33	220,220,220,220	0
60	MG	DA	3052	1/1	0.93	0.20	105,105,105,105	0
60	MG	DA	3120	1/1	0.93	0.14	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3090	1/1	0.93	0.14	93,93,93,93	0
60	MG	BA	3012	1/1	0.93	0.13	5,5,5,5	0
60	MG	DA	3034	1/1	0.93	0.21	156,156,156,156	0
60	MG	BA	3134	1/1	0.93	0.11	145,145,145,145	0
60	MG	BA	3003	1/1	0.94	0.13	44,44,44,44	0
60	MG	BA	3002	1/1	0.94	0.09	60,60,60,60	0
60	MG	BA	3055	1/1	0.94	0.36	240,240,240,240	0
60	MG	BA	3001	1/1	0.94	0.07	84,84,84,84	0
60	MG	CA	1620	1/1	0.94	0.20	209,209,209,209	0
60	MG	DA	3038	1/1	0.94	0.18	163,163,163,163	0
60	MG	DA	3081	1/1	0.94	0.22	143,143,143,143	0
60	MG	DA	3059	1/1	0.94	0.38	241,241,241,241	0
60	MG	DA	3123	1/1	0.94	0.14	65,65,65,65	0
60	MG	AA	1604	1/1	0.94	0.10	112,112,112,112	0
60	MG	AA	1607	1/1	0.94	0.10	98,98,98,98	0
60	MG	DA	3018	1/1	0.94	0.21	225,225,225,225	0
60	MG	AA	1629	1/1	0.94	0.14	227,227,227,227	0
60	MG	CA	1639	1/1	0.94	0.06	148,148,148,148	0
60	MG	DA	3128	1/1	0.94	0.26	138,138,138,138	0
60	MG	AA	1622	1/1	0.94	0.16	185,185,185,185	0
60	MG	BA	3075	1/1	0.94	0.19	74,74,74,74	0
60	MG	DA	3102	1/1	0.94	0.16	105,105,105,105	0
60	MG	DA	3016	1/1	0.95	0.12	75,75,75,75	0
60	MG	AA	1630	1/1	0.95	0.14	209,209,209,209	0
60	MG	DA	3009	1/1	0.95	0.11	75,75,75,75	0
60	MG	CA	1604	1/1	0.95	0.04	65,65,65,65	0
60	MG	BA	3041	1/1	0.95	0.14	12,12,12,12	0
60	MG	CA	1641	1/1	0.95	0.18	73,73,73,73	0
60	MG	DA	3106	1/1	0.95	0.10	55,55,55,55	0
60	MG	BA	3091	1/1	0.95	0.14	131,131,131,131	0
60	MG	CA	1613	1/1	0.95	0.08	116,116,116,116	0
60	MG	BA	3124	1/1	0.95	0.16	22,22,22,22	0
60	MG	CA	1636	1/1	0.95	0.10	130,130,130,130	0
60	MG	CA	1638	1/1	0.95	0.11	106,106,106,106	0
60	MG	BA	3123	1/1	0.95	0.56	112,112,112,112	0
60	MG	DA	3051	1/1	0.95	0.09	49,49,49,49	0
60	MG	BA	3073	1/1	0.95	0.09	116,116,116,116	0
60	MG	BA	3118	1/1	0.95	0.29	136,136,136,136	0
60	MG	AA	1609	1/1	0.95	0.10	47,47,47,47	0
60	MG	BA	3114	1/1	0.95	0.15	148,148,148,148	0
60	MG	BA	3104	1/1	0.95	0.18	27,27,27,27	0
60	MG	BA	3057	1/1	0.95	0.06	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3082	1/1	0.95	0.17	98,98,98,98	0
60	MG	DA	3093	1/1	0.95	0.30	166,166,166,166	0
60	MG	DA	3076	1/1	0.95	0.08	110,110,110,110	0
60	MG	BA	3033	1/1	0.95	0.16	89,89,89,89	0
60	MG	BA	3051	1/1	0.95	0.10	48,48,48,48	0
60	MG	DA	3092	1/1	0.95	0.12	209,209,209,209	0
60	MG	CA	1625	1/1	0.95	0.21	160,160,160,160	0
60	MG	BA	3046	1/1	0.95	0.12	142,142,142,142	0
60	MG	BA	3007	1/1	0.95	0.10	84,84,84,84	0
60	MG	AA	1608	1/1	0.95	0.14	38,38,38,38	0
60	MG	BA	3060	1/1	0.96	0.26	257,257,257,257	0
60	MG	BA	3122	1/1	0.96	0.12	25,25,25,25	0
60	MG	AA	1613	1/1	0.96	0.09	56,56,56,56	0
60	MG	BA	3008	1/1	0.96	0.16	29,29,29,29	0
60	MG	DA	3047	1/1	0.96	0.14	82,82,82,82	0
60	MG	AA	1601	1/1	0.96	0.15	93,93,93,93	0
60	MG	DA	3099	1/1	0.96	0.15	96,96,96,96	0
60	MG	BA	3014	1/1	0.96	0.17	75,75,75,75	0
60	MG	DA	3035	1/1	0.96	0.36	228,228,228,228	0
60	MG	DA	3111	1/1	0.96	0.11	89,89,89,89	0
60	MG	DA	3064	1/1	0.96	0.13	65,65,65,65	0
60	MG	BB	204	1/1	0.96	0.11	30,30,30,30	0
60	MG	DA	3036	1/1	0.96	0.15	111,111,111,111	0
60	MG	CA	1603	1/1	0.96	0.16	140,140,140,140	0
60	MG	DA	3033	1/1	0.96	0.07	91,91,91,91	0
62	ZN	B4	101	1/1	0.96	0.05	81,81,81,81	0
60	MG	BA	3056	1/1	0.96	0.12	86,86,86,86	0
60	MG	BA	3111	1/1	0.96	0.13	93,93,93,93	0
60	MG	BA	3010	1/1	0.96	0.09	48,48,48,48	0
60	MG	BA	3106	1/1	0.96	0.14	13,13,13,13	0
60	MG	BA	3115	1/1	0.96	0.18	8,8,8,8	0
60	MG	DA	3104	1/1	0.96	0.15	48,48,48,48	0
60	MG	CA	1633	1/1	0.96	0.07	82,82,82,82	0
60	MG	DA	3015	1/1	0.96	0.26	277,277,277,277	0
60	MG	BA	3005	1/1	0.96	0.07	60,60,60,60	0
60	MG	AA	1635	1/1	0.96	0.21	198,198,198,198	0
60	MG	DA	3021	1/1	0.96	0.15	169,169,169,169	0
60	MG	DA	3080	1/1	0.96	0.25	70,70,70,70	0
60	MG	BA	3100	1/1	0.96	0.17	26,26,26,26	0
60	MG	AA	1633	1/1	0.96	0.09	52,52,52,52	0
60	MG	AA	1636	1/1	0.96	0.18	149,149,149,149	0
60	MG	DA	3113	1/1	0.96	0.06	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	CA	1619	1/1	0.96	0.26	243,243,243,243	0
60	MG	BA	3083	1/1	0.96	0.10	52,52,52,52	0
60	MG	DA	3066	1/1	0.96	0.12	65,65,65,65	0
60	MG	AA	1619	1/1	0.96	0.06	165,165,165,165	0
60	MG	BA	3078	1/1	0.96	0.07	49,49,49,49	0
60	MG	BA	3085	1/1	0.97	0.13	24,24,24,24	0
60	MG	CA	1605	1/1	0.97	0.17	47,47,47,47	0
60	MG	BA	3045	1/1	0.97	0.12	13,13,13,13	0
60	MG	CA	1609	1/1	0.97	0.13	71,71,71,71	0
60	MG	CA	1635	1/1	0.97	0.09	85,85,85,85	0
60	MG	AA	1626	1/1	0.97	0.20	185,185,185,185	0
60	MG	DA	3114	1/1	0.97	0.24	166,166,166,166	0
60	MG	BA	3061	1/1	0.97	0.12	11,11,11,11	0
60	MG	AA	1628	1/1	0.97	0.06	70,70,70,70	0
60	MG	BA	3079	1/1	0.97	0.11	20,20,20,20	0
60	MG	DA	3116	1/1	0.97	0.10	59,59,59,59	0
60	MG	AA	1637	1/1	0.97	0.11	34,34,34,34	0
60	MG	BA	3015	1/1	0.97	0.07	30,30,30,30	0
60	MG	BA	3071	1/1	0.97	0.11	8,8,8,8	0
60	MG	AA	1616	1/1	0.97	0.13	123,123,123,123	0
60	MG	BA	3009	1/1	0.97	0.15	12,12,12,12	0
60	MG	BA	3049	1/1	0.97	0.11	72,72,72,72	0
60	MG	BA	3076	1/1	0.97	0.06	31,31,31,31	0
60	MG	BA	3048	1/1	0.97	0.14	18,18,18,18	0
60	MG	AA	1625	1/1	0.97	0.22	31,31,31,31	0
60	MG	AA	1632	1/1	0.97	0.10	53,53,53,53	0
60	MG	BA	3035	1/1	0.97	0.20	241,241,241,241	0
60	MG	DA	3039	1/1	0.97	0.15	59,59,59,59	0
60	MG	BA	3098	1/1	0.97	0.12	46,46,46,46	0
60	MG	BA	3084	1/1	0.97	0.13	9,9,9,9	0
60	MG	DA	3118	1/1	0.97	0.06	75,75,75,75	0
60	MG	BA	3107	1/1	0.97	0.19	8,8,8,8	0
60	MG	CA	1621	1/1	0.97	0.17	60,60,60,60	0
61	CLM	BA	3136	20/20	0.97	0.20	2,26,77,92	0
60	MG	AA	1612	1/1	0.97	0.14	103,103,103,103	0
60	MG	DA	3088	1/1	0.97	0.21	102,102,102,102	0
60	MG	BA	3030	1/1	0.97	0.13	34,34,34,34	0
60	MG	BA	3039	1/1	0.98	0.20	9,9,9,9	0
60	MG	BA	3101	1/1	0.98	0.06	105,105,105,105	0
60	MG	BA	3027	1/1	0.98	0.12	34,34,34,34	0
60	MG	BA	3096	1/1	0.98	0.17	59,59,59,59	0
60	MG	BA	3112	1/1	0.98	0.16	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3021	1/1	0.98	0.11	15,15,15,15	0
60	MG	BA	3059	1/1	0.98	0.16	147,147,147,147	0
60	MG	AA	1615	1/1	0.98	0.04	127,127,127,127	0
60	MG	BA	3119	1/1	0.98	0.14	15,15,15,15	0
60	MG	DA	3055	1/1	0.98	0.10	121,121,121,121	0
60	MG	BA	3025	1/1	0.98	0.10	38,38,38,38	0
60	MG	BA	3050	1/1	0.98	0.10	12,12,12,12	0
60	MG	BA	3081	1/1	0.98	0.04	41,41,41,41	0
60	MG	BA	3108	1/1	0.98	0.17	6,6,6,6	0
60	MG	BA	3102	1/1	0.98	0.10	14,14,14,14	0
60	MG	BA	3006	1/1	0.98	0.05	47,47,47,47	0
60	MG	BA	3064	1/1	0.98	0.08	8,8,8,8	0
60	MG	CA	1626	1/1	0.98	0.22	27,27,27,27	0
60	MG	BA	3029	1/1	0.98	0.20	10,10,10,10	0
60	MG	BA	3017	1/1	0.98	0.07	27,27,27,27	0
60	MG	DA	3020	1/1	0.98	0.19	36,36,36,36	0
60	MG	BA	3080	1/1	0.98	0.14	25,25,25,25	0
60	MG	BA	3125	1/1	0.98	0.11	26,26,26,26	0
60	MG	BA	3077	1/1	0.98	0.13	151,151,151,151	0
60	MG	AA	1624	1/1	0.98	0.07	139,139,139,139	0
60	MG	AA	1641	1/1	0.98	0.16	27,27,27,27	0
60	MG	DA	3089	1/1	0.98	0.06	81,81,81,81	0
60	MG	DA	3115	1/1	0.98	0.19	69,69,69,69	0
60	MG	AA	1640	1/1	0.98	0.25	189,189,189,189	0
60	MG	BA	3131	1/1	0.98	0.09	96,96,96,96	0
60	MG	DA	3065	1/1	0.98	0.12	40,40,40,40	0
60	MG	BA	3130	1/1	0.98	0.44	257,257,257,257	0
60	MG	AA	1606	1/1	0.98	0.11	58,58,58,58	0
60	MG	BA	3028	1/1	0.98	0.07	45,45,45,45	0
60	MG	DA	3054	1/1	0.98	0.13	125,125,125,125	0
60	MG	AA	1611	1/1	0.98	0.10	81,81,81,81	0
60	MG	AA	1634	1/1	0.98	0.07	58,58,58,58	0
60	MG	BA	3113	1/1	0.98	0.10	34,34,34,34	0
60	MG	BA	3109	1/1	0.98	0.10	105,105,105,105	0
60	MG	BA	3088	1/1	0.98	0.10	22,22,22,22	0
60	MG	BA	3074	1/1	0.98	0.17	15,15,15,15	0
60	MG	BA	3011	1/1	0.98	0.08	149,149,149,149	0
60	MG	BA	3127	1/1	0.98	0.10	21,21,21,21	0
60	MG	BA	3023	1/1	0.99	0.12	8,8,8,8	0
60	MG	BA	3121	1/1	0.99	0.14	5,5,5,5	0
60	MG	BA	3099	1/1	0.99	0.10	32,32,32,32	0
60	MG	AA	1621	1/1	0.99	0.14	35,35,35,35	0

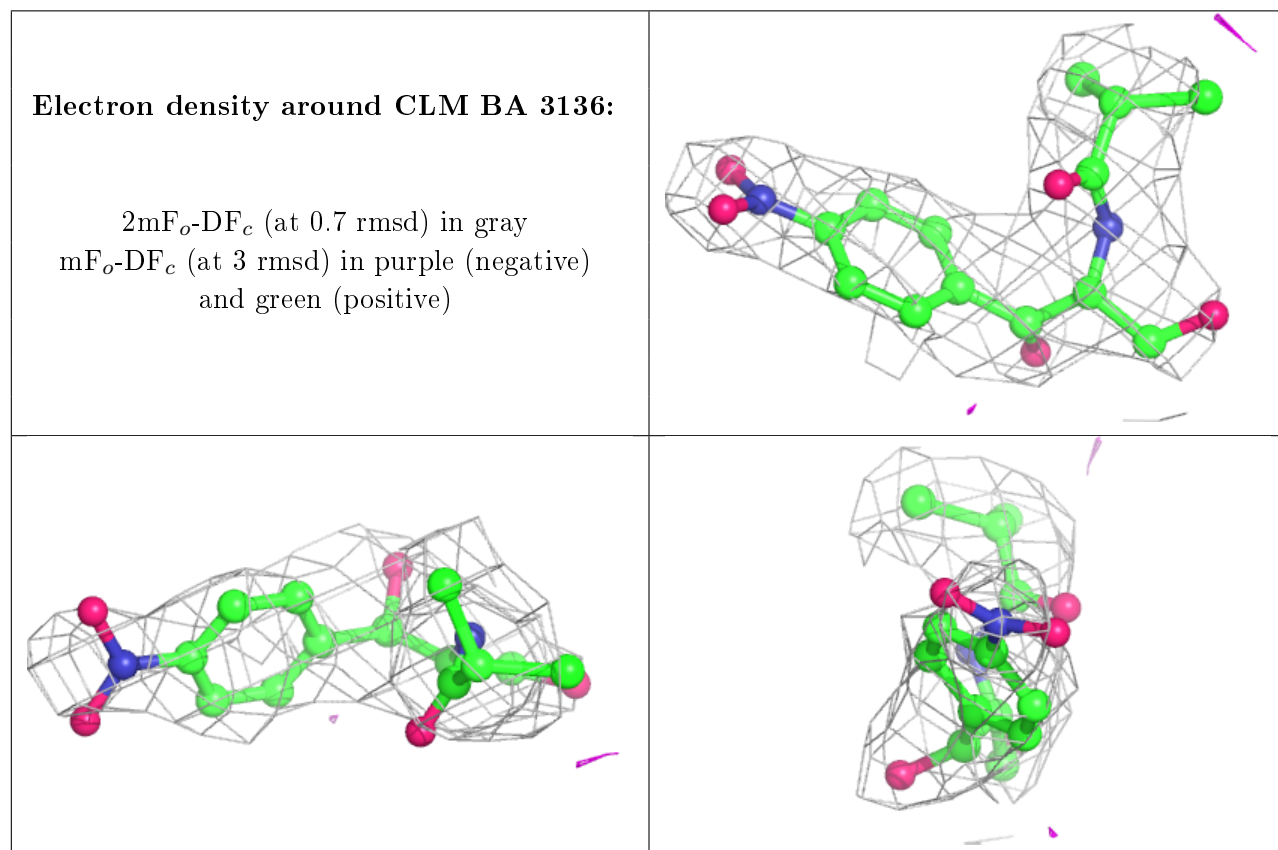
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3032	1/1	0.99	0.16	6,6,6,6	0
60	MG	BB	203	1/1	0.99	0.10	16,16,16,16	0
60	MG	BL	201	1/1	0.99	0.07	34,34,34,34	0
60	MG	BA	3036	1/1	0.99	0.15	30,30,30,30	0
60	MG	BA	3013	1/1	0.99	0.18	6,6,6,6	0
60	MG	BA	3095	1/1	0.99	0.12	13,13,13,13	0
60	MG	BA	3065	1/1	0.99	0.15	27,27,27,27	0
60	MG	BA	3129	1/1	0.99	0.15	15,15,15,15	0
60	MG	BA	3070	1/1	0.99	0.11	76,76,76,76	0
60	MG	BA	3072	1/1	0.99	0.16	81,81,81,81	0
60	MG	BA	3116	1/1	0.99	0.06	14,14,14,14	0
60	MG	BA	3052	1/1	0.99	0.09	12,12,12,12	0
60	MG	BA	3031	1/1	0.99	0.12	15,15,15,15	0
60	MG	BA	3126	1/1	0.99	0.14	32,32,32,32	0
60	MG	BA	3133	1/1	0.99	0.14	5,5,5,5	0
60	MG	AA	1605	1/1	0.99	0.12	30,30,30,30	0
60	MG	BA	3128	1/1	0.99	0.13	6,6,6,6	0
60	MG	BA	3120	1/1	0.99	0.06	44,44,44,44	0
60	MG	BA	3026	1/1	0.99	0.18	122,122,122,122	0
60	MG	BA	3053	1/1	0.99	0.10	35,35,35,35	0
60	MG	AA	1602	1/1	0.99	0.08	117,117,117,117	0
60	MG	BA	3093	1/1	0.99	0.10	68,68,68,68	0
60	MG	BA	3110	1/1	0.99	0.09	65,65,65,65	0
60	MG	BA	3043	1/1	0.99	0.25	19,19,19,19	0
60	MG	BA	3105	1/1	0.99	0.15	11,11,11,11	0
60	MG	BA	3067	1/1	0.99	0.11	22,22,22,22	0
60	MG	BA	3019	1/1	0.99	0.15	50,50,50,50	0
60	MG	BA	3038	1/1	0.99	0.17	21,21,21,21	0
60	MG	BA	3016	1/1	0.99	0.07	5,5,5,5	0
60	MG	BA	3034	1/1	0.99	0.09	9,9,9,9	0
60	MG	AA	1631	1/1	0.99	0.13	95,95,95,95	0
60	MG	BA	3066	1/1	0.99	0.11	14,14,14,14	0
60	MG	BA	3020	1/1	0.99	0.11	21,21,21,21	0
60	MG	BA	3042	1/1	0.99	0.13	34,34,34,34	0
60	MG	BA	3040	1/1	0.99	0.12	11,11,11,11	0
60	MG	AA	1642	1/1	0.99	0.09	42,42,42,42	0
60	MG	BA	3037	1/1	0.99	0.16	7,7,7,7	0
60	MG	BA	3018	1/1	1.00	0.30	10,10,10,10	0
60	MG	BA	3063	1/1	1.00	0.12	11,11,11,11	0
60	MG	BA	3062	1/1	1.00	0.13	9,9,9,9	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.