



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2023 – 04:07 AM EDT

PDB ID : 4V64
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with hygromycin B.
Authors : Borovinskaya, M.A.; Shoji, S.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2008-06-11
Resolution : 3.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

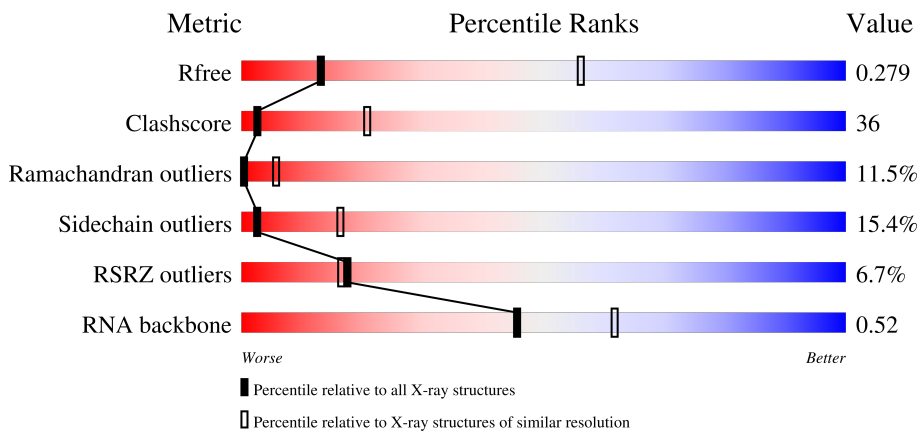
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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 of 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	1542	 22% 63% 14% ..
1	CA	1542	 21% 65% 13% ..
2	AC	232	 13% 31% 43% 13% • 11%
2	CC	232	 7% 31% 44% 13% • 11%

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Mol	Chain	Length	Quality of chain
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	5% 32% 54% 11% ..
16	AQ	83	22% 23% 61% 12% .
16	CQ	83	25% 60% 12% .
17	AR	74	4% 39% 32% . 26%
17	CR	74	7% 38% 34% . 26%
18	AS	91	24% 18% 53% 15% . 13%
18	CS	91	3% 19% 53% 15% . 12%
19	AT	86	3% 38% 47% 12% ..
19	CT	86	43% 42% 12% ..
20	AB	240	10% 25% 50% 15% . 9%
20	CB	240	30% 24% 48% 18% . 9%
21	AU	71	3% 20% 37% 13% . 28%
21	CU	71	11% 17% 39% 13% . 28%
22	BA	120	% 21% 63% 12% ..
22	DA	120	% 20% 65% 12% ..
23	BB	2904	% 24% 61% 12% ..
23	DB	2904	23% 62% 12% ..
24	BV	94	5% 26% 61% 14%
24	DV	94	3% 23% 65% 12%
25	BC	273	11% 25% 51% 22% ..
25	DC	273	8% 23% 51% 22% ..
26	BD	209	13% 25% 56% 17% .
26	DD	209	10% 24% 57% 17% .
27	BE	201	12% 29% 54% 17%
27	DE	201	6% 30% 53% 16%

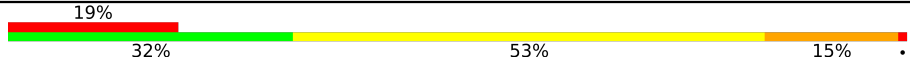
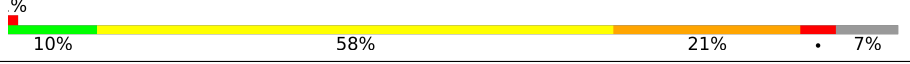
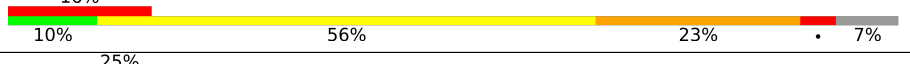
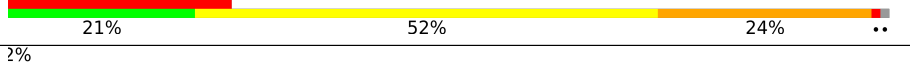
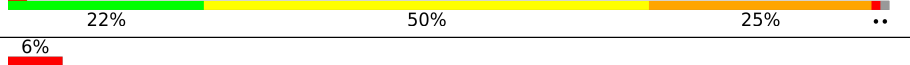
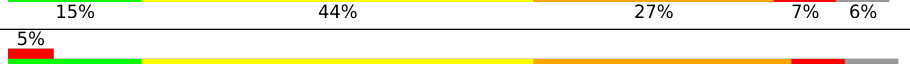
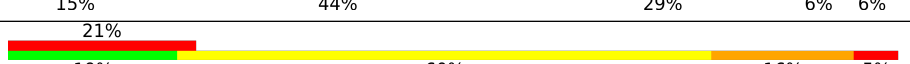
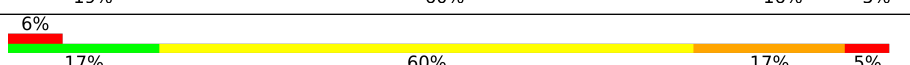
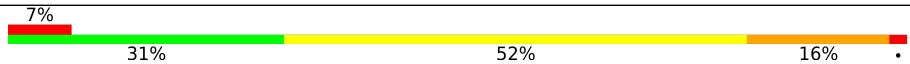

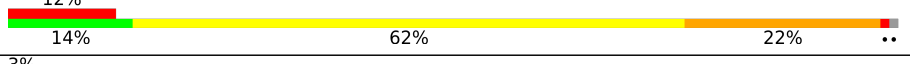
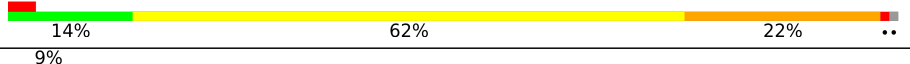
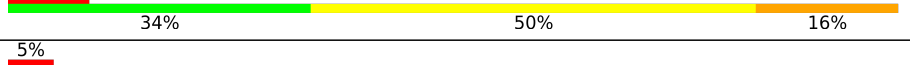

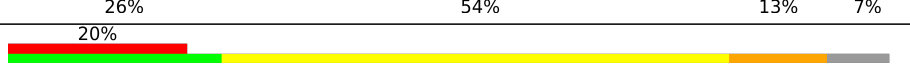
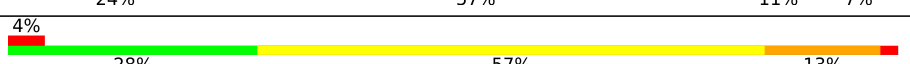
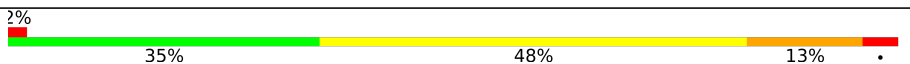
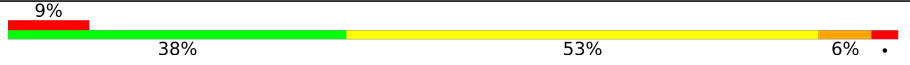
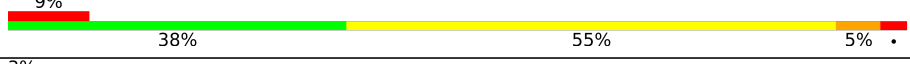
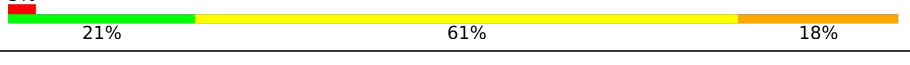
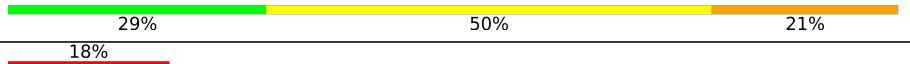

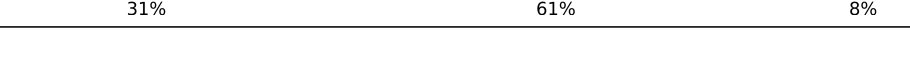


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Mol	Chain	Length	Quality of chain
28	BF	178	
28	DF	178	
29	BG	176	
29	DG	176	
30	BH	149	
30	DH	149	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	

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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	100	
41	DT	100	
42	BU	103	
42	DU	103	
43	BW	84	
43	DW	84	
44	BX	63	
44	DX	63	
45	BY	58	
45	DY	58	
46	BZ	78	
46	DZ	78	
47	B0	56	
47	D0	56	
48	B1	54	
48	D1	54	
49	B2	46	
49	D2	46	
50	B3	64	
50	D3	64	
51	B4	38	
51	D4	38	
52	BI	141	
52	DI	141	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284077 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 ribosomal RNA.

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

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AC	206	Total 1624	C 1028	N 305	O 288	S 3	0	0	0
2	CC	206	Total 1624	C 1028	N 305	O 288	S 3	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AE	150	Total 1105	C 687	N 211	O 201	S 6	0	0	0
4	CE	150	Total 1105	C 687	N 211	O 201	S 6	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
5	CF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
9	CJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AM	114	883	546	178	156	3	0	0	0
12	CM	113	876	541	177	155	3	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AN	96	774	483	160	128	3	0	0	0
13	CN	96	774	483	160	128	3	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AO	88	715	440	146	128	1	0	0	0
14	CO	88	715	440	146	128	1	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AP	82	649	406	128	114	1	0	0	0
15	CP	80	638	400	126	111	1	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
16	CQ	81	Total	C	N	O	S	0	0	0
			656	417	122	114	3			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
17	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
18	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
20	CB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- 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
			425	265	86	73	1			
21	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
22	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 23 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
23	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
25	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	BK	121	Total 930	C 582	N 179	O 164	S 5	0	0	0
32	DK	121	Total 930	C 582	N 179	O 164	S 5	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	BN	120	Total 960	C 593	N 196	O 166	S 5	0	0	0
35	DN	120	Total 960	C 593	N 196	O 166	S 5	0	0	0

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

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

- 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	S	0	0	0
			947	604	192	151				
38	DQ	117	Total	C	N	O	S	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			
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
			738	466	139	131	2			
41	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	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
			779	492	146	141			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	DU	102	779	492	146	141	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L27.

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

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	BX	63	509	313	99	95	2	0	0	0
44	DX	63	509	313	99	95	2	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BY	58	449	281	87	79	2	0	0	0
45	DY	58	449	281	87	79	2	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	BZ	77	625	388	129	106	2	0	0	0
46	DZ	77	625	388	129	106	2	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
48	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
48	D1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 49 is a protein called 50S ribosomal protein L34.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L36.

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

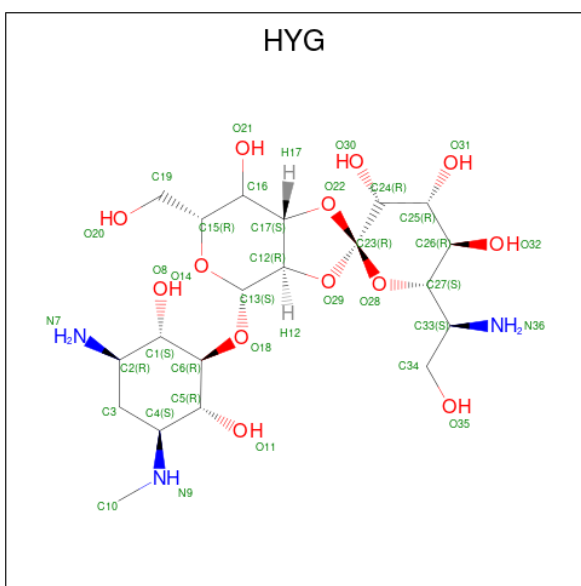
- Molecule 52 is a protein called 50S ribosomal protein L11.

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

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	AA	58	Total Mg 58 58	0	0
53	AE	1	Total Mg 1 1	0	0
53	AN	1	Total Mg 1 1	0	0
53	BB	110	Total Mg 110 110	0	0
53	CA	61	Total Mg 61 61	0	0
53	CE	1	Total Mg 1 1	0	0
53	DB	111	Total Mg 111 111	0	0

- Molecule 54 is HYGROMYCIN B (three-letter code: HYG) (formula: C₂₀H₃₇N₃O₁₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	AA	1	Total C N O 36 20 3 13	0	0
54	CA	1	Total C N O 36 20 3 13	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	B4	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	D4	1	Total 1	Zn 1	0	0

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	282	Total 282	O 282	0	0
56	AE	4	Total 4	O 4	0	0
56	AK	2	Total 2	O 2	0	0
56	AL	5	Total 5	O 5	0	0
56	AN	4	Total 4	O 4	0	0
56	AT	3	Total 3	O 3	0	0
56	BB	492	Total 492	O 492	0	0
56	BC	8	Total 8	O 8	0	0
56	BD	1	Total 1	O 1	0	0
56	BE	2	Total 2	O 2	0	0
56	BH	1	Total 1	O 1	0	0
56	BL	2	Total 2	O 2	0	0
56	B2	1	Total 1	O 1	0	0
56	CA	294	Total 294	O 294	0	0
56	CE	4	Total 4	O 4	0	0
56	CI	1	Total 1	O 1	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	3	Total 3	O 3	0	0

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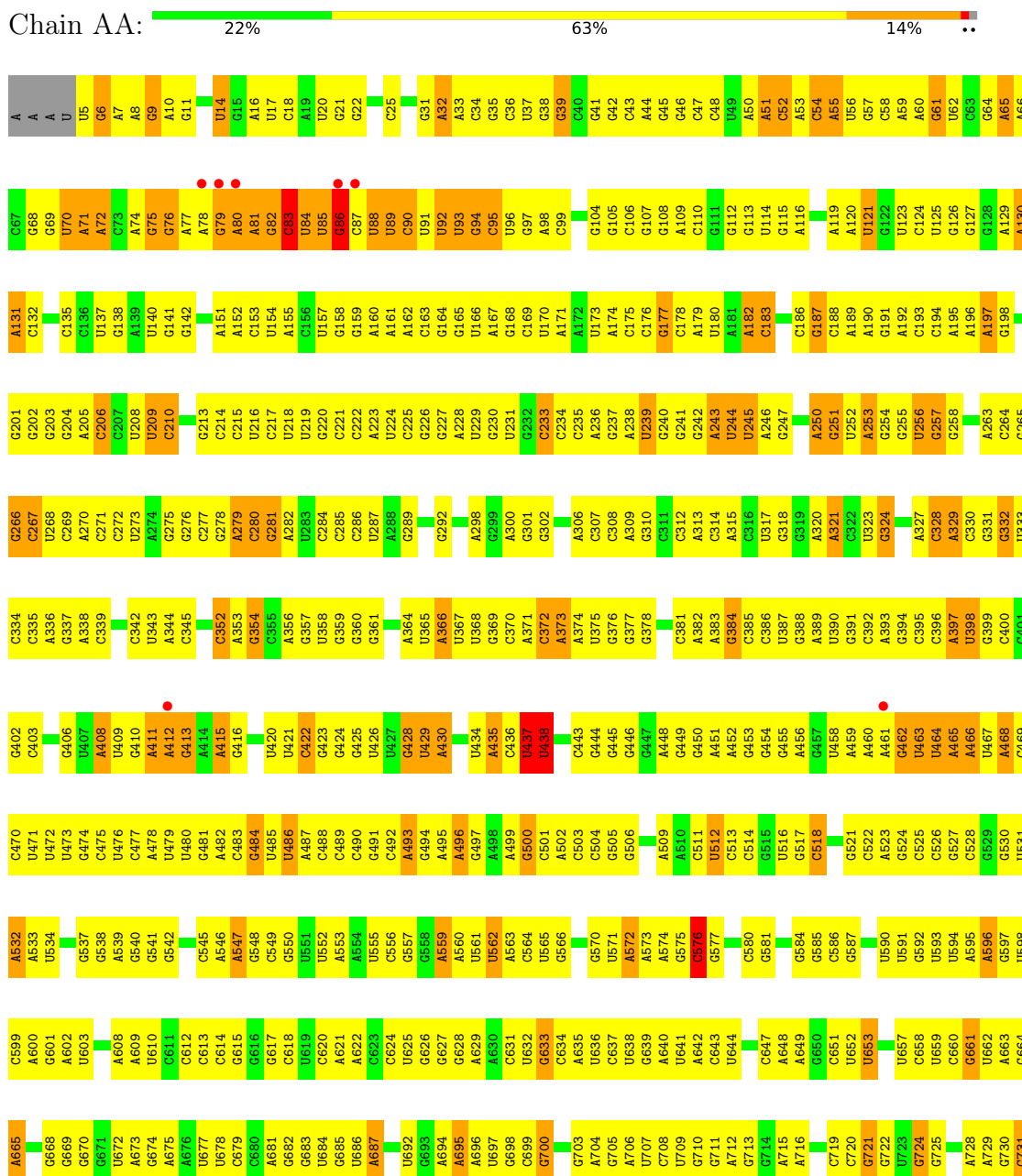
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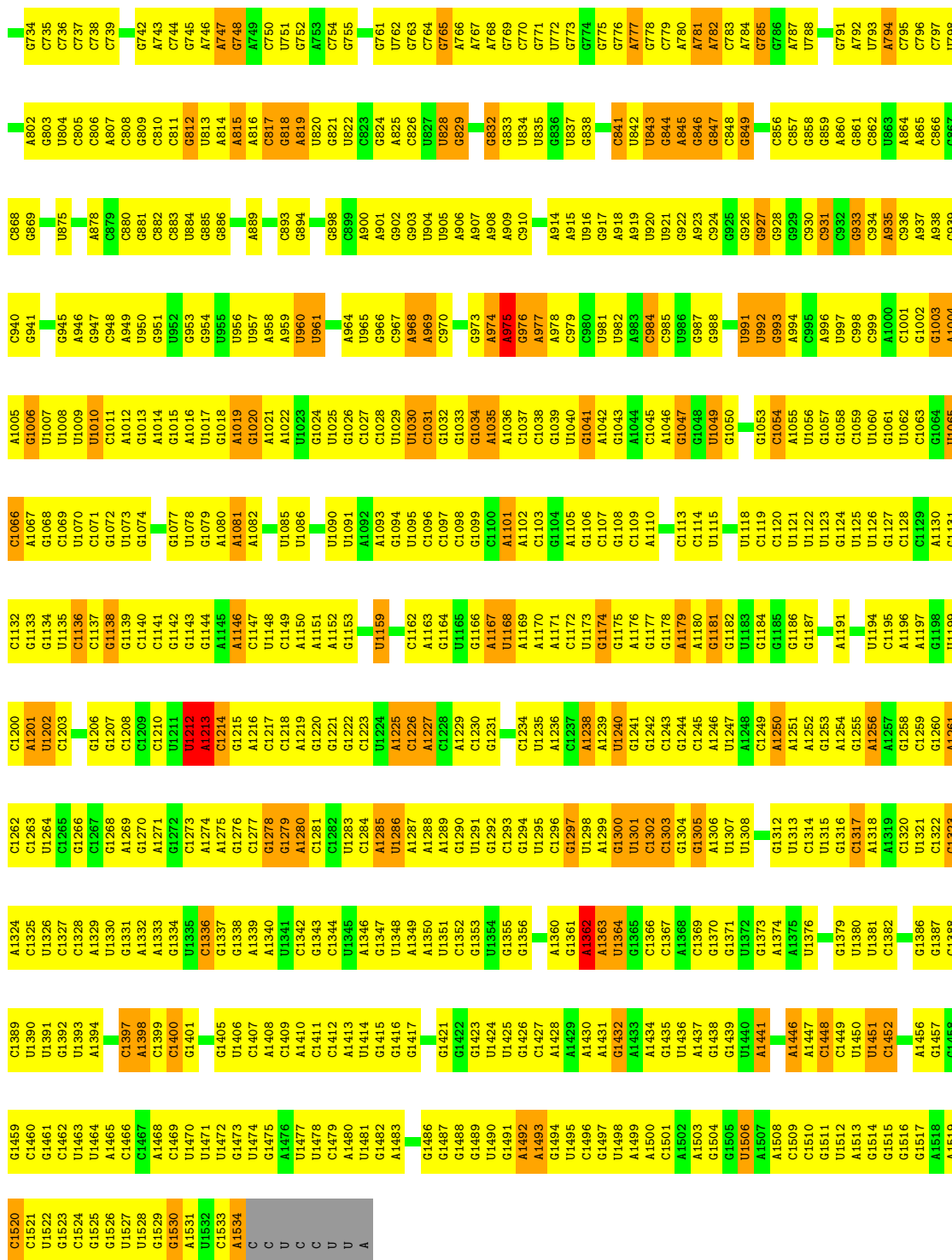
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	CN	3	Total O 3 3	0	0
56	CT	1	Total O 1 1	0	0
56	DB	499	Total O 499 499	0	0
56	DC	5	Total O 5 5	0	0
56	DD	1	Total O 1 1	0	0
56	DE	1	Total O 1 1	0	0
56	DL	5	Total O 5 5	0	0
56	DP	1	Total O 1 1	0	0
56	D2	1	Total O 1 1	0	0

3 Residue-property plots [\(i\)](#)

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

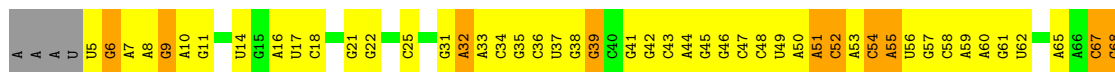
- Molecule 1: 16S ribosomal RNA



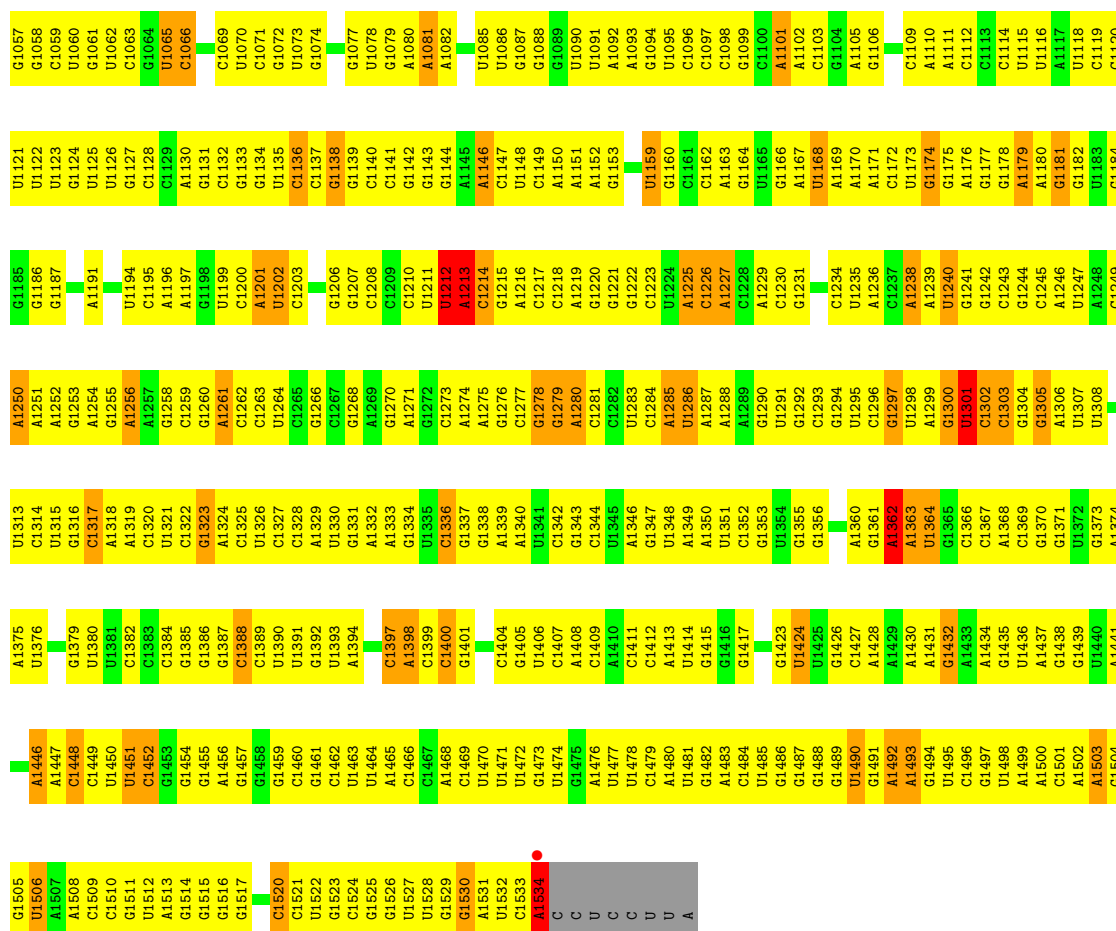


● Molecule 1: 16S ribosomal RNA

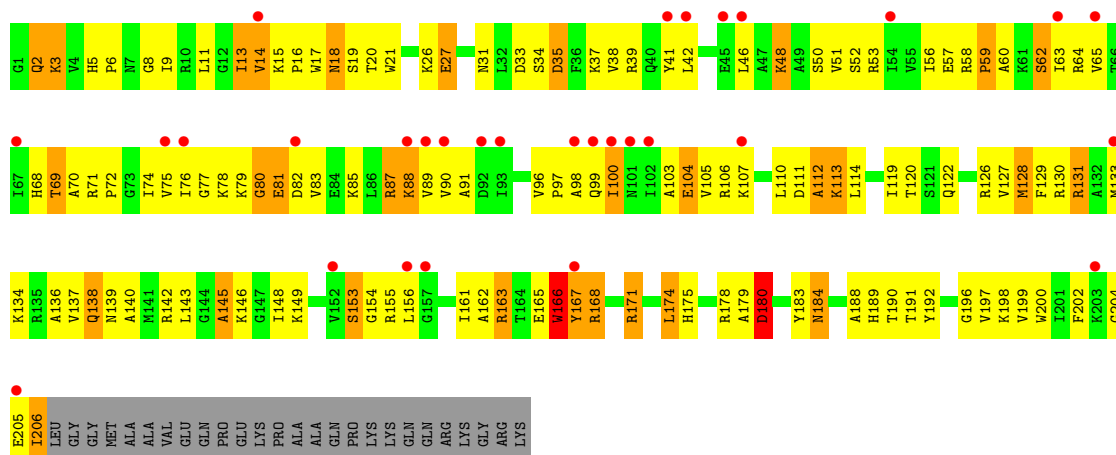
Chain CA: 21% 65% 13% ..



A996	U997	A998	C999	A1000	C1001	G1002	G1003	A1004	G1005	C1006	U1007	U1008	U1009	U1010	C1011	A1012	G1013	A1014	A1015	A1016	U1017	G1018	A1019	G1020	A1021	U1022	U1023	U1024	U1025	C1026	C1027	C1028	U1029	U1030	C1031	G1032	G1033	G1034	A1035	A1036	C1037	C1038	G1039	U1040	G1041	A1042	G1043	A1044	C1045	A1046	G1047	U1048	U1049	G1050	G1053	C1054	A1055	U1056																																																																																																																																																																																																					
C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995																																																																																																																																																																																															
A860	G861	C862	U863	A864	A865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930																																																																																																																																																																																									
U793	A794	C795	C796	C797	U798	A802	G803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900																																																																																																																																																							
G724	G725	A726	A727	G728	G729	G730	G731	G732	G733	G734	C735	C736	C737	C738	C739	G742	A743	A744	A745	A746	A747	A748	A749	C750	U751	C754	G755	U762	G763	C764	G765	A766	A767	G768	G769	C770	G771	U772	A773	G774	G775	G776	A777	G778	C779	A780	A781	C782	C783	A784	G785	G786	A787	U788	A790	U791	G792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900																																																																																										
A860	G861	C862	U863	A864	A865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930																																																																																																																																																																																									
U996	U997	A998	C999	A1000	C1001	G1002	G1003	A1004	G1005	C1006	U1007	U1008	U1009	U1010	C1011	A1012	G1013	A1014	A1015	A1016	U1017	G1018	A1019	G1020	A1021	U1022	U1023	U1024	U1025	C1026	C1027	C1028	U1029	U1030	C1031	G1032	G1033	G1034	A1035	A1036	C1037	C1038	G1039	U1040	G1041	A1042	G1043	A1044	C1045	A1046	G1047	U1048	U1049	G1050	G1053	C1054	A1055	U1056																																																																																																																																																																																																					
A996	U997	A998	C999	A1000	C1001	G1002	G1003	A1004	G1005	C1006	U1007	U1008	U1009	U1010	C1011	A1012	G1013	A1014	A1015	A1016	U1017	G1018	A1019	G1020	A1021	U1022	U1023	U1024	U1025	C1026	C1027	C1028	U1029	U1030	C1031	G1032	G1033	G1034	A1035	A1036	C1037	C1038	G1039	U1040	G1041	A1042	G1043	A1044	C1045	A1046	G1047	U1048	U1049	G1050	G1053	C1054	A1055	U1056																																																																																																																																																																																																					
C135	C136	U137	G138	G141	G142	A143	G144	G145	A149	U150	A151	A152	C153	U154	A155	C156	U157	G158	G159	U160	A161	C162	A163	G164	G165	A166	A167	G168	C169	G170	U171	C172	A173	C174	G175	C176	G177	G178	A179	U180	U181	A182	C183	C186	A187	U188	A189	A190	G191	G192	C193	U194	A195	A196	U197	C198	G199	A200	C201	G202	G203	U204	C205	C206	C207	U208	U209	C210	G211	C212	C213	C214	C215	C216	C217	C218	A219	U220	U221	C222	C223	A224	U225	A226	C227	C228	C229	A230	U231	U232	C233	C234	C235	A236	G237	A238	U239	G240	G241	G242	G243	U244	U245	A246	G247	A250	G251	U252	A253	G254	C255	U256	G257	A258	A259	G260	C261	A262																																																																																																																																									
A263	C264	G265	U266	C267	C268	C269	A270	C271	U272	U273	G274	G275	C276	C277	C278	A279	C280	G281	A282	U283	C284	C285	C286	U287	A288	G289	G292	A298	C299	A300	G301	G302	A306	C307	C308	A309	G310	G311	G312	G313	C314	C315	A316	U317	G318	C319	A320	A321	G322	U323	G324	A325	C326	C327	A328	A329	C330	G331	C332	C333	C334	C335	C336	C337	C338	C339	C340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	C356	C357	C358	C359	C360	C361	C362	A363	A364	A365	A366	U367	U368	G369	C370	A371	C372	A373	A374	U375	G376	G377	G378	C379	C380	C381	A382	A383	A384	C385	C386	U387	G388	A389	U390	U391	C392	A393	G394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528
G69	U70	A71	A72	C73	A77	A78	G79	A80	A81	G82	C83	U84	U85	G86	C87	U88	U89	C90	U91	U92	U93	G94	C95	U96	A97	A98	C99	G100	A101	G104	G105	C106	G107	G108	A109	C110	G111	G112	G113	U114	G115	A116	A119	A120	U121	G122	U123	G126	C127	A128	A129	A130	A131	C132																																																																																																																																																																																																									

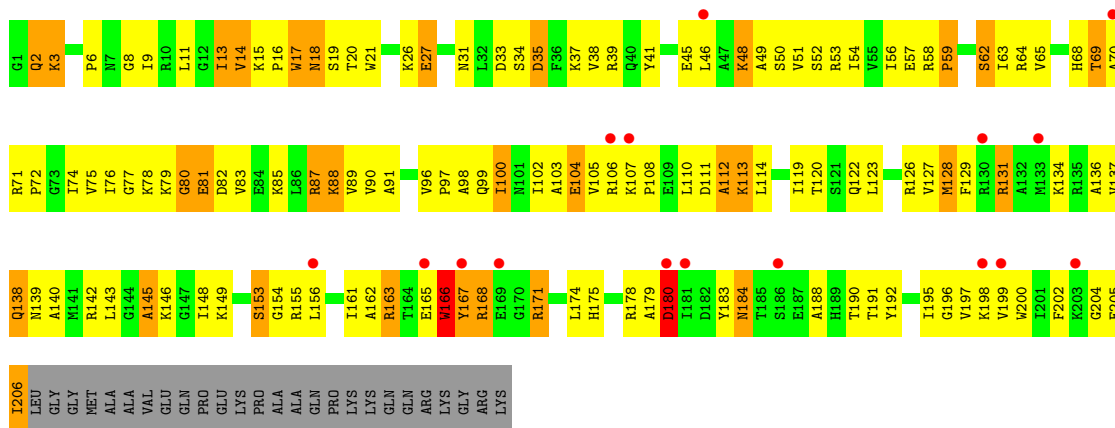


• Molecule 2: 30S ribosomal protein S3

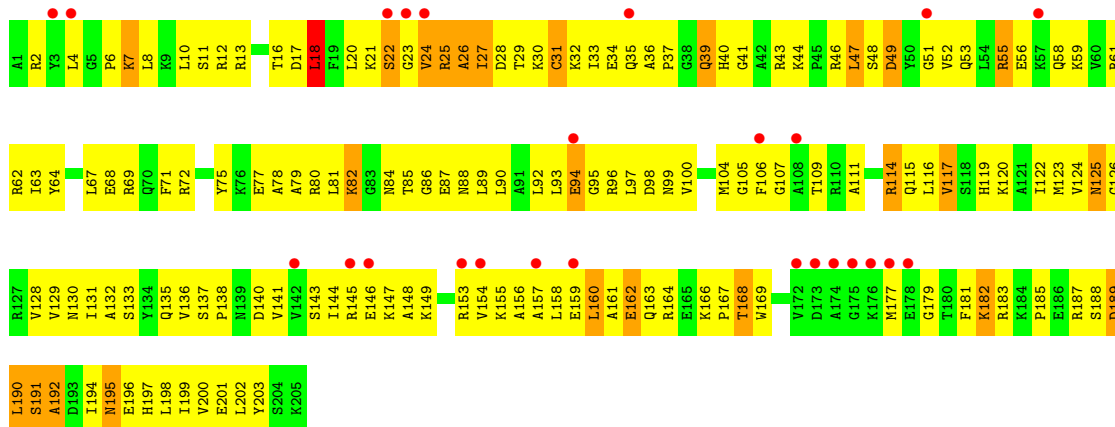


• Molecule 2: 30S ribosomal protein S3

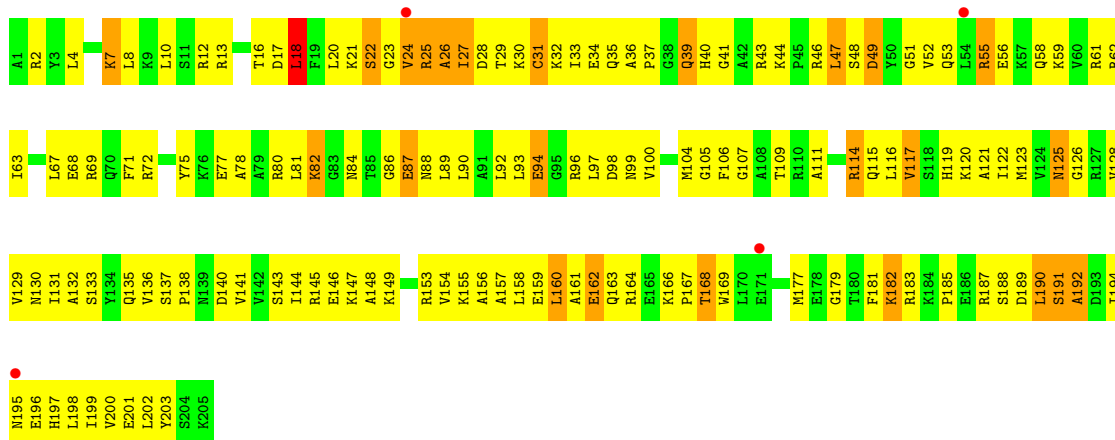




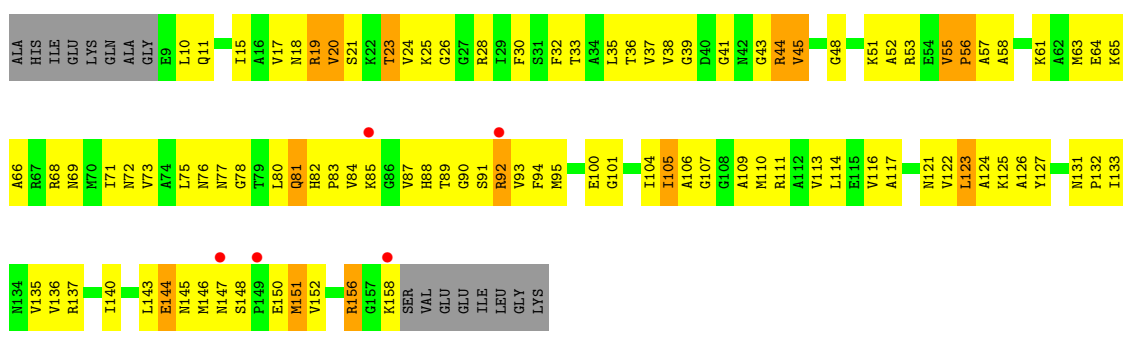
• Molecule 3: 30S ribosomal protein S4



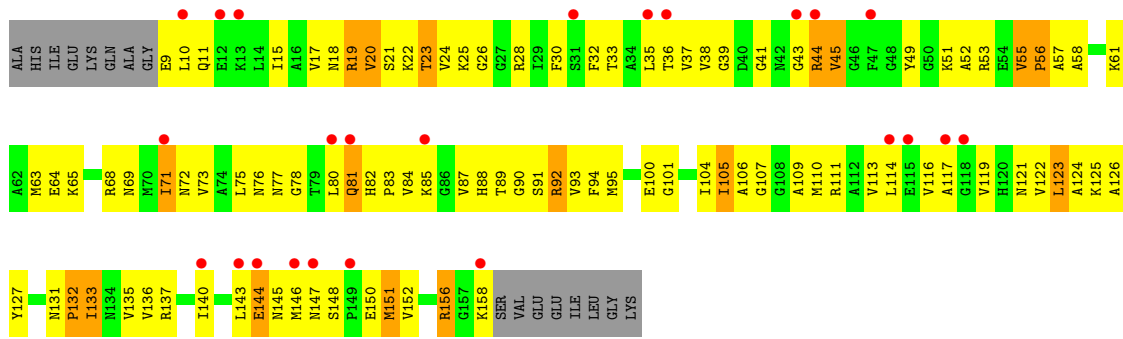
• Molecule 3: 30S ribosomal protein S4



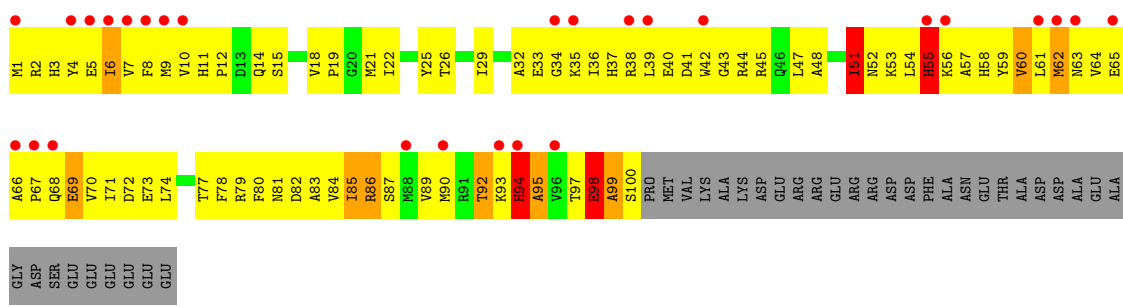
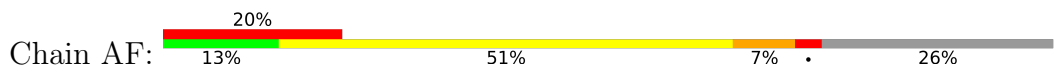
• Molecule 4: 30S ribosomal protein S5



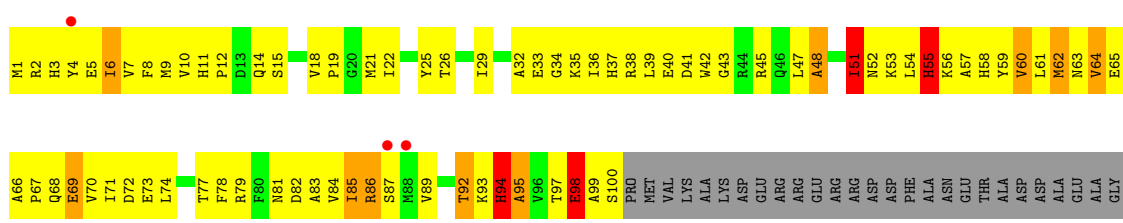
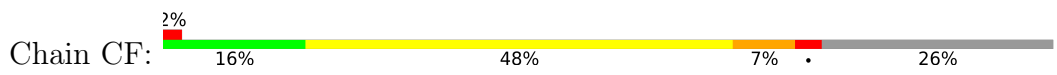
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6

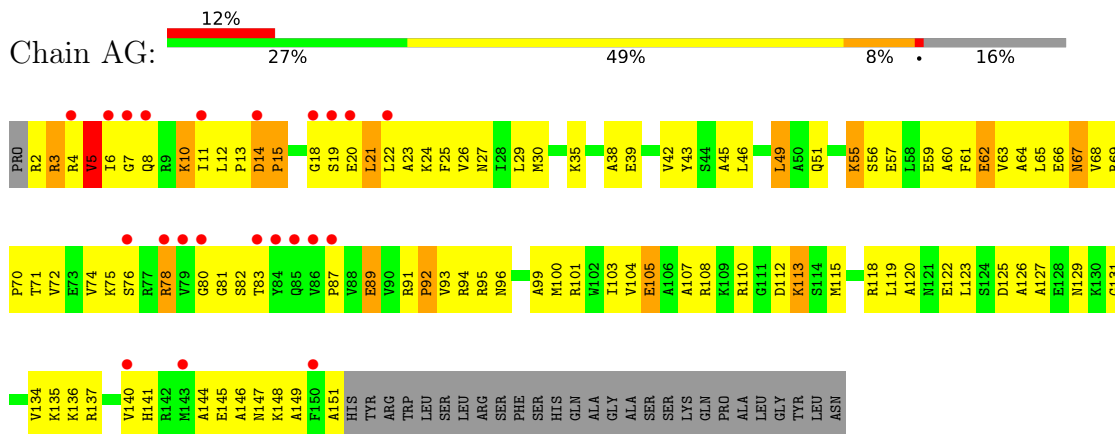


• Molecule 5: 30S ribosomal protein S6

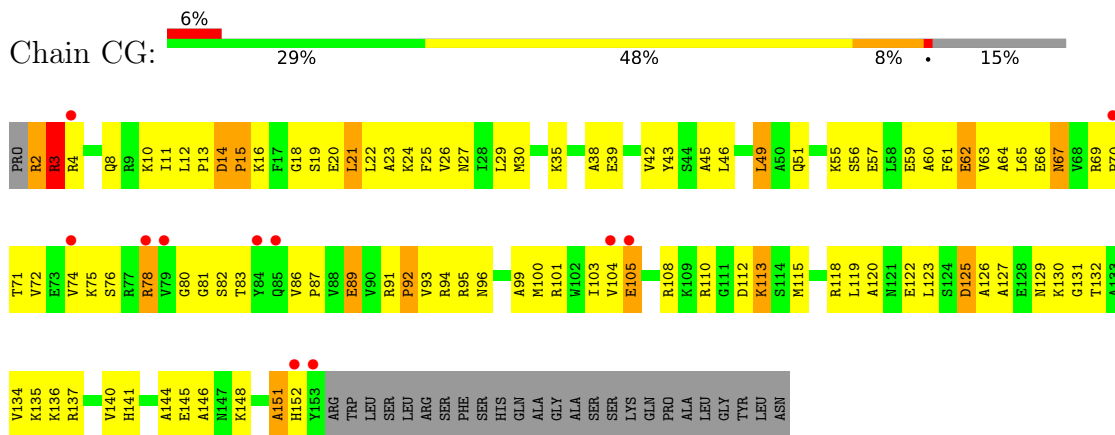


ASP
SER
GLU
GLU
GLU
GLU
GLU

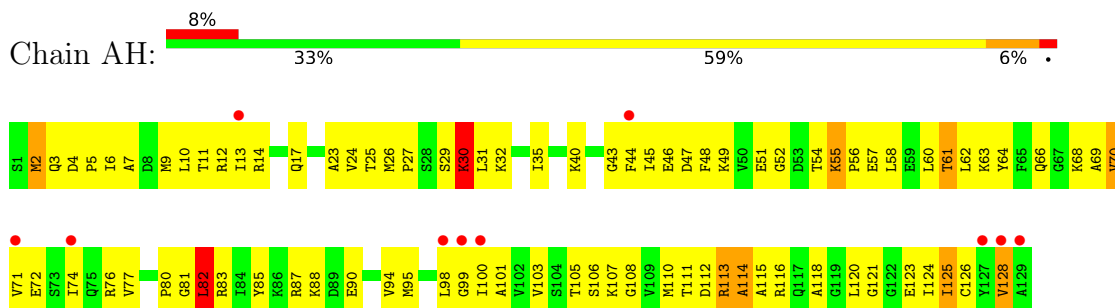
• Molecule 6: 30S ribosomal protein S7



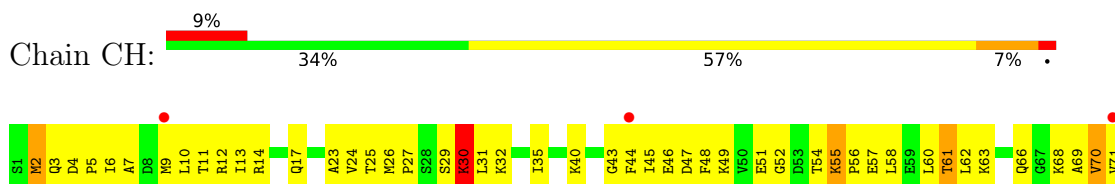
• Molecule 6: 30S ribosomal protein S7

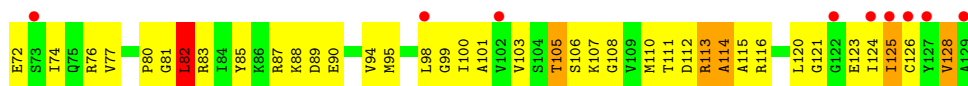


• Molecule 7: 30S ribosomal protein S8

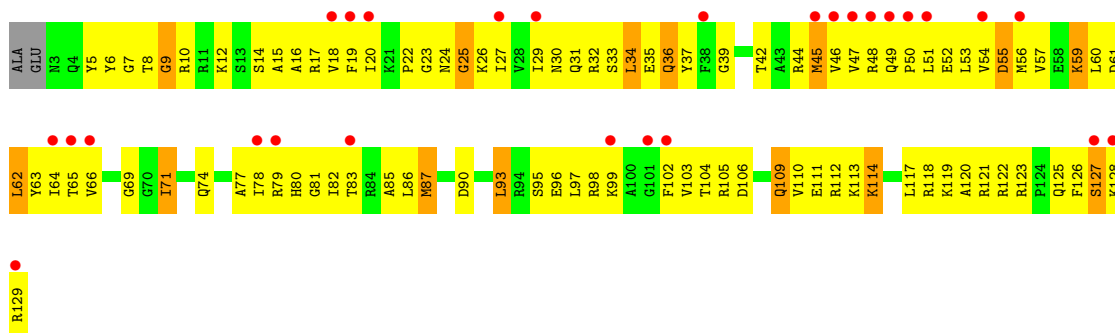


• Molecule 7: 30S ribosomal protein S8

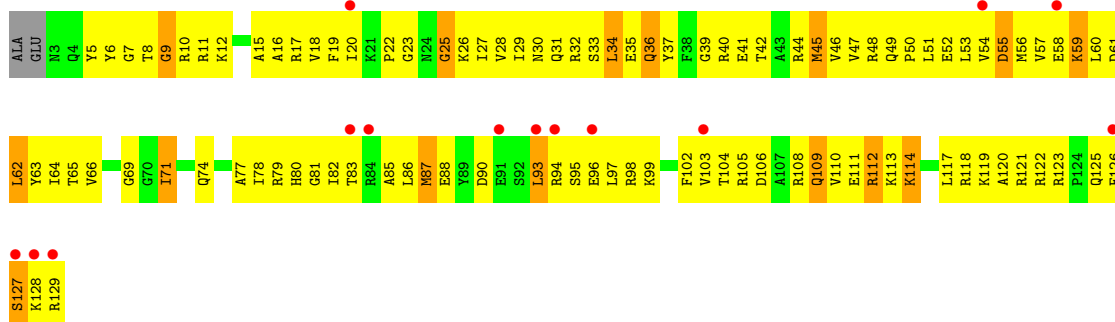




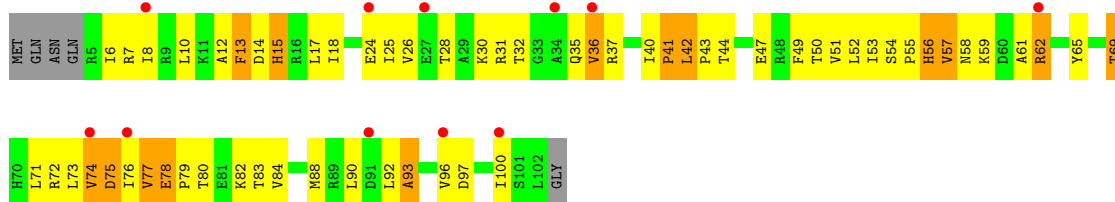
• Molecule 8: 30S ribosomal protein S9



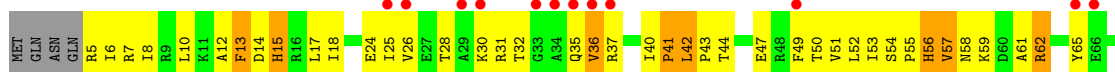
• Molecule 8: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S10

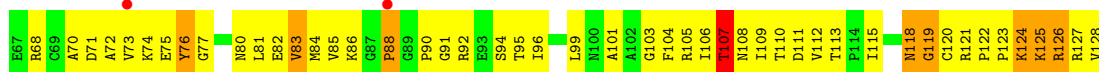


• Molecule 9: 30S ribosomal protein S10

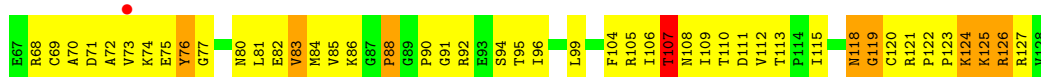




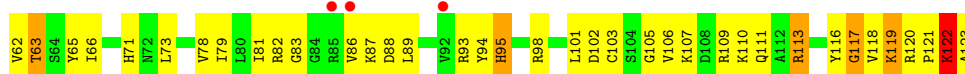
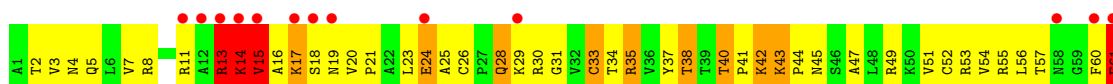
• Molecule 10: 30S ribosomal protein S11



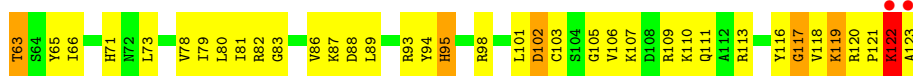
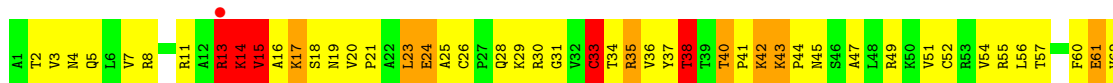
• Molecule 10: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S12

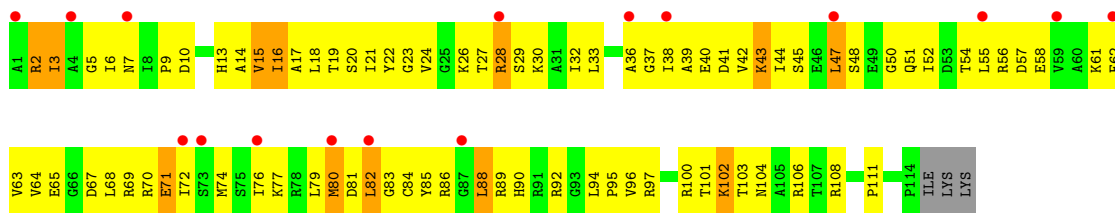


• Molecule 11: 30S ribosomal protein S12

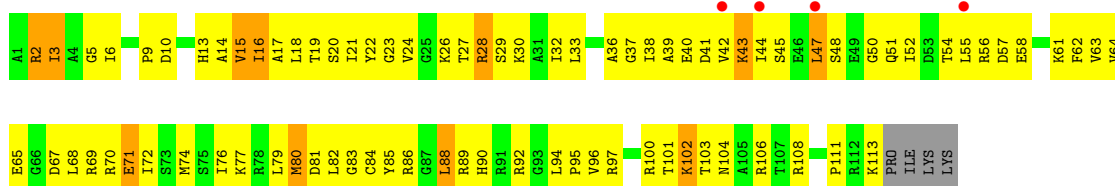


• Molecule 12: 30S ribosomal protein S13

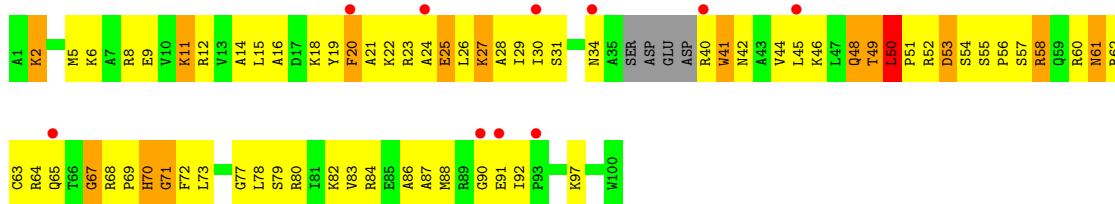




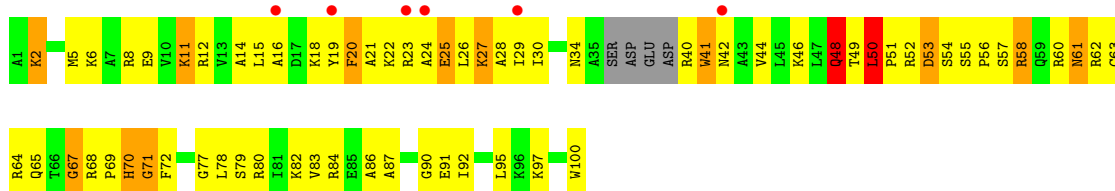
• Molecule 12: 30S ribosomal protein S13



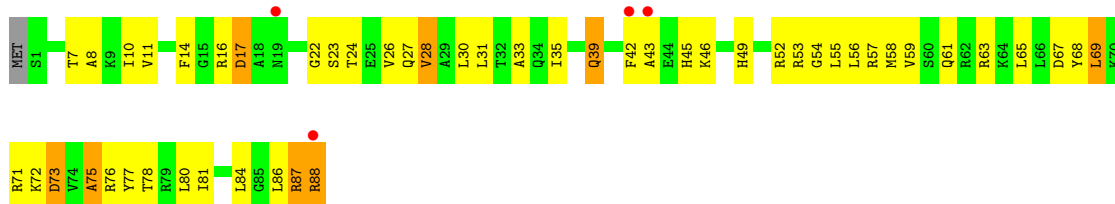
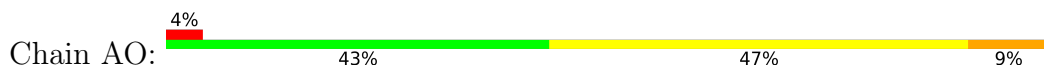
• Molecule 13: 30S ribosomal protein S14



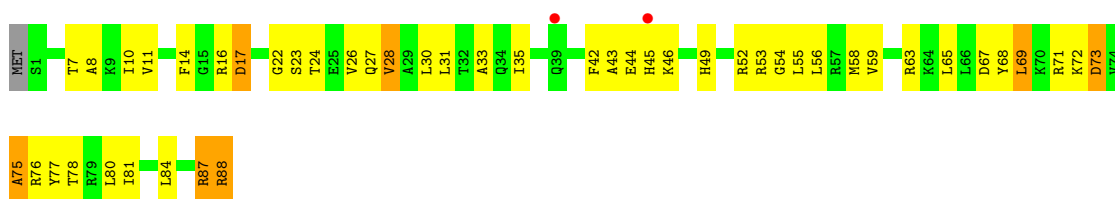
• Molecule 13: 30S ribosomal protein S14



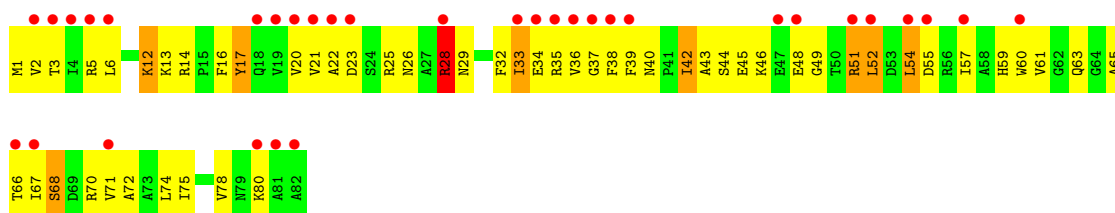
• Molecule 14: 30S ribosomal protein S15



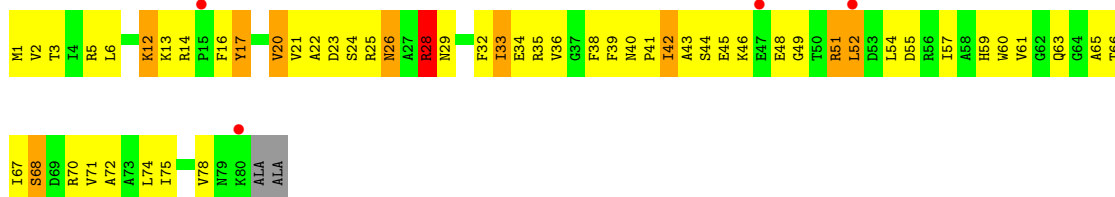
- Molecule 14: 30S ribosomal protein S15



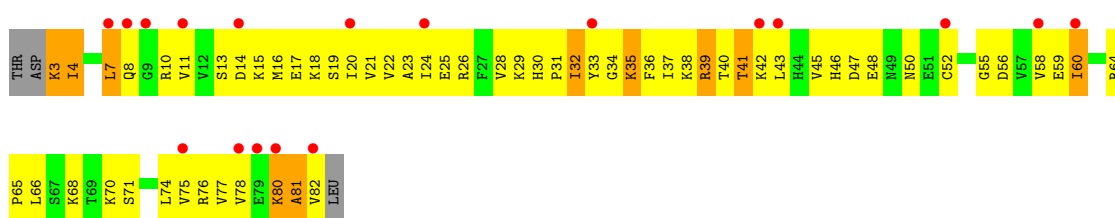
- Molecule 15: 30S ribosomal protein S16



- Molecule 15: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S17



- Molecule 16: 30S ribosomal protein S17



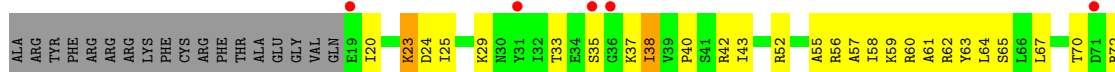


- Molecule 17: 30S ribosomal protein S18



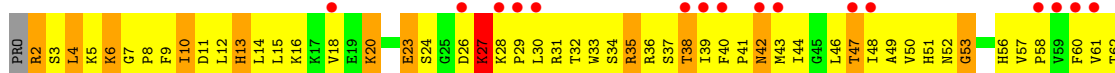
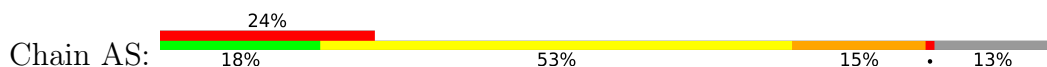
GLN

- Molecule 17: 30S ribosomal protein S18

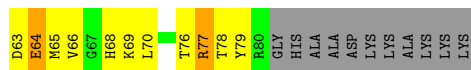
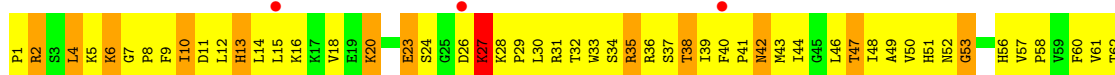
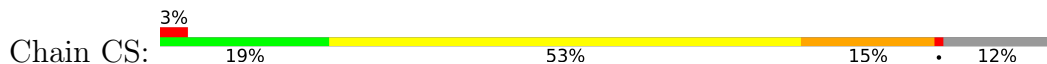


H73
GLN

- Molecule 18: 30S ribosomal protein S19

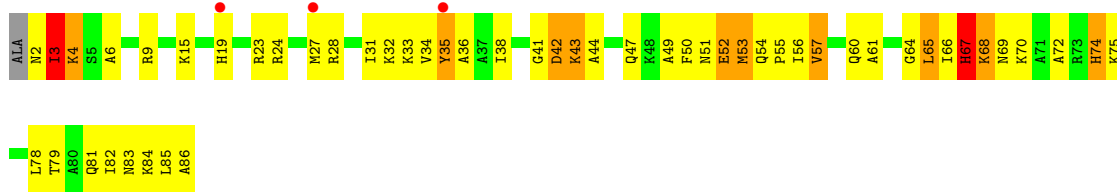


- Molecule 18: 30S ribosomal protein S19

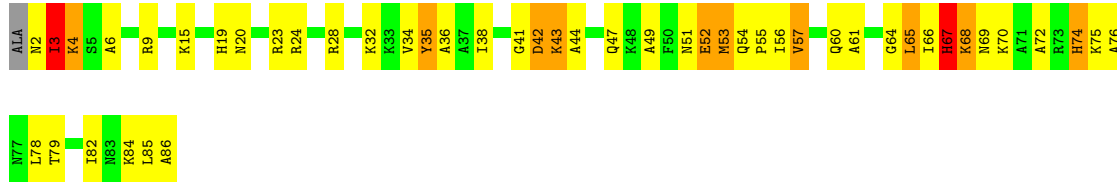


- Molecule 19: 30S ribosomal protein S20

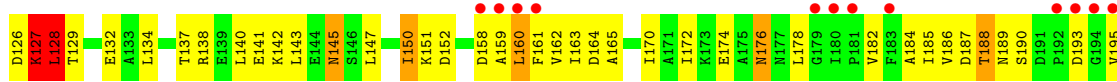
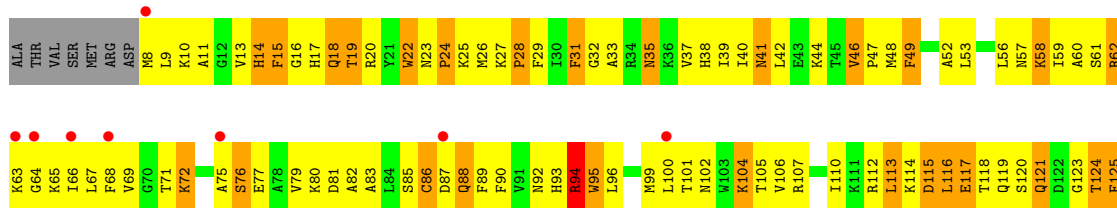




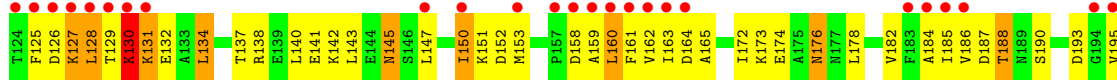
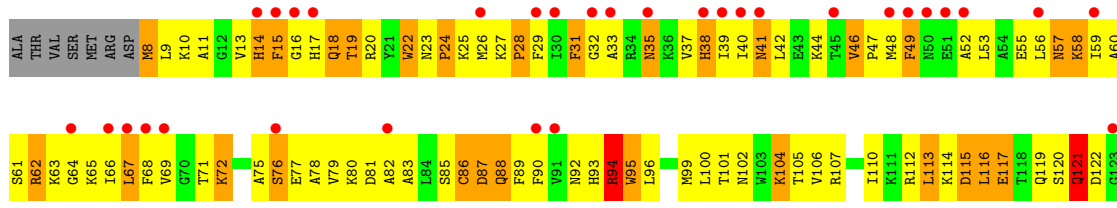
• Molecule 19: 30S ribosomal protein S20

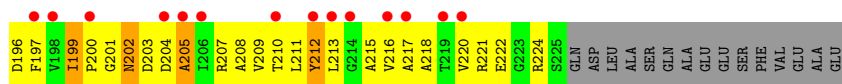


• Molecule 20: 30S ribosomal protein S2

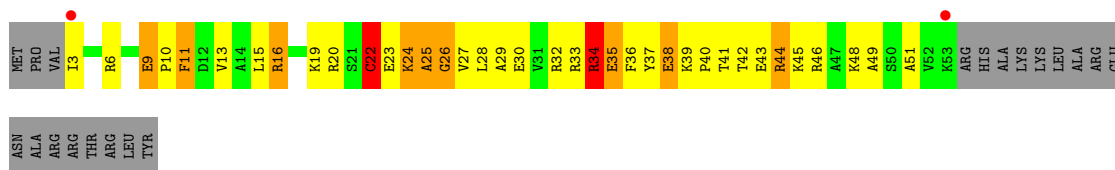
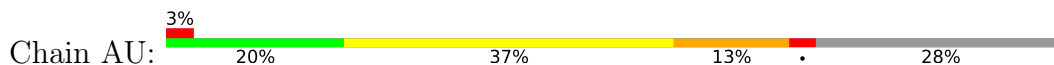


• Molecule 20: 30S ribosomal protein S2

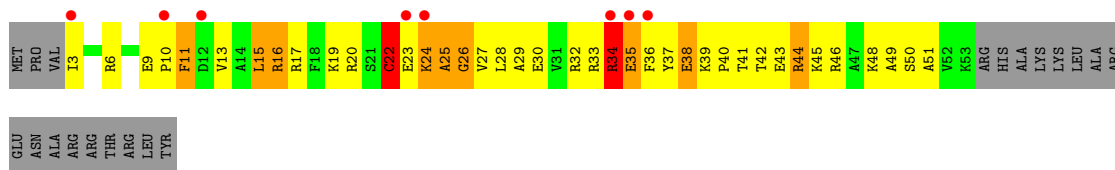
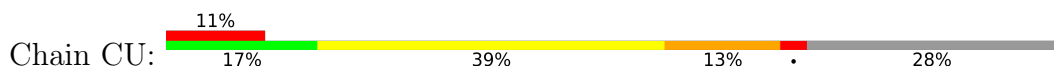




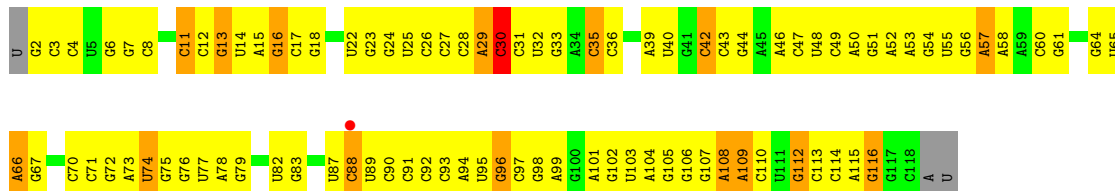
• Molecule 21: 30S ribosomal protein S21



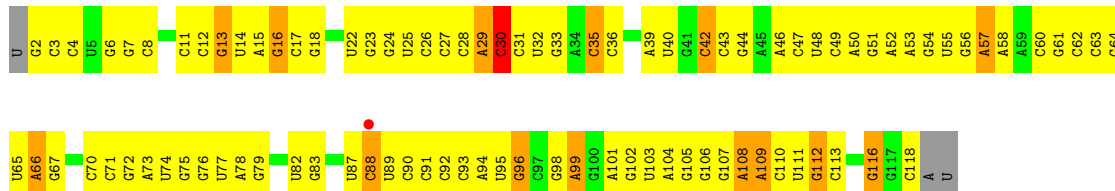
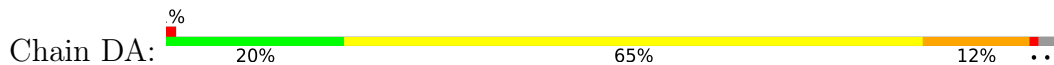
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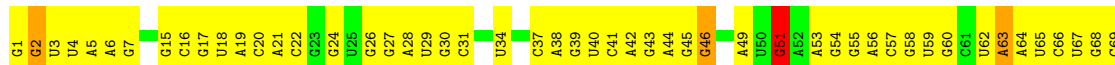
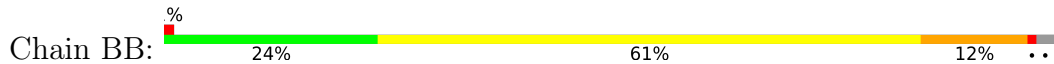
• Molecule 22: 5S ribosomal RNA



• Molecule 22: 5S ribosomal RNA



• Molecule 23: 23S ribosomal RNA



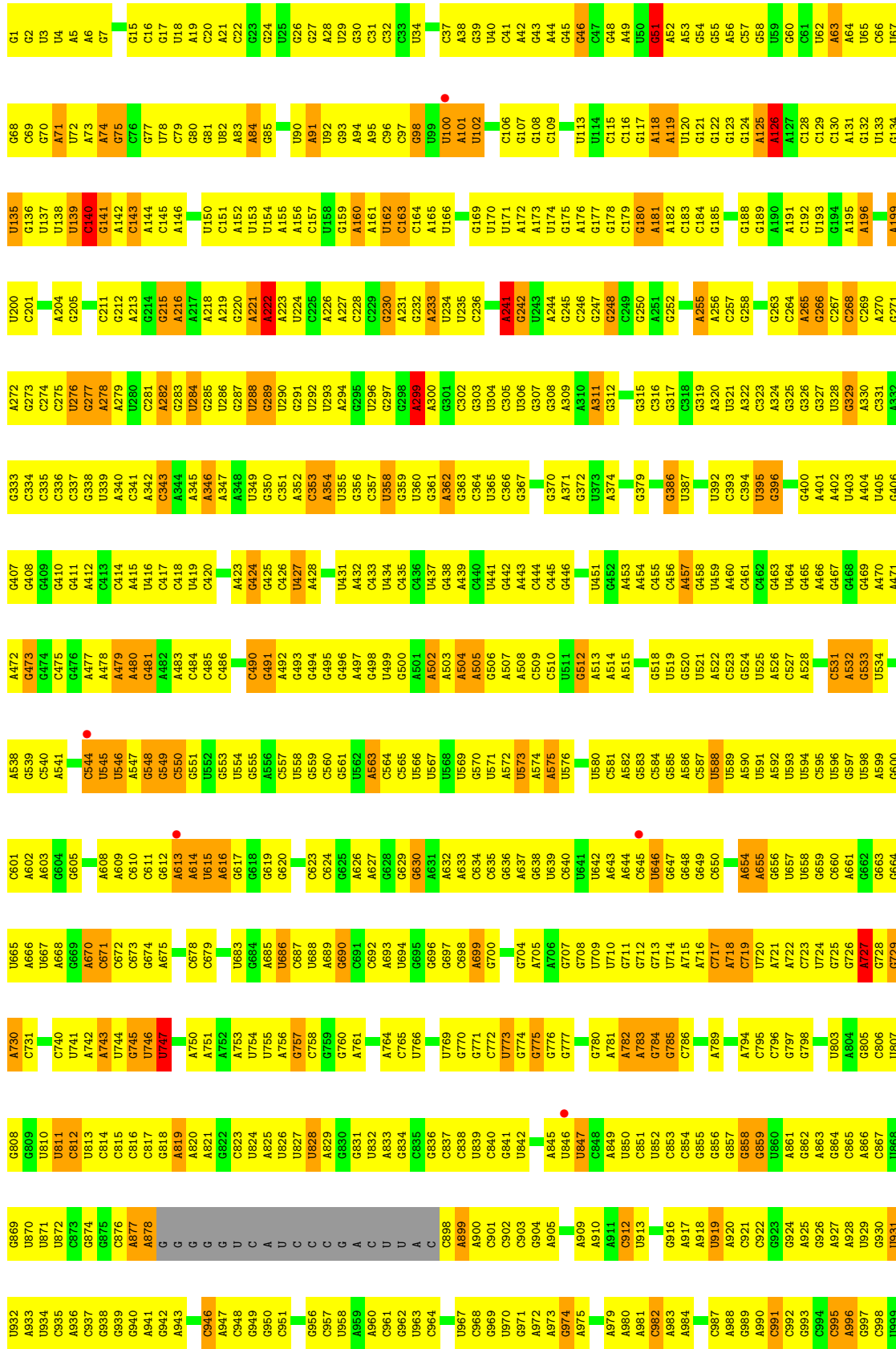
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G1017	A941	G	G818	A742	G669	A608	C943	G411	C334	A271	C202	U137	U72
U1018	G942	G	A819	A743	A670	A609	C944	G412	C335	A272	A204	U138	A73
U1019	G943	G	A820	A744	C671	A610	A475	C413	C336	G273	G205	U139	A74
A1020	C944	G	A821	G745	C672	C610	A480	C414	C337	C274	G206	U140	G75
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C946	C946	U	G823	U747	G674	G612	A482	U416	G339	U276	G212	A142	G77
A947	A947	C	U824	A750	A675	A613	A483	C417	U390	G277	A213	C143	U78
C948	C948	A	A825	A751	A676	A614	C484	C418	C341	A278	G214	A144	C79
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G950	G950	C	U827	G752	G681	A616	C486	C420	C343	U280	A216	G81	G81
C951	C951	C	G682	A753	G682	G617	G553	A344	C344	C281	A217	U82	U82
A1028	A1028	C	A829	U754	U685	G618	G554	A345	A345	A282	A218	U150	A83
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G1032	G961	G	U832	G757	U686	A621	C493	U348	A348	U286	A221	A152	U90
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A1039	U967	C	G836	C765	G690	G625	A497	U431	A352	U290	C225	C157	G93
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G1047	A975	G	A845	G774	C698	A633	A505	A439	A299	A299	A233	A165	A101
A979	A979	A	U846	G775	A699	C634	G506	U441	A300	A300	U234	U166	U102
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U1060	A990	U	A855	G712	G712	A644	A515	A453	G372	A309	A244	G175	G175
U1061	C991	U	U856	G713	U713	A645	A516	A454	U373	A310	G245	G177	G177
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C1079	C1013	U	U871	A727	A727	A661	A530	A470	U403	G326	G263	C129	C129
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			U874	A730	A730	U665	A533	A473	G406	G329	G286	A196	G132
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• Molecule 23: 23S ribosomal RNA



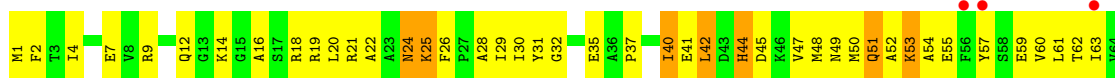


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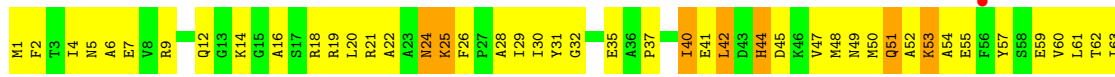
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• Molecule 24: 50S ribosomal protein L25

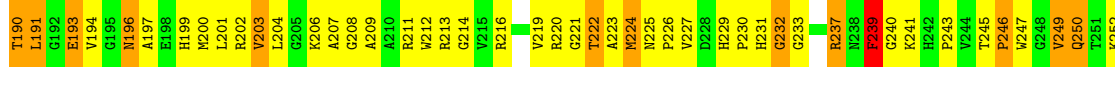
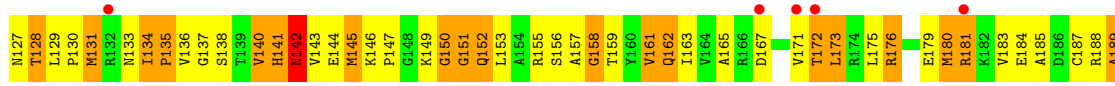
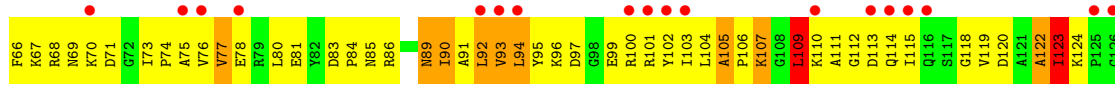
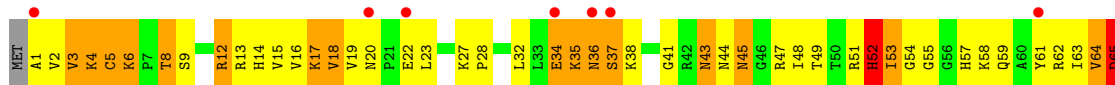




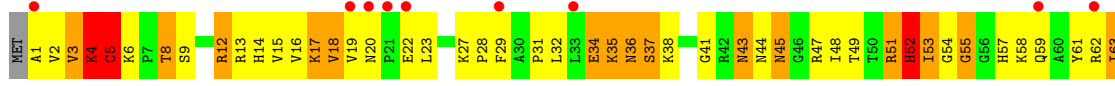
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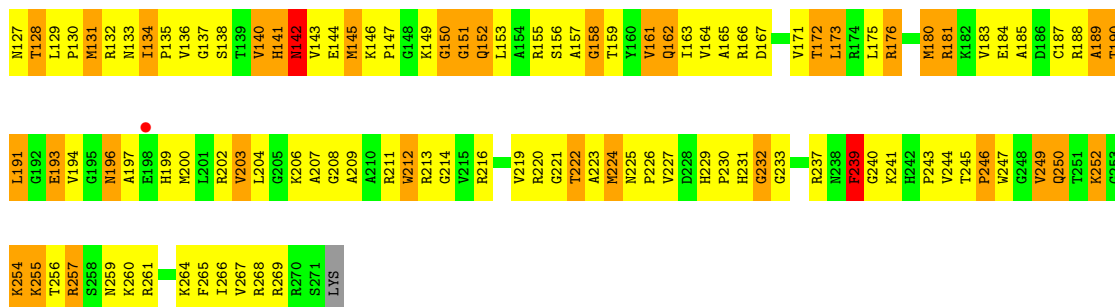


• Molecule 25: 50S ribosomal protein L2

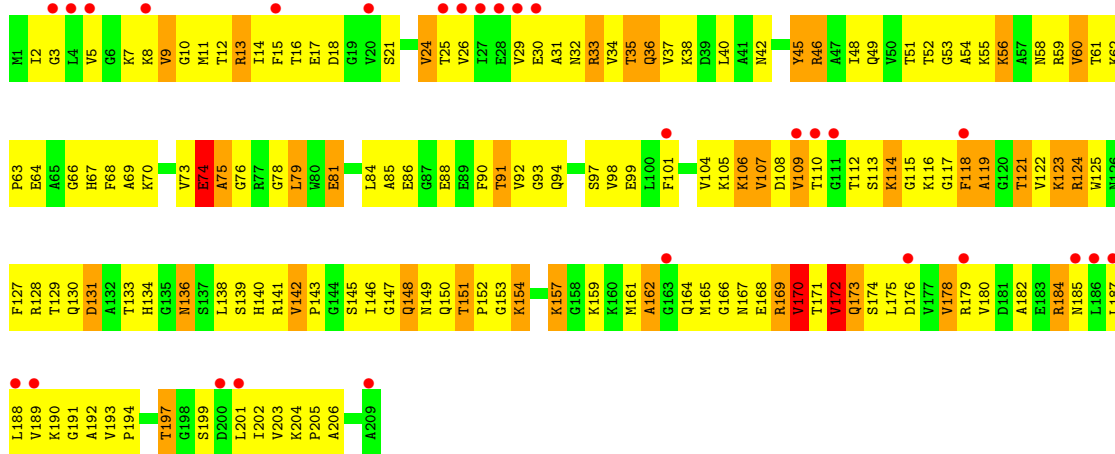


• Molecule 25: 50S ribosomal protein L2

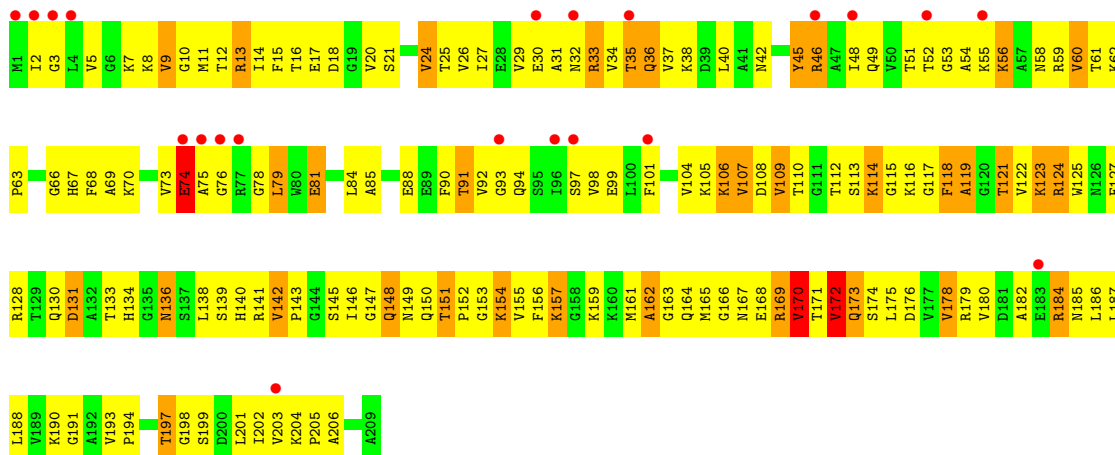




• Molecule 26: 50S ribosomal protein L3

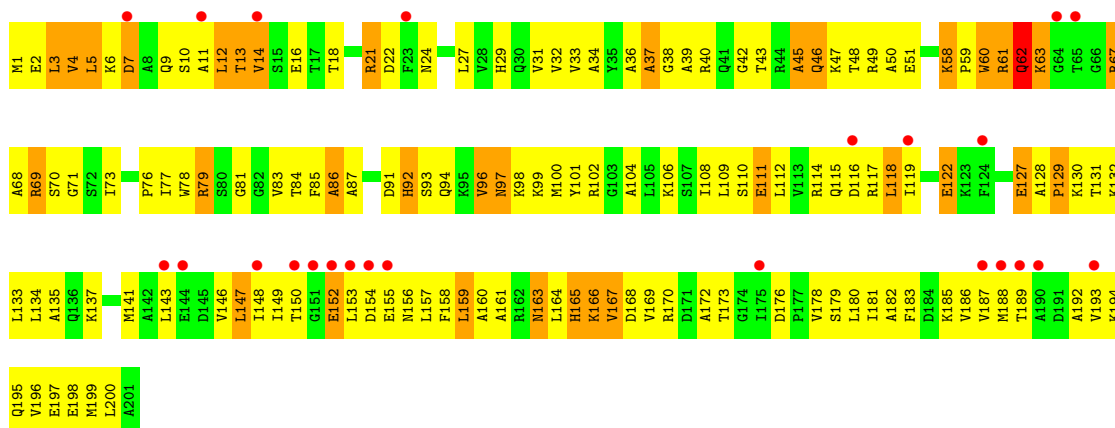


• Molecule 26: 50S ribosomal protein L3

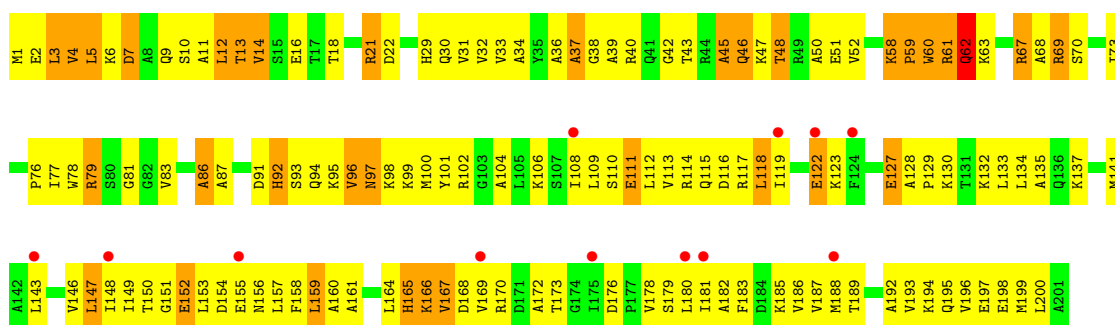


• Molecule 27: 50S ribosomal protein L4

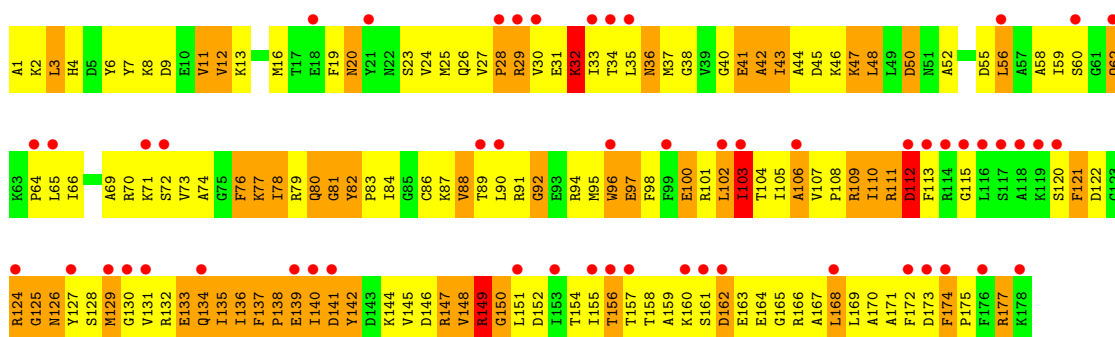
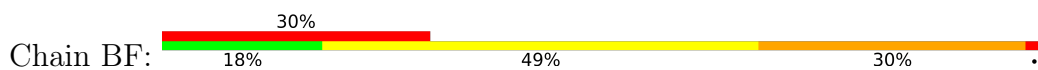




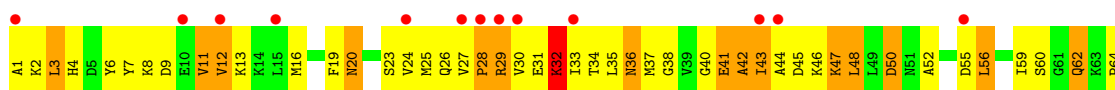
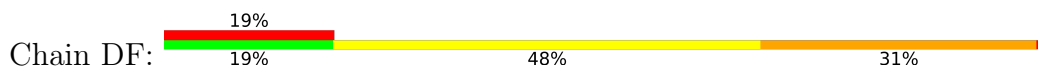
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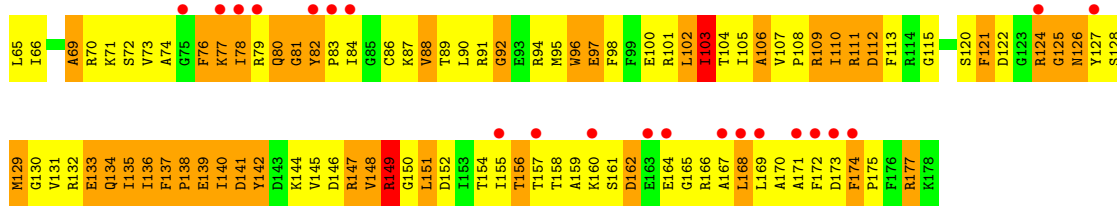


• Molecule 28: 50S ribosomal protein L5

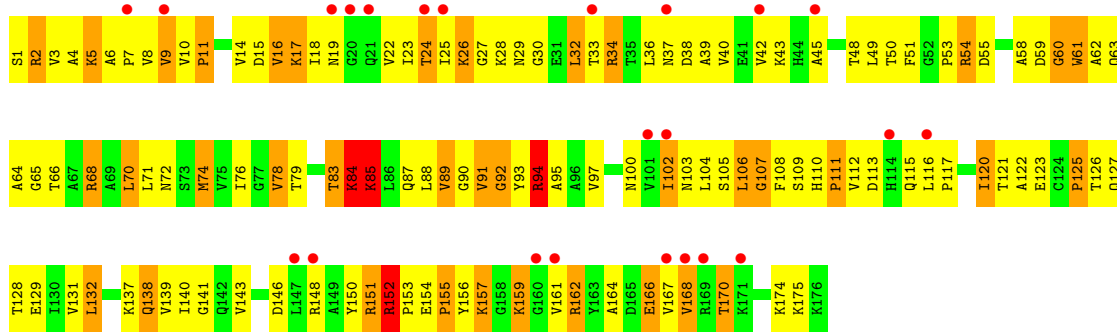


• Molecule 28: 50S ribosomal protein L5

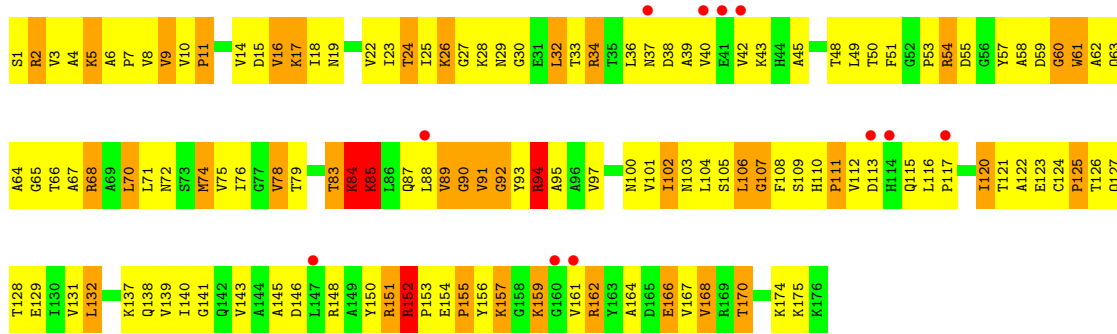




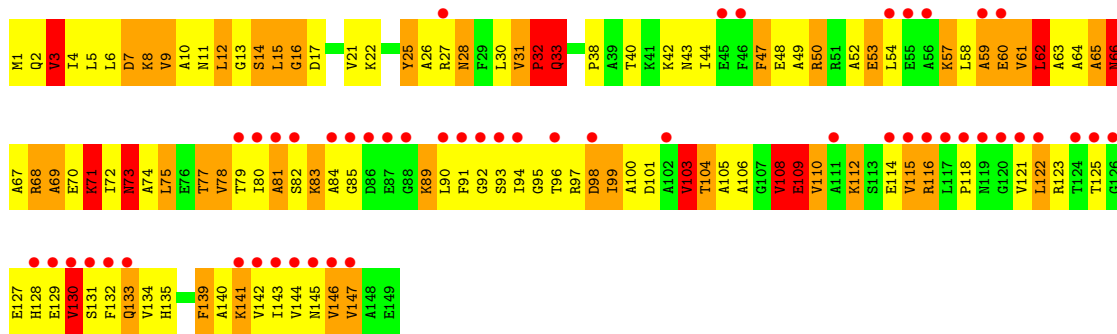
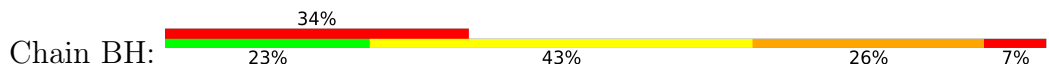
● Molecule 29: 50S ribosomal protein L6



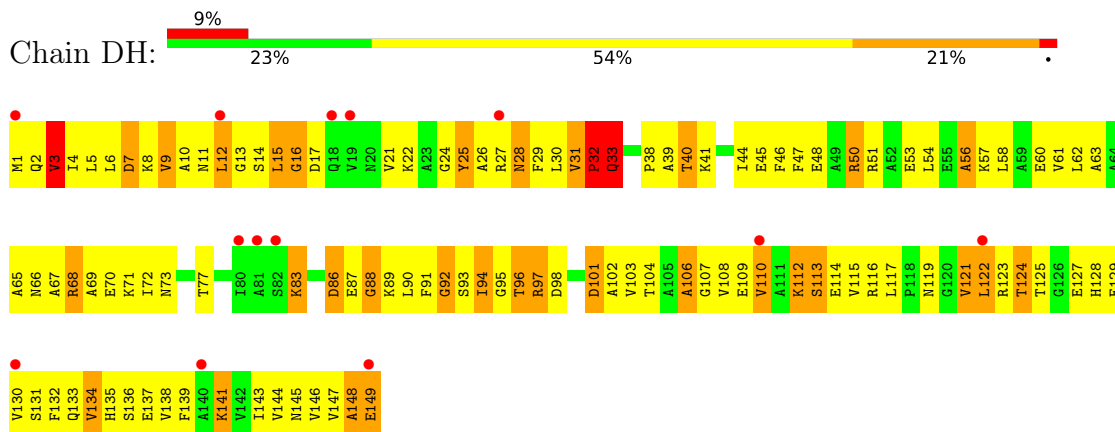
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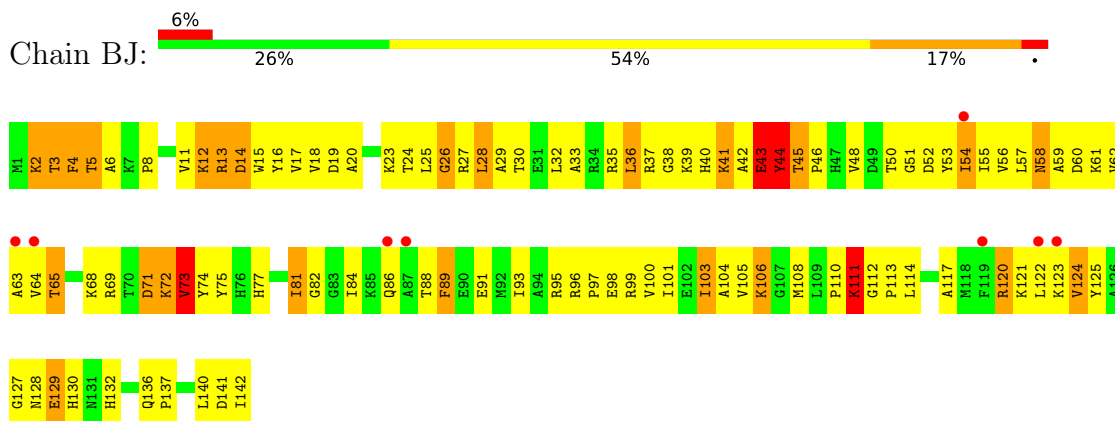
● Molecule 30: 50S ribosomal protein L9



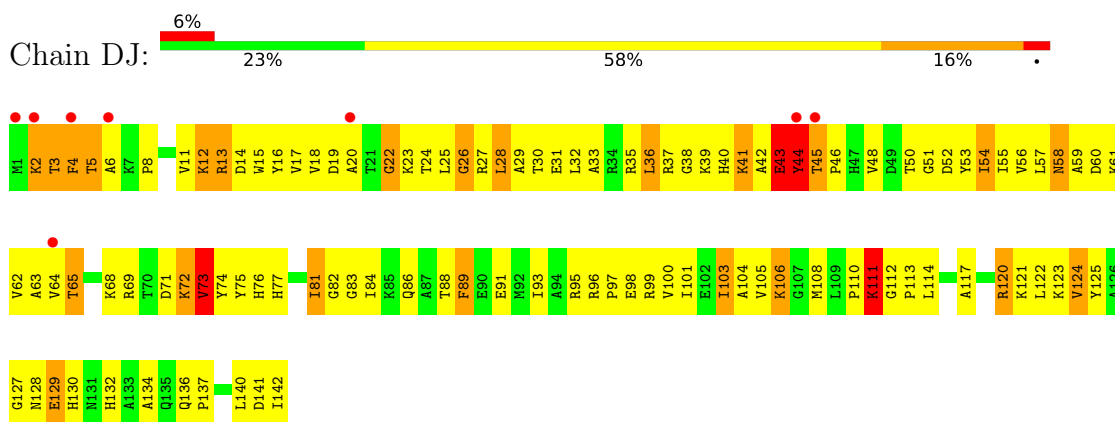
- Molecule 30: 50S ribosomal protein L9



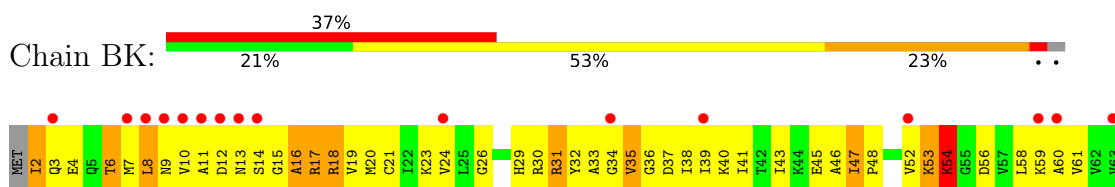
- Molecule 31: 50S ribosomal protein L13

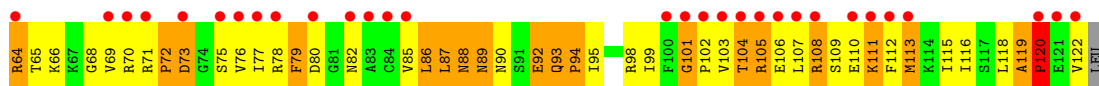


- Molecule 31: 50S ribosomal protein L13



- Molecule 32: 50S ribosomal protein L14

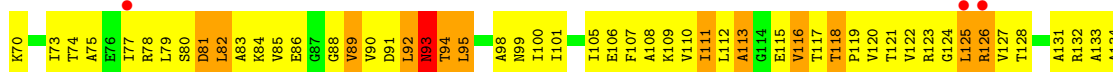
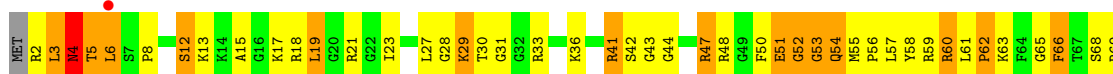




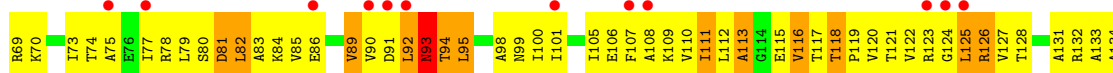
• Molecule 32: 50S ribosomal protein L14



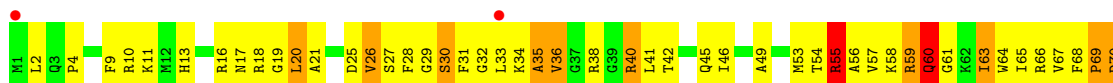
• Molecule 33: 50S ribosomal protein L15

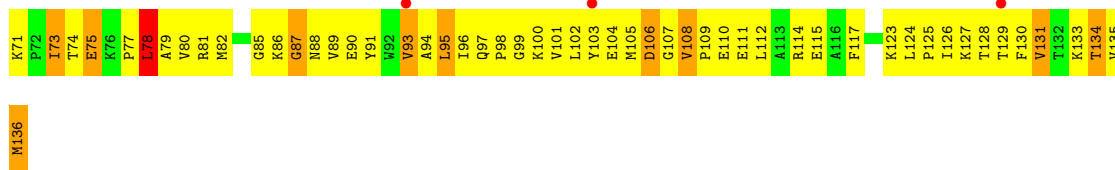


• Molecule 33: 50S ribosomal protein L15

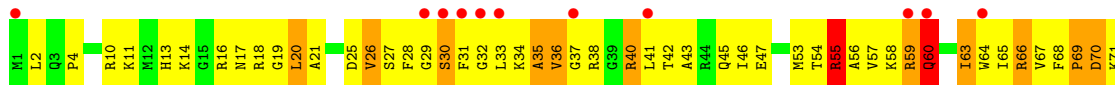


• Molecule 34: 50S ribosomal protein L16





• Molecule 34: 50S ribosomal protein L16



• Molecule 35: 50S ribosomal protein L17

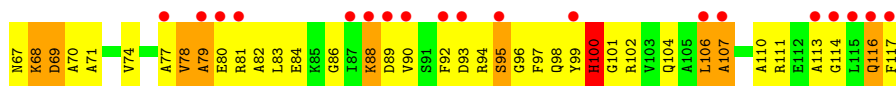


• Molecule 35: 50S ribosomal protein L17

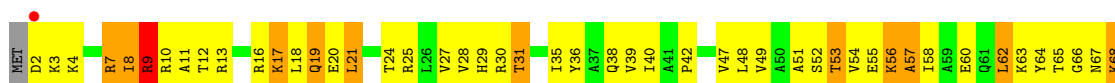


• Molecule 36: 50S ribosomal protein L18

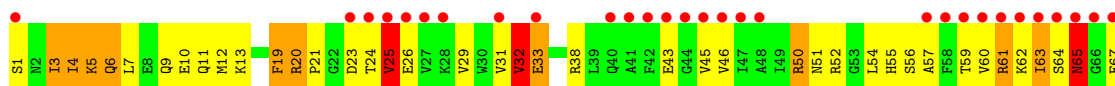




- Molecule 36: 50S ribosomal protein L18



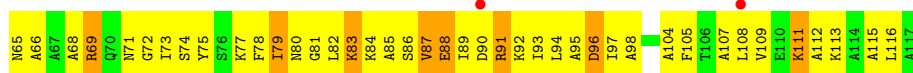
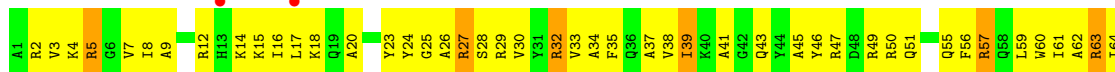
- Molecule 37: 50S ribosomal protein L19



- Molecule 37: 50S ribosomal protein L19

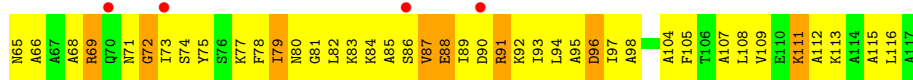


- Molecule 38: 50S ribosomal protein L20

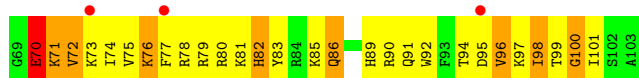


- Molecule 38: 50S ribosomal protein L20

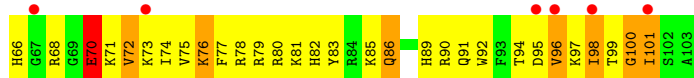
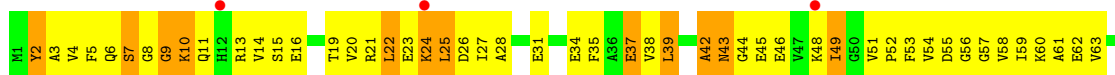
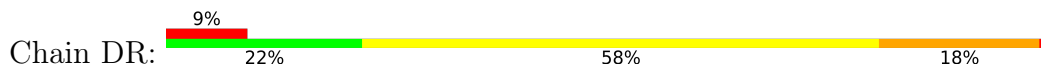




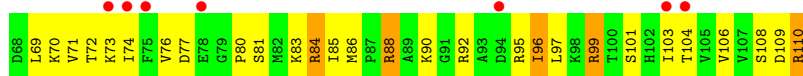
• Molecule 39: 50S ribosomal protein L21



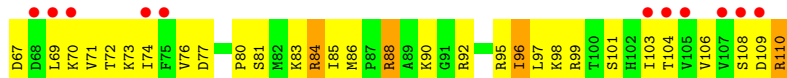
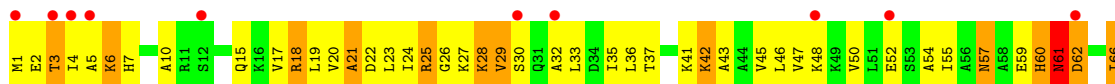
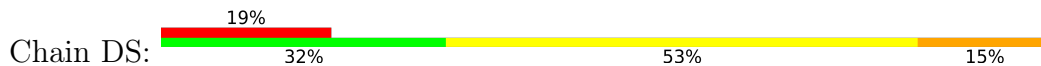
• Molecule 39: 50S ribosomal protein L21



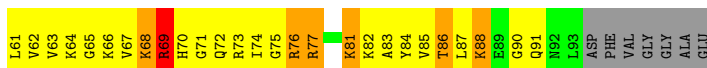
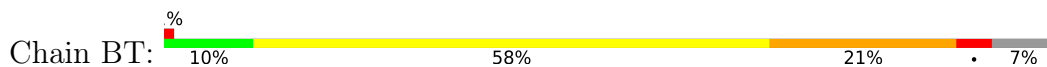
• Molecule 40: 50S ribosomal protein L22



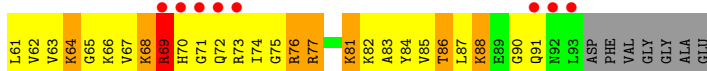
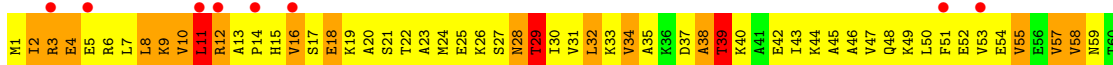
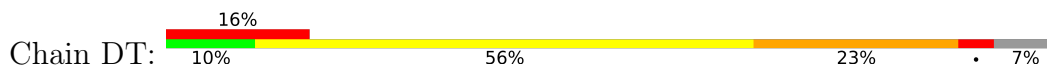
• Molecule 40: 50S ribosomal protein L22



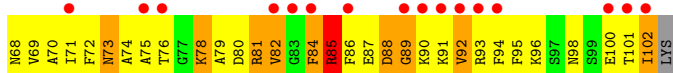
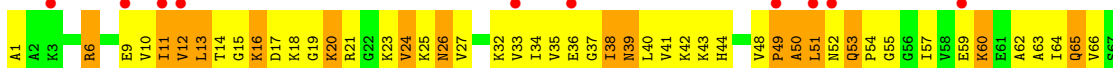
- Molecule 41: 50S ribosomal protein L23



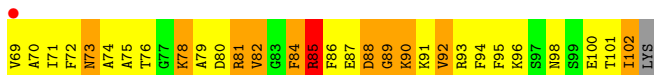
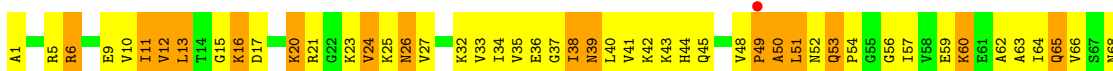
- Molecule 41: 50S ribosomal protein L23



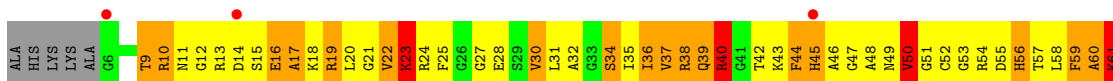
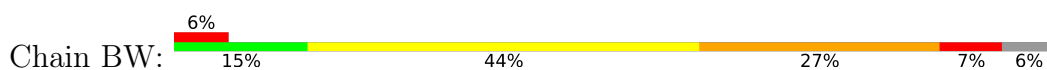
- Molecule 42: 50S ribosomal protein L24

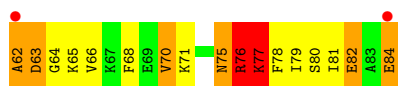


- Molecule 42: 50S ribosomal protein L24

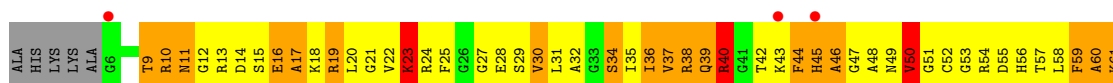
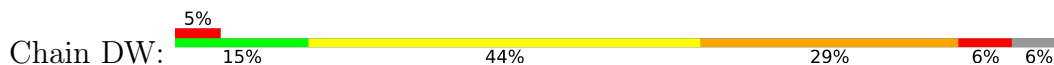


- Molecule 43: 50S ribosomal protein L27

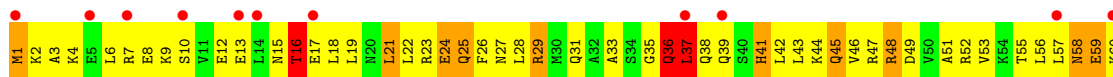




- Molecule 43: 50S ribosomal protein L27



- Molecule 44: 50S ribosomal protein L29



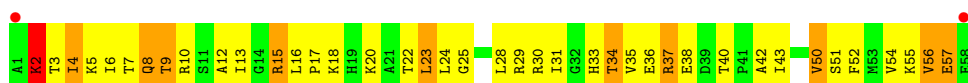
- Molecule 44: 50S ribosomal protein L29



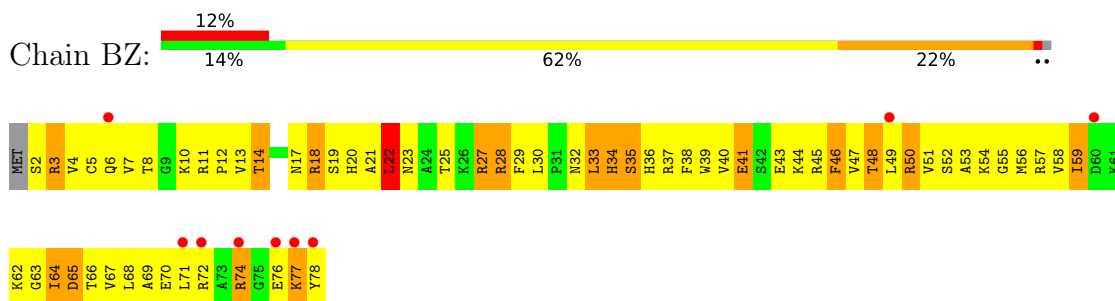
- Molecule 45: 50S ribosomal protein L30



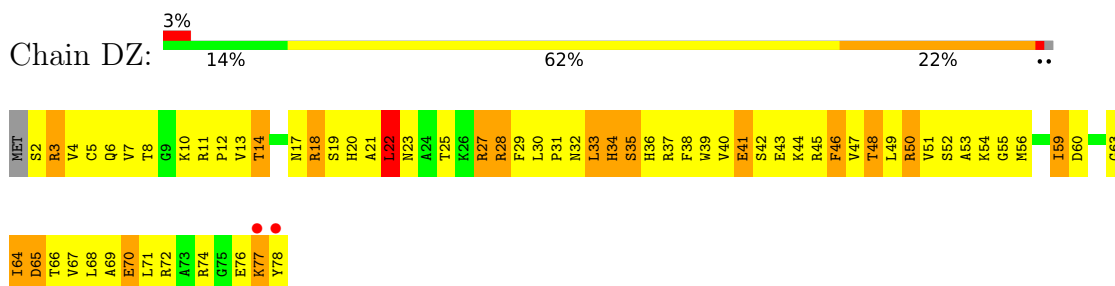
- Molecule 45: 50S ribosomal protein L30



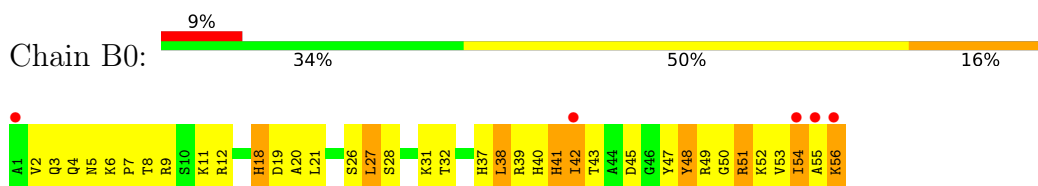
- Molecule 46: 50S ribosomal protein L28



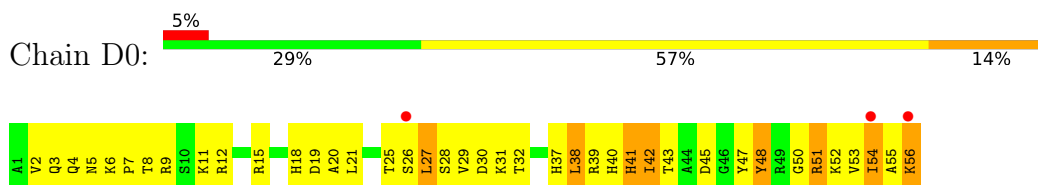
- Molecule 46: 50S ribosomal protein L28



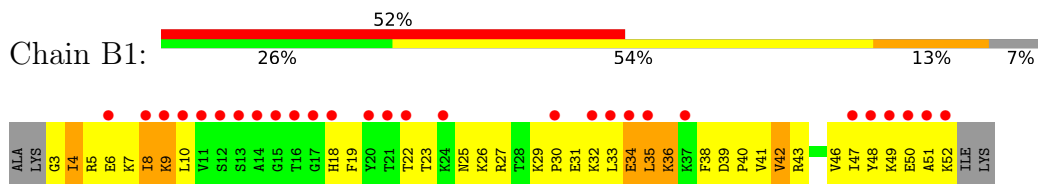
- Molecule 47: 50S ribosomal protein L32



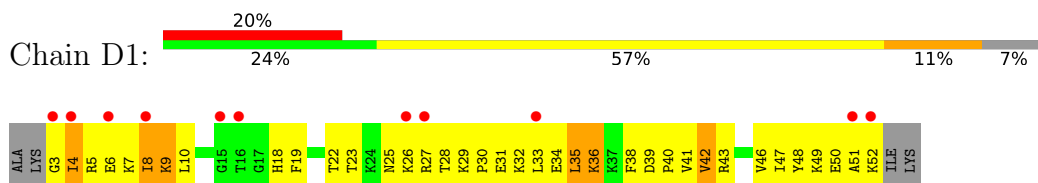
- Molecule 47: 50S ribosomal protein L32



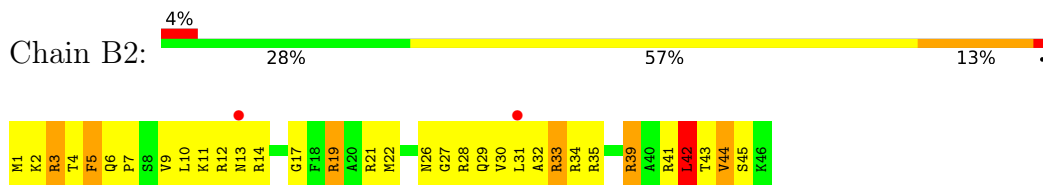
- Molecule 48: 50S ribosomal protein L33



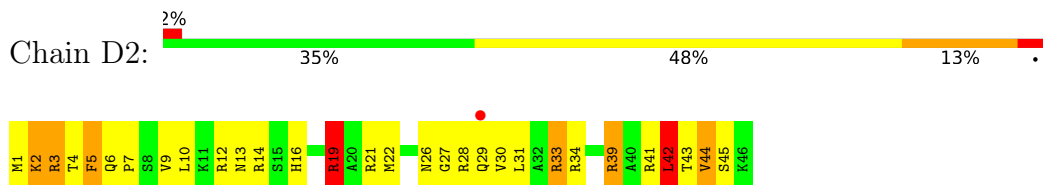
- Molecule 48: 50S ribosomal protein L33



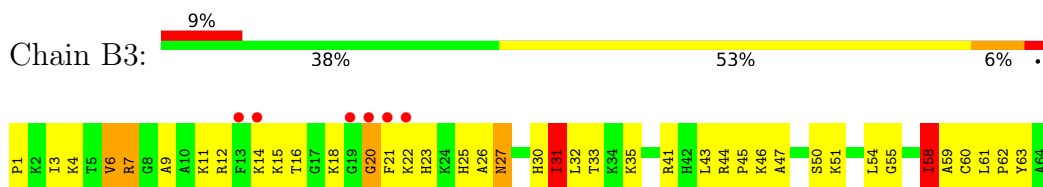
- Molecule 49: 50S ribosomal protein L34



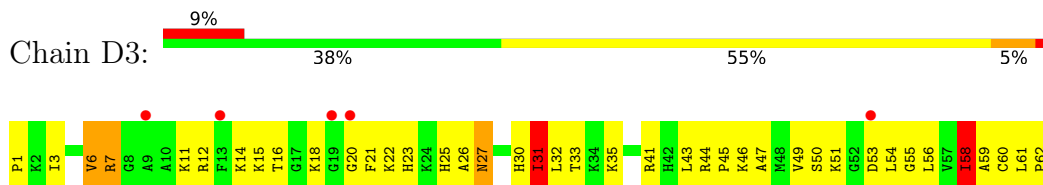
- Molecule 49: 50S ribosomal protein L34



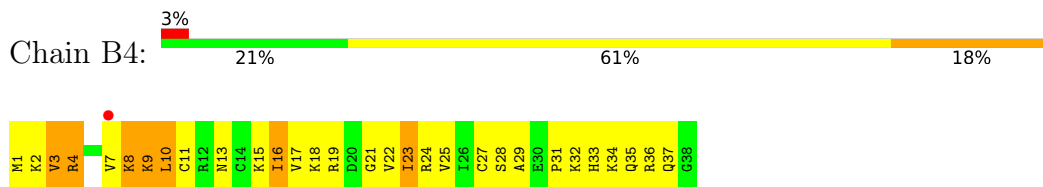
- Molecule 50: 50S ribosomal protein L35



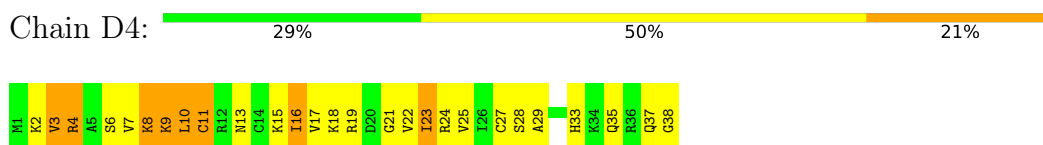
- Molecule 50: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L36

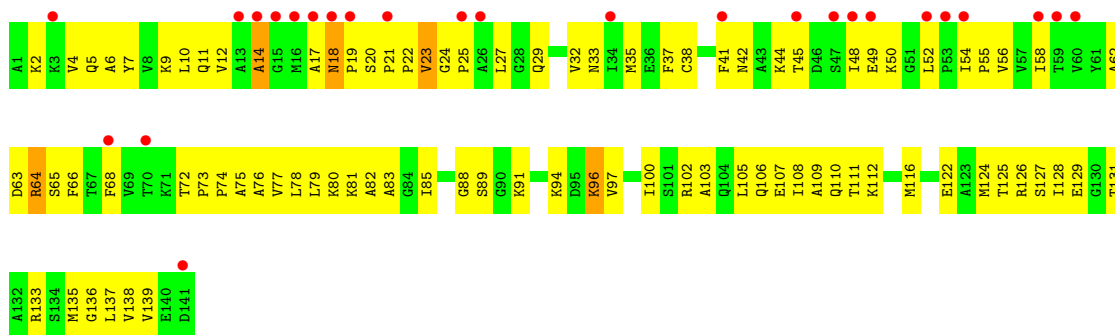


- Molecule 51: 50S ribosomal protein L36

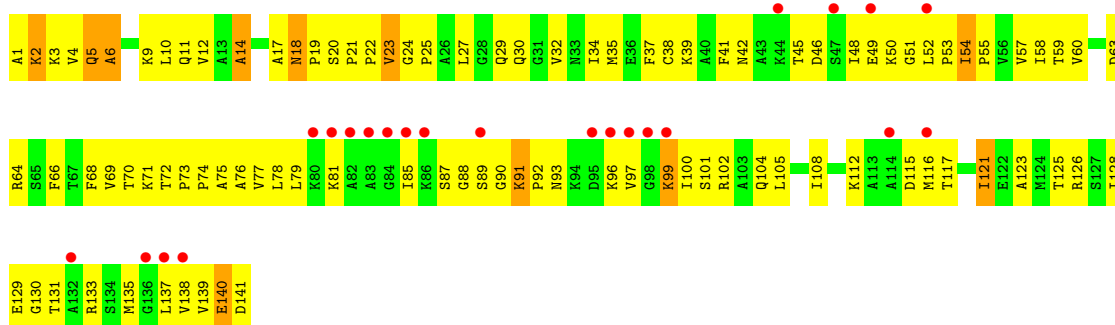


- Molecule 52: 50S ribosomal protein L11





● Molecule 52: 50S ribosomal protein L11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.70Å 379.50Å 739.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.50 137.77 – 3.50	Depositor EDS
% Data completeness (in resolution range)	62.1 (70.00-3.50) 62.3 (137.77-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.49Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.269 , 0.318 0.234 , 0.279	Depositor DCC
R_{free} test set	22229 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	117.9	Xtrriage
Anisotropy	0.294	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	284077	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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 i

5.1 Standard geometry i

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

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	0.26	1/36762 (0.0%)	0.77	13/57350 (0.0%)
1	CA	0.26	1/36762 (0.0%)	0.77	17/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.43	0/2227
3	CD	0.23	0/1665	0.43	0/2227
4	AE	0.23	0/1118	0.45	0/1504
4	CE	0.23	0/1118	0.45	0/1504
5	AF	0.24	0/835	0.44	0/1128
5	CF	0.24	0/835	0.44	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.44	0/1624
7	AH	0.23	0/989	0.45	0/1326
7	CH	0.23	0/989	0.45	0/1326
8	AI	0.24	0/1034	0.44	0/1375
8	CI	0.24	0/1034	0.44	0/1375
9	AJ	0.22	0/796	0.47	0/1077
9	CJ	0.22	0/796	0.47	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.47	0/1300
11	CL	0.22	0/969	0.47	0/1300
12	AM	0.21	0/892	0.45	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.43	0/1043
13	CN	0.24	0/785	0.43	0/1043
14	AO	0.22	0/723	0.44	0/966
14	CO	0.22	0/723	0.44	0/966
15	AP	0.25	0/659	0.45	0/884
15	CP	0.25	0/648	0.44	0/870
16	AQ	0.24	0/657	0.46	0/881
16	CQ	0.24	0/665	0.48	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.44	0/621
17	CR	0.23	0/462	0.44	0/621
18	AS	0.25	0/652	0.45	0/877
18	CS	0.25	0/660	0.46	0/888
19	AT	0.23	0/671	0.41	0/888
19	CT	0.24	0/671	0.41	0/888
20	AB	0.25	0/1735	0.44	0/2338
20	CB	0.25	0/1735	0.44	0/2338
21	AU	0.26	0/430	0.46	0/570
21	CU	0.26	0/430	0.46	0/570
22	BA	0.24	0/2803	0.75	2/4371 (0.0%)
22	DA	0.25	0/2803	0.75	1/4371 (0.0%)
23	BB	0.27	7/68314 (0.0%)	0.78	41/106569 (0.0%)
23	DB	0.28	7/68314 (0.0%)	0.78	49/106569 (0.0%)
24	BV	0.25	0/766	0.43	0/1025
24	DV	0.25	0/766	0.43	0/1025
25	BC	0.22	0/2121	0.47	0/2852
25	DC	0.22	0/2121	0.47	0/2852
26	BD	0.24	0/1586	0.46	0/2134
26	DD	0.24	0/1586	0.47	0/2134
27	BE	0.23	0/1571	0.49	0/2113
27	DE	0.24	0/1571	0.49	0/2113
28	BF	0.26	0/1444	0.51	0/1937
28	DF	0.26	0/1444	0.51	0/1937
29	BG	0.23	0/1343	0.46	0/1816
29	DG	0.23	0/1343	0.46	0/1816
30	BH	0.25	0/1122	0.46	0/1515
30	DH	0.25	0/1122	0.46	0/1515
31	BJ	0.23	0/1152	0.47	0/1551
31	DJ	0.23	0/1152	0.47	0/1551
32	BK	0.24	0/939	0.52	0/1258
32	DK	0.23	0/939	0.52	0/1258
33	BL	0.23	0/1054	0.47	0/1403
33	DL	0.23	0/1054	0.47	0/1403
34	BM	0.25	0/1093	0.47	0/1460
34	DM	0.25	0/1093	0.47	0/1460
35	BN	0.24	0/973	0.51	0/1301
35	DN	0.24	0/973	0.51	0/1301
36	BO	0.23	0/902	0.47	0/1209
36	DO	0.23	0/902	0.48	0/1209
37	BP	0.24	0/929	0.48	0/1242
37	DP	0.24	0/929	0.48	0/1242
38	BQ	0.25	0/960	0.46	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.25	0/960	0.46	0/1278
39	BR	0.25	0/829	0.48	0/1107
39	DR	0.25	0/829	0.48	0/1107
40	BS	0.22	0/864	0.49	0/1156
40	DS	0.22	0/864	0.49	0/1156
41	BT	0.23	0/744	0.52	0/994
41	DT	0.23	0/744	0.52	0/994
42	BU	0.25	0/787	0.45	0/1051
42	DU	0.25	0/787	0.45	0/1051
43	BW	0.28	0/603	0.48	0/797
43	DW	0.27	0/603	0.48	0/797
44	BX	0.23	0/510	0.51	0/677
44	DX	0.23	0/510	0.51	0/677
45	BY	0.23	0/453	0.49	0/605
45	DY	0.23	0/453	0.49	0/605
46	BZ	0.25	0/635	0.51	0/848
46	DZ	0.25	0/635	0.51	0/848
47	B0	0.22	0/450	0.52	0/599
47	D0	0.22	0/450	0.52	0/599
48	B1	0.27	0/416	0.47	0/554
48	D1	0.27	0/416	0.47	0/554
49	B2	0.25	0/380	0.49	0/498
49	D2	0.26	0/380	0.49	0/498
50	B3	0.24	0/513	0.46	0/676
50	D3	0.24	0/513	0.46	0/676
51	B4	0.22	0/303	0.46	0/397
51	D4	0.22	0/303	0.46	0/397
52	BI	0.24	0/1046	0.46	0/1410
52	DI	0.25	0/1046	0.47	0/1410
All	All	0.26	16/306361 (0.0%)	0.70	123/457973 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	13
1	CA	0	13
23	BB	0	36
23	DB	0	38
All	All	0	100

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	1086	A	C5-C6	-16.14	1.26	1.41
23	BB	1086	A	C5-C6	-16.11	1.26	1.41
23	BB	1088	A	C6-N1	-10.49	1.28	1.35
23	DB	1088	A	C6-N1	-10.45	1.28	1.35
23	DB	1060	U	C2-N3	7.89	1.43	1.37

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	2791	G	O5'-P-OP1	-31.87	72.45	110.70
23	DB	2791	G	O5'-P-OP2	-31.41	73.01	110.70
23	DB	2204	G	O5'-P-OP1	-29.65	75.12	110.70
1	AA	1213	A	O5'-P-OP2	-29.58	75.21	110.70
23	BB	2204	G	O5'-P-OP2	-28.34	76.69	110.70

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	83	C	Sidechain

5.2 Too-close contacts [i](#)

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	32831	0	16521	1355	0
1	CA	32831	0	16521	1385	0
2	AC	1624	0	1699	137	0
2	CC	1624	0	1699	145	0
3	AD	1643	0	1710	166	0
3	CD	1643	0	1710	156	0
4	AE	1105	0	1148	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CE	1105	0	1148	115	0
5	AF	817	0	808	98	0
5	CF	817	0	808	88	0
6	AG	1174	0	1230	118	0
6	CG	1196	0	1246	110	0
7	AH	979	0	1034	93	0
7	CH	979	0	1034	93	0
8	AI	1022	0	1070	153	0
8	CI	1022	0	1070	151	0
9	AJ	786	0	828	78	0
9	CJ	786	0	828	84	0
10	AK	877	0	887	100	0
10	CK	877	0	887	101	0
11	AL	955	0	1019	90	0
11	CL	955	0	1019	94	0
12	AM	883	0	944	110	0
12	CM	876	0	937	109	0
13	AN	774	0	827	96	0
13	CN	774	0	827	90	0
14	AO	715	0	742	48	0
14	CO	715	0	742	41	0
15	AP	649	0	666	53	0
15	CP	638	0	656	55	0
16	AQ	648	0	691	73	0
16	CQ	656	0	702	73	0
17	AR	455	0	478	34	0
17	CR	455	0	478	34	0
18	AS	637	0	665	101	0
18	CS	644	0	675	98	0
19	AT	665	0	714	49	0
19	CT	665	0	714	49	0
20	AB	1704	0	1732	205	0
20	CB	1704	0	1732	208	0
21	AU	425	0	449	75	0
21	CU	425	0	449	68	0
22	BA	2507	0	1270	109	0
22	DA	2507	0	1270	111	0
23	BB	60995	0	30678	2412	0
23	DB	60995	0	30677	2498	0
24	BV	753	0	780	89	0
24	DV	753	0	780	90	0
25	BC	2082	0	2157	261	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DC	2082	0	2157	274	0
26	BD	1565	0	1616	216	0
26	DD	1565	0	1616	220	0
27	BE	1552	0	1619	180	0
27	DE	1552	0	1619	170	0
28	BF	1420	0	1460	236	0
28	DF	1420	0	1460	238	0
29	BG	1323	0	1374	163	0
29	DG	1323	0	1374	161	0
30	BH	1111	0	1148	176	0
30	DH	1111	0	1148	146	0
31	BJ	1129	0	1162	150	0
31	DJ	1129	0	1162	154	0
32	BK	930	0	1000	122	0
32	DK	930	0	1000	134	0
33	BL	1045	0	1117	150	0
33	DL	1045	0	1117	155	0
34	BM	1074	0	1157	114	0
34	DM	1074	0	1157	112	0
35	BN	960	0	1000	135	0
35	DN	960	0	1000	129	0
36	BO	892	0	923	97	0
36	DO	892	0	923	104	0
37	BP	917	0	965	112	0
37	DP	917	0	965	113	0
38	BQ	947	0	1022	156	0
38	DQ	947	0	1022	167	0
39	BR	816	0	839	123	0
39	DR	816	0	839	138	0
40	BS	857	0	922	93	0
40	DS	857	0	922	93	0
41	BT	738	0	807	127	0
41	DT	738	0	807	122	0
42	BU	779	0	834	132	0
42	DU	779	0	834	121	0
43	BW	596	0	610	128	0
43	DW	596	0	610	137	0
44	BX	509	0	543	54	0
44	DX	509	0	543	50	0
45	BY	449	0	491	48	0
45	DY	449	0	491	50	0
46	BZ	625	0	652	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DZ	625	0	652	92	0
47	B0	444	0	461	40	0
47	D0	444	0	461	42	0
48	B1	409	0	440	57	0
48	D1	409	0	440	44	0
49	B2	377	0	418	43	0
49	D2	377	0	418	43	0
50	B3	504	0	574	40	0
50	D3	504	0	574	40	0
51	B4	302	0	340	40	0
51	D4	302	0	340	35	0
52	BI	1032	0	1088	111	0
52	DI	1032	0	1088	182	0
53	AA	58	0	0	0	0
53	AE	1	0	0	0	0
53	AN	1	0	0	0	0
53	BB	110	0	0	0	0
53	CA	61	0	0	0	0
53	CE	1	0	0	0	0
53	DB	111	0	0	0	0
54	AA	36	0	37	2	0
54	CA	36	0	37	1	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	282	0	0	4	0
56	AE	4	0	0	0	0
56	AK	2	0	0	0	0
56	AL	5	0	0	0	0
56	AN	4	0	0	0	0
56	AT	3	0	0	0	0
56	B2	1	0	0	0	0
56	BB	492	0	0	5	0
56	BC	8	0	0	0	0
56	BD	1	0	0	0	0
56	BE	2	0	0	0	0
56	BH	1	0	0	0	0
56	BL	2	0	0	0	0
56	CA	294	0	0	0	0
56	CE	4	0	0	0	0
56	CI	1	0	0	0	0
56	CK	1	0	0	0	0
56	CL	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CN	3	0	0	0	0
56	CT	1	0	0	0	0
56	D2	1	0	0	0	0
56	DB	499	0	0	8	0
56	DC	5	0	0	0	0
56	DD	1	0	0	0	0
56	DE	1	0	0	0	0
56	DL	5	0	0	1	0
56	DP	1	0	0	0	0
All	All	284077	0	190751	17232	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 36.

The worst 5 of 17232 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)
23:DB:1099:G:H8	52:DI:3:LYS:N	1.38	1.20
23:BB:855:G:H21	43:BW:23:LYS:HG2	1.08	1.15
42:DU:85:ARG:HD3	42:DU:86:PHE:H	1.13	1.14
41:DT:5:GLU:HA	41:DT:8:LEU:HB2	1.25	1.13
42:BU:85:ARG:HD3	42:BU:86:PHE:H	1.11	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	AC	204/232 (88%)	147 (72%)	40 (20%)	17 (8%)	1 9
2	CC	204/232 (88%)	148 (72%)	40 (20%)	16 (8%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	136 (67%)	52 (26%)	15 (7%)	1	11
3	CD	203/205 (99%)	134 (66%)	54 (27%)	15 (7%)	1	11
4	AE	148/166 (89%)	117 (79%)	27 (18%)	4 (3%)	5	33
4	CE	148/166 (89%)	117 (79%)	25 (17%)	6 (4%)	3	23
5	AF	98/135 (73%)	66 (67%)	21 (21%)	11 (11%)	0	6
5	CF	98/135 (73%)	67 (68%)	21 (21%)	10 (10%)	0	7
6	AG	148/178 (83%)	122 (82%)	18 (12%)	8 (5%)	2	17
6	CG	150/178 (84%)	124 (83%)	20 (13%)	6 (4%)	3	24
7	AH	127/129 (98%)	92 (72%)	26 (20%)	9 (7%)	1	12
7	CH	127/129 (98%)	90 (71%)	28 (22%)	9 (7%)	1	12
8	AI	125/129 (97%)	88 (70%)	29 (23%)	8 (6%)	1	14
8	CI	125/129 (97%)	88 (70%)	29 (23%)	8 (6%)	1	14
9	AJ	96/103 (93%)	69 (72%)	17 (18%)	10 (10%)	0	7
9	CJ	96/103 (93%)	68 (71%)	18 (19%)	10 (10%)	0	7
10	AK	115/128 (90%)	81 (70%)	26 (23%)	8 (7%)	1	12
10	CK	115/128 (90%)	80 (70%)	27 (24%)	8 (7%)	1	12
11	AL	121/123 (98%)	78 (64%)	29 (24%)	14 (12%)	0	5
11	CL	121/123 (98%)	79 (65%)	28 (23%)	14 (12%)	0	5
12	AM	112/117 (96%)	72 (64%)	36 (32%)	4 (4%)	3	26
12	CM	111/117 (95%)	69 (62%)	38 (34%)	4 (4%)	3	26
13	AN	92/100 (92%)	57 (62%)	25 (27%)	10 (11%)	0	6
13	CN	92/100 (92%)	56 (61%)	26 (28%)	10 (11%)	0	6
14	AO	86/89 (97%)	65 (76%)	16 (19%)	5 (6%)	1	16
14	CO	86/89 (97%)	65 (76%)	16 (19%)	5 (6%)	1	16
15	AP	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	0	6
15	CP	78/82 (95%)	53 (68%)	15 (19%)	10 (13%)	0	4
16	AQ	78/83 (94%)	56 (72%)	17 (22%)	5 (6%)	1	14
16	CQ	79/83 (95%)	56 (71%)	17 (22%)	6 (8%)	1	10
17	AR	53/74 (72%)	41 (77%)	10 (19%)	2 (4%)	3	25
17	CR	53/74 (72%)	41 (77%)	10 (19%)	2 (4%)	3	25
18	AS	77/91 (85%)	58 (75%)	17 (22%)	2 (3%)	5	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CS	78/91 (86%)	58 (74%)	18 (23%)	2 (3%)	5	33
19	AT	83/86 (96%)	59 (71%)	19 (23%)	5 (6%)	1	15
19	CT	83/86 (96%)	59 (71%)	19 (23%)	5 (6%)	1	15
20	AB	216/240 (90%)	143 (66%)	53 (24%)	20 (9%)	0	8
20	CB	216/240 (90%)	148 (68%)	46 (21%)	22 (10%)	0	7
21	AU	49/71 (69%)	28 (57%)	14 (29%)	7 (14%)	0	3
21	CU	49/71 (69%)	28 (57%)	14 (29%)	7 (14%)	0	3
24	BV	92/94 (98%)	63 (68%)	23 (25%)	6 (6%)	1	14
24	DV	92/94 (98%)	62 (67%)	24 (26%)	6 (6%)	1	14
25	BC	269/273 (98%)	158 (59%)	65 (24%)	46 (17%)	0	2
25	DC	269/273 (98%)	158 (59%)	65 (24%)	46 (17%)	0	2
26	BD	207/209 (99%)	121 (58%)	56 (27%)	30 (14%)	0	3
26	DD	207/209 (99%)	123 (59%)	52 (25%)	32 (16%)	0	3
27	BE	199/201 (99%)	120 (60%)	56 (28%)	23 (12%)	0	5
27	DE	199/201 (99%)	120 (60%)	56 (28%)	23 (12%)	0	5
28	BF	176/178 (99%)	103 (58%)	39 (22%)	34 (19%)	0	2
28	DF	176/178 (99%)	101 (57%)	41 (23%)	34 (19%)	0	2
29	BG	174/176 (99%)	105 (60%)	37 (21%)	32 (18%)	0	2
29	DG	174/176 (99%)	105 (60%)	36 (21%)	33 (19%)	0	2
30	BH	147/149 (99%)	68 (46%)	43 (29%)	36 (24%)	0	0
30	DH	147/149 (99%)	88 (60%)	32 (22%)	27 (18%)	0	2
31	BJ	140/142 (99%)	85 (61%)	39 (28%)	16 (11%)	0	6
31	DJ	140/142 (99%)	83 (59%)	40 (29%)	17 (12%)	0	5
32	BK	119/123 (97%)	70 (59%)	28 (24%)	21 (18%)	0	2
32	DK	119/123 (97%)	69 (58%)	27 (23%)	23 (19%)	0	2
33	BL	141/144 (98%)	75 (53%)	40 (28%)	26 (18%)	0	2
33	DL	141/144 (98%)	75 (53%)	40 (28%)	26 (18%)	0	2
34	BM	134/136 (98%)	77 (58%)	38 (28%)	19 (14%)	0	3
34	DM	134/136 (98%)	78 (58%)	35 (26%)	21 (16%)	0	2
35	BN	118/127 (93%)	73 (62%)	33 (28%)	12 (10%)	0	7
35	DN	118/127 (93%)	73 (62%)	32 (27%)	13 (11%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BO	114/117 (97%)	83 (73%)	21 (18%)	10 (9%)	1	8
36	DO	114/117 (97%)	83 (73%)	20 (18%)	11 (10%)	0	8
37	BP	112/114 (98%)	59 (53%)	35 (31%)	18 (16%)	0	2
37	DP	112/114 (98%)	58 (52%)	36 (32%)	18 (16%)	0	2
38	BQ	115/117 (98%)	79 (69%)	27 (24%)	9 (8%)	1	10
38	DQ	115/117 (98%)	75 (65%)	32 (28%)	8 (7%)	1	12
39	BR	101/103 (98%)	60 (59%)	31 (31%)	10 (10%)	0	7
39	DR	101/103 (98%)	61 (60%)	29 (29%)	11 (11%)	0	6
40	BS	108/110 (98%)	75 (69%)	21 (19%)	12 (11%)	0	6
40	DS	108/110 (98%)	75 (69%)	20 (18%)	13 (12%)	0	5
41	BT	91/100 (91%)	47 (52%)	25 (28%)	19 (21%)	0	1
41	DT	91/100 (91%)	47 (52%)	23 (25%)	21 (23%)	0	1
42	BU	100/103 (97%)	53 (53%)	35 (35%)	12 (12%)	0	5
42	DU	100/103 (97%)	51 (51%)	35 (35%)	14 (14%)	0	3
43	BW	77/84 (92%)	29 (38%)	23 (30%)	25 (32%)	0	0
43	DW	77/84 (92%)	29 (38%)	22 (29%)	26 (34%)	0	0
44	BX	61/63 (97%)	37 (61%)	14 (23%)	10 (16%)	0	2
44	DX	61/63 (97%)	37 (61%)	14 (23%)	10 (16%)	0	2
45	BY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	8
45	DY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	8
46	BZ	75/78 (96%)	47 (63%)	20 (27%)	8 (11%)	0	6
46	DZ	75/78 (96%)	48 (64%)	19 (25%)	8 (11%)	0	6
47	B0	54/56 (96%)	33 (61%)	16 (30%)	5 (9%)	0	8
47	D0	54/56 (96%)	33 (61%)	16 (30%)	5 (9%)	0	8
48	B1	48/54 (89%)	34 (71%)	12 (25%)	2 (4%)	3	23
48	D1	48/54 (89%)	34 (71%)	12 (25%)	2 (4%)	3	23
49	B2	44/46 (96%)	31 (70%)	9 (20%)	4 (9%)	1	8
49	D2	44/46 (96%)	30 (68%)	8 (18%)	6 (14%)	0	4
50	B3	62/64 (97%)	41 (66%)	15 (24%)	6 (10%)	0	7
50	D3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	0	7
51	B4	36/38 (95%)	21 (58%)	10 (28%)	5 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	D4	36/38 (95%)	21 (58%)	9 (25%)	6 (17%)	0	2
52	BI	139/141 (99%)	119 (86%)	16 (12%)	4 (3%)	4	31
52	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	3	26
All	All	11241/11918 (94%)	7279 (65%)	2673 (24%)	1289 (12%)	0	6

5 of 1289 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	112	ALA
2	AC	180	ASP
2	AC	205	GLU
4	AE	20	VAL
5	AF	98	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	AC	170/189 (90%)	144 (85%)	26 (15%)	2	17
2	CC	170/189 (90%)	145 (85%)	25 (15%)	3	18
3	AD	172/172 (100%)	148 (86%)	24 (14%)	3	19
3	CD	172/172 (100%)	149 (87%)	23 (13%)	4	21
4	AE	113/125 (90%)	100 (88%)	13 (12%)	5	26
4	CE	113/125 (90%)	98 (87%)	15 (13%)	4	21
5	AF	87/116 (75%)	76 (87%)	11 (13%)	4	22
5	CF	87/116 (75%)	75 (86%)	12 (14%)	3	20
6	AG	123/146 (84%)	108 (88%)	15 (12%)	5	23
6	CG	125/146 (86%)	108 (86%)	17 (14%)	3	20
7	AH	104/104 (100%)	96 (92%)	8 (8%)	13	42
7	CH	104/104 (100%)	96 (92%)	8 (8%)	13	42
8	AI	105/106 (99%)	94 (90%)	11 (10%)	7	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/106 (99%)	93 (89%)	12 (11%)	5	26
9	AJ	86/90 (96%)	79 (92%)	7 (8%)	11	41
9	CJ	86/90 (96%)	80 (93%)	6 (7%)	15	46
10	AK	90/98 (92%)	77 (86%)	13 (14%)	3	18
10	CK	90/98 (92%)	77 (86%)	13 (14%)	3	18
11	AL	103/103 (100%)	85 (82%)	18 (18%)	2	10
11	CL	103/103 (100%)	84 (82%)	19 (18%)	1	8
12	AM	92/95 (97%)	82 (89%)	10 (11%)	6	29
12	CM	91/95 (96%)	82 (90%)	9 (10%)	8	33
13	AN	79/83 (95%)	67 (85%)	12 (15%)	3	17
13	CN	79/83 (95%)	67 (85%)	12 (15%)	3	17
14	AO	76/77 (99%)	69 (91%)	7 (9%)	9	36
14	CO	76/77 (99%)	70 (92%)	6 (8%)	12	41
15	AP	65/65 (100%)	57 (88%)	8 (12%)	4	23
15	CP	65/65 (100%)	57 (88%)	8 (12%)	4	23
16	AQ	74/77 (96%)	65 (88%)	9 (12%)	5	23
16	CQ	75/77 (97%)	65 (87%)	10 (13%)	4	21
17	AR	48/64 (75%)	46 (96%)	2 (4%)	30	63
17	CR	48/64 (75%)	46 (96%)	2 (4%)	30	63
18	AS	70/78 (90%)	52 (74%)	18 (26%)	0	3
18	CS	71/78 (91%)	53 (75%)	18 (25%)	0	3
19	AT	65/65 (100%)	53 (82%)	12 (18%)	1	8
19	CT	65/65 (100%)	53 (82%)	12 (18%)	1	8
20	AB	180/198 (91%)	152 (84%)	28 (16%)	2	16
20	CB	180/198 (91%)	150 (83%)	30 (17%)	2	12
21	AU	44/61 (72%)	35 (80%)	9 (20%)	1	6
21	CU	44/61 (72%)	35 (80%)	9 (20%)	1	6
24	BV	78/78 (100%)	68 (87%)	10 (13%)	4	22
24	DV	78/78 (100%)	69 (88%)	9 (12%)	5	26
25	BC	216/218 (99%)	178 (82%)	38 (18%)	2	10
25	DC	216/218 (99%)	175 (81%)	41 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	164/164 (100%)	140 (85%)	24 (15%)	3	18
26	DD	164/164 (100%)	140 (85%)	24 (15%)	3	18
27	BE	165/165 (100%)	146 (88%)	19 (12%)	5	26
27	DE	165/165 (100%)	146 (88%)	19 (12%)	5	26
28	BF	149/149 (100%)	114 (76%)	35 (24%)	1	4
28	DF	149/149 (100%)	115 (77%)	34 (23%)	1	4
29	BG	137/137 (100%)	116 (85%)	21 (15%)	2	17
29	DG	137/137 (100%)	116 (85%)	21 (15%)	2	17
30	BH	114/114 (100%)	77 (68%)	37 (32%)	0	2
30	DH	114/114 (100%)	93 (82%)	21 (18%)	1	8
31	BJ	116/116 (100%)	98 (84%)	18 (16%)	2	16
31	DJ	116/116 (100%)	98 (84%)	18 (16%)	2	16
32	BK	102/104 (98%)	79 (78%)	23 (22%)	1	4
32	DK	102/104 (98%)	79 (78%)	23 (22%)	1	4
33	BL	102/103 (99%)	89 (87%)	13 (13%)	4	22
33	DL	102/103 (99%)	90 (88%)	12 (12%)	5	25
34	BM	109/109 (100%)	88 (81%)	21 (19%)	1	7
34	DM	109/109 (100%)	88 (81%)	21 (19%)	1	7
35	BN	100/103 (97%)	82 (82%)	18 (18%)	1	9
35	DN	100/103 (97%)	81 (81%)	19 (19%)	1	8
36	BO	86/87 (99%)	69 (80%)	17 (20%)	1	7
36	DO	86/87 (99%)	69 (80%)	17 (20%)	1	7
37	BP	99/99 (100%)	80 (81%)	19 (19%)	1	7
37	DP	99/99 (100%)	81 (82%)	18 (18%)	1	9
38	BQ	89/89 (100%)	79 (89%)	10 (11%)	6	27
38	DQ	89/89 (100%)	79 (89%)	10 (11%)	6	27
39	BR	84/84 (100%)	68 (81%)	16 (19%)	1	8
39	DR	84/84 (100%)	70 (83%)	14 (17%)	2	12
40	BS	93/93 (100%)	81 (87%)	12 (13%)	4	22
40	DS	93/93 (100%)	82 (88%)	11 (12%)	5	25
41	BT	80/84 (95%)	62 (78%)	18 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DT	80/84 (95%)	62 (78%)	18 (22%)	1	4
42	BU	83/84 (99%)	67 (81%)	16 (19%)	1	7
42	DU	83/84 (99%)	67 (81%)	16 (19%)	1	7
43	BW	59/62 (95%)	42 (71%)	17 (29%)	0	2
43	DW	59/62 (95%)	42 (71%)	17 (29%)	0	2
44	BX	55/55 (100%)	42 (76%)	13 (24%)	1	4
44	DX	55/55 (100%)	42 (76%)	13 (24%)	1	4
45	BY	48/48 (100%)	40 (83%)	8 (17%)	2	12
45	DY	48/48 (100%)	40 (83%)	8 (17%)	2	12
46	BZ	67/68 (98%)	54 (81%)	13 (19%)	1	7
46	DZ	67/68 (98%)	53 (79%)	14 (21%)	1	6
47	B0	47/47 (100%)	39 (83%)	8 (17%)	2	12
47	D0	47/47 (100%)	40 (85%)	7 (15%)	3	17
48	B1	45/48 (94%)	40 (89%)	5 (11%)	6	28
48	D1	45/48 (94%)	41 (91%)	4 (9%)	9	37
49	B2	38/38 (100%)	32 (84%)	6 (16%)	2	15
49	D2	38/38 (100%)	32 (84%)	6 (16%)	2	15
50	B3	51/51 (100%)	46 (90%)	5 (10%)	8	33
50	D3	51/51 (100%)	46 (90%)	5 (10%)	8	33
51	B4	34/34 (100%)	32 (94%)	2 (6%)	19	53
51	D4	34/34 (100%)	32 (94%)	2 (6%)	19	53
52	BI	109/109 (100%)	108 (99%)	1 (1%)	78	90
52	DI	109/109 (100%)	103 (94%)	6 (6%)	21	54
All	All	9333/9704 (96%)	7895 (85%)	1438 (15%)	2	16

5 of 1438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	CS	20	LYS
30	DH	68	ARG
20	CB	35	ASN
18	CS	13	HIS
26	DD	13	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 346 such sidechains are listed below:

Mol	Chain	Res	Type
18	CS	68	HIS
32	DK	89	ASN
20	CB	119	GLN
26	DD	136	ASN
36	DO	100	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	257 (16%)	27 (1%)
1	CA	1529/1542 (99%)	240 (15%)	27 (1%)
22	BA	116/120 (96%)	22 (18%)	0
22	DA	116/120 (96%)	22 (18%)	0
23	BB	2837/2904 (97%)	460 (16%)	17 (0%)
23	DB	2837/2904 (97%)	460 (16%)	21 (0%)
All	All	8964/9132 (98%)	1461 (16%)	92 (1%)

5 of 1461 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	975	A
23	DB	63	A
1	CA	1049	U
1	CA	1285	A
23	DB	544	C

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 347 ligands modelled in this entry, 345 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	HYG	CA	2062	-	35,39,39	1.38	6 (17%)	43,60,60	1.45	5 (11%)
54	HYG	AA	2059	-	35,39,39	1.36	6 (17%)	43,60,60	1.45	5 (11%)

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
54	HYG	CA	2062	-	-	9/12/87/87	0/4/4/4
54	HYG	AA	2059	-	-	9/12/87/87	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CA	2062	HYG	O28-C23	2.99	1.44	1.40
54	AA	2059	HYG	O28-C23	2.97	1.44	1.40
54	AA	2059	HYG	C27-C33	2.73	1.56	1.52
54	CA	2062	HYG	C27-C33	2.72	1.56	1.52
54	CA	2062	HYG	O22-C17	-2.49	1.38	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	2062	HYG	O22-C17-C16	4.52	122.21	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AA	2059	HYG	O22-C17-C16	4.46	122.08	111.22
54	CA	2062	HYG	O8-C1-C2	-4.38	101.78	109.81
54	AA	2059	HYG	O8-C1-C2	-4.36	101.81	109.81
54	CA	2062	HYG	O35-C34-C33	-3.56	103.94	111.43

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

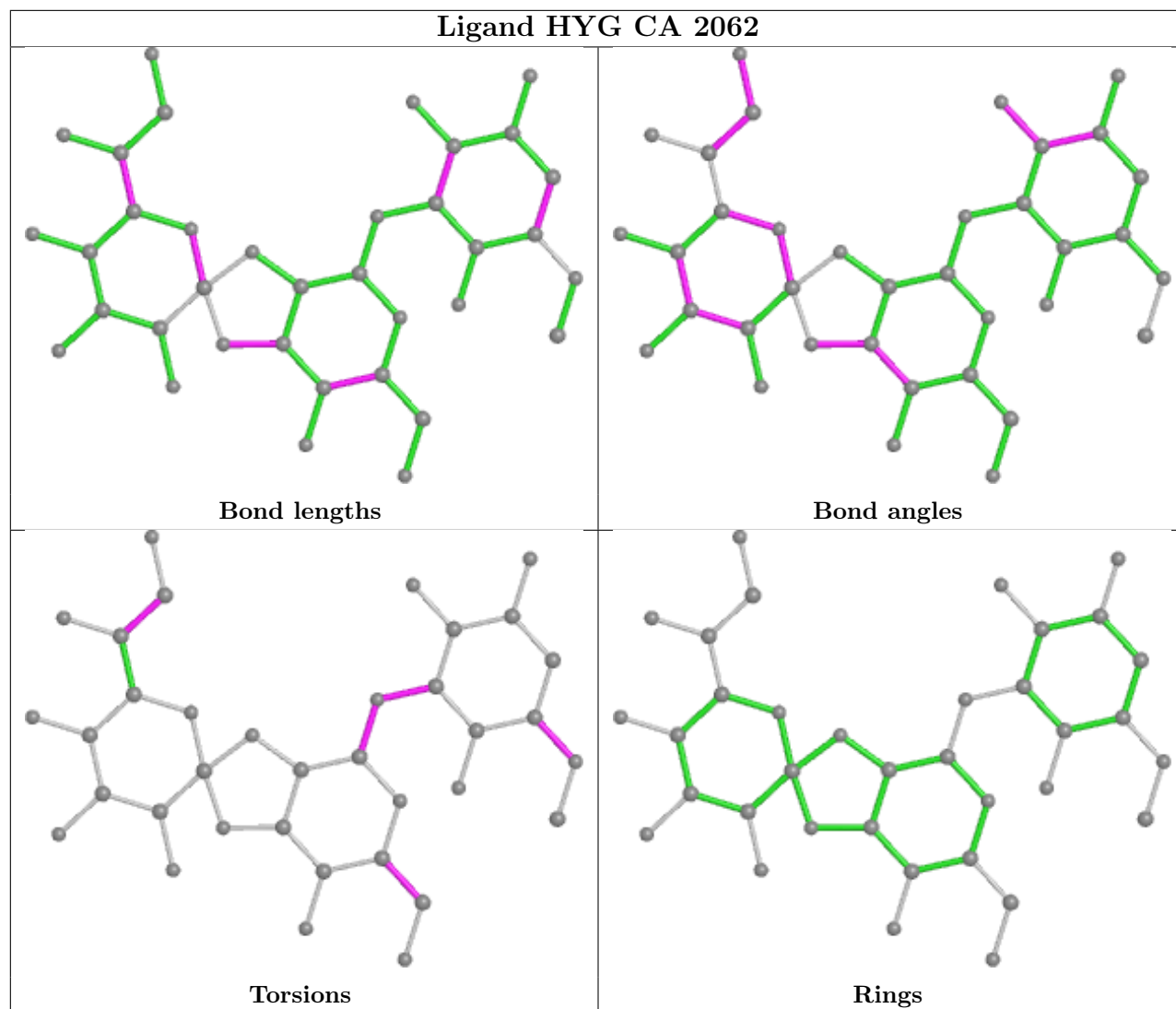
Mol	Chain	Res	Type	Atoms
54	AA	2059	HYG	C5-C4-N9-C10
54	AA	2059	HYG	N36-C33-C34-O35
54	CA	2062	HYG	C3-C4-N9-C10
54	CA	2062	HYG	C5-C4-N9-C10
54	CA	2062	HYG	N36-C33-C34-O35

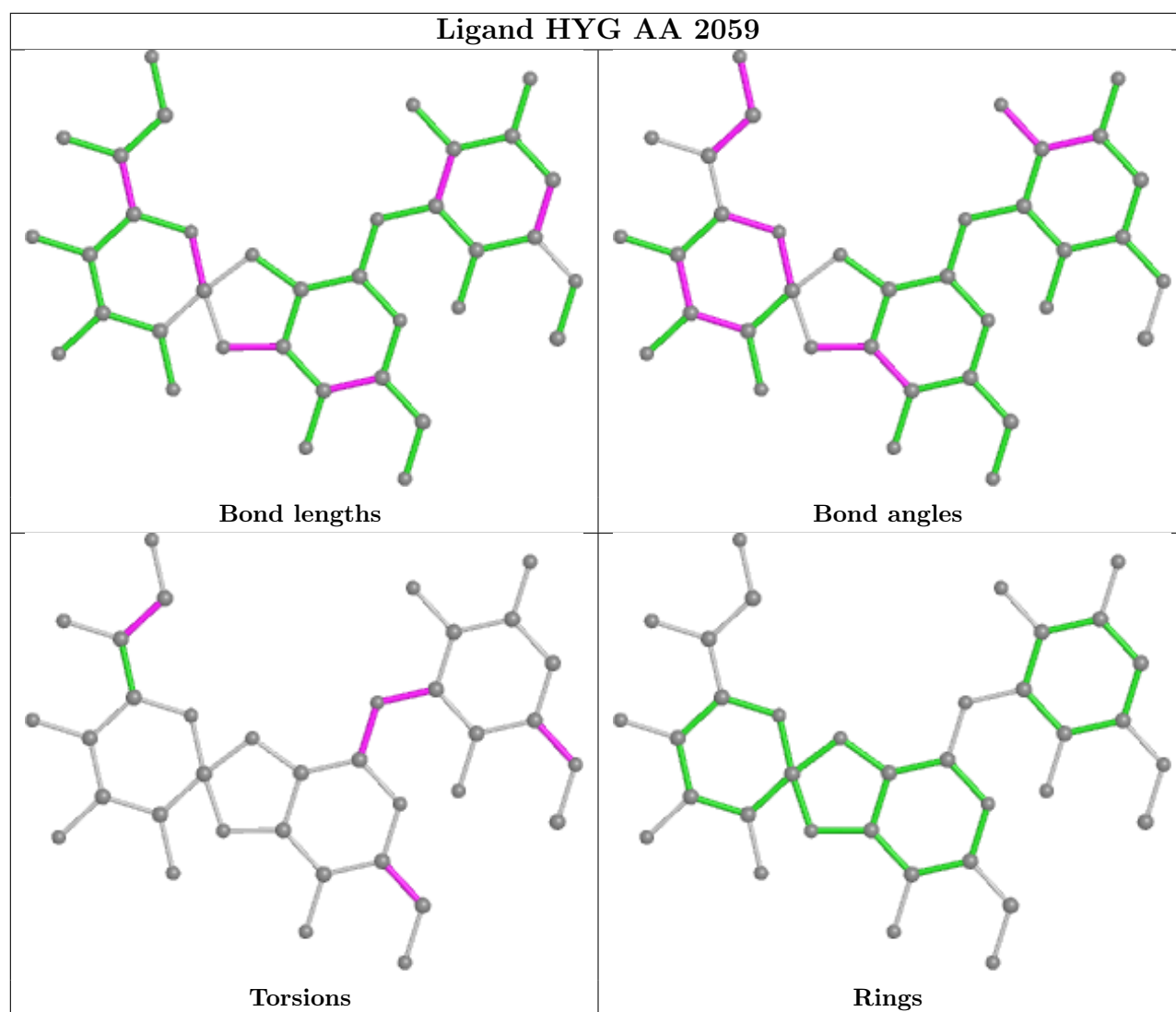
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	CA	2062	HYG	1	0
54	AA	2059	HYG	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1530/1542 (99%)	-0.72	7 (0%) 91 88	16, 85, 158, 180	0
1	CA	1530/1542 (99%)	-0.74	5 (0%) 94 91	8, 57, 142, 180	0
2	AC	206/232 (88%)	0.84	30 (14%) 2 3	8, 89, 145, 180	0
2	CC	206/232 (88%)	0.30	16 (7%) 13 13	15, 81, 138, 180	0
3	AD	205/205 (100%)	0.63	25 (12%) 4 5	19, 97, 160, 180	0
3	CD	205/205 (100%)	-0.03	4 (1%) 65 60	5, 63, 135, 180	0
4	AE	150/166 (90%)	0.16	5 (3%) 46 41	5, 76, 136, 167	0
4	CE	150/166 (90%)	0.86	24 (16%) 1 2	5, 62, 135, 175	0
5	AF	100/135 (74%)	1.19	27 (27%) 0 0	13, 81, 137, 180	0
5	CF	100/135 (74%)	0.34	3 (3%) 50 44	14, 78, 126, 166	0
6	AG	150/178 (84%)	0.38	22 (14%) 2 3	41, 110, 166, 180	0
6	CG	152/178 (85%)	0.16	11 (7%) 15 15	27, 98, 156, 177	0
7	AH	129/129 (100%)	0.24	10 (7%) 13 13	26, 91, 148, 180	0
7	CH	129/129 (100%)	0.28	12 (9%) 8 9	5, 53, 117, 153	0
8	AI	127/129 (98%)	0.85	27 (21%) 0 1	32, 103, 160, 180	0
8	CI	127/129 (98%)	0.66	14 (11%) 5 6	32, 103, 162, 180	0
9	AJ	98/103 (95%)	0.85	11 (11%) 5 6	34, 106, 162, 180	0
9	CJ	98/103 (95%)	1.22	28 (28%) 0 0	42, 107, 156, 180	0
10	AK	117/128 (91%)	-0.06	2 (1%) 70 64	5, 71, 122, 174	0
10	CK	117/128 (91%)	0.12	5 (4%) 35 31	5, 57, 112, 179	0
11	AL	123/123 (100%)	0.51	16 (13%) 3 4	15, 82, 132, 153	0
11	CL	123/123 (100%)	-0.04	3 (2%) 59 53	5, 44, 109, 165	0
12	AM	114/117 (97%)	0.68	16 (14%) 2 3	68, 130, 178, 180	0
12	CM	113/117 (96%)	0.02	4 (3%) 44 39	32, 108, 156, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.56	10 (10%) 6 7	32, 103, 161, 180	0
13	CN	96/100 (96%)	0.18	6 (6%) 20 18	38, 99, 137, 171	0
14	AO	88/89 (98%)	0.40	4 (4%) 33 29	35, 83, 132, 180	0
14	CO	88/89 (98%)	-0.03	2 (2%) 60 54	8, 54, 111, 165	0
15	AP	82/82 (100%)	1.81	33 (40%) 0 0	43, 99, 163, 180	0
15	CP	80/82 (97%)	0.07	4 (5%) 28 25	5, 51, 143, 164	0
16	AQ	80/83 (96%)	1.10	18 (22%) 0 0	49, 106, 156, 177	0
16	CQ	81/83 (97%)	-0.09	0 100 100	5, 51, 121, 157	0
17	AR	55/74 (74%)	0.29	3 (5%) 25 22	16, 78, 142, 152	0
17	CR	55/74 (74%)	0.72	5 (9%) 9 9	13, 69, 132, 149	0
18	AS	79/91 (86%)	1.07	22 (27%) 0 0	67, 128, 175, 180	0
18	CS	80/91 (87%)	-0.12	3 (3%) 40 36	49, 113, 171, 180	0
19	AT	85/86 (98%)	0.02	3 (3%) 44 39	43, 100, 153, 175	0
19	CT	85/86 (98%)	-0.17	0 100 100	14, 58, 121, 177	0
20	AB	218/240 (90%)	0.28	23 (10%) 6 7	30, 102, 152, 180	0
20	CB	218/240 (90%)	1.40	71 (32%) 0 0	26, 106, 160, 180	0
21	AU	51/71 (71%)	0.37	2 (3%) 39 35	26, 102, 172, 180	0
21	CU	51/71 (71%)	0.77	8 (15%) 2 2	19, 85, 151, 180	0
22	BA	117/120 (97%)	-0.77	1 (0%) 84 79	43, 83, 131, 172	0
22	DA	117/120 (97%)	-0.82	1 (0%) 84 79	32, 75, 118, 180	0
23	BB	2841/2904 (97%)	-0.49	15 (0%) 91 88	6, 56, 146, 180	0
23	DB	2841/2904 (97%)	-0.53	7 (0%) 95 93	5, 40, 139, 180	0
24	BV	94/94 (100%)	0.09	5 (5%) 26 24	11, 96, 146, 176	0
24	DV	94/94 (100%)	-0.10	3 (3%) 47 42	14, 86, 143, 180	0
25	BC	271/273 (99%)	0.66	30 (11%) 5 6	7, 48, 104, 170	0
25	DC	271/273 (99%)	0.47	23 (8%) 10 11	5, 28, 81, 120	0
26	BD	209/209 (100%)	0.52	28 (13%) 3 4	5, 73, 138, 180	0
26	DD	209/209 (100%)	0.43	21 (10%) 7 8	5, 42, 118, 180	0
27	BE	201/201 (100%)	0.79	24 (11%) 4 5	5, 65, 142, 180	0
27	DE	201/201 (100%)	0.35	12 (5%) 21 19	5, 67, 135, 180	0
28	BF	178/178 (100%)	1.40	54 (30%) 0 0	50, 116, 175, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	178/178 (100%)	1.08	34 (19%) 1 1	7, 101, 172, 180	0
29	BG	176/176 (100%)	0.64	23 (13%) 3 4	23, 102, 155, 180	0
29	DG	176/176 (100%)	0.19	11 (6%) 20 18	24, 90, 161, 180	0
30	BH	149/149 (100%)	1.71	51 (34%) 0 0	14, 117, 177, 180	0
30	DH	149/149 (100%)	0.52	13 (8%) 10 11	11, 100, 156, 180	0
31	BJ	142/142 (100%)	0.35	8 (5%) 24 22	6, 80, 141, 171	0
31	DJ	142/142 (100%)	0.31	8 (5%) 24 22	5, 60, 119, 164	0
32	BK	121/123 (98%)	1.75	46 (38%) 0 0	5, 73, 135, 180	0
32	DK	121/123 (98%)	0.56	11 (9%) 9 9	5, 35, 102, 145	0
33	BL	143/144 (99%)	0.03	5 (3%) 44 39	10, 64, 128, 180	0
33	DL	143/144 (99%)	0.54	18 (12%) 3 5	5, 54, 118, 162	0
34	BM	136/136 (100%)	0.07	5 (3%) 41 37	8, 70, 129, 172	0
34	DM	136/136 (100%)	0.75	19 (13%) 2 3	5, 51, 114, 168	0
35	BN	120/127 (94%)	0.50	12 (10%) 7 8	7, 66, 132, 163	0
35	DN	120/127 (94%)	-0.09	1 (0%) 86 81	5, 42, 86, 145	0
36	BO	116/117 (99%)	0.77	27 (23%) 0 0	27, 87, 135, 156	0
36	DO	116/117 (99%)	-0.04	1 (0%) 84 79	17, 78, 142, 180	0
37	BP	114/114 (100%)	1.71	46 (40%) 0 0	20, 85, 149, 178	0
37	DP	114/114 (100%)	0.14	4 (3%) 44 39	5, 48, 107, 159	0
38	BQ	117/117 (100%)	-0.18	4 (3%) 45 40	5, 63, 127, 180	0
38	DQ	117/117 (100%)	0.41	5 (4%) 35 31	5, 48, 116, 150	0
39	BR	103/103 (100%)	-0.02	5 (4%) 29 26	16, 82, 145, 158	0
39	DR	103/103 (100%)	0.54	9 (8%) 10 11	5, 73, 136, 180	0
40	BS	110/110 (100%)	0.40	7 (6%) 19 18	5, 53, 116, 142	0
40	DS	110/110 (100%)	0.98	21 (19%) 1 1	5, 42, 116, 146	0
41	BT	93/100 (93%)	0.00	1 (1%) 80 75	6, 72, 139, 179	0
41	DT	93/100 (93%)	0.79	16 (17%) 1 1	11, 64, 156, 180	0
42	BU	102/103 (99%)	1.23	26 (25%) 0 0	5, 78, 144, 178	0
42	DU	102/103 (99%)	0.08	2 (1%) 65 60	10, 90, 154, 180	0
43	BW	79/84 (94%)	0.36	5 (6%) 20 18	10, 79, 157, 163	0
43	DW	79/84 (94%)	0.16	4 (5%) 28 25	5, 75, 131, 174	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	63/63 (100%)	0.88	13 (20%) 1 1	9, 74, 146, 179	0
44	DX	63/63 (100%)	0.51	4 (6%) 20 18	17, 96, 147, 180	0
45	BY	58/58 (100%)	0.32	4 (6%) 16 16	14, 78, 135, 170	0
45	DY	58/58 (100%)	-0.08	2 (3%) 45 40	10, 73, 129, 160	0
46	BZ	77/78 (98%)	0.60	9 (11%) 4 5	5, 49, 121, 160	0
46	DZ	77/78 (98%)	-0.02	2 (2%) 56 49	5, 42, 107, 141	0
47	B0	56/56 (100%)	0.43	5 (8%) 9 10	5, 77, 144, 166	0
47	D0	56/56 (100%)	0.27	3 (5%) 25 23	8, 52, 128, 160	0
48	B1	50/54 (92%)	2.28	28 (56%) 0 0	51, 99, 149, 165	0
48	D1	50/54 (92%)	1.43	11 (22%) 0 0	43, 93, 138, 171	0
49	B2	46/46 (100%)	0.42	2 (4%) 35 31	7, 49, 103, 135	0
49	D2	46/46 (100%)	0.18	1 (2%) 62 56	5, 28, 99, 180	0
50	B3	64/64 (100%)	0.60	6 (9%) 8 9	16, 56, 110, 137	0
50	D3	64/64 (100%)	0.35	6 (9%) 8 9	5, 43, 112, 152	0
51	B4	38/38 (100%)	0.15	1 (2%) 56 49	33, 92, 143, 146	0
51	D4	38/38 (100%)	-0.41	0 100 100	5, 68, 112, 150	0
52	BI	141/141 (100%)	0.99	26 (18%) 1 1	67, 169, 180, 180	0
52	DI	141/141 (100%)	0.82	23 (16%) 1 2	91, 160, 180, 180	0
All	All	20417/21050 (96%)	0.03	1362 (6%) 17 16	5, 70, 153, 180	0

The worst 5 of 1362 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BH	84	ALA	9.6
15	AP	80	LYS	9.6
48	D1	52	LYS	9.6
15	AP	81	ALA	9.4
30	BH	45	GLU	8.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
53	MG	BB	3042	1/1	0.13	0.10	168,168,168,168	0
53	MG	AA	2023	1/1	0.54	0.36	66,66,66,66	1
53	MG	AA	2037	1/1	0.58	0.33	138,138,138,138	0
53	MG	AA	2057	1/1	0.62	0.17	141,141,141,141	0
53	MG	CA	2011	1/1	0.65	0.28	132,132,132,132	0
53	MG	AA	2014	1/1	0.68	0.22	112,112,112,112	0
53	MG	CA	2015	1/1	0.68	0.10	149,149,149,149	0
53	MG	CA	2027	1/1	0.69	0.13	50,50,50,50	1
53	MG	DB	3060	1/1	0.71	0.20	112,112,112,112	0
53	MG	AN	201	1/1	0.72	0.12	69,69,69,69	0
53	MG	BB	3100	1/1	0.72	0.20	129,129,129,129	0
53	MG	AA	2031	1/1	0.74	0.09	58,58,58,58	0
53	MG	AA	2047	1/1	0.74	0.04	100,100,100,100	0
53	MG	AA	2008	1/1	0.76	0.08	125,125,125,125	0
53	MG	CA	2059	1/1	0.78	0.12	94,94,94,94	0
53	MG	AA	2019	1/1	0.78	0.06	107,107,107,107	0
53	MG	CA	2023	1/1	0.79	0.20	137,137,137,137	0
53	MG	AA	2033	1/1	0.79	0.11	99,99,99,99	0
53	MG	AA	2056	1/1	0.79	0.12	124,124,124,124	0
53	MG	CA	2021	1/1	0.79	0.36	125,125,125,125	0
53	MG	AE	201	1/1	0.80	0.07	144,144,144,144	0
53	MG	DB	3059	1/1	0.80	0.12	180,180,180,180	0
53	MG	CA	2057	1/1	0.80	0.09	99,99,99,99	0
53	MG	DB	3066	1/1	0.80	0.08	146,146,146,146	0
53	MG	CA	2060	1/1	0.81	0.05	80,80,80,80	0
53	MG	BB	3080	1/1	0.81	0.18	39,39,39,39	0
53	MG	AA	2018	1/1	0.81	0.09	131,131,131,131	0
53	MG	AA	2012	1/1	0.81	0.09	84,84,84,84	0
53	MG	AA	2005	1/1	0.82	0.08	69,69,69,69	0
53	MG	BB	3010	1/1	0.82	0.10	44,44,44,44	0
53	MG	AA	2035	1/1	0.83	0.34	137,137,137,137	0
53	MG	CA	2026	1/1	0.83	0.20	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
53	MG	AA	2055	1/1	0.83	0.20	102,102,102,102	0
53	MG	CA	2038	1/1	0.83	0.12	128,128,128,128	0
53	MG	CA	2008	1/1	0.83	0.09	93,93,93,93	0
53	MG	BB	3099	1/1	0.85	0.17	40,40,40,40	0
53	MG	BB	3081	1/1	0.86	0.22	46,46,46,46	0
53	MG	BB	3037	1/1	0.86	0.11	23,23,23,23	0
53	MG	CE	201	1/1	0.86	0.15	127,127,127,127	0
53	MG	CA	2042	1/1	0.87	0.08	58,58,58,58	0
53	MG	DB	3045	1/1	0.87	0.06	57,57,57,57	0
53	MG	AA	2050	1/1	0.87	0.14	105,105,105,105	0
53	MG	AA	2024	1/1	0.87	0.08	5,5,5,5	1
53	MG	AA	2013	1/1	0.87	0.12	122,122,122,122	0
53	MG	DB	3095	1/1	0.87	0.15	89,89,89,89	0
53	MG	BB	3077	1/1	0.88	0.09	36,36,36,36	0
53	MG	BB	3097	1/1	0.88	0.18	114,114,114,114	0
53	MG	DB	3013	1/1	0.88	0.17	51,51,51,51	0
53	MG	DB	3090	1/1	0.88	0.08	37,37,37,37	0
53	MG	AA	2044	1/1	0.88	0.12	112,112,112,112	0
53	MG	AA	2026	1/1	0.89	0.08	65,65,65,65	0
53	MG	CA	2014	1/1	0.90	0.07	47,47,47,47	0
53	MG	CA	2029	1/1	0.90	0.05	23,23,23,23	1
53	MG	CA	2035	1/1	0.90	0.08	89,89,89,89	0
53	MG	DB	3023	1/1	0.90	0.08	32,32,32,32	0
53	MG	DB	3029	1/1	0.90	0.16	88,88,88,88	0
53	MG	AA	2030	1/1	0.90	0.09	99,99,99,99	0
53	MG	BB	3017	1/1	0.90	0.14	34,34,34,34	0
53	MG	CA	2052	1/1	0.90	0.09	73,73,73,73	0
53	MG	CA	2054	1/1	0.90	0.08	104,104,104,104	0
53	MG	BB	3052	1/1	0.90	0.08	38,38,38,38	0
53	MG	BB	3071	1/1	0.90	0.09	26,26,26,26	0
54	HYG	AA	2059	36/36	0.90	0.24	52,52,52,52	0
53	MG	DB	3036	1/1	0.91	0.09	30,30,30,30	0
53	MG	AA	2052	1/1	0.91	0.07	78,78,78,78	0
53	MG	AA	2049	1/1	0.91	0.06	75,75,75,75	0
53	MG	AA	2017	1/1	0.91	0.12	87,87,87,87	0
53	MG	BB	3014	1/1	0.91	0.05	50,50,50,50	0
53	MG	AA	2051	1/1	0.91	0.10	41,41,41,41	0
53	MG	DB	3092	1/1	0.91	0.13	66,66,66,66	0
53	MG	BB	3104	1/1	0.91	0.18	36,36,36,36	0
53	MG	CA	2007	1/1	0.91	0.04	46,46,46,46	0
54	HYG	CA	2062	36/36	0.91	0.22	45,45,45,45	0
53	MG	AA	2021	1/1	0.92	0.31	5,5,5,5	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	AA	2004	1/1	0.92	0.14	56,56,56,56	0
53	MG	AA	2045	1/1	0.92	0.64	92,92,92,92	0
53	MG	DB	3050	1/1	0.92	0.08	90,90,90,90	0
53	MG	BB	3048	1/1	0.92	0.10	44,44,44,44	0
53	MG	BB	3051	1/1	0.92	0.14	35,35,35,35	0
53	MG	BB	3046	1/1	0.93	0.11	22,22,22,22	0
53	MG	AA	2046	1/1	0.93	0.07	5,5,5,5	0
53	MG	BB	3049	1/1	0.93	0.10	10,10,10,10	0
53	MG	AA	2054	1/1	0.93	0.08	110,110,110,110	0
53	MG	AA	2015	1/1	0.93	0.06	24,24,24,24	0
53	MG	BB	3053	1/1	0.93	0.06	28,28,28,28	0
53	MG	BB	3054	1/1	0.93	0.06	77,77,77,77	0
53	MG	AA	2016	1/1	0.93	0.09	89,89,89,89	0
53	MG	DB	3044	1/1	0.93	0.11	24,24,24,24	0
53	MG	BB	3024	1/1	0.93	0.11	15,15,15,15	0
53	MG	BB	3031	1/1	0.93	0.14	41,41,41,41	0
53	MG	DB	3058	1/1	0.93	0.33	151,151,151,151	0
53	MG	CA	2028	1/1	0.93	0.07	75,75,75,75	0
53	MG	BB	3032	1/1	0.93	0.10	56,56,56,56	0
53	MG	BB	3085	1/1	0.93	0.17	103,103,103,103	0
53	MG	CA	2037	1/1	0.93	0.08	94,94,94,94	0
53	MG	BB	3093	1/1	0.93	0.24	71,71,71,71	0
53	MG	BB	3033	1/1	0.93	0.33	125,125,125,125	0
53	MG	AA	2032	1/1	0.93	0.08	62,62,62,62	0
53	MG	AA	2001	1/1	0.93	0.07	35,35,35,35	0
53	MG	CA	2036	1/1	0.94	0.17	101,101,101,101	0
53	MG	BB	3027	1/1	0.94	0.08	33,33,33,33	0
53	MG	CA	2019	1/1	0.94	0.10	73,73,73,73	0
53	MG	BB	3039	1/1	0.94	0.18	7,7,7,7	0
53	MG	AA	2002	1/1	0.94	0.06	99,99,99,99	0
53	MG	DB	3052	1/1	0.94	0.12	100,100,100,100	0
53	MG	CA	2024	1/1	0.94	0.06	29,29,29,29	0
53	MG	BB	3020	1/1	0.94	0.10	26,26,26,26	0
53	MG	CA	2058	1/1	0.94	0.11	106,106,106,106	0
53	MG	BB	3001	1/1	0.94	0.10	51,51,51,51	0
53	MG	CA	2010	1/1	0.94	0.08	33,33,33,33	0
53	MG	BB	3055	1/1	0.94	0.15	17,17,17,17	0
53	MG	CA	2033	1/1	0.94	0.15	56,56,56,56	0
53	MG	DB	3015	1/1	0.94	0.07	33,33,33,33	0
53	MG	BB	3057	1/1	0.94	0.19	28,28,28,28	0
53	MG	AA	2022	1/1	0.95	0.07	82,82,82,82	0
53	MG	BB	3083	1/1	0.95	0.22	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
53	MG	AA	2028	1/1	0.95	0.17	100,100,100,100	0
53	MG	DB	3005	1/1	0.95	0.12	10,10,10,10	0
53	MG	BB	3088	1/1	0.95	0.06	28,28,28,28	0
53	MG	BB	3036	1/1	0.95	0.11	42,42,42,42	0
53	MG	AA	2029	1/1	0.95	0.06	39,39,39,39	0
53	MG	AA	2006	1/1	0.95	0.03	60,60,60,60	0
53	MG	DB	3035	1/1	0.95	0.06	55,55,55,55	0
53	MG	AA	2007	1/1	0.95	0.06	31,31,31,31	0
53	MG	DB	3041	1/1	0.95	0.11	29,29,29,29	0
53	MG	BB	3102	1/1	0.95	0.12	20,20,20,20	0
53	MG	BB	3045	1/1	0.95	0.10	31,31,31,31	0
53	MG	DB	3046	1/1	0.95	0.09	24,24,24,24	0
53	MG	BB	3061	1/1	0.95	0.04	48,48,48,48	0
53	MG	BB	3063	1/1	0.95	0.09	11,11,11,11	0
53	MG	CA	2009	1/1	0.95	0.06	67,67,67,67	0
53	MG	BB	3064	1/1	0.95	0.08	35,35,35,35	0
53	MG	CA	2043	1/1	0.95	0.04	19,19,19,19	0
53	MG	CA	2047	1/1	0.95	0.06	121,121,121,121	0
53	MG	DB	3072	1/1	0.95	0.12	18,18,18,18	0
53	MG	DB	3073	1/1	0.95	0.10	14,14,14,14	0
53	MG	DB	3074	1/1	0.95	0.09	12,12,12,12	0
53	MG	DB	3080	1/1	0.95	0.10	10,10,10,10	0
53	MG	CA	2049	1/1	0.95	0.06	74,74,74,74	0
53	MG	AA	2025	1/1	0.95	0.17	58,58,58,58	0
53	MG	BB	3047	1/1	0.95	0.06	75,75,75,75	0
53	MG	DB	3097	1/1	0.95	0.14	38,38,38,38	0
53	MG	DB	3110	1/1	0.95	0.14	21,21,21,21	0
53	MG	BB	3008	1/1	0.95	0.10	89,89,89,89	0
53	MG	CA	2016	1/1	0.95	0.04	53,53,53,53	0
53	MG	BB	3056	1/1	0.96	0.08	26,26,26,26	0
53	MG	BB	3098	1/1	0.96	0.15	35,35,35,35	0
53	MG	DB	3021	1/1	0.96	0.23	11,11,11,11	0
53	MG	AA	2058	1/1	0.96	0.14	86,86,86,86	0
53	MG	DB	3026	1/1	0.96	0.08	34,34,34,34	0
53	MG	AA	2038	1/1	0.96	0.11	71,71,71,71	0
53	MG	DB	3032	1/1	0.96	0.09	63,63,63,63	0
53	MG	DB	3034	1/1	0.96	0.16	52,52,52,52	0
53	MG	BB	3021	1/1	0.96	0.08	30,30,30,30	0
53	MG	AA	2039	1/1	0.96	0.12	64,64,64,64	0
53	MG	BB	3109	1/1	0.96	0.09	54,54,54,54	0
53	MG	BB	3068	1/1	0.96	0.12	53,53,53,53	0
53	MG	AA	2041	1/1	0.96	0.07	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	CA	2040	1/1	0.96	0.09	48,48,48,48	0
53	MG	DB	3047	1/1	0.96	0.17	14,14,14,14	0
53	MG	CA	2041	1/1	0.96	0.05	46,46,46,46	0
53	MG	BB	3003	1/1	0.96	0.07	32,32,32,32	0
53	MG	DB	3054	1/1	0.96	0.04	19,19,19,19	0
53	MG	DB	3057	1/1	0.96	0.06	71,71,71,71	0
53	MG	BB	3078	1/1	0.96	0.15	70,70,70,70	0
53	MG	CA	2044	1/1	0.96	0.07	59,59,59,59	0
53	MG	AA	2048	1/1	0.96	0.03	99,99,99,99	0
53	MG	CA	2048	1/1	0.96	0.11	58,58,58,58	0
53	MG	DB	3071	1/1	0.96	0.06	16,16,16,16	0
53	MG	AA	2042	1/1	0.96	0.09	69,69,69,69	0
53	MG	BB	3082	1/1	0.96	0.16	46,46,46,46	0
53	MG	BB	3034	1/1	0.96	0.10	35,35,35,35	0
53	MG	AA	2009	1/1	0.96	0.10	7,7,7,7	0
53	MG	CA	2020	1/1	0.96	0.21	73,73,73,73	0
53	MG	BB	3087	1/1	0.96	0.16	57,57,57,57	0
53	MG	DB	3093	1/1	0.96	0.22	11,11,11,11	0
53	MG	BB	3016	1/1	0.96	0.07	38,38,38,38	0
53	MG	BB	3038	1/1	0.96	0.03	71,71,71,71	0
53	MG	DB	3108	1/1	0.96	0.09	37,37,37,37	0
53	MG	DB	3003	1/1	0.96	0.19	63,63,63,63	0
53	MG	DB	3111	1/1	0.96	0.09	38,38,38,38	0
53	MG	CA	2025	1/1	0.96	0.12	50,50,50,50	0
53	MG	DB	3011	1/1	0.96	0.16	17,17,17,17	0
53	MG	AA	2036	1/1	0.97	0.04	31,31,31,31	0
53	MG	DB	3022	1/1	0.97	0.08	25,25,25,25	0
53	MG	BB	3013	1/1	0.97	0.10	43,43,43,43	0
53	MG	DB	3025	1/1	0.97	0.15	5,5,5,5	0
53	MG	BB	3035	1/1	0.97	0.07	15,15,15,15	0
53	MG	DB	3028	1/1	0.97	0.06	24,24,24,24	0
53	MG	BB	3090	1/1	0.97	0.12	112,112,112,112	0
53	MG	DB	3030	1/1	0.97	0.17	6,6,6,6	0
53	MG	BB	3091	1/1	0.97	0.09	16,16,16,16	0
53	MG	DB	3033	1/1	0.97	0.08	9,9,9,9	0
53	MG	AA	2043	1/1	0.97	0.08	96,96,96,96	0
53	MG	CA	2034	1/1	0.97	0.11	6,6,6,6	0
53	MG	BB	3096	1/1	0.97	0.11	34,34,34,34	0
53	MG	DB	3038	1/1	0.97	0.12	5,5,5,5	0
53	MG	DB	3039	1/1	0.97	0.04	22,22,22,22	0
53	MG	AA	2011	1/1	0.97	0.07	85,85,85,85	0
53	MG	BB	3058	1/1	0.97	0.10	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	BB	3060	1/1	0.97	0.13	19,19,19,19	0
53	MG	AA	2027	1/1	0.97	0.09	36,36,36,36	0
53	MG	BB	3062	1/1	0.97	0.17	14,14,14,14	0
53	MG	AA	2034	1/1	0.97	0.06	68,68,68,68	0
53	MG	AA	2040	1/1	0.97	0.10	83,83,83,83	0
53	MG	CA	2004	1/1	0.97	0.09	8,8,8,8	0
53	MG	DB	3055	1/1	0.97	0.11	26,26,26,26	0
53	MG	DB	3056	1/1	0.97	0.09	5,5,5,5	0
53	MG	CA	2046	1/1	0.97	0.09	57,57,57,57	0
53	MG	CA	2005	1/1	0.97	0.09	24,24,24,24	0
53	MG	BB	3065	1/1	0.97	0.06	29,29,29,29	0
53	MG	BB	3066	1/1	0.97	0.12	23,23,23,23	0
53	MG	DB	3061	1/1	0.97	0.09	69,69,69,69	0
53	MG	BB	3043	1/1	0.97	0.05	104,104,104,104	0
53	MG	DB	3070	1/1	0.97	0.08	45,45,45,45	0
53	MG	BB	3069	1/1	0.97	0.11	17,17,17,17	0
53	MG	BB	3023	1/1	0.97	0.14	5,5,5,5	0
53	MG	BB	3074	1/1	0.97	0.07	28,28,28,28	0
53	MG	BB	3075	1/1	0.97	0.21	40,40,40,40	0
53	MG	DB	3078	1/1	0.97	0.08	27,27,27,27	0
53	MG	BB	3004	1/1	0.97	0.06	32,32,32,32	0
53	MG	DB	3082	1/1	0.97	0.10	30,30,30,30	0
53	MG	DB	3086	1/1	0.97	0.15	11,11,11,11	0
53	MG	DB	3087	1/1	0.97	0.15	53,53,53,53	0
53	MG	DB	3088	1/1	0.97	0.14	25,25,25,25	0
53	MG	CA	2061	1/1	0.97	0.08	23,23,23,23	0
53	MG	BB	3026	1/1	0.97	0.08	39,39,39,39	0
53	MG	BB	3005	1/1	0.97	0.19	5,5,5,5	0
53	MG	DB	3094	1/1	0.97	0.03	29,29,29,29	0
53	MG	BB	3029	1/1	0.97	0.07	14,14,14,14	0
53	MG	DB	3007	1/1	0.97	0.14	18,18,18,18	0
53	MG	DB	3100	1/1	0.97	0.16	13,13,13,13	0
53	MG	DB	3102	1/1	0.97	0.09	12,12,12,12	0
53	MG	DB	3103	1/1	0.97	0.13	27,27,27,27	0
53	MG	DB	3105	1/1	0.97	0.14	23,23,23,23	0
53	MG	DB	3009	1/1	0.97	0.07	29,29,29,29	0
53	MG	DB	3109	1/1	0.97	0.10	9,9,9,9	0
53	MG	DB	3010	1/1	0.97	0.08	8,8,8,8	0
53	MG	CA	2022	1/1	0.97	0.10	63,63,63,63	0
53	MG	AA	2010	1/1	0.97	0.04	60,60,60,60	0
53	MG	BB	3009	1/1	0.97	0.04	46,46,46,46	0
55	ZN	B4	101	1/1	0.97	0.04	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	BB	3067	1/1	0.98	0.09	44,44,44,44	0
53	MG	BB	3022	1/1	0.98	0.26	34,34,34,34	0
53	MG	DB	3040	1/1	0.98	0.16	5,5,5,5	0
53	MG	CA	2013	1/1	0.98	0.08	73,73,73,73	0
53	MG	DB	3042	1/1	0.98	0.10	6,6,6,6	0
53	MG	DB	3043	1/1	0.98	0.11	5,5,5,5	0
53	MG	BB	3089	1/1	0.98	0.15	56,56,56,56	0
53	MG	CA	2051	1/1	0.98	0.05	39,39,39,39	0
53	MG	BB	3044	1/1	0.98	0.15	53,53,53,53	0
53	MG	AA	2020	1/1	0.98	0.07	5,5,5,5	0
53	MG	DB	3048	1/1	0.98	0.12	28,28,28,28	0
53	MG	DB	3049	1/1	0.98	0.09	36,36,36,36	0
53	MG	CA	2055	1/1	0.98	0.07	11,11,11,11	0
53	MG	DB	3051	1/1	0.98	0.19	23,23,23,23	0
53	MG	CA	2056	1/1	0.98	0.05	5,5,5,5	0
53	MG	CA	2017	1/1	0.98	0.11	5,5,5,5	0
53	MG	BB	3072	1/1	0.98	0.12	17,17,17,17	0
53	MG	BB	3094	1/1	0.98	0.07	28,28,28,28	0
53	MG	BB	3095	1/1	0.98	0.07	33,33,33,33	0
53	MG	BB	3073	1/1	0.98	0.09	39,39,39,39	0
53	MG	BB	3006	1/1	0.98	0.07	5,5,5,5	0
53	MG	DB	3002	1/1	0.98	0.07	12,12,12,12	0
53	MG	BB	3059	1/1	0.98	0.12	26,26,26,26	0
53	MG	DB	3062	1/1	0.98	0.04	77,77,77,77	0
53	MG	DB	3063	1/1	0.98	0.12	43,43,43,43	0
53	MG	DB	3064	1/1	0.98	0.05	20,20,20,20	0
53	MG	DB	3065	1/1	0.98	0.05	37,37,37,37	0
53	MG	DB	3004	1/1	0.98	0.11	6,6,6,6	0
53	MG	DB	3067	1/1	0.98	0.07	5,5,5,5	0
53	MG	DB	3068	1/1	0.98	0.10	5,5,5,5	0
53	MG	DB	3069	1/1	0.98	0.18	11,11,11,11	0
53	MG	BB	3025	1/1	0.98	0.13	30,30,30,30	0
53	MG	DB	3006	1/1	0.98	0.10	5,5,5,5	0
53	MG	BB	3011	1/1	0.98	0.19	5,5,5,5	0
53	MG	DB	3008	1/1	0.98	0.18	6,6,6,6	0
53	MG	BB	3101	1/1	0.98	0.09	24,24,24,24	0
53	MG	DB	3075	1/1	0.98	0.10	57,57,57,57	0
53	MG	DB	3077	1/1	0.98	0.21	54,54,54,54	0
53	MG	BB	3079	1/1	0.98	0.04	19,19,19,19	0
53	MG	DB	3079	1/1	0.98	0.14	28,28,28,28	0
53	MG	BB	3103	1/1	0.98	0.08	5,5,5,5	0
53	MG	CA	2030	1/1	0.98	0.12	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
53	MG	DB	3083	1/1	0.98	0.16	85,85,85,85	0
53	MG	DB	3084	1/1	0.98	0.17	5,5,5,5	0
53	MG	CA	2032	1/1	0.98	0.17	33,33,33,33	0
53	MG	DB	3016	1/1	0.98	0.05	15,15,15,15	0
53	MG	DB	3017	1/1	0.98	0.10	13,13,13,13	0
53	MG	DB	3089	1/1	0.98	0.17	7,7,7,7	0
53	MG	BB	3019	1/1	0.98	0.05	22,22,22,22	0
53	MG	BB	3105	1/1	0.98	0.08	20,20,20,20	0
53	MG	BB	3108	1/1	0.98	0.10	47,47,47,47	0
53	MG	DB	3024	1/1	0.98	0.13	63,63,63,63	0
53	MG	BB	3028	1/1	0.98	0.20	86,86,86,86	0
53	MG	DB	3096	1/1	0.98	0.12	6,6,6,6	0
53	MG	CA	2001	1/1	0.98	0.05	5,5,5,5	0
53	MG	DB	3099	1/1	0.98	0.19	7,7,7,7	0
53	MG	DB	3027	1/1	0.98	0.15	6,6,6,6	0
53	MG	BB	3012	1/1	0.98	0.09	32,32,32,32	0
53	MG	CA	2039	1/1	0.98	0.12	16,16,16,16	0
53	MG	DB	3104	1/1	0.98	0.08	33,33,33,33	0
53	MG	BB	3040	1/1	0.98	0.18	26,26,26,26	0
53	MG	DB	3106	1/1	0.98	0.13	23,23,23,23	0
53	MG	DB	3107	1/1	0.98	0.07	10,10,10,10	0
53	MG	DB	3031	1/1	0.98	0.18	8,8,8,8	0
53	MG	CA	2006	1/1	0.98	0.05	95,95,95,95	0
53	MG	BB	3084	1/1	0.98	0.16	24,24,24,24	0
53	MG	AA	2053	1/1	0.98	0.07	79,79,79,79	0
53	MG	BB	3086	1/1	0.98	0.26	42,42,42,42	0
53	MG	CA	2045	1/1	0.98	0.16	48,48,48,48	0
53	MG	DB	3037	1/1	0.98	0.16	28,28,28,28	0
55	ZN	D4	101	1/1	0.98	0.06	46,46,46,46	0
53	MG	DB	3001	1/1	0.99	0.10	5,5,5,5	0
53	MG	BB	3007	1/1	0.99	0.14	82,82,82,82	0
53	MG	DB	3085	1/1	0.99	0.12	5,5,5,5	0
53	MG	BB	3092	1/1	0.99	0.06	54,54,54,54	0
53	MG	BB	3018	1/1	0.99	0.14	32,32,32,32	0
53	MG	BB	3041	1/1	0.99	0.08	7,7,7,7	0
53	MG	CA	2012	1/1	0.99	0.08	93,93,93,93	0
53	MG	BB	3106	1/1	0.99	0.12	62,62,62,62	0
53	MG	DB	3091	1/1	0.99	0.18	13,13,13,13	0
53	MG	CA	2031	1/1	0.99	0.06	28,28,28,28	0
53	MG	CA	2050	1/1	0.99	0.11	8,8,8,8	0
53	MG	BB	3107	1/1	0.99	0.11	6,6,6,6	0
53	MG	AA	2003	1/1	0.99	0.17	39,39,39,39	0

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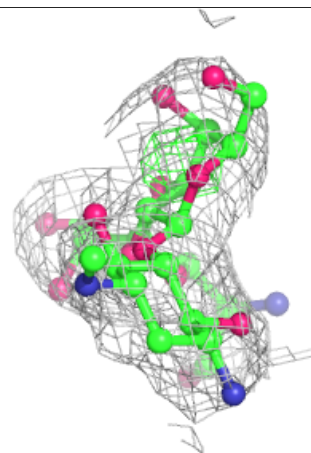
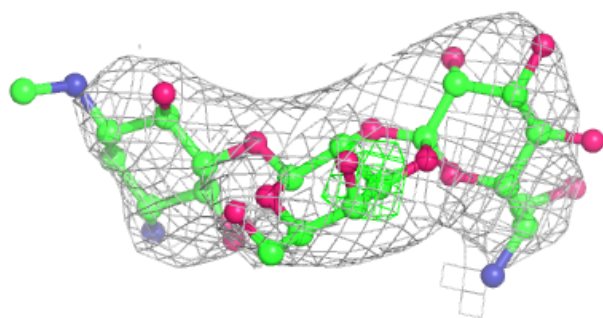
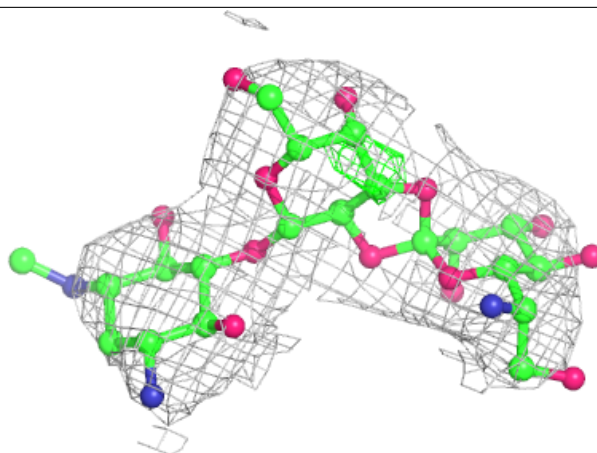
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	DB	3012	1/1	0.99	0.20	9,9,9,9	0
53	MG	CA	2053	1/1	0.99	0.06	30,30,30,30	0
53	MG	DB	3098	1/1	0.99	0.22	44,44,44,44	0
53	MG	DB	3014	1/1	0.99	0.05	5,5,5,5	0
53	MG	BB	3050	1/1	0.99	0.12	28,28,28,28	0
53	MG	DB	3101	1/1	0.99	0.20	5,5,5,5	0
53	MG	BB	3110	1/1	0.99	0.15	23,23,23,23	0
53	MG	CA	2018	1/1	0.99	0.03	6,6,6,6	0
53	MG	DB	3018	1/1	0.99	0.07	22,22,22,22	0
53	MG	DB	3019	1/1	0.99	0.09	5,5,5,5	0
53	MG	DB	3020	1/1	0.99	0.15	5,5,5,5	0
53	MG	BB	3076	1/1	0.99	0.05	38,38,38,38	0
53	MG	CA	2003	1/1	0.99	0.04	35,35,35,35	0
53	MG	DB	3076	1/1	0.99	0.10	5,5,5,5	0
53	MG	BB	3030	1/1	0.99	0.03	35,35,35,35	0
53	MG	BB	3015	1/1	0.99	0.09	13,13,13,13	0
53	MG	BB	3002	1/1	0.99	0.07	5,5,5,5	0
53	MG	BB	3070	1/1	0.99	0.14	37,37,37,37	0
53	MG	DB	3081	1/1	0.99	0.13	18,18,18,18	0
53	MG	DB	3053	1/1	0.99	0.07	35,35,35,35	0
53	MG	CA	2002	1/1	1.00	0.11	5,5,5,5	0

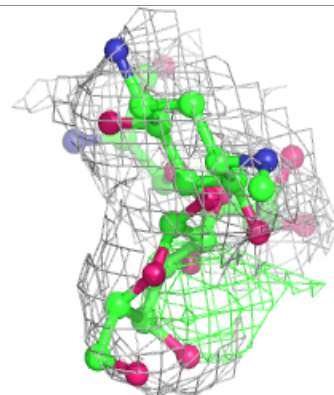
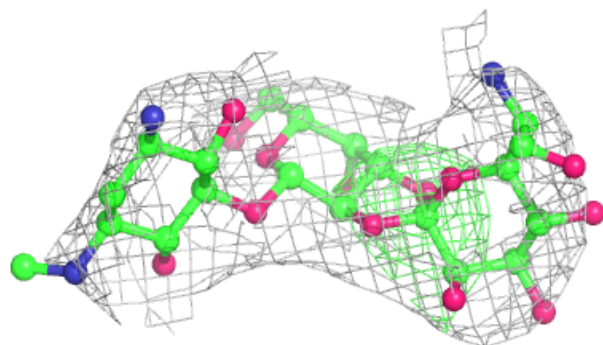
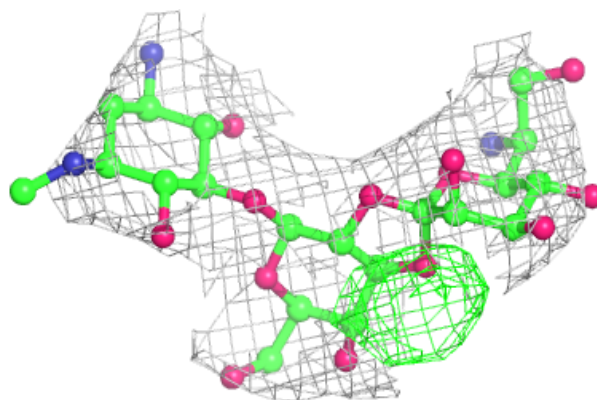
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HYG AA 2059:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around HYG CA 2062:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.