



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 09:55 am BST

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](mailto: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.

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

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

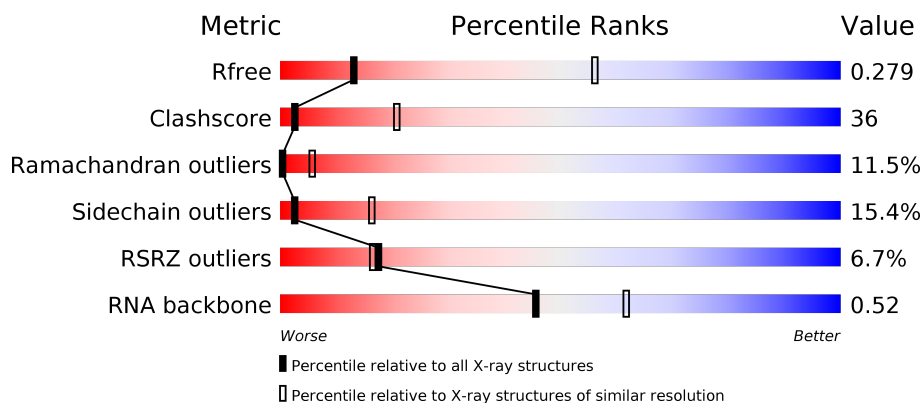
# 1 Overall quality at a glance

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

Mol	Chain	Length	Quality of chain
1	AA	1542	<div> <div>22%</div> <div>63%</div> <div>14%</div> <div>..</div> </div>
1	CA	1542	<div> <div>21%</div> <div>65%</div> <div>13%</div> <div>..</div> </div>
2	AC	232	<div> <div>13%</div> <div>31%</div> <div>43%</div> <div>13%</div> <div>11%</div> </div>
2	CC	232	<div> <div>7%</div> <div>31%</div> <div>44%</div> <div>13%</div> <div>11%</div> </div>

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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	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	71	
21	CU	71	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BV	94	
24	DV	94	
25	BC	273	
25	DC	273	
26	BD	209	
26	DD	209	
27	BE	201	
27	DE	201	

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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
1	AA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

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

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

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

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

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

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

- 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
10	CK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

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

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

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

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

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

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

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

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

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

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

- 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
26	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BQ	117	Total	C	N	O	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	S	0	0	0
			779	492	146	141				

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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
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
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
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			

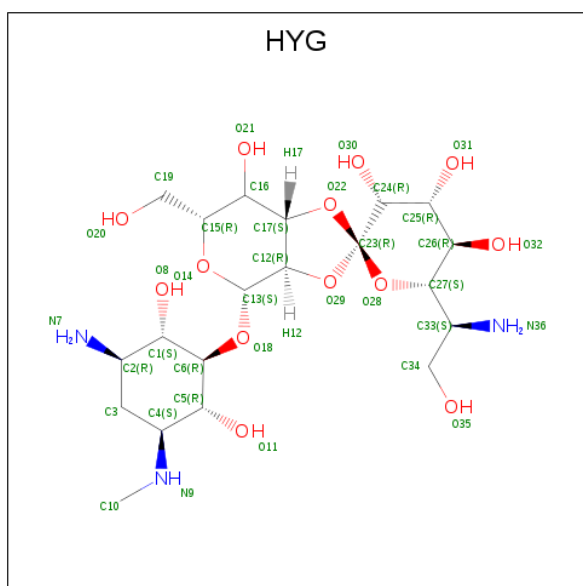
- Molecule 52 is a protein called 50S ribosomal protein L11.

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

- Molecule 54 is HYGROMYCIN B (three-letter code: HYG) (formula:  $C_{20}H_{37}N_3O_{13}$ ).



*Continued from previous page...*

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

- Molecule 56 is water.

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

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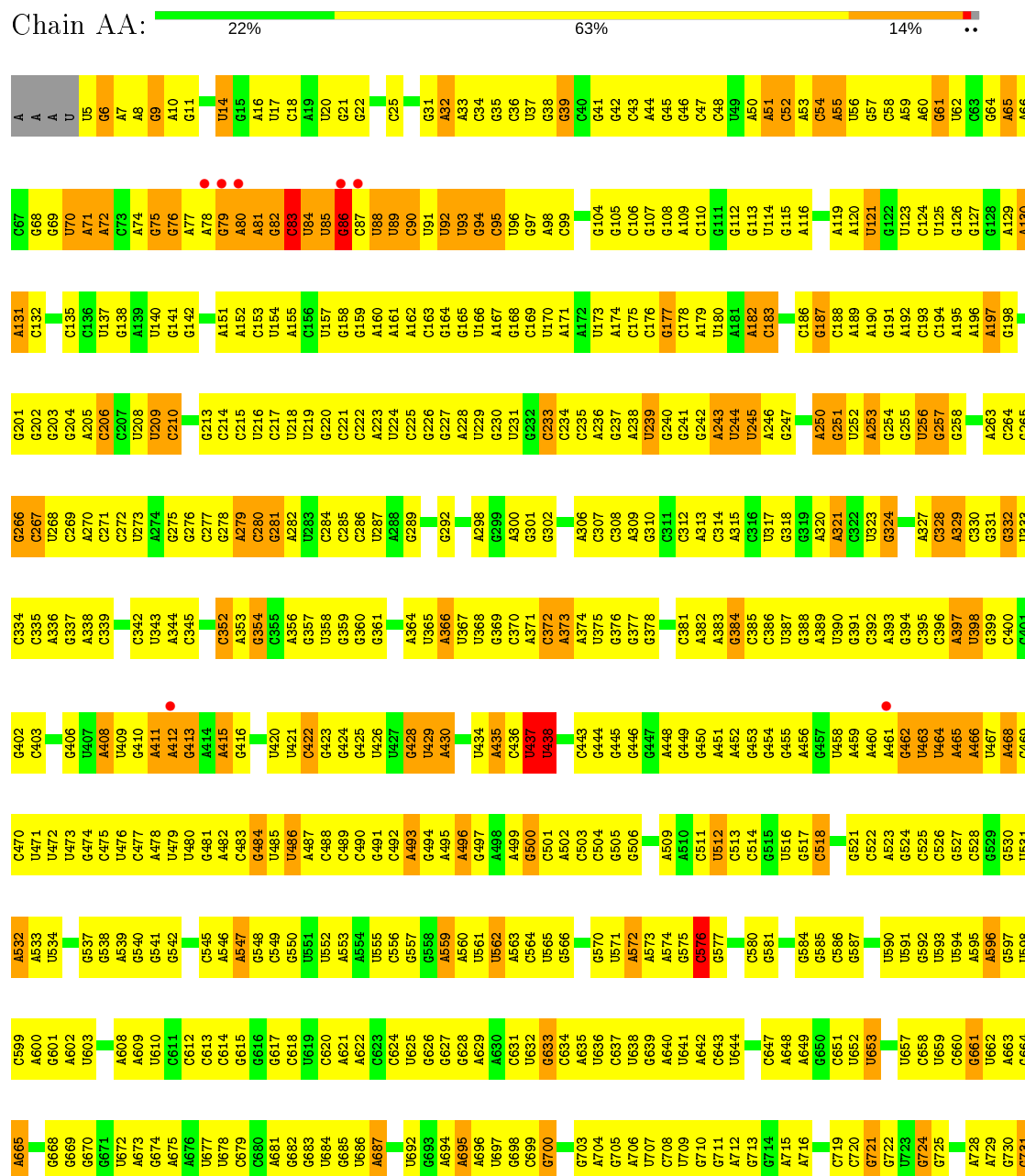
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CN	3	Total 3	O 3	0	0
56	CT	1	Total 1	O 1	0	0
56	DB	499	Total 499	O 499	0	0
56	DC	5	Total 5	O 5	0	0
56	DD	1	Total 1	O 1	0	0
56	DE	1	Total 1	O 1	0	0
56	DL	5	Total 5	O 5	0	0
56	DP	1	Total 1	O 1	0	0
56	D2	1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

### 3 Residue-property plots

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

- Molecule 1: 16S ribosomal RNA



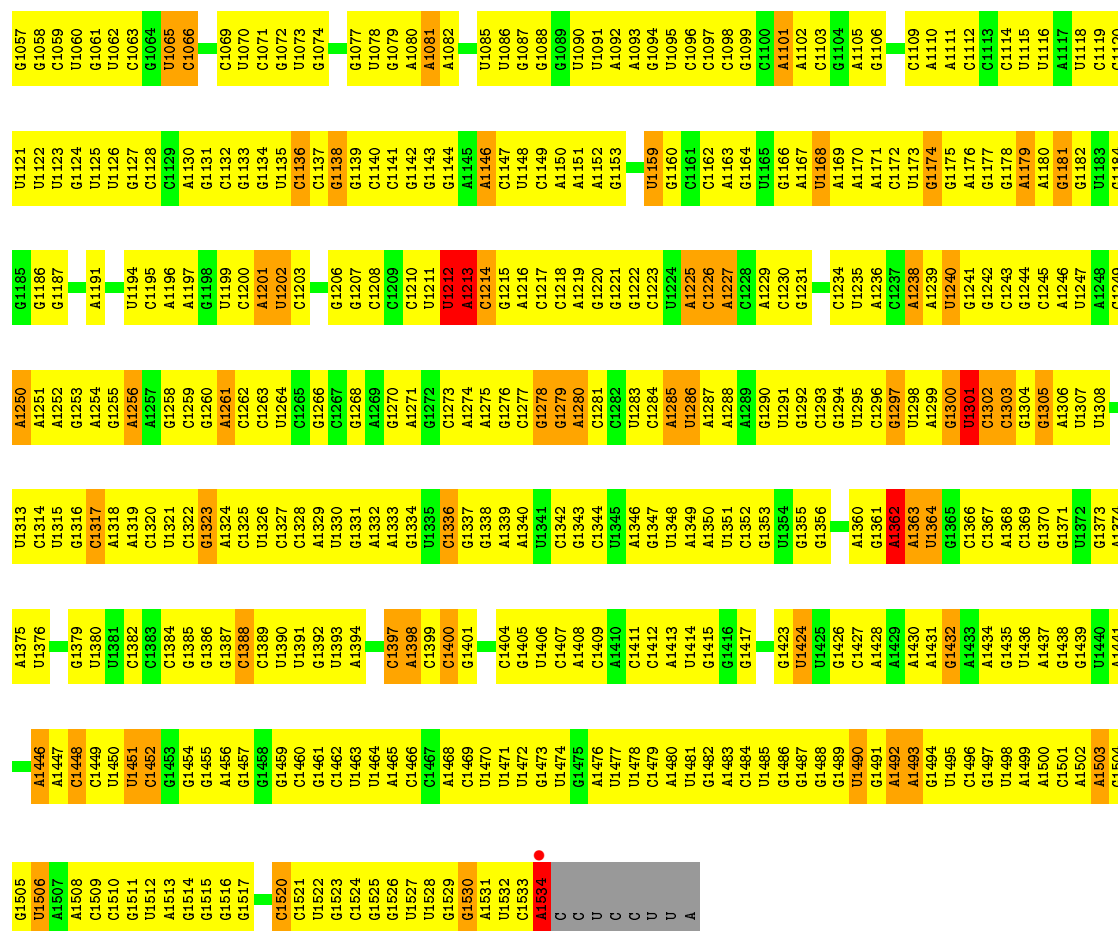
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G1459	C1460	G1461	G1462	G1463	G1464	G1465	G1466	C1467	A1468	C1469	G1470	G1471	U1472	G1473	U1474	G1475	A1476	C1477	G1478	A1479	G1480	G1481	G1482	A1483																																			
C1389	U1390	U1391	G1392	U1393	A1394	C1397	A1398	C1399	G1400	G1401	G1405	C1336	G1337	G1338	C1339	A1340	U1341	C1342	G1343	C1344	U1345	A1346	G1347	U1348	A1349	A1350	U1351	C1352	G1353	U1354	G1355	G1356	A1360	G1361	A1362	A1363	G1364	C1365	C1366	C1367	A1368	C1369	G1370	G1371	U1372	G1373	A1374	A1375	U1376	G1379	U1380	U1381	C1382	G1386	C1387	C1388			
C1262	C1263	U1264	C1265	G1266	C1267	G1268	A1269	G1270	C1271	G1272	C1273	A1274	G1275	G1276	C1277	G1278	C1279	A1280	C1281	C1282	U1283	C1284	U1285	A1286	G1287	A1288	A1289	G1290	U1291	C1292	C1293	G1294	U1295	C1296	G1297	U1298	A1299	G1300	U1301	C1302	C1303	G1304	G1305	A1306	U1307	U1308	G1312	U1313	C1314	U1315	G1316	C1317	U1318	A1319	C1320	U1321	C1322	G1323	
C1200	A1201	U1202	C1203	G1206	G1207	G1208	G1209	C1210	U1211	U1212	C1213	A1214	G1215	A1216	C1217	G1218	A1219	G1220	C1221	G1222	C1223	U1224	A1225	C1226	A1227	G1228	C1229	C1230	C1231	C1234	U1235	U1236	G1237	A1238	C1239	A1240	G1241	C1242	C1243	G1244	C1245	A1246	U1247	U1248	A1249	A1250	A1251	A1252	G1253	A1254	G1255	A1256	A1257	G1258	C1259	G1260	A1261		
C1132	G1133	U1134	U1135	C1136	C1137	G1138	G1139	C1140	G1141	G1142	G1143	G1144	A1145	A1146	C1147	U1148	C1149	A1150	A1151	A1152	G1153	U1159	C1162	A1163	G1164	U1165	G1166	A1167	U1168	A1169	A1170	A1171	C1172	C1173	U1174	G1175	A1176	G1177	G1178	A1179	A1180	G1181	G1182	U1183	G1184	U1185	G1186	G1187	A1191	U1194	C1195	A1196	A1197	G1198	U1199				
A1005	G1006	U1007	U1008	U1009	U1010	C1011	A1012	G1013	A1014	G1015	A1016	U1017	G1018	A1019	G1020	A1021	A1022	U1023	G1024	U1025	G1026	C1027	U1028	C1029	U1030	C1031	C1032	G1033	G1034	A1035	A1036	C1037	C1038	G1039	U1040	G1041	A1042	G1043	A1044	C1045	A1046	G1047	G1048	U1049	G1050	G1053	C1054	A1055	U1056	G1057	G1058	C1059	U1060	G1061	U1062	G1063	U1065		
C940	G941	G945	A946	G947	C948	A949	U950	C951	U952	G953	A954	G955	U956	U957	A958	A959	U960	U961	A964	U965	G966	C967	A968	A969	C970	G973	A974	A975	G976	A977	A978	C979	C980	U981	U982	A983	C984	C985	U986	G987	G988	U991	U992	G993	A994	C995	A996	U997	C998	C999	A1000	C1001	G1002	G1003	A1004				
C868	G869	U875	A878	C879	C880	G881	C882	C883	U884	G885	G886	U887	C888	A889	C893	G894	G898	C899	A900	G824	A901	G902	G903	U904	U905	A906	A907	A908	A909	C910	A914	A915	U916	G917	A918	U920	C984	U921	G922	A923	C924	G925	G926	G927	G928	G929	C930	C931	G932	G933	U934	A935	C936	A937	A938	G939			
C734	C735	U804	C737	C738	C739	G742	A743	C744	G745	U812	A746	A747	A815	A816	C750	G817	G818	U751	G752	A753	G761	U762	G763	C764	U827	U828	G829	A766	A767	A768	G832	A775	G776	C841	U842	A777	U843	U844	U845	U846	U847	C848	G849	A784	G785	G786	A787	U788	G791	A792	U793	C794	A794	C795	G796	C797	C866	G867	U798

## ● Molecule 1: 16S ribosomal RNA

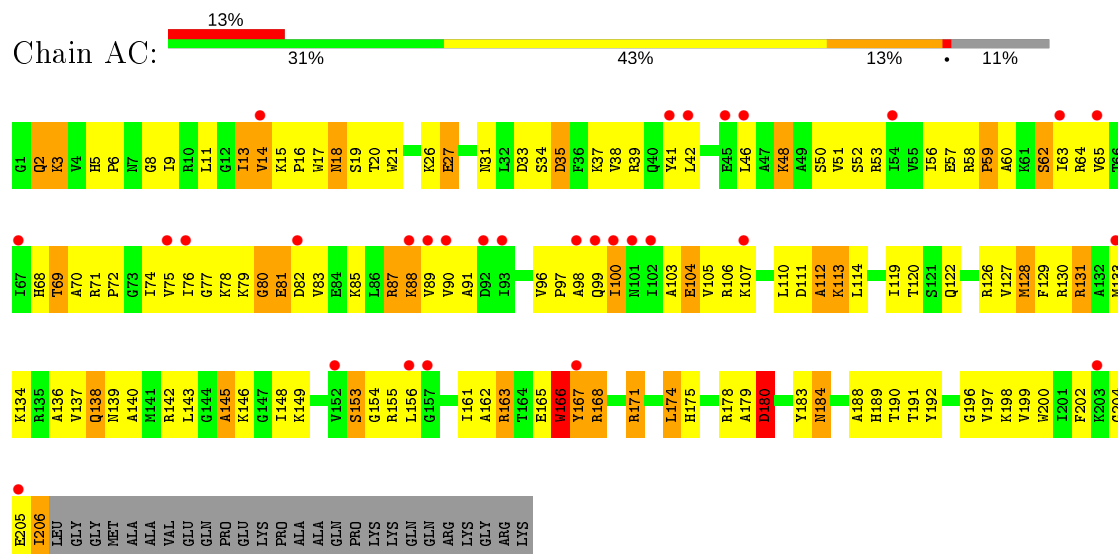
Chain CA:  21% 65% 13% \*\*

A	A	U	U	U5	G6	A7	A8	G9	A10	G11	U14	G15	A16	U17	C18	G21	G22	C25	G31	A32	A33	C34	G35	C36	U37	G38	C39	C40	G41	G42	C43	A44	G45	G46	C47	C48	U49	A50	A51	C52	C54	A53	A55	U56	G57	C58	A59	A60	G61	U62	A65	A66	C67	G68
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A996	U997	C931	A860	U793	G724	C660	A595	G539	U464	A397	C332	A263	G201	C135	G69
C998	C998	C934	G861	A794	G725	G661	A596	G530	A465	U998	U333	C264	G202	C136	U70
C999	A935	A935	U862	C795	A728	U662	G597	U531	A466	C399	C394	G265	G203	G137	A71
A1000	A864	A936	G863	C796	A729	A663	U598	A532	U467	C400	C335	G266	G204	G138	A72
C1001	A937	A937	A865	C797	A730	A664	C599	A533	A468	G401	A336	C267	A205	C139	C73
G1002	A938	A938	C866	U798	G731	A665	A600	U534	C469	G402	A337	U268	C206	G141	
G1003	G939	G939	G867				G601		C470	C403	A338	C269	C207	G142	A77
A1004	C940	C940	C868	A802	G734	G668	A602	G537	U471	G406	C339	A270	U208	A143	A78
G1005	G941	G941	G869	G803	C735	G669	U603	A538	U472	U407	U340	C271	U209	G144	G79
A1006			G870	U804	C736	G670		A539	U473	U408	C341	C272	U209	G145	A80
U1007	G945	G945	U875	C805	A737	G671	A607	A540	U474	A408	C342	U273			A81
A946	A946	A946	C876	C806	C737	U672	A608	G541	C475	U409	U343	A274	G213	A149	G82
G947	G947	G947	G877	A807	C738	A673	A609	G542	U476	G410	U344	G275	G214	U150	C83
U1009	C948	C948	A878	C808	C739	G674	U610	U543	C477	A411	C345	G276	C215	A151	U84
U1010	A949	A949	C879	G809		A675	G611	G544	U478	A412					
C949	C949	C949	C880	C810	G742	A676	C612	C545	U479	A413	C352		G216	A152	
G950	G950	G950	C881	C811	A743	U677	C613	A546	U480	A414	A353	A279	U218	A153	G86
A1011	U952	U952	C882	G812	C744	U678	C614	A547	G481	A415	G354	C280	U218	C154	U87
A1014	U953	U953	C883	U813	G745	C679	G615	G548	A482	G416	C355	G281	U219	A155	U88
G953	G953	G953	U884	A814	A746	G680	G616	C549	C483		A356	A282	G220	C156	U89
G954	G954	G954	U885	A815	A747	A681	G617	G550	A484	U420	G357	A283	C221	U157	C90
A1016	G955	G955	C886	C816	C748	U682	U618	U551	U485	U421	U358	A284	A223	G158	U91
U1017	U956	U956	G887	C817	A749	G683	U619	U552	U486	C422	C359	C285	A224	G159	U92
G1018	U957	U957		C818	C750	U684	C620	A553	A487	G423	G360	C286	G225	A161	U93
A1019	A958	A958	U889	G819	U751	G685	A621	A554	C488	G424	G361	U287	G226	A162	G94
G1020	A959	A959		A819		U686	A622	U555	C489	G425	G362	A288	G227	C163	G95
A1021	U960	U960	C893	U820	C754	A687	C623	C556	C490	U426	A363	G289	A228	G164	G97
U1022	U961	U961	G894	G821	G755	G688	C624		C491	U427	A364	G289	U229	G165	A98
G1024				U822			U625	A559	C492	G428	U365	G292	U230	U166	C99
U1025	A964	A964	G898	C823	U762	U692	G626	A560	A493	U429	A366	A298	U231	A167	G100
G1026	U965	U965	C899	A825	G763	G693	G627	U561	G494	A430	U367	G298	G232	G168	A101
C1027	G966	G966	A900	C826	C764	A694	G628	U562	A495	A431	U368	C299	C233	C169	
C1028	C967	C967	A901	U827	A765	A695	A629	A563	A496		G369	A300	C234	U170	G104
U1029	A968	A968	G902	U828	A766	A696	A630	C564	G497	U434	C370	G301	C235	G105	C106
U1030	A969	A969	G903	C829	A767	U697	C631	U565	A498	C436	A371	G302	A236	G107	G108
G1031	C970	C970	U904	G829	C768	G698	U632	G566	A499	C437	C372	G237	G237	C175	A109
G971	G971	G971	U905		G769	C699	G633		G500	U437	A373	A306	A238	C176	
C972	C972	C972	A906	G833	C770	G700	C634	G570	C501	U438	A374	C307	U239	G177	G110
G973	G973	G973	U916	U842	G771	U701	A635	U571	A502		U375	C308	G240	C178	G111
A1035	A974	A974	G917	U834	U772	A702	G636	A572	C503	C443	G376	A309	G241	A179	G112
A1036	A975	A975	U982	U835	G773	G703	C637	A573	C504	G444	G377	G310	G242	G113	
C1037	G976	G976	A909	G836	G774	A704	U638	A574	G505	G445	G378	A243	G243	U180	
G1038	A977	A977	C910	U837	G775	G705	G639	G575	G506	G446	C379	C312	U244	A181	U114
C1039	A978	A978		G838	G776	A706	A640	G576		G447	A313	U245	U245	A182	G115
U1040	C979	C979	A914		A777	U707	U641	G577	C511	A448	C381	C314	A246	C183	A116
G1041	C980	C980	U916	U841		U707	U642	C578	U512	G449	A382	C315	G247	C186	A119
A1042	U981	U981	G917	U843	G778	C708	A642	A579	C513	G450	A383	G316	A250	G187	A120
G1043	U982	U982	A918	G844	A780	U709	C643	C580		A451	G384	U317	G251	C188	U121
A1044	A983	A983	A919	A845	A781	G711	U644	G581	U516	A452	C385	G319	U252	A189	G122
C1045	C984	C984	U920	G846	A782	A712		G584	G517	G453	C386	A320	A253	A190	U123
A1046	C985	C985	U921	G847	C783	G713	A646	G585		G454	U387	A321	G254	G191	
G1047	U986	U986	G922	C948	A784	G714	A649	C586	G521	G455	G388	C322	G255	A192	G126
U1048	C987	C987	A923	U849	G785	A715	U650	G587	C522	A456	A389	U323	U256	C193	G127
U1049	G988	G988	C924		G786	A716	G651	G587	C523	G457	U390	G391	G257	C194	G128
G1050			G925	C953	A787		U652		U590	U458	G392	G324	G258	A195	A129
	U991	U991	G926	U854		C719	U663		C525	A459	C393		G259	A196	A130
G1053	U992	U992	G927	U854		C720	U637		C526	A460	A394	C328	G260	A197	A131
C1054	G993	G993	G928	A790		G721	U657		C527	A461	G395	A329	G261	A198	C132
A1055	A994	A994	G929	G722		U722	U658		U594		C396	G331	A262	G198	
U1056	C995	C995	C930	U723		U723	U659								

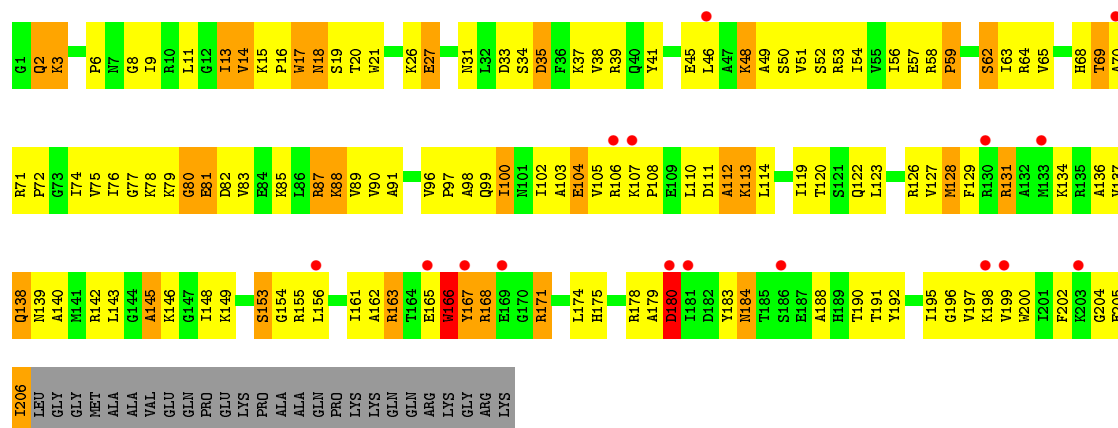


### • Molecule 2: 30S ribosomal protein S3

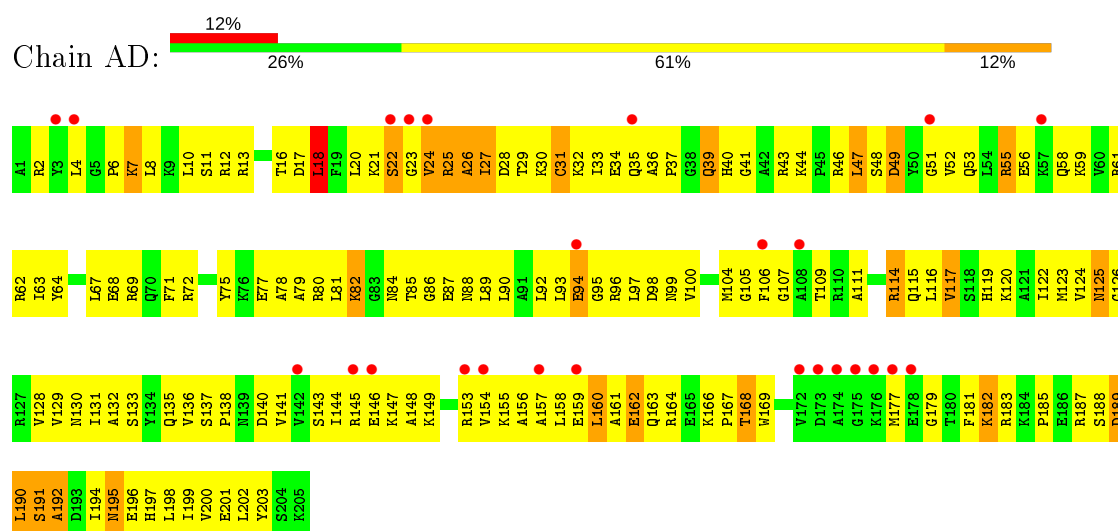


### • Molecule 2: 30S ribosomal protein S3

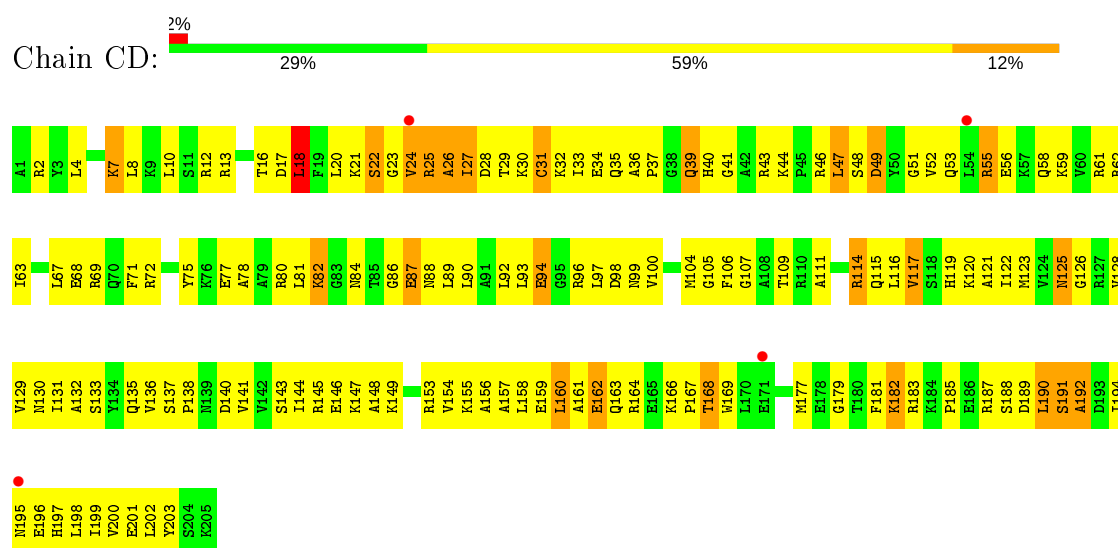




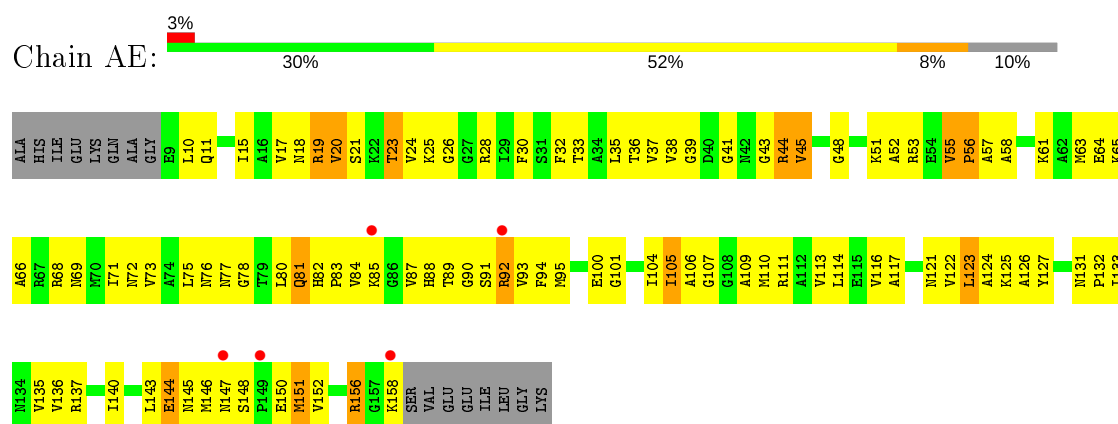
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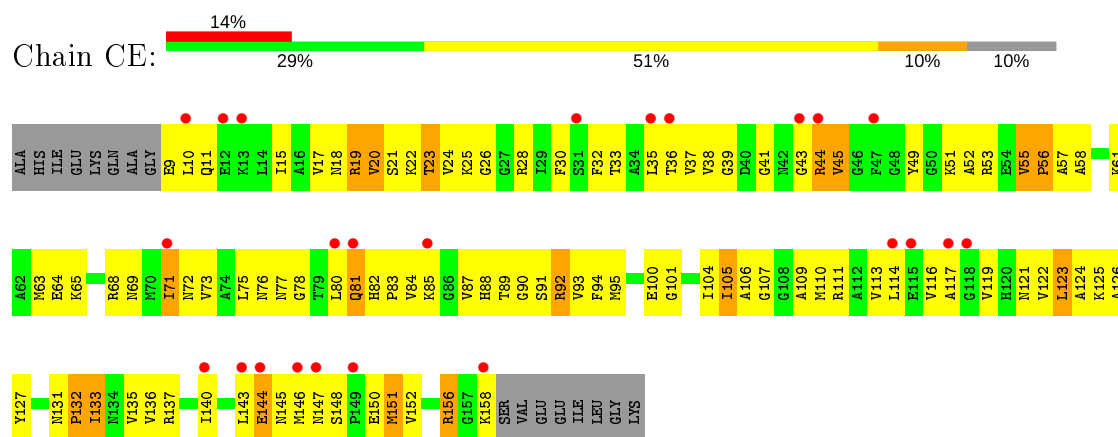
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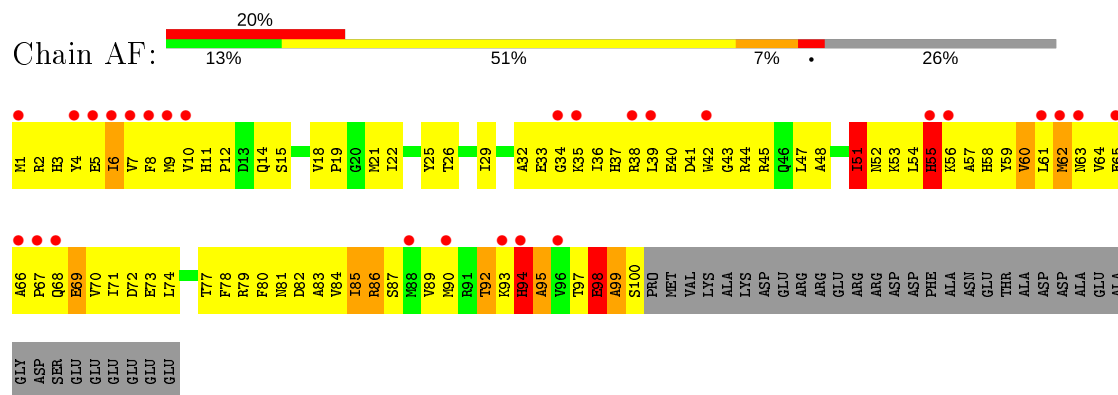
• Molecule 4: 30S ribosomal protein S5



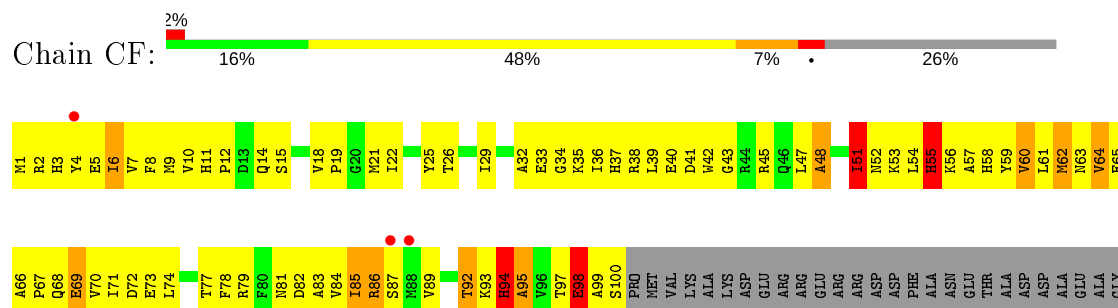
- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



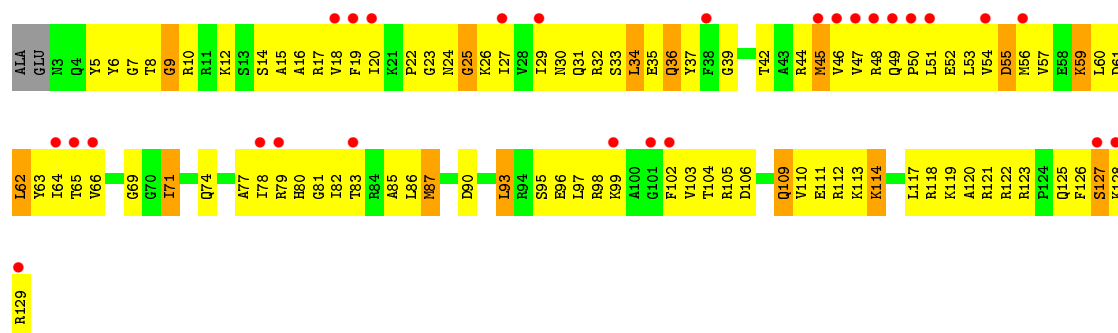
- Molecule 5: 30S ribosomal protein S6



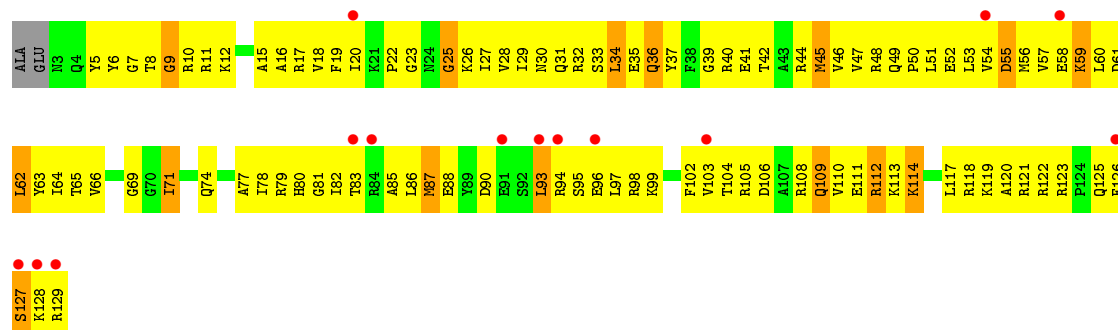




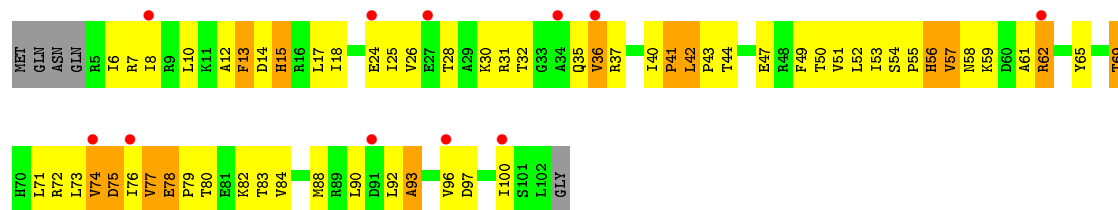
• Molecule 8: 30S ribosomal protein S9



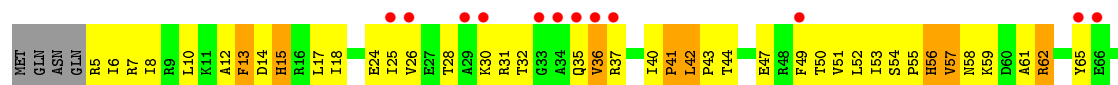
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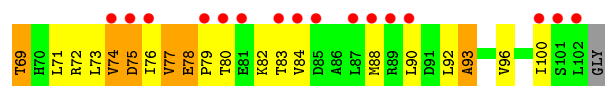


• Molecule 9: 30S ribosomal protein S10

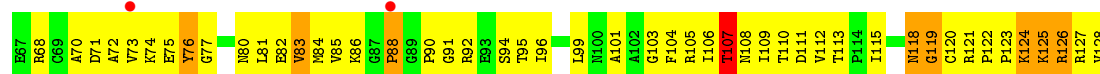


• Molecule 9: 30S ribosomal protein S10

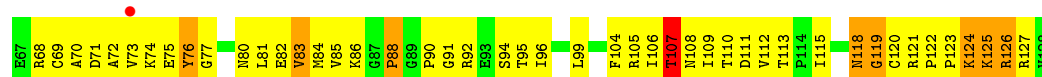




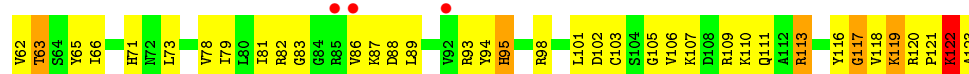
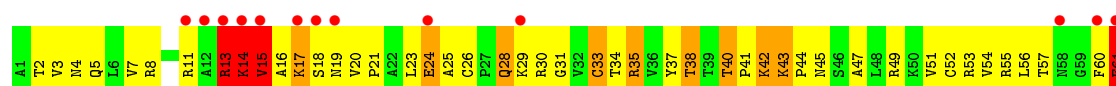
• Molecule 10: 30S ribosomal protein S11



• Molecule 10: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S12

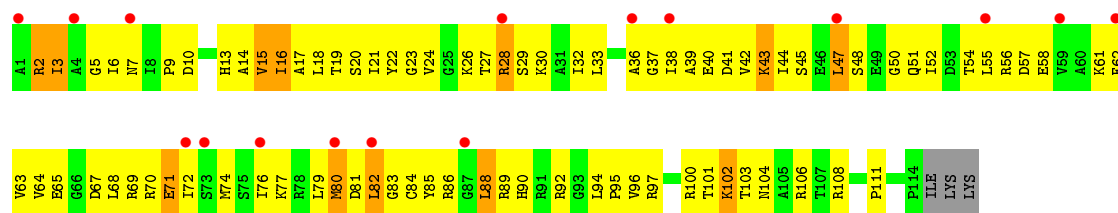


• Molecule 11: 30S ribosomal protein S12

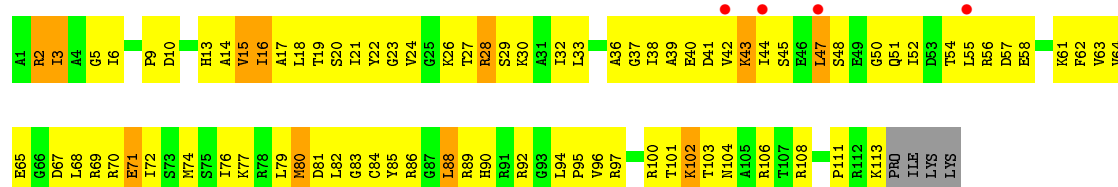


• Molecule 12: 30S ribosomal protein S13

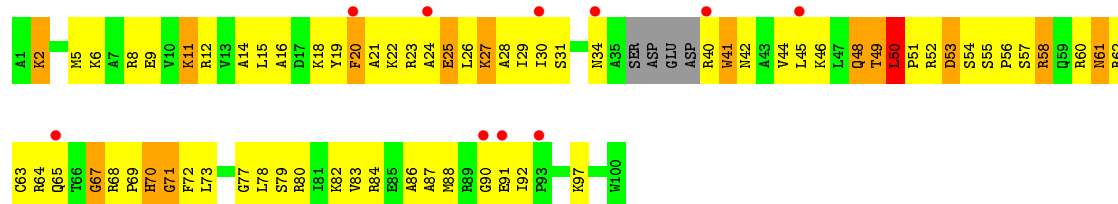




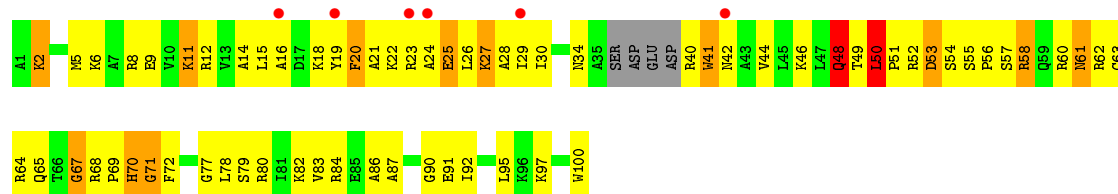
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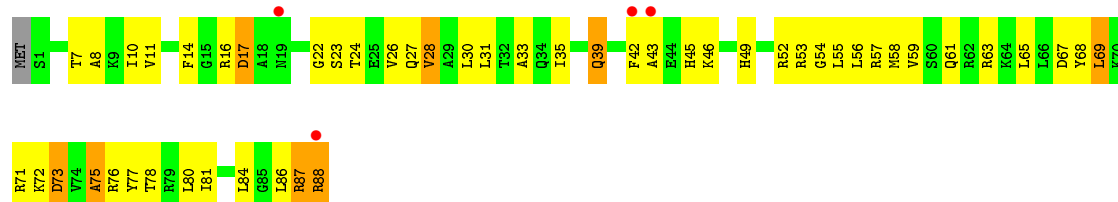
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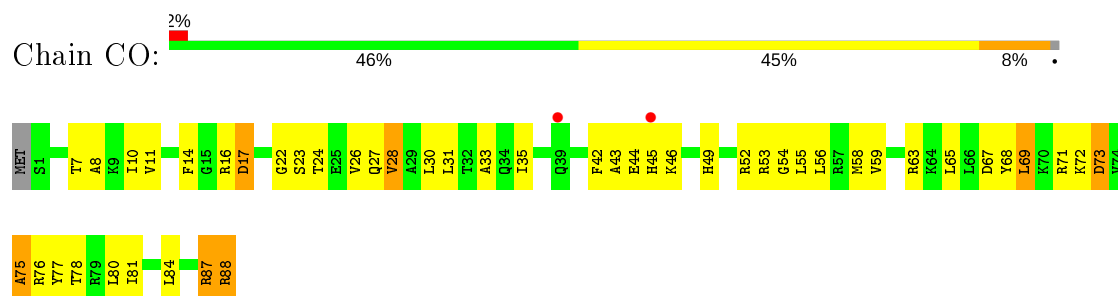
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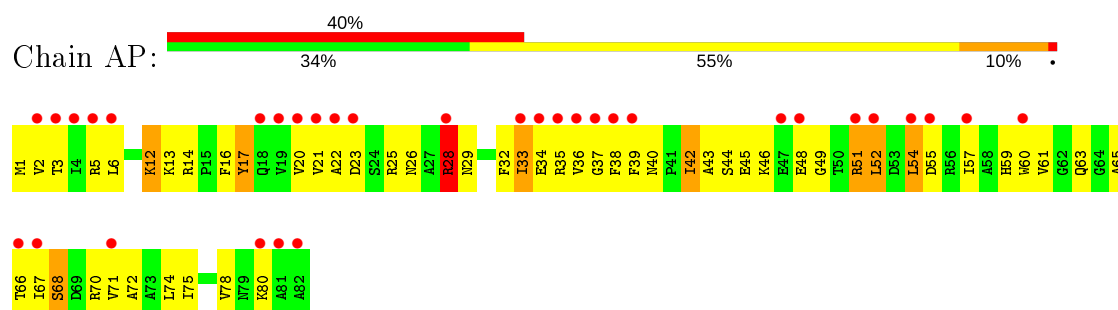
• Molecule 14: 30S ribosomal protein S15



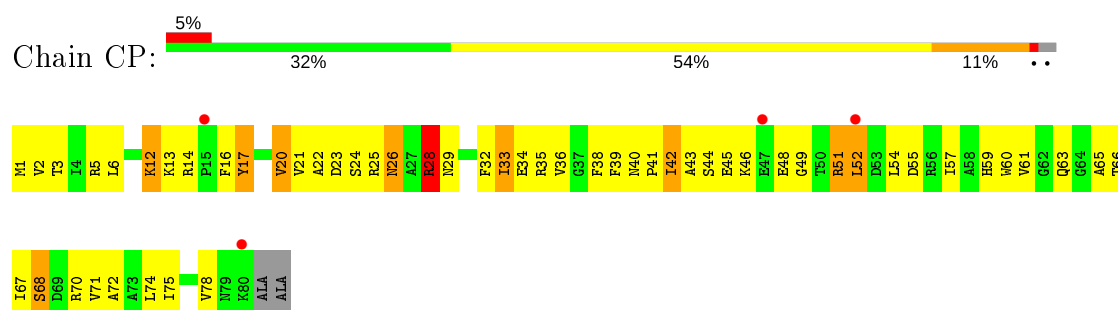
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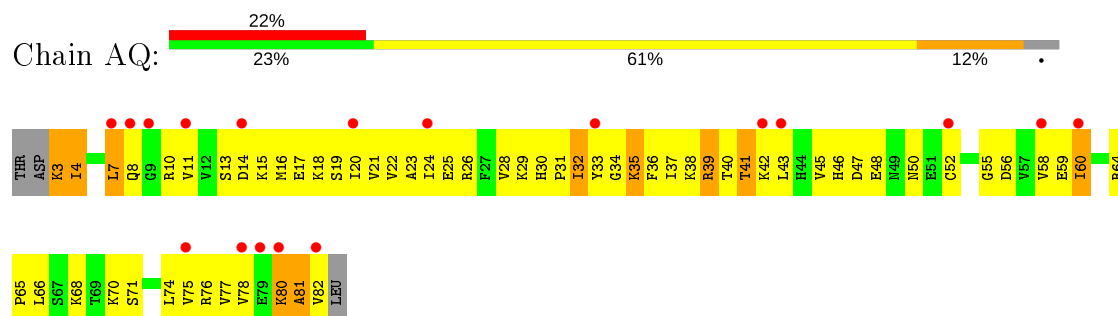
- Molecule 15: 30S ribosomal protein S16



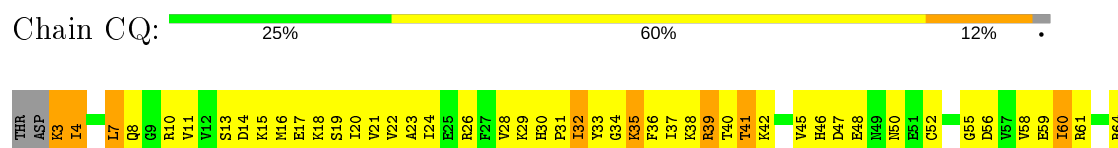
- Molecule 15: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S17

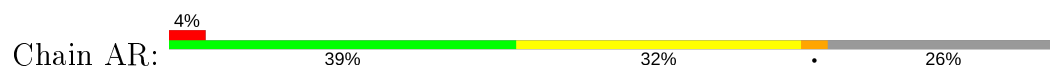


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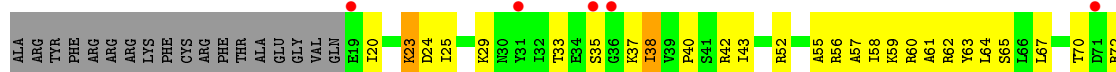




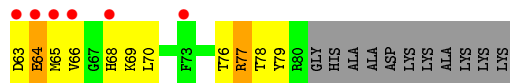
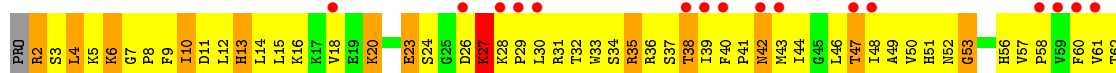
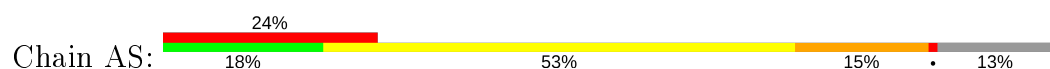
- Molecule 17: 30S ribosomal protein S18



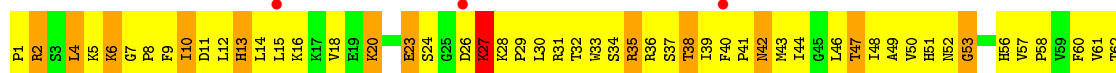
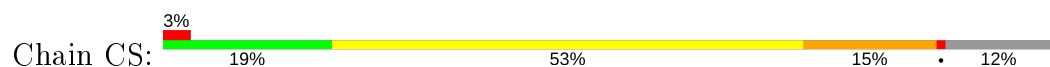
- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19

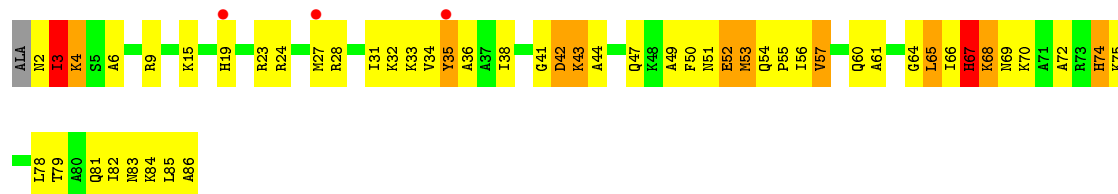


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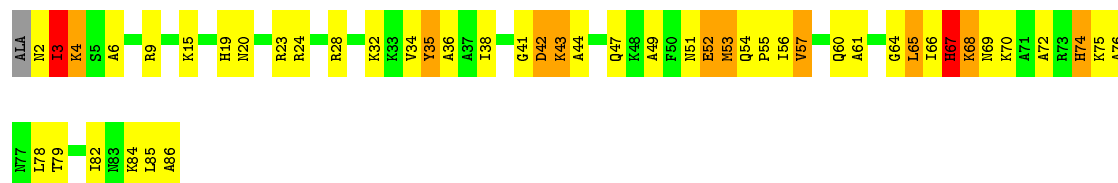
- Molecule 19: 30S ribosomal protein S20





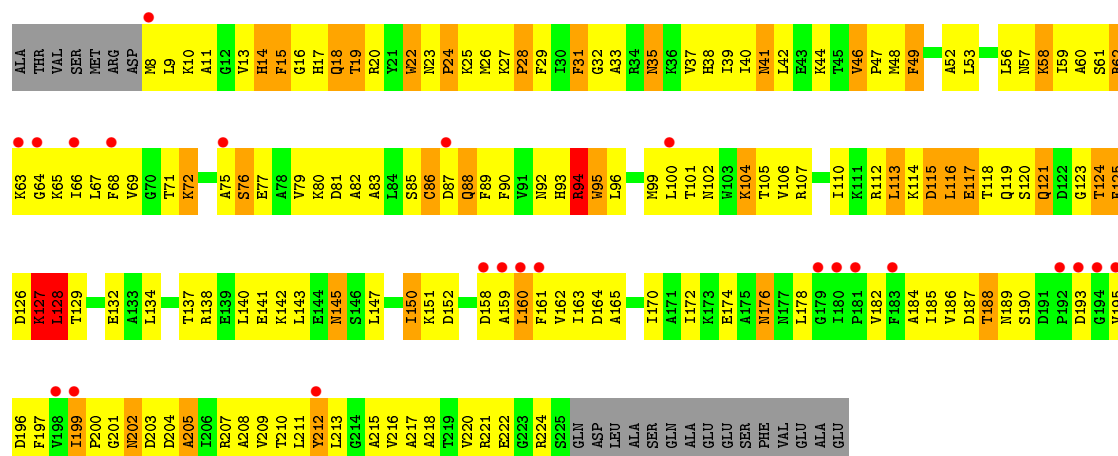
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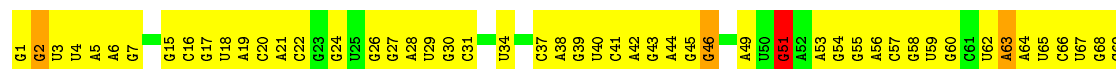
Chain CT: 43% 42% 12% ..



• Molecule 20: 30S ribosomal protein S2

Chain AB: 10% 25% 50% 15% • 9%



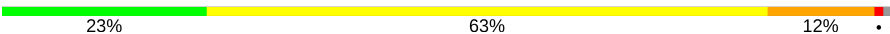


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U1018	G942	G	A819	A743	A670	A608	C544	A478	G412	C335	A272	A204	U138	A73
U1019	A943	G	A820	G744	A671	A609	U545	A479	C413	C336	G273	G205	U139	A74
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A1022	C946	C	C823	U747	G674	G612	G548	A482	U416	U339	G276	C212	A142	G77
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C2025	G1946	U1880	G1813	C1741	A1676	U1599	G1538	G1475	A1412	A1269	G1202	G1202	G1138
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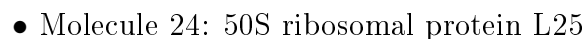
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G2038	A2108	A	U2231	A2298	G2428	G2429	U2493	U2563	G2628	G2693	A2758	G2824	G2886
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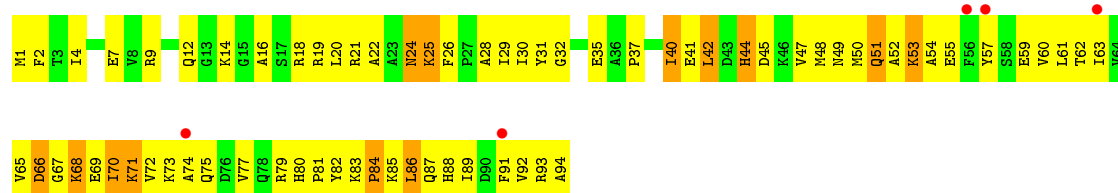
• Molecule 23: 23S ribosomal RNA

Chain DB:  23% 63% 12% ..

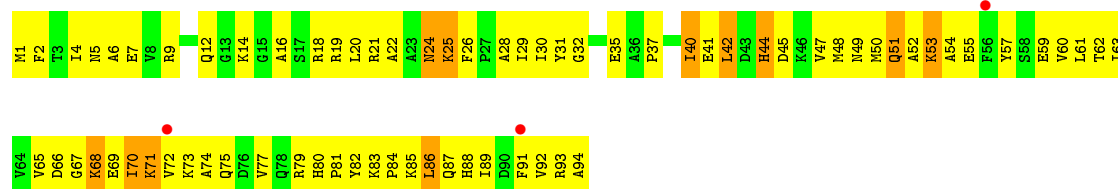
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C935	U872	U811	C740	A668	G604	A541	C475	G410	C336	G275	A204	U138	A71	U4
C936	C873	C812	U741	G669	G605	C544	G476	G411	C337	U276	G205	U139	U72	A5
C937	G874	U813	A742	A670		U545	A477	A412	G338	G277		G140	A73	A6
C938	C875	C814	A743	C671	A808	U546	A478	G413	U339	A278	G211	G141	A74	G7
G939	C876	C815	U744	C672	A609	U547	A479	C414	A340	A279		A142	G75	
G940	A877	C816	G745	C673	C610	A547	A480	A415	C341	U280	A213	C143	G76	G15
A941	A878	C817	U746	G674	C611	U548	G481	U416	A342	G281	G214	A144	G77	C16
G942	G	G818	U747	A675	G612	U549	A482	C417	C343	A282	G215	C145	U78	G17
A943	G	A819			A613	C550	A483	C418	A344	G283	A216	A146	C79	U18
	G	A820	A750	C678	A614	G551	C484	U419	A345	U284			G80	A19
C946	G	A821	A751	C679	U615	U552	C485	C420	A346	G285	A218	U150	G81	C20
A947	U	G822	A752		A616	G553	C486		A347	U286	A219	C151	U82	A21
C948	G	G823	A753	U683	G617	U554		A423	A348	G287	G220	A152	A83	C22
G949	C	U824	U754	G684	G618	U555	C490	G424	U349	U288	A221	U153	A84	G23
G950	A	A825	U755	A685	G619	A556	C491	G425	G350	G289	A222	U154		G24
C951	U	U826	A756	U686	G620	C557	A492	C426	C351	U290	A223	A155	G85	U25
	C	U827	G757	C687		U558	G493	U427	A352	G291	U224	A156		G26
G956	C	U828	C758	U688	C623	G559	G494	A428	C353	U292	G225	U157	U90	G27
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G971	G903	U842	G774	U573	A637	U574	A508	A443	C367	U306	G242	U172	G107	A42
A972	G904		G775	A705	G638	A574	C509	C444		G307	U243	A173	G108	G43
G973	A905		G776	A706	U639	A575	C510	C445	G370	G308	A244	U174	C109	A44
C974		U846	G777	G707	C640	U576	U511	G446	A371	A309	G245	G175		G45
A975	A909	U847		G708	U641	U580	G512		G372	A310	C246	A176	U113	G46
		C848	G780	U709	U642	U581	A513	U451	U373	A311	G247	G177	U114	C47
A979	A911	A849	A781	U710	A643	C581	A514	G452	A374	G312	G248	G178	C115	G48
U980	C912	U850	A782	G711	A644	A582	A515	A453		G315	C249	G179	C116	A49
A981	U913	C851	G783	G712	C645	G583		A454	G379	G316	G250	A118	A118	U50
C982		U852	G784	G713	U646	C584	G518	C455		G317	A251	A181	A119	G51
A983	G916	C853	G785	U714	G647	G585	U519	C456	G386	C318	G252	A182	A120	A52
A984	A917	C854		U715	G648	A586	G520	A457	U387	G319		C183	U120	A53
C987	U918	G855	C786	A716	G649	C587	U521	G458		A320	A255	C184	G121	G54
A988	A920	G856	A789	C717	C650	U588	A522	U459	U392	U321	C257	G185	G122	G55
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C990	C922	G858	A794	C719	C651	U590	U525	G462	U395	C323		G189	G124	C57
G991	G923	U860	C795	U720	A654	U591	A526	A653	G396	A324	G263	A126	A126	G58
C992		C861	C796	A721	A655	A592	A527	U464		G325	C264	A127	A127	U59
G993	A925	G862	G797	C723	U656	U593	A528	G465	G400	G326	A265	C128	G60	G60
C994	G926	A863	G798	G724	G659	C595		A466		G327	G266	C129	U62	U62
G995	A927	G864		G725	C660	U596	C531	G467		U328	C267	G194	C130	A63
A996	A928	C865	U803	G726	A661	G597	A532	G468	U403	G329	C268	A195	A131	A64
G997	U929	A866	A804	G727	G662	U598	A533	G469	A404	C330	C269	A196	G132	U65
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G1945	U1880	A1815	A1746	G1682	G1537	U1474	U1411	G1344	A1274	C1208	C1146	A1080	A1001
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	C1894	C1830	G1762	G1690	C1550	U1487	G1426	G1356	C1289		U1173	U1094	
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C1972	C1904	C1843	U1636	C1709		U1496	A1435	U1373	G1298		U1182	A1103	
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		A1847	G1776	U1712	C1564		A1438	U1376	A1237		U1174	U1107	U1032
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	C1914	U1851	A1780	U1716	A1569	A1505	U1442	G1381	U1438		C1179	A1111	G1042
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C1994	G1922	A1858	G1724	G1724	C1577	U1513	G1450	G1389	G1250		G1124	G1125	A1054
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	G1929	U1865	G1731		U1584		G1459	U1397	G1257		G1135	U1067	
C2008	U1930	A1866	C1732	G1666	C1585	U1523	U1460	C1398	U1258		G1136	U1068	
A2009	G1931	G1867	G1733	G1667	G1524	G1524	A1461	U1329	G1259		G1137	U1069	
G2010	A1932	C1868	G1734	A1668	A1525	A1525	C1462	C1330	U1260		G1138	U1070	
G2011	G1933	G1869	A1735	A1669	U1589	C1526	C1463	G1331	C1261		G1139	A1141	
G2012	C1934	C1870	U1736	C1670	A1590	G1527	G1464	U1401	A1262		G1140	U1203	
A2013	A1871	G1871	G1737	A1528	A1591	U1528	G1465	U1402	G1333		G1141	U1204	
A2014	G1935	A1872	C1738	C1592	C1592	G1529	U1466	A1403	C1200		G1142	U1205	
A2015	A1937	G1873	A1739	G1673	A1593	G1530	U1467	C1404	U1267		G1143	U1206	
U2016	C1938	C1874	G1740	G1674	U1594	C1531	U1468	U1405	G1268		G1144	U1207	
U2017	U1939	G1875	C1741	G1675	C1595	A1532	A1469	U1406	A1269		G1145	U1208	
G2018	A1876	U1811	U1742	A1676	A1596	C1533	A1470	G1407	G1338		G1146	U1209	
A2019	U1940	G1877	G1743	A1677	A1597	U1534	G1471	G1408	G1271		G1147	U1210	
G2020		G1878	A1744	A1678	A1598	A1535	C1472	U1409	A1272		G1148	U1211	

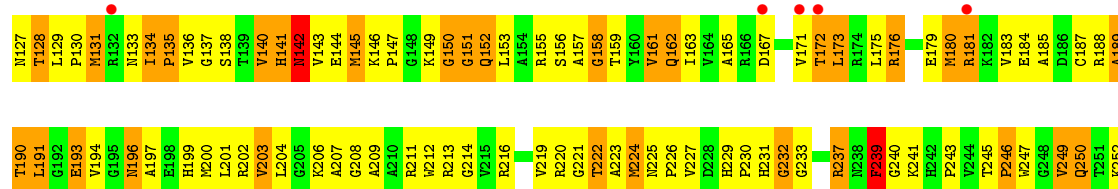
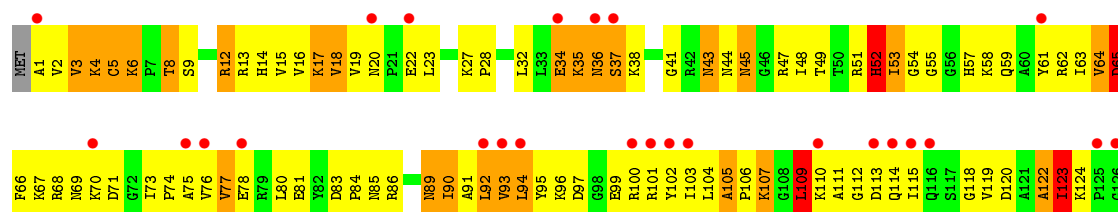




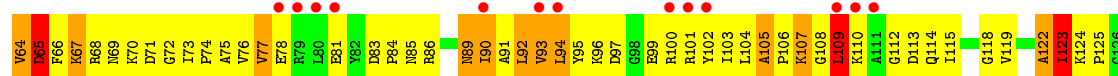
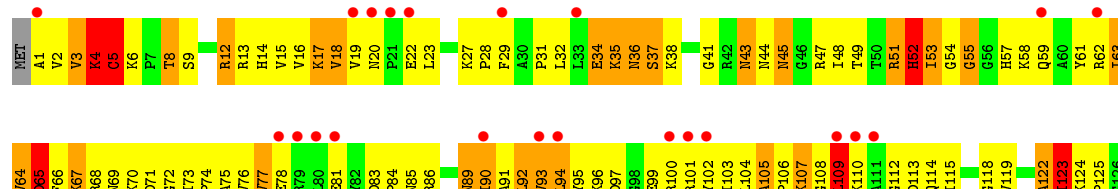
• Molecule 24: 50S ribosomal protein L25

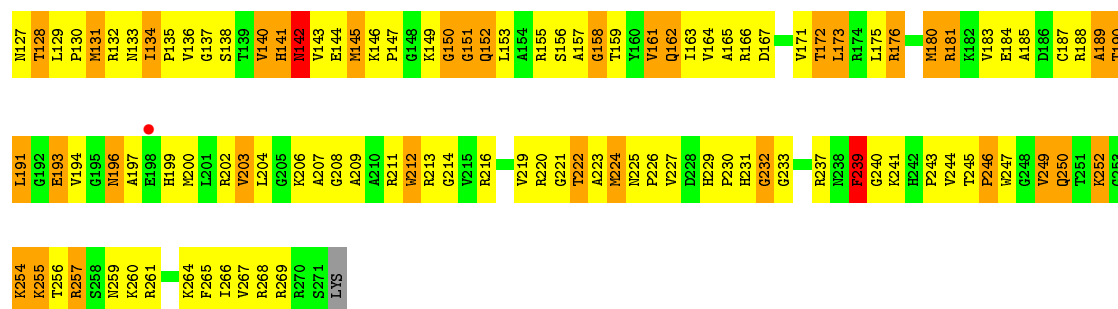


• Molecule 25: 50S ribosomal protein L2

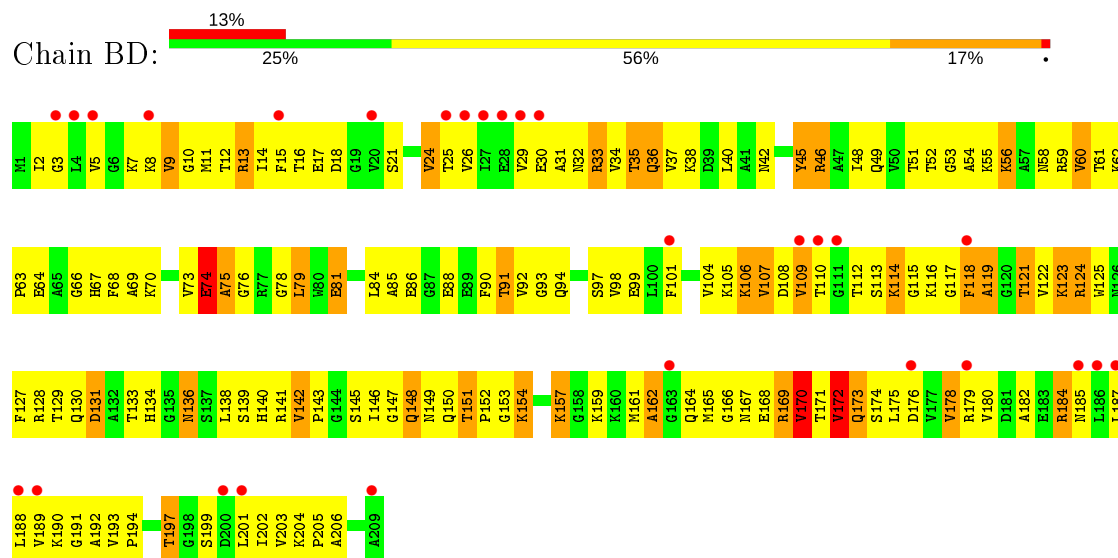


• Molecule 25: 50S ribosomal protein L2

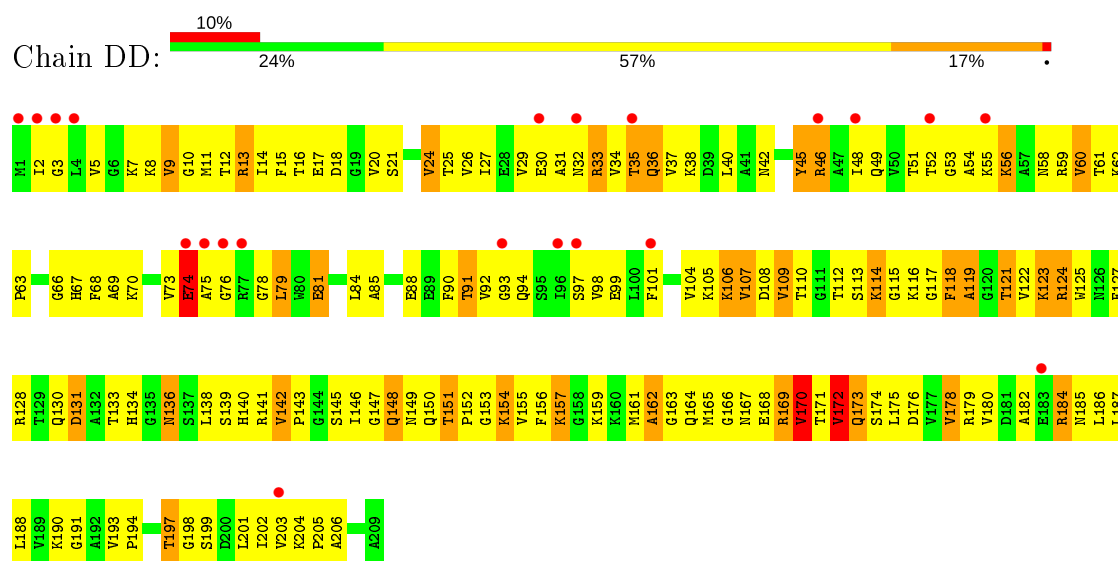




• Molecule 26: 50S ribosomal protein L3

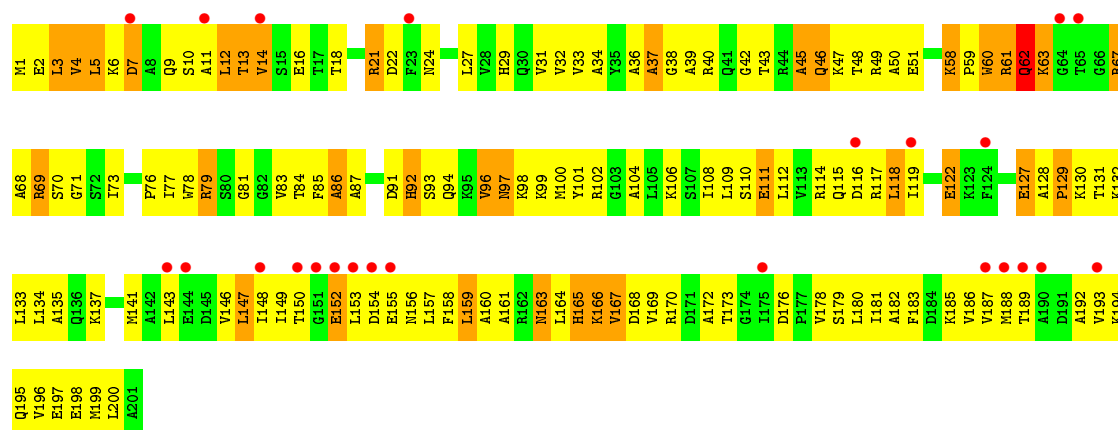


• Molecule 26: 50S ribosomal protein L3

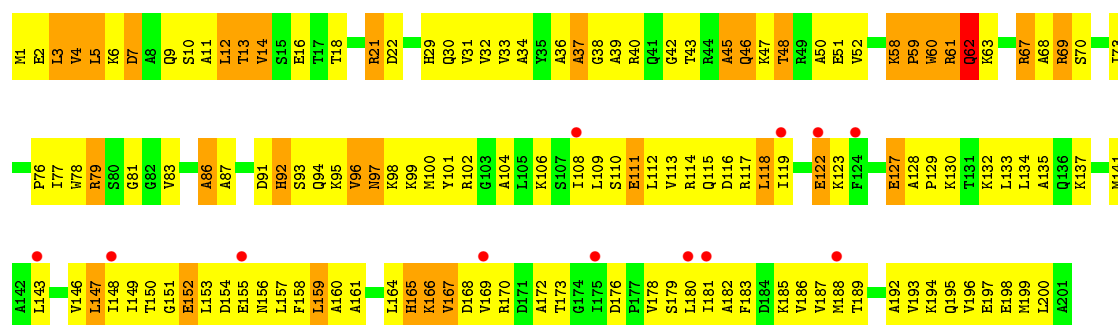


• Molecule 27: 50S ribosomal protein L4

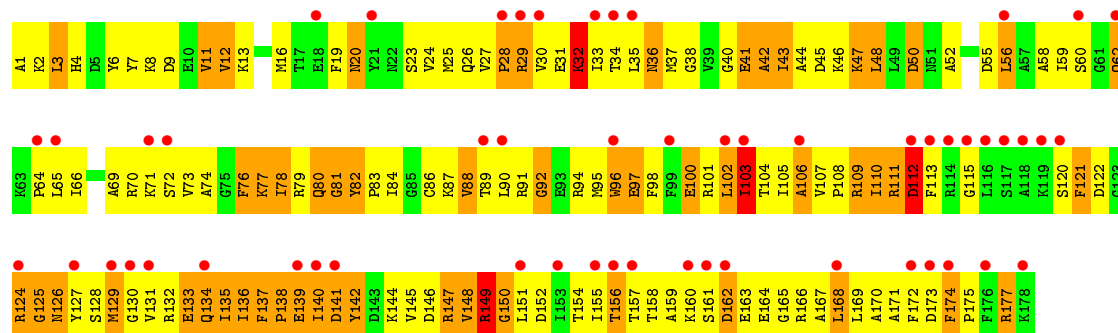
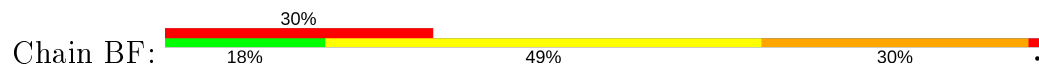




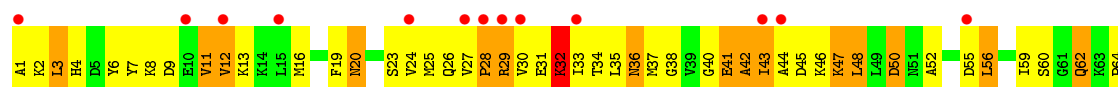
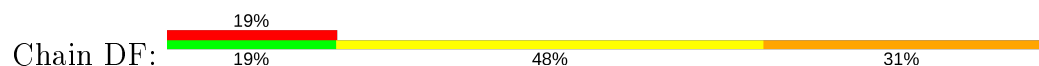
• Molecule 27: 50S ribosomal protein L4

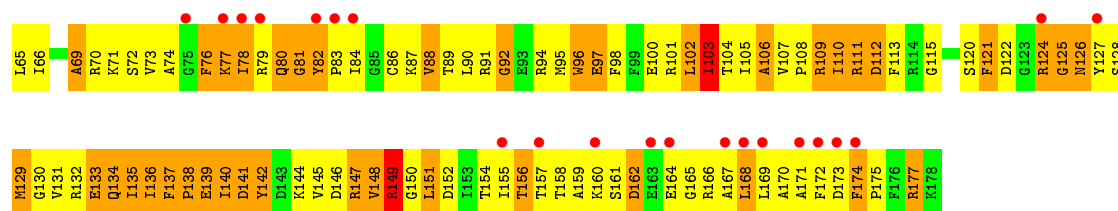


• Molecule 28: 50S ribosomal protein L5

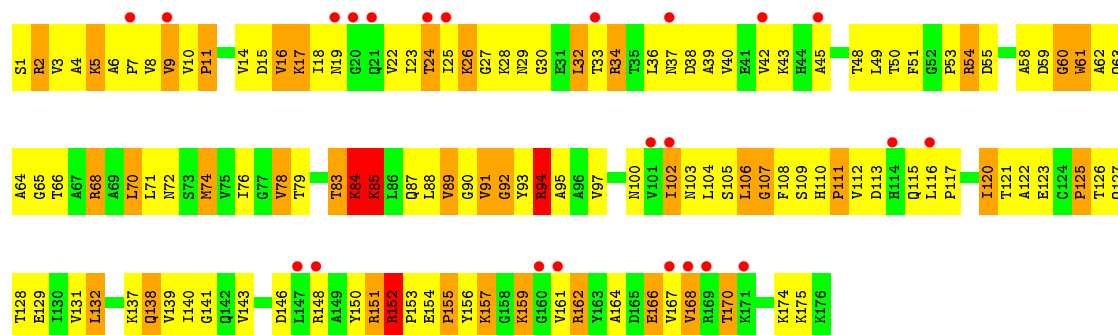


• Molecule 28: 50S ribosomal protein L5

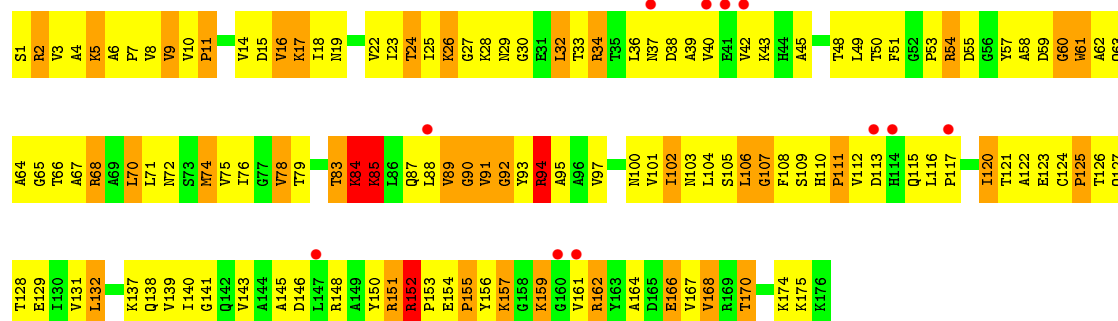




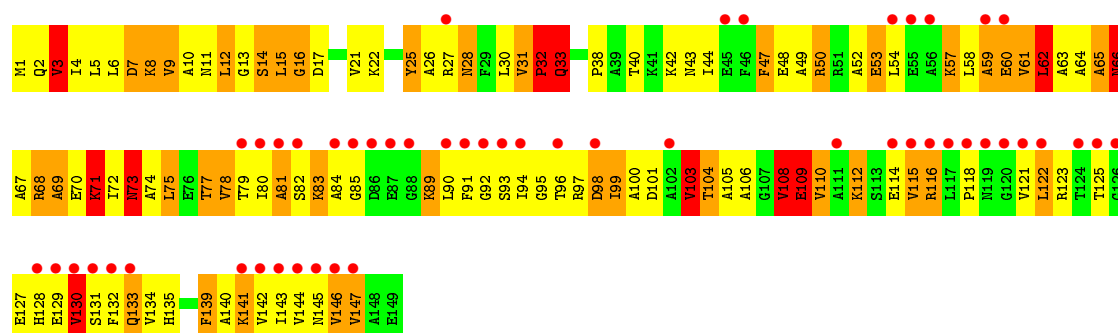
• Molecule 29: 50S ribosomal protein L6



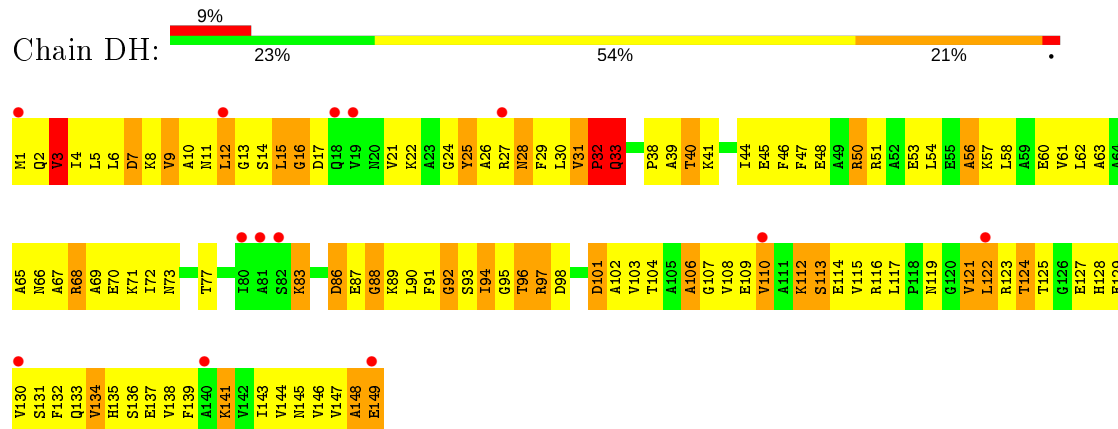
• Molecule 29: 50S ribosomal protein L6



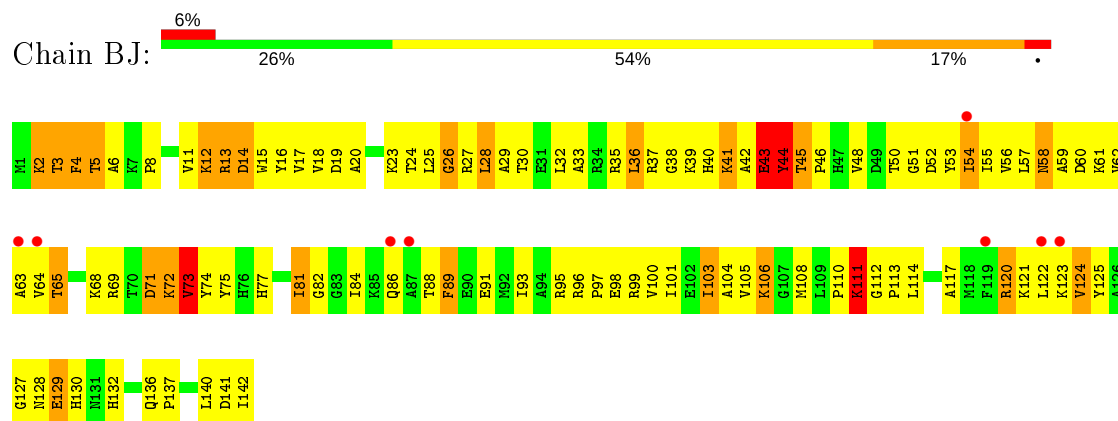
• Molecule 30: 50S ribosomal protein L9



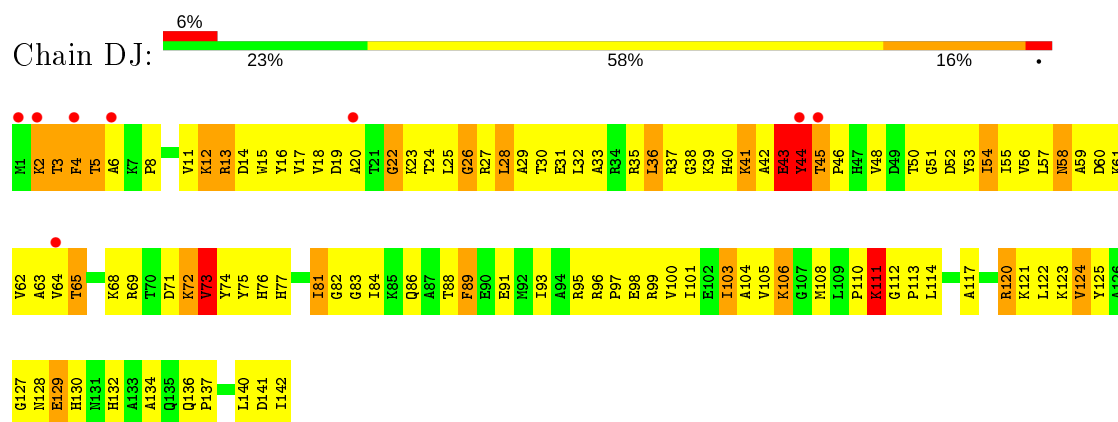
- Molecule 30: 50S ribosomal protein L9



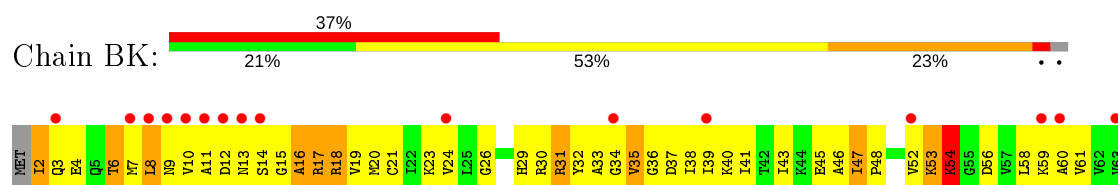
- Molecule 31: 50S ribosomal protein L13

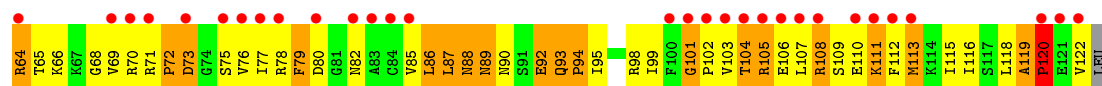


- Molecule 31: 50S ribosomal protein L13

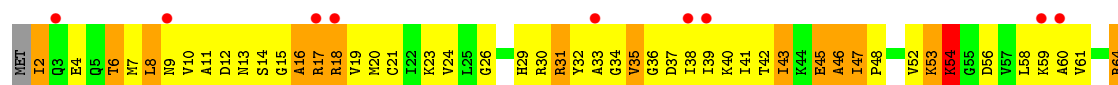


- Molecule 32: 50S ribosomal protein L14

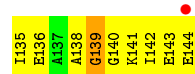
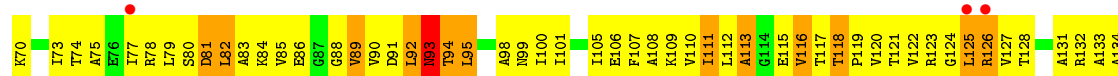
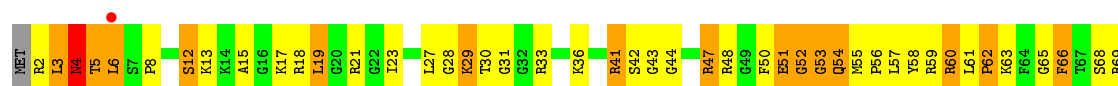




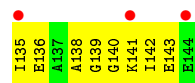
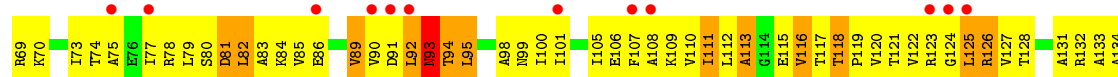
- Molecule 32: 50S ribosomal protein L14



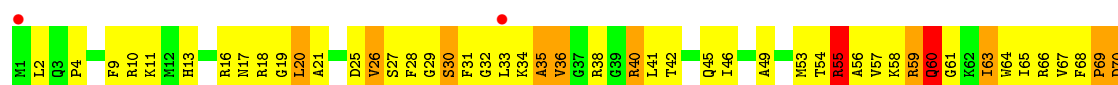
- Molecule 33: 50S ribosomal protein L15

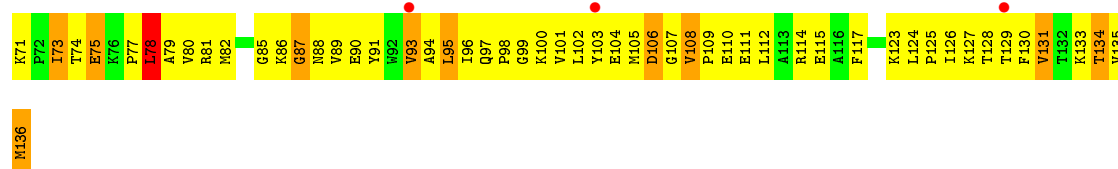


- Molecule 33: 50S ribosomal protein L15

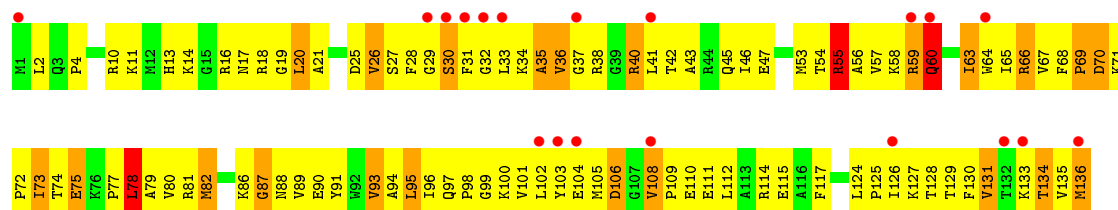


- Molecule 34: 50S ribosomal protein L16

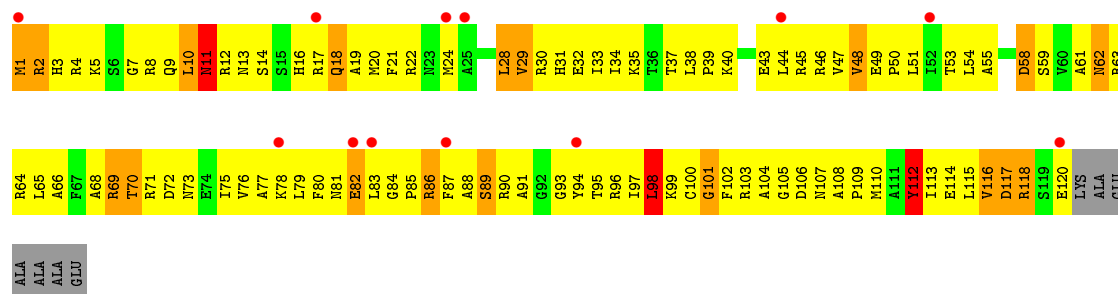




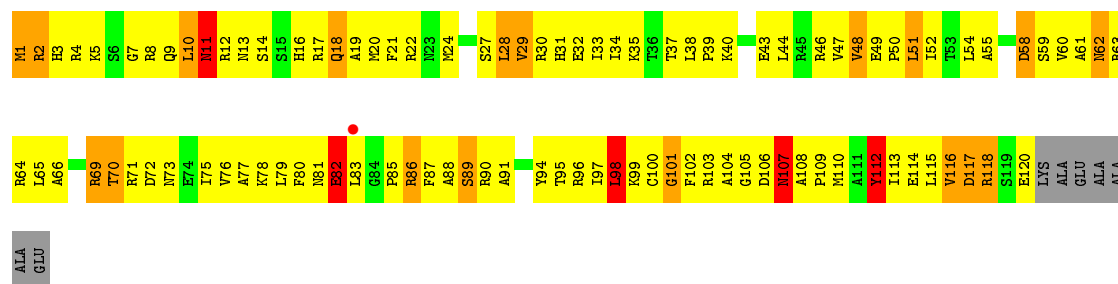
- Molecule 34: 50S ribosomal protein L16



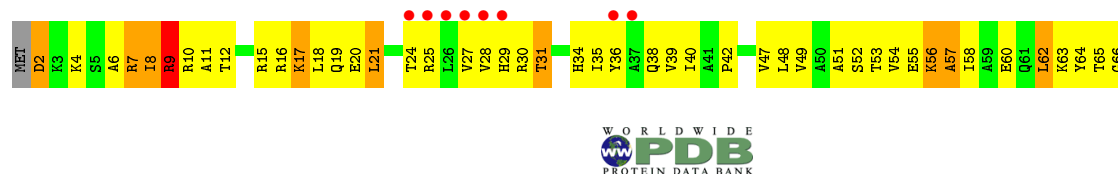
- Molecule 35: 50S ribosomal protein L17

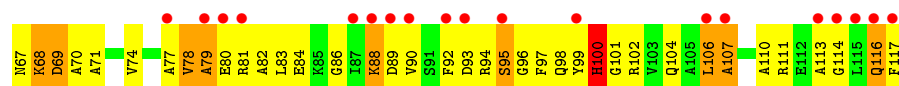


- Molecule 35: 50S ribosomal protein L17

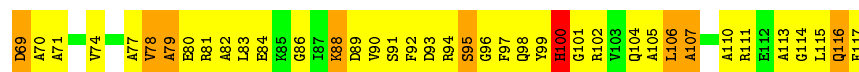
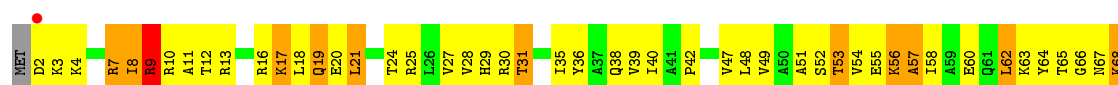


- Molecule 36: 50S ribosomal protein L18

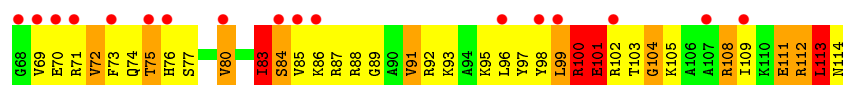




- Molecule 36: 50S ribosomal protein L18



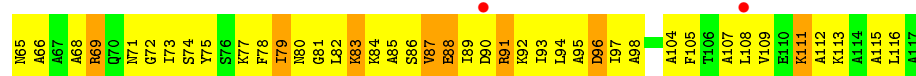
- Molecule 37: 50S ribosomal protein L19



- Molecule 37: 50S ribosomal protein L19

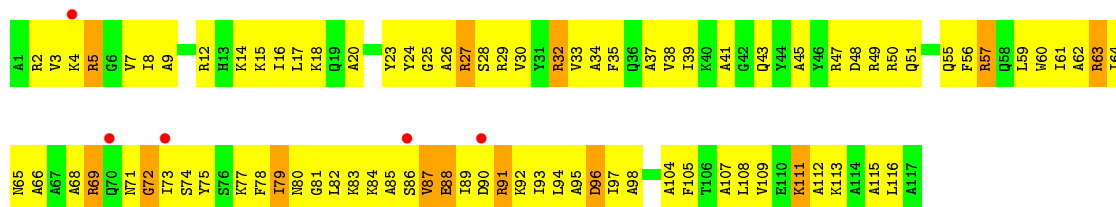


- Molecule 38: 50S ribosomal protein L20

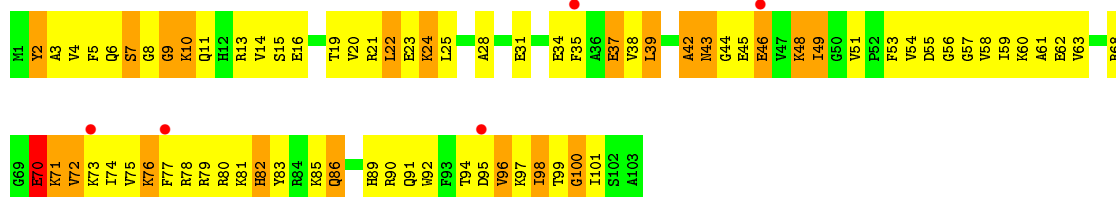


- Molecule 38: 50S ribosomal protein L20

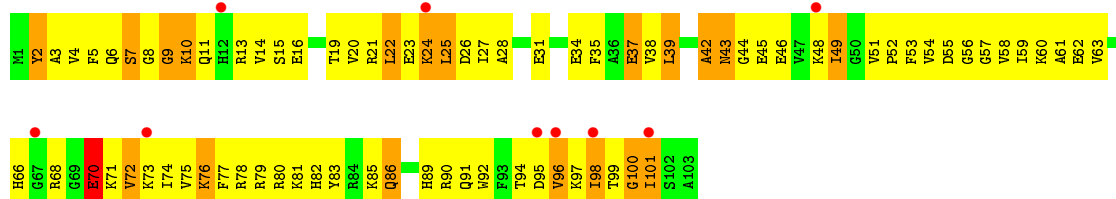




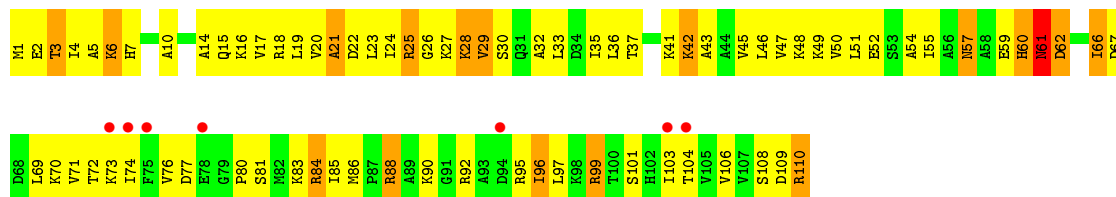
• Molecule 39: 50S ribosomal protein L21



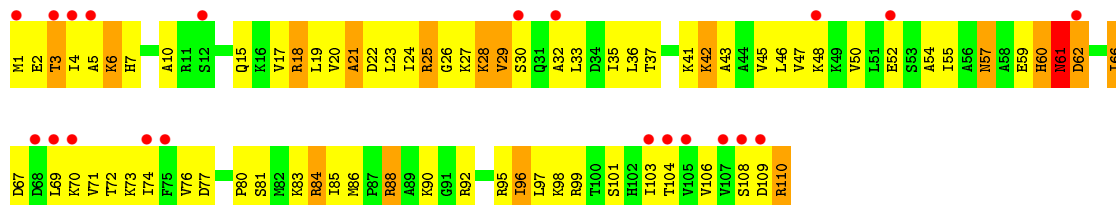
• Molecule 39: 50S ribosomal protein L21



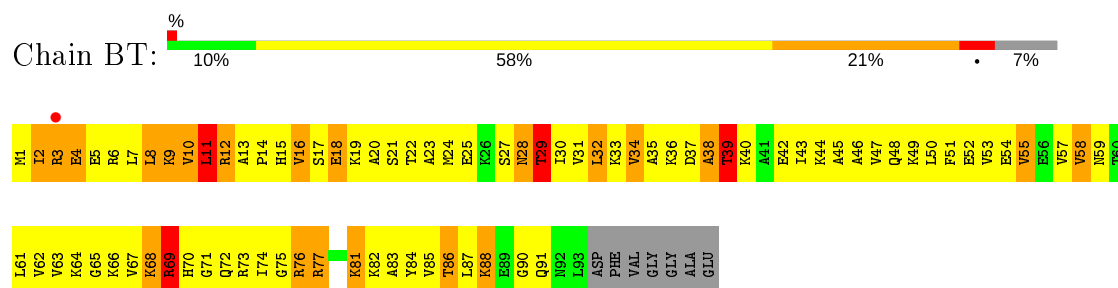
• Molecule 40: 50S ribosomal protein L22



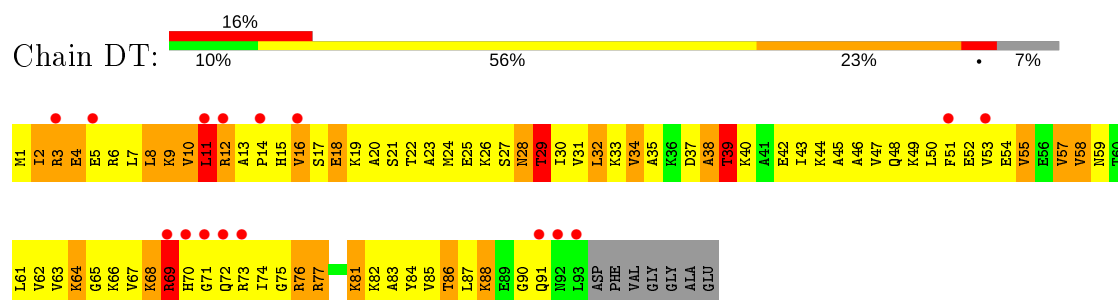
• Molecule 40: 50S ribosomal protein L22



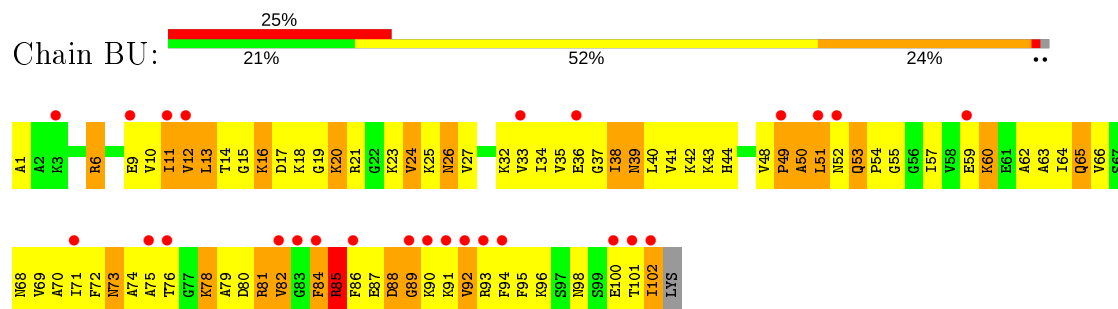
- Molecule 41: 50S ribosomal protein L23



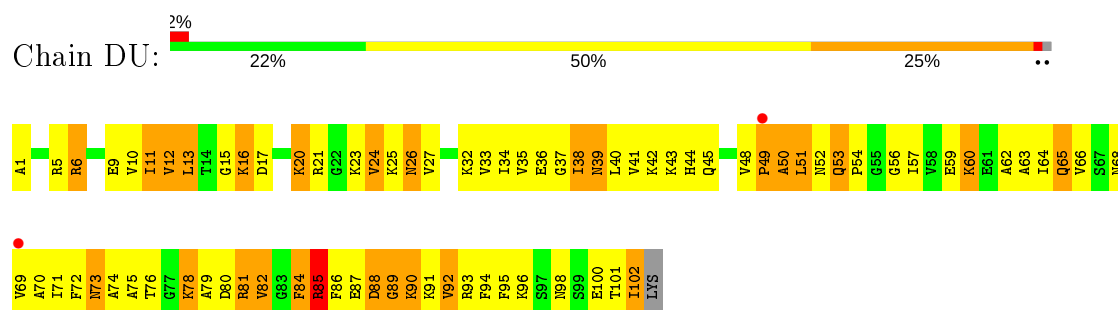
- Molecule 41: 50S ribosomal protein L23



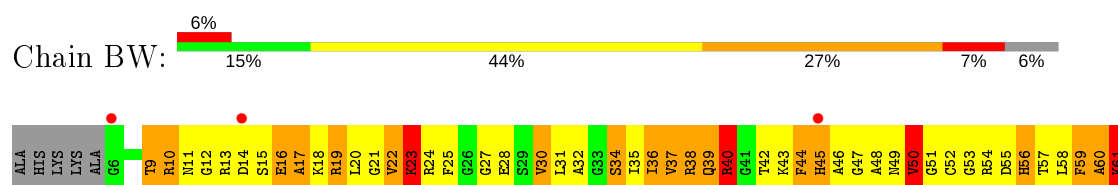
- Molecule 42: 50S ribosomal protein L24

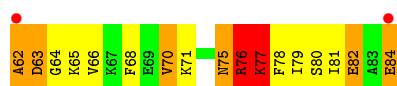


- Molecule 42: 50S ribosomal protein L24

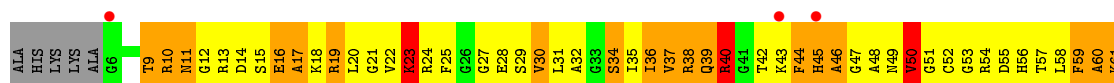
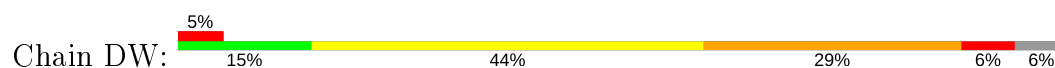


- Molecule 43: 50S ribosomal protein L27





- Molecule 43: 50S ribosomal protein L27



- Molecule 44: 50S ribosomal protein L29



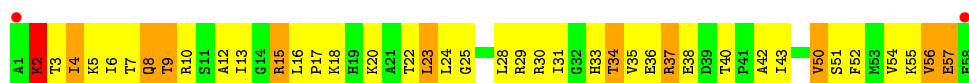
- Molecule 44: 50S ribosomal protein L29



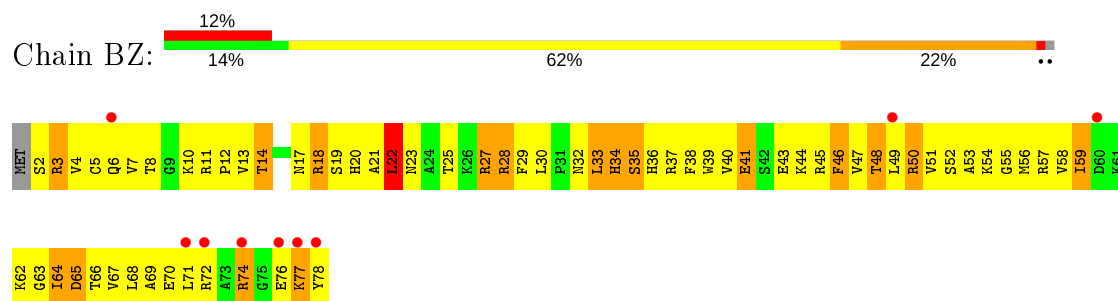
- Molecule 45: 50S ribosomal protein L30



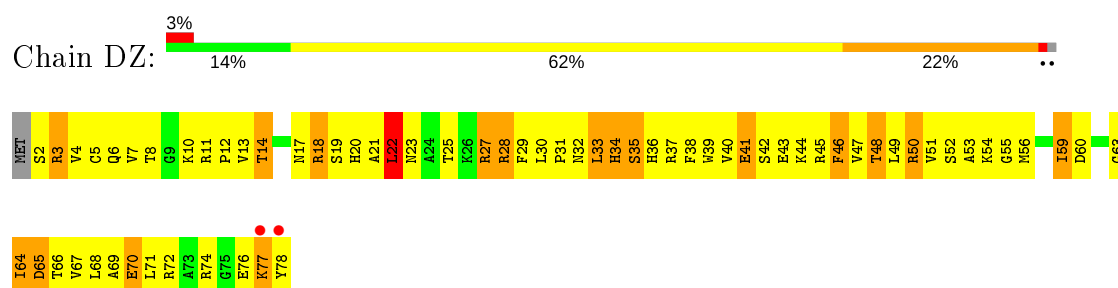
- Molecule 45: 50S ribosomal protein L30



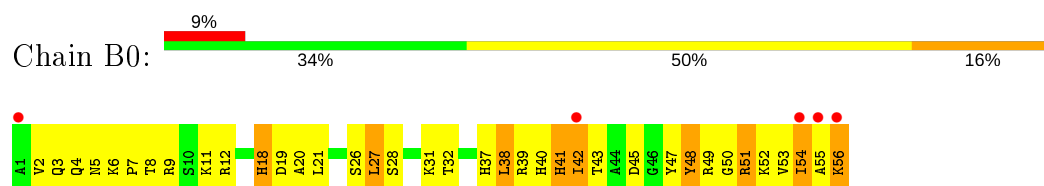
- Molecule 46: 50S ribosomal protein L28



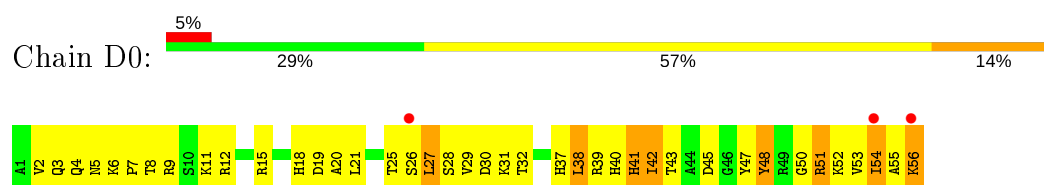
- Molecule 46: 50S ribosomal protein L28



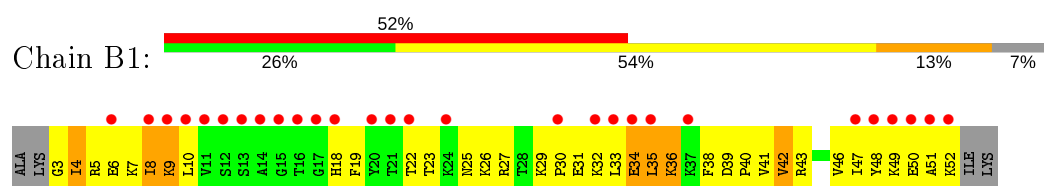
- Molecule 47: 50S ribosomal protein L32



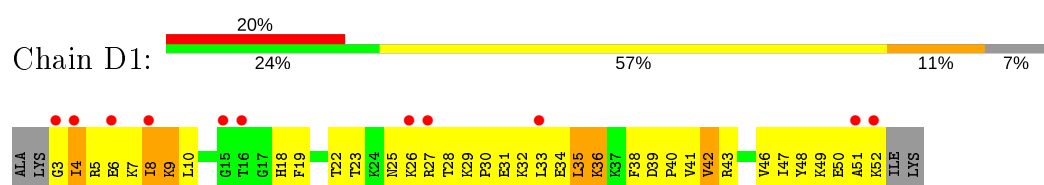
- Molecule 47: 50S ribosomal protein L32



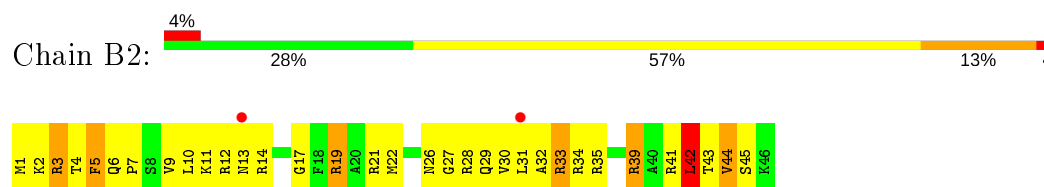
- Molecule 48: 50S ribosomal protein L33



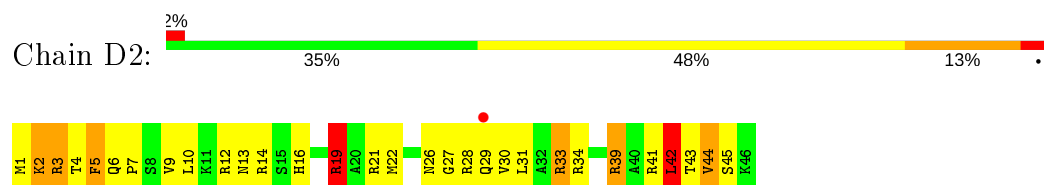
- Molecule 48: 50S ribosomal protein L33



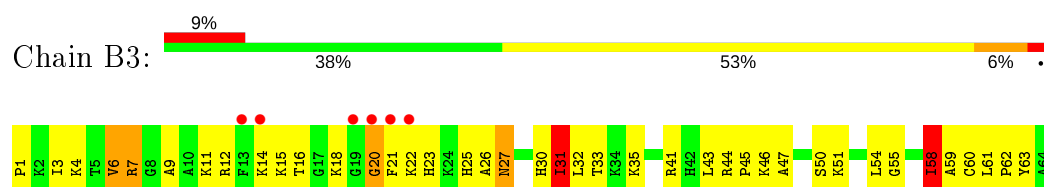
- Molecule 49: 50S ribosomal protein L34



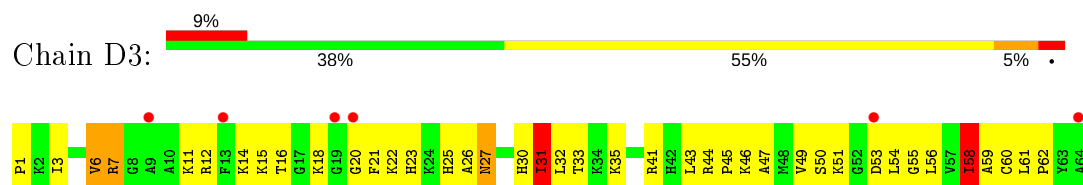
- Molecule 49: 50S ribosomal protein L34



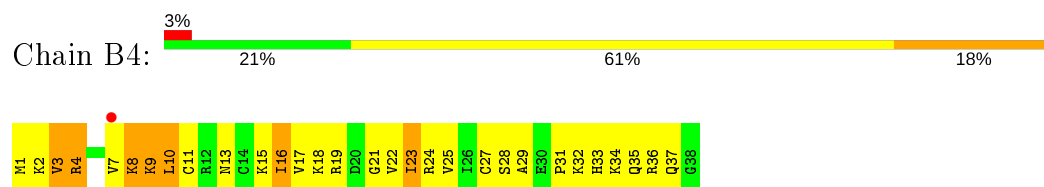
- Molecule 50: 50S ribosomal protein L35



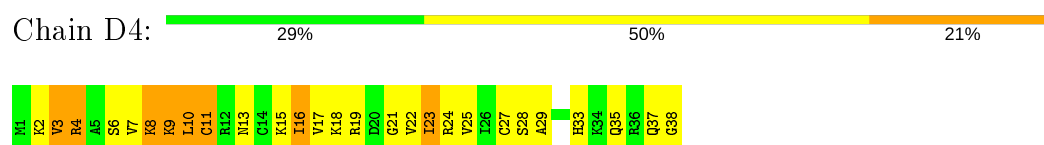
- Molecule 50: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L36

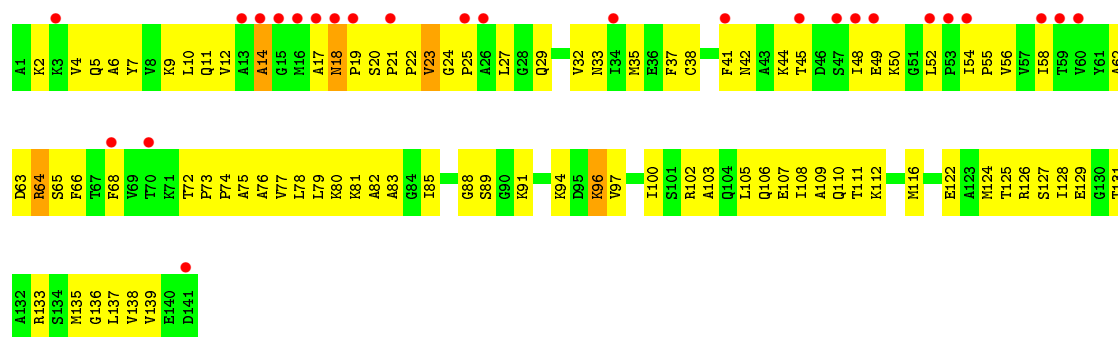


- Molecule 51: 50S ribosomal protein L36

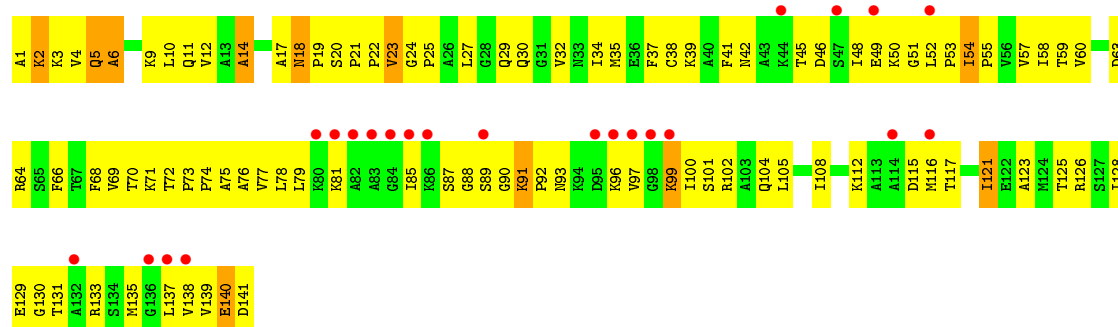


- Molecule 52: 50S ribosomal protein L11





● 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, $\alpha$ , $\beta$ , $\gamma$	208.70 Å   379.50 Å   739.30 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 3.49 Å)	Xtriage
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 <sup>2</sup> )	117.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	284077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

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%)	<a href="#">1</a> <a href="#">9</a>
2	CC	204/232 (88%)	148 (72%)	40 (20%)	16 (8%)	<a href="#">1</a> <a href="#">10</a>

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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 ⓘ

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
43	BW	38	ARG
6	CG	49	LEU
41	DT	24	MET
44	BX	28	LEU
2	CC	35	ASP

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

Mol	Chain	Res	Type
44	BX	25	GLN
6	CG	129	ASN
42	DU	26	ASN
45	BY	48	ASN
2	CC	7	ASN

### 5.3.3 RNA ⓘ

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
23	BB	2756	U
1	CA	372	C
23	DB	2282	G
23	BB	2808	G
1	CA	243	A

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	CA	2062	HYG	C3-C4-N9-C10
54	CA	2062	HYG	C5-C4-N9-C10
54	CA	2062	HYG	N36-C33-C34-O35
54	AA	2059	HYG	C5-C4-N9-C10
54	AA	2059	HYG	N36-C33-C34-O35

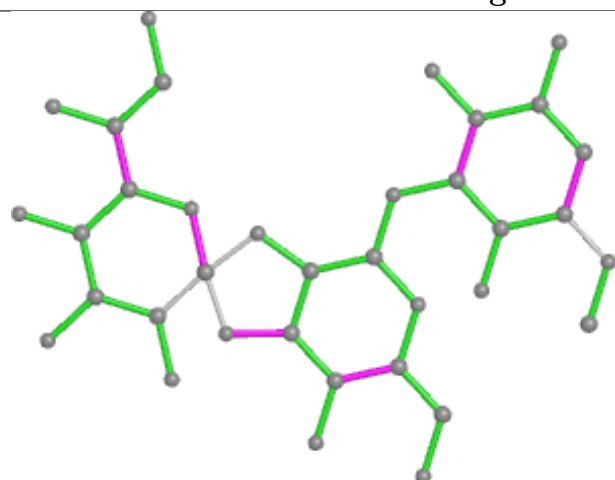
There are no ring outliers.

2 monomers are involved in 3 short contacts:

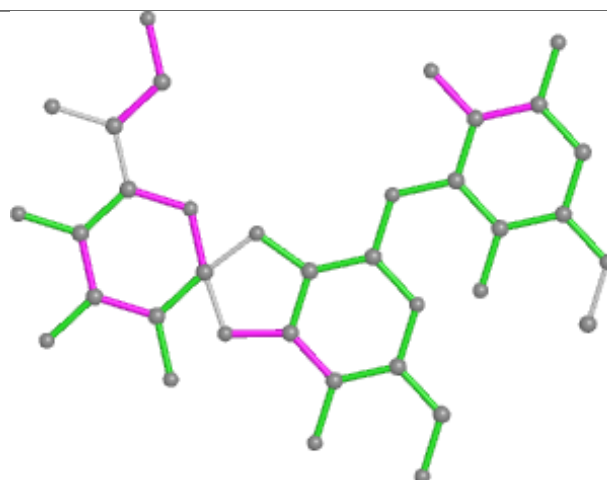
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	CA	2062	HYG	1	0
54	AA	2059	HYG	2	0

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.

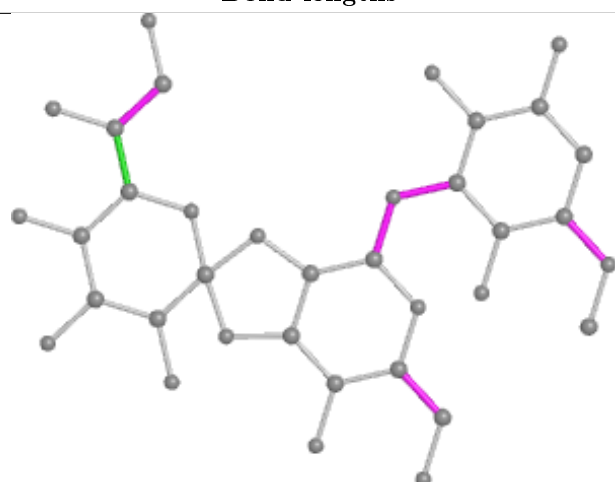
## Ligand HYG CA 2062



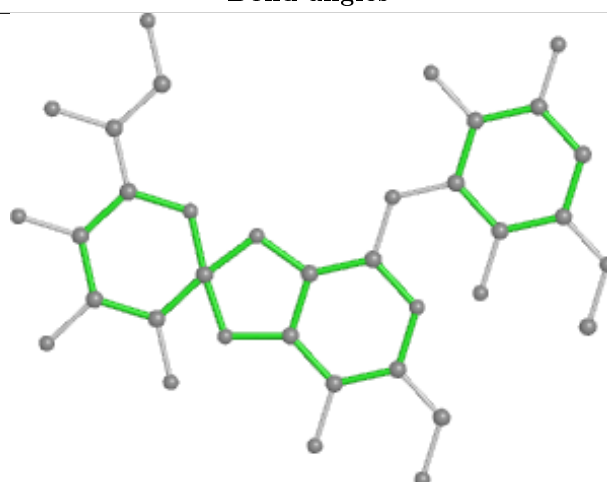
Bond lengths



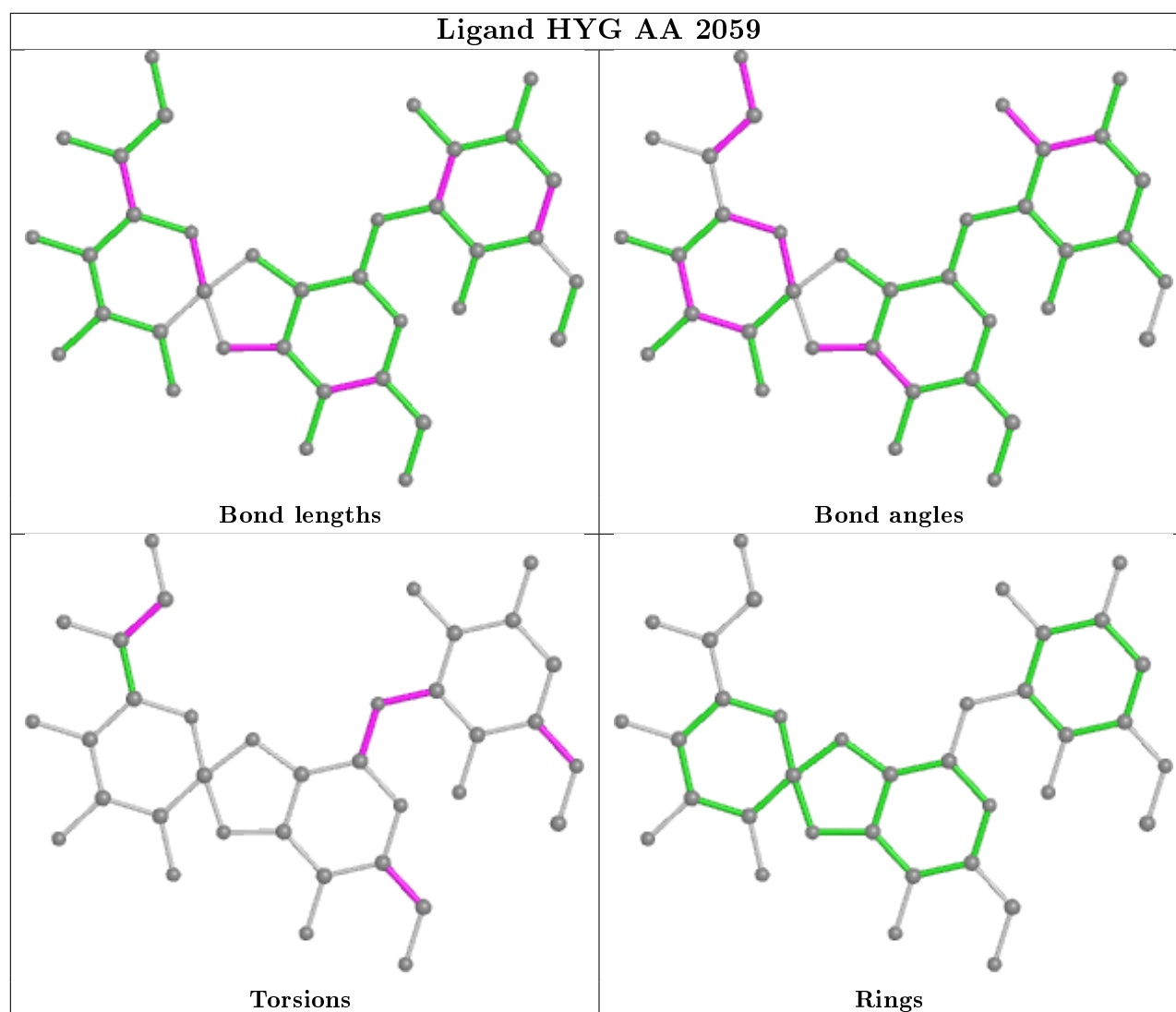
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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(Å²)	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 <sup>2</sup> )	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, 173	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 <sup>2</sup> )	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, 165	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, 67, 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 <sup>2</sup> )	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 ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	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	CA	2015	1/1	0.68	0.10	149,149,149,149	0
53	MG	AA	2014	1/1	0.68	0.22	112,112,112,112	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	BB	3100	1/1	0.72	0.20	129,129,129,129	0
53	MG	AN	201	1/1	0.72	0.12	69,69,69,69	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	AA	2019	1/1	0.78	0.06	107,107,107,107	0
53	MG	CA	2059	1/1	0.78	0.12	94,94,94,94	0
53	MG	AA	2033	1/1	0.79	0.11	99,99,99,99	0
53	MG	CA	2021	1/1	0.79	0.36	125,125,125,125	0
53	MG	AA	2056	1/1	0.79	0.12	124,124,124,124	0
53	MG	CA	2023	1/1	0.79	0.20	137,137,137,137	0
53	MG	DB	3066	1/1	0.80	0.08	146,146,146,146	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	AE	201	1/1	0.80	0.07	144,144,144,144	0
53	MG	AA	2012	1/1	0.81	0.09	84,84,84,84	0
53	MG	CA	2060	1/1	0.81	0.05	80,80,80,80	0
53	MG	AA	2018	1/1	0.81	0.09	131,131,131,131	0
53	MG	BB	3080	1/1	0.81	0.18	39,39,39,39	0
53	MG	BB	3010	1/1	0.82	0.10	44,44,44,44	0
53	MG	AA	2005	1/1	0.82	0.08	69,69,69,69	0
53	MG	CA	2026	1/1	0.83	0.20	26,26,26,26	1
53	MG	AA	2055	1/1	0.83	0.20	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	CA	2008	1/1	0.83	0.09	93,93,93,93	0
53	MG	AA	2035	1/1	0.83	0.34	137,137,137,137	0
53	MG	CA	2038	1/1	0.83	0.12	128,128,128,128	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	CE	201	1/1	0.86	0.15	127,127,127,127	0
53	MG	BB	3037	1/1	0.86	0.11	23,23,23,23	0
53	MG	AA	2050	1/1	0.87	0.14	105,105,105,105	0
53	MG	DB	3045	1/1	0.87	0.06	57,57,57,57	0
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	CA	2042	1/1	0.87	0.08	58,58,58,58	0
53	MG	AA	2024	1/1	0.87	0.08	5,5,5,5	1
53	MG	BB	3097	1/1	0.88	0.18	114,114,114,114	0
53	MG	AA	2044	1/1	0.88	0.12	112,112,112,112	0
53	MG	BB	3077	1/1	0.88	0.09	36,36,36,36	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	2026	1/1	0.89	0.08	65,65,65,65	0
53	MG	BB	3017	1/1	0.90	0.14	34,34,34,34	0
54	HYG	AA	2059	36/36	0.90	0.24	52,52,52,52	0
53	MG	DB	3023	1/1	0.90	0.08	32,32,32,32	0
53	MG	CA	2052	1/1	0.90	0.09	73,73,73,73	0
53	MG	DB	3029	1/1	0.90	0.16	88,88,88,88	0
53	MG	CA	2035	1/1	0.90	0.08	89,89,89,89	0
53	MG	BB	3071	1/1	0.90	0.09	26,26,26,26	0
53	MG	CA	2029	1/1	0.90	0.05	23,23,23,23	1
53	MG	CA	2014	1/1	0.90	0.07	47,47,47,47	0
53	MG	BB	3052	1/1	0.90	0.08	38,38,38,38	0
53	MG	AA	2030	1/1	0.90	0.09	99,99,99,99	0
53	MG	CA	2054	1/1	0.90	0.08	104,104,104,104	0
53	MG	DB	3036	1/1	0.91	0.09	30,30,30,30	0
53	MG	AA	2049	1/1	0.91	0.06	75,75,75,75	0
54	HYG	CA	2062	36/36	0.91	0.22	45,45,45,45	0
53	MG	AA	2017	1/1	0.91	0.12	87,87,87,87	0
53	MG	CA	2007	1/1	0.91	0.04	46,46,46,46	0
53	MG	AA	2051	1/1	0.91	0.10	41,41,41,41	0
53	MG	AA	2052	1/1	0.91	0.07	78,78,78,78	0
53	MG	BB	3014	1/1	0.91	0.05	50,50,50,50	0
53	MG	BB	3104	1/1	0.91	0.18	36,36,36,36	0
53	MG	DB	3092	1/1	0.91	0.13	66,66,66,66	0
53	MG	DB	3050	1/1	0.92	0.08	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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	AA	2045	1/1	0.92	0.64	92,92,92,92	0
53	MG	AA	2021	1/1	0.92	0.31	5,5,5,5	1
53	MG	AA	2004	1/1	0.92	0.14	56,56,56,56	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	3049	1/1	0.93	0.10	10,10,10,10	0
53	MG	AA	2046	1/1	0.93	0.07	5,5,5,5	0
53	MG	BB	3024	1/1	0.93	0.11	15,15,15,15	0
53	MG	BB	3093	1/1	0.93	0.24	71,71,71,71	0
53	MG	DB	3044	1/1	0.93	0.11	24,24,24,24	0
53	MG	BB	3053	1/1	0.93	0.06	28,28,28,28	0
53	MG	AA	2001	1/1	0.93	0.07	35,35,35,35	0
53	MG	DB	3058	1/1	0.93	0.33	151,151,151,151	0
53	MG	CA	2037	1/1	0.93	0.08	94,94,94,94	0
53	MG	AA	2016	1/1	0.93	0.09	89,89,89,89	0
53	MG	BB	3033	1/1	0.93	0.33	125,125,125,125	0
53	MG	BB	3046	1/1	0.93	0.11	22,22,22,22	0
53	MG	AA	2015	1/1	0.93	0.06	24,24,24,24	0
53	MG	AA	2054	1/1	0.93	0.08	110,110,110,110	0
53	MG	BB	3085	1/1	0.93	0.17	103,103,103,103	0
53	MG	BB	3031	1/1	0.93	0.14	41,41,41,41	0
53	MG	AA	2032	1/1	0.93	0.08	62,62,62,62	0
53	MG	BB	3054	1/1	0.93	0.06	77,77,77,77	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	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	3039	1/1	0.94	0.18	7,7,7,7	0
53	MG	CA	2010	1/1	0.94	0.08	33,33,33,33	0
53	MG	CA	2024	1/1	0.94	0.06	29,29,29,29	0
53	MG	BB	3057	1/1	0.94	0.19	28,28,28,28	0
53	MG	DB	3052	1/1	0.94	0.12	100,100,100,100	0
53	MG	BB	3027	1/1	0.94	0.08	33,33,33,33	0
53	MG	CA	2036	1/1	0.94	0.17	101,101,101,101	0
53	MG	AA	2002	1/1	0.94	0.06	99,99,99,99	0
53	MG	CA	2019	1/1	0.94	0.10	73,73,73,73	0
53	MG	BB	3001	1/1	0.94	0.10	51,51,51,51	0
53	MG	DB	3097	1/1	0.95	0.14	38,38,38,38	0
53	MG	DB	3046	1/1	0.95	0.09	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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	CA	2016	1/1	0.95	0.04	53,53,53,53	0
53	MG	DB	3035	1/1	0.95	0.06	55,55,55,55	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
53	MG	DB	3041	1/1	0.95	0.11	29,29,29,29	0
53	MG	DB	3072	1/1	0.95	0.12	18,18,18,18	0
53	MG	CA	2009	1/1	0.95	0.06	67,67,67,67	0
53	MG	DB	3005	1/1	0.95	0.12	10,10,10,10	0
53	MG	BB	3063	1/1	0.95	0.09	11,11,11,11	0
53	MG	DB	3074	1/1	0.95	0.09	12,12,12,12	0
53	MG	BB	3102	1/1	0.95	0.12	20,20,20,20	0
53	MG	CA	2047	1/1	0.95	0.06	121,121,121,121	0
53	MG	AA	2029	1/1	0.95	0.06	39,39,39,39	0
53	MG	BB	3088	1/1	0.95	0.06	28,28,28,28	0
53	MG	BB	3045	1/1	0.95	0.10	31,31,31,31	0
53	MG	DB	3073	1/1	0.95	0.10	14,14,14,14	0
53	MG	BB	3008	1/1	0.95	0.10	89,89,89,89	0
53	MG	BB	3047	1/1	0.95	0.06	75,75,75,75	0
53	MG	AA	2028	1/1	0.95	0.17	100,100,100,100	0
53	MG	AA	2007	1/1	0.95	0.06	31,31,31,31	0
53	MG	CA	2043	1/1	0.95	0.04	19,19,19,19	0
53	MG	DB	3110	1/1	0.95	0.14	21,21,21,21	0
53	MG	DB	3080	1/1	0.95	0.10	10,10,10,10	0
53	MG	BB	3061	1/1	0.95	0.04	48,48,48,48	0
53	MG	BB	3064	1/1	0.95	0.08	35,35,35,35	0
53	MG	BB	3036	1/1	0.95	0.11	42,42,42,42	0
53	MG	AA	2006	1/1	0.95	0.03	60,60,60,60	0
53	MG	DB	3003	1/1	0.96	0.19	63,63,63,63	0
53	MG	BB	3016	1/1	0.96	0.07	38,38,38,38	0
53	MG	CA	2048	1/1	0.96	0.11	58,58,58,58	0
53	MG	CA	2040	1/1	0.96	0.09	48,48,48,48	0
53	MG	BB	3068	1/1	0.96	0.12	53,53,53,53	0
53	MG	DB	3108	1/1	0.96	0.09	37,37,37,37	0
53	MG	AA	2042	1/1	0.96	0.09	69,69,69,69	0
53	MG	AA	2039	1/1	0.96	0.12	64,64,64,64	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	AA	2009	1/1	0.96	0.10	7,7,7,7	0
53	MG	DB	3026	1/1	0.96	0.08	34,34,34,34	0
53	MG	DB	3071	1/1	0.96	0.06	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	DB	3032	1/1	0.96	0.09	63,63,63,63	0
53	MG	BB	3078	1/1	0.96	0.15	70,70,70,70	0
53	MG	DB	3057	1/1	0.96	0.06	71,71,71,71	0
53	MG	BB	3098	1/1	0.96	0.15	35,35,35,35	0
53	MG	BB	3038	1/1	0.96	0.03	71,71,71,71	0
53	MG	DB	3021	1/1	0.96	0.23	11,11,11,11	0
53	MG	DB	3111	1/1	0.96	0.09	38,38,38,38	0
53	MG	BB	3034	1/1	0.96	0.10	35,35,35,35	0
53	MG	CA	2020	1/1	0.96	0.21	73,73,73,73	0
53	MG	DB	3047	1/1	0.96	0.17	14,14,14,14	0
53	MG	BB	3087	1/1	0.96	0.16	57,57,57,57	0
53	MG	AA	2041	1/1	0.96	0.07	83,83,83,83	0
53	MG	DB	3011	1/1	0.96	0.16	17,17,17,17	0
53	MG	BB	3003	1/1	0.96	0.07	32,32,32,32	0
53	MG	CA	2025	1/1	0.96	0.12	50,50,50,50	0
53	MG	BB	3021	1/1	0.96	0.08	30,30,30,30	0
53	MG	DB	3093	1/1	0.96	0.22	11,11,11,11	0
53	MG	BB	3056	1/1	0.96	0.08	26,26,26,26	0
53	MG	DB	3034	1/1	0.96	0.16	52,52,52,52	0
53	MG	CA	2041	1/1	0.96	0.05	46,46,46,46	0
53	MG	DB	3054	1/1	0.96	0.04	19,19,19,19	0
53	MG	BB	3109	1/1	0.96	0.09	54,54,54,54	0
53	MG	AA	2038	1/1	0.96	0.11	71,71,71,71	0
53	MG	AA	2058	1/1	0.96	0.14	86,86,86,86	0
53	MG	BB	3082	1/1	0.96	0.16	46,46,46,46	0
53	MG	AA	2011	1/1	0.97	0.07	85,85,85,85	0
53	MG	DB	3025	1/1	0.97	0.15	5,5,5,5	0
53	MG	BB	3075	1/1	0.97	0.21	40,40,40,40	0
53	MG	CA	2005	1/1	0.97	0.09	24,24,24,24	0
53	MG	AA	2040	1/1	0.97	0.10	83,83,83,83	0
53	MG	DB	3070	1/1	0.97	0.08	45,45,45,45	0
53	MG	CA	2034	1/1	0.97	0.11	6,6,6,6	0
53	MG	BB	3029	1/1	0.97	0.07	14,14,14,14	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	BB	3062	1/1	0.97	0.17	14,14,14,14	0
53	MG	CA	2004	1/1	0.97	0.09	8,8,8,8	0
53	MG	BB	3069	1/1	0.97	0.11	17,17,17,17	0
53	MG	DB	3086	1/1	0.97	0.15	11,11,11,11	0
53	MG	DB	3033	1/1	0.97	0.08	9,9,9,9	0
53	MG	BB	3043	1/1	0.97	0.05	104,104,104,104	0
53	MG	AA	2034	1/1	0.97	0.06	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	BB	3009	1/1	0.97	0.04	46,46,46,46	0
53	MG	BB	3035	1/1	0.97	0.07	15,15,15,15	0
53	MG	DB	3109	1/1	0.97	0.10	9,9,9,9	0
53	MG	DB	3102	1/1	0.97	0.09	12,12,12,12	0
53	MG	DB	3082	1/1	0.97	0.10	30,30,30,30	0
53	MG	BB	3058	1/1	0.97	0.10	22,22,22,22	0
53	MG	DB	3100	1/1	0.97	0.16	13,13,13,13	0
53	MG	DB	3088	1/1	0.97	0.14	25,25,25,25	0
53	MG	DB	3022	1/1	0.97	0.08	25,25,25,25	0
53	MG	BB	3026	1/1	0.97	0.08	39,39,39,39	0
53	MG	AA	2043	1/1	0.97	0.08	96,96,96,96	0
53	MG	BB	3090	1/1	0.97	0.12	112,112,112,112	0
55	ZN	B4	101	1/1	0.97	0.04	80,80,80,80	0
53	MG	DB	3087	1/1	0.97	0.15	53,53,53,53	0
53	MG	CA	2061	1/1	0.97	0.08	23,23,23,23	0
53	MG	BB	3023	1/1	0.97	0.14	5,5,5,5	0
53	MG	DB	3055	1/1	0.97	0.11	26,26,26,26	0
53	MG	AA	2010	1/1	0.97	0.04	60,60,60,60	0
53	MG	DB	3094	1/1	0.97	0.03	29,29,29,29	0
53	MG	DB	3078	1/1	0.97	0.08	27,27,27,27	0
53	MG	CA	2046	1/1	0.97	0.09	57,57,57,57	0
53	MG	BB	3013	1/1	0.97	0.10	43,43,43,43	0
53	MG	BB	3005	1/1	0.97	0.19	5,5,5,5	0
53	MG	AA	2036	1/1	0.97	0.04	31,31,31,31	0
53	MG	BB	3004	1/1	0.97	0.06	32,32,32,32	0
53	MG	DB	3010	1/1	0.97	0.08	8,8,8,8	0
53	MG	BB	3065	1/1	0.97	0.06	29,29,29,29	0
53	MG	DB	3009	1/1	0.97	0.07	29,29,29,29	0
53	MG	DB	3038	1/1	0.97	0.12	5,5,5,5	0
53	MG	DB	3007	1/1	0.97	0.14	18,18,18,18	0
53	MG	DB	3061	1/1	0.97	0.09	69,69,69,69	0
53	MG	CA	2022	1/1	0.97	0.10	63,63,63,63	0
53	MG	DB	3028	1/1	0.97	0.06	24,24,24,24	0
53	MG	BB	3060	1/1	0.97	0.13	19,19,19,19	0
53	MG	BB	3074	1/1	0.97	0.07	28,28,28,28	0
53	MG	DB	3039	1/1	0.97	0.04	22,22,22,22	0
53	MG	BB	3096	1/1	0.97	0.11	34,34,34,34	0
53	MG	DB	3030	1/1	0.97	0.17	6,6,6,6	0
53	MG	BB	3066	1/1	0.97	0.12	23,23,23,23	0
53	MG	BB	3091	1/1	0.97	0.09	16,16,16,16	0
53	MG	AA	2027	1/1	0.97	0.09	36,36,36,36	0
53	MG	DB	3056	1/1	0.97	0.09	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	BB	3040	1/1	0.98	0.18	26,26,26,26	0
53	MG	BB	3079	1/1	0.98	0.04	19,19,19,19	0
53	MG	DB	3063	1/1	0.98	0.12	43,43,43,43	0
53	MG	CA	2056	1/1	0.98	0.05	5,5,5,5	0
53	MG	DB	3089	1/1	0.98	0.17	7,7,7,7	0
53	MG	BB	3028	1/1	0.98	0.20	86,86,86,86	0
53	MG	DB	3043	1/1	0.98	0.11	5,5,5,5	0
53	MG	BB	3105	1/1	0.98	0.08	20,20,20,20	0
53	MG	BB	3101	1/1	0.98	0.09	24,24,24,24	0
53	MG	BB	3025	1/1	0.98	0.13	30,30,30,30	0
53	MG	DB	3049	1/1	0.98	0.09	36,36,36,36	0
53	MG	DB	3031	1/1	0.98	0.18	8,8,8,8	0
53	MG	BB	3086	1/1	0.98	0.26	42,42,42,42	0
53	MG	DB	3069	1/1	0.98	0.18	11,11,11,11	0
55	ZN	D4	101	1/1	0.98	0.06	46,46,46,46	0
53	MG	CA	2013	1/1	0.98	0.08	73,73,73,73	0
53	MG	DB	3040	1/1	0.98	0.16	5,5,5,5	0
53	MG	DB	3104	1/1	0.98	0.08	33,33,33,33	0
53	MG	DB	3042	1/1	0.98	0.10	6,6,6,6	0
53	MG	CA	2032	1/1	0.98	0.17	33,33,33,33	0
53	MG	BB	3012	1/1	0.98	0.09	32,32,32,32	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	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	DB	3008	1/1	0.98	0.18	6,6,6,6	0
53	MG	BB	3108	1/1	0.98	0.10	47,47,47,47	0
53	MG	DB	3004	1/1	0.98	0.11	6,6,6,6	0
53	MG	DB	3065	1/1	0.98	0.05	37,37,37,37	0
53	MG	DB	3017	1/1	0.98	0.10	13,13,13,13	0
53	MG	DB	3075	1/1	0.98	0.10	57,57,57,57	0
53	MG	BB	3103	1/1	0.98	0.08	5,5,5,5	0
53	MG	CA	2017	1/1	0.98	0.11	5,5,5,5	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	3094	1/1	0.98	0.07	28,28,28,28	0
53	MG	AA	2053	1/1	0.98	0.07	79,79,79,79	0
53	MG	DB	3051	1/1	0.98	0.19	23,23,23,23	0
53	MG	DB	3107	1/1	0.98	0.07	10,10,10,10	0
53	MG	CA	2045	1/1	0.98	0.16	48,48,48,48	0
53	MG	BB	3059	1/1	0.98	0.12	26,26,26,26	0
53	MG	CA	2055	1/1	0.98	0.07	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	DB	3064	1/1	0.98	0.05	20,20,20,20	0
53	MG	BB	3089	1/1	0.98	0.15	56,56,56,56	0
53	MG	DB	3106	1/1	0.98	0.13	23,23,23,23	0
53	MG	DB	3024	1/1	0.98	0.13	63,63,63,63	0
53	MG	CA	2006	1/1	0.98	0.05	95,95,95,95	0
53	MG	CA	2039	1/1	0.98	0.12	16,16,16,16	0
53	MG	BB	3011	1/1	0.98	0.19	5,5,5,5	0
53	MG	DB	3079	1/1	0.98	0.14	28,28,28,28	0
53	MG	DB	3062	1/1	0.98	0.04	77,77,77,77	0
53	MG	DB	3027	1/1	0.98	0.15	6,6,6,6	0
53	MG	CA	2001	1/1	0.98	0.05	5,5,5,5	0
53	MG	DB	3006	1/1	0.98	0.10	5,5,5,5	0
53	MG	DB	3083	1/1	0.98	0.16	85,85,85,85	0
53	MG	AA	2020	1/1	0.98	0.07	5,5,5,5	0
53	MG	DB	3016	1/1	0.98	0.05	15,15,15,15	0
53	MG	DB	3048	1/1	0.98	0.12	28,28,28,28	0
53	MG	DB	3037	1/1	0.98	0.16	28,28,28,28	0
53	MG	BB	3072	1/1	0.98	0.12	17,17,17,17	0
53	MG	DB	3068	1/1	0.98	0.10	5,5,5,5	0
53	MG	DB	3077	1/1	0.98	0.21	54,54,54,54	0
53	MG	DB	3099	1/1	0.98	0.19	7,7,7,7	0
53	MG	BB	3022	1/1	0.98	0.26	34,34,34,34	0
53	MG	CA	2030	1/1	0.98	0.12	7,7,7,7	0
53	MG	DB	3096	1/1	0.98	0.12	6,6,6,6	0
53	MG	BB	3067	1/1	0.98	0.09	44,44,44,44	0
53	MG	BB	3084	1/1	0.98	0.16	24,24,24,24	0
53	MG	BB	3019	1/1	0.98	0.05	22,22,22,22	0
53	MG	DB	3067	1/1	0.98	0.07	5,5,5,5	0
53	MG	DB	3084	1/1	0.98	0.17	5,5,5,5	0
53	MG	AA	2003	1/1	0.99	0.17	39,39,39,39	0
53	MG	CA	2018	1/1	0.99	0.03	6,6,6,6	0
53	MG	DB	3076	1/1	0.99	0.10	5,5,5,5	0
53	MG	DB	3020	1/1	0.99	0.15	5,5,5,5	0
53	MG	CA	2050	1/1	0.99	0.11	8,8,8,8	0
53	MG	BB	3092	1/1	0.99	0.06	54,54,54,54	0
53	MG	DB	3098	1/1	0.99	0.22	44,44,44,44	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	BB	3050	1/1	0.99	0.12	28,28,28,28	0
53	MG	BB	3110	1/1	0.99	0.15	23,23,23,23	0
53	MG	BB	3015	1/1	0.99	0.09	13,13,13,13	0
53	MG	DB	3014	1/1	0.99	0.05	5,5,5,5	0

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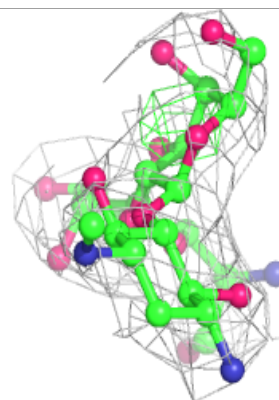
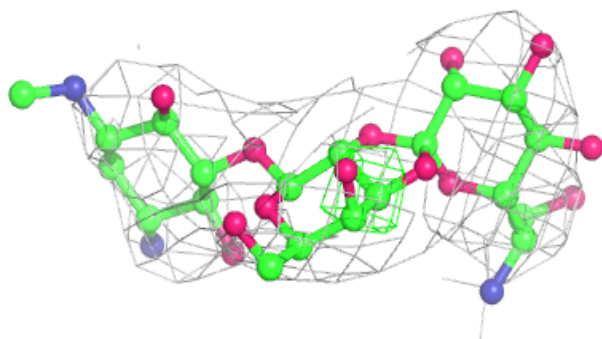
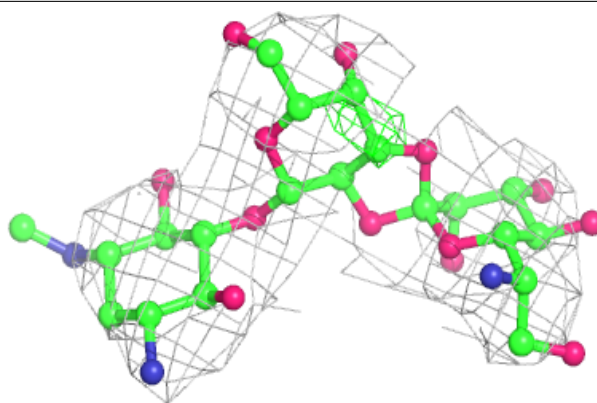
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	CA	2031	1/1	0.99	0.06	28,28,28,28	0
53	MG	CA	2053	1/1	0.99	0.06	30,30,30,30	0
53	MG	DB	3053	1/1	0.99	0.07	35,35,35,35	0
53	MG	BB	3076	1/1	0.99	0.05	38,38,38,38	0
53	MG	CA	2003	1/1	0.99	0.04	35,35,35,35	0
53	MG	BB	3106	1/1	0.99	0.12	62,62,62,62	0
53	MG	DB	3001	1/1	0.99	0.10	5,5,5,5	0
53	MG	BB	3041	1/1	0.99	0.08	7,7,7,7	0
53	MG	DB	3085	1/1	0.99	0.12	5,5,5,5	0
53	MG	BB	3002	1/1	0.99	0.07	5,5,5,5	0
53	MG	BB	3107	1/1	0.99	0.11	6,6,6,6	0
53	MG	DB	3091	1/1	0.99	0.18	13,13,13,13	0
53	MG	DB	3012	1/1	0.99	0.20	9,9,9,9	0
53	MG	BB	3030	1/1	0.99	0.03	35,35,35,35	0
53	MG	CA	2012	1/1	0.99	0.08	93,93,93,93	0
53	MG	DB	3019	1/1	0.99	0.09	5,5,5,5	0
53	MG	DB	3018	1/1	0.99	0.07	22,22,22,22	0
53	MG	BB	3007	1/1	0.99	0.14	82,82,82,82	0
53	MG	DB	3101	1/1	0.99	0.20	5,5,5,5	0
53	MG	BB	3018	1/1	0.99	0.14	32,32,32,32	0
53	MG	CA	2002	1/1	1.00	0.11	5,5,5,5	0

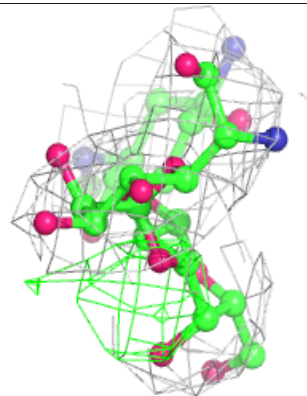
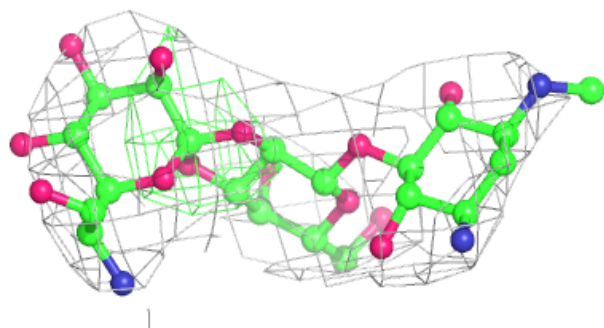
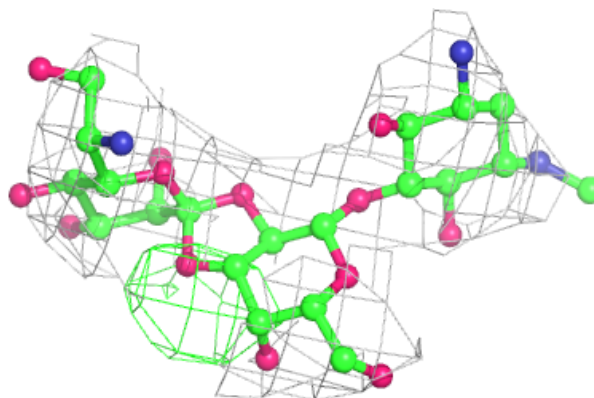
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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