



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 05:22 PM EST

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 : unknown
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

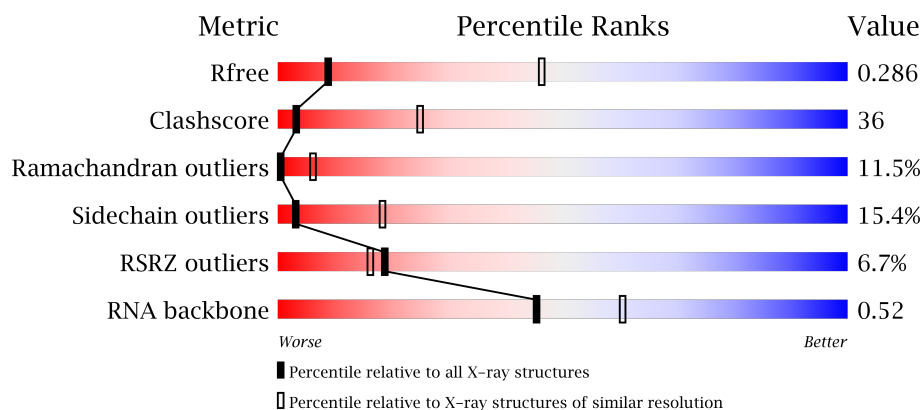
1 Overall quality at a glance

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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)
RNA backbone	2435	1024 (4.10-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>.</div> </div>
2	CC	232	<div> <div>7%</div> <div>31%</div> <div>44%</div> <div>13%</div> <div>11%</div> <div>.</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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	AA	2023	-	-	-	X
53	MG	BB	3086	-	-	-	X
53	MG	BB	3097	-	-	-	X
53	MG	CA	2020	-	-	-	X
53	MG	CA	2045	-	-	-	X
54	HYG	CA	2062	-	-	-	X

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			

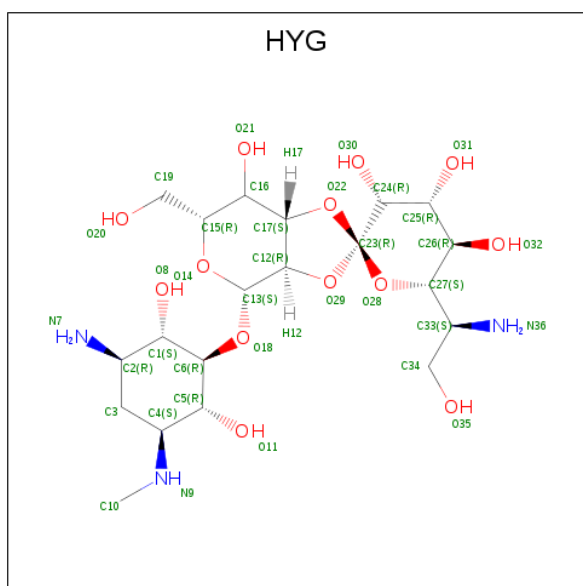
- Molecule 52 is a protein called 50S ribosomal protein L11.

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: $C_{20}H_{37}N_3O_{13}$).



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

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

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

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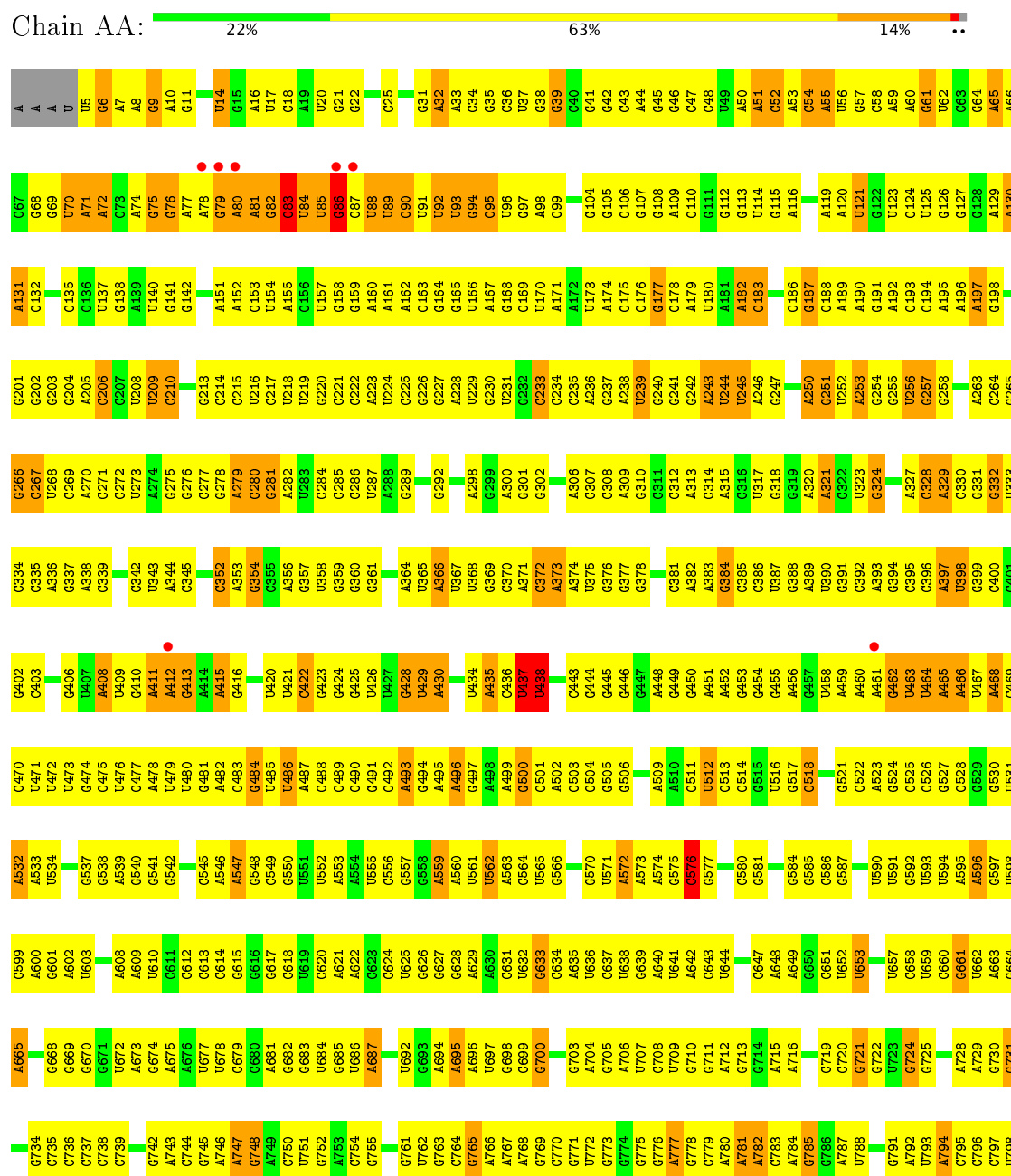
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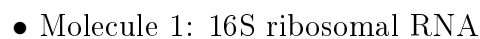
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CN	3	Total 3	O 3	0	0
56	CT	1	Total 1	O 1	0	0
56	DB	499	Total 499	O 499	0	0
56	DC	5	Total 5	O 5	0	0
56	DD	1	Total 1	O 1	0	0
56	DE	1	Total 1	O 1	0	0
56	DL	5	Total 5	O 5	0	0
56	DP	1	Total 1	O 1	0	0
56	D2	1	Total 1	O 1	0	0

3 Residue-property plots

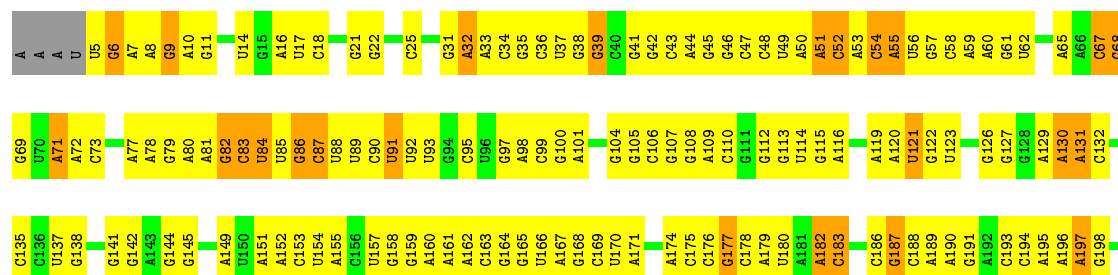
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

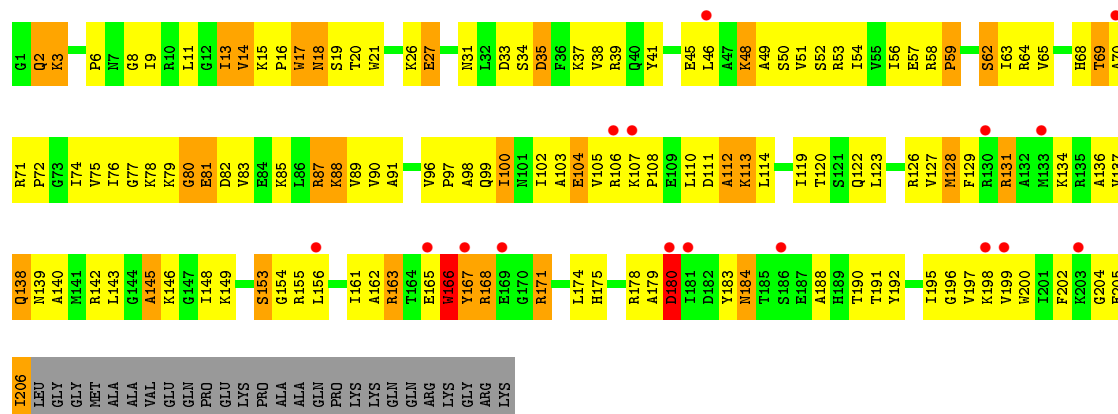




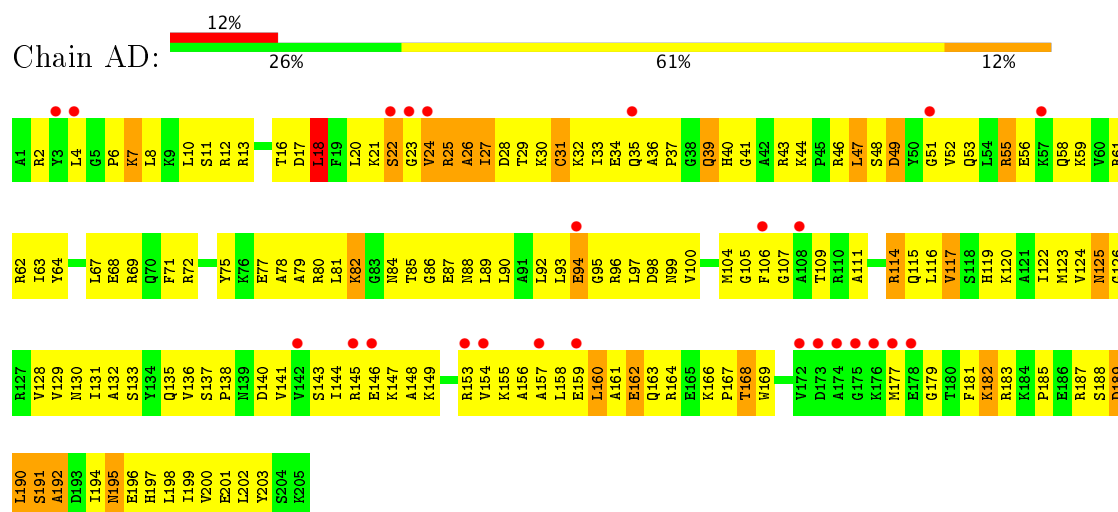
Chain CA:  21% 65% 13% ..



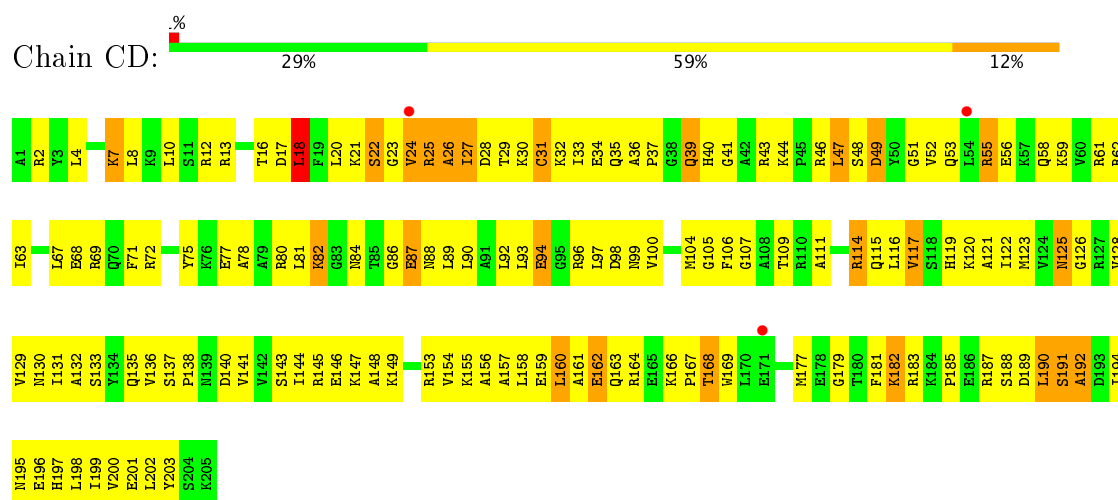
G1185	G1057	U1121	G1065	A996	C931	A860	U793	G724	C660	A595	G539	U464	A397	G332	A263	G201
G1186	G1058	U1122	U1065	U997	C934	G861	A794	G725	G661	A596	G530	A465	U398	U333	C264	G202
G1187	C1059	G1123	C1059	C998	C998	G862	C795		U62	G597	U531	A466	G399	C334	G265	G203
A1191	U1060	G1124	U1060	C999	A935	U863	A728		A663	U598	A532	U467	C400	C335	G266	G204
	G1061	U1125	G1061	A1000	C936	A864	A729		G664	C599	A468	A469	C401	A336	C267	A205
U1194	U1062	U1126	U1062	G1001	A937	A865	G730		A665	A600	U534	C469	G402	G337	U268	C206
C1195	C1063	G1127	C1063	G1002	A938	C866	G731			G801		C470	C403	A338	C269	C207
A1196	U1064	C1128	U1065	G1003	G939	G867			G668	A602	G537	U471		A339	A270	U208
A1197	U1065	C1129	C1065	A1004	C940	C868	G734		G669	U603		U472	G406	U340	C271	U209
C1198	A1005	G1130	A1005	G1006	G941	G670	C735		G671			U473	U407	C272	U273	C210
U1199	U1007	G1131	G1007	U1007	G945	U875	C736		A607			U474	U408	C342	U274	G213
C1200	U1008	G1132	U1070	U1008	A946	C876	C737		U672	A608	G541	C475	U409	U343	G275	G214
A1201	C1071	G1133	A807	U1009	G947	G877	C738		U673	A609	G542	U476		G410	G276	C215
	U1072	G1134	C1071	U1010	C948	C878	C739		U674	U610	U543	C477	A411	A344	C277	U216
U1202	U1073	C1135	U1073	C1011	A949	C879			A675	C612	G545	U478	A412	A413	G278	C217
C1203	G1074	G1137	U1074	A1012	C880	U676	G742			G618	G544	U479	A414		C279	U218
G1206		G1138		G1013	C881	U677	A743			G619	A546	U480	A415	A353	C280	U219
G1207	U1077	G1139	U1077	A1014	C882	U678	C744			G615	A547	G481	A416	C355	G281	G220
C1208	U1078	G1140	G1078	G1015	C883	U679	G745			G616	C549	U482		A356	A282	C221
G1209	U1079	G1141	U1079	A1016	C884	A681	A746			G617	G550	C484	U420	G357	U283	C222
C1210	A1080	G1142	U1017	U1017	G885	U682	A748			G618	U551	U485	U421	U358	C284	A223
U1211	U1081	G1143	U1081	G1018	G886	U683	A749			U619	U552	U486	U422	G359	C285	U224
U1212	A1082	G1144		A1019	G887	U684	C750			G620	A553	A487	G423	G360	C286	C225
A1213		A1145		G1020	A889	U685	U751			A621	A584	C488	G424	G361	U287	G226
C1214	U1085	A1146		A1021	A890	U686				A622	U555	C489	G425	G362	A288	G227
G1215	U1086	C1147	U1086	U1022	C893	U687	C754			G623	C556	C490	U426	A363	G289	U228
A1216	G1087	G1148	G1087	U1023	G894	U688	G755			G624		C491	U427	U365		G230
C1217	U1088	G1149	U1088	G1024	C895	U689				U625	A559	C492	G428	U366	G292	G231
G1218	G1089	A1150	G1089	U1025	G898	U692	U762			G626	A560	A493	U429	U367	A298	C232
A1219	U1090	G1151	U1090	G1026	C899	G693	G763			G627	U561	G494	A430	U368	C233	G233
U1151	U1091	A1152	U1091	C1027	A900	A694	C764			G628	U562	A495		A300	C234	C234
G1153	U1092	G1153	U1092	C1028	C901	U696	A766			A629	A563	A496	U434	C370	G302	A236
	U1093		G1093	U1029	A968	U697	A767			G630	C564	A498	U435	U371		G237
U1159	G1094	U1159	G1094	U1030	A969	U698	A768			U632	C566	A500	C436	C372	A238	
G1161	U1095	G1161	U1095	C1031	C970	C699	G769			G633	G570	C501	U437	A373	C307	U239
C1162	C1096	G1162	C1096	G1032	G971	G700	C770			C634	U571	A502	U438	A374	C308	G240
A1163	C1097	A1163	C1097	G1033	C972	U701				A635	A572	C503		U375	G241	
G1164	C1098	G1164	C1098	G1034	G973	A702	U772			U636	A573	C504	C443	G376	A309	G242
U1165	G1099	U1165	G1099	A1035	A974	G703	G773			G637	A574	G505	G444	G377	G311	A243
C1223	C1100	G1166	C1100	C1037	G975	A704	G774			U638	G575	G506	G445	G378	C312	U244
C1230	A1101	A1167	A1101	U1038	A977	G705	G775			G639	G576		G446	C379	A313	U245
G1231	A1102	U1168	A1102	G1039	A978	A706	G776			A640	C577	C511		C380	A314	
	C1103		C1103	U1040	A979	U707	A777			U641	A448	C512		C381	C315	A246
C1234	G1104	A1169	G1104	G1041	C979	U708	G778			A642	G578	U512	G449	A382	A316	G247
U1235	A1105	U1170	A1105	U1042	U981	G709	C779			C643	A579	C513	G450	A383	U317	A250
A1236	G1106	C1171	G1106	G1043	U982	A844	A780			U644	C580	U516		G384	G318	U252
C1237	U1109	U1173	U1109	A1044	A983	A781	A781				G581	C517	A451	A385	G319	A253
G1238	A1110	G1174	A1110	C1045	C984	A845	A782			C647	G584	C518		C386	A320	G254
A1239	A1111	G1175	A1111	U1046	C985	U920	C783			A648	G585	G521	G452	A387	A321	U256
U1240	C1112	A1176	C1112	G1047	U986	G922	A784			U649	C586	C522	A453	U388	G324	G257
G1241	G1113	G1177	G1113	U1048	A987	A715	G785			G650	G587	G523	G454	U389	C322	U258
C1242	C1114	C1178	C1114	U1049	C924	A716	G786			U652	G589	C524		U390	U323	G259
G1243	U1115	A1179	U1115	G1050	G925	A717	G787			U653	U590	G525		G391	G324	G260
A1244	U1116	A1180	U1116		C926	C719	A788			U654	U591	A459		U458	C392	G261
C1245	A1117	G1181	A1117	G1053	G927	C720	U789			U657	U592	C526		G393	C328	G262
A1246	C1118	U1182	C1118	A1054	G928	G721	A790			G658	G593	C527		U459	A329	U261
U1247	G1183	U1183	G1183	C1055	G929	G722	G791			U659	U594	C528		G395	C330	
A1248	U1184	G1184	U1184	U1056	C930	U723	A792						U463	C396	G331	A262



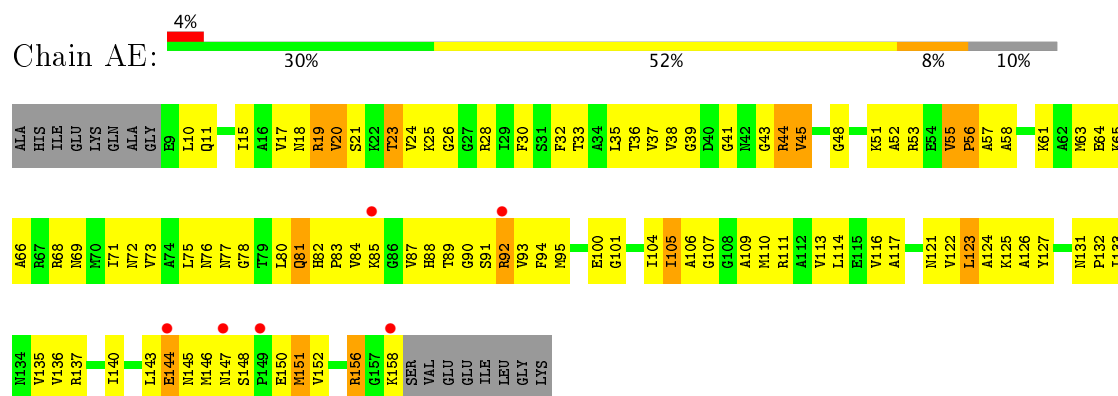
- Molecule 3: 30S ribosomal protein S4



- Molecule 3: 30S ribosomal protein S4



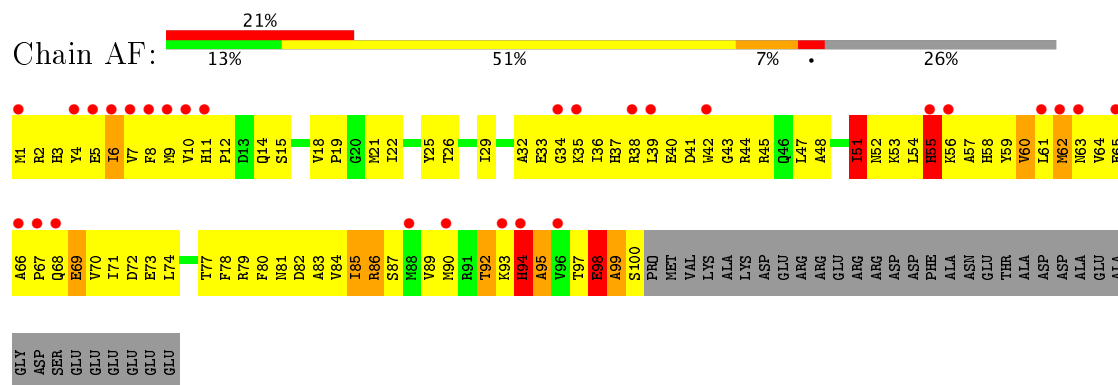
- Molecule 4: 30S ribosomal protein S5



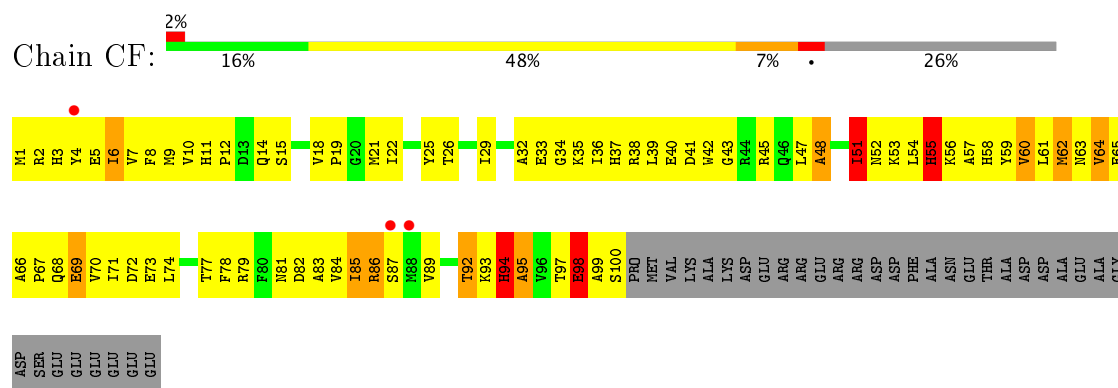
- Molecule 4: 30S ribosomal protein S5



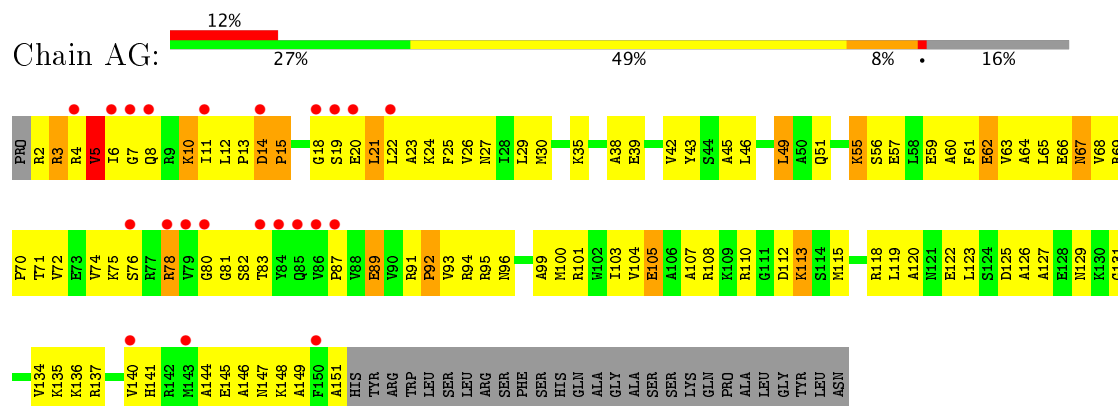
- Molecule 5: 30S ribosomal protein S6



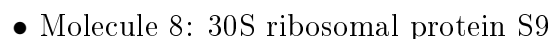
- Molecule 5: 30S ribosomal protein S6

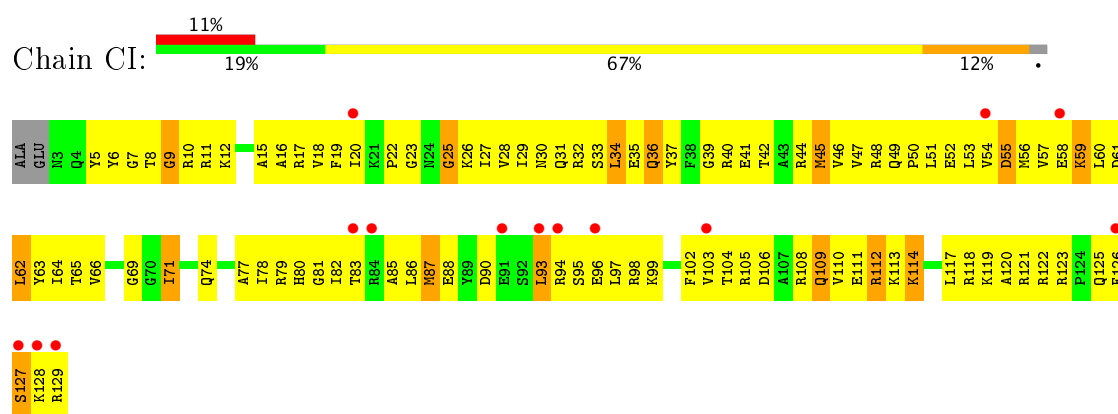


- Molecule 6: 30S ribosomal protein S7

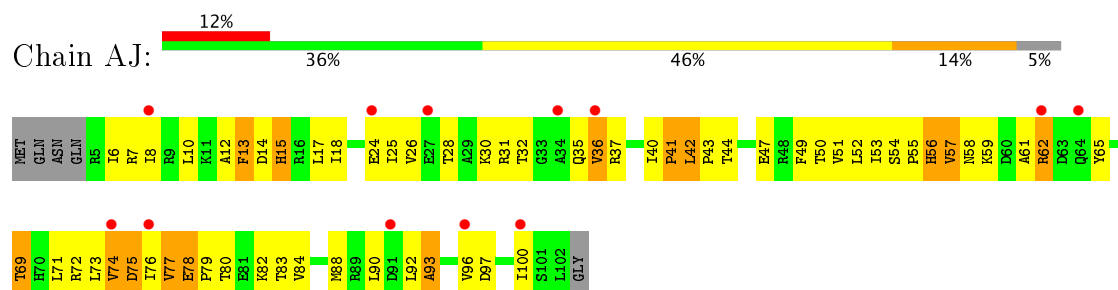


- Chain CG: 

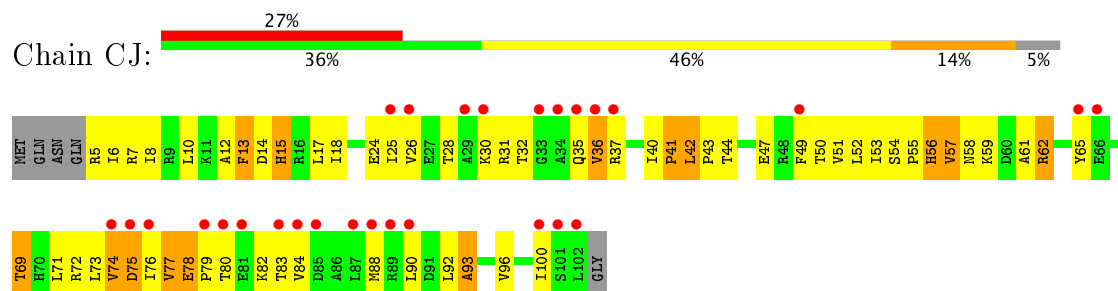




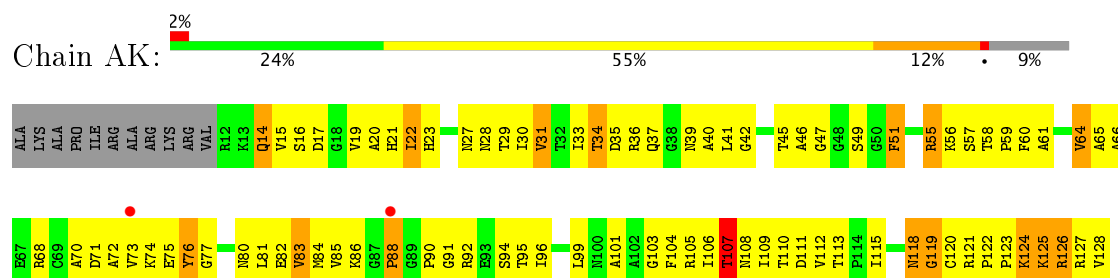
• Molecule 9: 30S ribosomal protein S10



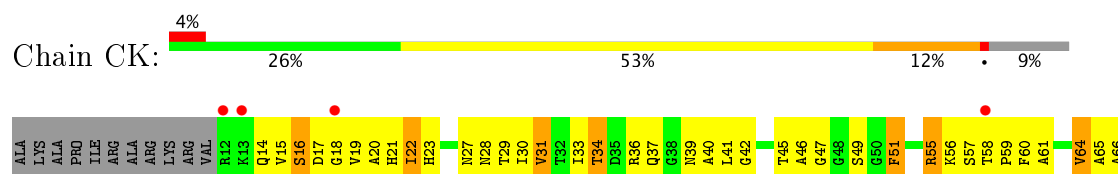
• Molecule 9: 30S ribosomal protein S10



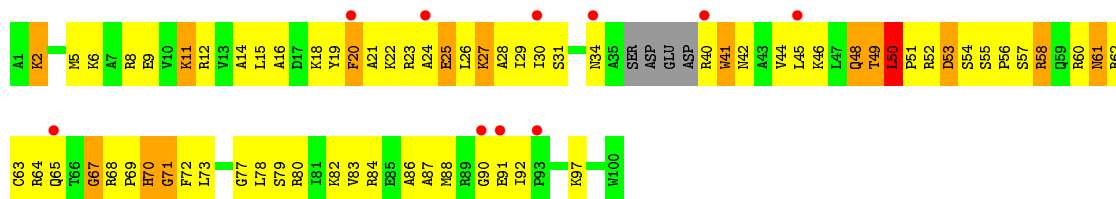
• Molecule 10: 30S ribosomal protein S11



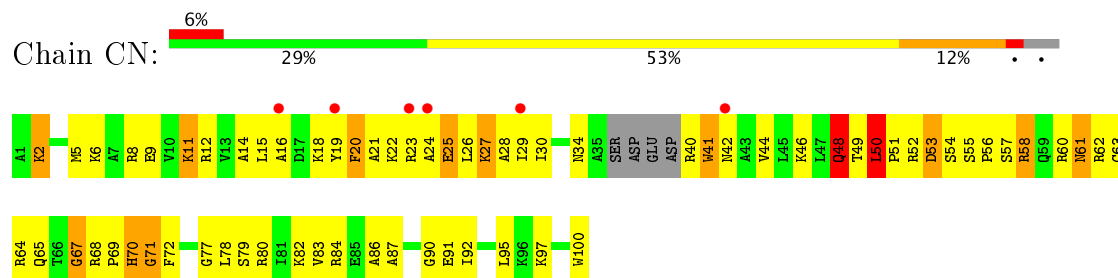
• Molecule 10: 30S ribosomal protein S11



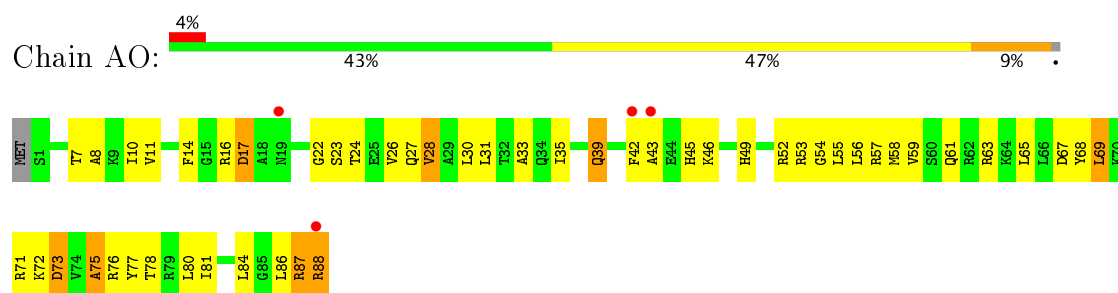




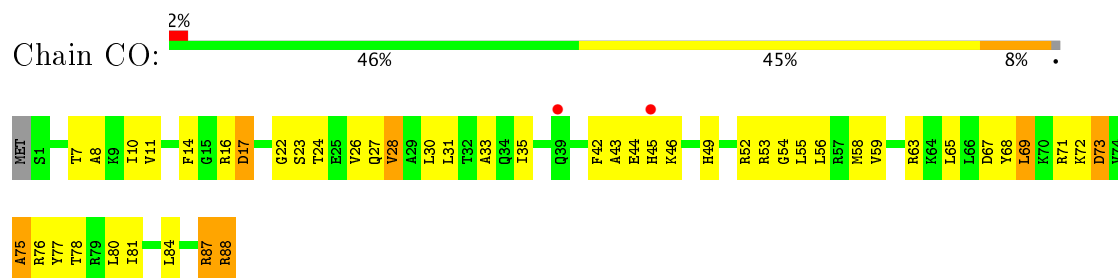
• Molecule 13: 30S ribosomal protein S14



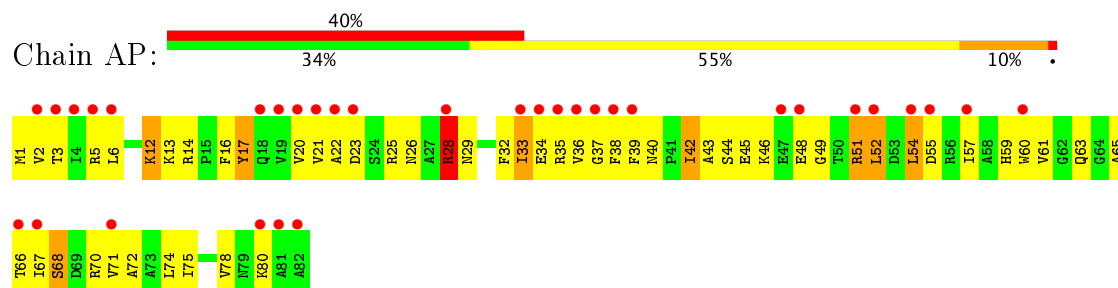
• Molecule 14: 30S ribosomal protein S15



• Molecule 14: 30S ribosomal protein S15

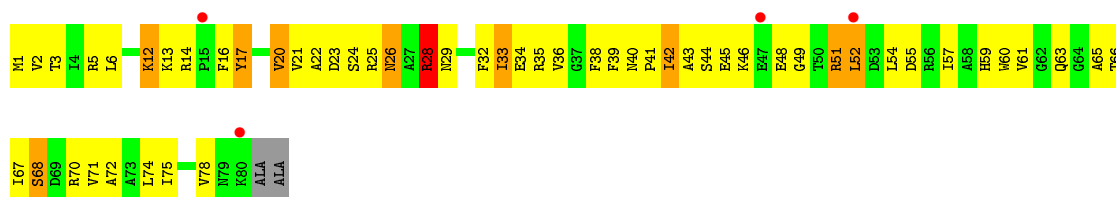


• Molecule 15: 30S ribosomal protein S16

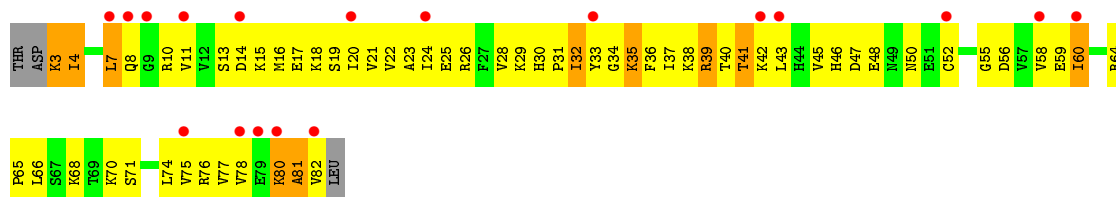


• Molecule 15: 30S ribosomal protein S16

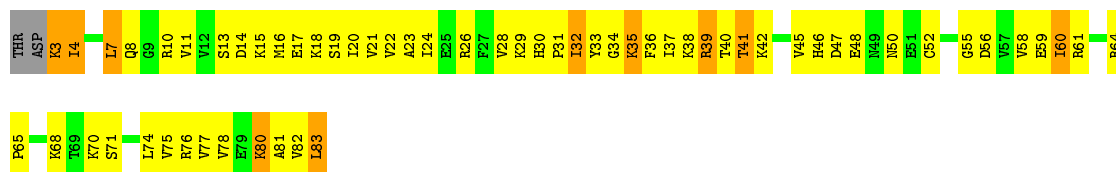




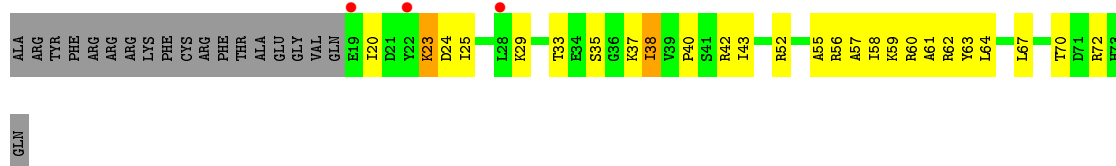
- Molecule 16: 30S ribosomal protein S17



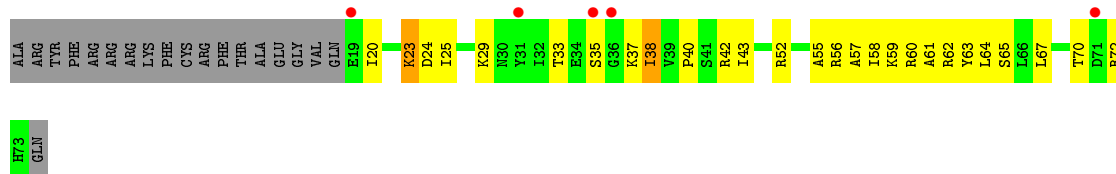
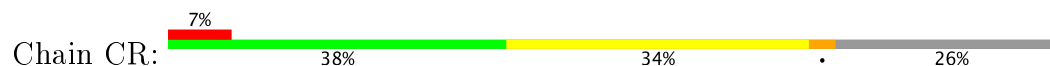
- Molecule 16: 30S ribosomal protein S17



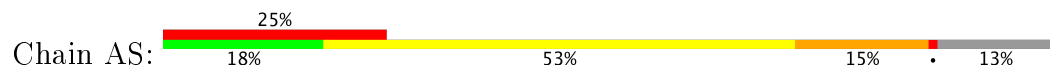
- Molecule 17: 30S ribosomal protein S18

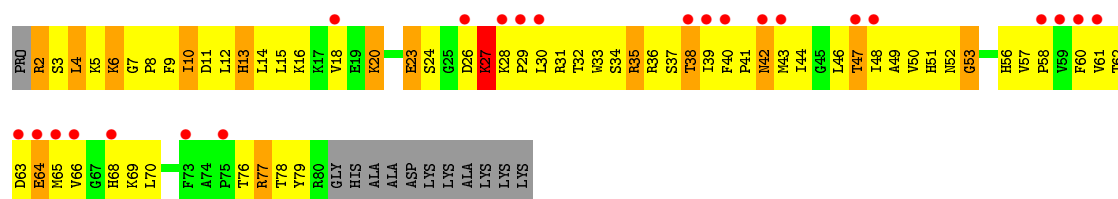


- Molecule 17: 30S ribosomal protein S18

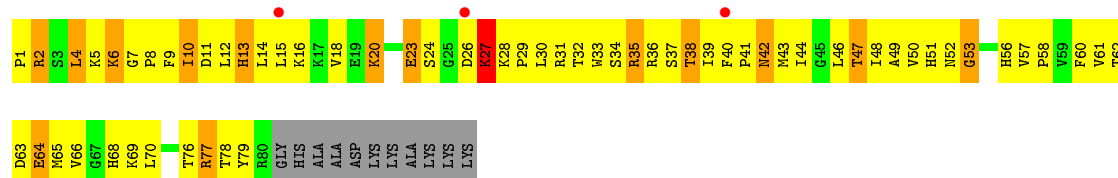
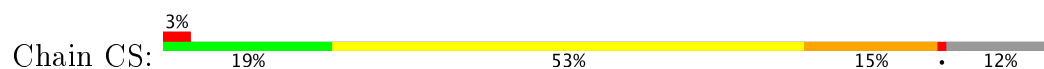


- Molecule 18: 30S ribosomal protein S19

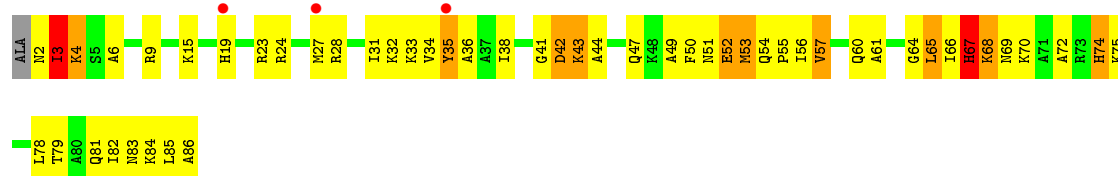
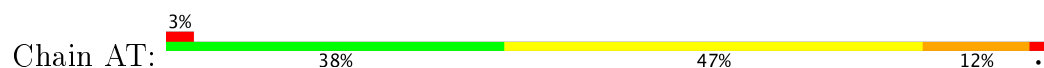




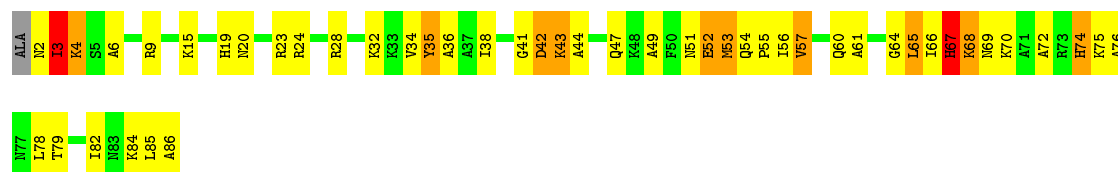
• Molecule 18: 30S ribosomal protein S19



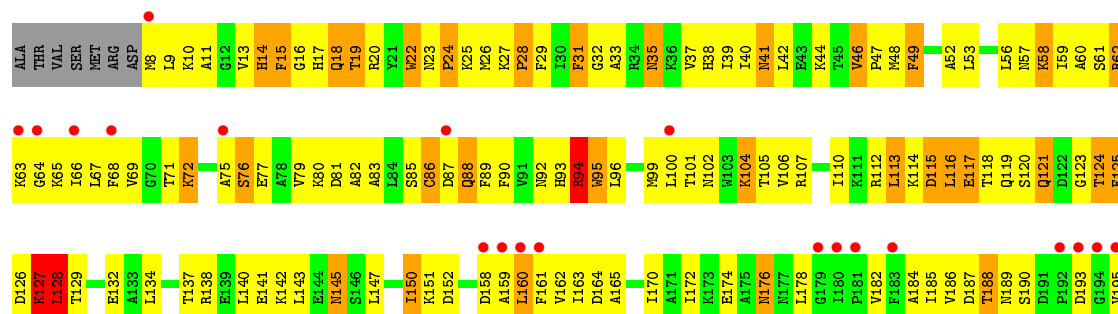
• Molecule 19: 30S ribosomal protein S20

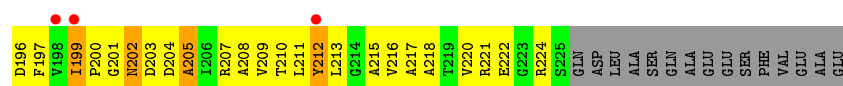


• Molecule 19: 30S ribosomal protein S20

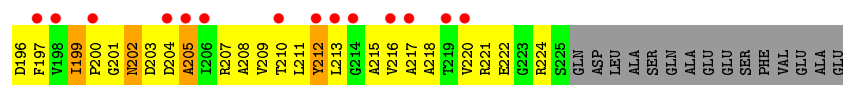
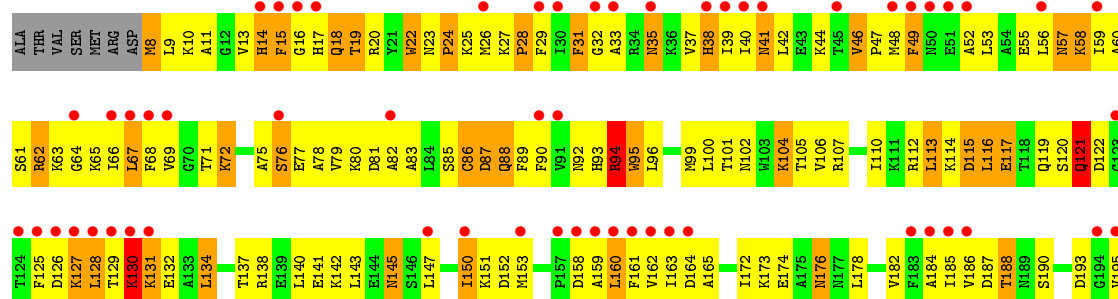


• Molecule 20: 30S ribosomal protein S2

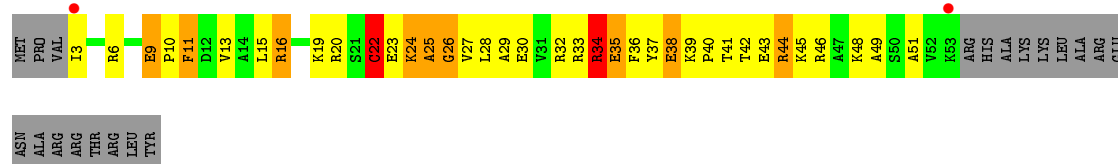
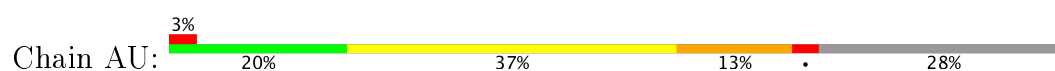




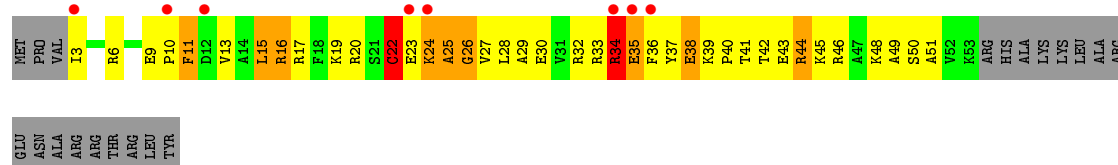
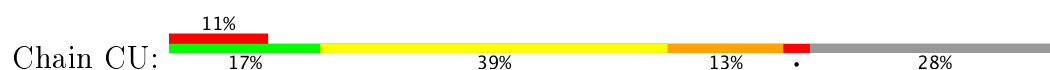
• Molecule 20: 30S ribosomal protein S2



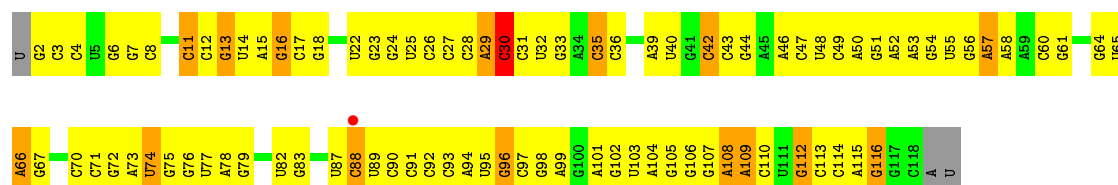
• Molecule 21: 30S ribosomal protein S21



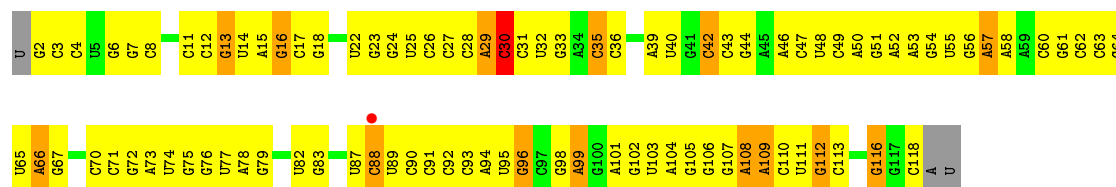
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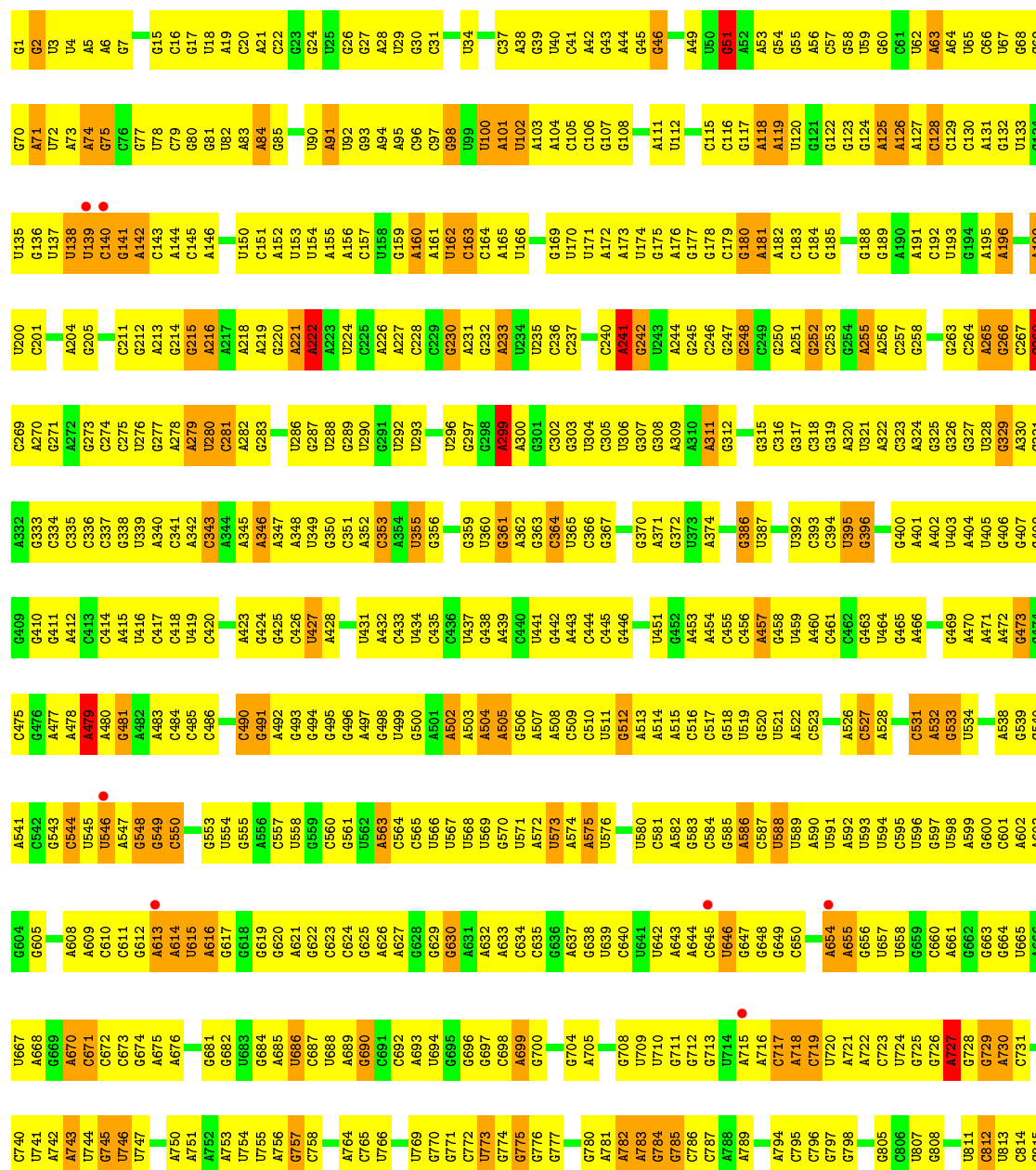
• Molecule 22: 5S ribosomal RNA



• Molecule 22: 5S ribosomal RNA



• Molecule 23: 23S ribosomal RNA

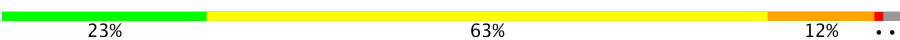


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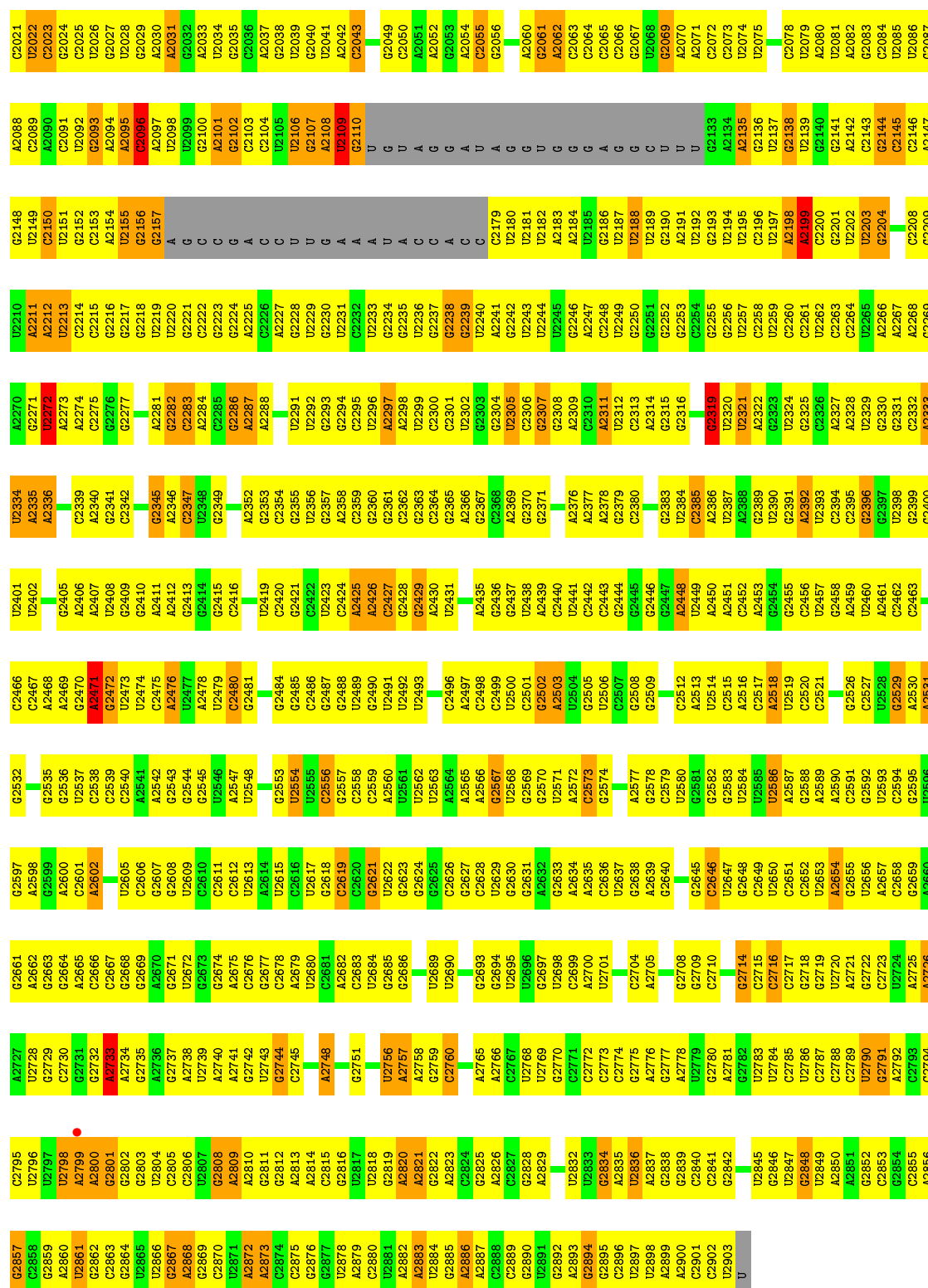
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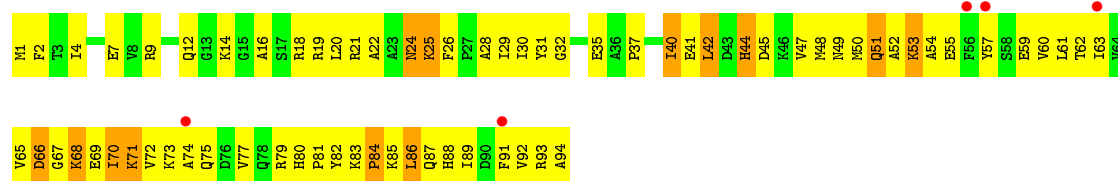
• Molecule 23: 23S ribosomal RNA

Chain DB:  23% 63% 12% ..

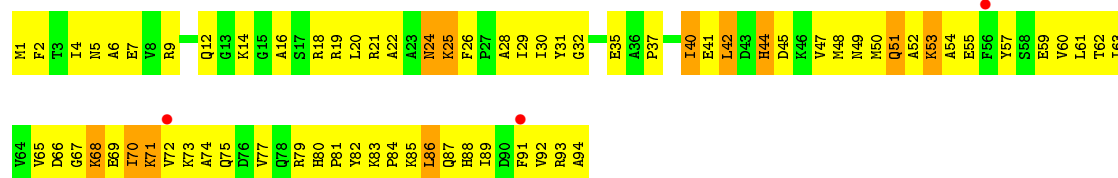
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A272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000

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C1958	A1829	G1761	G1689	G1619	C1550	U1486	G1425	G1355	G1221	C1221	U1160	C1093	U1019	A947
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G1961	G1832	U1766	G1702	G1624	U1553	C1489	G1428	A1366	G1291	U1224	G1163	U1098	G1022	G950
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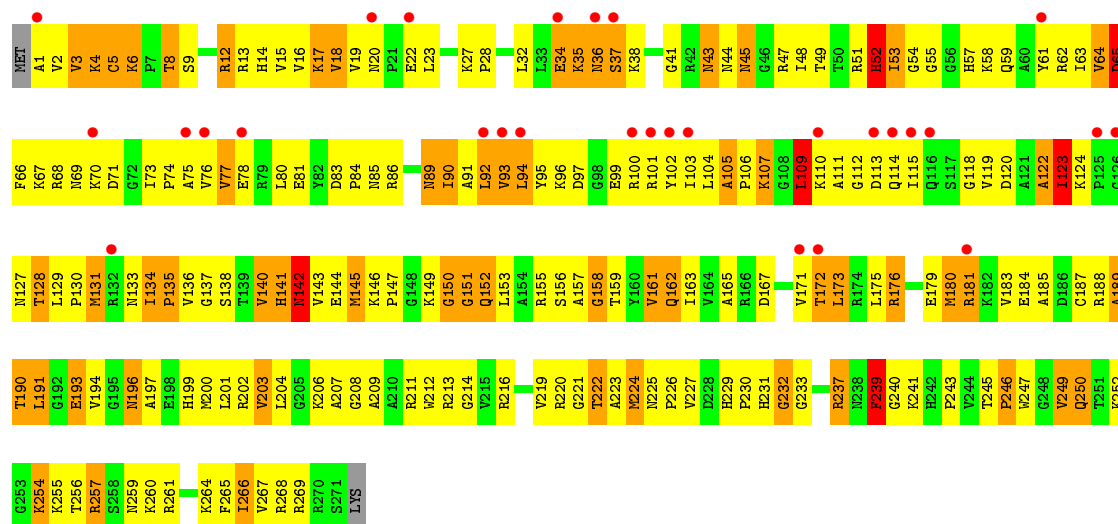




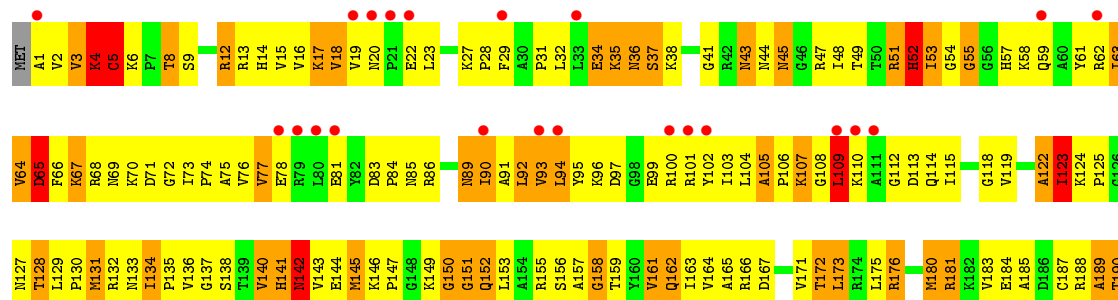
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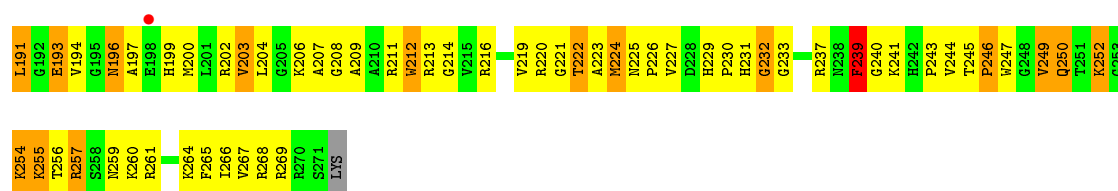


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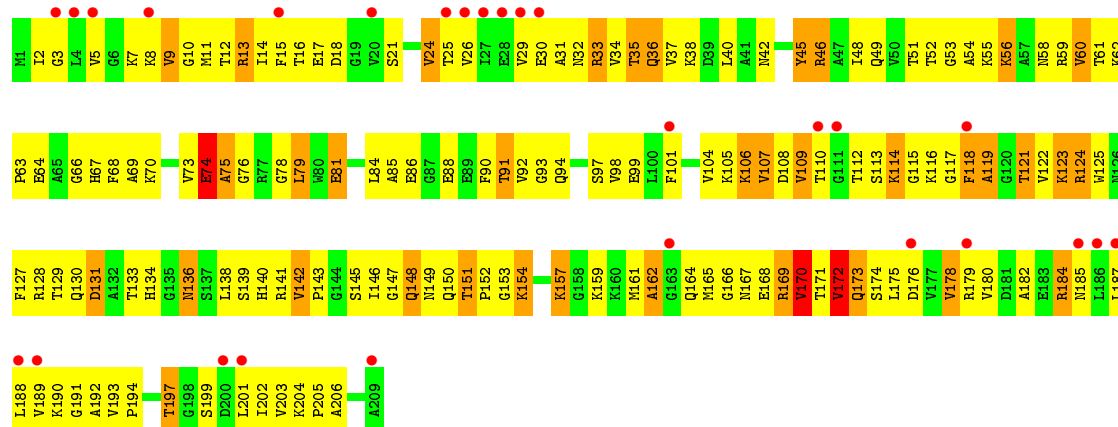


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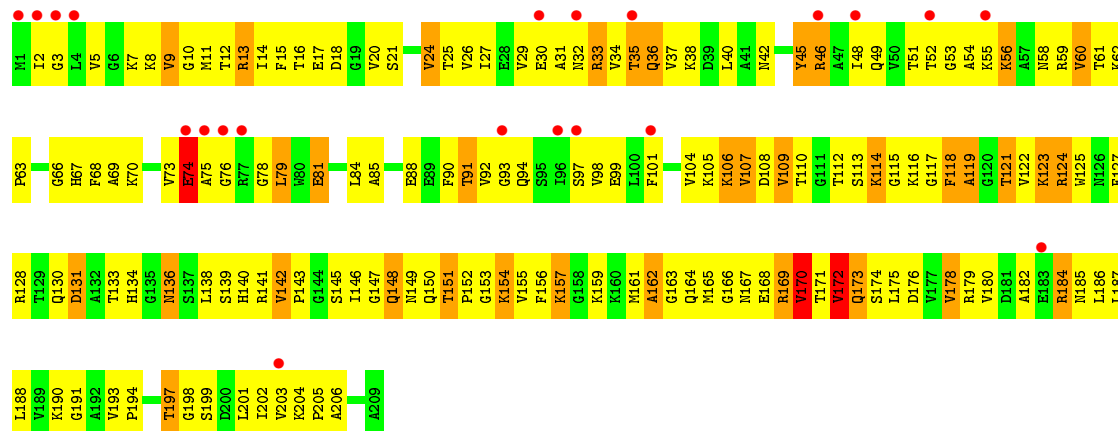




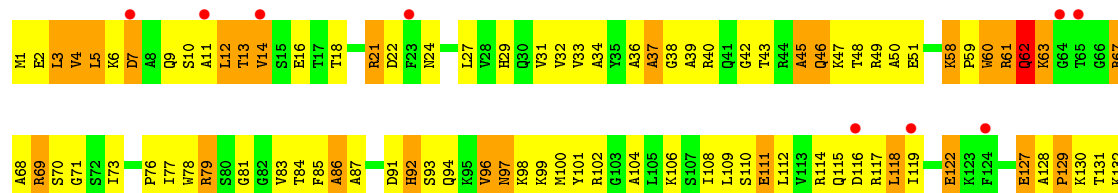
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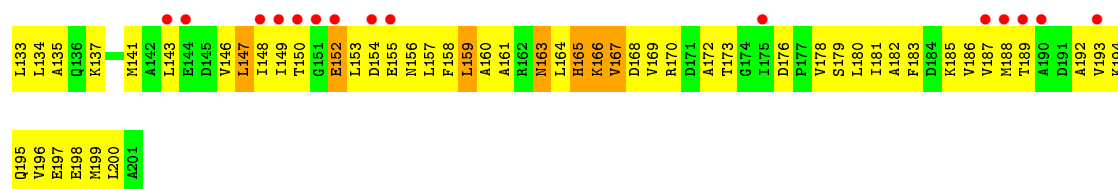


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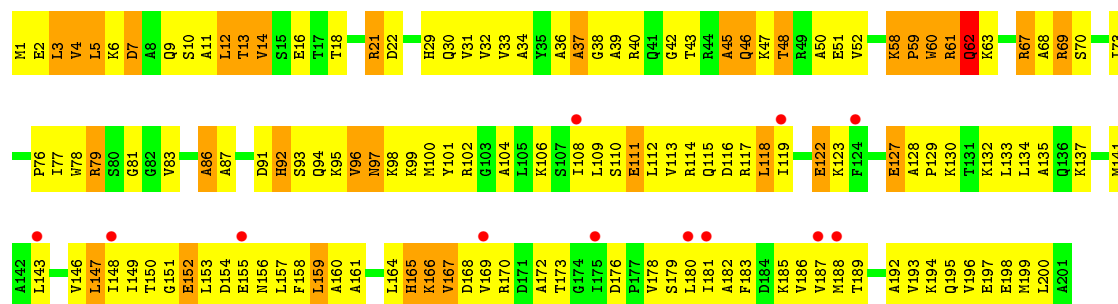


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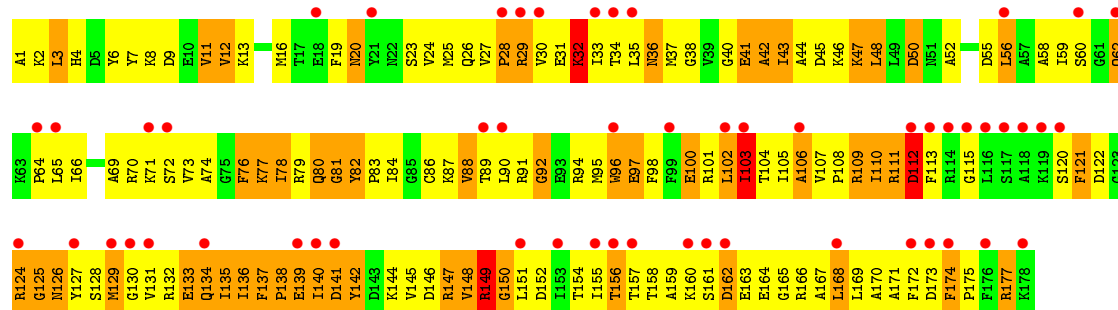
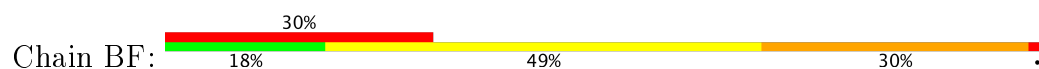




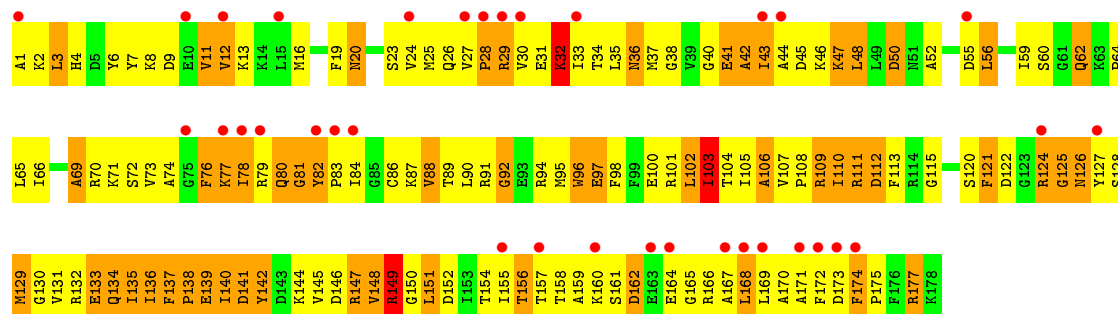
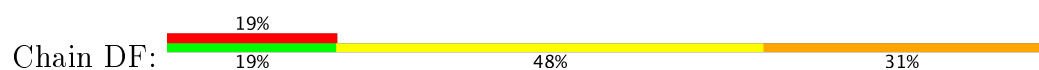
• Molecule 27: 50S ribosomal protein L4



• Molecule 28: 50S ribosomal protein L5

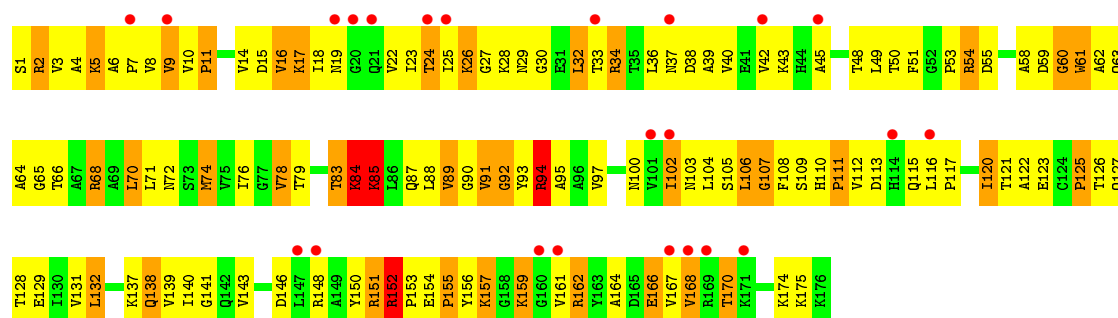


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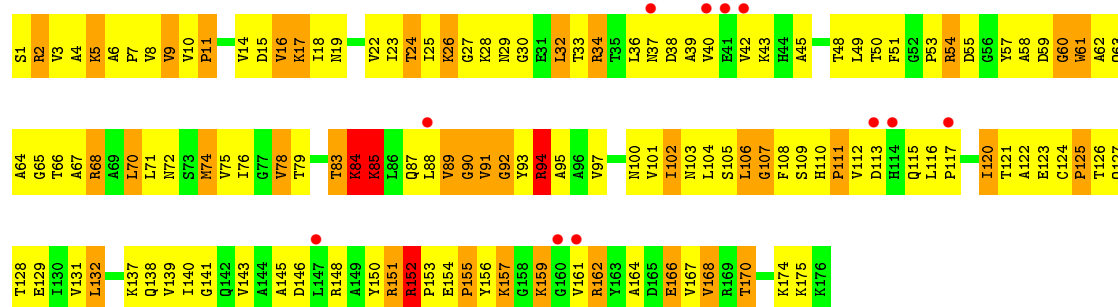


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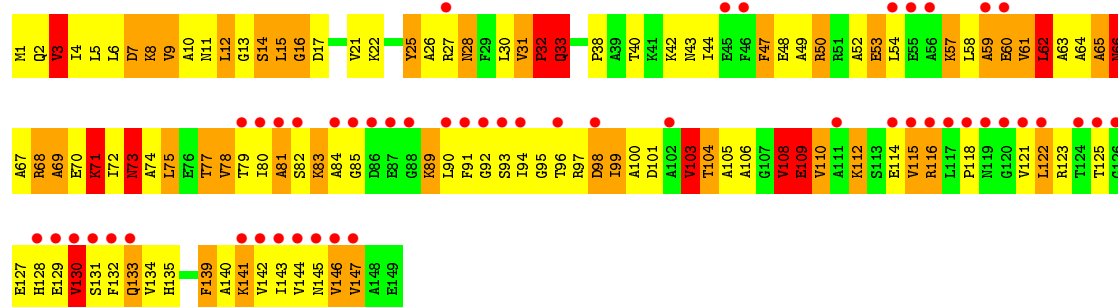
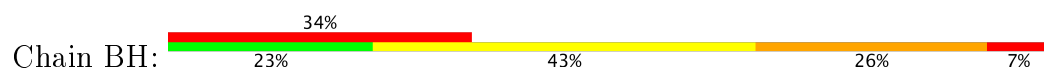




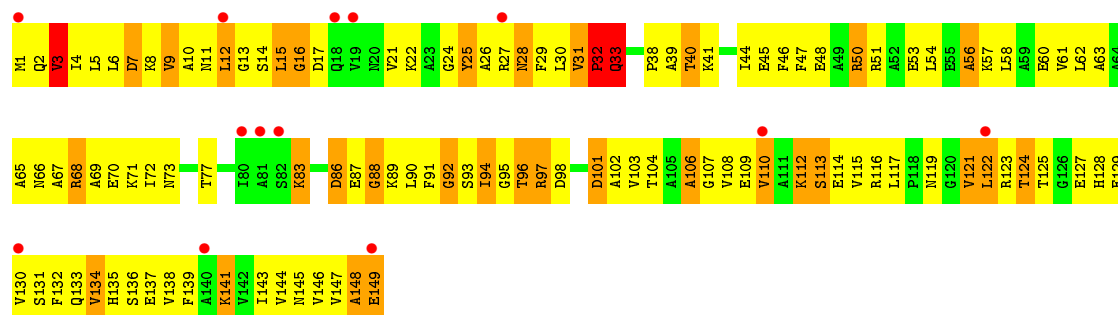
• Molecule 29: 50S ribosomal protein L6



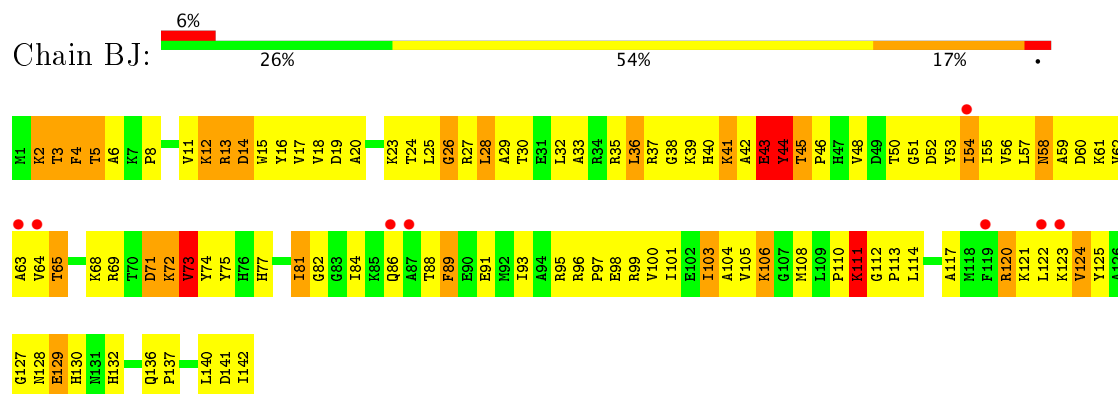
• Molecule 30: 50S ribosomal protein L9



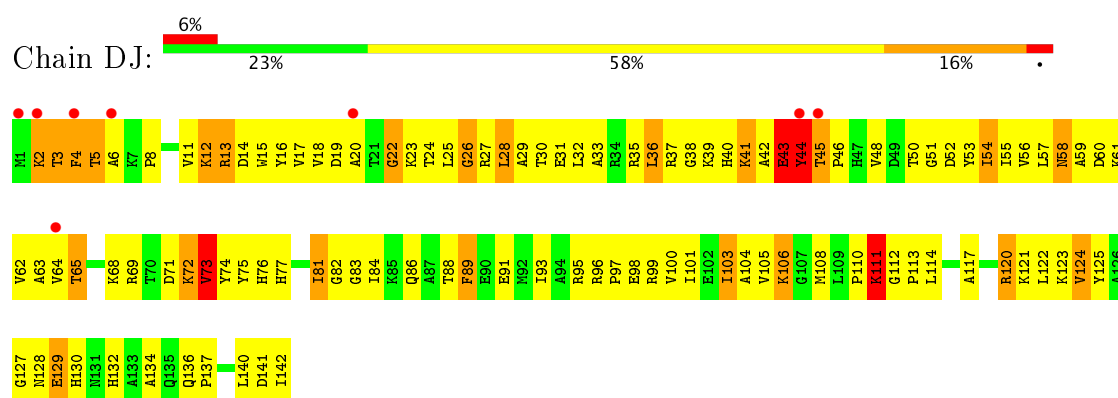
• Molecule 30: 50S ribosomal protein L9



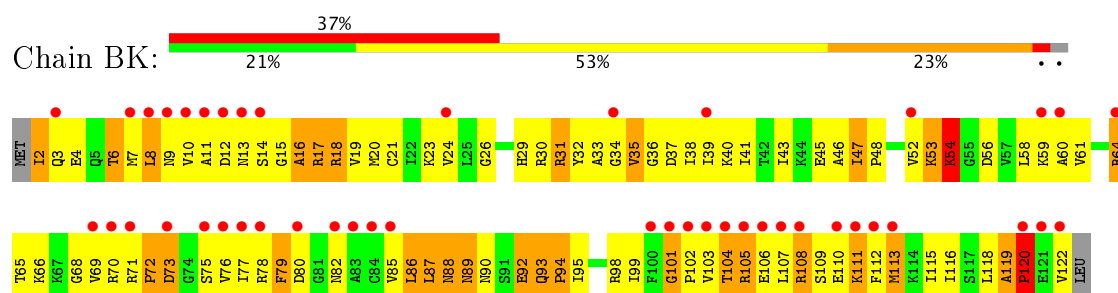
- Molecule 31: 50S ribosomal protein L13



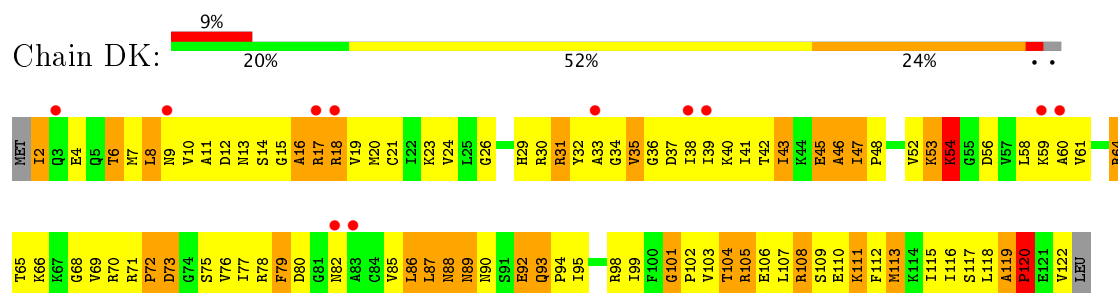
- Molecule 31: 50S ribosomal protein L13



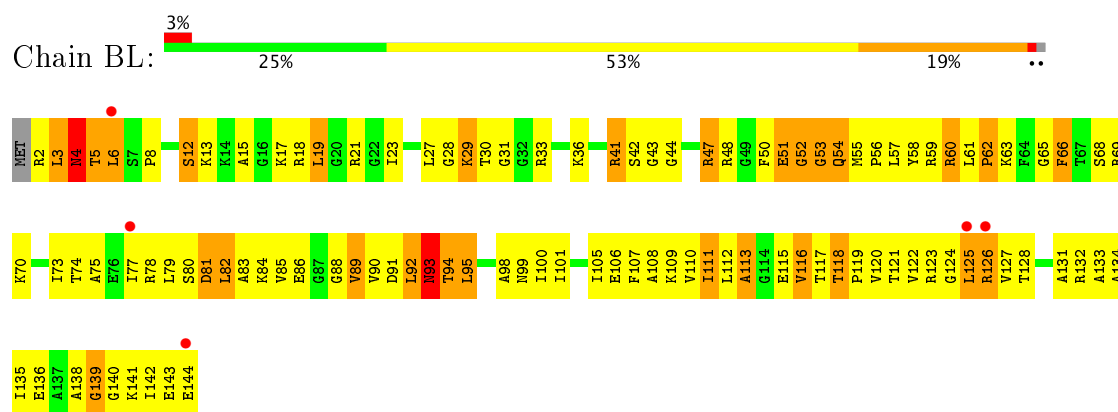
- Molecule 32: 50S ribosomal protein L14



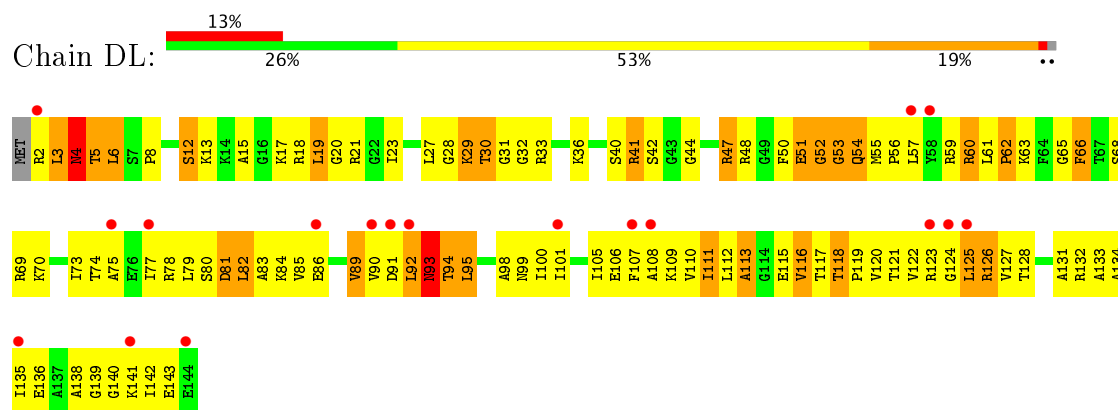
- Molecule 32: 50S ribosomal protein L14



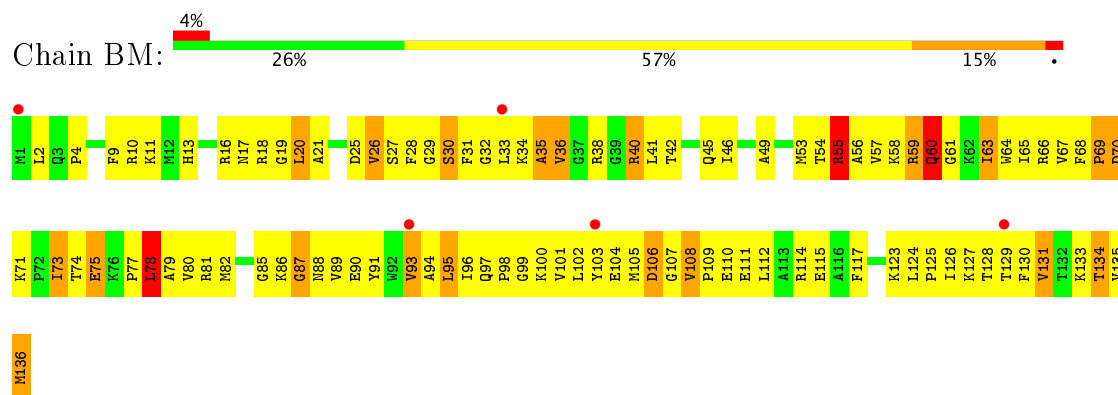
- Molecule 33: 50S ribosomal protein L15



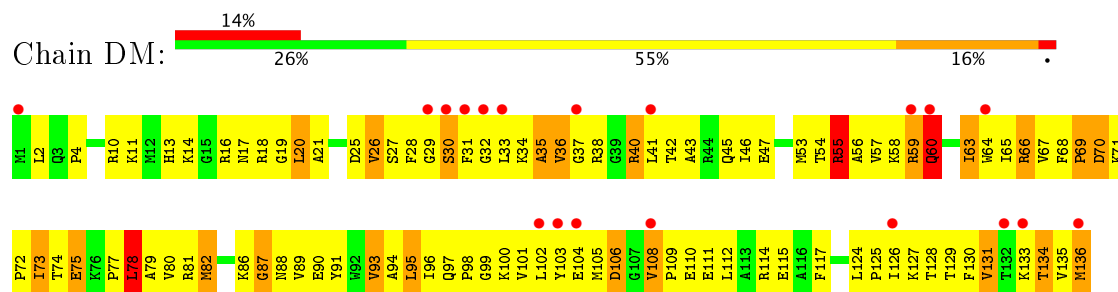
• Molecule 33: 50S ribosomal protein L15



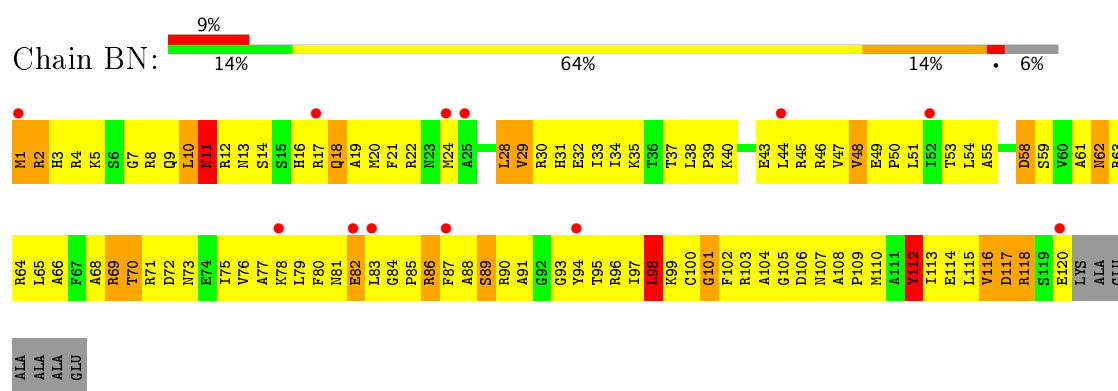
• Molecule 34: 50S ribosomal protein L16



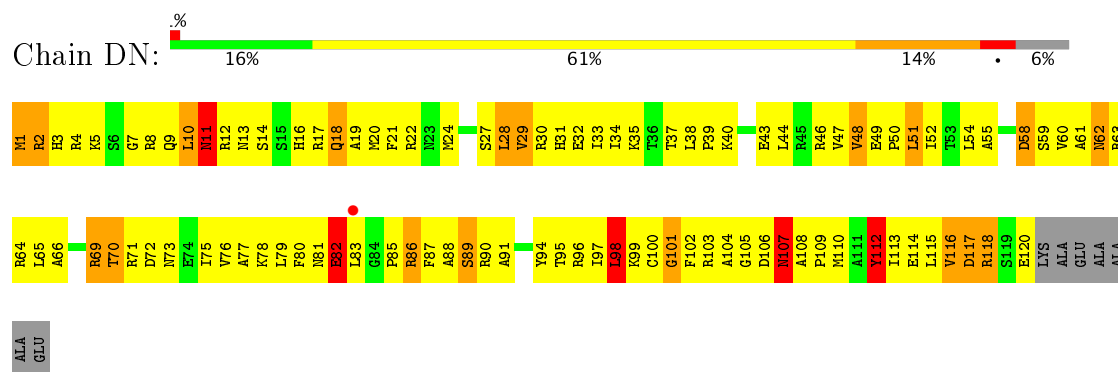
• Molecule 34: 50S ribosomal protein L16



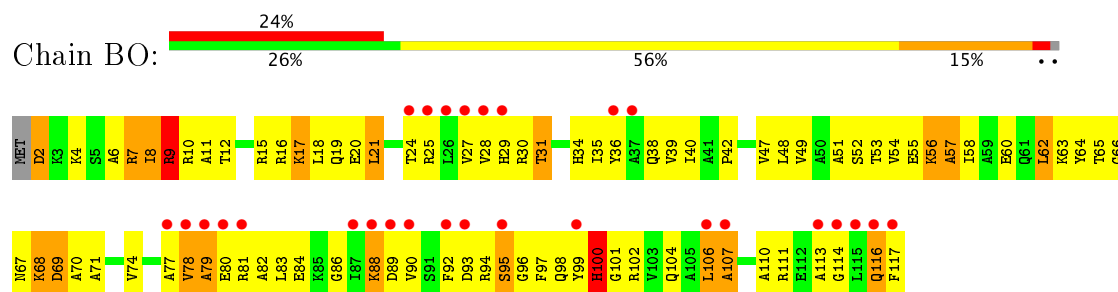
• Molecule 35: 50S ribosomal protein L17



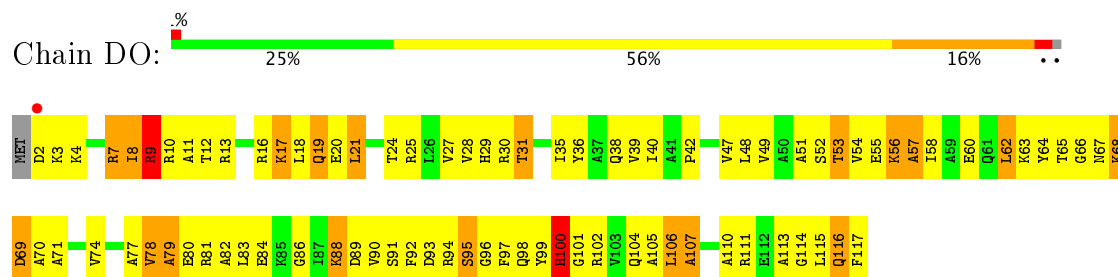
- Molecule 35: 50S ribosomal protein L17



- Molecule 36: 50S ribosomal protein L18

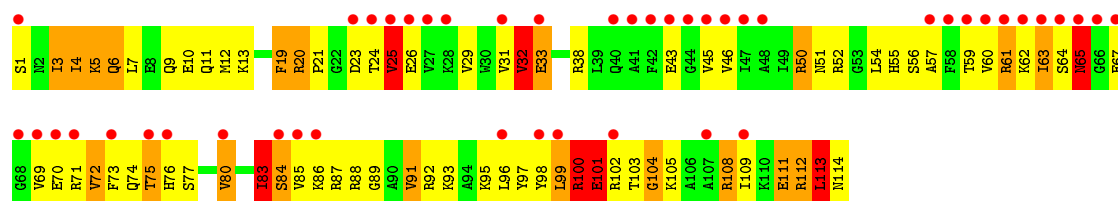


- Molecule 36: 50S ribosomal protein L18

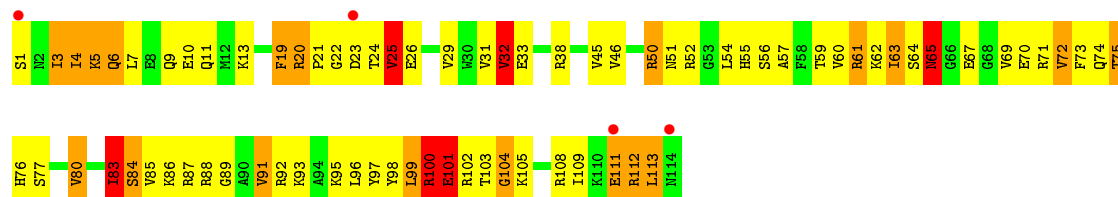


- Molecule 37: 50S ribosomal protein L19

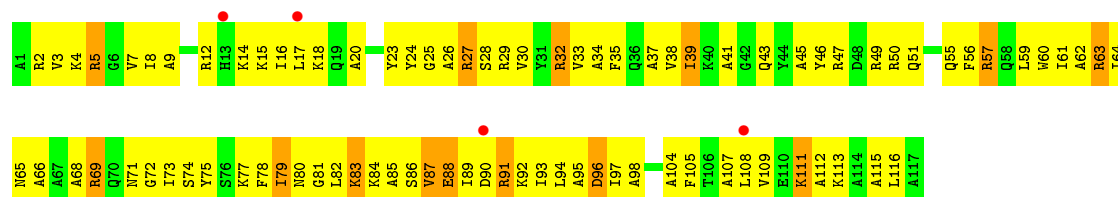




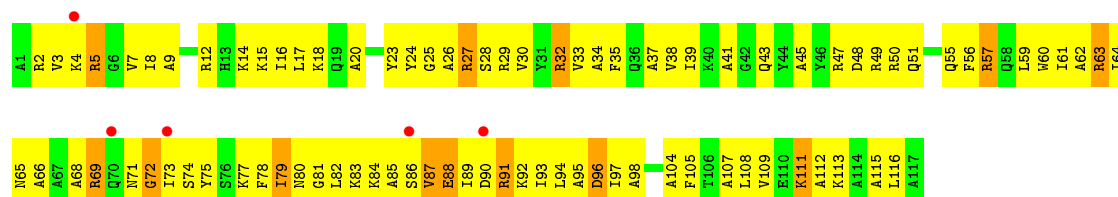
• Molecule 37: 50S ribosomal protein L19



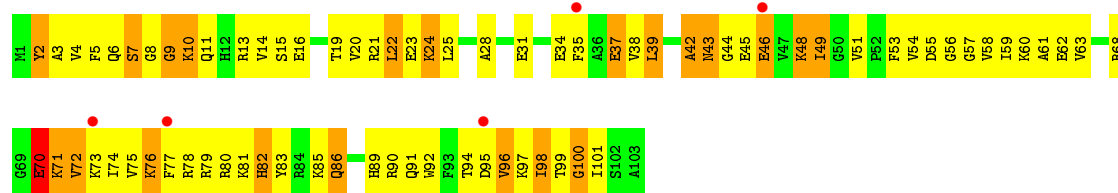
• Molecule 38: 50S ribosomal protein L20



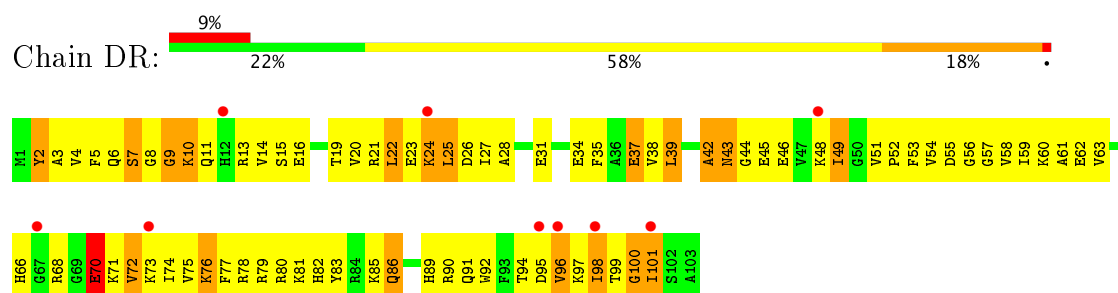
• Molecule 38: 50S ribosomal protein L20



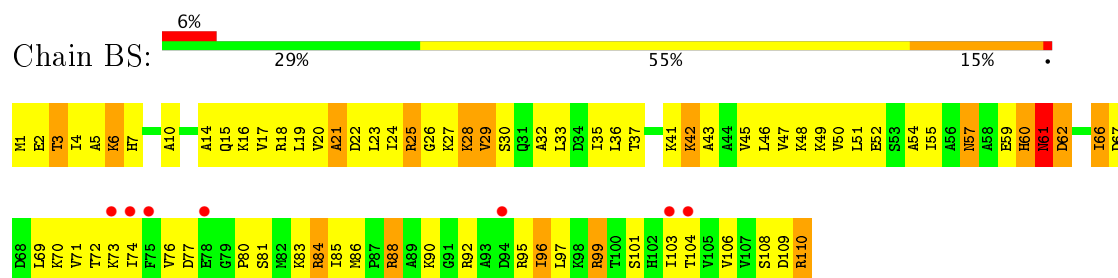
• Molecule 39: 50S ribosomal protein L21



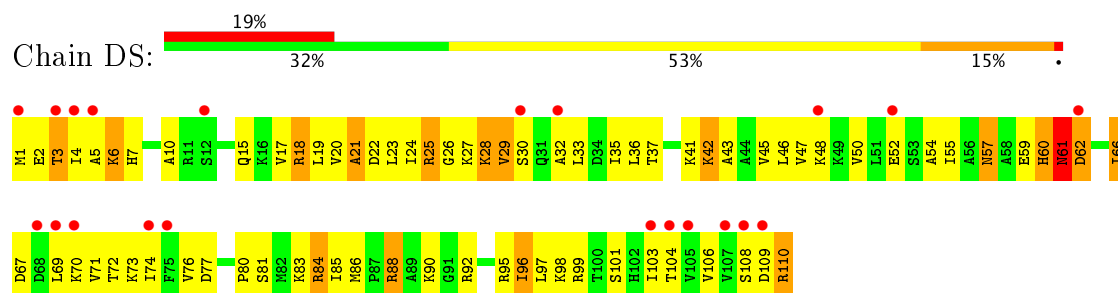
• Molecule 39: 50S ribosomal protein L21



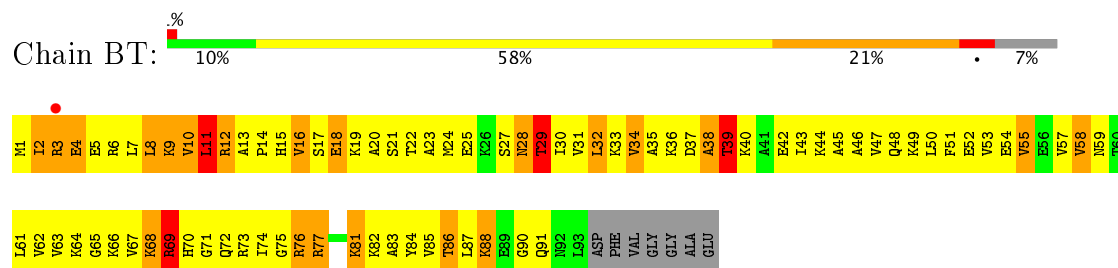
• Molecule 40: 50S ribosomal protein L22



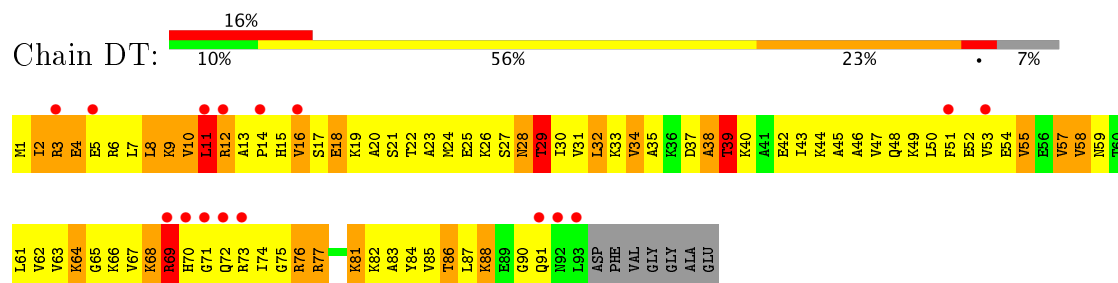
• Molecule 40: 50S ribosomal protein L22



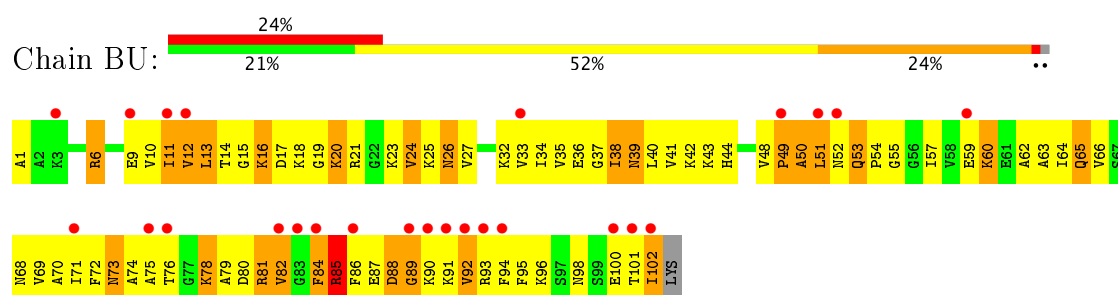
• Molecule 41: 50S ribosomal protein L23



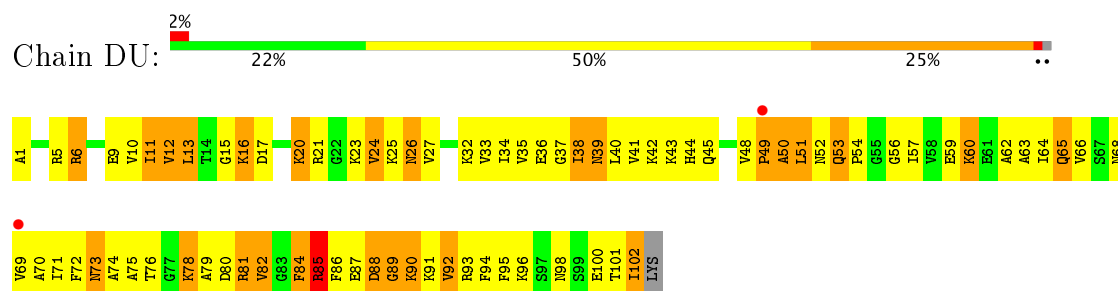
• Molecule 41: 50S ribosomal protein L23



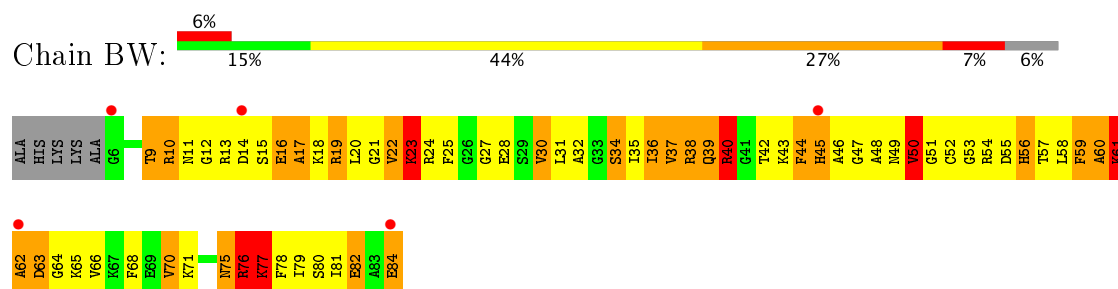
• Molecule 42: 50S ribosomal protein L24



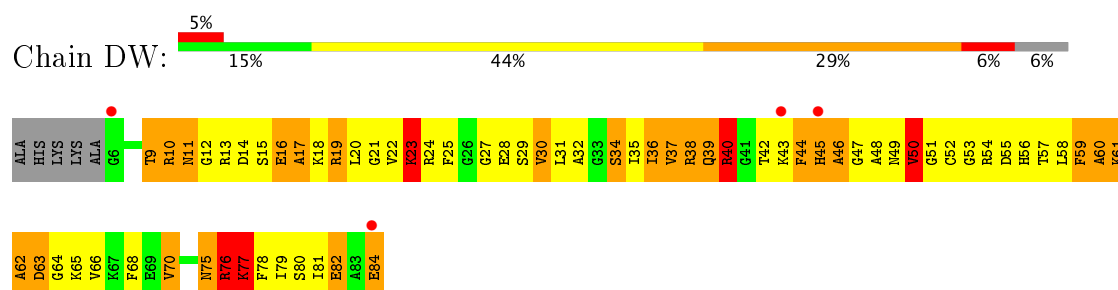
- Molecule 42: 50S ribosomal protein L24



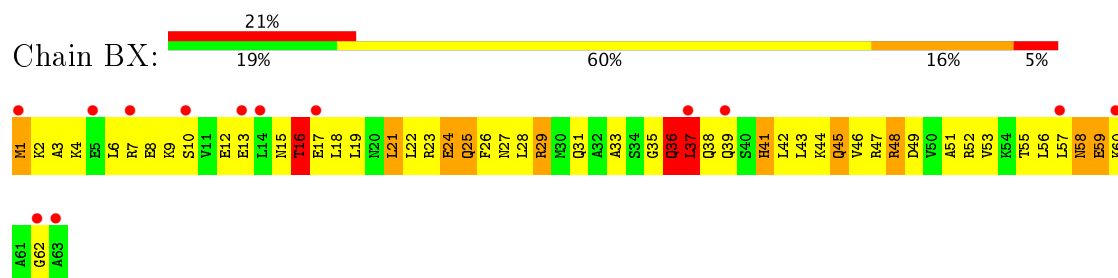
- Molecule 43: 50S ribosomal protein L27



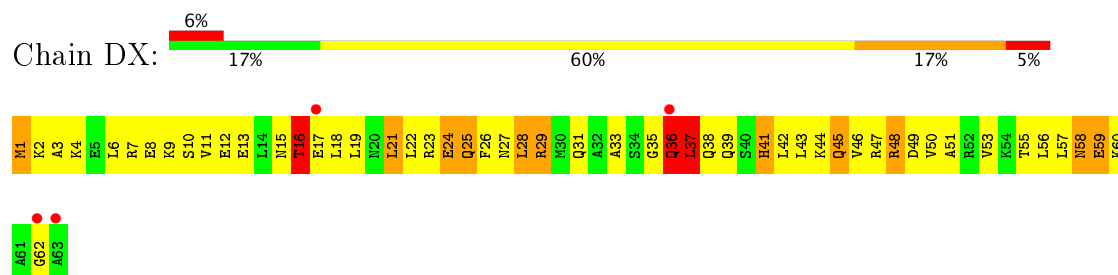
- Molecule 43: 50S ribosomal protein L27



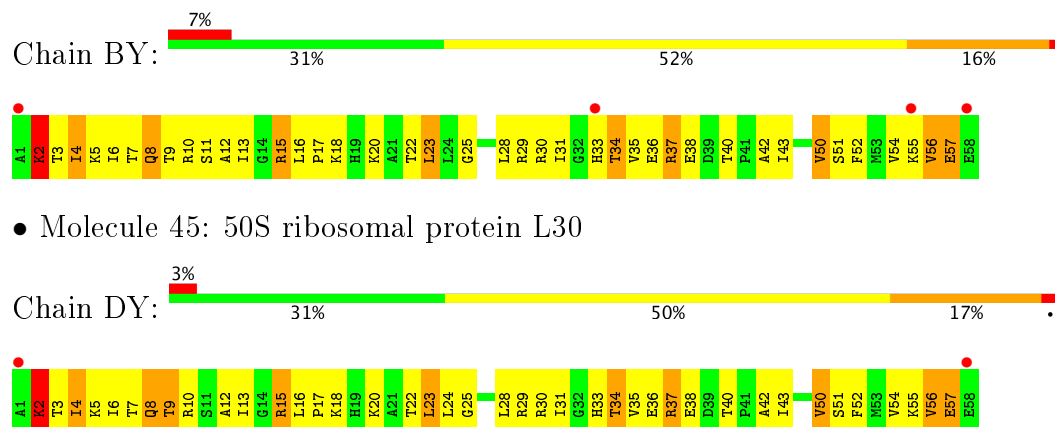
- Molecule 44: 50S ribosomal protein L29



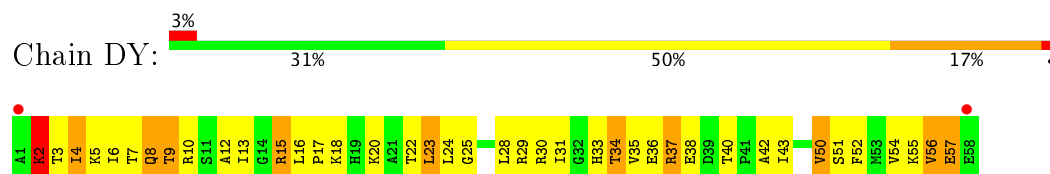
- Molecule 44: 50S ribosomal protein L29



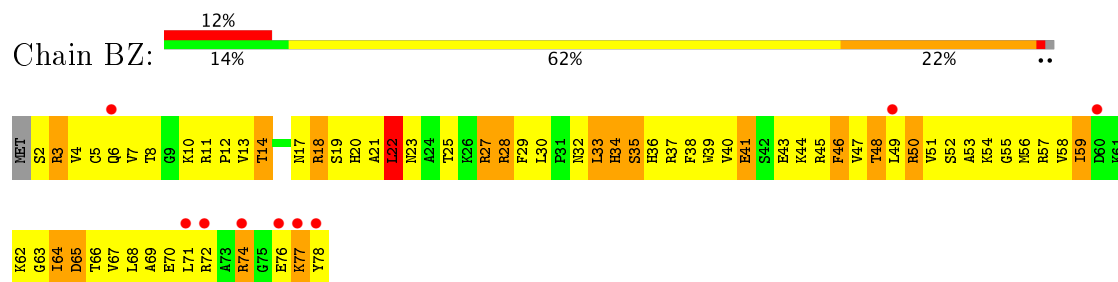
- Molecule 45: 50S ribosomal protein L30



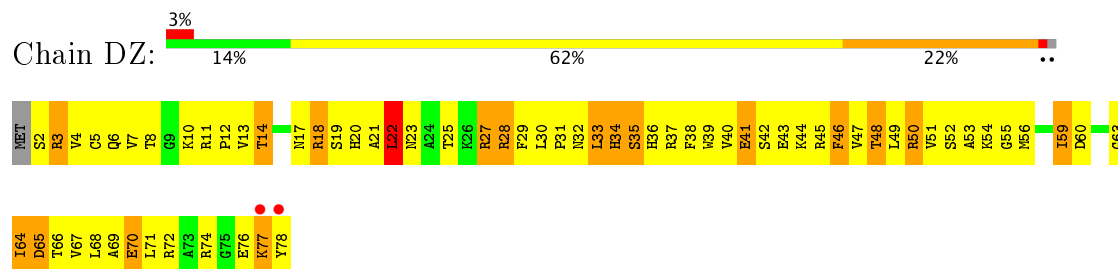
- Molecule 45: 50S ribosomal protein L30



- Molecule 46: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L32





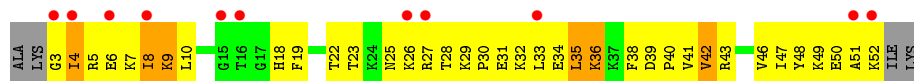
- Molecule 47: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L33



- Molecule 48: 50S ribosomal protein L33



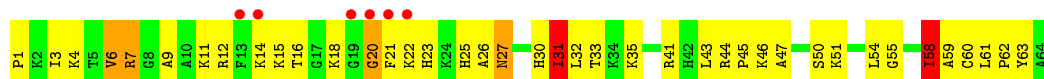
- Molecule 49: 50S ribosomal protein L34



- Molecule 49: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L35



- Molecule 50: 50S ribosomal protein L35

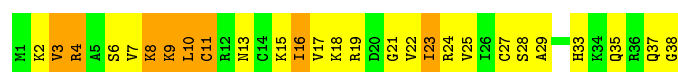




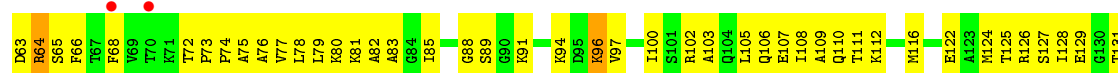
- Molecule 51: 50S ribosomal protein L36



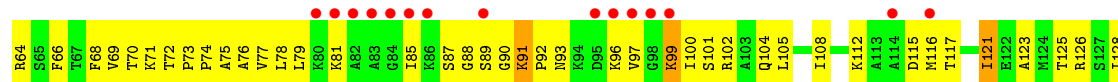
- Molecule 51: 50S ribosomal protein L36



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.49 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.269 , 0.318 0.241 , 0.286	Depositor DCC
R_{free} test set	22227 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	117.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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%)	1 11
2	CC	204/232 (88%)	148 (72%)	40 (20%)	16 (8%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	136 (67%)	52 (26%)	15 (7%)	1	14
3	CD	203/205 (99%)	134 (66%)	54 (27%)	15 (7%)	1	14
4	AE	148/166 (89%)	117 (79%)	27 (18%)	4 (3%)	6	40
4	CE	148/166 (89%)	117 (79%)	25 (17%)	6 (4%)	3	29
5	AF	98/135 (73%)	66 (67%)	21 (21%)	11 (11%)	0	6
5	CF	98/135 (73%)	67 (68%)	21 (21%)	10 (10%)	1	8
6	AG	148/178 (83%)	122 (82%)	18 (12%)	8 (5%)	2	22
6	CG	150/178 (84%)	124 (83%)	20 (13%)	6 (4%)	3	30
7	AH	127/129 (98%)	92 (72%)	26 (20%)	9 (7%)	1	15
7	CH	127/129 (98%)	90 (71%)	28 (22%)	9 (7%)	1	15
8	AI	125/129 (97%)	88 (70%)	29 (23%)	8 (6%)	1	18
8	CI	125/129 (97%)	88 (70%)	29 (23%)	8 (6%)	1	18
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	15
10	CK	115/128 (90%)	80 (70%)	27 (24%)	8 (7%)	1	15
11	AL	121/123 (98%)	78 (64%)	29 (24%)	14 (12%)	0	6
11	CL	121/123 (98%)	79 (65%)	28 (23%)	14 (12%)	0	6
12	AM	112/117 (96%)	72 (64%)	36 (32%)	4 (4%)	4	33
12	CM	111/117 (95%)	69 (62%)	38 (34%)	4 (4%)	4	33
13	AN	92/100 (92%)	57 (62%)	25 (27%)	10 (11%)	0	7
13	CN	92/100 (92%)	56 (61%)	26 (28%)	10 (11%)	0	7
14	AO	86/89 (97%)	65 (76%)	16 (19%)	5 (6%)	2	20
14	CO	86/89 (97%)	65 (76%)	16 (19%)	5 (6%)	2	20
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	5
16	AQ	78/83 (94%)	56 (72%)	17 (22%)	5 (6%)	1	18
16	CQ	79/83 (95%)	56 (71%)	17 (22%)	6 (8%)	1	13
17	AR	53/74 (72%)	41 (77%)	10 (19%)	2 (4%)	4	31
17	CR	53/74 (72%)	41 (77%)	10 (19%)	2 (4%)	4	31
18	AS	77/91 (85%)	58 (75%)	17 (22%)	2 (3%)	6	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CS	78/91 (86%)	58 (74%)	18 (23%)	2 (3%)	6	40
19	AT	83/86 (96%)	59 (71%)	19 (23%)	5 (6%)	2	19
19	CT	83/86 (96%)	59 (71%)	19 (23%)	5 (6%)	2	19
20	AB	216/240 (90%)	143 (66%)	53 (24%)	20 (9%)	1	9
20	CB	216/240 (90%)	148 (68%)	46 (21%)	22 (10%)	1	8
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	18
24	DV	92/94 (98%)	62 (67%)	24 (26%)	6 (6%)	1	18
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	6
27	DE	199/201 (99%)	120 (60%)	56 (28%)	23 (12%)	0	6
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	1
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	4
34	DM	134/136 (98%)	78 (58%)	35 (26%)	21 (16%)	0	3
35	BN	118/127 (93%)	73 (62%)	33 (28%)	12 (10%)	1	8
35	DN	118/127 (93%)	73 (62%)	32 (27%)	13 (11%)	0	7

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

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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%)	5	38
52	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	4	33
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%)	3	19
2	CC	170/189 (90%)	145 (85%)	25 (15%)	3	20
3	AD	172/172 (100%)	148 (86%)	24 (14%)	4	22
3	CD	172/172 (100%)	149 (87%)	23 (13%)	4	24
4	AE	113/125 (90%)	100 (88%)	13 (12%)	6	30
4	CE	113/125 (90%)	98 (87%)	15 (13%)	4	24
5	AF	87/116 (75%)	76 (87%)	11 (13%)	5	26
5	CF	87/116 (75%)	75 (86%)	12 (14%)	4	23
6	AG	123/146 (84%)	108 (88%)	15 (12%)	6	27
6	CG	125/146 (86%)	108 (86%)	17 (14%)	4	23
7	AH	104/104 (100%)	96 (92%)	8 (8%)	15	50
7	CH	104/104 (100%)	96 (92%)	8 (8%)	15	50
8	AI	105/106 (99%)	94 (90%)	11 (10%)	8	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/106 (99%)	93 (89%)	12 (11%)	7	31
9	AJ	86/90 (96%)	79 (92%)	7 (8%)	14	48
9	CJ	86/90 (96%)	80 (93%)	6 (7%)	18	55
10	AK	90/98 (92%)	77 (86%)	13 (14%)	4	21
10	CK	90/98 (92%)	77 (86%)	13 (14%)	4	21
11	AL	103/103 (100%)	85 (82%)	18 (18%)	2	13
11	CL	103/103 (100%)	84 (82%)	19 (18%)	2	10
12	AM	92/95 (97%)	82 (89%)	10 (11%)	7	33
12	CM	91/95 (96%)	82 (90%)	9 (10%)	9	38
13	AN	79/83 (95%)	67 (85%)	12 (15%)	3	19
13	CN	79/83 (95%)	67 (85%)	12 (15%)	3	19
14	AO	76/77 (99%)	69 (91%)	7 (9%)	11	41
14	CO	76/77 (99%)	70 (92%)	6 (8%)	14	49
15	AP	65/65 (100%)	57 (88%)	8 (12%)	5	27
15	CP	65/65 (100%)	57 (88%)	8 (12%)	5	27
16	AQ	74/77 (96%)	65 (88%)	9 (12%)	6	27
16	CQ	75/77 (97%)	65 (87%)	10 (13%)	4	24
17	AR	48/64 (75%)	46 (96%)	2 (4%)	34	70
17	CR	48/64 (75%)	46 (96%)	2 (4%)	34	70
18	AS	70/78 (90%)	52 (74%)	18 (26%)	0	4
18	CS	71/78 (91%)	53 (75%)	18 (25%)	0	4
19	AT	65/65 (100%)	53 (82%)	12 (18%)	2	10
19	CT	65/65 (100%)	53 (82%)	12 (18%)	2	10
20	AB	180/198 (91%)	152 (84%)	28 (16%)	3	18
20	CB	180/198 (91%)	150 (83%)	30 (17%)	2	14
21	AU	44/61 (72%)	35 (80%)	9 (20%)	1	7
21	CU	44/61 (72%)	35 (80%)	9 (20%)	1	7
24	BV	78/78 (100%)	68 (87%)	10 (13%)	5	25
24	DV	78/78 (100%)	69 (88%)	9 (12%)	6	30
25	BC	216/218 (99%)	178 (82%)	38 (18%)	2	12
25	DC	216/218 (99%)	175 (81%)	41 (19%)	2	9

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DT	80/84 (95%)	62 (78%)	18 (22%)	1	5
42	BU	83/84 (99%)	67 (81%)	16 (19%)	1	9
42	DU	83/84 (99%)	67 (81%)	16 (19%)	1	9
43	BW	59/62 (95%)	42 (71%)	17 (29%)	0	3
43	DW	59/62 (95%)	42 (71%)	17 (29%)	0	3
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	14
45	DY	48/48 (100%)	40 (83%)	8 (17%)	2	14
46	BZ	67/68 (98%)	54 (81%)	13 (19%)	1	8
46	DZ	67/68 (98%)	53 (79%)	14 (21%)	1	7
47	B0	47/47 (100%)	39 (83%)	8 (17%)	2	14
47	D0	47/47 (100%)	40 (85%)	7 (15%)	3	20
48	B1	45/48 (94%)	40 (89%)	5 (11%)	7	32
48	D1	45/48 (94%)	41 (91%)	4 (9%)	11	43
49	B2	38/38 (100%)	32 (84%)	6 (16%)	3	17
49	D2	38/38 (100%)	32 (84%)	6 (16%)	3	17
50	B3	51/51 (100%)	46 (90%)	5 (10%)	9	38
50	D3	51/51 (100%)	46 (90%)	5 (10%)	9	38
51	B4	34/34 (100%)	32 (94%)	2 (6%)	23	61
51	D4	34/34 (100%)	32 (94%)	2 (6%)	23	61
52	BI	109/109 (100%)	108 (99%)	1 (1%)	82	93
52	DI	109/109 (100%)	103 (94%)	6 (6%)	25	62
All	All	9333/9704 (96%)	7895 (85%)	1438 (15%)	3	18

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	AA	2059	-	35,39,39	1.33	4 (11%)	41,60,60	1.51	6 (14%)
54	HYG	CA	2062	-	35,39,39	1.36	6 (17%)	41,60,60	1.51	6 (14%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CA	2062	HYG	O22-C17	-2.41	1.38	1.43
54	CA	2062	HYG	C3-C4	2.01	1.56	1.53
54	CA	2062	HYG	C1-C6	2.04	1.57	1.52
54	AA	2059	HYG	C1-C6	2.05	1.57	1.52
54	AA	2059	HYG	C16-C15	2.11	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	2062	HYG	O8-C1-C2	-4.36	101.78	109.82
54	AA	2059	HYG	O8-C1-C2	-4.34	101.81	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	2062	HYG	O35-C34-C33	-3.50	103.94	111.44
54	AA	2059	HYG	O35-C34-C33	-3.48	103.97	111.44
54	AA	2059	HYG	C26-C25-C24	-2.20	108.22	111.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	AA	1530/1542 (99%)	-0.72	7 (0%)	90	86	16, 85, 158, 180	0
1	CA	1530/1542 (99%)	-0.74	5 (0%)	93	90	8, 57, 142, 180	0
2	AC	206/232 (88%)	0.84	29 (14%)	3	4	8, 89, 145, 180	0
2	CC	206/232 (88%)	0.31	16 (7%)	14	13	15, 81, 138, 180	0
3	AD	205/205 (100%)	0.63	25 (12%)	5	6	19, 97, 160, 180	0
3	CD	205/205 (100%)	-0.03	3 (1%)	74	66	5, 63, 135, 180	0
4	AE	150/166 (90%)	0.16	6 (4%)	39	32	5, 76, 136, 167	0
4	CE	150/166 (90%)	0.86	24 (16%)	2	3	5, 62, 135, 175	0
5	AF	100/135 (74%)	1.19	28 (28%)	1	1	13, 81, 137, 180	0
5	CF	100/135 (74%)	0.35	3 (3%)	51	42	14, 78, 126, 166	0
6	AG	150/178 (84%)	0.38	22 (14%)	3	3	41, 110, 166, 180	0
6	CG	152/178 (85%)	0.17	12 (7%)	13	13	27, 98, 156, 177	0
7	AH	129/129 (100%)	0.24	10 (7%)	14	13	26, 91, 148, 180	0
7	CH	129/129 (100%)	0.28	12 (9%)	9	10	5, 53, 117, 153	0
8	AI	127/129 (98%)	0.85	27 (21%)	1	1	32, 103, 160, 180	0
8	CI	127/129 (98%)	0.65	14 (11%)	6	7	32, 103, 162, 180	0
9	AJ	98/103 (95%)	0.85	12 (12%)	5	6	34, 106, 162, 180	0
9	CJ	98/103 (95%)	1.22	28 (28%)	1	1	42, 107, 156, 180	0
10	AK	117/128 (91%)	-0.06	2 (1%)	70	62	5, 71, 122, 174	0
10	CK	117/128 (91%)	0.12	5 (4%)	36	29	5, 57, 112, 179	0
11	AL	123/123 (100%)	0.52	16 (13%)	4	5	15, 82, 132, 153	0
11	CL	123/123 (100%)	-0.04	3 (2%)	59	50	5, 44, 109, 165	0
12	AM	114/117 (97%)	0.68	17 (14%)	3	3	68, 130, 178, 180	0
12	CM	113/117 (96%)	0.02	4 (3%)	44	38	32, 108, 156, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.56	10 (10%) 7 8	32, 103, 161, 180	0
13	CN	96/100 (96%)	0.18	6 (6%) 21 17	38, 99, 137, 171	0
14	AO	88/89 (98%)	0.40	4 (4%) 34 27	35, 83, 132, 180	0
14	CO	88/89 (98%)	-0.03	2 (2%) 61 51	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%)	0.08	4 (5%) 30 24	5, 51, 143, 164	0
16	AQ	80/83 (96%)	1.10	18 (22%) 1 1	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%) 26 21	16, 78, 142, 152	0
17	CR	55/74 (74%)	0.72	5 (9%) 10 10	13, 69, 132, 149	0
18	AS	79/91 (86%)	1.08	23 (29%) 1 1	67, 128, 175, 180	0
18	CS	80/91 (87%)	-0.12	3 (3%) 41 35	49, 113, 171, 180	0
19	AT	85/86 (98%)	0.02	3 (3%) 44 38	43, 100, 153, 175	0
19	CT	85/86 (98%)	-0.18	0 100 100	14, 58, 121, 177	0
20	AB	218/240 (90%)	0.28	23 (10%) 7 8	30, 102, 152, 180	0
20	CB	218/240 (90%)	1.41	71 (32%) 0 0	26, 106, 160, 180	0
21	AU	51/71 (71%)	0.37	2 (3%) 40 33	26, 102, 172, 180	0
21	CU	51/71 (71%)	0.77	8 (15%) 2 3	19, 85, 151, 180	0
22	BA	117/120 (97%)	-0.77	1 (0%) 84 77	43, 83, 131, 173	0
22	DA	117/120 (97%)	-0.82	1 (0%) 84 77	32, 75, 118, 180	0
23	BB	2841/2904 (97%)	-0.49	15 (0%) 90 86	6, 56, 146, 180	0
23	DB	2841/2904 (97%)	-0.53	7 (0%) 94 93	5, 40, 139, 180	0
24	BV	94/94 (100%)	0.09	5 (5%) 27 22	11, 96, 146, 176	0
24	DV	94/94 (100%)	-0.10	3 (3%) 48 40	14, 86, 143, 180	0
25	BC	271/273 (99%)	0.66	29 (10%) 7 7	7, 48, 104, 170	0
25	DC	271/273 (99%)	0.46	23 (8%) 11 12	5, 28, 81, 120	0
26	BD	209/209 (100%)	0.52	27 (12%) 4 5	5, 73, 138, 180	0
26	DD	209/209 (100%)	0.43	21 (10%) 8 8	5, 42, 118, 180	0
27	BE	201/201 (100%)	0.80	24 (11%) 5 6	5, 65, 142, 180	0
27	DE	201/201 (100%)	0.35	12 (5%) 23 19	5, 67, 135, 180	0
28	BF	178/178 (100%)	1.40	54 (30%) 0 1	50, 116, 175, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	178/178 (100%)	1.08	34 (19%) 1 1	7, 101, 172, 180	0
29	BG	176/176 (100%)	0.64	23 (13%) 4 5	23, 102, 155, 180	0
29	DG	176/176 (100%)	0.19	11 (6%) 21 17	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%)	0.53	13 (8%) 11 11	11, 100, 156, 180	0
31	BJ	142/142 (100%)	0.35	8 (5%) 25 21	6, 80, 141, 171	0
31	DJ	142/142 (100%)	0.31	8 (5%) 25 21	5, 60, 119, 165	0
32	BK	121/123 (98%)	1.75	45 (37%) 0 0	5, 73, 135, 180	0
32	DK	121/123 (98%)	0.56	11 (9%) 10 10	5, 35, 102, 145	0
33	BL	143/144 (99%)	0.03	5 (3%) 44 38	10, 64, 128, 180	0
33	DL	143/144 (99%)	0.54	18 (12%) 4 5	5, 54, 118, 162	0
34	BM	136/136 (100%)	0.07	5 (3%) 42 35	8, 70, 129, 172	0
34	DM	136/136 (100%)	0.75	19 (13%) 3 4	5, 51, 114, 168	0
35	BN	120/127 (94%)	0.49	12 (10%) 8 8	7, 67, 132, 163	0
35	DN	120/127 (94%)	-0.09	1 (0%) 86 79	5, 42, 86, 145	0
36	BO	116/117 (99%)	0.77	28 (24%) 1 1	27, 87, 135, 156	0
36	DO	116/117 (99%)	-0.04	1 (0%) 84 77	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%)	0.15	4 (3%) 44 38	5, 48, 107, 159	0
38	BQ	117/117 (100%)	-0.18	4 (3%) 46 38	5, 63, 127, 180	0
38	DQ	117/117 (100%)	0.41	5 (4%) 36 29	5, 48, 116, 150	0
39	BR	103/103 (100%)	-0.02	5 (4%) 30 24	16, 82, 145, 158	0
39	DR	103/103 (100%)	0.54	9 (8%) 11 11	5, 73, 136, 180	0
40	BS	110/110 (100%)	0.40	7 (6%) 20 17	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%)	0.01	1 (1%) 80 72	6, 72, 139, 179	0
41	DT	93/100 (93%)	0.79	16 (17%) 2 2	11, 64, 156, 180	0
42	BU	102/103 (99%)	1.23	25 (24%) 1 1	5, 78, 144, 178	0
42	DU	102/103 (99%)	0.08	2 (1%) 65 57	10, 90, 154, 180	0
43	BW	79/84 (94%)	0.35	5 (6%) 21 17	10, 79, 157, 163	0
43	DW	79/84 (94%)	0.16	4 (5%) 29 23	5, 75, 131, 174	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	63/63 (100%)	0.89	13 (20%) 1 1	9, 74, 146, 179	0
44	DX	63/63 (100%)	0.51	4 (6%) 21 17	17, 96, 147, 180	0
45	BY	58/58 (100%)	0.32	4 (6%) 18 15	14, 78, 135, 170	0
45	DY	58/58 (100%)	-0.08	2 (3%) 46 38	10, 73, 129, 160	0
46	BZ	77/78 (98%)	0.60	9 (11%) 5 6	5, 49, 121, 160	0
46	DZ	77/78 (98%)	-0.02	2 (2%) 56 47	5, 42, 107, 141	0
47	B0	56/56 (100%)	0.43	5 (8%) 10 10	5, 77, 144, 166	0
47	D0	56/56 (100%)	0.27	3 (5%) 26 22	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%)	1.44	11 (22%) 1 1	43, 93, 138, 171	0
49	B2	46/46 (100%)	0.42	2 (4%) 36 29	7, 49, 103, 135	0
49	D2	46/46 (100%)	0.18	1 (2%) 62 53	5, 28, 99, 180	0
50	B3	64/64 (100%)	0.60	6 (9%) 9 9	16, 56, 110, 137	0
50	D3	64/64 (100%)	0.35	5 (7%) 14 13	5, 43, 112, 152	0
51	B4	38/38 (100%)	0.15	1 (2%) 56 47	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 2	67, 169, 180, 180	0
52	DI	141/141 (100%)	0.83	23 (16%) 2 2	91, 160, 180, 180	0
All	All	20417/21050 (96%)	0.03	1362 (6%) 19 16	5, 70, 153, 180	0

The worst 5 of 1362 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	AP	80	LYS	9.6
48	D1	52	LYS	9.6
30	BH	84	ALA	9.6
15	AP	81	ALA	9.4
30	BH	45	GLU	8.9

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
53	MG	AA	2023	1/1	0.54	0.35	9.31	66,66,66,66	1
53	MG	BB	3097	1/1	0.88	0.18	4.08	114,114,114,114	0
53	MG	CA	2045	1/1	0.98	0.16	2.97	48,48,48,48	0
53	MG	CA	2020	1/1	0.96	0.21	2.72	73,73,73,73	0
54	HYG	CA	2062	36/36	0.91	0.22	2.29	45,45,45,45	0
53	MG	BB	3086	1/1	0.98	0.25	2.05	42,42,42,42	0
53	MG	CA	2038	1/1	0.83	0.12	1.73	128,128,128,128	0
53	MG	BB	3083	1/1	0.95	0.22	1.40	12,12,12,12	0
53	MG	DB	3099	1/1	0.98	0.19	1.37	7,7,7,7	0
54	HYG	AA	2059	36/36	0.90	0.24	1.10	52,52,52,52	0
53	MG	AA	2033	1/1	0.79	0.11	0.90	99,99,99,99	0
53	MG	BB	3040	1/1	0.98	0.18	0.90	26,26,26,26	0
53	MG	AA	2028	1/1	0.95	0.17	0.47	100,100,100,100	0
53	MG	BB	3081	1/1	0.86	0.22	0.43	46,46,46,46	0
53	MG	CA	2036	1/1	0.94	0.17	0.34	101,101,101,101	0
53	MG	CA	2033	1/1	0.94	0.15	0.34	56,56,56,56	0
53	MG	DB	3003	1/1	0.96	0.19	0.27	63,63,63,63	0
53	MG	AA	2014	1/1	0.68	0.22	0.22	112,112,112,112	0
53	MG	DB	3051	1/1	0.98	0.19	-0.02	23,23,23,23	0
53	MG	DB	3089	1/1	0.98	0.17	-0.32	7,7,7,7	0
53	MG	BB	3011	1/1	0.98	0.19	-0.37	5,5,5,5	0
53	MG	BB	3087	1/1	0.96	0.16	-0.40	57,57,57,57	0
53	MG	AA	2031	1/1	0.75	0.09	-0.46	58,58,58,58	0
53	MG	BB	3062	1/1	0.97	0.17	-0.52	14,14,14,14	0
53	MG	AN	201	1/1	0.72	0.12	-0.53	69,69,69,69	0
53	MG	DB	3110	1/1	0.95	0.14	-0.57	21,21,21,21	0
53	MG	DB	3087	1/1	0.97	0.15	-0.61	53,53,53,53	0
53	MG	BB	3005	1/1	0.97	0.19	-0.75	5,5,5,5	0
53	MG	BB	3085	1/1	0.93	0.17	-0.78	103,103,103,103	0
53	MG	CA	2039	1/1	0.98	0.12	-0.82	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3099	1/1	0.85	0.17	-0.90	40,40,40,40	0
53	MG	DB	3030	1/1	0.97	0.17	-0.97	6,6,6,6	0
53	MG	DB	3007	1/1	0.97	0.14	-1.02	18,18,18,18	0
53	MG	BB	3098	1/1	0.96	0.15	-1.03	35,35,35,35	0
53	MG	DB	3100	1/1	0.97	0.16	-1.15	13,13,13,13	0
53	MG	BB	3090	1/1	0.97	0.12	-1.16	112,112,112,112	0
53	MG	BB	3018	1/1	0.99	0.14	-1.25	32,32,32,32	0
53	MG	DB	3084	1/1	0.98	0.17	-1.25	5,5,5,5	0
53	MG	DB	3092	1/1	0.91	0.13	-1.26	66,66,66,66	0
53	MG	AA	2049	1/1	0.91	0.06	-1.26	75,75,75,75	0
53	MG	DB	3088	1/1	0.97	0.14	-1.41	25,25,25,25	0
53	MG	CA	2053	1/1	0.99	0.06	-1.42	30,30,30,30	0
53	MG	CA	2016	1/1	0.95	0.04	-1.50	53,53,53,53	0
53	MG	AA	2034	1/1	0.97	0.06	-1.54	68,68,68,68	0
53	MG	BB	3037	1/1	0.86	0.11	-1.54	23,23,23,23	0
53	MG	DB	3078	1/1	0.97	0.08	-1.54	27,27,27,27	0
53	MG	DB	3047	1/1	0.96	0.17	-1.57	14,14,14,14	0
53	MG	CA	2012	1/1	0.99	0.08	-1.62	93,93,93,93	0
53	MG	CA	2014	1/1	0.90	0.07	-1.66	47,47,47,47	0
53	MG	CA	2017	1/1	0.98	0.11	-1.74	5,5,5,5	0
53	MG	DB	3096	1/1	0.98	0.12	-1.76	6,6,6,6	0
53	MG	AA	2040	1/1	0.97	0.09	-1.80	83,83,83,83	0
53	MG	BB	3013	1/1	0.97	0.10	-1.86	43,43,43,43	0
55	ZN	B4	101	1/1	0.97	0.04	-1.91	80,80,80,80	0
53	MG	AA	2007	1/1	0.95	0.06	-1.92	31,31,31,31	0
53	MG	BB	3082	1/1	0.96	0.16	-1.94	46,46,46,46	0
53	MG	DB	3069	1/1	0.98	0.18	-2.02	11,11,11,11	0
53	MG	BB	3059	1/1	0.98	0.12	-2.05	26,26,26,26	0
53	MG	BB	3023	1/1	0.97	0.14	-2.15	5,5,5,5	0
55	ZN	D4	101	1/1	0.98	0.06	-2.18	46,46,46,46	0
53	MG	BB	3012	1/1	0.98	0.09	-2.39	32,32,32,32	0
53	MG	BB	3048	1/1	0.92	0.11	-2.45	44,44,44,44	0
53	MG	BB	3021	1/1	0.95	0.08	-2.46	30,30,30,30	0
53	MG	AA	2009	1/1	0.96	0.10	-2.51	7,7,7,7	0
53	MG	CA	2005	1/1	0.97	0.09	-2.78	24,24,24,24	0
53	MG	BB	3103	1/1	0.98	0.08	-2.82	5,5,5,5	0
53	MG	DB	3006	1/1	0.98	0.10	-2.87	5,5,5,5	0
53	MG	DB	3022	1/1	0.97	0.08	-2.93	25,25,25,25	0
53	MG	CA	2056	1/1	0.98	0.05	-2.98	5,5,5,5	0
53	MG	DB	3070	1/1	0.97	0.08	-3.00	45,45,45,45	0
53	MG	DB	3074	1/1	0.95	0.09	-3.00	12,12,12,12	0
53	MG	AA	2001	1/1	0.93	0.07	-3.01	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	2040	1/1	0.96	0.09	-3.01	48,48,48,48	0
53	MG	BB	3032	1/1	0.93	0.10	-3.05	56,56,56,56	0
53	MG	BB	3066	1/1	0.97	0.12	-3.10	23,23,23,23	0
53	MG	DB	3103	1/1	0.97	0.13	-3.11	27,27,27,27	0
53	MG	AA	2051	1/1	0.91	0.10	-3.12	41,41,41,41	0
53	MG	DB	3111	1/1	0.96	0.09	-3.18	38,38,38,38	0
53	MG	AA	2036	1/1	0.97	0.04	-3.39	31,31,31,31	0
53	MG	CA	2004	1/1	0.97	0.09	-3.42	8,8,8,8	0
53	MG	DB	3044	1/1	0.93	0.11	-3.49	24,24,24,24	0
53	MG	DB	3035	1/1	0.96	0.06	-3.58	55,55,55,55	0
53	MG	DB	3019	1/1	0.99	0.09	-3.58	5,5,5,5	0
53	MG	BB	3001	1/1	0.94	0.10	-3.64	51,51,51,51	0
53	MG	BB	3108	1/1	0.98	0.10	-3.71	47,47,47,47	0
53	MG	DB	3085	1/1	0.99	0.12	-3.76	5,5,5,5	0
53	MG	DB	3080	1/1	0.95	0.10	-3.83	10,10,10,10	0
53	MG	BB	3069	1/1	0.97	0.11	-3.86	17,17,17,17	0
53	MG	DB	3014	1/1	0.99	0.05	-3.87	5,5,5,5	0
53	MG	BB	3088	1/1	0.95	0.06	-3.95	28,28,28,28	0
53	MG	BB	3065	1/1	0.97	0.06	-3.99	29,29,29,29	0
53	MG	AA	2052	1/1	0.91	0.07	-4.00	78,78,78,78	0
53	MG	DB	3090	1/1	0.88	0.08	-4.02	37,37,37,37	0
53	MG	BB	3056	1/1	0.96	0.08	-4.09	26,26,26,26	0
53	MG	DB	3055	1/1	0.97	0.11	-4.13	26,26,26,26	0
53	MG	DB	3001	1/1	0.99	0.10	-4.81	5,5,5,5	0
53	MG	DB	3068	1/1	0.98	0.10	-4.96	5,5,5,5	0
53	MG	DB	3056	1/1	0.97	0.09	-5.10	5,5,5,5	0
53	MG	BB	3029	1/1	0.97	0.07	-5.19	14,14,14,14	0
53	MG	BB	3052	1/1	0.90	0.08	-5.71	38,38,38,38	0
53	MG	CA	2044	1/1	0.96	0.07	-5.89	59,59,59,59	0
53	MG	BB	3019	1/1	0.98	0.05	-6.02	22,22,22,22	0
53	MG	CA	2018	1/1	0.99	0.03	-6.04	6,6,6,6	0
53	MG	AA	2010	1/1	0.97	0.04	-6.26	60,60,60,60	0
53	MG	CA	2001	1/1	0.98	0.05	-7.01	5,5,5,5	0
53	MG	AA	2041	1/1	0.96	0.07	-7.04	83,83,83,83	0
53	MG	DB	3002	1/1	0.98	0.07	-8.03	12,12,12,12	0
53	MG	BB	3035	1/1	0.97	0.07	-8.14	15,15,15,15	0
53	MG	BB	3002	1/1	0.99	0.07	-8.43	5,5,5,5	0
53	MG	DB	3010	1/1	0.97	0.08	-9.61	8,8,8,8	0
53	MG	CA	2055	1/1	0.98	0.07	-9.77	11,11,11,11	0
53	MG	BB	3094	1/1	0.98	0.07	-10.47	28,28,28,28	0
53	MG	DB	3009	1/1	0.97	0.07	-14.19	29,29,29,29	0
53	MG	AA	2035	1/1	0.83	0.34	-	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	2037	1/1	0.58	0.33	-	138,138,138,138	0
53	MG	DB	3095	1/1	0.86	0.15	-	89,89,89,89	0
53	MG	CA	2050	1/1	0.99	0.11	-	8,8,8,8	0
53	MG	BB	3067	1/1	0.98	0.09	-	44,44,44,44	0
53	MG	DB	3036	1/1	0.91	0.09	-	30,30,30,30	0
53	MG	AA	2056	1/1	0.79	0.12	-	124,124,124,124	0
53	MG	AE	201	1/1	0.79	0.07	-	144,144,144,144	0
53	MG	BB	3079	1/1	0.98	0.04	-	19,19,19,19	0
53	MG	CA	2031	1/1	0.99	0.06	-	28,28,28,28	0
53	MG	DB	3033	1/1	0.97	0.08	-	9,9,9,9	0
53	MG	DB	3058	1/1	0.93	0.33	-	151,151,151,151	0
53	MG	BB	3101	1/1	0.98	0.09	-	24,24,24,24	0
53	MG	DB	3102	1/1	0.98	0.09	-	12,12,12,12	0
53	MG	BB	3063	1/1	0.95	0.09	-	11,11,11,11	0
53	MG	CA	2037	1/1	0.93	0.09	-	94,94,94,94	0
53	MG	AA	2022	1/1	0.95	0.07	-	82,82,82,82	0
53	MG	DB	3104	1/1	0.98	0.08	-	33,33,33,33	0
53	MG	BB	3096	1/1	0.97	0.11	-	34,34,34,34	0
53	MG	AA	2047	1/1	0.74	0.04	-	100,100,100,100	0
53	MG	BB	3046	1/1	0.93	0.11	-	22,22,22,22	0
53	MG	CA	2051	1/1	0.98	0.05	-	39,39,39,39	0
53	MG	DB	3057	1/1	0.96	0.06	-	71,71,71,71	0
53	MG	DB	3017	1/1	0.98	0.10	-	13,13,13,13	0
53	MG	AA	2042	1/1	0.96	0.09	-	69,69,69,69	0
53	MG	DB	3023	1/1	0.90	0.08	-	32,32,32,32	0
53	MG	DB	3091	1/1	0.99	0.18	-	13,13,13,13	0
53	MG	DB	3105	1/1	0.97	0.14	-	23,23,23,23	0
53	MG	BB	3084	1/1	0.98	0.16	-	24,24,24,24	0
53	MG	BB	3030	1/1	0.99	0.03	-	35,35,35,35	0
53	MG	DB	3052	1/1	0.94	0.12	-	100,100,100,100	0
53	MG	DB	3076	1/1	0.99	0.10	-	5,5,5,5	0
53	MG	CA	2013	1/1	0.97	0.08	-	73,73,73,73	0
53	MG	BB	3055	1/1	0.94	0.15	-	17,17,17,17	0
53	MG	CA	2035	1/1	0.90	0.08	-	89,89,89,89	0
53	MG	DB	3081	1/1	0.99	0.13	-	18,18,18,18	0
53	MG	CA	2027	1/1	0.69	0.13	-	50,50,50,50	1
53	MG	DB	3106	1/1	0.98	0.13	-	23,23,23,23	0
53	MG	DB	3005	1/1	0.95	0.12	-	10,10,10,10	0
53	MG	BB	3071	1/1	0.90	0.09	-	26,26,26,26	0
53	MG	CA	2003	1/1	0.99	0.04	-	35,35,35,35	0
53	MG	BB	3014	1/1	0.91	0.05	-	50,50,50,50	0
53	MG	BB	3042	1/1	0.13	0.10	-	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	2022	1/1	0.97	0.10	-	63,63,63,63	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	CA	2060	1/1	0.81	0.05	-	80,80,80,80	0
53	MG	BB	3102	1/1	0.95	0.12	-	20,20,20,20	0
53	MG	AA	2046	1/1	0.93	0.07	-	5,5,5,5	0
53	MG	BB	3061	1/1	0.95	0.04	-	48,48,48,48	0
53	MG	DB	3071	1/1	0.96	0.06	-	16,16,16,16	0
53	MG	DB	3098	1/1	0.99	0.22	-	44,44,44,44	0
53	MG	BB	3073	1/1	0.98	0.09	-	39,39,39,39	0
53	MG	BB	3036	1/1	0.95	0.11	-	42,42,42,42	0
53	MG	AA	2018	1/1	0.82	0.09	-	131,131,131,131	0
53	MG	BB	3058	1/1	0.97	0.10	-	22,22,22,22	0
53	MG	BB	3041	1/1	0.99	0.08	-	7,7,7,7	0
53	MG	AA	2025	1/1	0.95	0.17	-	58,58,58,58	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	DB	3093	1/1	0.96	0.22	-	11,11,11,11	0
53	MG	BB	3109	1/1	0.96	0.09	-	54,54,54,54	0
53	MG	AA	2050	1/1	0.87	0.14	-	105,105,105,105	0
53	MG	DB	3094	1/1	0.97	0.03	-	29,29,29,29	0
53	MG	CA	2021	1/1	0.79	0.36	-	125,125,125,125	0
53	MG	DB	3079	1/1	0.98	0.14	-	28,28,28,28	0
53	MG	AA	2039	1/1	0.96	0.12	-	64,64,64,64	0
53	MG	BB	3039	1/1	0.94	0.18	-	7,7,7,7	0
53	MG	BB	3092	1/1	0.99	0.06	-	54,54,54,54	0
53	MG	CA	2054	1/1	0.91	0.08	-	104,104,104,104	0
53	MG	BB	3095	1/1	0.98	0.07	-	33,33,33,33	0
53	MG	BB	3054	1/1	0.93	0.06	-	77,77,77,77	0
53	MG	DB	3061	1/1	0.97	0.09	-	69,69,69,69	0
53	MG	AA	2044	1/1	0.88	0.12	-	112,112,112,112	0
53	MG	BB	3049	1/1	0.93	0.10	-	10,10,10,10	0
53	MG	DB	3107	1/1	0.98	0.07	-	10,10,10,10	0
53	MG	BB	3076	1/1	0.99	0.05	-	38,38,38,38	0
53	MG	BB	3106	1/1	0.99	0.12	-	62,62,62,62	0
53	MG	BB	3074	1/1	0.97	0.07	-	28,28,28,28	0
53	MG	DB	3043	1/1	0.98	0.11	-	5,5,5,5	0
53	MG	DB	3031	1/1	0.98	0.18	-	8,8,8,8	0
53	MG	CA	2008	1/1	0.83	0.09	-	93,93,93,93	0
53	MG	DB	3086	1/1	0.97	0.14	-	11,11,11,11	0
53	MG	CA	2007	1/1	0.91	0.05	-	46,46,46,46	0
53	MG	DB	3062	1/1	0.98	0.04	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	2027	1/1	0.97	0.09	-	36,36,36,36	0
53	MG	CA	2042	1/1	0.87	0.08	-	58,58,58,58	0
53	MG	AA	2003	1/1	0.99	0.17	-	39,39,39,39	0
53	MG	BB	3044	1/1	0.98	0.15	-	53,53,53,53	0
53	MG	AA	2020	1/1	0.98	0.07	-	5,5,5,5	0
53	MG	AA	2011	1/1	0.97	0.07	-	85,85,85,85	0
53	MG	BB	3038	1/1	0.96	0.03	-	71,71,71,71	0
53	MG	BB	3047	1/1	0.95	0.06	-	75,75,75,75	0
53	MG	DB	3013	1/1	0.88	0.17	-	51,51,51,51	0
53	MG	DB	3046	1/1	0.95	0.09	-	24,24,24,24	0
53	MG	DB	3075	1/1	0.98	0.10	-	57,57,57,57	0
53	MG	DB	3038	1/1	0.97	0.12	-	5,5,5,5	0
53	MG	CA	2015	1/1	0.68	0.10	-	149,149,149,149	0
53	MG	BB	3072	1/1	0.98	0.12	-	17,17,17,17	0
53	MG	CA	2048	1/1	0.96	0.11	-	58,58,58,58	0
53	MG	DB	3063	1/1	0.98	0.12	-	43,43,43,43	0
53	MG	CA	2025	1/1	0.96	0.12	-	50,50,50,50	0
53	MG	BB	3051	1/1	0.92	0.14	-	35,35,35,35	0
53	MG	AA	2053	1/1	0.98	0.07	-	79,79,79,79	0
53	MG	AA	2048	1/1	0.96	0.03	-	99,99,99,99	0
53	MG	BB	3105	1/1	0.98	0.08	-	20,20,20,20	0
53	MG	CE	201	1/1	0.86	0.15	-	127,127,127,127	0
53	MG	BB	3025	1/1	0.98	0.13	-	30,30,30,30	0
53	MG	AA	2021	1/1	0.92	0.31	-	5,5,5,5	1
53	MG	BB	3075	1/1	0.97	0.21	-	40,40,40,40	0
53	MG	DB	3034	1/1	0.96	0.16	-	52,52,52,52	0
53	MG	BB	3064	1/1	0.95	0.07	-	35,35,35,35	0
53	MG	DB	3027	1/1	0.98	0.15	-	6,6,6,6	0
53	MG	AA	2006	1/1	0.95	0.03	-	60,60,60,60	0
53	MG	DB	3020	1/1	0.99	0.15	-	5,5,5,5	0
53	MG	DB	3083	1/1	0.98	0.16	-	85,85,85,85	0
53	MG	AA	2029	1/1	0.95	0.07	-	39,39,39,39	0
53	MG	DB	3077	1/1	0.98	0.21	-	54,54,54,54	0
53	MG	BB	3010	1/1	0.82	0.10	-	44,44,44,44	0
53	MG	CA	2049	1/1	0.95	0.06	-	74,74,74,74	0
53	MG	AA	2026	1/1	0.89	0.08	-	65,65,65,65	0
53	MG	DB	3108	1/1	0.96	0.09	-	37,37,37,37	0
53	MG	BB	3104	1/1	0.91	0.18	-	36,36,36,36	0
53	MG	DB	3015	1/1	0.94	0.07	-	33,33,33,33	0
53	MG	AA	2054	1/1	0.93	0.08	-	110,110,110,110	0
53	MG	AA	2019	1/1	0.79	0.05	-	107,107,107,107	0
53	MG	BB	3020	1/1	0.94	0.10	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	2058	1/1	0.94	0.11	-	106,106,106,106	0
53	MG	DB	3072	1/1	0.96	0.12	-	18,18,18,18	0
53	MG	BB	3017	1/1	0.90	0.14	-	34,34,34,34	0
53	MG	BB	3078	1/1	0.96	0.15	-	70,70,70,70	0
53	MG	DB	3109	1/1	0.97	0.10	-	9,9,9,9	0
53	MG	CA	2009	1/1	0.95	0.06	-	67,67,67,67	0
53	MG	BB	3026	1/1	0.97	0.08	-	39,39,39,39	0
53	MG	BB	3068	1/1	0.96	0.12	-	53,53,53,53	0
53	MG	DB	3064	1/1	0.98	0.05	-	20,20,20,20	0
53	MG	DB	3018	1/1	0.99	0.07	-	22,22,22,22	0
53	MG	AA	2017	1/1	0.91	0.12	-	87,87,87,87	0
53	MG	DB	3021	1/1	0.96	0.23	-	11,11,11,11	0
53	MG	AA	2045	1/1	0.92	0.64	-	92,92,92,92	0
53	MG	AA	2057	1/1	0.62	0.18	-	141,141,141,141	0
53	MG	DB	3039	1/1	0.97	0.04	-	22,22,22,22	0
53	MG	CA	2047	1/1	0.95	0.06	-	121,121,121,121	0
53	MG	CA	2061	1/1	0.97	0.08	-	23,23,23,23	0
53	MG	DB	3041	1/1	0.95	0.11	-	29,29,29,29	0
53	MG	CA	2057	1/1	0.79	0.10	-	99,99,99,99	0
53	MG	CA	2010	1/1	0.94	0.07	-	33,33,33,33	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	BB	3091	1/1	0.97	0.09	-	16,16,16,16	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	CA	2023	1/1	0.78	0.20	-	137,137,137,137	0
53	MG	CA	2024	1/1	0.95	0.06	-	29,29,29,29	0
53	MG	DB	3042	1/1	0.98	0.10	-	6,6,6,6	0
53	MG	CA	2019	1/1	0.94	0.10	-	73,73,73,73	0
53	MG	AA	2012	1/1	0.81	0.09	-	84,84,84,84	0
53	MG	DB	3050	1/1	0.92	0.08	-	90,90,90,90	0
53	MG	BB	3107	1/1	0.99	0.11	-	6,6,6,6	0
53	MG	BB	3100	1/1	0.72	0.20	-	129,129,129,129	0
53	MG	CA	2034	1/1	0.97	0.11	-	6,6,6,6	0
53	MG	AA	2038	1/1	0.96	0.11	-	71,71,71,71	0
53	MG	BB	3004	1/1	0.97	0.06	-	32,32,32,32	0
53	MG	BB	3028	1/1	0.98	0.20	-	86,86,86,86	0
53	MG	DB	3029	1/1	0.90	0.15	-	88,88,88,88	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	3057	1/1	0.94	0.20	-	28,28,28,28	0
53	MG	DB	3066	1/1	0.81	0.08	-	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3016	1/1	0.96	0.07	-	38,38,38,38	0
53	MG	DB	3049	1/1	0.98	0.09	-	36,36,36,36	0
53	MG	DB	3097	1/1	0.95	0.14	-	38,38,38,38	0
53	MG	AA	2004	1/1	0.92	0.13	-	56,56,56,56	0
53	MG	BB	3043	1/1	0.97	0.05	-	104,104,104,104	0
53	MG	BB	3031	1/1	0.93	0.14	-	41,41,41,41	0
53	MG	BB	3070	1/1	0.99	0.14	-	37,37,37,37	0
53	MG	BB	3009	1/1	0.97	0.04	-	46,46,46,46	0
53	MG	DB	3040	1/1	0.98	0.16	-	5,5,5,5	0
53	MG	AA	2032	1/1	0.93	0.08	-	62,62,62,62	0
53	MG	BB	3015	1/1	0.99	0.09	-	13,13,13,13	0
53	MG	AA	2055	1/1	0.83	0.20	-	102,102,102,102	0
53	MG	CA	2032	1/1	0.98	0.17	-	33,33,33,33	0
53	MG	CA	2028	1/1	0.93	0.07	-	75,75,75,75	0
53	MG	DB	3053	1/1	0.99	0.07	-	35,35,35,35	0
53	MG	DB	3082	1/1	0.97	0.10	-	30,30,30,30	0
53	MG	BB	3077	1/1	0.88	0.09	-	36,36,36,36	0
53	MG	BB	3006	1/1	0.98	0.07	-	5,5,5,5	0
53	MG	BB	3027	1/1	0.94	0.08	-	33,33,33,33	0
53	MG	BB	3093	1/1	0.93	0.23	-	71,71,71,71	0
53	MG	CA	2059	1/1	0.78	0.12	-	94,94,94,94	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	3026	1/1	0.96	0.08	-	34,34,34,34	0
53	MG	AA	2002	1/1	0.94	0.06	-	99,99,99,99	0
53	MG	AA	2043	1/1	0.97	0.08	-	96,96,96,96	0
53	MG	DB	3032	1/1	0.96	0.09	-	63,63,63,63	0
53	MG	CA	2011	1/1	0.66	0.28	-	132,132,132,132	0
53	MG	BB	3024	1/1	0.93	0.12	-	15,15,15,15	0
53	MG	AA	2005	1/1	0.82	0.08	-	69,69,69,69	0
53	MG	BB	3060	1/1	0.97	0.13	-	19,19,19,19	0
53	MG	AA	2016	1/1	0.93	0.09	-	89,89,89,89	0
53	MG	AA	2058	1/1	0.96	0.14	-	86,86,86,86	0
53	MG	BB	3053	1/1	0.93	0.06	-	28,28,28,28	0
53	MG	CA	2026	1/1	0.83	0.19	-	26,26,26,26	1
53	MG	CA	2046	1/1	0.97	0.10	-	57,57,57,57	0
53	MG	DB	3008	1/1	0.98	0.18	-	6,6,6,6	0
53	MG	DB	3025	1/1	0.97	0.15	-	5,5,5,5	0
53	MG	BB	3089	1/1	0.98	0.15	-	56,56,56,56	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	2052	1/1	0.90	0.09	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3050	1/1	0.99	0.12	-	28,28,28,28	0
53	MG	DB	3059	1/1	0.80	0.12	-	180,180,180,180	0
53	MG	DB	3060	1/1	0.71	0.20	-	112,112,112,112	0
53	MG	BB	3110	1/1	0.99	0.15	-	23,23,23,23	0
53	MG	BB	3008	1/1	0.95	0.10	-	89,89,89,89	0
53	MG	BB	3033	1/1	0.93	0.34	-	125,125,125,125	0
53	MG	AA	2008	1/1	0.76	0.08	-	125,125,125,125	0
53	MG	AA	2024	1/1	0.87	0.08	-	5,5,5,5	1
53	MG	DB	3028	1/1	0.97	0.06	-	24,24,24,24	0
53	MG	CA	2043	1/1	0.95	0.04	-	19,19,19,19	0
53	MG	AA	2015	1/1	0.93	0.06	-	24,24,24,24	0
53	MG	CA	2029	1/1	0.90	0.05	-	23,23,23,23	1
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	DB	3012	1/1	0.99	0.20	-	9,9,9,9	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	BB	3080	1/1	0.81	0.18	-	39,39,39,39	0
53	MG	BB	3034	1/1	0.96	0.10	-	35,35,35,35	0
53	MG	AA	2030	1/1	0.90	0.09	-	99,99,99,99	0
53	MG	DB	3037	1/1	0.98	0.16	-	28,28,28,28	0
53	MG	DB	3067	1/1	0.98	0.07	-	5,5,5,5	0
53	MG	CA	2002	1/1	1.00	0.11	-	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.