



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 08:50 PM UTC

PDB ID : 4V55 / pdb_00004v55
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin and ribosome recycling factor (RRF).
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-17
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

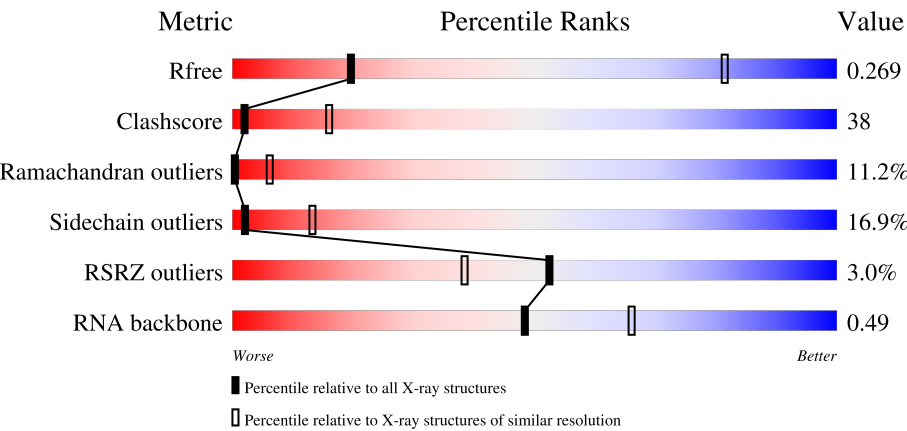
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	24%62%12%..
1	CA	1542	22%65%12%..
2	AC	232	2% 28%48%12%.11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	CC	232	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	AP	82	
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	70	
21	CU	70	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	DK	123	
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
38	DM	136	
39	BX	63	
39	DX	63	

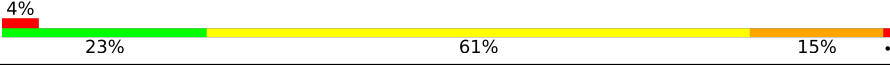
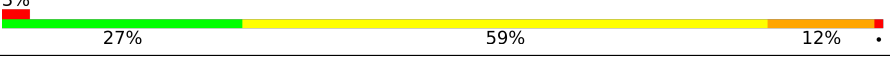
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	BH	149	
40	DH	149	
41	BJ	142	
41	DJ	142	
42	BN	127	
42	DN	127	
43	BO	117	
43	DO	117	
44	BQ	117	
44	DQ	117	
45	BS	110	
45	DS	110	
46	BU	103	
46	DU	103	
47	BF	178	
47	DF	178	
48	BG	176	
48	DG	176	
49	BR	103	
49	DR	103	
50	BT	100	
50	DT	100	
51	BZ	78	
51	DZ	78	
52	BW	84	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	DW	84	
53	B6	185	
53	D6	185	

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
54	MG	AA	1623	-	-	-	X
54	MG	AA	1637	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 287083 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	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
			1021	634	206	178	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			

Continued on next page...

Continued from previous page...

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
			714	439	144	130	1			
14	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	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
			657	417	122	115	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 rRNA.

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 rRNA.

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 L11.

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

- 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			

Continued on next page...

Continued from previous page...

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 L14.

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

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L29.

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

- Molecule 40 is a protein called 50S ribosomal protein L9.

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

- Molecule 41 is a protein called 50S ribosomal protein L13.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

Continued on next page...

Continued from previous page...

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L5.

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

- Molecule 48 is a protein called 50S ribosomal protein L6.

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

- Molecule 49 is a protein called 50S ribosomal protein L21.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
50	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L27.

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

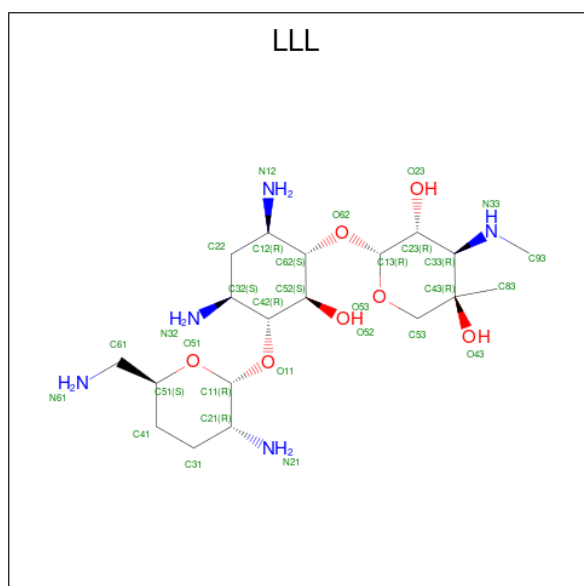
- Molecule 53 is a protein called 50S ribosomal protein RRF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			
53	D6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AA	60	Total	Mg	0	0
			60	60		
54	BB	110	Total	Mg	0	0
			110	110		
54	CA	61	Total	Mg	0	0
			61	61		
54	CE	1	Total	Mg	0	0
			1	1		
54	DB	111	Total	Mg	0	0
			111	111		

- Molecule 55 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (CCD ID: LLL) (formula: C₁₉H₃₉N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	AA	1	Total	C	N	O	0	0
			31	19	5	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BB	1	Total	C	N	O	0	0
			31	19	5	7		
55	CA	1	Total	C	N	O	0	0
			31	19	5	7		
55	DB	1	Total	C	N	O	0	0
			31	19	5	7		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	287	Total	O	0	0
			287	287		
57	AE	3	Total	O	0	0
			3	3		
57	AK	1	Total	O	0	0
			1	1		
57	AL	3	Total	O	0	0
			3	3		
57	AN	4	Total	O	0	0
			4	4		
57	AT	2	Total	O	0	0
			2	2		
57	BB	492	Total	O	0	0
			492	492		
57	BC	6	Total	O	0	0
			6	6		
57	BD	1	Total	O	0	0
			1	1		
57	BE	3	Total	O	0	0
			3	3		
57	BL	3	Total	O	0	0
			3	3		
57	BT	1	Total	O	0	0
			1	1		

Continued on next page...

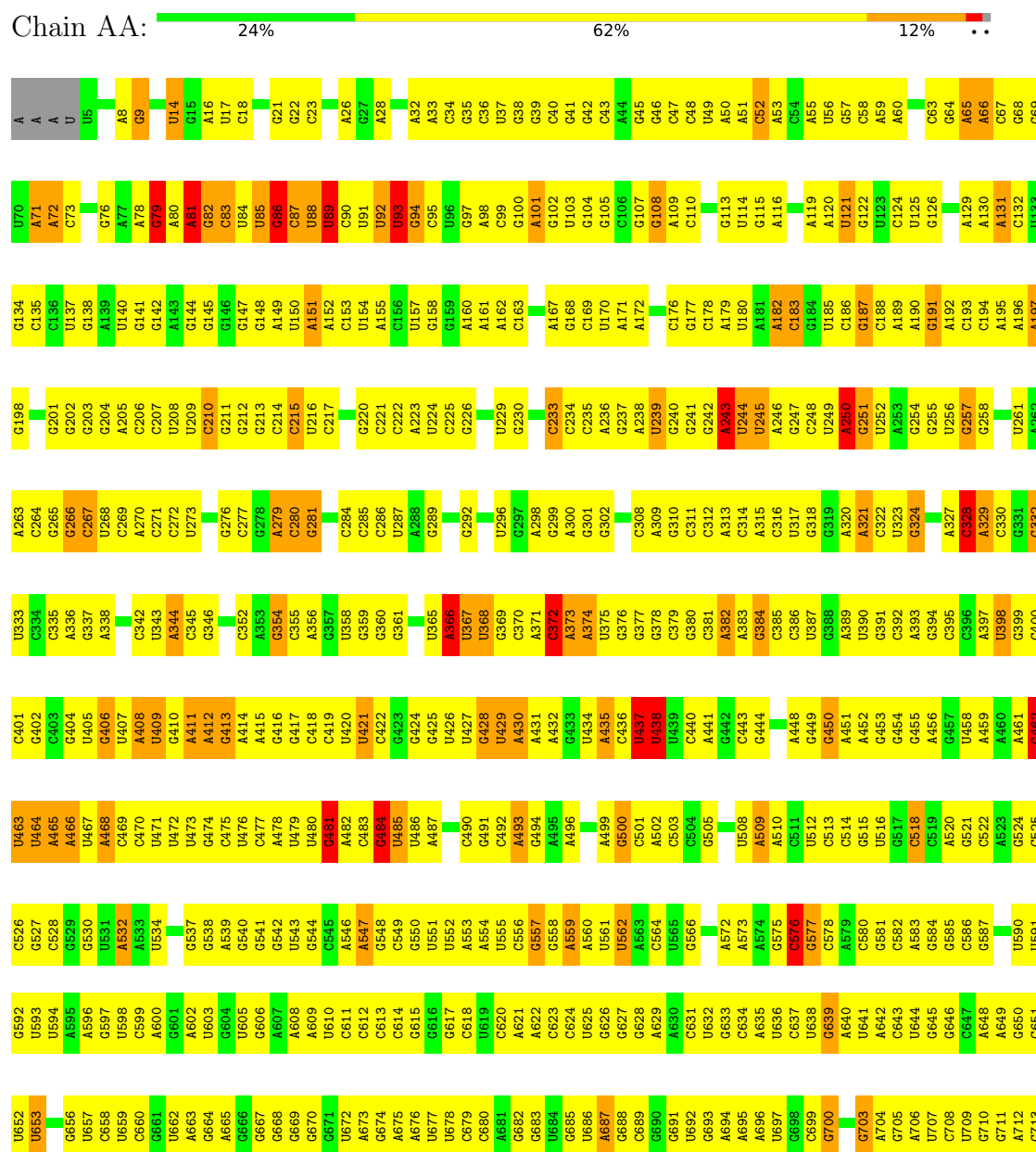
Continued from previous page...

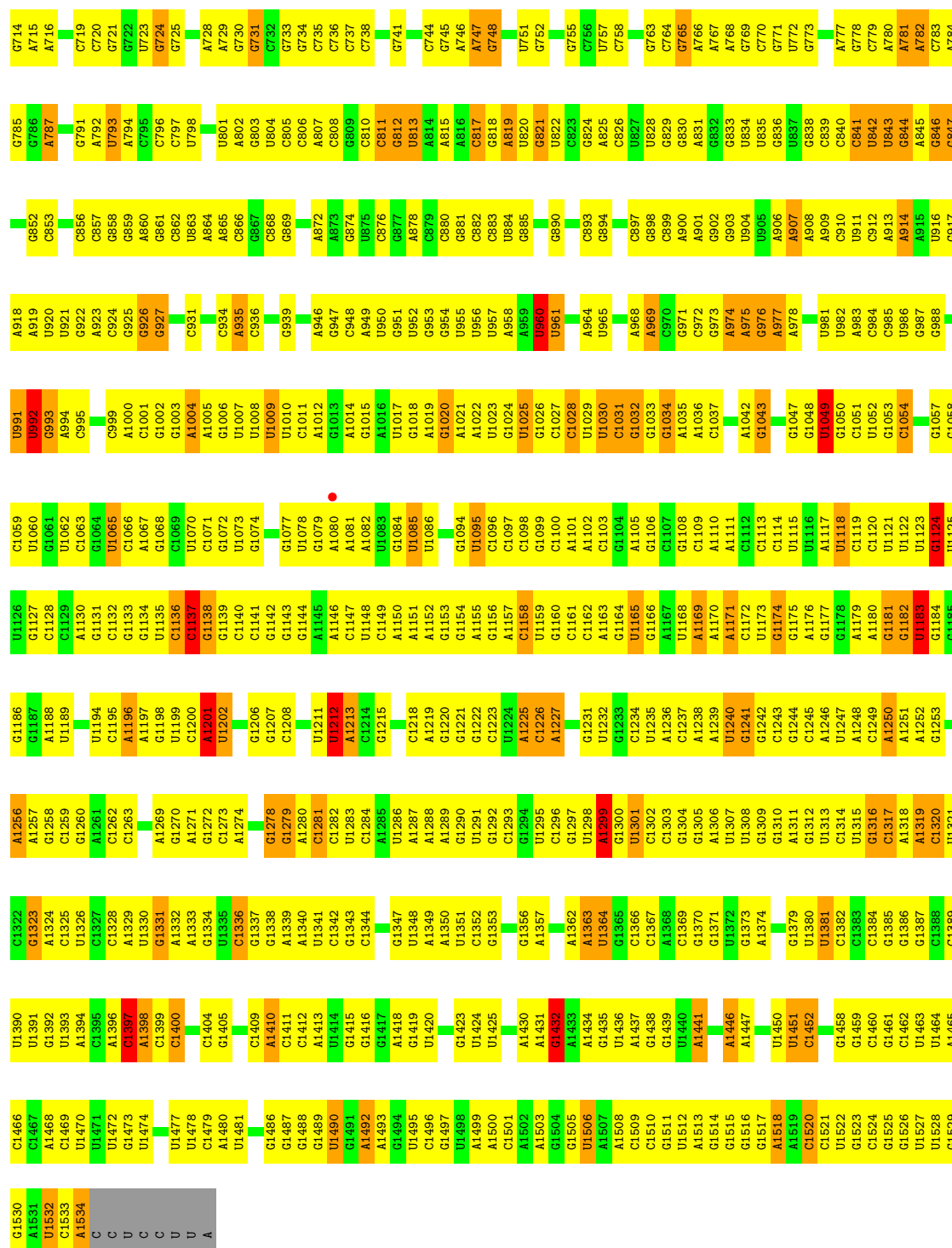
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CA	296	Total 296	O 296	0	0
57	CE	3	Total 3	O 3	0	0
57	CK	1	Total 1	O 1	0	0
57	CL	3	Total 3	O 3	0	0
57	CN	4	Total 4	O 4	0	0
57	CT	2	Total 2	O 2	0	0
57	DB	500	Total 500	O 500	0	0
57	DC	6	Total 6	O 6	0	0
57	DE	2	Total 2	O 2	0	0
57	DL	2	Total 2	O 2	0	0
57	DR	1	Total 1	O 1	0	0
57	DT	1	Total 1	O 1	0	0

3 Residue-property plots

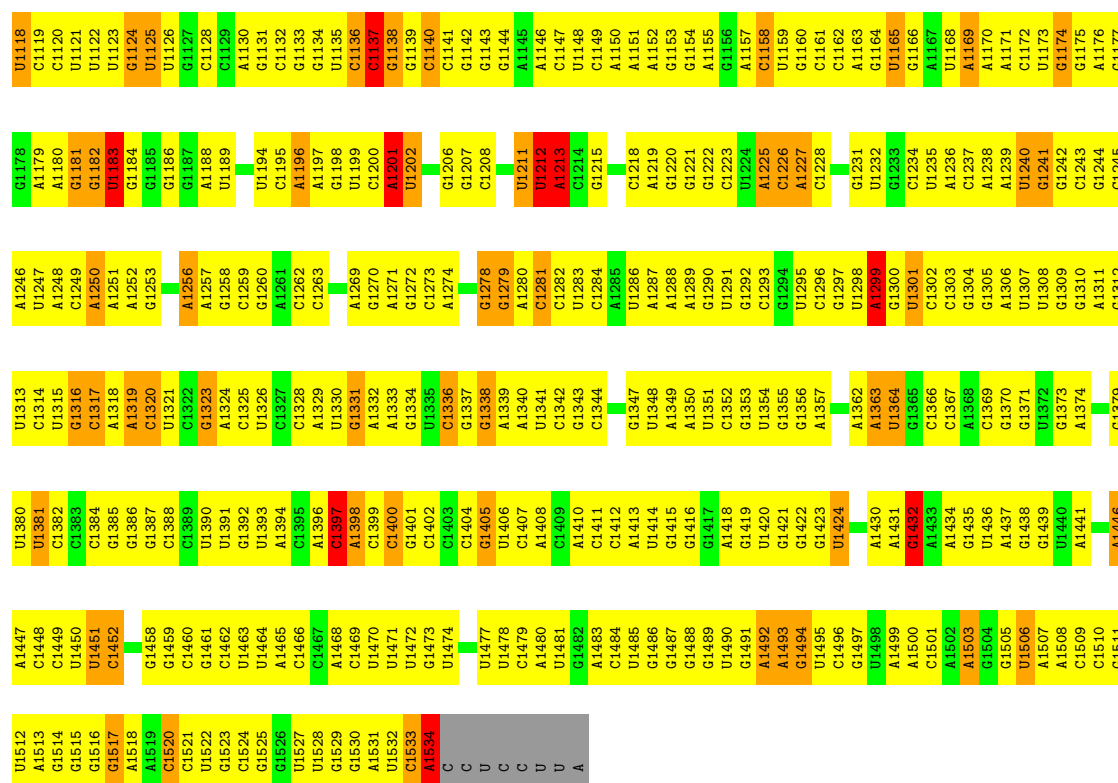
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

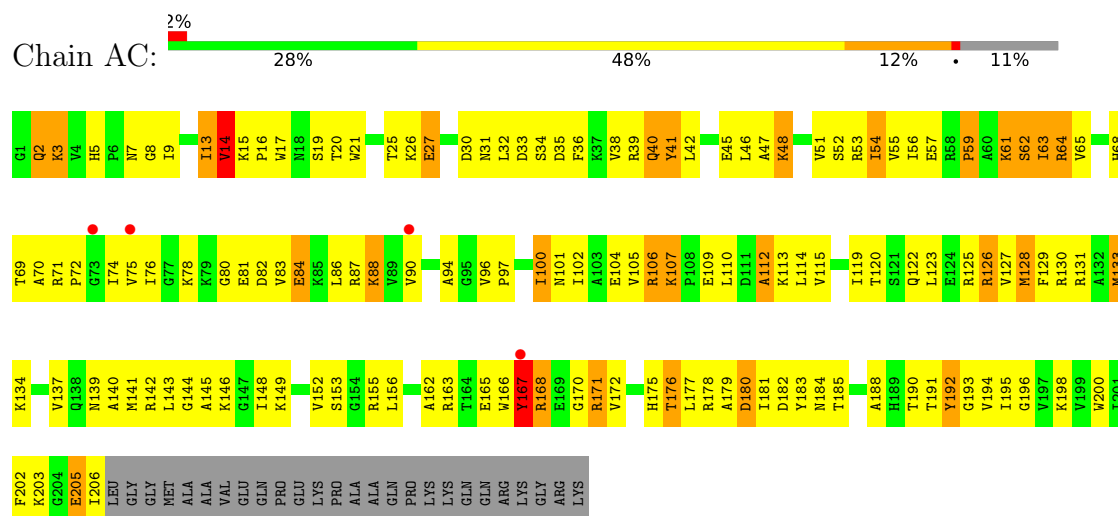




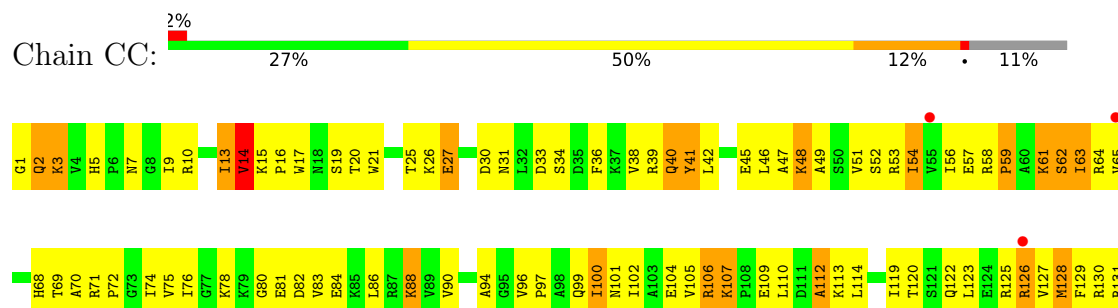
G1047	G1048	U1049	A983	G984	G985	A918	A919	G987	G988	U981	U982	U983	U984	U985	U986	G987	G988	U991	U992	G993	A994	G1061	U1062	G1063	U997	G998	U999	U1065	U1066	A1067	G1068	G1069	U1070	U1071	G1072	U1073	G1074	U1075	U1076	G1077	U1078	U1079	A1080	A1081	G1084	U1085	U1086	G1094	U1095	G1096	G1097	G1098	G1099	C1100	A1101	A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	C1113	C1114	A1117																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
C135	C136	U137	A138	G139	A139	U140	A141	G142	G143	A144	G145	G146	C147	U148	A149	U150	C151	U152	U153	A154	C155	U156	U157	C158	U159	U160	C161	U162	A163	U164	C165	U166	U167	C168	U169	A170	U171	C172	U173	U174	U175	U176	U177	U178	U179	U180	U181	U182	U183	U184	U185	U186	U187	U188	U189	U190	U191	U192	U193	U194	U195																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
A196	A197	G198	U201	G202	G203	U204	A205	G206	A207	C207	U208	U209	C210	A211	U212	U213	C214	C215	C216	C217	G218	U219	U220	C221	C222	A223	U224	C225	U226	U227	U228	U229	U230	G231	G232	A233	C234	C235	A236	U237	A238	U239	C240	G241	U242	A243	U244	U245	A246	C247	C248	U249	A250	G251	U252	A253	G254	U255	U256	A257	C258	U259	U260																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
U261	A262	U263	U264	U265	U266	U267	U268	U269	U270	C271	U272	U273	C274	U275	U276	U277	U278	A279	C280	U281	U282	U283	U284	C285	U286	A287	U288	U289	U290	U291	U292	U293	U294	U295	U296	U297	U298	U299	C300	G301	C302	A303	A304	U305	C306	U307	C308	A309	G310	C311	C312	A313	C314	A315	C316	U317	C318	U319	A320	U321	U322	U323	G324	U325	U326	U327	U328	U329	U330																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
A329	C330	U331	U332	U333	U334	U335	U336	U337	U338	U339	U340	U341	U342	U343	U344	U345	U346	C347	A348	U349	U350	U351	U352	U353	U354	U355	U356	U357	U358	U359	U360	U361	U362	U363	U364	U365	U366	U367	U368	U369	U370	U371	U372	U373	U374	U375	U376	U377	U378	U379	U380	U381	U382	U383	U384	U385	U386	U387	U388	U389	U390	U391	U392	U393	U394	U395	U396	U397	U398	U399	U400	U401	U402	U403	U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117

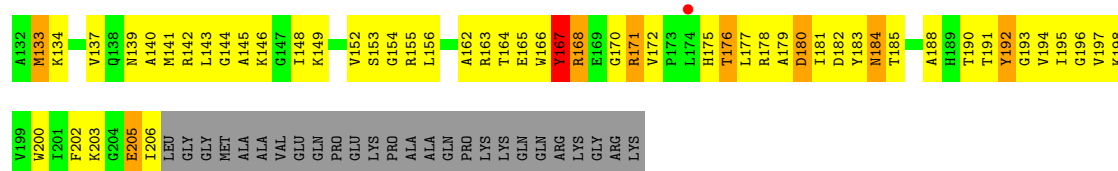


• Molecule 2: 30S ribosomal protein S3

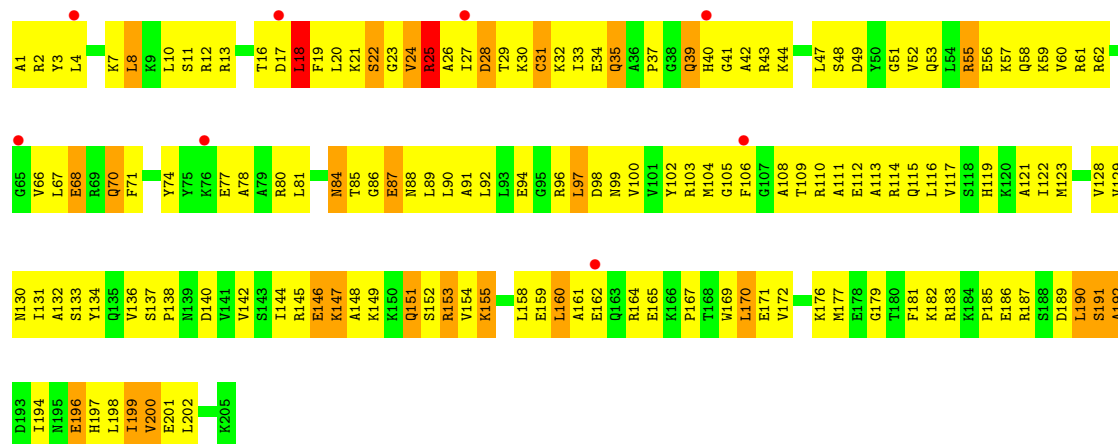


• Molecule 2: 30S ribosomal protein S3

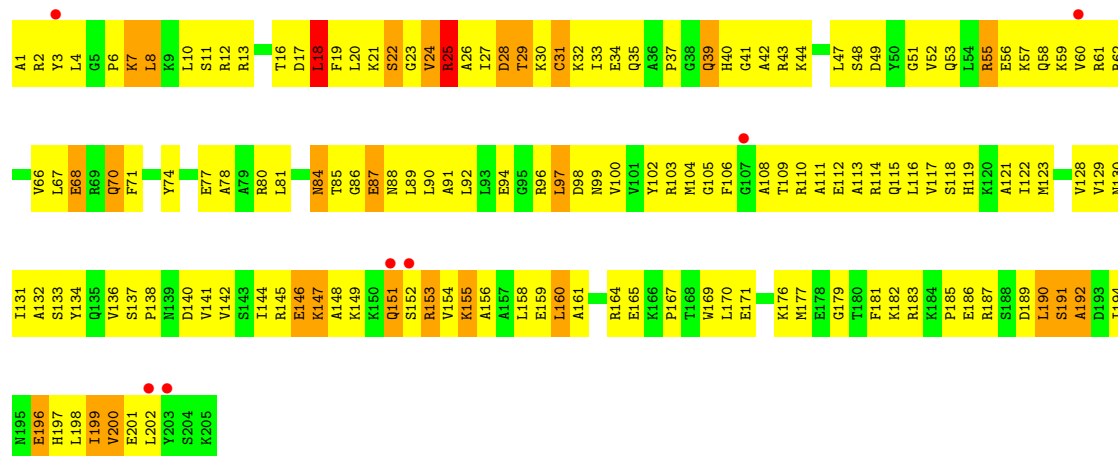




• Molecule 3: 30S ribosomal protein S4

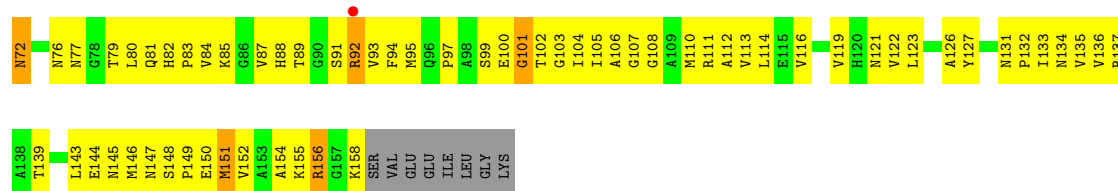


• Molecule 3: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S5

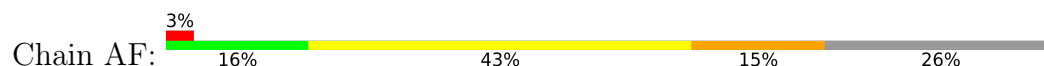




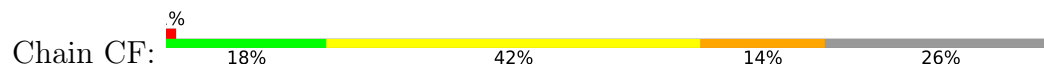
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6

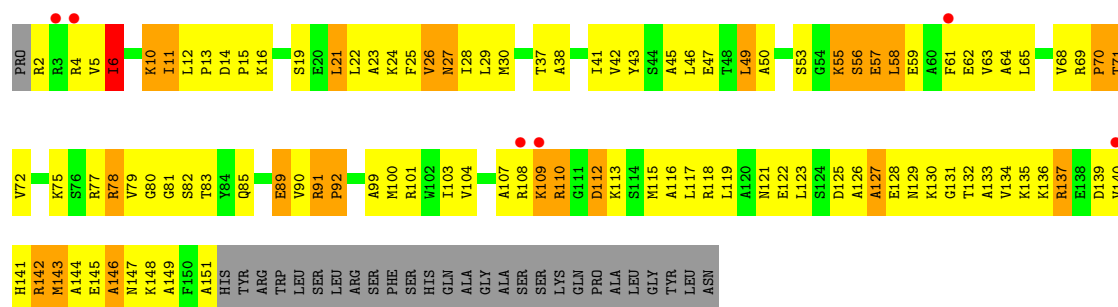


• Molecule 5: 30S ribosomal protein S6

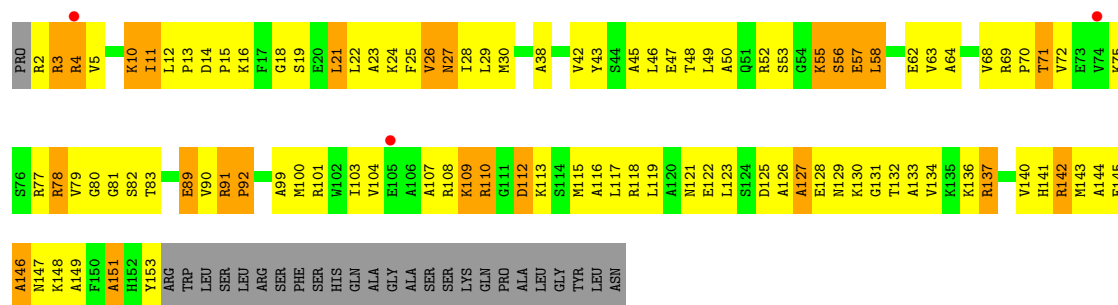


• Molecule 6: 30S ribosomal protein S7

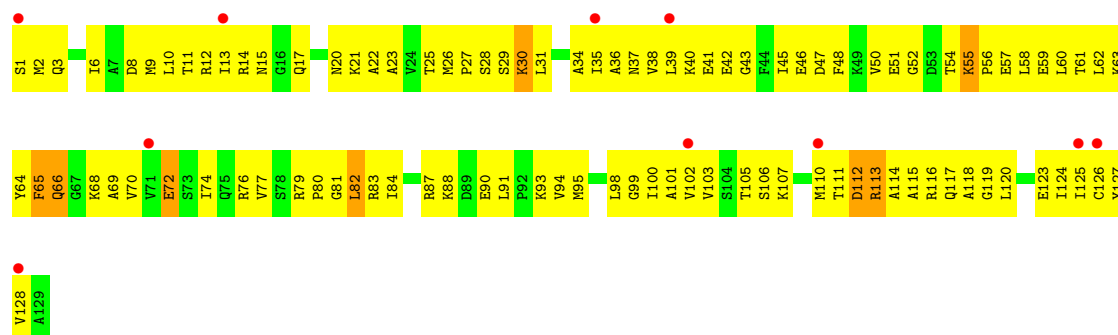




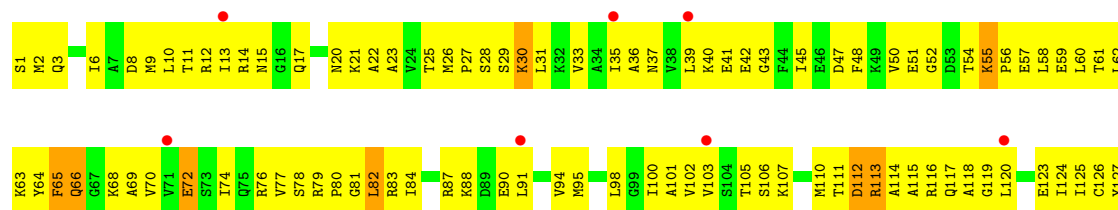
• Molecule 6: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S8

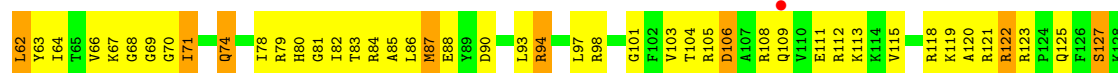
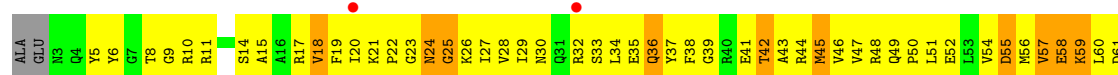


• Molecule 7: 30S ribosomal protein S8

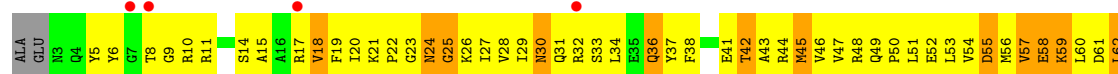




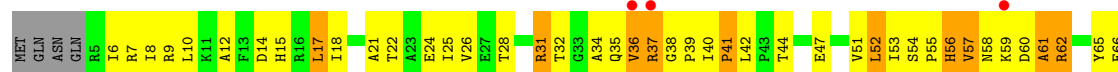
• Molecule 8: 30S ribosomal protein S9



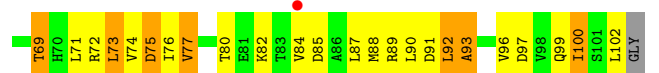
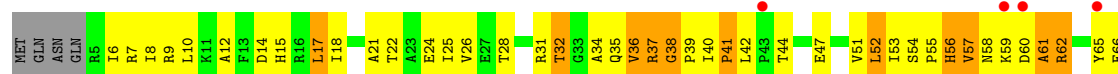
• Molecule 8: 30S ribosomal protein S9



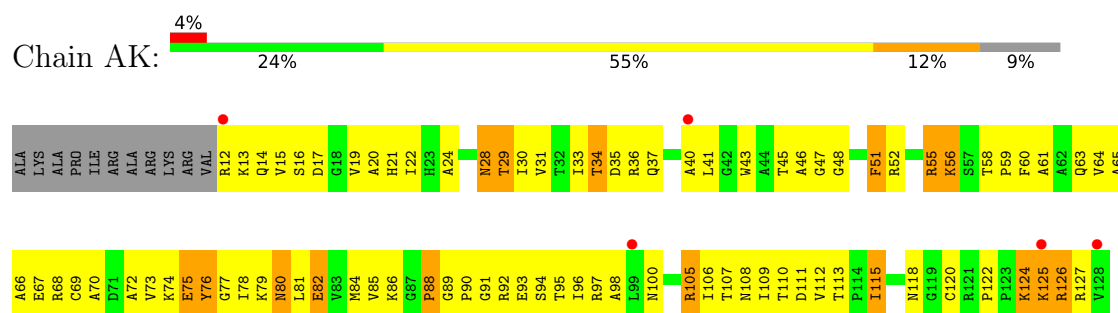
• Molecule 9: 30S ribosomal protein S10



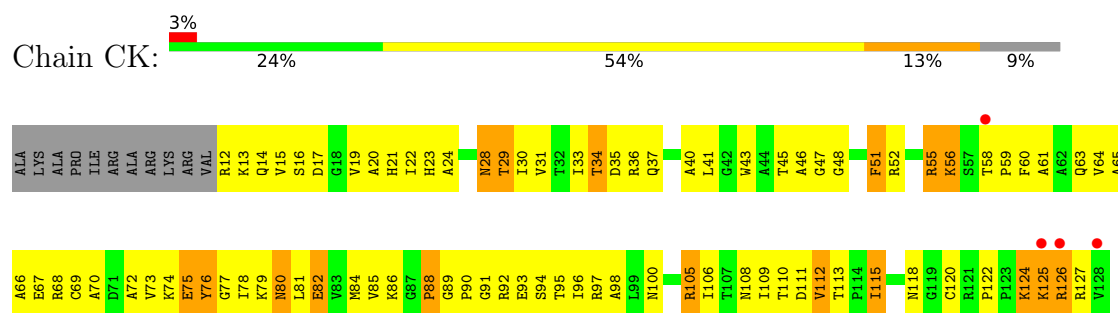
• Molecule 9: 30S ribosomal protein S10



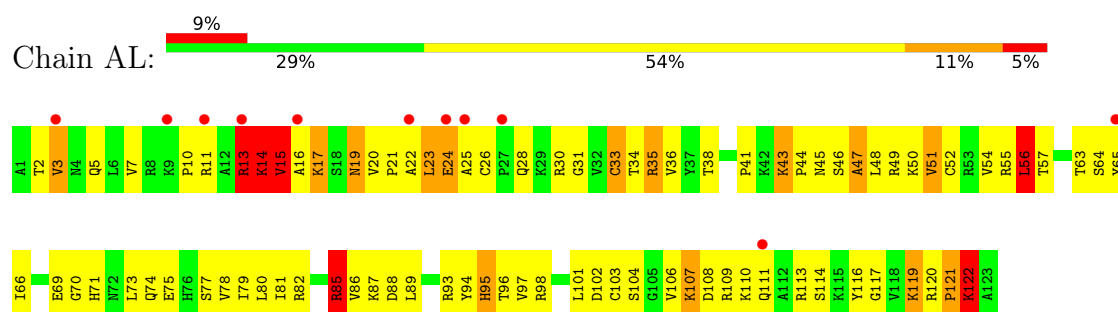
- Molecule 10: 30S ribosomal protein S11



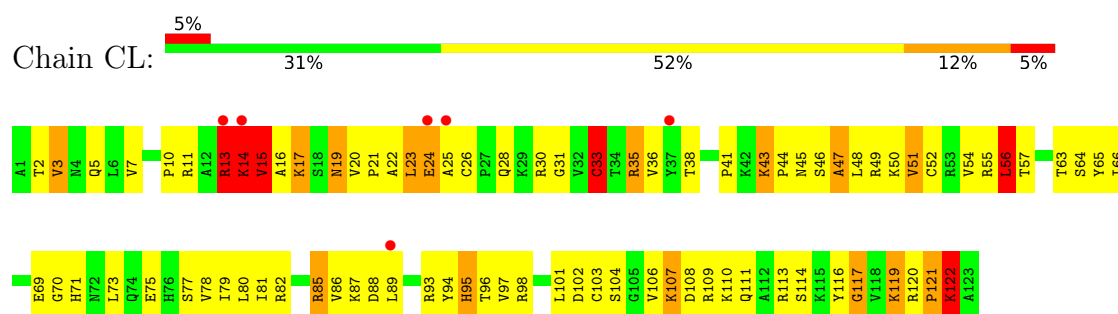
- Molecule 10: 30S ribosomal protein S11



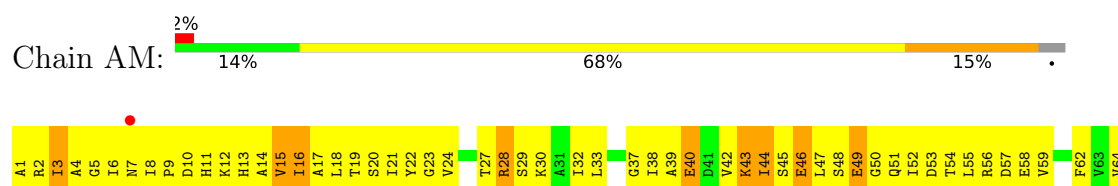
- Molecule 11: 30S ribosomal protein S12



- Molecule 11: 30S ribosomal protein S12

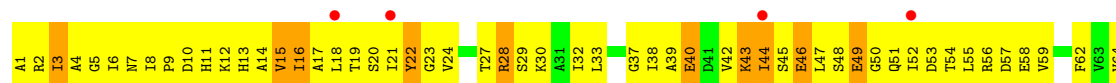


- Molecule 12: 30S ribosomal protein S13

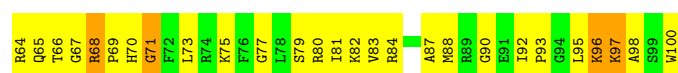
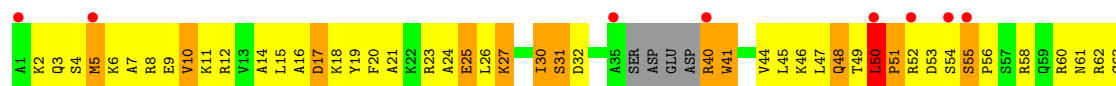




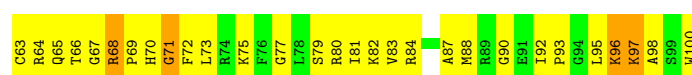
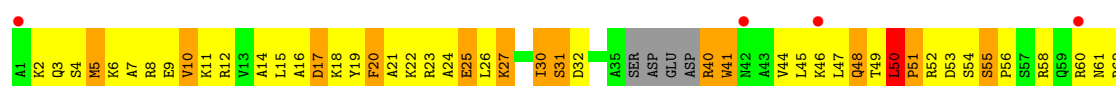
• Molecule 12: 30S ribosomal protein S13



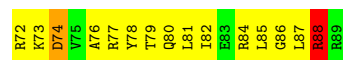
• Molecule 13: 30S ribosomal protein S14



• Molecule 13: 30S ribosomal protein S14

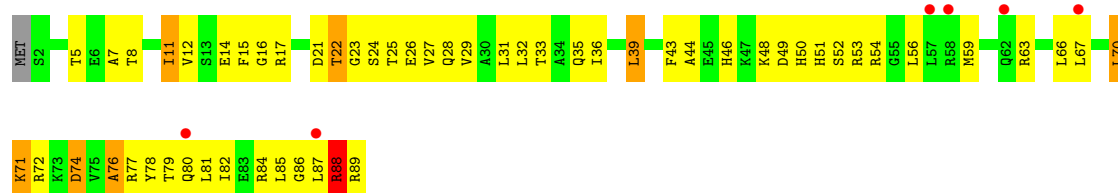


• Molecule 14: 30S ribosomal protein S15

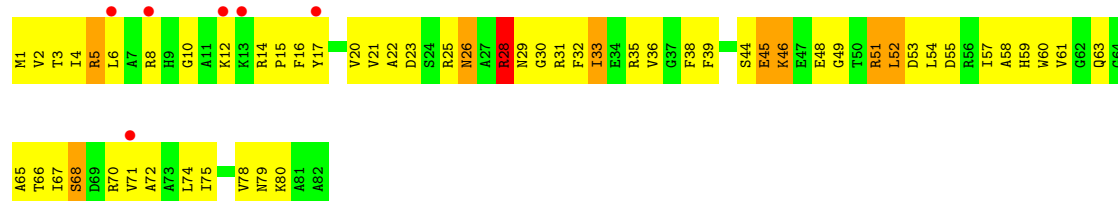


• Molecule 14: 30S ribosomal protein S15

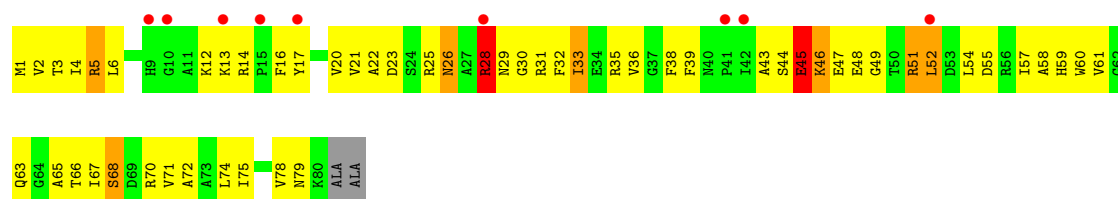




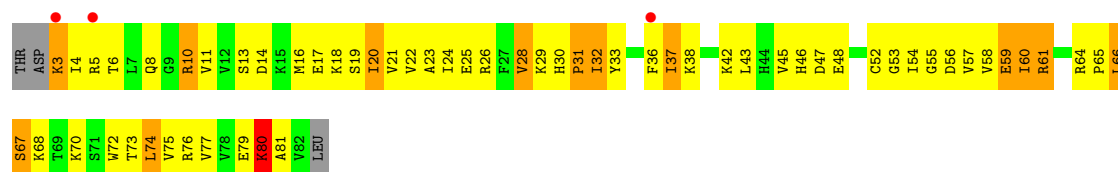
• Molecule 15: 30S ribosomal protein S16



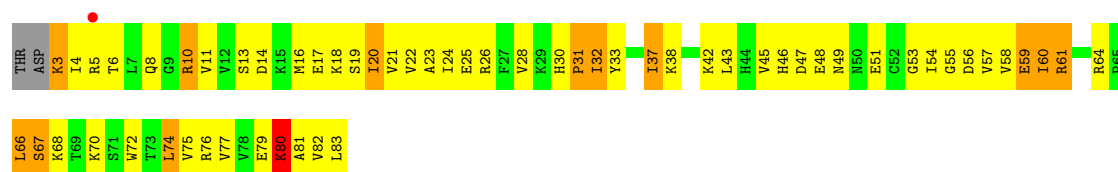
• Molecule 15: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S17



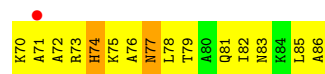
• Molecule 16: 30S ribosomal protein S17



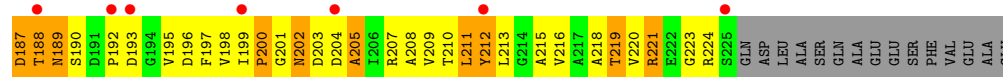
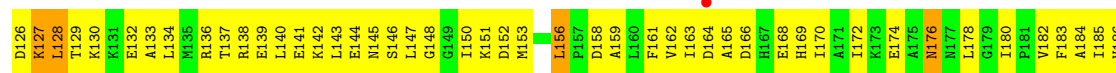
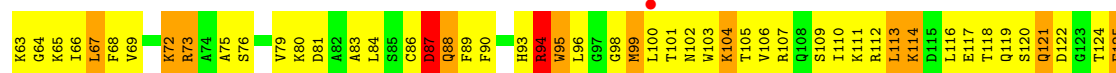
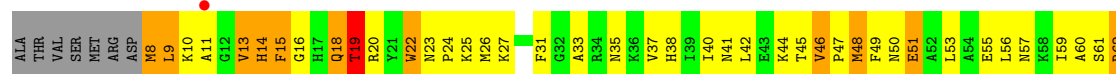
• Molecule 17: 30S ribosomal protein S18



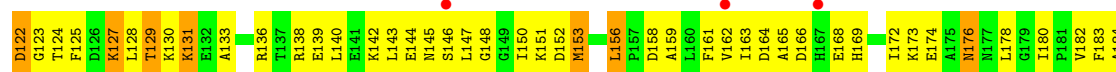
• Molecule 19: 30S ribosomal protein S20



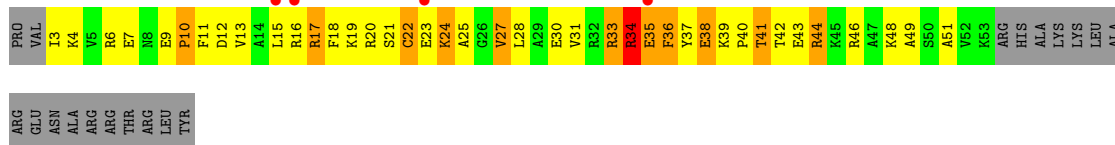
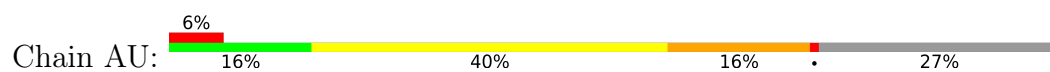
• Molecule 20: 30S ribosomal protein S2



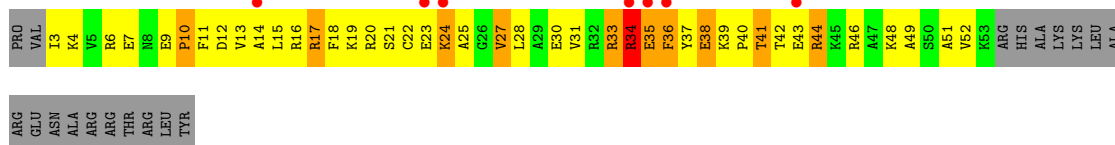
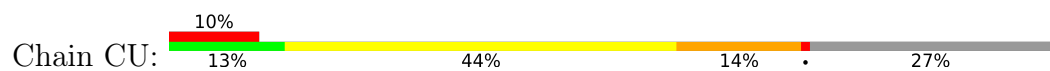
• Molecule 20: 30S ribosomal protein S2



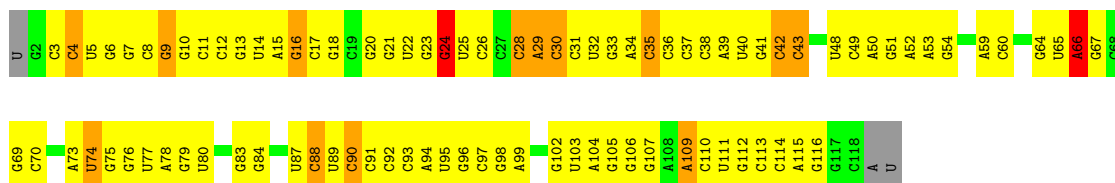
• Molecule 21: 30S ribosomal protein S21



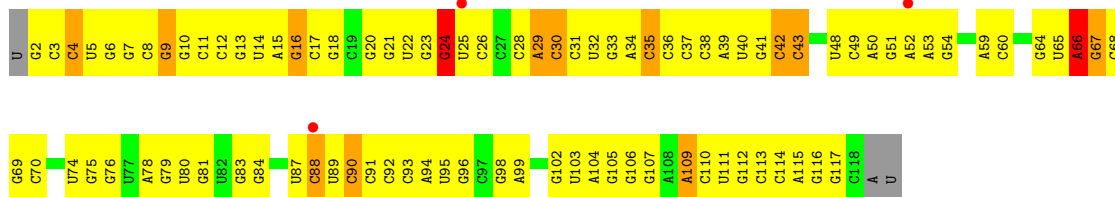
• Molecule 21: 30S ribosomal protein S21



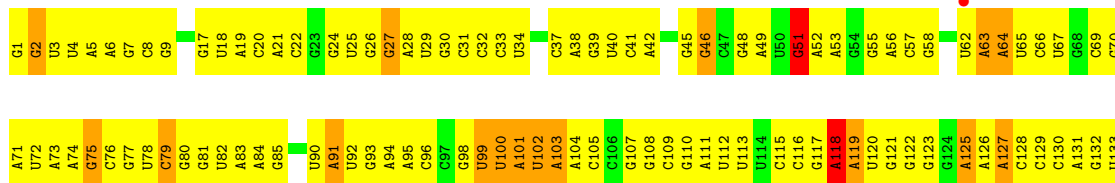
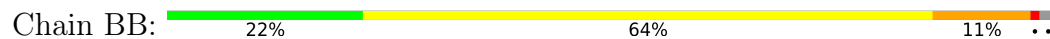
• Molecule 22: 5S rRNA



• Molecule 22: 5S rRNA

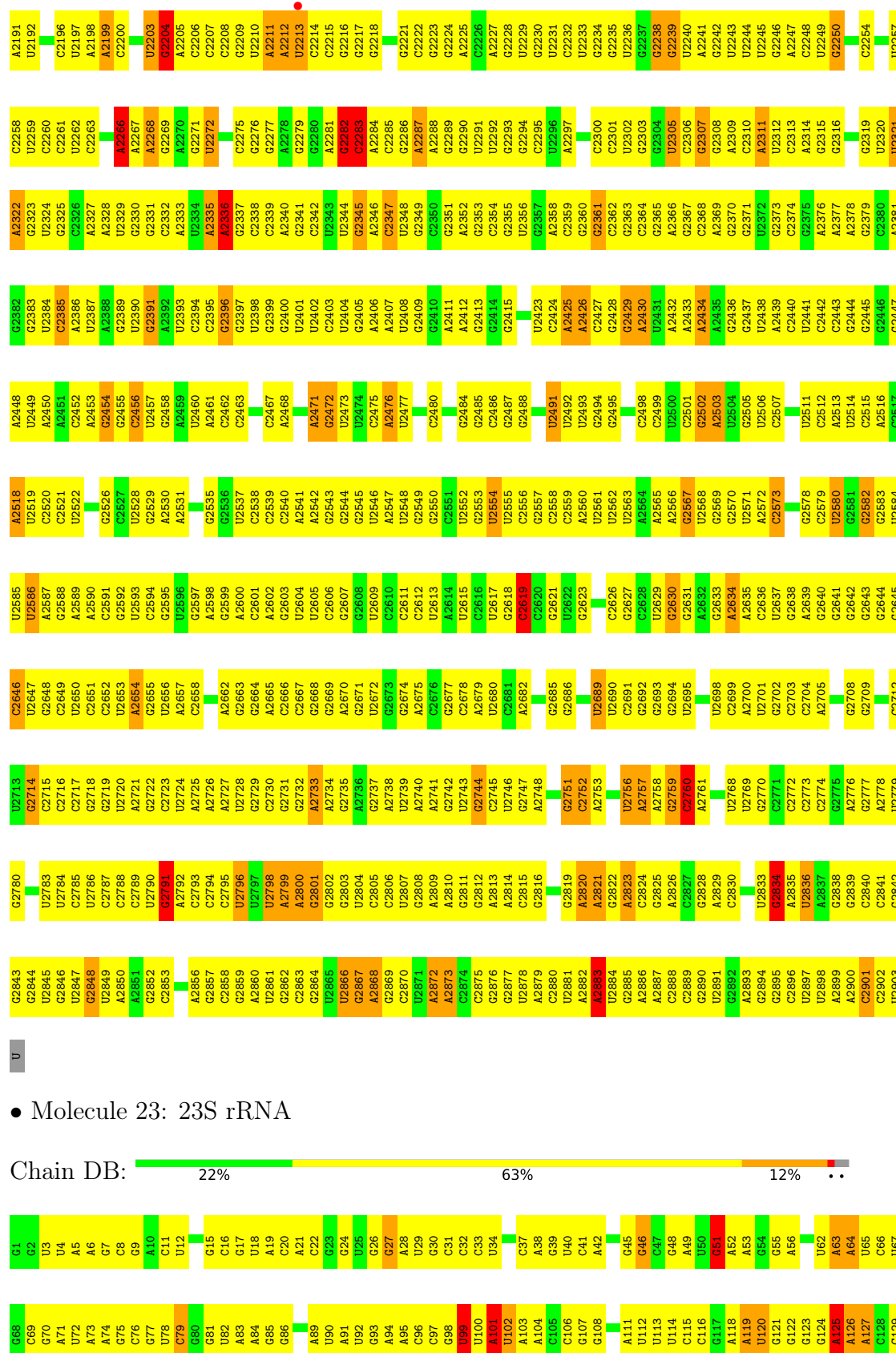


• Molecule 23: 23S rRNA



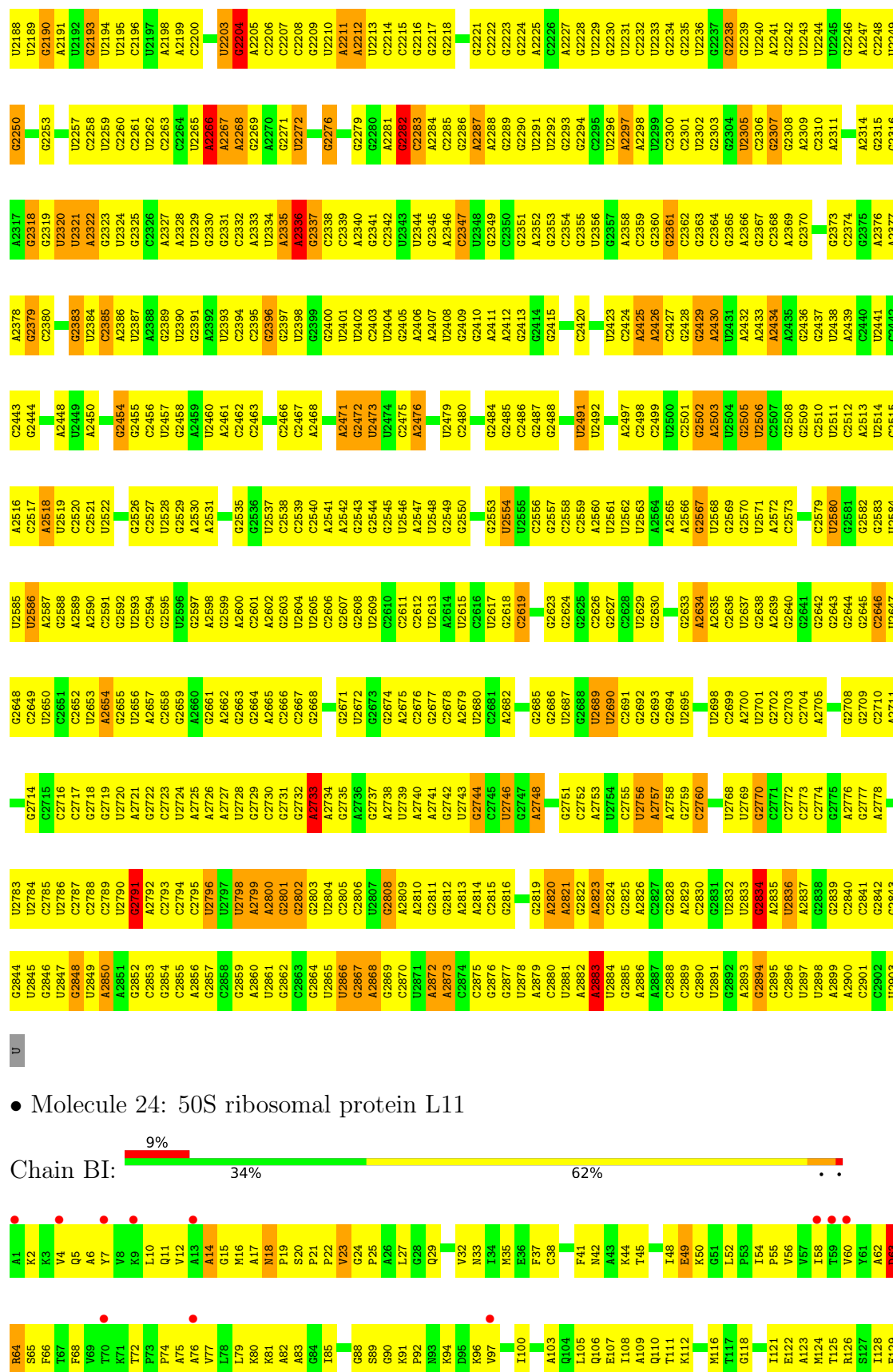
A1134	C1135	G1136	G1137	G1138	G1139	C1140	U1141	A1142	A1143	A1144	C1145	C1146	A1147	U1148	G1149	C1150	A1151	C1152	C1153		G1157		C1161	G1162	G1163	C1164	A1165	G1166	C1167		G1171	C1172	U1173	U1174	A1175	C1176	G1177	G1178	U1179	G1180	G1181	C1182	U1183	U1184	G1185	G1186	G1187	U1188	A1189	G1190	G1191	G1192	G1193	A1194	G1195	C1196	U1197	U1198	U1199																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
G134	U135	G136	U137	U138	U139	C140	G141	A142	C143	A144	C145	A146	C147	U148	G149	C208	C209		G215	A216	A217	A218	A149	U150	C151	A152	U153	U154	A155	A156		G159	A160	A161	U162	C163	C164	A165	U166																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		

C	C2067	G2068	C1996	G1930	A1858	G1791	C1726	U1662	U1589	G1464	U1402	A1336	A1268	C1200
U	G2069	U2068	C1997	U1931	U1859	G1792	C1727	G1663	A1590	G1465	A1403	G1357	A1269	U1201
U	G2070	A1860	G1932	A1932	G1860	G1793	C1728	A1664	C1591	U1466	C1405	G1338	G1271	G1202
U	G2071	G1862	G1933	G1933	G1861	A1794	C1729	A1665	C1592	U1467	C1406	G1339	G1270	U1203
A2134	C2072	G1863	U2007	G1935	G1863	U1796	C1730	G1666	A1593	U1468	U1407	G1341	A1272	A1204
A2135	C2073	G1864	C2008	A1936	U1864	G1797	G1731	G1667	U1594	A1469	G1408	G1340	U1273	A1205
G2136	U2074	U1865	C2009	A1937	U1865	U1798	C1732	A1668	C1595	A1470		G1345	A1274	G1206
U2137	U2075	A1866	U2010	A1938	U1866	G1799	G1733	A1669	A1596	G1471		G1346	A1275	C1267
G2138	U2076	G1867	U2011	G1939	U1867	C1800	G1734	U1671	A1598	U1472	U1411	A1347	A1276	C1208
	A2077	C1868	G2012	U1940	C1868	A1901	G1735	A1672	U1599	U1473	A1413	A1348	C1278	U1209
C2142	C2078	G1869	A2013	G1941	C1869	A1902	U1736	G1673	C1600	U1474		C1349	G1279	G1210
C2143	U2079	C1870	A2014	C1942	C1870	A1903	G1737	G1674		U1475	G1416	C1350	G1280	C1211
G2144	A2080	A1871	A2015	U1943	A1871	C1804	G1738	C1675	A1603	A1477	C1417	C1351	G1281	G1212
C2145	U2081	A1872	A2016	A1944	A1872	A1905	A1739	A1676	C1604	G1478	A1418	A1352	U1282	G1215
C2146	A2082	G1873	U2017	G1945	G1873	C1806	G1740	A1677	C1605	G1479	G1419	A1353	G1283	G1216
A2147	G2018	G1874	U2018	U1946	C1874	G1907	C1741	A1678	C1606	A1480	A1420	A1354	A1284	U1217
G2148	U2019	C1947	A2019	C1947	G1875	A1908	U1742	A1679	C1607	U1481	G1421	G1355	A1285	G1218
U2149	U2086	A1876	A2020	G1948	A1876	A1909	G1743	U1680	A1608	G1482	G1422	G1356	A1286	U1219
C2150	G2087	A1877	C2021	G1949	A1877	A1810	A1744	G1681	A1609	G1483	G1423	C1357	A1287	G1220
U2151	A2088	G1878	U2022	G1950	G1878	G1811	A1745	G1682	A1610	U1484	G1424	G1358	G1288	C1221
G2152	C2089	C1879	C2023	U1951	C1879	U1812	A1746	U1683	C1611	U1485	G1425		U1222	U1222
A2154	A2090	G1880	G2024	A1952	G1880	G1813		U1684	C1612	U1486	G1426	A1359	G1223	G1223
U2155	U2092	C1881	C2025	A1953	C1881	G1814	G1752	C1685	G1613	U1487	A1427		C1291	U1224
G2156	G2093	U1882	U2026	G1954	U1882	A1815	G1753	C1686	A1553	C1488	G1428	A1366	G1292	G1292
G2157	A2094	U1883	C2027	U1955	U1883	C1816	A1754	G1687	U1554	C1489	G1429	A1367	U1294	G1228
A	C2095	A1884	U2028	U1956	A1884	G1817	A1755	G1688	G1555	A1490	G1430	G1368	U1295	C1229
C	C2096	G1885	G2029	C1957	G1885	U1818		A1689	G1556	A1491	A1431	G1369	G1296	U1230
G	C2097	U1886	A2030	C1958	U1886	A1819	U1758	A1689	C1557	G1492	G1432	C1370	G1297	U1231
C	U2098	C1887	A2031	G1959	C1887	U1820	A1759	C1691	C1558	G1493	A1433	G1371	C1298	
G	U2099	G1888	G2032		G1888	A1821	C1760	U1692	U1559	A1494	A1434	U1372	G1299	G1236
		A1889			A1889	C1822	C1761	U1693	G1560	A1495	A1435	A1373	G1300	A1237
	G2102	G1964	G2035	G1964	A1890	G1823	C1762	C1694	C1561	U1496	G1436	A1374	A1301	U1240
C	C2103	C2036	A2037	C1965	G1891	G1824	G1763	G1695	U1562	U1497	U1437	U1375	A1302	U1241
C	C2104	A1966	G2038	C1967	C1892	U1825	C1764	U1696	C1563		U1438	G1376	U1242	U1242
U	U2105	C1968	U2039	G1968	C1894	G1826	U1765	G1766	C1564		A1439	G1377	C1309	U1243
U	U2106	A1969	G2040	A1969		U1827	G1766	G1699	C1565	A1502	U1440	A1378	U1244	A1244
G	G2107	U2041	U2041	A1970	A1899	G1828	G1767	A1700	A1634	A1503	G1441	U1379	G1245	G1245
A	A2108	U1971	A2042	U1971	A1900	A1829	C1768	G1702	A1635	A1504	U1442	G1380	C1314	C1314
A	U2109	G1972	C2043	G1972	A1901	C1830	U1769	G1703	U1636	A1505	U1443	G1381	G1315	G1315
U	G2110	C1973		G1973	G1902	G1831	G1770	C1704	C1638	U1506	G1444	A1247	U1316	U1316
A		C1974			G1903	C1833		A1705	C1639	C1507	G1445	A1383	G1317	G1248
C	G		C2047	C1974	G1904	U1834	C1774		A1640	A1508	C1446	A1384	U1249	U1249
C	U		G2048		C1905		U1775	C1708	A1641	A1509	C1447	A1385	G1250	G1250
A	A		G2049		G1906	U1841	U1776	U1709	G1642	G1510	G1448	C1386	C1320	C1320
C	C		A2051			G1842	G1777	G1710		C1512	G1449	A1387	A1322	A1253
C	G		U1981			C1843	U1778	U1712	U1647	U1513	G1451	G1389	A1254	U1254
G	A		G1982		A1913	C1844	U1779	A1711	U1648	G1514	G1452	U1390	G1324	U1255
U	U2180	G2053	A2052	G1983	C1914	C1845	U1780	U1712	G1649	C1577	A1453	U1391	U1256	G1256
U	U2181	A2054	C2055	G1984	U1915	G1846	U1781	U1713	A1650	G1516	C1454	A1392	G1325	G1257
A		C2055		C1985	A1916		U1782	U1714	G1651	U1579	U1455	A1393	U1326	U1326
G	G	G2056		C1986		A1847	U1783	G1715	A1652	A1580	G1456	U1394	A1327	U1298
U	U2182	U1987	A2060	G1987	G1921	A1848	A1784	U1716	G1653	G1581	U1457	A1395	U1328	A1259
C	A2183	U1988	G2061	G1988	G1922	G1849	A1785	A1717	A1654	C1582	G1458	U1396	A1260	A1260
G	G		C2062		G1925	U1851	A1786	G1718	A1655	A1583	U1459	U1397	C1330	C1261
C	U2185	U1989	A2063		C1926	U1852	A1787	G1719	C1656	U1584	G1459	U1397	G1331	A1262
G	U2186	G1992	C2063		U1986	U1853	A1788	U1720	U1657	C1585	U1460	G1396	G1332	U1263
A	U2187	C1993	C2064		U1987	G1854	A1789	G1721	C1658	A1586	C1461	A1399	G1333	G1266
G	U2188	A1928	C2065		A1928	A1854	C1789	G1722	G1688	G1587	U1462	U1400	G1334	G1266
G	G2190	U1995	C2066		G1929	G1723	C1790	G1723	G1661	A1525	C1463	G1401	G1335	U1267



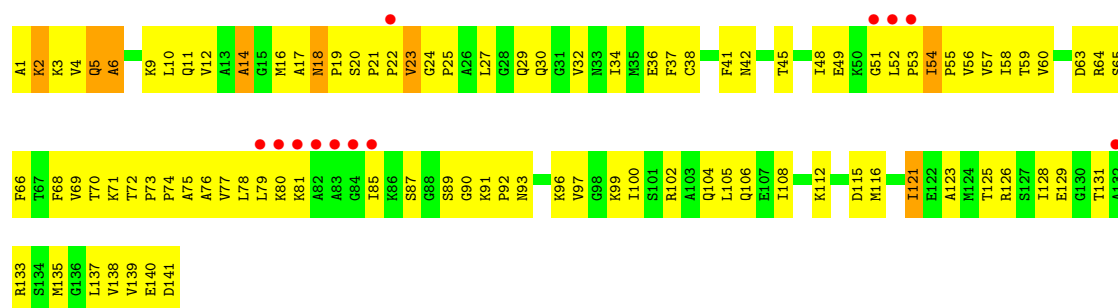
A1134	C1064	A996	U932	C965	A800	U667	G604	G543	A470	U405	G333	A270	C130
C1136	U1065	G997	A933	A966	G805	A668	G605	C544	A471	C406	C334	G271	A131
G1137	G1068	U999	U934	C998	U606	G669	U607	U545	A472	C408	C335	C274	G132
G1138	A1069	U999	C935	C969	U670	A670	A608	U546	G477	G409	C336	C275	U133
G1139	A1070	U999	A936	U870	C671	A609	A609	A547	A478	G410	C337	U276	G134
C1140	G1002	A1001	C937	U871	C672	A609	A609	A548	A479	G411	C338	G277	U135
U1141	C1076	G1002	G938	U872	C673	A609	A609	A549	A480	G412	C339	G278	G136
U1142	A1077	C1007	G939	C873	C610	A609	A609	A550	A481	G413	C340	A278	U137
A1143	G940	G874	U941	G874	C611	A609	A609	A551	A482	C414	C341	U279	U138
A1144	A941	C875	G942	C875	C612	A609	A609	A552	A483	C415	C342	U280	U139
A1145	A1010	C876	U943	C876	A613	A609	A609	U553	A484	C416	C343	U281	C140
C1146	U1081	A877	A943	A877	U615	A609	A609	U554	A485	U416	C344	U282	A141
A1147	U1082	A878	C944	A878	U616	A609	A609	U555	A486	U417	C345	U283	A142
U1148	U1083	C1013	A945	C945	G617	A609	A609	A556	A487	U418	C346	U284	C143
A1149	A1084	A1014	C946	G946	G620	A609	A609	C557	A488	U419	C347	U285	A144
G1149	A1085	A947	A947	G947	G621	A609	A609	U558	A489	U420	C348	U286	A145
C1150	A1086	G1016	C948	G948	A622	A609	A609	U559	A490	C423	C349	U287	C146
A1151	G1017	A819	G949	G949	G623	A609	A609	C560	A491	C424	C350	U288	A147
G1152	A1088	U1018	G950	G950	C624	A609	A609	C561	A492	U425	C351	U289	G220
C1153	A1089	U1019	C951	C951	G625	A609	A609	U562	A493	U426	C352	U290	A221
U1157	A1090	U1020	G952	G952	G626	A609	A609	A563	A494	U427	C353	U291	A222
G1158	G1091	A1021	G953	G953	A626	A609	A609	C564	A495	U428	C354	U292	A223
C1159	G1092	U1022	G954	G954	A627	A609	A609	C565	A496	U429	C355	U293	U150
U1160	G1093	U1023	U955	C955	G630	A609	A609	C566	A497	A430	C356	U294	A152
C1161	U1094	G1024	G956	C956	G631	A609	A609	U567	A498	U431	C357	U295	U153
G1162	A1095	G1025	C957	C957	A632	A609	A609	U568	A499	U432	C358	U296	U154
U1163	U1096	U1097	U958	C958	A633	A609	A609	C569	A500	A433	C359	U297	A155
C1164	A1098	A1029	G959	C959	A634	A609	A609	U569	A501	U434	C360	U298	A156
A1165	G1099	C1030	C960	C960	C635	A609	A609	C570	A502	C435	C361	U299	G159
G1166	U1100	G1031	G961	G961	C636	A609	A609	U571	A503	U436	C362	U300	A160
C1167	U1101	A1032	U962	C962	C637	A609	A609	A572	A504	C437	C363	U301	A161
G1168	U1102	U1033	C963	C963	A638	A609	A609	U573	A505	U438	C364	U302	U162
U1169	A1103	G1036	G964	C964	C639	A609	A609	A574	A506	U439	C365	U303	C163
C1170	U1104	U1037	U965	C965	C640	A609	A609	A575	A507	U440	C366	U304	C164
G1171	U1105	G1038	G966	C966	U641	A609	A609	U576	A508	C441	C367	U305	A165
C1172	U1106	A1039	U967	C967	U642	A609	A609	C581	A509	U442	C368	U306	U166
U1173	U1107	G1040	G968	C968	A643	A609	A609	U580	A510	U443	C369	U307	U170
A1174	U1108	G1041	A969	C969	A644	A609	A609	C582	A511	C444	C370	U308	A171
U1175	C1109	U1042	G971	C971	A645	A609	A609	U583	A512	C445	C371	U309	A172
G1176	U1110	C1043	A972	C972	U646	A609	A609	U584	A513	U446	C372	U310	A173
C1177	U1111	A910	A973	C973	U647	A609	A609	C585	A514	C447	C373	U311	U174
U1178	G1112	C1045	G974	C974	U648	A609	A609	U586	A515	U448	C374	U312	G175
G1179	A1046	U1046	C975	C975	U649	A609	A609	U587	A516	C449	C375	U313	A176
U1180	G1116	G1047	A979	C979	C650	A609	A609	C588	A517	U450	C376	U314	G177
C1181	U1117	A1048	A980	C980	C651	A609	A609	U589	A518	A453	C377	U315	G178
G1182	U1118	C1049	A981	C981	U652	A609	A609	U590	A519	A454	C378	U316	C179
U1183	U1119	A918	U982	C982	U653	A609	A609	A591	A520	C455	C379	U317	C180
A1184	G1120	G1051	A983	C983	U654	A609	A609	U592	A521	C456	C380	U318	G181
C1185	U1121	C1052	A984	C984	A655	A609	A609	U593	A522	C457	C381	U319	A182
G1186	G1122	C1053	G985	C985	U656	A609	A609	U594	A523	C458	C382	U320	C183
U1187	U1123	A1054	C986	C986	U657	A609	A609	U595	A524	U459	C383	U321	G184
C1188	G1124	G1055	C987	C987	U658	A609	A609	U596	A525	U460	C384	U322	C185
A1189	U1125	U1056	A988	C988	U659	A609	A609	U597	A526	C461	C385	U323	G186
G1190	A1126	A1057	G926	C926	C660	A609	A609	U598	A527	U462	C386	U324	A187
C1191	U1127	U1057	G927	C927	A661	A609	A609	U599	A528	U463	C387	U325	C188
G1192	U1128	U1058	C928	C928	U662	A609	A609	U600	A529	U464	C388	U326	G189
A1193	G1131	U1060	C929	C929	U663	A609	A609	U601	A530	U465	C389	U327	A190
C1194	U1132	U1061	G930	C930	U664	A609	A609	U602	A531	U466	C390	U328	C191
G1195	U1133	U1062	C931	C931	U665	A609	A609	U603	A532	U467	C391	U329	C192
		U1063	U931	C931	U666	A609	A609	U604	A533	U468	C392	U330	A193
					U667	A609	A609	U605	A534	U469	C393	U331	C194
					U668	A609	A609	U606	A535	U470	C394	U332	G195
					U669	A609	A609	U607	A536	U471	C395	U333	
					U670	A609	A609	U608	A537	U472	C396	U334	
					U671	A609	A609	U609	A538	U473	C397	U335	
					U672	A609	A609	U610	A539	U474	C398	U336	
					U673	A609	A609	U611	A540	U475	C399	U337	
					U674	A609	A609	U612	A541	U476	C400	U338	
					U675	A609	A609	U613	A542	U477	C401	U339	
					U676	A609	A609	U614	A543	U478	C402	U340	
					U677	A609	A609	U615	A544	U479	C403	U341	
					U678	A609	A609	U616	A545	U480	C404	U342	
					U679	A609	A609	U617	A546	U481	C405	U343	
					U680	A609	A609	U618	A547	U482	C406	U344	
					U681	A609	A609	U619	A548	U483	C407	U345	
					U682	A609	A609	U620	A549	U484	C408	U346	
					U683	A609	A609	U621	A550	U485	C409	U347	
					U684	A609	A609	U622	A551	U486	C410	U348	
					U685	A609	A609	U623	A552	U487	C411	U349	
					U686	A609	A609	U624	A553	U488	C412	U350	
					U687	A609	A609	U625	A554	U489	C413	U351	
					U688	A609	A609	U626	A555	U490	C414	U352	
					U689	A609	A609	U627	A556	U491	C415	U353	
					U690	A609	A609	U628	A557	U492	C416	U354	
					U691	A609	A609	U629	A558	U493	C417	U355	
					U692	A609	A609	U630	A559	U494	C418	U356	
					U693	A609	A609	U631	A560	U495	C419	U357	
					U694	A609	A609	U632	A561	U496	C420	U358	
					U695	A609	A609	U633	A562	U497	C421	U359	
					U696	A609	A609	U634	A563	U498	C422	U360	
					U697	A609	A609	U635	A564	U499	C423	U361	
					U698	A609	A609	U636	A565	U500	C424	U362	
					U699	A609	A609	U637	A566	U501	C425	U363	
					U700	A609	A609	U638	A567	U502	C426	U364	
					U701	A609	A609	U639	A568	U503	C427	U365	
					U702	A609	A609	U640	A569	U504	C428	U366	
					U703	A609	A609	U641	A570	U505	C429	U367	
					U704	A609	A609	U642	A571	U506	C430	U368	
					U705	A609	A609	U643	A572	U507	C431	U369	
					U706	A609	A609	U644	A573	U508	C432	U370	
					U707	A609	A609	U645	A574	U509	C433	U371	
					U708	A609	A609	U646	A575	U510	C434	U372	
					U709	A609	A609	U647	A576	U511	C435	U373	
					U710	A609	A609	U648	A577	U512	C436	U374	
					U711	A609	A609	U649	A578	U513	C437	U375	
					U712	A609	A609	U650	A579	U514	C438	U376	
					U713	A609	A609	U651	A580	U515	C439	U377	
					U714	A609	A609	U652	A581	U516	C440	U378	
					U715	A609	A609	U653	A582	U517	C441	U379	
					U716	A609	A609	U654	A583	U518	C442	U380	
					U717	A609	A609	U655	A584	U519	C443	U381	

G	U2068	A1998	U1925	U1864	C1795	C1726	C1858	A1583	U1520	U1458	U1394	U1329	C1261	C1196
C	G2069	A1927	A1925	U1865	U1796	C1727	G1661	U1584	G1521	G1489	A1395	C1330	A1262	G1197
U	A2071	C2001	A1928	A1866	G1797	C1728	G1662	C1585	U1522	U1460	U1396	C1331	U1263	U1198
U	C2072	U2007	G1929	A1867	U1798	G1729	G1663	A1586	U1523	U1461	U1397	G1332	A1264	U1199
	C2073	C2008	C1868	G1869	G1799	C1730	G1664		G1524	C1462	C1398	G1333	A1265	C1200
	U2074	A2009	U1931	C1870	C1800	G1731	A1665	A1590	A1525	C1463	C1399	G1334	G1266	U1201
	U2075	A2010	A1932	C1871	A1802	G1732	G1666	A1591	C1526	G1464	U1400	C1335	U1267	G1202
	U2076	U2011	G1933	A1872	A1803	C1733	G1667	C1592	G1527	U1401	U1402	C1336	A1268	U1203
	A2077	G2012	C1935	C1873	C1804	G1734	A1668	A1593	A1528	U1402	A1403	G1337	A1269	A1204
	G2078	A2013	A1936	C1874	C1805	A1735	A1669	U1594	G1529	U1403	G1271	G1338	C1270	G1205
	U2079	A2014	A1937	A1875	C1806	G1736	G1670	A1596	C1533	U1405	U1406	G1340	A1272	G1206
	A2080	A2015	G1937	A1876	G1807	G1737	U1671	A1597	U1534	U1406	U1273	G1341	C1207	C1208
	U2081	U2016	U1939	A1877	G1807	G1738	G1674	A1598	A1535	G1407	A1274	U1342	U1269	U1209
	A2082	A2017	C1940	C1878	G1811	A1739	G1675	U1599	C1536	G1408	A1275	C1345	A1276	G1210
	G2083	C2019	C1941	C1879	U1812	G1740	A1676	C1600		G1472	A1276	G1346	A1277	C1211
	U2084	A2020	U1942	U1880	G1813	G1741	A1677	U1603	U1539	U1411	A1277	G1347	G1278	G1212
	C2085	C2021	U1943	C1881	G1814	U1742	A1678	A1604	G1540	U1412	C1277	C1348	C1279	A1213
	U2086	U2022	U1944	U1882	A1815	G1743	A1679	C1605	C1541	U1413	G1278	C1349	G1279	A1214
	C2087	C2023	G1945	U1883	C1816	A1744	A1679	C1606	U1542	A1477	G1280	C1350	G1281	G1215
	A2088	G2024	U1946	G1884	G1817	A1745	U1680	C1607	G1543	U1478	A1286	C1351	G1282	G1216
	C2089	C2025	C1947	U1885	U1818	A1746	G1681	C1608	A1544	G1479	A1287	U1352	U1282	U1217
	A2090	U2026	G1948	U1886	A1819	A1746	G1682	A1608	A1545	U1486	G1288	C1353	G1289	G1218
	C2091	G2027	G1949	C1887	U1820		U1683	A1609	G1546	U1481	C1290	A1354	C1291	U1219
	U2092	U2028		G1888	A1821		G1684	A1610	C1547	G1482	A1287	G1355	G1292	G1220
	C2093	C2029	U1955	A1889	C1822	U1758	C1685	C1611	A1548	G1483	A1287	G1356	C1221	G1221
	A2094	A2030	U1956	A1890	G1823	A1759	C1686	C1612	A1549	U1484	G1288	C1357	U1222	U1222
	U2095	C2031	C1957	U1891	G1824	G1760	G1687	G1613	U1550	U1485	G1289	C1358	G1223	G1223
	C2096	G2032	C1958	C1892	U1825	C1761	U1688	A1551	A1551	U1486	C1290	G1361	U1224	U1224
	A2097	A2033	G1959	C1893	G1826	A1762	A1689	A1616	A1552	U1487	C1291	C1362	G1228	G1228
	U2098	U2034		C1894	U1827	G1763	A1690	G1620	G1553	C1488	A1292	C1362	C1229	C1229
	C2099	G2035	U1963	C1895	G1828	C1764	C1691	U1620	U1554	C1489	U1294	A1365	U1231	U1231
	G2100	C2036	G1964	G1896	A1829	U1765	U1692	G1623	G1555	A1490	G1295	G1368	G1235	G1235
	A2101	A2037	C1965	A1897	C1830	G1766	U1693	U1624	C1556	G1491	G1296	G1369	A1237	A1237
	C2102	G2038	A1966	U1898	G1831	G1767	C1694	U1624	C1557	A1431	G1297	C1370	G1238	G1238
	A2103	C2039	C1967	A1899	C1832	C1768	G1695	G1628	C1558	G1493	G1298	C1371	G1239	G1239
	C2104	G2040	G1968	A1900	C1833	U1769	G1696	G1628	U1559	A1494	G1299	G1372	A1241	A1241
	U2105	U2041	A1969	A1901	U1834	G1770	G1699	G1633	G1560	A1495	G1300	U1373	U1240	U1240
	U2106	A2042	A1970	C1902	U1841	C1771	G1700	A1634	C1561	A1496	A1302	U1374	G1309	G1309
	G2107	C2043	U1971	G1903	G1842	A1772	A1700	A1634	U1562	U1497	A1301	U1375	U1242	U1242
	A2108	G1972	G1972	G1904	C1843	A1773	C1704	U1635	U1563	G1501	A1241	U1376	C1243	C1243
	U2109	C1973	C1973	C1905	C1844	C1774	A1705	U1636	C1564	A1502	G1314	U1377	G1245	G1245
	A2110	C1974	C1974	G1906	C1844	U1775	G1705	C1637	C1565	U1503	G1315	G1377	A1247	A1247
	U			G1907	G1845	G1776		C1638	A1566	A1504	U1316	G1378	G1248	G1248
	G	A1977		C1908	G1846	U1777	C1708	C1639	G1567	U1504	U1317	G1379	U1249	U1249
	U	C2060		C1909	A1847	U1778	U1709	A1640	U1568	A1505	C1320	U1379	G1250	G1250
	A	A2051		G1910	A1848	U1779	G1710	A1641	A1569	U1506	A1321	U1380	C1251	C1251
	C	G2052		U1911	G1849		A1711	G1642	A1570	C1507	A1322	G1381	A1253	A1253
	A	A2053		A1912	A1853	A1783	U1712		A1571	A1508	G1323	G1382	G1256	G1256
	C	C2054		A1913	A1854	U1784	A1713	U1647	A1572	U1509	G1324	G1383	C1257	C1257
	A	C2055		U1914	A1854	A1785	U1714	U1648	C1573	A1509	U1325	A1384	U1258	U1258
	U	G1987		C1915	U1855	A1786	G1715	G1649	C1574	U1510	G1326	G1385	A1327	A1327
	G	G1988		A1916	U1856	A1787	U1716	U1650	C1575	C1512	U1326	U1386	U1259	U1259
	U	U1991		C1917	G1857	C1788	A1717	G1651	U1576	G1514	G1327	C1387	G1260	G1260
	A	A2062		A1918	U1858	G1789	G1718	A1652	C1577	G1514	G1328	G1388	G1261	G1261
	C	C2063		A1919	U1859	C1790	G1719	G1653	U1578	A1515	G1329	G1389	G1262	G1262
	G	C2064		U1923	G1860	A1791	U1720	A1654	A1579	G1516	U1329	U1390	G1263	G1263
	A	U1995		G1961	G1861	G1792	G1721	A1655	A1580	G1517	U1326	U1391	C1257	C1257
	C	C1996		C1962	G1862	C1793	A1722	A1656	G1518	C1518	U1327	U1392	U1259	U1259
	G	C1997		C1963	G1863	A1794	G1723	U1657	C1582	U1519	U1328	A1393	A1260	A1260

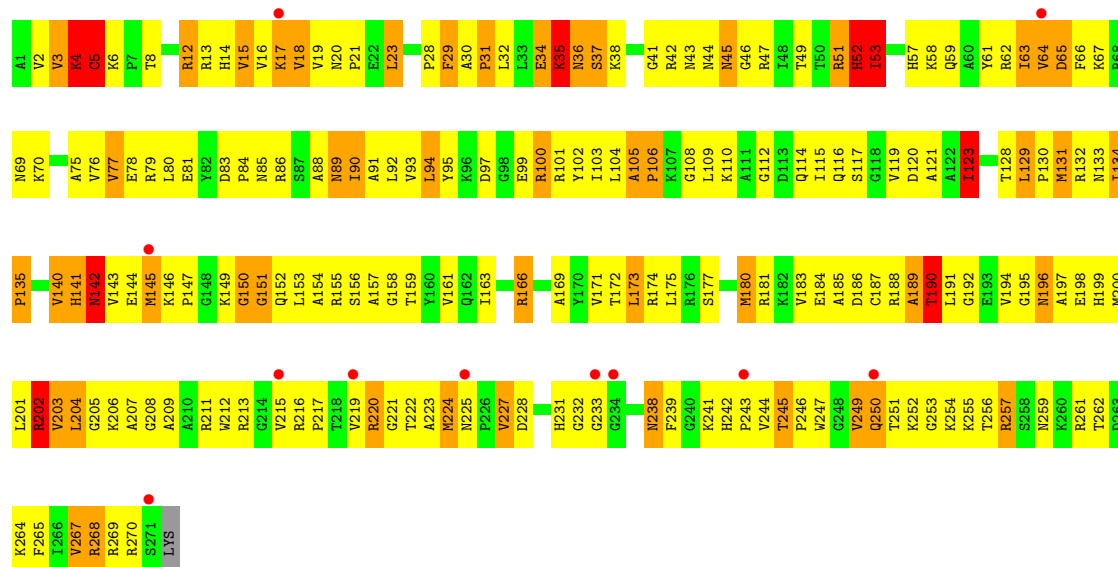




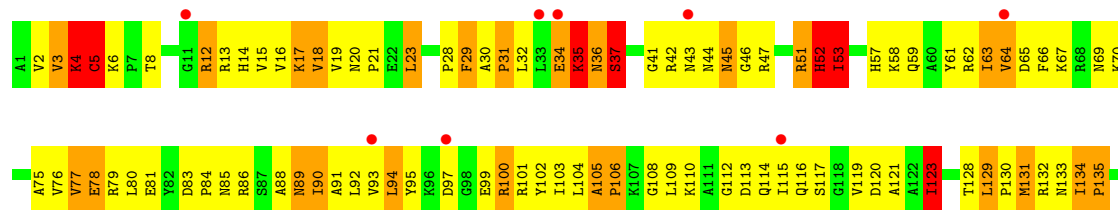
• Molecule 24: 50S ribosomal protein L11

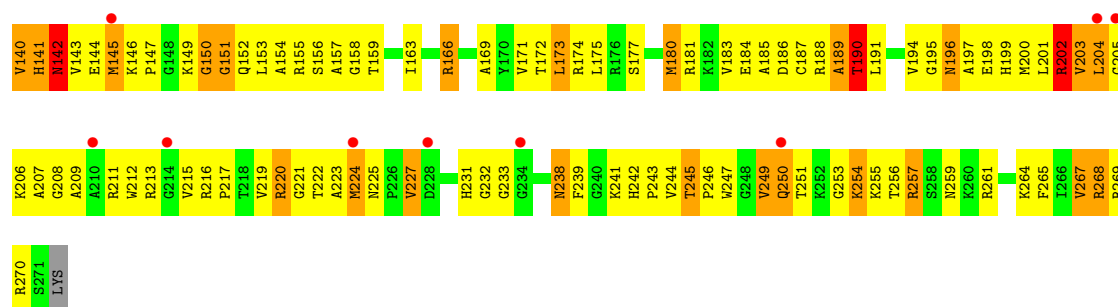


• Molecule 25: 50S ribosomal protein L2

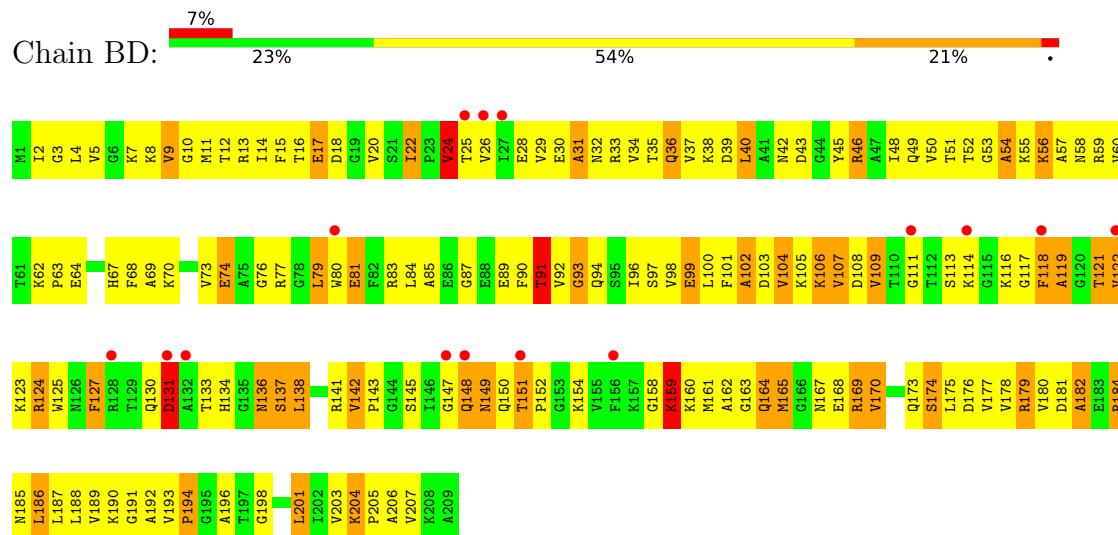


• Molecule 25: 50S ribosomal protein L2

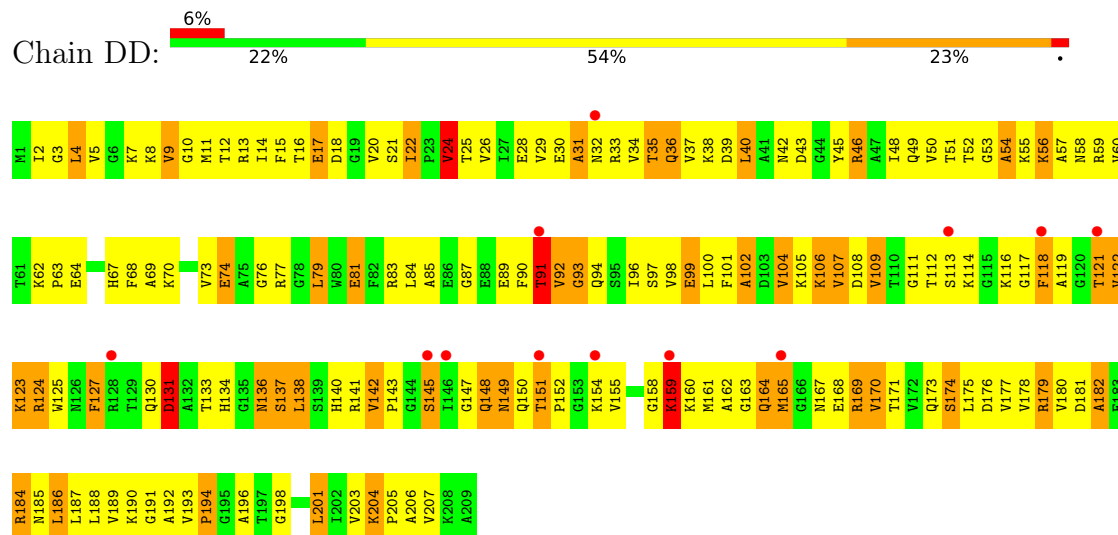




• Molecule 26: 50S ribosomal protein L3

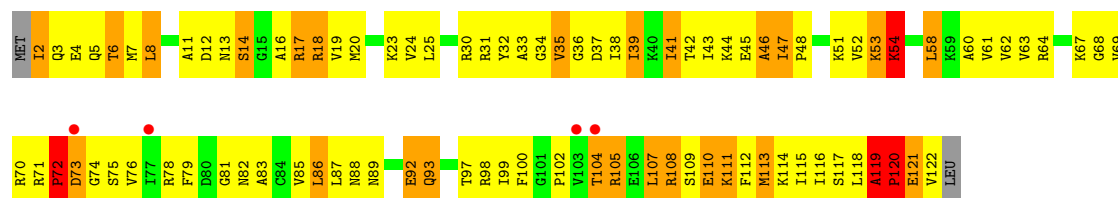


• Molecule 26: 50S ribosomal protein L3

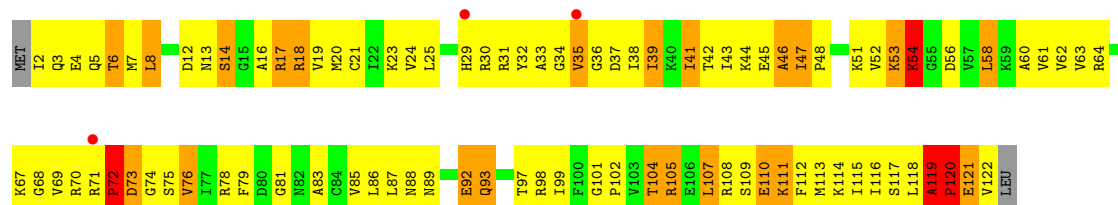


• Molecule 27: 50S ribosomal protein L14

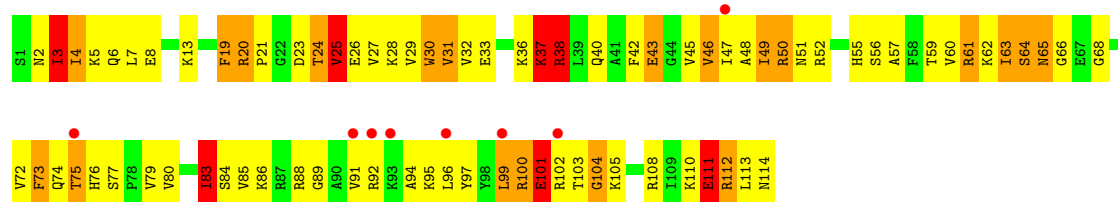




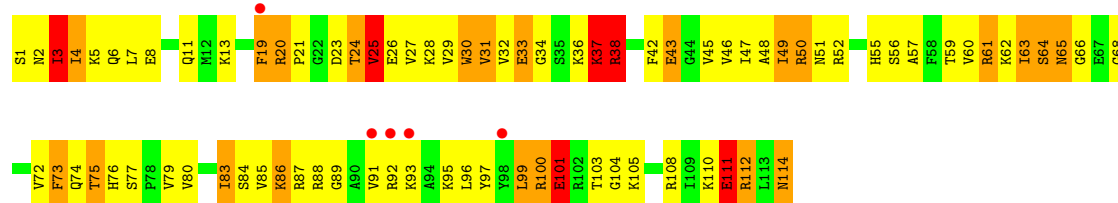
• Molecule 27: 50S ribosomal protein L14



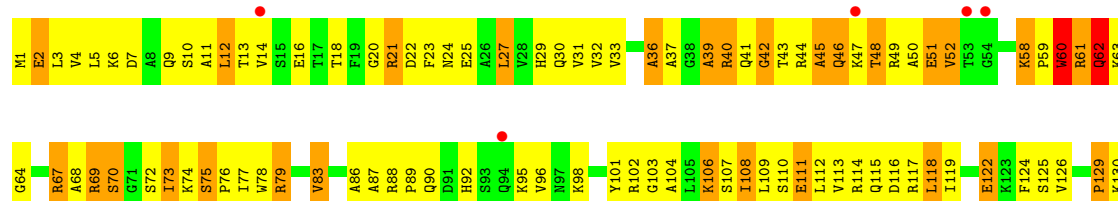
• Molecule 28: 50S ribosomal protein L19

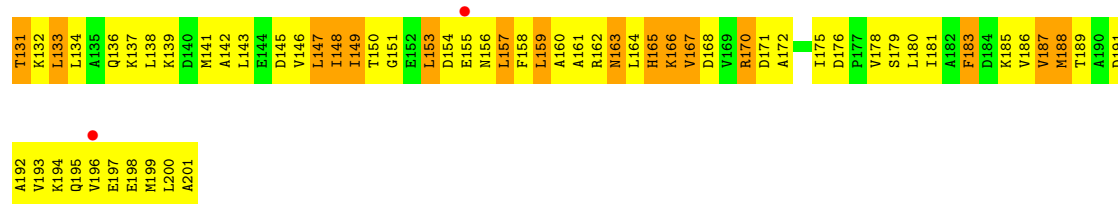


• Molecule 28: 50S ribosomal protein L19

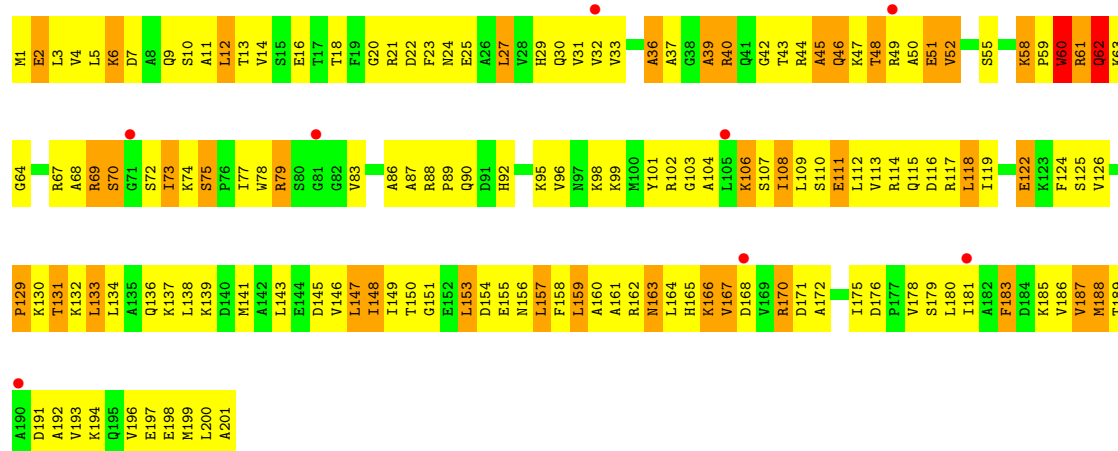


• Molecule 29: 50S ribosomal protein L4

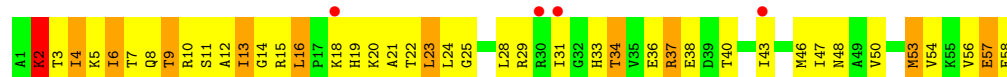
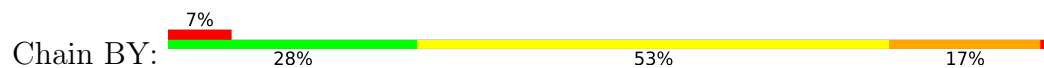




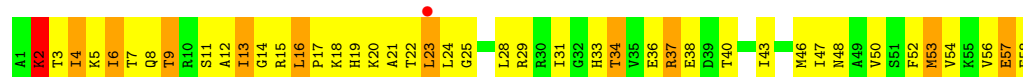
• Molecule 29: 50S ribosomal protein L4



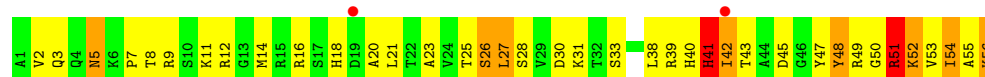
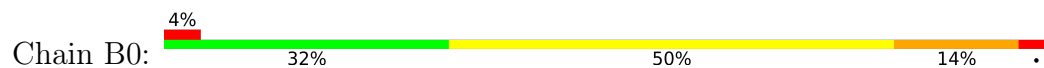
• Molecule 30: 50S ribosomal protein L30



• Molecule 30: 50S ribosomal protein L30



• Molecule 31: 50S ribosomal protein L32

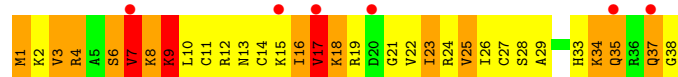
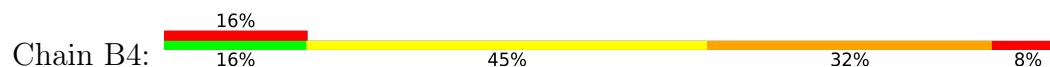


• Molecule 31: 50S ribosomal protein L32

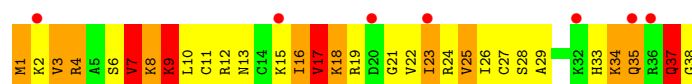
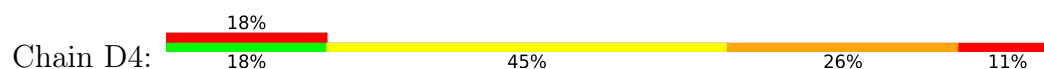




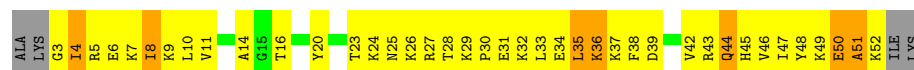
• Molecule 32: 50S ribosomal protein L36



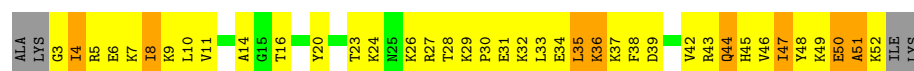
• Molecule 32: 50S ribosomal protein L36



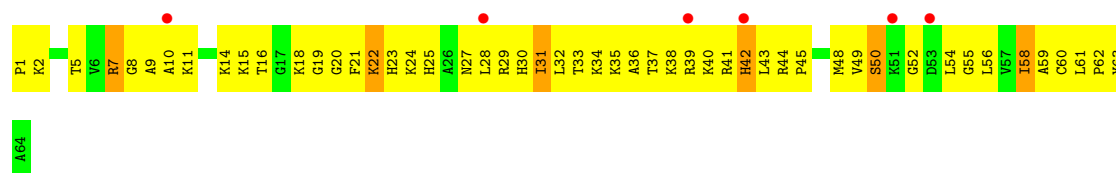
• Molecule 33: 50S ribosomal protein L33



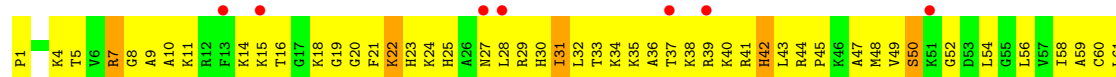
• Molecule 33: 50S ribosomal protein L33



• Molecule 34: 50S ribosomal protein L35



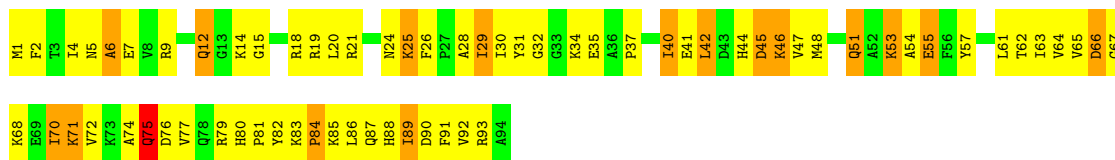
• Molecule 34: 50S ribosomal protein L35





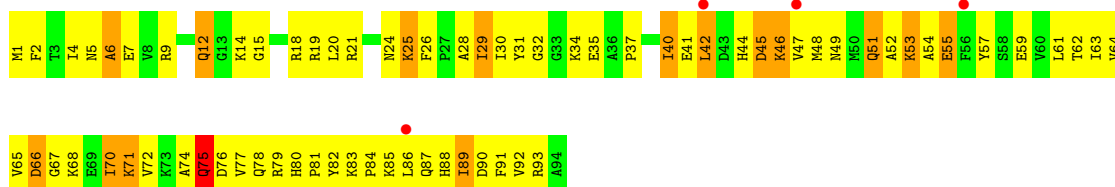
• Molecule 35: 50S ribosomal protein L25

Chain BV: 28% 54% 17%



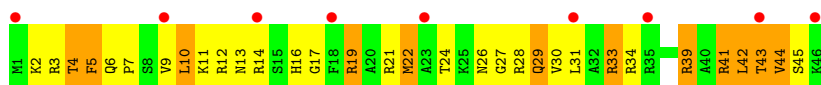
• Molecule 35: 50S ribosomal protein L25

Chain DV: 4% 23% 60% 16%



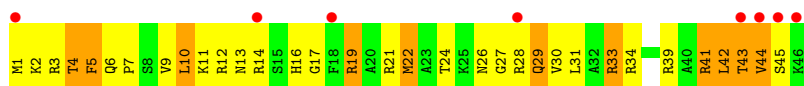
• Molecule 36: 50S ribosomal protein L34

Chain B2: 20% 30% 43% 26%



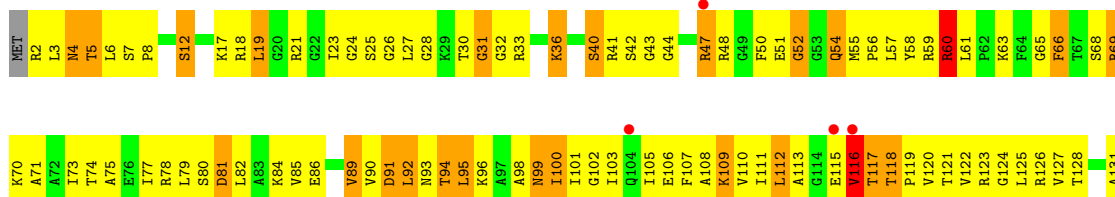
• Molecule 36: 50S ribosomal protein L34

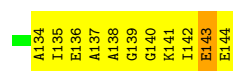
Chain D2: 17% 28% 48% 24%



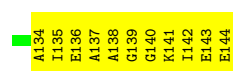
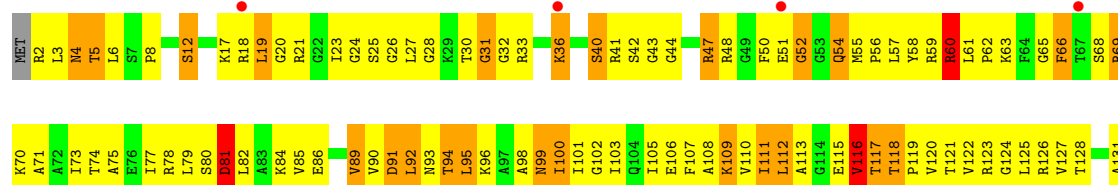
• Molecule 37: 50S ribosomal protein L15

Chain BL: 3% 24% 57% 17%

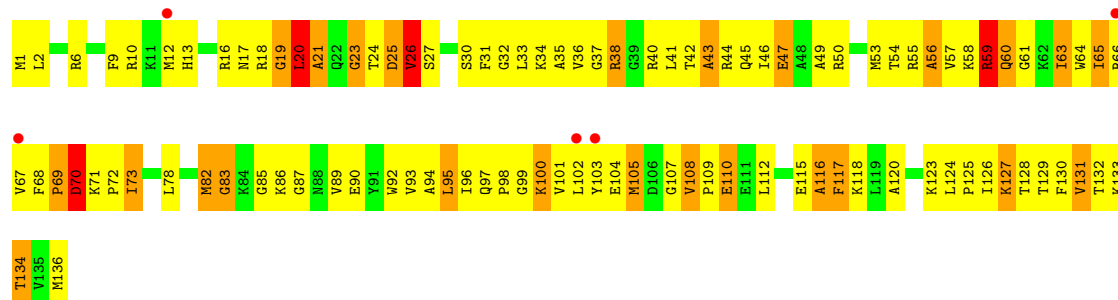




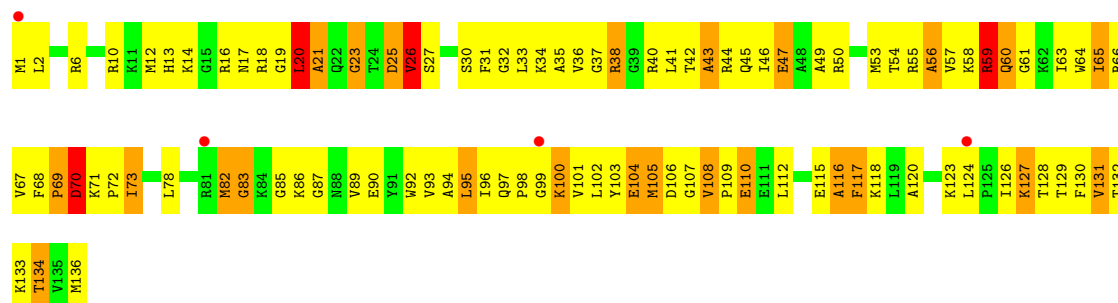
• Molecule 37: 50S ribosomal protein L15



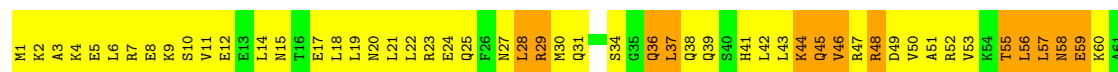
• Molecule 38: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L16



• Molecule 39: 50S ribosomal protein L29



G62
A63

• Molecule 39: 50S ribosomal protein L29

Chain DX: 13% 63% 24%

M1 K2 A3 K4 E5 L6 R7 E8 K9 S10 V11 N12 E13 L14 M15 T16 E17 L18 L19 N20 L21 L22 R23 R24 E25 Q26 F26 N27 L28 L29 R30 M31 Q32 S34 G35 Q36 L37 Q38 Q39 H41 L42 L43 K44 Q45 Q46 R47 R48 D49 V50 A51 A52 V53 K54 T55 L56 L57 N58 E59 K60 A61

G62
A63

• Molecule 40: 50S ribosomal protein L9

Chain BH: 3% 17% 50% 28% 5%

M1 Q2 V3 I4 L5 L6 D7 K8 V9 A10 N11 L12 G13 S14 L15 G16 E17 D18 Q19 V20 G24 Y25 D26 A27 R27 N28 F29 L30 V31 P32 Q33 V37 P38 A39 T40 K41 K42 M43 I44 E45 F46 F47 A48 A49 R50 R51 A52 E53 L54 E55 A56 K57 L58 A59 E60 V61 L62 A63 A64

A65 M66 A67 R68 A69 E70 D71 K72 V73 W74 L75 E76 T77 V78 I80 A81 S82 K83 A84 G85 D86 E87 K88 K89 L90 F91 I94 D98 I99 A100 D101 A102 V103 T104 A105 A106 G107 V108 E109 V110 A111 K112 S113 E114 V115 R116 L117 V121 L122 R123 T124 T125 G126 E127 H128 E129

V130 S131 F132 Q133 H135 S136 E137 V138 F139 A140 N141 K142 V143 I144 M145 V146 V147 A148 E149

• Molecule 40: 50S ribosomal protein L9

Chain DH: % 21% 56% 19% .

M1 Q2 V3 I4 L5 L6 D7 K8 V9 A10 N11 L12 G13 S14 L15 G16 E17 D18 Q19 V20 G24 Y25 D26 A27 R27 N28 F29 L30 V31 P32 Q33 V37 P38 A39 T40 K41 K42 M43 I44 E45 F46 F47 A48 A49 R50 R51 A52 E53 L54 K57 L58 L62 A63 A64 A65

M66 A67 R68 A69 E70 D71 K72 V73 W74 L75 E76 T77 V78 I80 A81 S82 K83 A84 G85 D86 E87 K88 K89 L90 F91 I94 D98 I99 A100 D101 A102 V103 T104 A105 A106 G107 V108 E109 V110 A111 K112 S113 E114 V115 R116 L117 V121 L122 R123 T124 T125 G126 E127 H128 E129 S131

F132 Q133 H135 S136 E137 V138 F139 A140 N141 K142 V143 I144 M145 V146 E149

• Molecule 41: 50S ribosomal protein L13

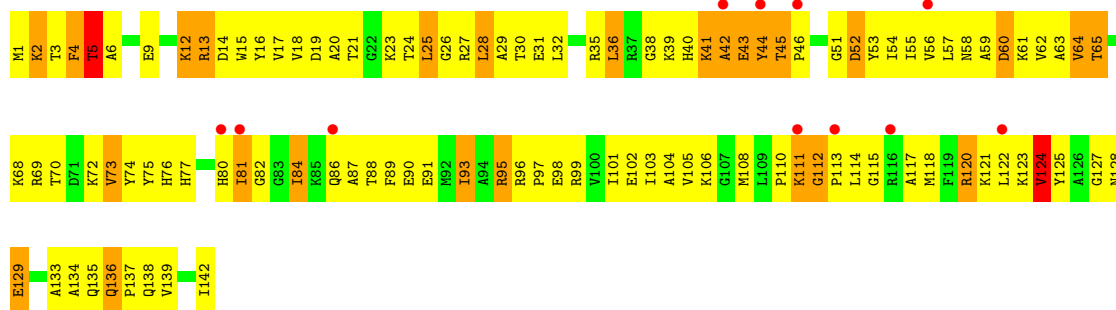
Chain BJ: 8% 23% 59% 16% .

M1 K2 T3 F4 T5 A6 E9 K12 R13 D14 V15 V16 V17 V18 D19 A20 T21 G22 K23 T24 L25 G26 R27 L28 A29 T30 E31 P32 R35 L36 R37 G38 K39 H40 K41 A42 E43 Y44 T45 P46 G51 D52 Y53 I54 T55 V56 L57 N58 A59 D60 G61 V62 A63 V64 T65 G66

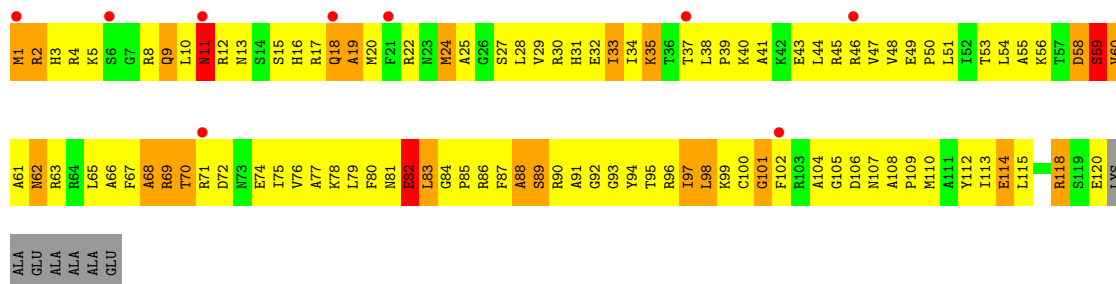
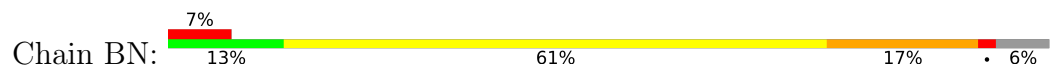
K68 R69 T70 F71 D72 V73 W74 L75 E76 T77 V78 I80 A81 S82 K83 A84 G85 D86 E87 K88 K89 L90 F91 I94 D98 I99 A100 D101 A102 V103 T104 A105 A106 G107 V108 E109 V110 A111 K112 S113 E114 V115 R116 L117 V121 L122 R123 T124 T125 G126 E127 H128 E129 S131



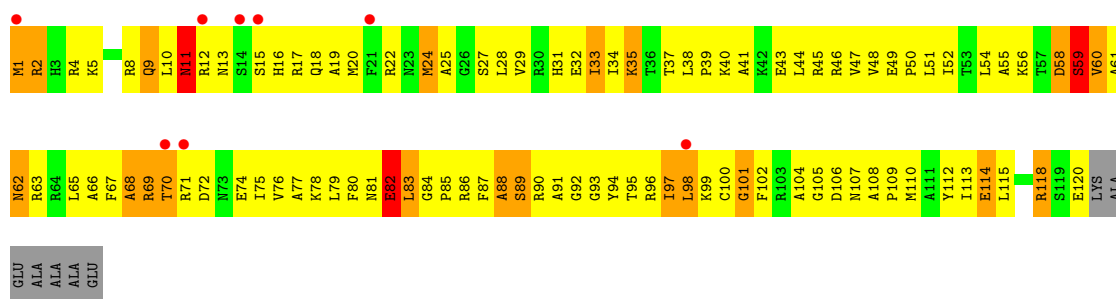
- Molecule 41: 50S ribosomal protein L13



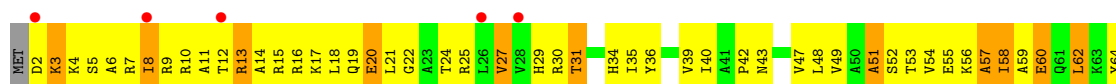
- Molecule 42: 50S ribosomal protein L17



- Molecule 42: 50S ribosomal protein L17

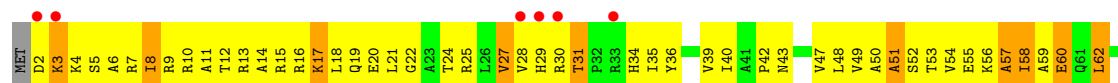


- Molecule 43: 50S ribosomal protein L18

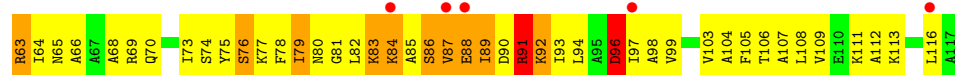
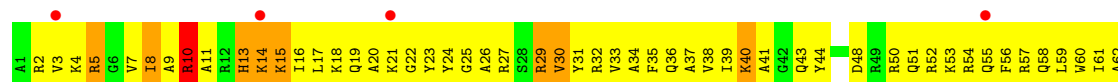




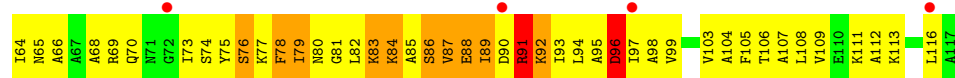
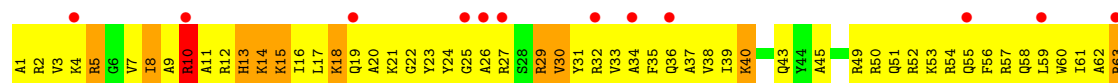
• Molecule 43: 50S ribosomal protein L18



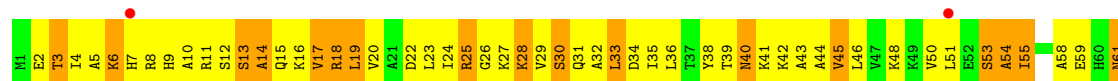
• Molecule 44: 50S ribosomal protein L20



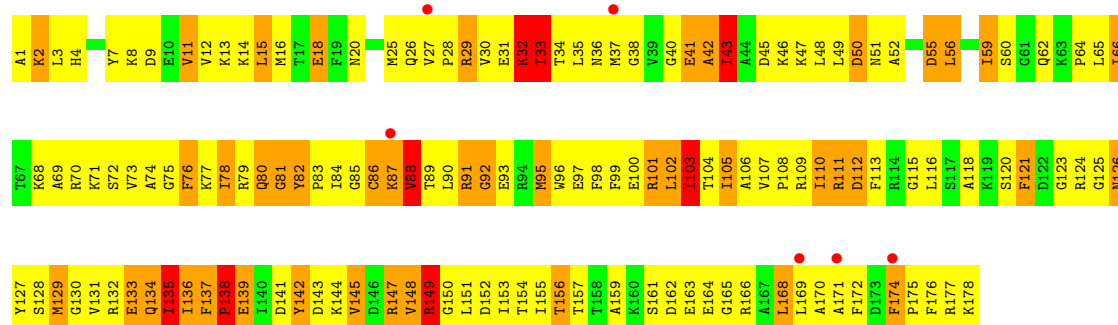
• Molecule 44: 50S ribosomal protein L20



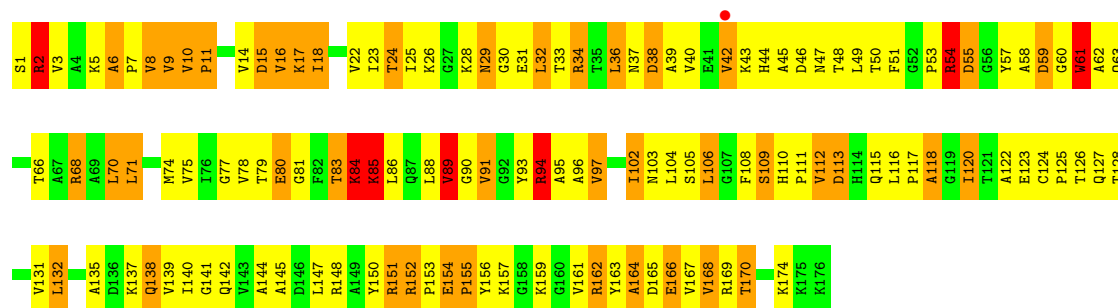
• Molecule 45: 50S ribosomal protein L22



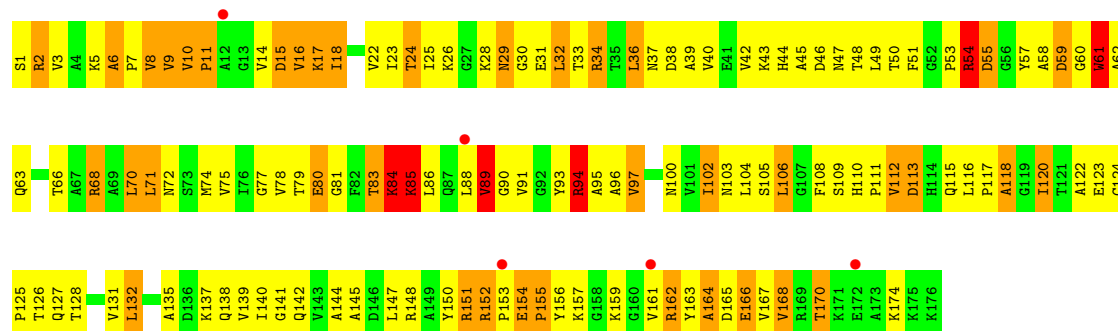
• Molecule 45: 50S ribosomal protein L22



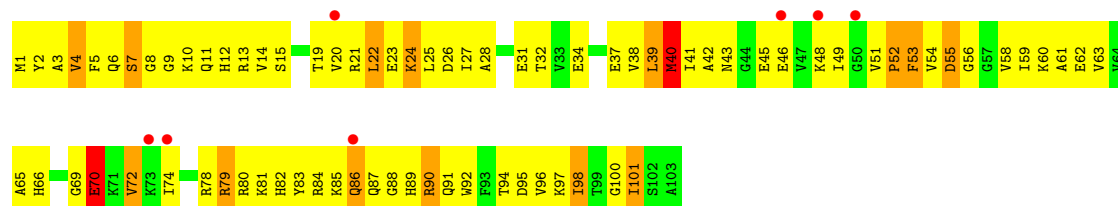
• Molecule 48: 50S ribosomal protein L6



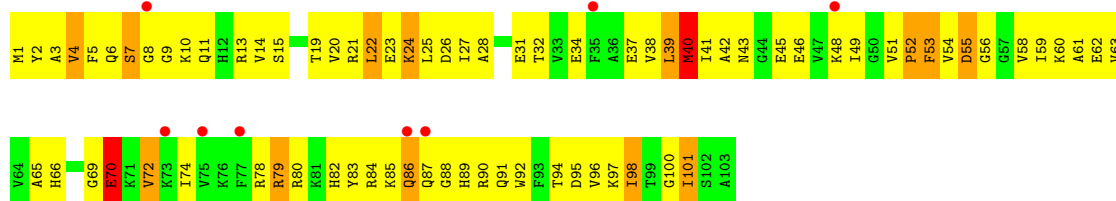
• Molecule 48: 50S ribosomal protein L6



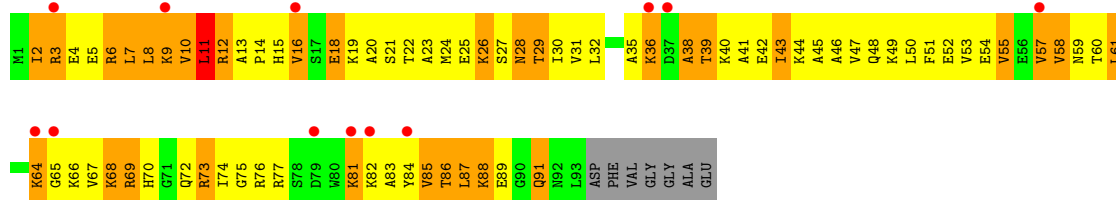
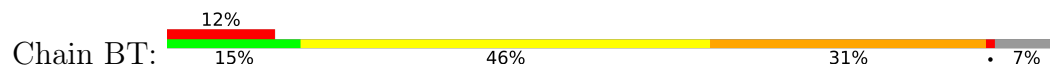
• Molecule 49: 50S ribosomal protein L21



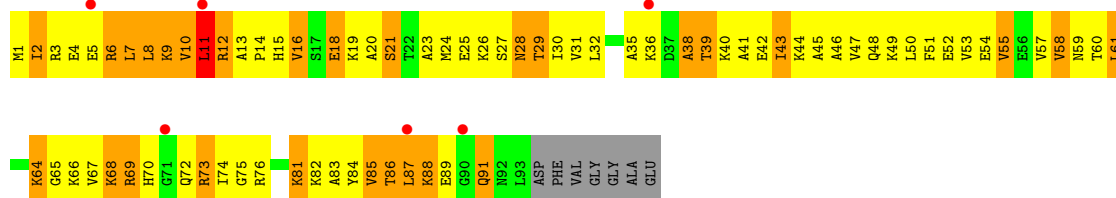
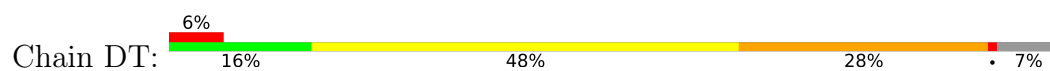
• Molecule 49: 50S ribosomal protein L21



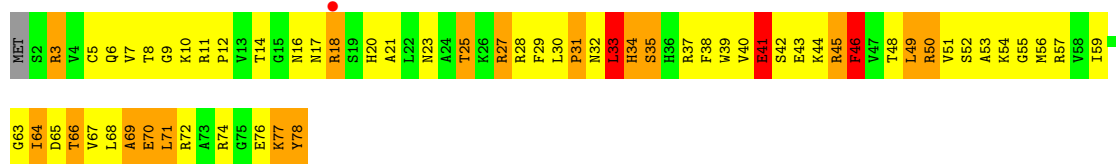
- Molecule 50: 50S ribosomal protein L23



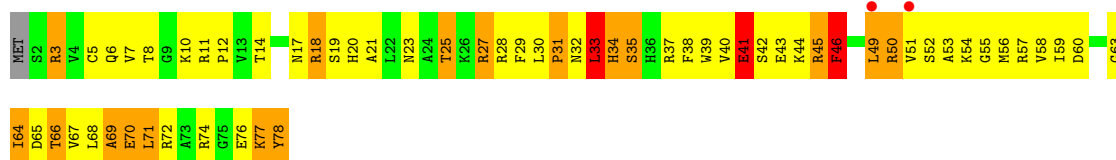
- Molecule 50: 50S ribosomal protein L23



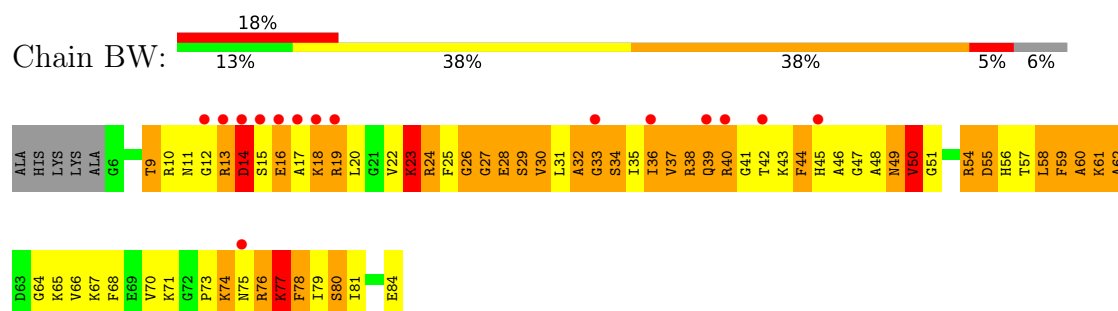
- Molecule 51: 50S ribosomal protein L28



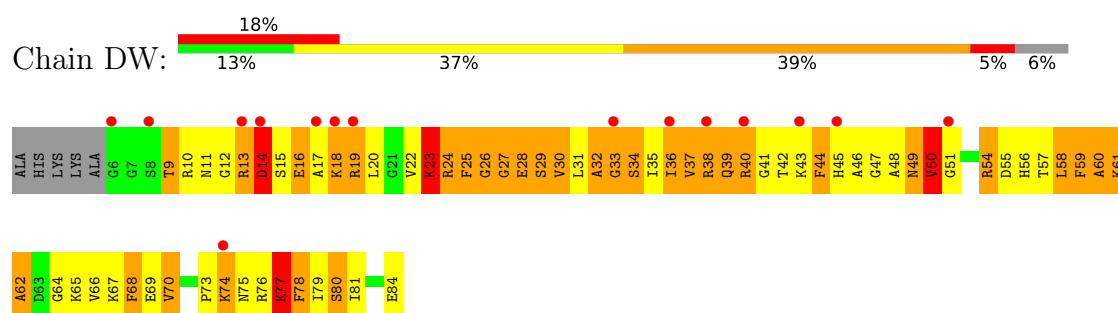
- Molecule 51: 50S ribosomal protein L28



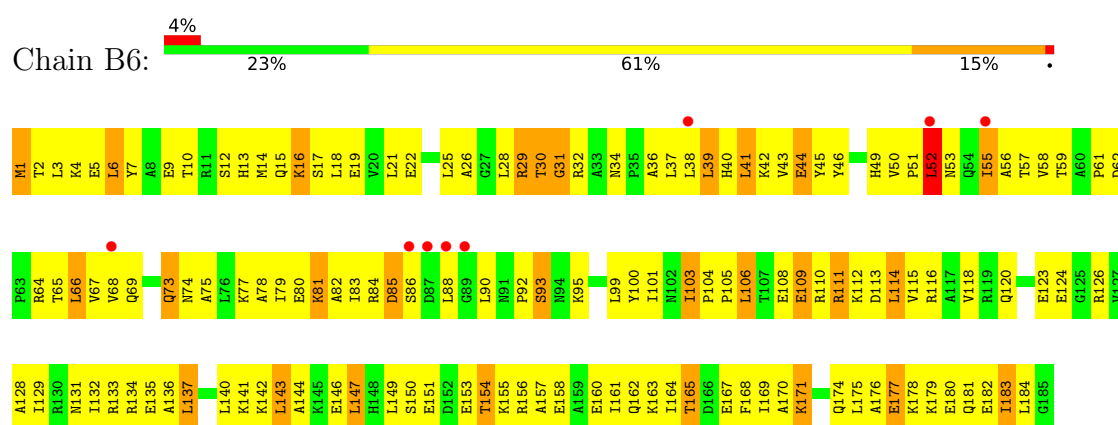
- Molecule 52: 50S ribosomal protein L27



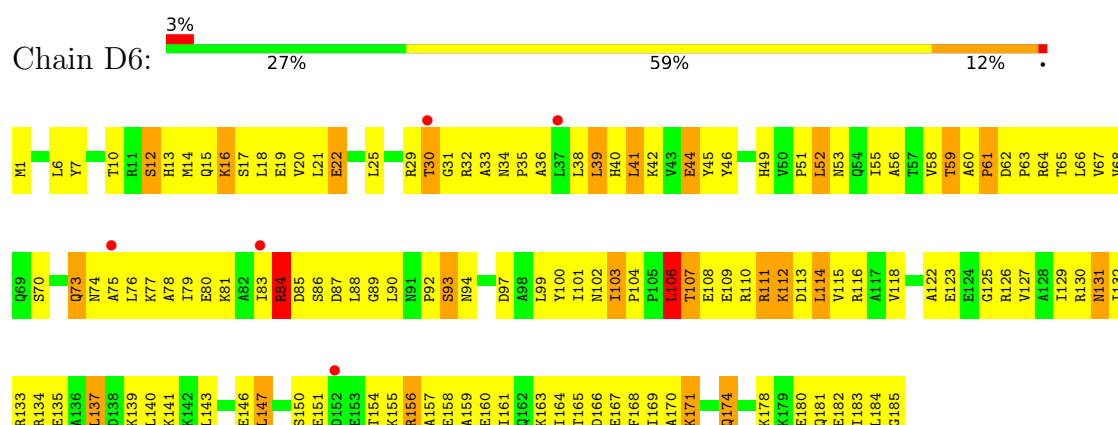
- Molecule 52: 50S ribosomal protein L27



- Molecule 53: 50S ribosomal protein RRF



- Molecule 53: 50S ribosomal protein RRF



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.54Å 378.89Å 736.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 40.00 – 4.15	Depositor EDS
% Data completeness (in resolution range)	87.4 (40.00-4.00) 87.3 (40.00-4.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 4.15Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.305 0.232 , 0.269	Depositor DCC
R_{free} test set	18876 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	133.1	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	287083	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.29	1/36762 (0.0%)	0.67	52/57350 (0.1%)
1	CA	0.28	2/36762 (0.0%)	0.67	46/57350 (0.1%)
2	AC	0.27	0/1651	0.69	0/2225
2	CC	0.27	0/1651	0.69	0/2225
3	AD	0.26	0/1665	0.71	0/2227
3	CD	0.27	0/1665	0.71	0/2227
4	AE	0.27	0/1118	0.74	0/1504
4	CE	0.27	0/1118	0.74	0/1504
5	AF	0.28	0/835	0.70	0/1128
5	CF	0.28	0/835	0.70	0/1128
6	AG	0.28	0/1187	0.77	2/1591 (0.1%)
6	CG	0.28	0/1211	0.76	2/1624 (0.1%)
7	AH	0.28	0/989	0.73	0/1326
7	CH	0.28	0/989	0.73	0/1326
8	AI	0.27	0/1034	0.70	0/1375
8	CI	0.27	0/1033	0.71	0/1375
9	AJ	0.29	0/796	0.76	0/1077
9	CJ	0.29	0/796	0.76	0/1077
10	AK	0.30	0/893	0.78	0/1205
10	CK	0.31	0/893	0.78	0/1205
11	AL	0.27	0/969	0.79	0/1300
11	CL	0.27	0/969	0.78	0/1300
12	AM	0.27	0/892	0.73	0/1193
12	CM	0.27	0/884	0.73	0/1181
13	AN	0.28	0/785	0.75	0/1043
13	CN	0.28	0/785	0.75	0/1043
14	AO	0.26	0/722	0.76	3/964 (0.3%)
14	CO	0.26	0/722	0.75	3/964 (0.3%)
15	AP	0.29	0/659	0.76	1/884 (0.1%)
15	CP	0.29	0/648	0.76	1/870 (0.1%)
16	AQ	0.27	0/657	0.66	0/881
16	CQ	0.27	0/666	0.66	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.28	0/462	0.71	0/621
17	CR	0.28	0/462	0.71	0/621
18	AS	0.27	0/652	0.72	0/877
18	CS	0.27	0/660	0.77	1/888 (0.1%)
19	AT	0.28	0/671	0.68	0/888
19	CT	0.28	0/671	0.67	0/888
20	AB	0.30	0/1735	0.73	0/2338
20	CB	0.28	0/1735	0.71	0/2338
21	AU	0.28	0/430	0.76	0/570
21	CU	0.28	0/430	0.77	1/570 (0.2%)
22	BA	0.29	0/2803	0.67	4/4371 (0.1%)
22	DA	0.29	0/2803	0.68	3/4371 (0.1%)
23	BB	0.27	1/68314 (0.0%)	0.65	64/106569 (0.1%)
23	DB	0.29	2/68314 (0.0%)	0.68	83/106569 (0.1%)
24	BI	0.32	0/1046	0.82	1/1410 (0.1%)
24	DI	0.34	0/1046	0.85	0/1410
25	BC	0.27	0/2121	0.76	1/2852 (0.0%)
25	DC	0.27	0/2121	0.76	1/2852 (0.0%)
26	BD	0.28	0/1586	0.77	3/2134 (0.1%)
26	DD	0.28	0/1586	0.76	2/2134 (0.1%)
27	BK	0.29	0/939	0.83	2/1258 (0.2%)
27	DK	0.29	0/939	0.83	2/1258 (0.2%)
28	BP	0.27	0/929	0.81	2/1242 (0.2%)
28	DP	0.27	0/929	0.79	2/1242 (0.2%)
29	BE	0.27	0/1571	0.85	5/2113 (0.2%)
29	DE	0.28	0/1571	0.85	6/2113 (0.3%)
30	BY	0.29	0/453	0.78	0/605
30	DY	0.29	0/453	0.78	0/605
31	B0	0.27	0/450	0.80	1/599 (0.2%)
31	D0	0.28	0/450	0.86	1/599 (0.2%)
32	B4	0.27	0/303	0.75	0/397
32	D4	0.27	0/303	0.76	0/397
33	B1	0.29	0/416	0.73	0/554
33	D1	0.29	0/416	0.73	0/554
34	B3	0.28	0/513	0.74	0/676
34	D3	0.28	0/513	0.74	0/676
35	BV	0.27	0/766	0.75	0/1025
35	DV	0.27	0/766	0.74	0/1025
36	B2	0.29	0/380	0.86	1/498 (0.2%)
36	D2	0.29	0/380	0.86	1/498 (0.2%)
37	BL	0.28	0/1054	0.78	0/1403
37	DL	0.28	0/1054	0.79	0/1403
38	BM	0.29	0/1093	0.78	1/1460 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.29	0/1093	0.78	1/1460 (0.1%)
39	BX	0.26	0/510	0.85	2/677 (0.3%)
39	DX	0.25	0/510	0.85	2/677 (0.3%)
40	BH	0.29	0/1122	0.73	1/1515 (0.1%)
40	DH	0.29	0/1122	0.74	1/1515 (0.1%)
41	BJ	0.29	0/1152	0.75	1/1551 (0.1%)
41	DJ	0.29	0/1152	0.75	1/1551 (0.1%)
42	BN	0.28	0/973	0.88	1/1301 (0.1%)
42	DN	0.28	0/973	0.88	1/1301 (0.1%)
43	BO	0.27	0/902	0.84	2/1209 (0.2%)
43	DO	0.27	0/902	0.84	3/1209 (0.2%)
44	BQ	0.27	0/960	0.90	5/1278 (0.4%)
44	DQ	0.27	0/960	0.90	5/1278 (0.4%)
45	BS	0.28	0/864	0.86	3/1156 (0.3%)
45	DS	0.28	0/864	0.87	3/1156 (0.3%)
46	BU	0.27	0/787	0.72	0/1051
46	DU	0.27	0/787	0.73	0/1051
47	BF	0.28	0/1444	0.83	1/1937 (0.1%)
47	DF	0.28	0/1444	0.83	1/1937 (0.1%)
48	BG	0.29	0/1343	0.80	4/1816 (0.2%)
48	DG	0.30	0/1343	0.79	4/1816 (0.2%)
49	BR	0.25	0/829	0.68	0/1107
49	DR	0.25	0/829	0.68	0/1107
50	BT	0.27	0/744	0.93	3/994 (0.3%)
50	DT	0.27	0/744	0.92	3/994 (0.3%)
51	BZ	0.27	0/635	0.85	1/848 (0.1%)
51	DZ	0.27	0/635	0.85	1/848 (0.1%)
52	BW	0.30	0/603	0.79	1/797 (0.1%)
52	DW	0.30	0/603	0.80	1/797 (0.1%)
53	B6	0.29	0/1497	0.82	2/2017 (0.1%)
53	D6	0.38	0/1497	0.88	3/2017 (0.1%)
All	All	0.28	6/309353 (0.0%)	0.70	355/462003 (0.1%)

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	16
1	CA	0	17
23	BB	0	35

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
23	DB	0	47
All	All	0	115

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1213	A	P-OP1	-8.17	1.32	1.49
1	AA	1213	A	P-OP2	-8.05	1.32	1.49
23	BB	1086	A	C5-C6	-7.45	1.26	1.41
23	DB	1086	A	C5-C6	-7.44	1.26	1.41
1	CA	1125	U	P-OP1	-6.09	1.36	1.49

The worst 5 of 355 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1124	G	OP1-P-O3'	-15.61	61.16	108.00
1	CA	366	A	C2'-C3'-O3'	12.65	128.47	109.50
1	AA	366	A	C2'-C3'-O3'	12.61	128.41	109.50
1	CA	1213	A	O5'-P-OP1	-11.86	72.42	108.00
1	AA	1213	A	O5'-P-OP2	-11.15	74.56	108.00

There are no chirality outliers.

5 of 115 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	86	G	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	1298	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	32831	0	16521	1352	0
2	AC	1624	0	1699	148	0
2	CC	1624	0	1699	150	0
3	AD	1643	0	1710	177	0
3	CD	1643	0	1710	173	0
4	AE	1105	0	1148	100	0
4	CE	1105	0	1148	103	0
5	AF	817	0	808	98	0
5	CF	817	0	808	97	0
6	AG	1174	0	1230	120	0
6	CG	1196	0	1246	112	0
7	AH	979	0	1034	104	0
7	CH	979	0	1034	107	0
8	AI	1022	0	1070	151	0
8	CI	1021	0	1070	153	0
9	AJ	786	0	828	78	0
9	CJ	786	0	828	80	0
10	AK	877	0	887	114	0
10	CK	877	0	887	118	0
11	AL	955	0	1019	102	0
11	CL	955	0	1019	99	0
12	AM	883	0	944	128	0
12	CM	876	0	937	126	0
13	AN	774	0	827	124	0
13	CN	774	0	827	134	0
14	AO	714	0	734	64	0
14	CO	714	0	734	59	0
15	AP	649	0	666	58	0
15	CP	638	0	656	58	0
16	AQ	648	0	691	73	0
16	CQ	657	0	702	72	0
17	AR	455	0	478	53	0
17	CR	455	0	478	60	0
18	AS	637	0	665	88	0
18	CS	644	0	675	90	0
19	AT	665	0	714	71	0
19	CT	665	0	714	74	0
20	AB	1704	0	1732	234	0
20	CB	1704	0	1732	225	0
21	AU	425	0	449	83	0
21	CU	425	0	449	92	0
22	BA	2507	0	1270	107	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	2507	0	1270	109	0
23	BB	60995	0	30678	2534	0
23	DB	60995	0	30678	2547	0
24	BI	1032	0	1088	126	0
24	DI	1032	0	1088	189	0
25	BC	2082	0	2157	255	0
25	DC	2082	0	2157	253	0
26	BD	1565	0	1616	217	0
26	DD	1565	0	1616	231	0
27	BK	930	0	1000	131	0
27	DK	930	0	1000	128	0
28	BP	917	0	965	102	0
28	DP	917	0	965	109	0
29	BE	1552	0	1619	201	0
29	DE	1552	0	1619	188	0
30	BY	449	0	491	52	0
30	DY	449	0	491	57	0
31	B0	444	0	461	54	0
31	D0	444	0	461	51	0
32	B4	302	0	340	39	0
32	D4	302	0	340	46	0
33	B1	409	0	440	58	0
33	D1	409	0	440	55	0
34	B3	504	0	574	60	0
34	D3	504	0	574	54	0
35	BV	753	0	780	100	0
35	DV	753	0	780	105	0
36	B2	377	0	418	40	0
36	D2	377	0	418	39	0
37	BL	1045	0	1117	155	0
37	DL	1045	0	1117	162	0
38	BM	1074	0	1157	136	0
38	DM	1074	0	1157	131	0
39	BX	509	0	543	60	0
39	DX	509	0	543	63	0
40	BH	1111	0	1148	194	0
40	DH	1111	0	1148	166	0
41	BJ	1129	0	1162	145	0
41	DJ	1129	0	1162	148	0
42	BN	960	0	1000	139	0
42	DN	960	0	1000	133	0
43	BO	892	0	923	99	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DO	892	0	923	104	0
44	BQ	947	0	1022	176	0
44	DQ	947	0	1022	182	0
45	BS	857	0	922	106	0
45	DS	857	0	922	104	0
46	BU	779	0	834	120	0
46	DU	779	0	834	115	0
47	BF	1420	0	1460	236	0
47	DF	1420	0	1460	229	0
48	BG	1323	0	1374	227	0
48	DG	1323	0	1374	198	0
49	BR	816	0	839	116	0
49	DR	816	0	839	130	0
50	BT	738	0	807	132	0
50	DT	738	0	807	129	0
51	BZ	625	0	652	86	0
51	DZ	625	0	652	87	0
52	BW	596	0	610	123	0
52	DW	596	0	610	130	0
53	B6	1478	0	1526	195	0
53	D6	1478	0	1526	161	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	61	0	0	0	0
54	CE	1	0	0	0	0
54	DB	111	0	0	0	0
55	AA	31	0	39	0	0
55	BB	31	0	39	2	0
55	CA	31	0	39	3	0
55	DB	31	0	39	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	287	0	0	1	0
57	AE	3	0	0	0	0
57	AK	1	0	0	0	0
57	AL	3	0	0	0	0
57	AN	4	0	0	0	0
57	AT	2	0	0	0	0
57	BB	492	0	0	8	0
57	BC	6	0	0	0	0
57	BD	1	0	0	0	0
57	BE	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	BL	3	0	0	0	0
57	BT	1	0	0	0	0
57	CA	296	0	0	2	0
57	CE	3	0	0	0	0
57	CK	1	0	0	0	0
57	CL	3	0	0	0	0
57	CN	4	0	0	0	0
57	CT	2	0	0	0	0
57	DB	500	0	0	7	0
57	DC	6	0	0	0	0
57	DE	2	0	0	0	0
57	DL	2	0	0	0	0
57	DR	1	0	0	0	0
57	DT	1	0	0	0	0
All	All	287083	0	193870	18347	0

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

The worst 5 of 18347 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	24:DI:3:LYS:N	1.36	1.20
40:BH:31:VAL:HB	40:BH:32:PRO:HD2	1.23	1.17
21:CU:36:PHE:HB3	21:CU:40:PRO:HD3	1.28	1.14
21:AU:36:PHE:HB3	21:AU:40:PRO:HD3	1.29	1.11
25:DC:144:GLU:HA	25:DC:151:GLY:HA2	1.33	1.11

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%)	151 (74%)	38 (19%)	15 (7%)	1	13
2	CC	204/232 (88%)	152 (74%)	37 (18%)	15 (7%)	1	13
3	AD	203/205 (99%)	151 (74%)	39 (19%)	13 (6%)	1	15
3	CD	203/205 (99%)	148 (73%)	42 (21%)	13 (6%)	1	15
4	AE	148/166 (89%)	117 (79%)	25 (17%)	6 (4%)	2	21
4	CE	148/166 (89%)	117 (79%)	25 (17%)	6 (4%)	2	21
5	AF	98/135 (73%)	64 (65%)	25 (26%)	9 (9%)	0	10
5	CF	98/135 (73%)	65 (66%)	24 (24%)	9 (9%)	0	10
6	AG	148/178 (83%)	106 (72%)	33 (22%)	9 (6%)	1	15
6	CG	150/178 (84%)	112 (75%)	29 (19%)	9 (6%)	1	16
7	AH	127/129 (98%)	98 (77%)	23 (18%)	6 (5%)	2	19
7	CH	127/129 (98%)	96 (76%)	25 (20%)	6 (5%)	2	19
8	AI	125/129 (97%)	99 (79%)	17 (14%)	9 (7%)	1	13
8	CI	125/129 (97%)	98 (78%)	18 (14%)	9 (7%)	1	13
9	AJ	96/103 (93%)	70 (73%)	13 (14%)	13 (14%)	0	3
9	CJ	96/103 (93%)	71 (74%)	12 (12%)	13 (14%)	0	3
10	AK	115/128 (90%)	87 (76%)	22 (19%)	6 (5%)	1	18
10	CK	115/128 (90%)	87 (76%)	22 (19%)	6 (5%)	1	18
11	AL	121/123 (98%)	73 (60%)	33 (27%)	15 (12%)	0	4
11	CL	121/123 (98%)	75 (62%)	31 (26%)	15 (12%)	0	4
12	AM	112/117 (96%)	79 (70%)	24 (21%)	9 (8%)	1	12
12	CM	111/117 (95%)	76 (68%)	25 (22%)	10 (9%)	0	10
13	AN	92/100 (92%)	59 (64%)	26 (28%)	7 (8%)	1	13
13	CN	92/100 (92%)	60 (65%)	24 (26%)	8 (9%)	0	10
14	AO	86/89 (97%)	59 (69%)	22 (26%)	5 (6%)	1	16
14	CO	86/89 (97%)	60 (70%)	22 (26%)	4 (5%)	2	19
15	AP	80/82 (98%)	59 (74%)	16 (20%)	5 (6%)	1	15
15	CP	78/82 (95%)	56 (72%)	16 (20%)	6 (8%)	1	12
16	AQ	78/83 (94%)	58 (74%)	15 (19%)	5 (6%)	1	15
16	CQ	79/83 (95%)	59 (75%)	15 (19%)	5 (6%)	1	15
17	AR	53/74 (72%)	41 (77%)	9 (17%)	3 (6%)	1	17
17	CR	53/74 (72%)	41 (77%)	9 (17%)	3 (6%)	1	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AS	77/91 (85%)	60 (78%)	12 (16%)	5 (6%)	1	15
18	CS	78/91 (86%)	61 (78%)	11 (14%)	6 (8%)	1	12
19	AT	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	1	16
19	CT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	1	16
20	AB	216/240 (90%)	142 (66%)	57 (26%)	17 (8%)	1	12
20	CB	216/240 (90%)	134 (62%)	65 (30%)	17 (8%)	1	12
21	AU	49/70 (70%)	28 (57%)	11 (22%)	10 (20%)	0	1
21	CU	49/70 (70%)	28 (57%)	12 (24%)	9 (18%)	0	2
24	BI	139/141 (99%)	120 (86%)	14 (10%)	5 (4%)	2	23
24	DI	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	2	23
25	BC	269/272 (99%)	155 (58%)	66 (24%)	48 (18%)	0	2
25	DC	269/272 (99%)	155 (58%)	65 (24%)	49 (18%)	0	2
26	BD	207/209 (99%)	122 (59%)	54 (26%)	31 (15%)	0	3
26	DD	207/209 (99%)	124 (60%)	51 (25%)	32 (16%)	0	3
27	BK	119/123 (97%)	78 (66%)	24 (20%)	17 (14%)	0	3
27	DK	119/123 (97%)	78 (66%)	24 (20%)	17 (14%)	0	3
28	BP	112/114 (98%)	61 (54%)	32 (29%)	19 (17%)	0	2
28	DP	112/114 (98%)	61 (54%)	34 (30%)	17 (15%)	0	3
29	BE	199/201 (99%)	125 (63%)	50 (25%)	24 (12%)	0	4
29	DE	199/201 (99%)	125 (63%)	51 (26%)	23 (12%)	0	5
30	BY	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	0	10
30	DY	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	0	10
31	B0	54/56 (96%)	39 (72%)	8 (15%)	7 (13%)	0	4
31	D0	54/56 (96%)	39 (72%)	8 (15%)	7 (13%)	0	4
32	B4	36/38 (95%)	16 (44%)	10 (28%)	10 (28%)	0	0
32	D4	36/38 (95%)	16 (44%)	10 (28%)	10 (28%)	0	0
33	B1	48/54 (89%)	37 (77%)	7 (15%)	4 (8%)	0	11
33	D1	48/54 (89%)	36 (75%)	8 (17%)	4 (8%)	0	11
34	B3	62/64 (97%)	35 (56%)	21 (34%)	6 (10%)	0	9
34	D3	62/64 (97%)	34 (55%)	22 (36%)	6 (10%)	0	9
35	BV	92/94 (98%)	64 (70%)	22 (24%)	6 (6%)	1	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	DV	92/94 (98%)	62 (67%)	24 (26%)	6 (6%)	1	15
36	B2	44/46 (96%)	30 (68%)	10 (23%)	4 (9%)	0	10
36	D2	44/46 (96%)	30 (68%)	10 (23%)	4 (9%)	0	10
37	BL	141/144 (98%)	89 (63%)	31 (22%)	21 (15%)	0	3
37	DL	141/144 (98%)	89 (63%)	32 (23%)	20 (14%)	0	3
38	BM	134/136 (98%)	84 (63%)	29 (22%)	21 (16%)	0	3
38	DM	134/136 (98%)	83 (62%)	31 (23%)	20 (15%)	0	3
39	BX	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	3
39	DX	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	3
40	BH	147/149 (99%)	76 (52%)	46 (31%)	25 (17%)	0	2
40	DH	147/149 (99%)	91 (62%)	33 (22%)	23 (16%)	0	3
41	BJ	140/142 (99%)	85 (61%)	37 (26%)	18 (13%)	0	4
41	DJ	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	3
42	BN	118/127 (93%)	76 (64%)	29 (25%)	13 (11%)	0	6
42	DN	118/127 (93%)	77 (65%)	28 (24%)	13 (11%)	0	6
43	BO	114/117 (97%)	74 (65%)	29 (25%)	11 (10%)	0	9
43	DO	114/117 (97%)	75 (66%)	27 (24%)	12 (10%)	0	7
44	BQ	115/117 (98%)	75 (65%)	31 (27%)	9 (8%)	1	12
44	DQ	115/117 (98%)	75 (65%)	29 (25%)	11 (10%)	0	9
45	BS	108/110 (98%)	68 (63%)	29 (27%)	11 (10%)	0	8
45	DS	108/110 (98%)	66 (61%)	31 (29%)	11 (10%)	0	8
46	BU	100/103 (97%)	58 (58%)	23 (23%)	19 (19%)	0	2
46	DU	100/103 (97%)	59 (59%)	22 (22%)	19 (19%)	0	2
47	BF	176/178 (99%)	103 (58%)	44 (25%)	29 (16%)	0	3
47	DF	176/178 (99%)	105 (60%)	42 (24%)	29 (16%)	0	3
48	BG	174/176 (99%)	99 (57%)	42 (24%)	33 (19%)	0	2
48	DG	174/176 (99%)	101 (58%)	41 (24%)	32 (18%)	0	2
49	BR	101/103 (98%)	72 (71%)	20 (20%)	9 (9%)	0	10
49	DR	101/103 (98%)	74 (73%)	18 (18%)	9 (9%)	0	10
50	BT	91/100 (91%)	48 (53%)	23 (25%)	20 (22%)	0	1
50	DT	91/100 (91%)	46 (50%)	27 (30%)	18 (20%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BZ	75/78 (96%)	50 (67%)	13 (17%)	12 (16%)	0	3
51	DZ	75/78 (96%)	50 (67%)	13 (17%)	12 (16%)	0	3
52	BW	77/84 (92%)	28 (36%)	23 (30%)	26 (34%)	0	0
52	DW	77/84 (92%)	28 (36%)	24 (31%)	25 (32%)	0	0
53	B6	183/185 (99%)	162 (88%)	16 (9%)	5 (3%)	4	28
53	D6	183/185 (99%)	152 (83%)	24 (13%)	7 (4%)	2	22
All	All	11607/12284 (94%)	7731 (67%)	2581 (22%)	1295 (11%)	0	6

5 of 1295 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	54	ILE
2	AC	205	GLU
3	AD	24	VAL
3	AD	25	ARG

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%)	142 (84%)	28 (16%)	2	13
2	CC	170/189 (90%)	143 (84%)	27 (16%)	2	15
3	AD	172/172 (100%)	145 (84%)	27 (16%)	2	15
3	CD	172/172 (100%)	145 (84%)	27 (16%)	2	15
4	AE	113/125 (90%)	95 (84%)	18 (16%)	2	15
4	CE	113/125 (90%)	95 (84%)	18 (16%)	2	15
5	AF	87/116 (75%)	73 (84%)	14 (16%)	2	14
5	CF	87/116 (75%)	73 (84%)	14 (16%)	2	14
6	AG	123/146 (84%)	100 (81%)	23 (19%)	1	11
6	CG	125/146 (86%)	103 (82%)	22 (18%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AH	104/104 (100%)	98 (94%)	6 (6%)	18	42
7	CH	104/104 (100%)	98 (94%)	6 (6%)	18	42
8	AI	105/106 (99%)	90 (86%)	15 (14%)	3	17
8	CI	105/106 (99%)	89 (85%)	16 (15%)	3	15
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	3	17
9	CJ	86/90 (96%)	74 (86%)	12 (14%)	3	17
10	AK	90/98 (92%)	75 (83%)	15 (17%)	2	13
10	CK	90/98 (92%)	74 (82%)	16 (18%)	2	12
11	AL	103/103 (100%)	85 (82%)	18 (18%)	2	13
11	CL	103/103 (100%)	85 (82%)	18 (18%)	2	13
12	AM	92/95 (97%)	79 (86%)	13 (14%)	3	17
12	CM	91/95 (96%)	78 (86%)	13 (14%)	3	17
13	AN	79/83 (95%)	64 (81%)	15 (19%)	1	10
13	CN	79/83 (95%)	64 (81%)	15 (19%)	1	10
14	AO	76/77 (99%)	69 (91%)	7 (9%)	8	30
14	CO	76/77 (99%)	69 (91%)	7 (9%)	8	30
15	AP	65/65 (100%)	58 (89%)	7 (11%)	6	24
15	CP	65/65 (100%)	58 (89%)	7 (11%)	6	24
16	AQ	74/77 (96%)	62 (84%)	12 (16%)	2	14
16	CQ	75/77 (97%)	63 (84%)	12 (16%)	2	14
17	AR	48/64 (75%)	40 (83%)	8 (17%)	2	13
17	CR	48/64 (75%)	40 (83%)	8 (17%)	2	13
18	AS	70/78 (90%)	58 (83%)	12 (17%)	2	13
18	CS	71/78 (91%)	58 (82%)	13 (18%)	2	12
19	AT	65/65 (100%)	56 (86%)	9 (14%)	3	17
19	CT	65/65 (100%)	56 (86%)	9 (14%)	3	17
20	AB	180/198 (91%)	148 (82%)	32 (18%)	2	12
20	CB	180/198 (91%)	150 (83%)	30 (17%)	2	13
21	AU	44/60 (73%)	35 (80%)	9 (20%)	1	8
21	CU	44/60 (73%)	35 (80%)	9 (20%)	1	8
24	BI	109/109 (100%)	108 (99%)	1 (1%)	70	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	DI	109/109 (100%)	105 (96%)	4 (4%)	30	52
25	BC	216/217 (100%)	181 (84%)	35 (16%)	2	14
25	DC	216/217 (100%)	182 (84%)	34 (16%)	2	15
26	BD	164/164 (100%)	131 (80%)	33 (20%)	1	9
26	DD	164/164 (100%)	130 (79%)	34 (21%)	1	7
27	BK	102/104 (98%)	83 (81%)	19 (19%)	1	11
27	DK	102/104 (98%)	83 (81%)	19 (19%)	1	11
28	BP	99/99 (100%)	82 (83%)	17 (17%)	2	13
28	DP	99/99 (100%)	82 (83%)	17 (17%)	2	13
29	BE	165/165 (100%)	139 (84%)	26 (16%)	2	15
29	DE	165/165 (100%)	140 (85%)	25 (15%)	3	15
30	BY	48/48 (100%)	40 (83%)	8 (17%)	2	13
30	DY	48/48 (100%)	40 (83%)	8 (17%)	2	13
31	B0	47/47 (100%)	39 (83%)	8 (17%)	2	13
31	D0	47/47 (100%)	38 (81%)	9 (19%)	1	10
32	B4	34/34 (100%)	24 (71%)	10 (29%)	0	3
32	D4	34/34 (100%)	25 (74%)	9 (26%)	0	4
33	B1	45/48 (94%)	42 (93%)	3 (7%)	15	39
33	D1	45/48 (94%)	41 (91%)	4 (9%)	9	31
34	B3	51/51 (100%)	47 (92%)	4 (8%)	11	35
34	D3	51/51 (100%)	47 (92%)	4 (8%)	11	35
35	BV	78/78 (100%)	64 (82%)	14 (18%)	2	12
35	DV	78/78 (100%)	64 (82%)	14 (18%)	2	12
36	B2	38/38 (100%)	29 (76%)	9 (24%)	1	5
36	D2	38/38 (100%)	29 (76%)	9 (24%)	1	5
37	BL	102/103 (99%)	90 (88%)	12 (12%)	5	21
37	DL	102/103 (99%)	89 (87%)	13 (13%)	4	20
38	BM	109/109 (100%)	85 (78%)	24 (22%)	1	6
38	DM	109/109 (100%)	85 (78%)	24 (22%)	1	6
39	BX	55/55 (100%)	45 (82%)	10 (18%)	2	12
39	DX	55/55 (100%)	45 (82%)	10 (18%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BH	114/114 (100%)	76 (67%)	38 (33%)	0	2
40	DH	114/114 (100%)	92 (81%)	22 (19%)	1	10
41	BJ	116/116 (100%)	101 (87%)	15 (13%)	4	19
41	DJ	116/116 (100%)	101 (87%)	15 (13%)	4	19
42	BN	100/103 (97%)	81 (81%)	19 (19%)	1	10
42	DN	100/103 (97%)	81 (81%)	19 (19%)	1	10
43	BO	86/87 (99%)	70 (81%)	16 (19%)	1	11
43	DO	86/87 (99%)	70 (81%)	16 (19%)	1	11
44	BQ	89/89 (100%)	76 (85%)	13 (15%)	3	16
44	DQ	89/89 (100%)	76 (85%)	13 (15%)	3	16
45	BS	93/93 (100%)	75 (81%)	18 (19%)	1	10
45	DS	93/93 (100%)	75 (81%)	18 (19%)	1	10
46	BU	83/84 (99%)	64 (77%)	19 (23%)	1	6
46	DU	83/84 (99%)	63 (76%)	20 (24%)	1	5
47	BF	149/149 (100%)	112 (75%)	37 (25%)	1	4
47	DF	149/149 (100%)	112 (75%)	37 (25%)	1	4
48	BG	137/137 (100%)	108 (79%)	29 (21%)	1	7
48	DG	137/137 (100%)	109 (80%)	28 (20%)	1	8
49	BR	84/84 (100%)	71 (84%)	13 (16%)	2	15
49	DR	84/84 (100%)	72 (86%)	12 (14%)	3	17
50	BT	80/84 (95%)	63 (79%)	17 (21%)	1	7
50	DT	80/84 (95%)	63 (79%)	17 (21%)	1	7
51	BZ	67/68 (98%)	55 (82%)	12 (18%)	2	12
51	DZ	67/68 (98%)	56 (84%)	11 (16%)	2	14
52	BW	59/62 (95%)	41 (70%)	18 (30%)	0	2
52	DW	59/62 (95%)	41 (70%)	18 (30%)	0	2
53	B6	157/157 (100%)	130 (83%)	27 (17%)	2	13
53	D6	157/157 (100%)	130 (83%)	27 (17%)	2	13
All	All	9647/10014 (96%)	8014 (83%)	1633 (17%)	2	13

5 of 1633 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	CG	109	LYS
25	DC	172	THR
52	DW	49	ASN
8	CI	123	ARG
6	CG	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 353 such sidechains are listed below:

Mol	Chain	Res	Type
20	CB	14	HIS
37	DL	54	GLN
24	DI	5	GLN
27	DK	88	ASN
40	DH	18	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	244 (15%)	21 (1%)
1	CA	1529/1542 (99%)	235 (15%)	19 (1%)
22	BA	116/120 (96%)	17 (14%)	0
22	DA	116/120 (96%)	16 (13%)	0
23	BB	2837/2904 (97%)	458 (16%)	17 (0%)
23	DB	2837/2904 (97%)	436 (15%)	22 (0%)
All	All	8964/9132 (98%)	1406 (15%)	79 (0%)

5 of 1406 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	DB	63	A
23	DB	2148	G
23	DB	139	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	DB	1205	A
23	DB	2756	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 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
55	LLL	CA	1662	-	31,33,33	2.58	14 (45%)	33,49,49	1.32	5 (15%)
55	LLL	DB	3112	-	31,33,33	2.59	14 (45%)	33,49,49	1.28	5 (15%)
55	LLL	AA	1661	-	31,33,33	2.58	13 (41%)	33,49,49	1.32	4 (12%)
55	LLL	BB	3111	-	31,33,33	2.54	13 (41%)	33,49,49	1.26	4 (12%)

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
55	LLL	CA	1662	-	-	1/11/65/65	0/3/3/3
55	LLL	DB	3112	-	-	1/11/65/65	0/3/3/3
55	LLL	AA	1661	-	-	1/11/65/65	0/3/3/3
55	LLL	BB	3111	-	-	1/11/65/65	0/3/3/3

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	CA	1662	LLL	O53-C53	6.60	1.52	1.43
55	AA	1661	LLL	O53-C53	6.58	1.52	1.43
55	DB	3112	LLL	O53-C53	6.57	1.52	1.43
55	BB	3111	LLL	O53-C53	6.52	1.52	1.43
55	CA	1662	LLL	C53-C43	4.68	1.56	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	CA	1662	LLL	C53-O53-C13	3.96	117.62	111.53
55	DB	3112	LLL	C53-O53-C13	3.93	117.59	111.53
55	AA	1661	LLL	C53-O53-C13	3.85	117.45	111.53
55	BB	3111	LLL	C53-O53-C13	3.85	117.45	111.53
55	AA	1661	LLL	C13-O62-C62	2.75	124.50	117.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	CA	1662	LLL	C23-C33-N33-C93
55	DB	3112	LLL	C23-C33-N33-C93
55	AA	1661	LLL	C23-C33-N33-C93
55	BB	3111	LLL	C23-C33-N33-C93

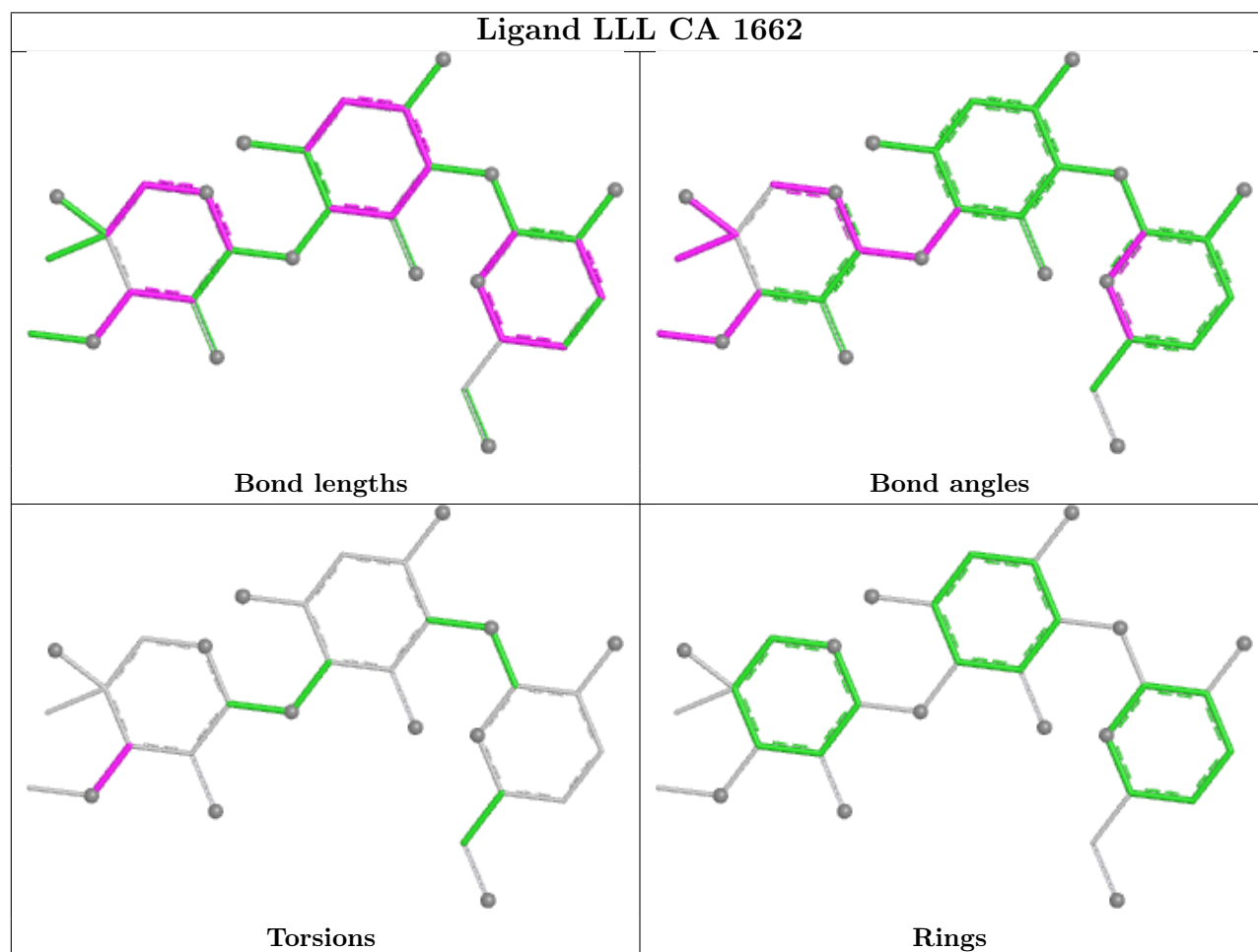
There are no ring outliers.

2 monomers are involved in 5 short contacts:

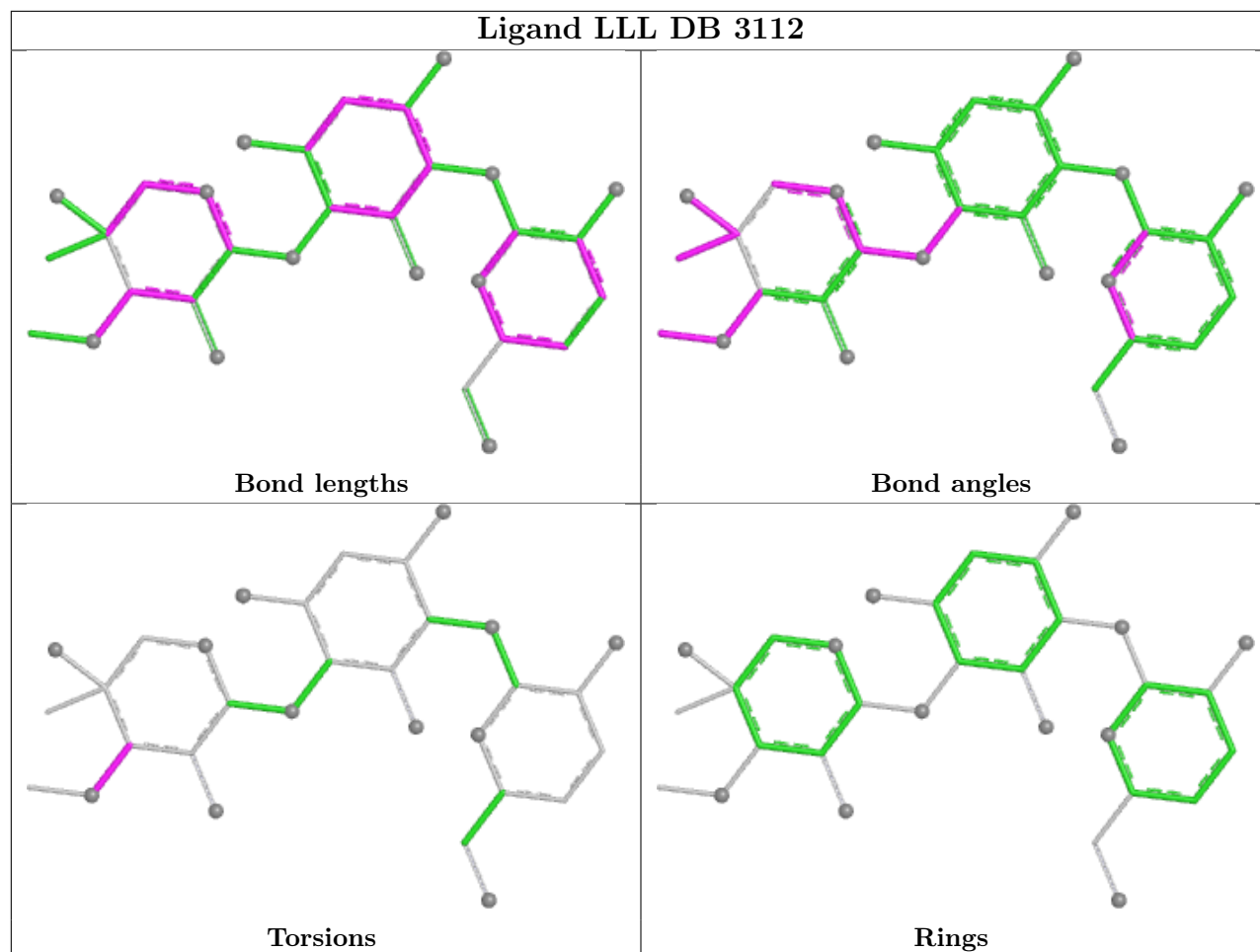
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	CA	1662	LLL	3	0
55	BB	3111	LLL	2	0

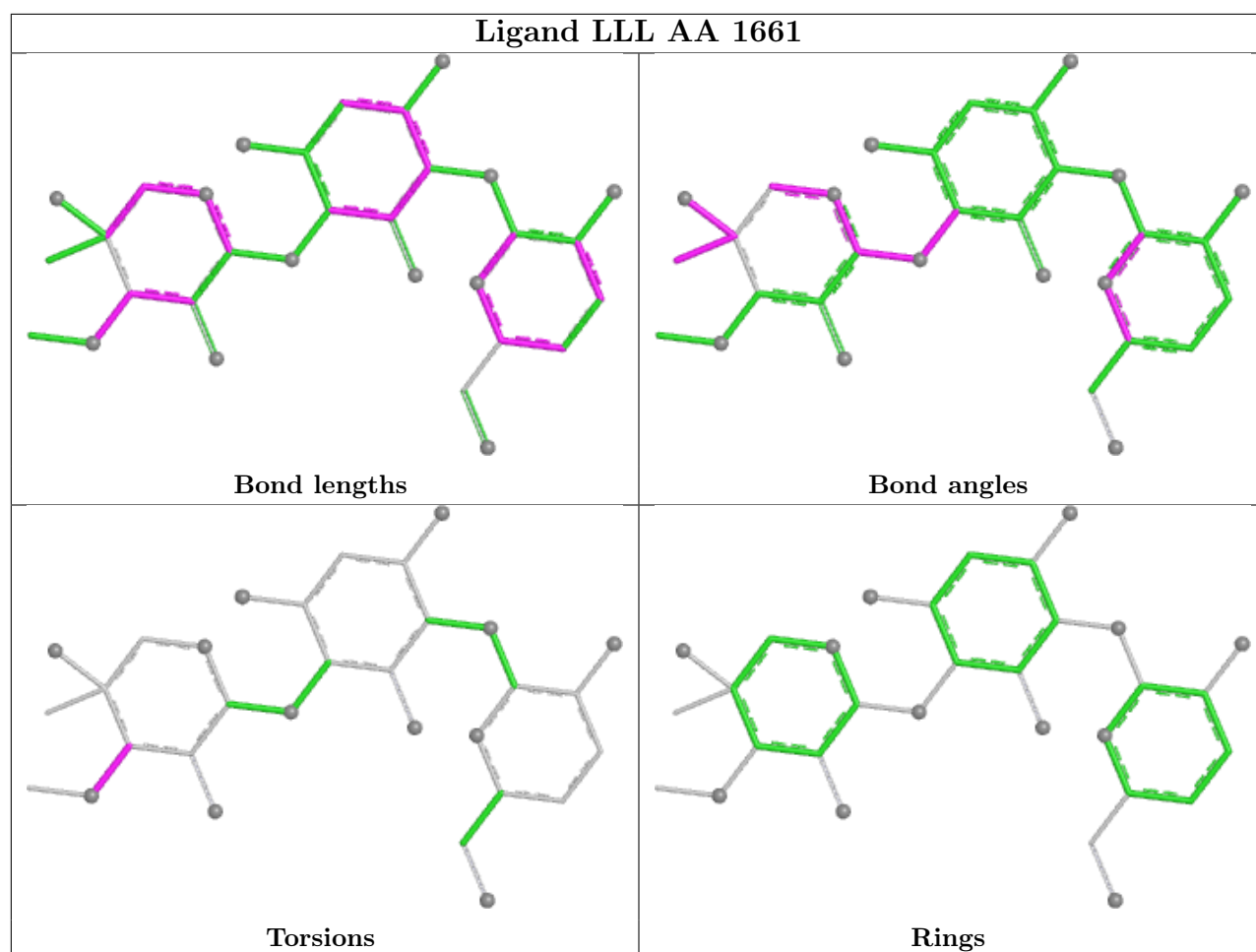
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

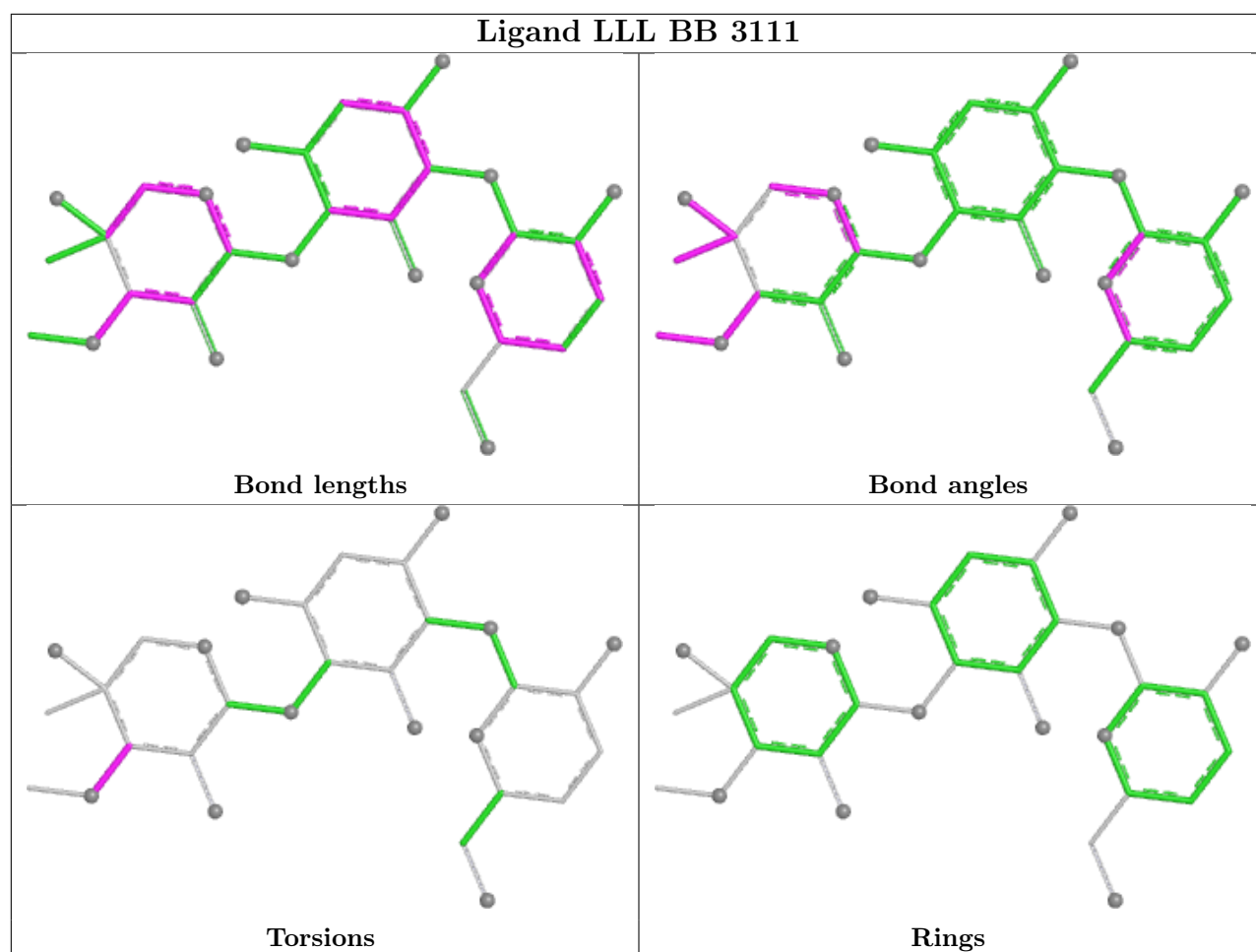
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand LLL DB 3112







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	-0.37	1 (0%) 92 87	13, 75, 157, 180	0
1	CA	1530/1542 (99%)	-0.45	0 100 100	8, 52, 139, 180	0
2	AC	206/232 (88%)	0.03	4 (1%) 66 49	5, 72, 147, 180	0
2	CC	206/232 (88%)	-0.09	4 (1%) 66 49	6, 72, 131, 180	0
3	AD	205/205 (100%)	0.36	8 (3%) 43 33	20, 95, 159, 180	0
3	CD	205/205 (100%)	0.23	7 (3%) 48 35	5, 56, 145, 180	0
4	AE	150/166 (90%)	0.19	11 (7%) 21 20	7, 69, 146, 180	0
4	CE	150/166 (90%)	0.02	1 (0%) 84 68	5, 49, 112, 180	0
5	AF	100/135 (74%)	0.07	4 (4%) 42 33	5, 69, 150, 177	0
5	CF	100/135 (74%)	0.18	2 (2%) 65 48	5, 72, 143, 166	0
6	AG	150/178 (84%)	0.18	6 (4%) 42 33	20, 97, 159, 175	0
6	CG	152/178 (85%)	0.09	3 (1%) 65 48	29, 85, 147, 180	0
7	AH	129/129 (100%)	0.30	10 (7%) 19 19	26, 80, 143, 177	0
7	CH	129/129 (100%)	0.24	7 (5%) 31 27	6, 49, 117, 174	0
8	AI	127/129 (98%)	0.26	4 (3%) 51 37	18, 89, 171, 180	0
8	CI	127/129 (98%)	0.42	10 (7%) 18 19	22, 92, 160, 180	0
9	AJ	98/103 (95%)	0.34	4 (4%) 41 32	16, 92, 169, 180	0
9	CJ	98/103 (95%)	0.42	5 (5%) 33 27	26, 87, 153, 180	0
10	AK	117/128 (91%)	0.15	5 (4%) 40 31	7, 59, 119, 180	0
10	CK	117/128 (91%)	0.15	4 (3%) 48 35	5, 52, 120, 180	0
11	AL	123/123 (100%)	0.58	11 (8%) 15 17	14, 78, 152, 180	0
11	CL	123/123 (100%)	0.45	6 (4%) 35 29	5, 46, 127, 170	0
12	AM	114/117 (97%)	0.15	2 (1%) 67 50	40, 114, 180, 180	0
12	CM	113/117 (96%)	0.37	5 (4%) 39 31	27, 100, 173, 180	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.49	8 (8%)	17 18	8, 86, 158, 180	0
13	CN	96/100 (96%)	0.42	4 (4%)	40 31	14, 87, 147, 178	0
14	AO	88/89 (98%)	0.10	1 (1%)	78 60	5, 76, 128, 180	0
14	CO	88/89 (98%)	0.41	6 (6%)	23 22	10, 63, 132, 159	0
15	AP	82/82 (100%)	0.47	6 (7%)	21 20	24, 94, 154, 180	0
15	CP	80/82 (97%)	0.57	9 (11%)	10 13	5, 46, 128, 180	0
16	AQ	80/83 (96%)	0.21	3 (3%)	44 34	36, 96, 168, 180	0
16	CQ	81/83 (97%)	0.04	1 (1%)	76 59	5, 52, 135, 180	0
17	AR	55/74 (74%)	0.38	4 (7%)	21 20	14, 70, 148, 180	0
17	CR	55/74 (74%)	0.75	9 (16%)	4 8	12, 64, 136, 180	0
18	AS	79/91 (86%)	0.36	7 (8%)	15 17	44, 120, 176, 180	0
18	CS	80/91 (87%)	0.22	2 (2%)	58 43	34, 107, 180, 180	0
19	AT	85/86 (98%)	0.41	5 (5%)	28 25	34, 101, 168, 180	0
19	CT	85/86 (98%)	0.69	10 (11%)	9 12	5, 62, 140, 180	0
20	AB	218/240 (90%)	0.28	10 (4%)	37 30	18, 97, 160, 180	0
20	CB	218/240 (90%)	0.22	9 (4%)	41 32	16, 93, 160, 180	0
21	AU	51/70 (72%)	0.78	4 (7%)	19 19	27, 89, 171, 180	0
21	CU	51/70 (72%)	0.79	7 (13%)	6 10	23, 81, 137, 180	0
22	BA	117/120 (97%)	-0.35	0	100 100	49, 85, 136, 180	0
22	DA	117/120 (97%)	-0.23	3 (2%)	57 42	36, 88, 148, 180	0
23	BB	2841/2904 (97%)	-0.39	2 (0%)	92 87	6, 60, 150, 180	0
23	DB	2841/2904 (97%)	-0.39	3 (0%)	92 87	5, 46, 154, 180	0
24	BI	141/141 (100%)	0.79	12 (8%)	16 18	72, 166, 180, 180	0
24	DI	141/141 (100%)	0.75	12 (8%)	16 18	63, 162, 180, 180	0
25	BC	271/272 (99%)	0.30	11 (4%)	41 32	5, 47, 107, 156	0
25	DC	271/272 (99%)	0.38	17 (6%)	26 23	5, 38, 99, 145	0
26	BD	209/209 (100%)	0.47	15 (7%)	21 20	8, 72, 145, 180	0
26	DD	209/209 (100%)	0.39	12 (5%)	29 26	5, 51, 131, 180	0
27	BK	121/123 (98%)	0.25	4 (3%)	49 36	16, 62, 142, 180	0
27	DK	121/123 (98%)	0.15	3 (2%)	58 43	5, 42, 103, 180	0
28	BP	114/114 (100%)	0.41	8 (7%)	22 21	28, 86, 155, 173	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.26	5 (4%)	39 31	5, 52, 119, 161	0
29	BE	201/201 (100%)	0.30	7 (3%)	47 35	5, 76, 143, 180	0
29	DE	201/201 (100%)	0.32	8 (3%)	42 33	5, 66, 138, 180	0
30	BY	58/58 (100%)	0.34	4 (6%)	23 21	22, 84, 137, 180	0
30	DY	58/58 (100%)	0.29	1 (1%)	69 51	10, 66, 149, 158	0
31	B0	56/56 (100%)	0.12	2 (3%)	46 35	5, 81, 149, 180	0
31	D0	56/56 (100%)	0.15	2 (3%)	46 35	9, 54, 119, 180	0
32	B4	38/38 (100%)	1.12	6 (15%)	5 9	5, 71, 153, 168	0
32	D4	38/38 (100%)	1.03	7 (18%)	3 6	17, 62, 132, 171	0
33	B1	50/54 (92%)	-0.12	0	100 100	32, 87, 132, 174	0
33	D1	50/54 (92%)	-0.04	0	100 100	24, 73, 125, 155	0
34	B3	64/64 (100%)	0.69	6 (9%)	14 16	19, 64, 105, 133	0
34	D3	64/64 (100%)	0.84	7 (10%)	10 13	6, 49, 107, 180	0
35	BV	94/94 (100%)	0.04	0	100 100	37, 92, 143, 180	0
35	DV	94/94 (100%)	0.20	4 (4%)	40 31	27, 94, 160, 180	0
36	B2	46/46 (100%)	0.93	9 (19%)	3 5	5, 50, 123, 143	0
36	D2	46/46 (100%)	0.87	8 (17%)	4 7	7, 43, 103, 180	0
37	BL	143/144 (99%)	0.45	4 (2%)	55 40	7, 72, 131, 180	0
37	DL	143/144 (99%)	0.38	4 (2%)	55 40	5, 61, 128, 162	0
38	BM	136/136 (100%)	0.33	5 (3%)	45 34	16, 68, 144, 165	0
38	DM	136/136 (100%)	0.45	4 (2%)	53 39	5, 63, 134, 171	0
39	BX	63/63 (100%)	0.24	0	100 100	24, 92, 169, 180	0
39	DX	63/63 (100%)	0.11	0	100 100	38, 94, 166, 180	0
40	BH	149/149 (100%)	0.37	5 (3%)	48 35	13, 125, 180, 180	0
40	DH	149/149 (100%)	0.16	1 (0%)	84 68	5, 109, 171, 180	0
41	BJ	142/142 (100%)	0.46	12 (8%)	16 18	13, 77, 132, 166	0
41	DJ	142/142 (100%)	0.45	11 (7%)	19 19	5, 65, 128, 180	0
42	BN	120/127 (94%)	0.42	9 (7%)	20 20	5, 68, 136, 180	0
42	DN	120/127 (94%)	0.26	8 (6%)	24 22	5, 44, 116, 141	0
43	BO	116/117 (99%)	0.36	7 (6%)	27 24	29, 94, 144, 180	0
43	DO	116/117 (99%)	0.48	7 (6%)	27 24	5, 93, 156, 180	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	0.47	9 (7%) 19 19	5, 72, 134, 171	0
44	DQ	117/117 (100%)	0.77	16 (13%) 6 10	5, 50, 131, 156	0
45	BS	110/110 (100%)	0.35	4 (3%) 46 35	5, 67, 129, 180	0
45	DS	110/110 (100%)	0.16	1 (0%) 81 64	5, 50, 120, 157	0
46	BU	102/103 (99%)	0.44	6 (5%) 28 25	13, 88, 148, 177	0
46	DU	102/103 (99%)	0.29	3 (2%) 53 39	26, 93, 154, 180	0
47	BF	178/178 (100%)	0.10	1 (0%) 85 71	39, 115, 174, 180	0
47	DF	178/178 (100%)	0.40	6 (3%) 48 35	22, 106, 175, 180	0
48	BG	176/176 (100%)	0.10	1 (0%) 85 71	8, 102, 172, 180	0
48	DG	176/176 (100%)	0.25	5 (2%) 55 40	32, 104, 164, 180	0
49	BR	103/103 (100%)	0.44	7 (6%) 23 22	18, 99, 151, 173	0
49	DR	103/103 (100%)	0.43	8 (7%) 19 19	5, 85, 144, 180	0
50	BT	93/100 (93%)	0.65	12 (12%) 7 11	13, 83, 160, 180	0
50	DT	93/100 (93%)	0.57	6 (6%) 25 23	15, 79, 167, 180	0
51	BZ	77/78 (98%)	0.22	1 (1%) 75 57	12, 57, 112, 152	0
51	DZ	77/78 (98%)	0.20	2 (2%) 57 42	5, 56, 101, 131	0
52	BW	79/84 (94%)	0.74	15 (18%) 3 6	19, 88, 139, 180	0
52	DW	79/84 (94%)	0.95	15 (18%) 3 6	5, 79, 143, 180	0
53	B6	185/185 (100%)	0.38	8 (4%) 40 31	23, 123, 180, 180	0
53	D6	185/185 (100%)	0.36	5 (2%) 56 41	5, 104, 180, 180	0
All	All	20787/21416 (97%)	0.02	615 (2%) 52 38	5, 69, 159, 180	0

The worst 5 of 615 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	DI	83	ALA	8.1
8	CI	129	ARG	7.6
43	DO	2	ASP	7.2
11	AL	111	GLN	6.3
44	DQ	90	ASP	6.1

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	AA	1626	1/1	-0.00	0.24	49,49,49,49	1
54	MG	AA	1623	1/1	0.07	0.55	73,73,73,73	1
54	MG	AA	1622	1/1	0.26	0.23	163,163,163,163	0
54	MG	AA	1608	1/1	0.45	0.16	147,147,147,147	0
54	MG	AA	1647	1/1	0.53	0.22	180,180,180,180	0
54	MG	AA	1656	1/1	0.54	0.34	161,161,161,161	0
54	MG	CA	1627	1/1	0.57	0.14	69,69,69,69	1
54	MG	DB	3066	1/1	0.64	0.13	158,158,158,158	0
54	MG	CA	1626	1/1	0.67	0.25	41,41,41,41	1
54	MG	BB	3033	1/1	0.71	0.09	141,141,141,141	0
54	MG	AA	1602	1/1	0.72	0.11	147,147,147,147	0
54	MG	AA	1637	1/1	0.72	0.44	151,151,151,151	0
54	MG	AA	1635	1/1	0.73	0.11	103,103,103,103	0
54	MG	AA	1625	1/1	0.73	0.26	84,84,84,84	1
54	MG	CA	1629	1/1	0.78	0.17	65,65,65,65	1
54	MG	AA	1639	1/1	0.78	0.12	134,134,134,134	0
54	MG	BB	3093	1/1	0.79	0.11	131,131,131,131	0
54	MG	CA	1608	1/1	0.80	0.14	139,139,139,139	0
54	MG	AA	1659	1/1	0.82	0.27	180,180,180,180	0
54	MG	BB	3042	1/1	0.83	0.06	135,135,135,135	0
54	MG	CA	1623	1/1	0.84	0.08	173,173,173,173	0
54	MG	DB	3060	1/1	0.85	0.08	104,104,104,104	0
54	MG	AA	1619	1/1	0.85	0.12	180,180,180,180	0
54	MG	DB	3100	1/1	0.85	0.12	46,46,46,46	0
54	MG	AA	1645	1/1	0.86	0.09	95,95,95,95	0
54	MG	BB	3038	1/1	0.86	0.10	152,152,152,152	0
54	MG	CA	1657	1/1	0.87	0.13	89,89,89,89	0
54	MG	CA	1614	1/1	0.87	0.09	90,90,90,90	0
54	MG	CA	1615	1/1	0.88	0.12	180,180,180,180	0
54	MG	AA	1646	1/1	0.88	0.09	104,104,104,104	0
54	MG	DB	3058	1/1	0.88	0.39	162,162,162,162	0
54	MG	CA	1621	1/1	0.89	0.21	110,110,110,110	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3013	1/1	0.89	0.08	92,92,92,92	0
54	MG	AA	1657	1/1	0.89	0.09	124,124,124,124	0
54	MG	AA	1644	1/1	0.89	0.07	98,98,98,98	0
54	MG	BB	3004	1/1	0.89	0.13	73,73,73,73	0
55	LLL	DB	3112	31/31	0.89	0.32	121,121,121,121	0
54	MG	BB	3099	1/1	0.90	0.09	56,56,56,56	0
54	MG	DB	3059	1/1	0.90	0.09	166,166,166,166	0
54	MG	CA	1635	1/1	0.90	0.09	98,98,98,98	0
54	MG	BB	3082	1/1	0.90	0.18	5,5,5,5	0
54	MG	CA	1658	1/1	0.90	0.28	53,53,53,53	0
54	MG	DB	3050	1/1	0.90	0.10	123,123,123,123	0
54	MG	CA	1649	1/1	0.91	0.13	127,127,127,127	0
55	LLL	BB	3111	31/31	0.91	0.18	107,107,107,107	0
54	MG	BB	3080	1/1	0.91	0.07	77,77,77,77	0
54	MG	CA	1638	1/1	0.92	0.11	98,98,98,98	0
54	MG	AA	1651	1/1	0.92	0.06	112,112,112,112	0
54	MG	BB	3078	1/1	0.92	0.07	101,101,101,101	0
54	MG	AA	1620	1/1	0.92	0.07	113,113,113,113	0
54	MG	DB	3034	1/1	0.93	0.05	69,69,69,69	0
54	MG	CA	1606	1/1	0.93	0.07	138,138,138,138	0
54	MG	AA	1614	1/1	0.93	0.06	113,113,113,113	0
54	MG	AA	1627	1/1	0.94	0.10	68,68,68,68	0
54	MG	BB	3072	1/1	0.94	0.07	79,79,79,79	0
54	MG	BB	3035	1/1	0.94	0.07	82,82,82,82	0
54	MG	DB	3052	1/1	0.94	0.06	113,113,113,113	0
54	MG	DB	3057	1/1	0.94	0.06	77,77,77,77	0
54	MG	BB	3031	1/1	0.94	0.08	63,63,63,63	0
54	MG	BB	3071	1/1	0.95	0.07	89,89,89,89	0
54	MG	DB	3097	1/1	0.95	0.08	64,64,64,64	0
54	MG	AA	1658	1/1	0.95	0.06	85,85,85,85	0
55	LLL	AA	1661	31/31	0.95	0.07	21,21,21,21	0
54	MG	BB	3010	1/1	0.95	0.06	40,40,40,40	0
55	LLL	CA	1662	31/31	0.95	0.09	14,14,14,14	0
54	MG	BB	3043	1/1	0.95	0.05	122,122,122,122	0
54	MG	BB	3012	1/1	0.96	0.06	53,53,53,53	0
54	MG	BB	3100	1/1	0.96	0.05	151,151,151,151	0
54	MG	BB	3108	1/1	0.96	0.09	44,44,44,44	0
54	MG	CA	1659	1/1	0.96	0.07	90,90,90,90	0
54	MG	CA	1660	1/1	0.96	0.18	63,63,63,63	0
54	MG	DB	3011	1/1	0.96	0.09	33,33,33,33	0
54	MG	DB	3033	1/1	0.96	0.06	43,43,43,43	0
54	MG	BB	3047	1/1	0.96	0.06	116,116,116,116	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3037	1/1	0.96	0.11	54,54,54,54	0
54	MG	DB	3045	1/1	0.96	0.05	68,68,68,68	0
54	MG	BB	3061	1/1	0.96	0.09	56,56,56,56	0
54	MG	CA	1609	1/1	0.96	0.03	84,84,84,84	0
54	MG	AA	1601	1/1	0.96	0.07	41,41,41,41	0
54	MG	AA	1630	1/1	0.96	0.05	88,88,88,88	0
54	MG	CA	1616	1/1	0.96	0.06	88,88,88,88	0
54	MG	AA	1650	1/1	0.96	0.07	122,122,122,122	0
54	MG	BB	3079	1/1	0.96	0.06	63,63,63,63	0
54	MG	DB	3071	1/1	0.96	0.06	37,37,37,37	0
54	MG	DB	3076	1/1	0.96	0.08	104,104,104,104	0
54	MG	AA	1632	1/1	0.96	0.21	62,62,62,62	0
54	MG	BB	3009	1/1	0.96	0.08	96,96,96,96	0
54	MG	DB	3106	1/1	0.96	0.07	64,64,64,64	0
54	MG	BB	3087	1/1	0.96	0.07	114,114,114,114	0
54	MG	AA	1615	1/1	0.96	0.07	106,106,106,106	0
54	MG	BB	3097	1/1	0.96	0.05	88,88,88,88	0
54	MG	CA	1642	1/1	0.96	0.05	108,108,108,108	0
54	MG	CA	1646	1/1	0.97	0.10	99,99,99,99	0
54	MG	BB	3051	1/1	0.97	0.06	65,65,65,65	0
54	MG	CA	1654	1/1	0.97	0.07	59,59,59,59	0
54	MG	DB	3053	1/1	0.97	0.05	80,80,80,80	0
54	MG	BB	3026	1/1	0.97	0.08	43,43,43,43	0
54	MG	BB	3063	1/1	0.97	0.07	28,28,28,28	0
54	MG	BB	3070	1/1	0.97	0.05	59,59,59,59	0
54	MG	AA	1652	1/1	0.97	0.07	90,90,90,90	0
54	MG	CE	201	1/1	0.97	0.07	113,113,113,113	0
54	MG	DB	3006	1/1	0.97	0.06	15,15,15,15	0
54	MG	DB	3073	1/1	0.97	0.12	67,67,67,67	0
54	MG	BB	3095	1/1	0.97	0.04	81,81,81,81	0
54	MG	DB	3083	1/1	0.97	0.07	83,83,83,83	0
54	MG	DB	3095	1/1	0.97	0.06	88,88,88,88	0
54	MG	DB	3013	1/1	0.97	0.05	41,41,41,41	0
54	MG	DB	3022	1/1	0.97	0.06	71,71,71,71	0
54	MG	DB	3029	1/1	0.97	0.06	59,59,59,59	0
54	MG	AA	1617	1/1	0.97	0.04	100,100,100,100	0
54	MG	CA	1641	1/1	0.97	0.12	42,42,42,42	0
54	MG	DB	3035	1/1	0.97	0.06	75,75,75,75	0
54	MG	BB	3016	1/1	0.97	0.08	91,91,91,91	0
54	MG	BB	3018	1/1	0.98	0.08	50,50,50,50	0
54	MG	DB	3028	1/1	0.98	0.08	58,58,58,58	0
54	MG	BB	3019	1/1	0.98	0.04	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3090	1/1	0.98	0.05	91,91,91,91	0
54	MG	BB	3091	1/1	0.98	0.05	37,37,37,37	0
54	MG	BB	3053	1/1	0.98	0.07	79,79,79,79	0
54	MG	CA	1630	1/1	0.98	0.07	52,52,52,52	0
54	MG	DB	3039	1/1	0.98	0.03	69,69,69,69	0
54	MG	CA	1631	1/1	0.98	0.04	40,40,40,40	0
54	MG	BB	3094	1/1	0.98	0.05	47,47,47,47	0
54	MG	CA	1636	1/1	0.98	0.06	92,92,92,92	0
54	MG	CA	1637	1/1	0.98	0.03	92,92,92,92	0
54	MG	AA	1624	1/1	0.98	0.08	77,77,77,77	0
54	MG	BB	3096	1/1	0.98	0.07	67,67,67,67	0
54	MG	BB	3008	1/1	0.98	0.06	75,75,75,75	0
54	MG	BB	3064	1/1	0.98	0.05	37,37,37,37	0
54	MG	DB	3064	1/1	0.98	0.04	19,19,19,19	0
54	MG	CA	1647	1/1	0.98	0.04	65,65,65,65	0
54	MG	DB	3070	1/1	0.98	0.11	38,38,38,38	0
54	MG	AA	1654	1/1	0.98	0.04	82,82,82,82	0
54	MG	CA	1652	1/1	0.98	0.07	65,65,65,65	0
54	MG	BB	3106	1/1	0.98	0.09	39,39,39,39	0
54	MG	DB	3081	1/1	0.98	0.04	19,19,19,19	0
54	MG	AA	1612	1/1	0.98	0.09	88,88,88,88	0
54	MG	DB	3085	1/1	0.98	0.06	49,49,49,49	0
54	MG	DB	3089	1/1	0.98	0.09	61,61,61,61	0
54	MG	DB	3090	1/1	0.98	0.14	64,64,64,64	0
54	MG	DB	3092	1/1	0.98	0.06	56,56,56,56	0
54	MG	AA	1631	1/1	0.98	0.05	88,88,88,88	0
54	MG	BB	3077	1/1	0.98	0.05	83,83,83,83	0
54	MG	AA	1640	1/1	0.98	0.07	56,56,56,56	0
54	MG	AA	1611	1/1	0.98	0.05	77,77,77,77	0
54	MG	DB	3109	1/1	0.98	0.05	83,83,83,83	0
54	MG	DB	3110	1/1	0.98	0.11	38,38,38,38	0
54	MG	BB	3044	1/1	0.98	0.08	52,52,52,52	0
54	MG	BB	3081	1/1	0.98	0.06	16,16,16,16	0
54	MG	CA	1619	1/1	0.98	0.07	70,70,70,70	0
54	MG	DB	3020	1/1	0.98	0.10	13,13,13,13	0
56	ZN	B4	101	1/1	0.98	0.04	64,64,64,64	0
56	ZN	D4	101	1/1	0.98	0.04	45,45,45,45	0
54	MG	BB	3059	1/1	0.99	0.04	60,60,60,60	0
54	MG	AA	1610	1/1	0.99	0.04	62,62,62,62	0
54	MG	BB	3011	1/1	0.99	0.04	29,29,29,29	0
54	MG	AA	1648	1/1	0.99	0.04	40,40,40,40	0
54	MG	BB	3067	1/1	0.99	0.03	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1643	1/1	0.99	0.03	32,32,32,32	0
54	MG	CA	1644	1/1	0.99	0.03	68,68,68,68	0
54	MG	CA	1645	1/1	0.99	0.03	66,66,66,66	0
54	MG	AA	1649	1/1	0.99	0.03	82,82,82,82	0
54	MG	BB	3014	1/1	0.99	0.07	58,58,58,58	0
54	MG	BB	3015	1/1	0.99	0.11	42,42,42,42	0
54	MG	CA	1650	1/1	0.99	0.04	33,33,33,33	0
54	MG	CA	1651	1/1	0.99	0.13	38,38,38,38	0
54	MG	BB	3073	1/1	0.99	0.06	38,38,38,38	0
54	MG	CA	1653	1/1	0.99	0.04	51,51,51,51	0
54	MG	BB	3074	1/1	0.99	0.03	13,13,13,13	0
54	MG	AA	1634	1/1	0.99	0.03	67,67,67,67	0
54	MG	BB	3017	1/1	0.99	0.03	73,73,73,73	0
54	MG	AA	1606	1/1	0.99	0.03	47,47,47,47	0
54	MG	AA	1636	1/1	0.99	0.06	93,93,93,93	0
54	MG	CA	1661	1/1	0.99	0.03	48,48,48,48	0
54	MG	BB	3020	1/1	0.99	0.03	36,36,36,36	0
54	MG	DB	3003	1/1	0.99	0.05	33,33,33,33	0
54	MG	DB	3004	1/1	0.99	0.06	69,69,69,69	0
54	MG	BB	3021	1/1	0.99	0.09	51,51,51,51	0
54	MG	DB	3008	1/1	0.99	0.04	17,17,17,17	0
54	MG	DB	3009	1/1	0.99	0.07	18,18,18,18	0
54	MG	BB	3084	1/1	0.99	0.04	77,77,77,77	0
54	MG	BB	3085	1/1	0.99	0.03	43,43,43,43	0
54	MG	DB	3014	1/1	0.99	0.08	43,43,43,43	0
54	MG	DB	3015	1/1	0.99	0.10	24,24,24,24	0
54	MG	BB	3022	1/1	0.99	0.05	37,37,37,37	0
54	MG	DB	3021	1/1	0.99	0.04	51,51,51,51	0
54	MG	BB	3024	1/1	0.99	0.10	44,44,44,44	0
54	MG	DB	3024	1/1	0.99	0.04	45,45,45,45	0
54	MG	DB	3025	1/1	0.99	0.04	42,42,42,42	0
54	MG	DB	3026	1/1	0.99	0.03	54,54,54,54	0
54	MG	DB	3027	1/1	0.99	0.09	28,28,28,28	0
54	MG	AA	1653	1/1	0.99	0.13	87,87,87,87	0
54	MG	BB	3092	1/1	0.99	0.04	45,45,45,45	0
54	MG	DB	3030	1/1	0.99	0.06	10,10,10,10	0
54	MG	BB	3027	1/1	0.99	0.09	42,42,42,42	0
54	MG	BB	3028	1/1	0.99	0.05	61,61,61,61	0
54	MG	BB	3030	1/1	0.99	0.02	70,70,70,70	0
54	MG	AA	1618	1/1	0.99	0.07	93,93,93,93	0
54	MG	DB	3038	1/1	0.99	0.05	37,37,37,37	0
54	MG	BB	3032	1/1	0.99	0.03	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3042	1/1	0.99	0.07	23,23,23,23	0
54	MG	DB	3043	1/1	0.99	0.05	32,32,32,32	0
54	MG	AA	1607	1/1	0.99	0.03	42,42,42,42	0
54	MG	DB	3048	1/1	0.99	0.06	34,34,34,34	0
54	MG	AA	1613	1/1	0.99	0.03	71,71,71,71	0
54	MG	DB	3051	1/1	0.99	0.06	32,32,32,32	0
54	MG	BB	3105	1/1	0.99	0.03	60,60,60,60	0
54	MG	BB	3036	1/1	0.99	0.10	62,62,62,62	0
54	MG	DB	3054	1/1	0.99	0.06	29,29,29,29	0
54	MG	DB	3055	1/1	0.99	0.05	41,41,41,41	0
54	MG	BB	3037	1/1	0.99	0.04	44,44,44,44	0
54	MG	BB	3109	1/1	0.99	0.05	59,59,59,59	0
54	MG	CA	1605	1/1	0.99	0.04	18,18,18,18	0
54	MG	AA	1641	1/1	0.99	0.04	69,69,69,69	0
54	MG	DB	3061	1/1	0.99	0.03	69,69,69,69	0
54	MG	DB	3062	1/1	0.99	0.03	67,67,67,67	0
54	MG	BB	3041	1/1	0.99	0.05	8,8,8,8	0
54	MG	AA	1642	1/1	0.99	0.03	41,41,41,41	0
54	MG	DB	3068	1/1	0.99	0.07	22,22,22,22	0
54	MG	CA	1610	1/1	0.99	0.05	75,75,75,75	0
54	MG	CA	1611	1/1	0.99	0.05	57,57,57,57	0
54	MG	DB	3072	1/1	0.99	0.05	54,54,54,54	0
54	MG	CA	1612	1/1	0.99	0.04	72,72,72,72	0
54	MG	DB	3074	1/1	0.99	0.03	17,17,17,17	0
54	MG	DB	3075	1/1	0.99	0.05	35,35,35,35	0
54	MG	BB	3003	1/1	0.99	0.06	51,51,51,51	0
54	MG	DB	3078	1/1	0.99	0.04	32,32,32,32	0
54	MG	AA	1628	1/1	0.99	0.04	59,59,59,59	0
54	MG	DB	3082	1/1	0.99	0.03	57,57,57,57	0
54	MG	BB	3046	1/1	0.99	0.03	64,64,64,64	0
54	MG	DB	3084	1/1	0.99	0.04	16,16,16,16	0
54	MG	CA	1618	1/1	0.99	0.09	30,30,30,30	0
54	MG	DB	3086	1/1	0.99	0.09	52,52,52,52	0
54	MG	DB	3088	1/1	0.99	0.04	46,46,46,46	0
54	MG	BB	3007	1/1	0.99	0.04	53,53,53,53	0
54	MG	CA	1620	1/1	0.99	0.04	37,37,37,37	0
54	MG	BB	3049	1/1	0.99	0.04	35,35,35,35	0
54	MG	DB	3094	1/1	0.99	0.04	55,55,55,55	0
54	MG	AA	1621	1/1	0.99	0.16	26,26,26,26	0
54	MG	CA	1624	1/1	0.99	0.09	56,56,56,56	0
54	MG	CA	1625	1/1	0.99	0.12	6,6,6,6	0
54	MG	DB	3101	1/1	0.99	0.08	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3104	1/1	0.99	0.09	71,71,71,71	0
54	MG	BB	3052	1/1	0.99	0.05	36,36,36,36	0
54	MG	AA	1605	1/1	0.99	0.05	47,47,47,47	0
54	MG	BB	3054	1/1	0.99	0.06	46,46,46,46	0
54	MG	DB	3111	1/1	0.99	0.07	32,32,32,32	0
54	MG	BB	3055	1/1	0.99	0.07	53,53,53,53	0
54	MG	BB	3056	1/1	0.99	0.06	31,31,31,31	0
54	MG	CA	1632	1/1	0.99	0.04	18,18,18,18	0
54	MG	CA	1633	1/1	0.99	0.08	50,50,50,50	0
54	MG	CA	1634	1/1	0.99	0.03	23,23,23,23	0
54	MG	BB	3057	1/1	0.99	0.09	65,65,65,65	0
54	MG	CA	1617	1/1	1.00	0.03	5,5,5,5	0
54	MG	DB	3023	1/1	1.00	0.02	17,17,17,17	0
54	MG	BB	3025	1/1	1.00	0.05	42,42,42,42	0
54	MG	AA	1609	1/1	1.00	0.00	5,5,5,5	0
54	MG	BB	3048	1/1	1.00	0.09	7,7,7,7	0
54	MG	AA	1633	1/1	1.00	0.06	48,48,48,48	0
54	MG	CA	1622	1/1	1.00	0.02	18,18,18,18	0
54	MG	BB	3050	1/1	1.00	0.06	33,33,33,33	0
54	MG	BB	3083	1/1	1.00	0.04	28,28,28,28	0
54	MG	DB	3031	1/1	1.00	0.06	24,24,24,24	0
54	MG	DB	3032	1/1	1.00	0.02	51,51,51,51	0
54	MG	AA	1616	1/1	1.00	0.04	42,42,42,42	0
54	MG	BB	3029	1/1	1.00	0.03	17,17,17,17	0
54	MG	BB	3086	1/1	1.00	0.03	18,18,18,18	0
54	MG	DB	3036	1/1	1.00	0.03	20,20,20,20	0
54	MG	CA	1628	1/1	1.00	0.02	44,44,44,44	0
54	MG	AA	1629	1/1	1.00	0.02	26,26,26,26	0
54	MG	BB	3088	1/1	1.00	0.04	36,36,36,36	0
54	MG	DB	3040	1/1	1.00	0.03	18,18,18,18	0
54	MG	DB	3041	1/1	1.00	0.05	34,34,34,34	0
54	MG	BB	3089	1/1	1.00	0.02	25,25,25,25	0
54	MG	AA	1660	1/1	1.00	0.04	37,37,37,37	0
54	MG	DB	3044	1/1	1.00	0.03	21,21,21,21	0
54	MG	BB	3001	1/1	1.00	0.06	29,29,29,29	0
54	MG	DB	3046	1/1	1.00	0.06	11,11,11,11	0
54	MG	DB	3047	1/1	1.00	0.02	19,19,19,19	0
54	MG	BB	3002	1/1	1.00	0.05	30,30,30,30	0
54	MG	DB	3049	1/1	1.00	0.01	9,9,9,9	0
54	MG	BB	3034	1/1	1.00	0.07	59,59,59,59	0
54	MG	BB	3058	1/1	1.00	0.03	11,11,11,11	0
54	MG	AA	1643	1/1	1.00	0.08	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3060	1/1	1.00	0.04	22,22,22,22	0
54	MG	CA	1639	1/1	1.00	0.01	7,7,7,7	0
54	MG	CA	1640	1/1	1.00	0.09	5,5,5,5	0
54	MG	DB	3056	1/1	1.00	0.03	12,12,12,12	0
54	MG	AA	1603	1/1	1.00	0.04	14,14,14,14	0
54	MG	BB	3098	1/1	1.00	0.03	16,16,16,16	0
54	MG	BB	3062	1/1	1.00	0.07	27,27,27,27	0
54	MG	BB	3005	1/1	1.00	0.03	20,20,20,20	0
54	MG	BB	3101	1/1	1.00	0.05	5,5,5,5	0
54	MG	BB	3102	1/1	1.00	0.07	31,31,31,31	0
54	MG	DB	3063	1/1	1.00	0.02	19,19,19,19	0
54	MG	BB	3103	1/1	1.00	0.07	20,20,20,20	0
54	MG	DB	3065	1/1	1.00	0.06	45,45,45,45	0
54	MG	CA	1648	1/1	1.00	0.10	14,14,14,14	0
54	MG	DB	3067	1/1	1.00	0.02	16,16,16,16	0
54	MG	BB	3104	1/1	1.00	0.02	28,28,28,28	0
54	MG	DB	3069	1/1	1.00	0.09	14,14,14,14	0
54	MG	BB	3006	1/1	1.00	0.05	20,20,20,20	0
54	MG	BB	3065	1/1	1.00	0.06	5,5,5,5	0
54	MG	BB	3107	1/1	1.00	0.03	30,30,30,30	0
54	MG	BB	3066	1/1	1.00	0.03	25,25,25,25	0
54	MG	BB	3039	1/1	1.00	0.07	5,5,5,5	0
54	MG	CA	1655	1/1	1.00	0.04	25,25,25,25	0
54	MG	CA	1656	1/1	1.00	0.05	11,11,11,11	0
54	MG	DB	3077	1/1	1.00	0.06	15,15,15,15	0
54	MG	BB	3110	1/1	1.00	0.02	40,40,40,40	0
54	MG	DB	3079	1/1	1.00	0.02	34,34,34,34	0
54	MG	DB	3080	1/1	1.00	0.04	5,5,5,5	0
54	MG	CA	1601	1/1	1.00	0.03	5,5,5,5	0
54	MG	CA	1602	1/1	1.00	0.01	11,11,11,11	0
54	MG	CA	1603	1/1	1.00	0.03	29,29,29,29	0
54	MG	CA	1604	1/1	1.00	0.04	16,16,16,16	0
54	MG	BB	3068	1/1	1.00	0.08	61,61,61,61	0
54	MG	DB	3001	1/1	1.00	0.04	6,6,6,6	0
54	MG	DB	3087	1/1	1.00	0.04	75,75,75,75	0
54	MG	DB	3002	1/1	1.00	0.09	6,6,6,6	0
54	MG	BB	3069	1/1	1.00	0.02	10,10,10,10	0
54	MG	CA	1607	1/1	1.00	0.02	83,83,83,83	0
54	MG	DB	3091	1/1	1.00	0.04	5,5,5,5	0
54	MG	DB	3005	1/1	1.00	0.03	45,45,45,45	0
54	MG	DB	3093	1/1	1.00	0.03	10,10,10,10	0
54	MG	BB	3040	1/1	1.00	0.03	27,27,27,27	0

Continued on next page...

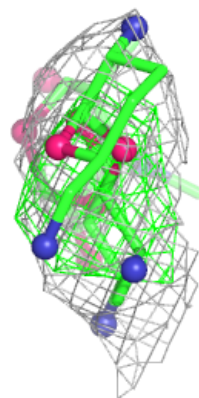
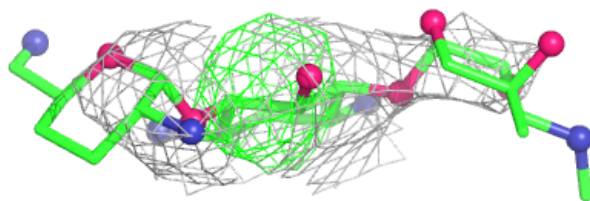
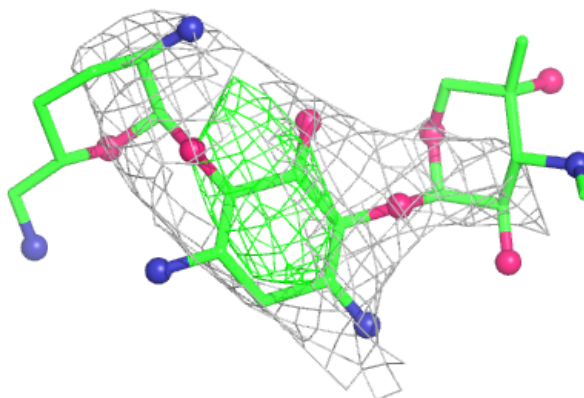
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3007	1/1	1.00	0.02	13,13,13,13	0
54	MG	DB	3096	1/1	1.00	0.03	20,20,20,20	0
54	MG	AA	1604	1/1	1.00	0.02	19,19,19,19	0
54	MG	DB	3098	1/1	1.00	0.02	28,28,28,28	0
54	MG	DB	3099	1/1	1.00	0.06	5,5,5,5	0
54	MG	AA	1638	1/1	1.00	0.09	20,20,20,20	0
54	MG	DB	3010	1/1	1.00	0.03	16,16,16,16	0
54	MG	DB	3102	1/1	1.00	0.03	22,22,22,22	0
54	MG	DB	3103	1/1	1.00	0.03	42,42,42,42	0
54	MG	BB	3023	1/1	1.00	0.03	11,11,11,11	0
54	MG	DB	3105	1/1	1.00	0.05	30,30,30,30	0
54	MG	DB	3012	1/1	1.00	0.05	12,12,12,12	0
54	MG	DB	3107	1/1	1.00	0.01	11,11,11,11	0
54	MG	DB	3108	1/1	1.00	0.05	5,5,5,5	0
54	MG	AA	1655	1/1	1.00	0.02	54,54,54,54	0
54	MG	CA	1613	1/1	1.00	0.02	40,40,40,40	0
54	MG	BB	3075	1/1	1.00	0.04	29,29,29,29	0
54	MG	DB	3016	1/1	1.00	0.01	25,25,25,25	0
54	MG	DB	3017	1/1	1.00	0.01	5,5,5,5	0
54	MG	DB	3018	1/1	1.00	0.04	22,22,22,22	0
54	MG	DB	3019	1/1	1.00	0.04	5,5,5,5	0
54	MG	BB	3076	1/1	1.00	0.07	20,20,20,20	0
54	MG	BB	3045	1/1	1.00	0.03	38,38,38,38	0

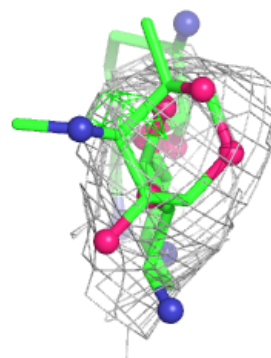
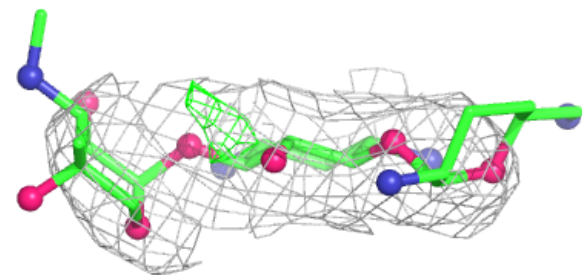
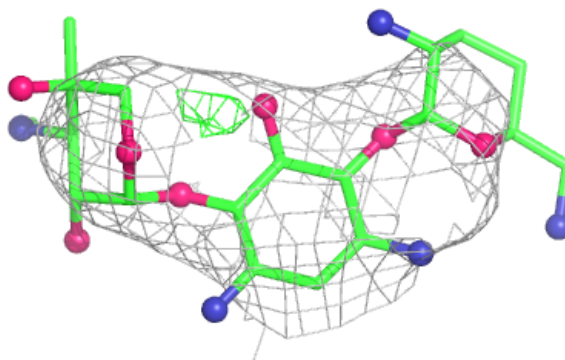
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LLL DB 3112:

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

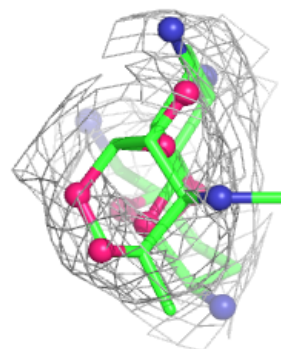
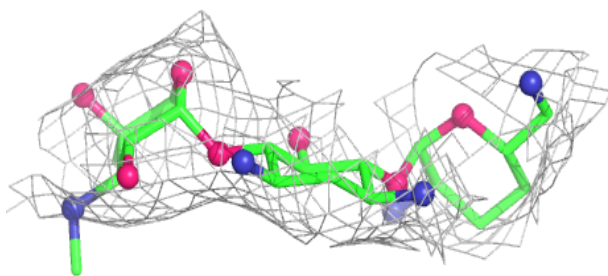
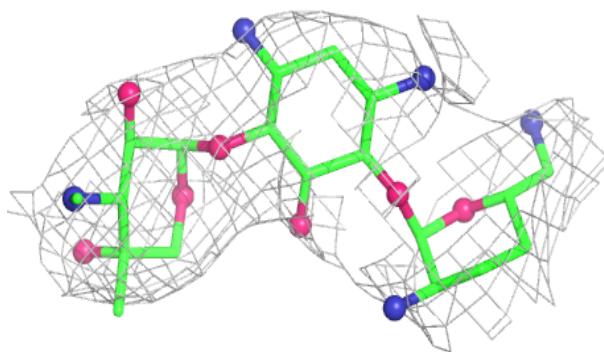
**Electron density around LLL BB 3111:**

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

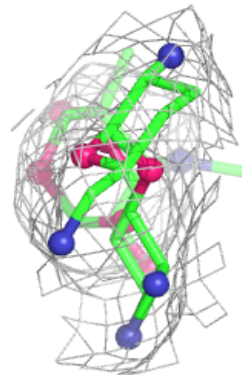
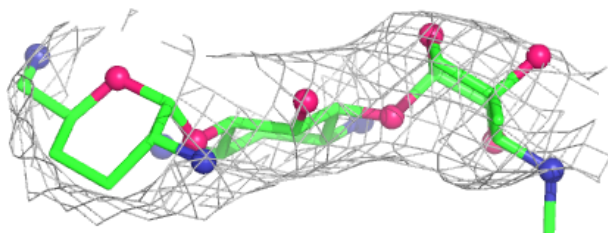
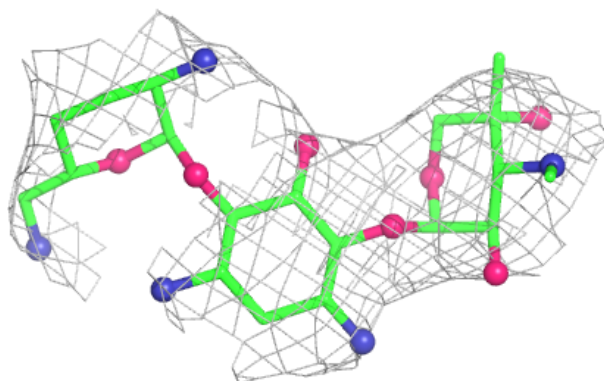


Electron density around LLL AA 1661:

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

**Electron density around LLL CA 1662:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.