



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 10:29 am BST

PDB ID : 4V53
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin.
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 : 2007-06-16
Resolution : 3.54 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

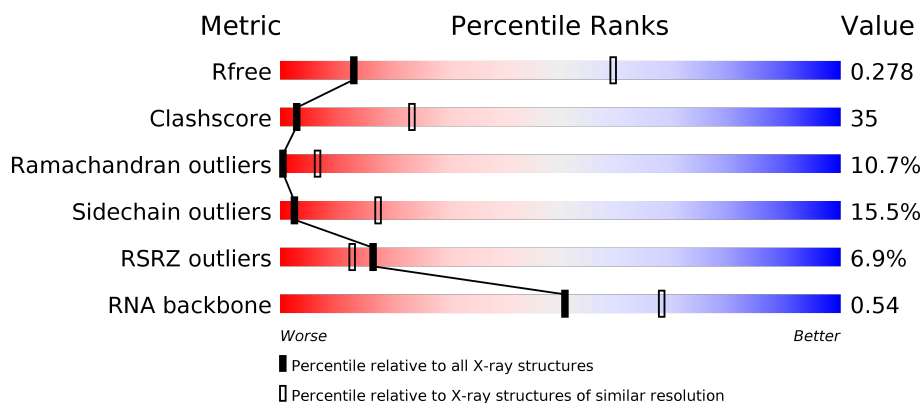
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)
RNA backbone	3102	1003 (4.02-3.00)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	<div> <div>25%</div> <div>60%</div> <div>13%</div> <div>..</div> </div>
1	CA	1542	<div> <div>24%</div> <div>63%</div> <div>12%</div> <div>.</div> </div>
2	AC	232	<div> <div>30%</div> <div>47%</div> <div>11%</div> <div>11%</div> </div>
2	CC	232	<div> <div>6%</div> <div>31%</div> <div>48%</div> <div>10%</div> <div>11%</div> </div>

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	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	
27	DK	123	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
40	BH	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
52	DW	84	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	AA	2023	-	-	-	X
53	MG	AA	2037	-	-	-	X
53	MG	DB	3059	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284252 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
			1022	634	206	179	3			

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

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

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

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

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			

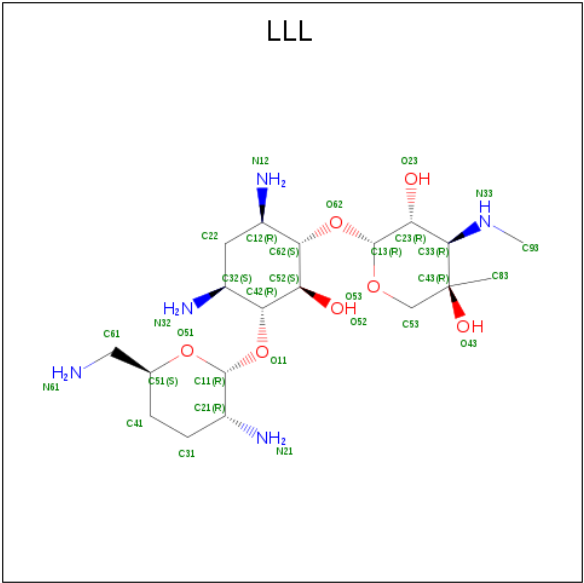
- Molecule 52 is a protein called 50S ribosomal protein L27.

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

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

- Molecule 54 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-O-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C₁₉H₃₉N₅O₇).



Continued from previous page...

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

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

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	292	Total	O	0	0
			292	292		
56	AE	1	Total	O	0	0
			1	1		
56	AK	1	Total	O	0	0
			1	1		
56	AL	2	Total	O	0	0
			2	2		
56	AN	2	Total	O	0	0
			2	2		
56	AT	2	Total	O	0	0
			2	2		
56	BB	492	Total	O	0	0
			492	492		
56	BC	7	Total	O	0	0
			7	7		
56	BE	3	Total	O	0	0
			3	3		
56	B2	1	Total	O	0	0
			1	1		
56	BL	3	Total	O	0	0
			3	3		
56	BH	1	Total	O	0	0
			1	1		

Continued on next page...

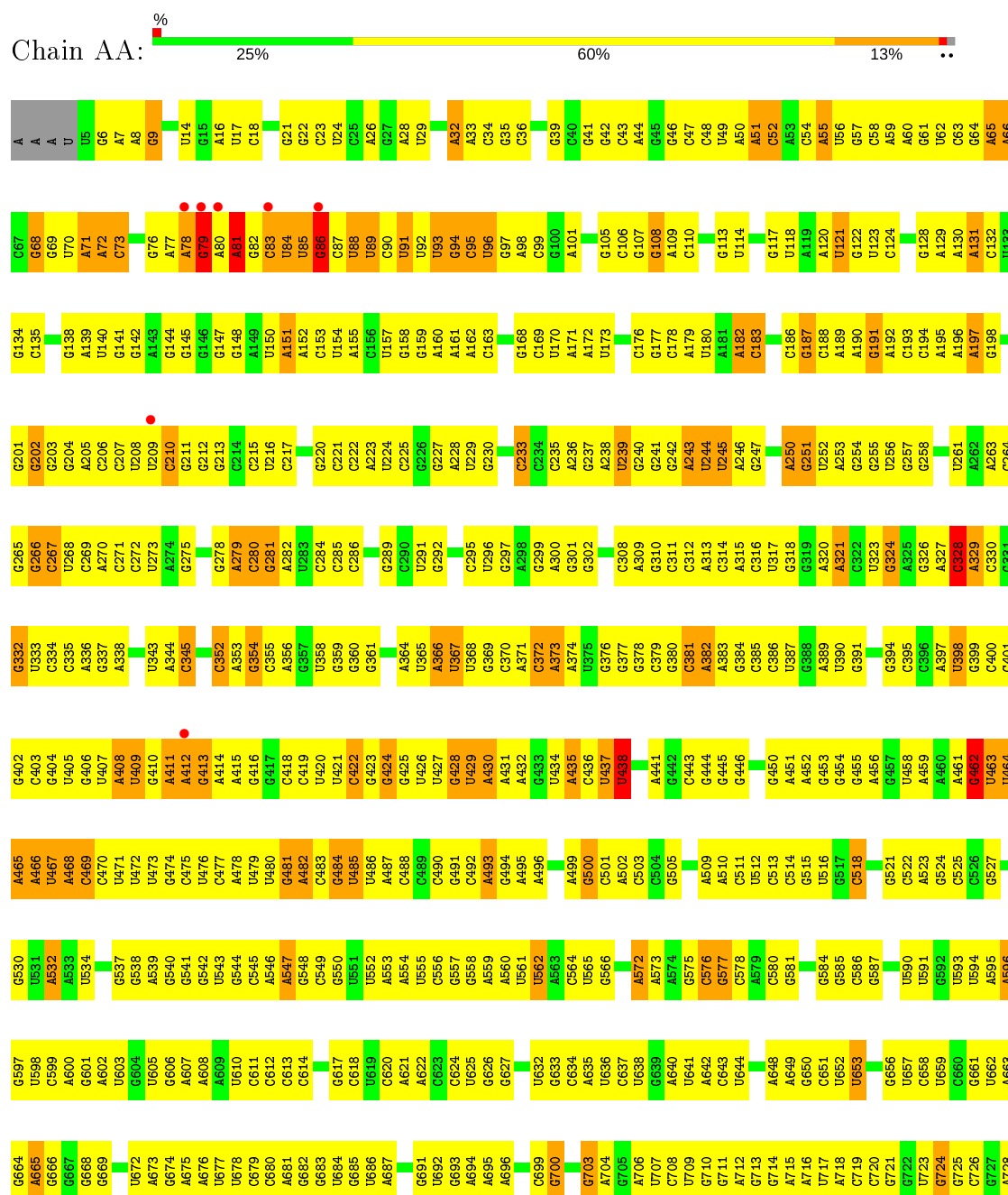
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CA	297	Total 297	O 297	0	0
56	CE	2	Total 2	O 2	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	2	Total 2	O 2	0	0
56	CN	4	Total 4	O 4	0	0
56	CT	2	Total 2	O 2	0	0
56	DB	502	Total 502	O 502	0	0
56	DC	4	Total 4	O 4	0	0
56	DE	2	Total 2	O 2	0	0
56	DL	4	Total 4	O 4	0	0

3 Residue-property plots

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

• Molecule 1: 16S rRNA

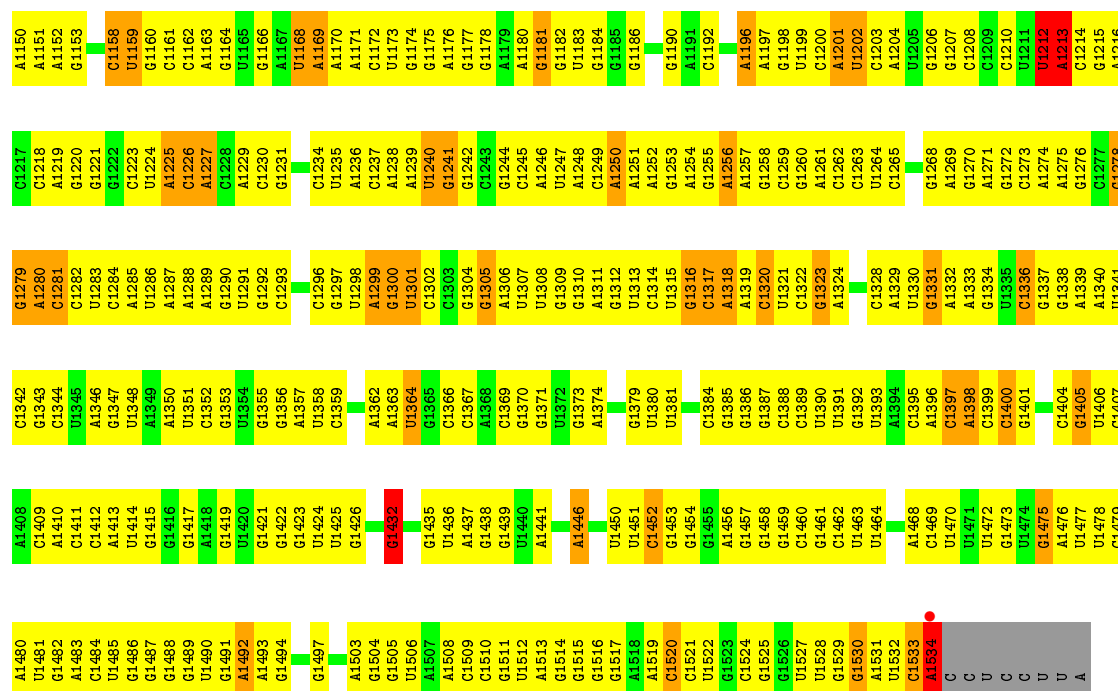




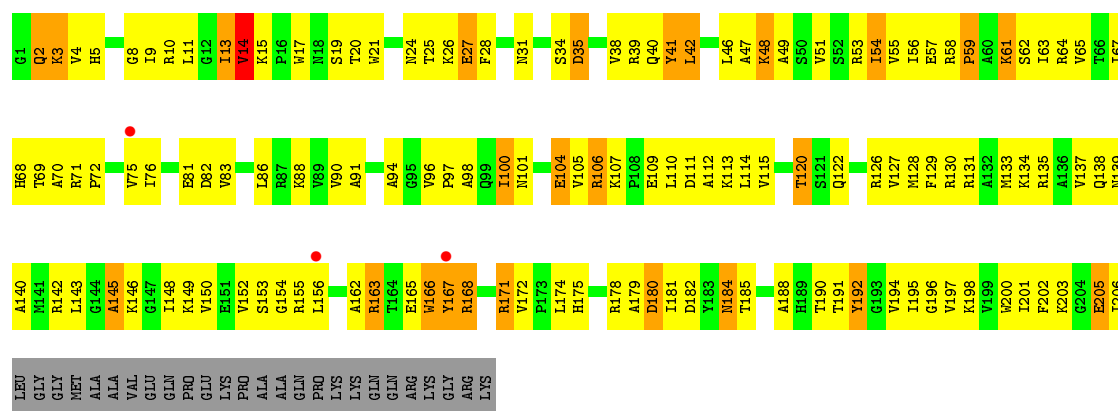
Chain CA:



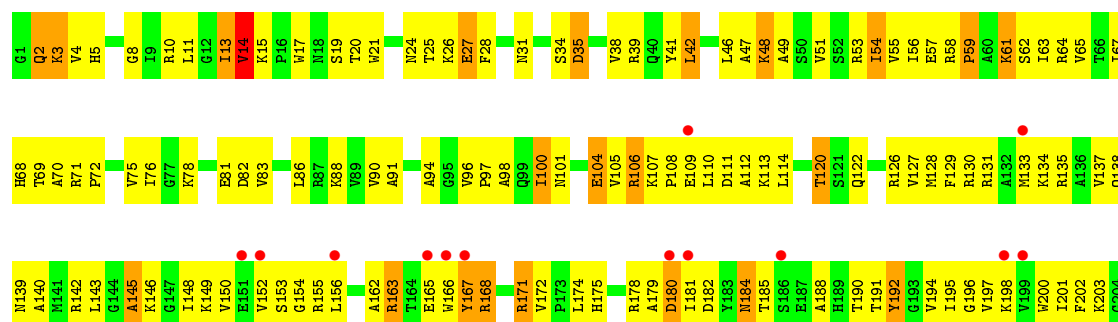
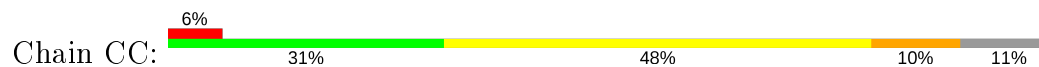
U1085	A958	A1019	A889	C811	G734	G601	U534	C469	G406	A336	U268	G202	G138
U1086	A959	G1020	G890	G812	C735	A602	G537	C470	U407	G337	C269	G203	A139
U1090	U960	A1021	G894	U813	C736	U603	G538	U471	A408	A338	A408	G204	G141
U1091	U961	A1022	G894	A814	C737	G604	A539	U472	U409	U343	C271	A205	G142
A1092	G962	G1023	G895	A815	C738	U605	A540	U473	G410	U344	C272	C206	G143
A1093	G963	U1024	G896	A816	C739	G606	G541	G474	A411	A344	U273	C207	U150
A1094	G964	U1025	G897	U817	U740	A607	G542	C475	A412	C345	G274	U208	G144
A1095	G965	G1026	G900	G818	G741	A608	G543	U476	A413	C352	G275	U209	G145
U1096	G967	U1028	G903	U820	A742	A609	U544	C477	A414	G353	G278	C210	G146
U1097	A968	A1029	G904	G821	C743	U610	G545	A478	A415	A354	G279	G211	G147
C1098	A969	U1030	U904	G822	C744	C611	C546	U479	G416	G355	G280	G212	G148
G1099	C970	C1031	U905	G823	A747	C612	A547	U480	A417	C356	C281	G213	A149
G1100	G971	G1032	A906	G824	G748	C613	G548	A481	C418	G357	A282	C214	A151
C1101	C972	G1033	A907	A825	U684	C614	G549	A482	C419	U358	G283	C215	A152
A1101	G973	A1034	A908	C826	G685	G617	C550	G483	U420	G359	C284	U216	C153
A1102	A974	A1035	A909	U827	A687	C618	U551	U484	G422	G360	C285	U217	U154
C1103	A975	U1036	C910	U828	G754	U619	U552	U485	G423	G361	U287	G220	A155
G1104	G976	C1037	U911	G829	G755	G620	A553	U486	G424	G364	A288	C221	C156
A1105	A977	G1038	G912	G833	G763	A621	A554	C488	G425	A364	G289	C222	U157
G1106	A978	U1039	A913	U834	C764	G622	U555	G489	U426	U365	G290	A223	G158
G1107	C979	G1040	A914	U835	G765	C623	C556	C490	U427	U366	C291	U224	G159
G1108	C980	U1041	G915	U836	A766	G624	G557	G491	G428	U367	G292	C225	A160
C1109	U981	A1042	G917	G836	A767	U625	G558	C492	U429	U368	C295	A228	A161
G1110	U982	U1043	A918	G837	G768	U632	A559	A493	A430	G369	U296	U229	A162
A1111	A983	C1045	A919	C839	A768	G633	A560	G494	A431	C370	G296	G230	C163
G1112	C984	A1046	U920	C840	G769	G634	U561	A495	A432	A371	G299	U231	A167
U1118	C985	A1047	U921	C841	C770	A635	A563	A496	G433	C372	G300	G232	G168
C1119	U986	G1048	G922	U842	A772	U636	C564	A499	U434	A373	A301	G233	C169
C1120	G987	U1049	A923	U843	G773	G637	U565	G500	A435	A374	G302	C234	U170
U1121	G988	G1050	G925	A845	A777	U638	G566	C501	U437	U375	A303	C235	A171
U1122	U989	G1051	G926	G846	G778	G639	A572	A502	U438	G377	C308	A236	A172
G1123	U991	C1052	G927	C847	C779	U640	A573	C503	C440	G378	A309	G237	U173
U1124	U992	A1053	G928	C848	A780	U641	C504	C504	A441	G379	G380	A238	G176
G1125	G993	U1055	G929	C857	A781	G642	G574	G505	G442	G381	U239	U239	G177
U1126	A994	A1056	C932	C858	C783	U644	G575	A509	C443	A382	G240	G241	C178
G1127	C995	G1057	G933	G859	A784	A648	G577	A510	G444	A383	G242	G242	A179
C1128	A996	U1058	C934	A860	G785	U649	C578	C511	G449	G384	A243	U244	U180
G1129	U997	C1059	A935	G861	G786	G650	A579	U512	G450	C385	U245	U245	A181
A1130	C998	U1060	A936	G862	A787	C651	C580	C513	A451	C386	G318	A246	A182
G1131	C999	G1061	C936	C862	G788	U652	G581	C514	A452	U387	A246	G247	C183
C1132	A1000	U1062	C936	U863	A791	U653	G584	G515	A453	G388	G319	G247	G186
G1133	C1001	C1063	G939	A864	A792	U654	G585	U516	G453	A389	A320	C186	C187
G1134	G1002	U1064	C940	A865	A793	G656	G586	C517	G454	U390	A321	A250	C188
U1135	U1003	C1065	G941	C868	U794	U657	G587	C518	G455	G391	C322	G251	C189
C1136	A1004	U1066	G945	G869	C795	U658	G590	C520	A456	G394	U323	U252	A189
G1137	U1005	G1067	A946	U870	G796	C658	C581	C521	G457	C395	G324	A253	A190
C1138	G1006	U1070	G947	U871	C797	U659	G591	C522	U458	C396	A325	G254	G191
G1139	U1007	U1008	C948	G874	U798	G724	U590	A523	A459	A397	G326	G255	A192
C1140	U1008	C1009	C949	U875	A802	G725	U591	C524	A460	U398	A327	U256	C193
G1141	U1009	U1010	A949	G876	C726	U661	G592	C525	A461	G399	C328	U257	C194
G1142	U1010	G1072	G950	U877	G727	U662	U593	C526	A462	G400	G329	G258	A195
G1143	C1011	U1073	G951	G803	G728	U663	U594	C527	U463	C401	G330	G259	A196
G1144	U1012	G1074	U952	G804	A729	G664	A595	G527	U464	G402	G331	A263	A197
A1145	G1013	U1075	G953	C882	A730	A665	A596	G530	U465	C403	G332	C264	G198
A1146	A1014	U1076	G954	C883	G731	G666	G597	U531	A466	G404	U333	G265	A199
C1147	U1015	G1077	U955	U884	C732	G667	U598	A532	U467	G200	G334	G266	G199
U1148	A1080	U1078	C732	G808	G733	G668	A600	A533	A468	G201	C335	C267	G201

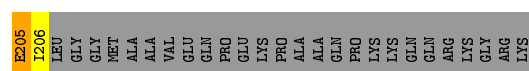


• Molecule 2: 30S ribosomal protein S3



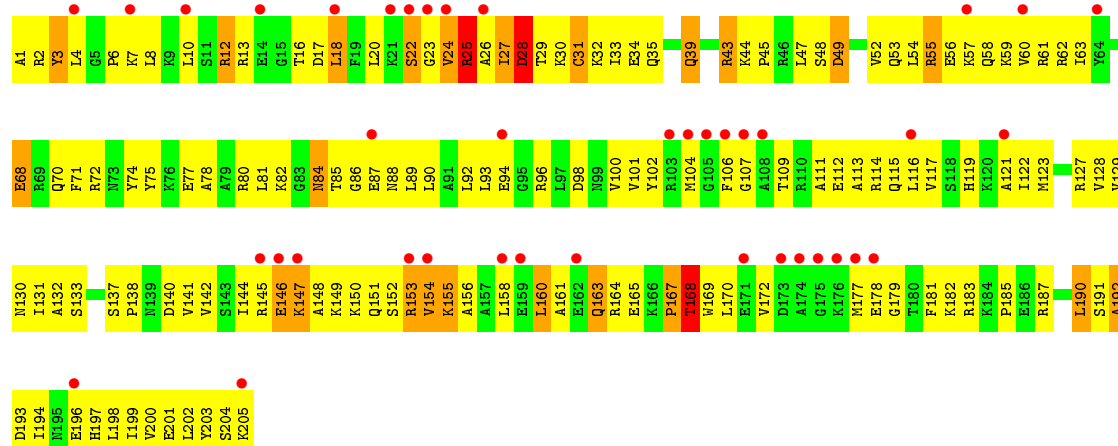
• Molecule 2: 30S ribosomal protein S3





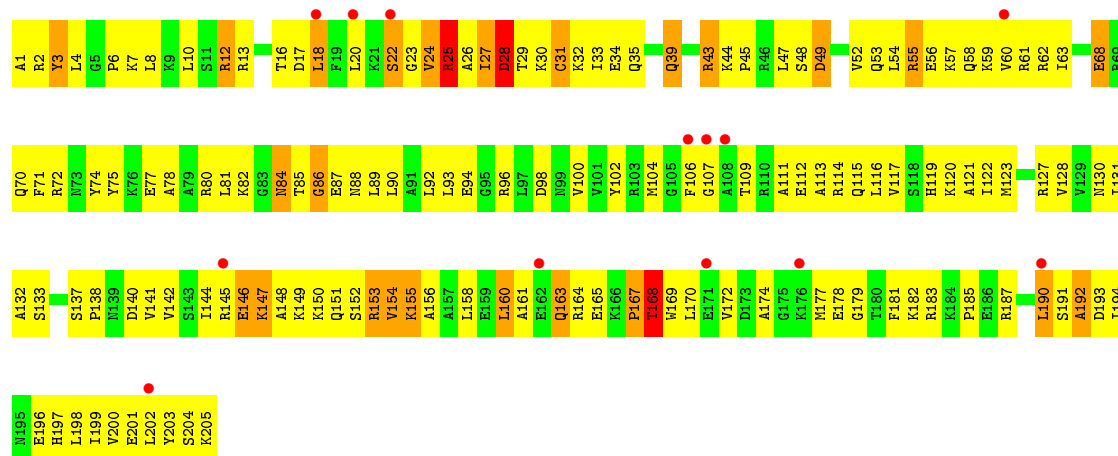
• Molecule 3: 30S ribosomal protein S4

Chain AD: 20% 28% 59% 11%



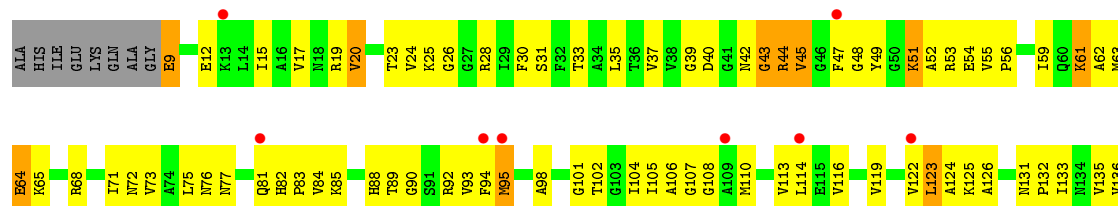
• Molecule 3: 30S ribosomal protein S4

Chain CD: 6% 28% 59% 12%



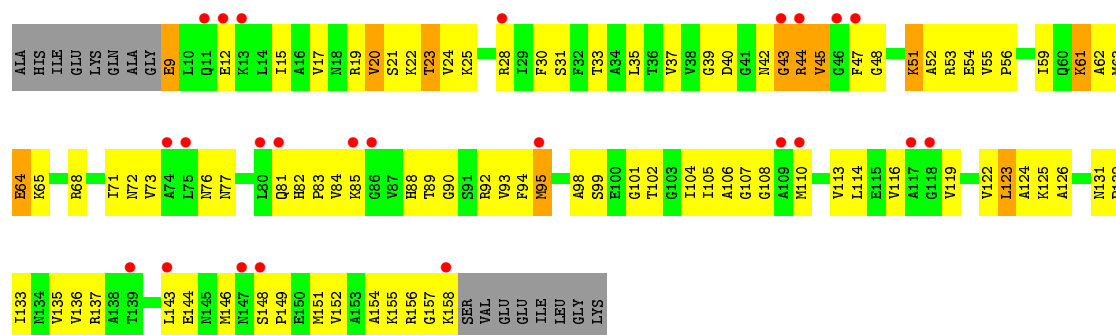
• Molecule 4: 30S ribosomal protein S5

Chain AE: 7% 34% 50% 6% 10%

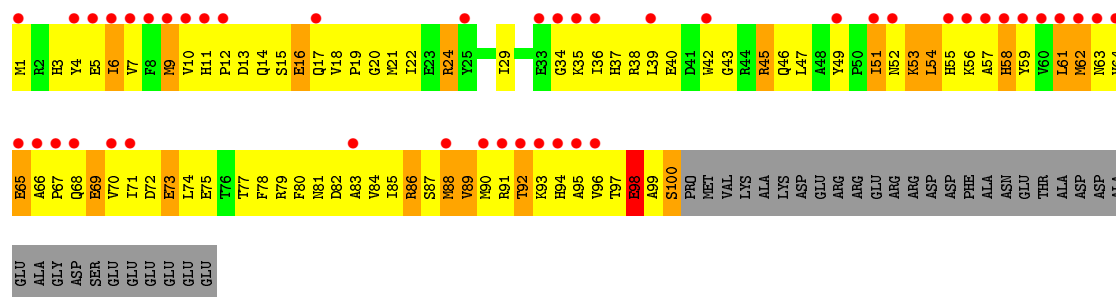
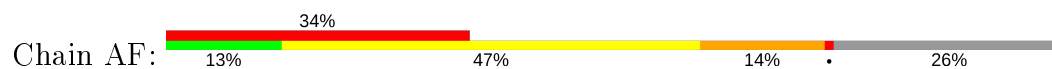




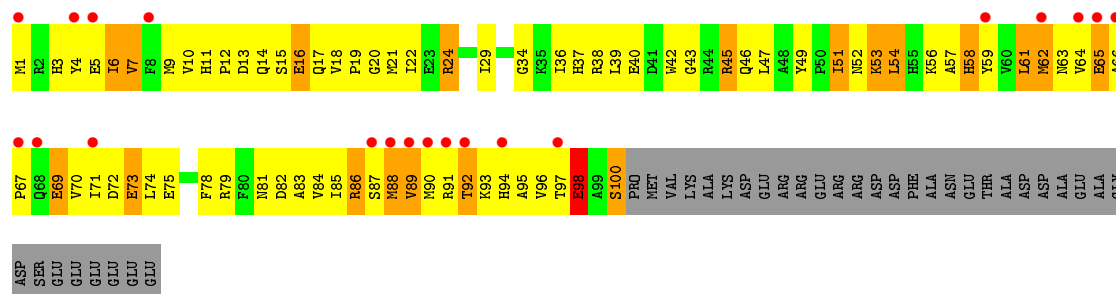
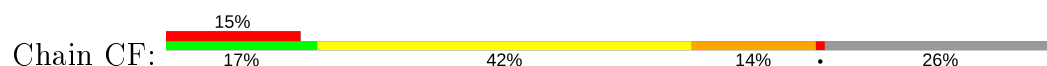
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6

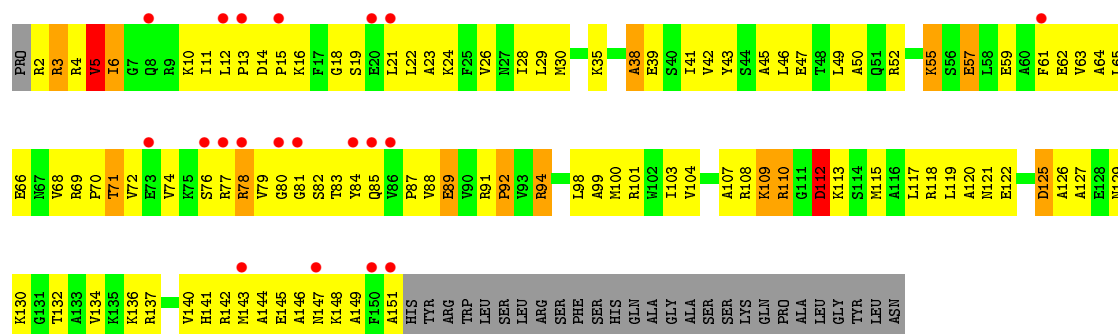


• Molecule 5: 30S ribosomal protein S6

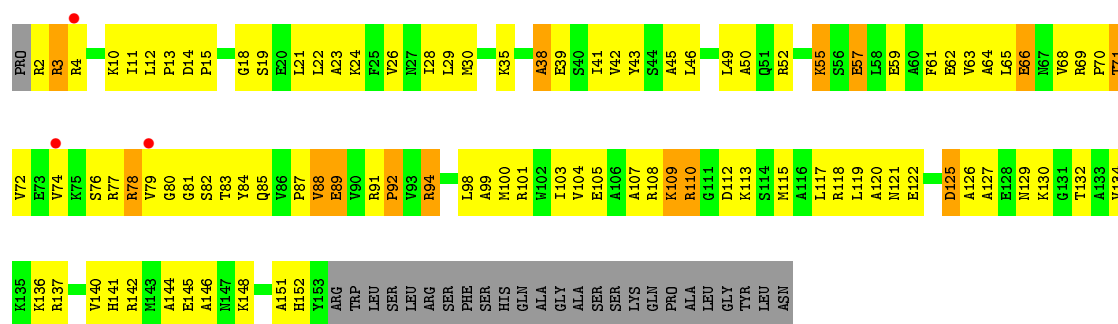


• Molecule 6: 30S ribosomal protein S7

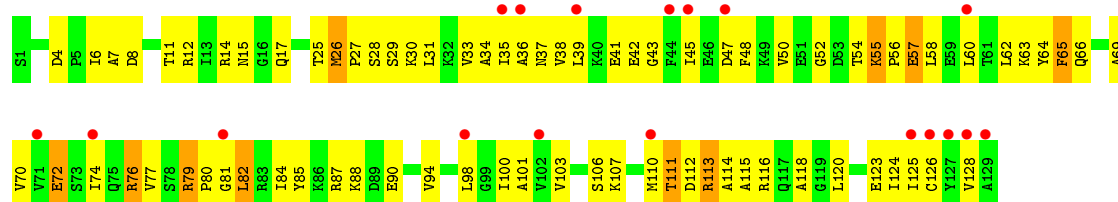




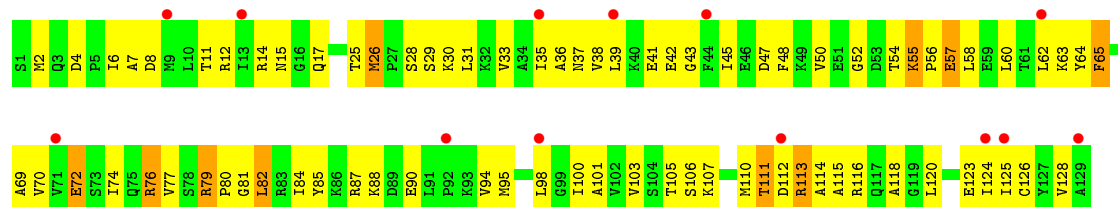
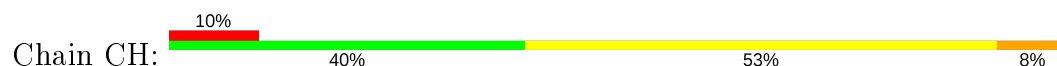
• Molecule 6: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S8

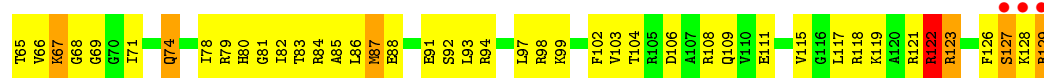
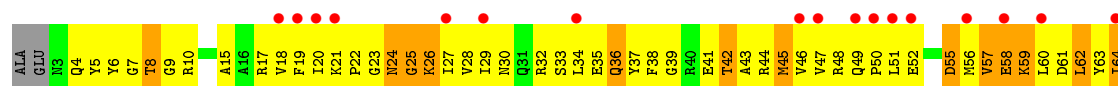


• Molecule 7: 30S ribosomal protein S8

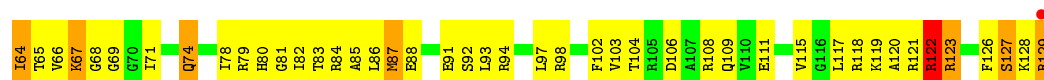


• Molecule 8: 30S ribosomal protein S9

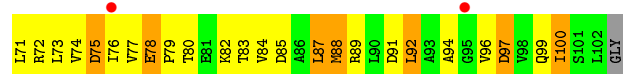
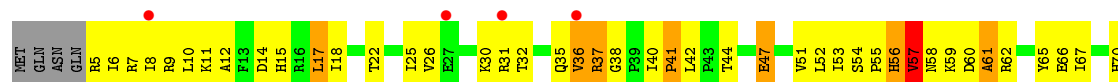




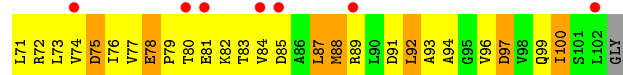
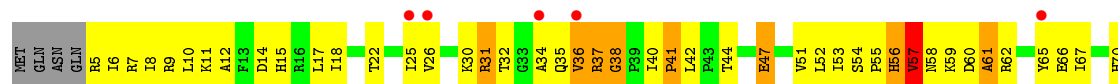
• Molecule 8: 30S ribosomal protein S9



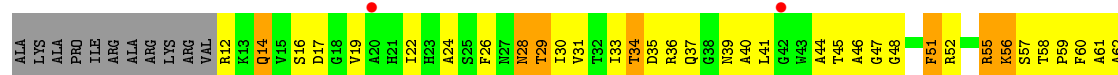
• Molecule 9: 30S ribosomal protein S10



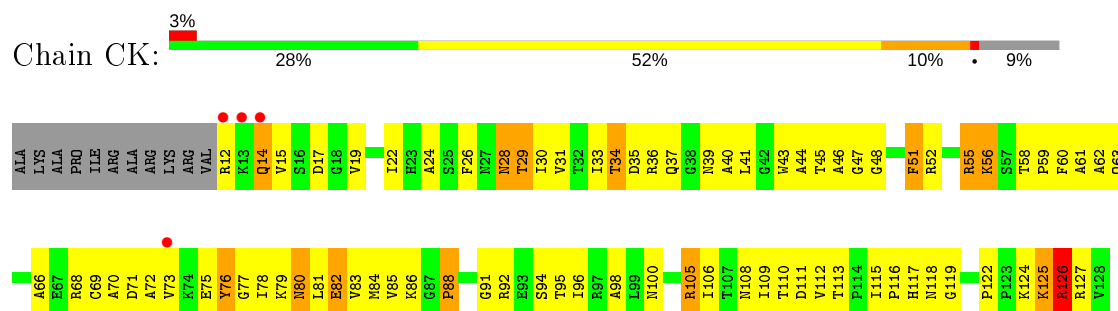
• Molecule 9: 30S ribosomal protein S10



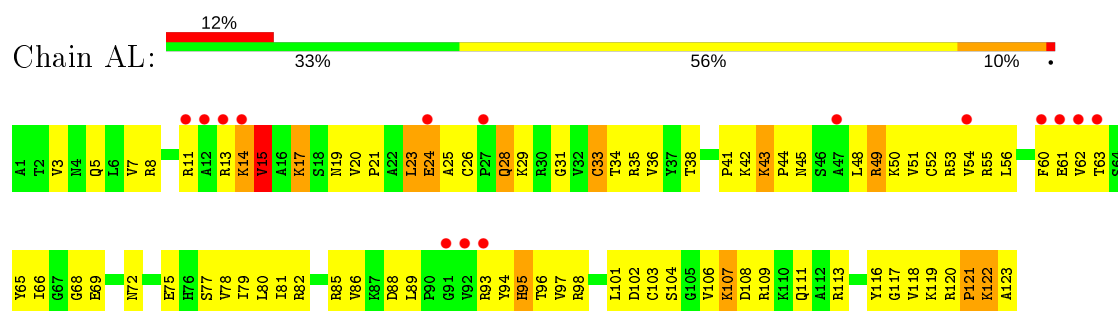
• Molecule 10: 30S ribosomal protein S11



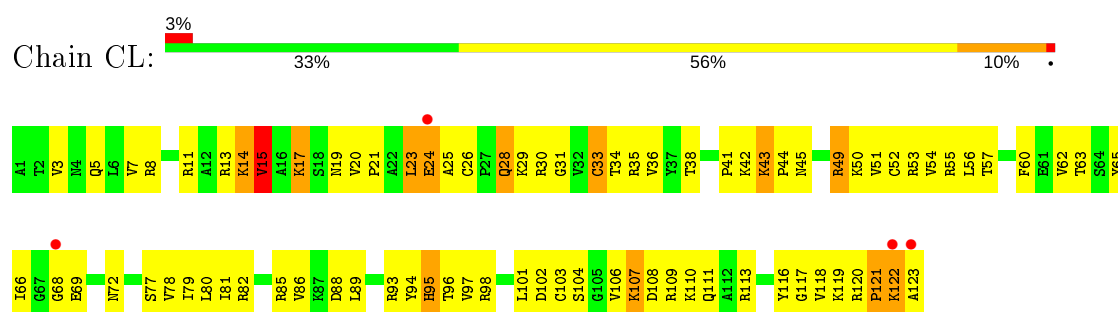
- Molecule 10: 30S ribosomal protein S11



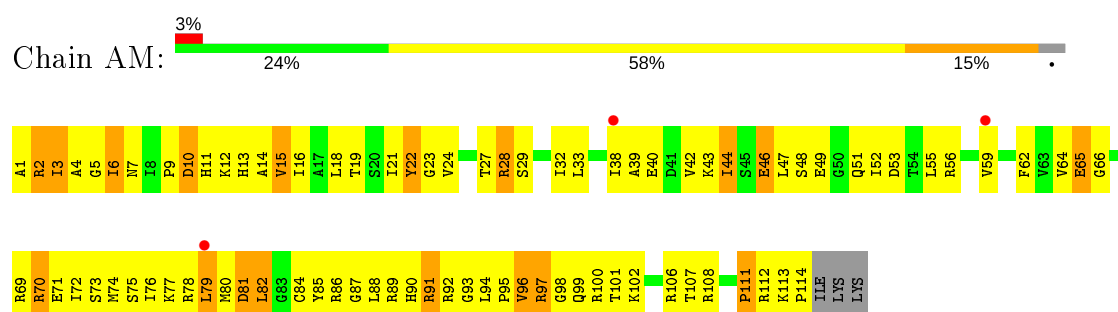
- Molecule 11: 30S ribosomal protein S12



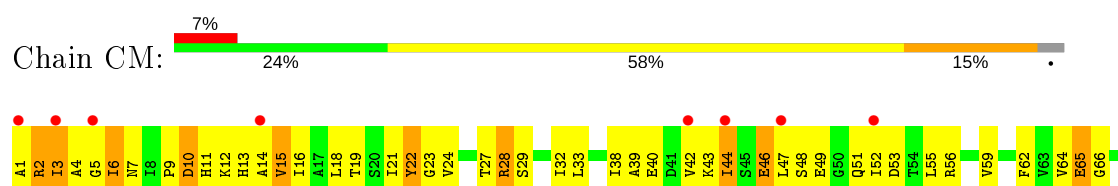
- Molecule 11: 30S ribosomal protein S12

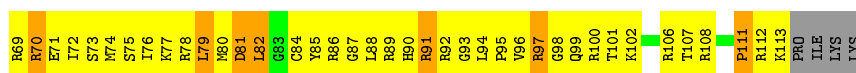


- Molecule 12: 30S ribosomal protein S13



- Molecule 12: 30S ribosomal protein S13

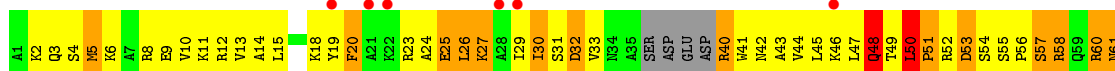




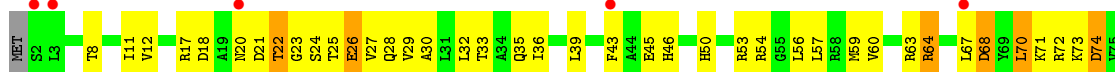
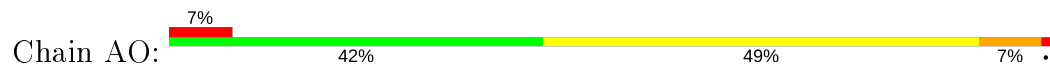
- Molecule 13: 30S ribosomal protein S14



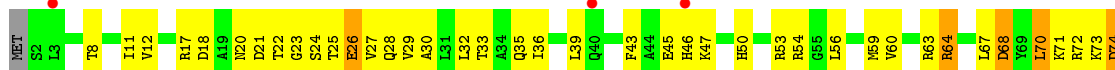
- Molecule 13: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S15

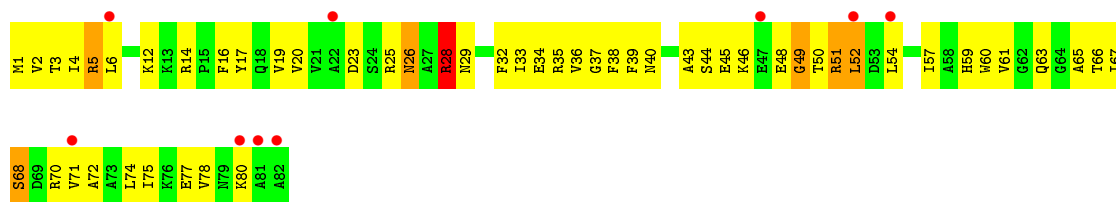


- Molecule 14: 30S ribosomal protein S15

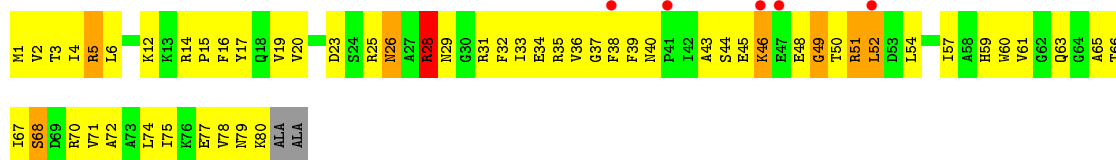


- Molecule 15: 30S ribosomal protein S16

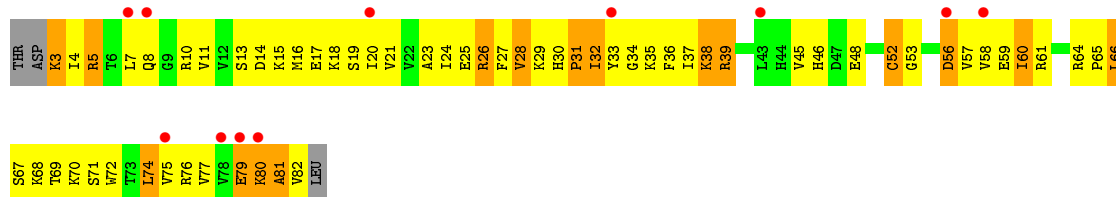




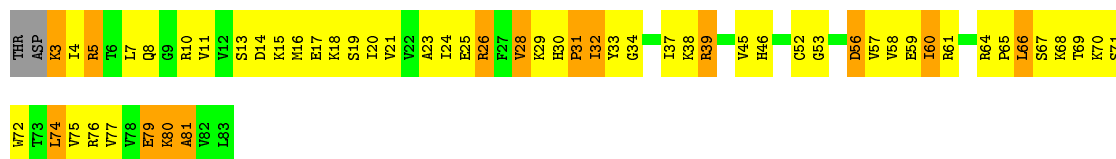
• Molecule 15: 30S ribosomal protein S16



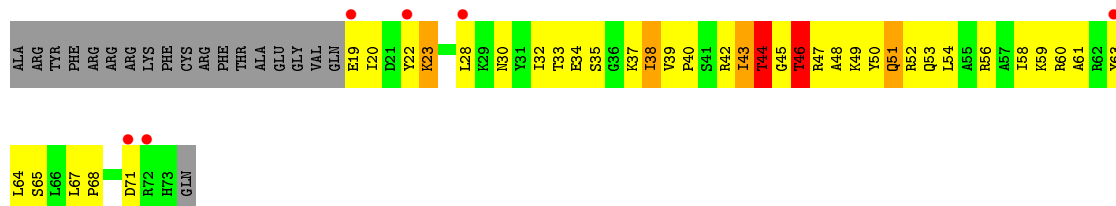
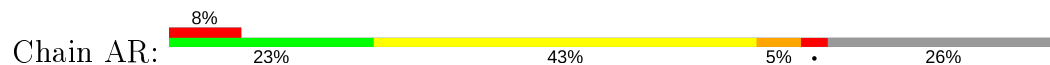
• Molecule 16: 30S ribosomal protein S17



• Molecule 16: 30S ribosomal protein S17

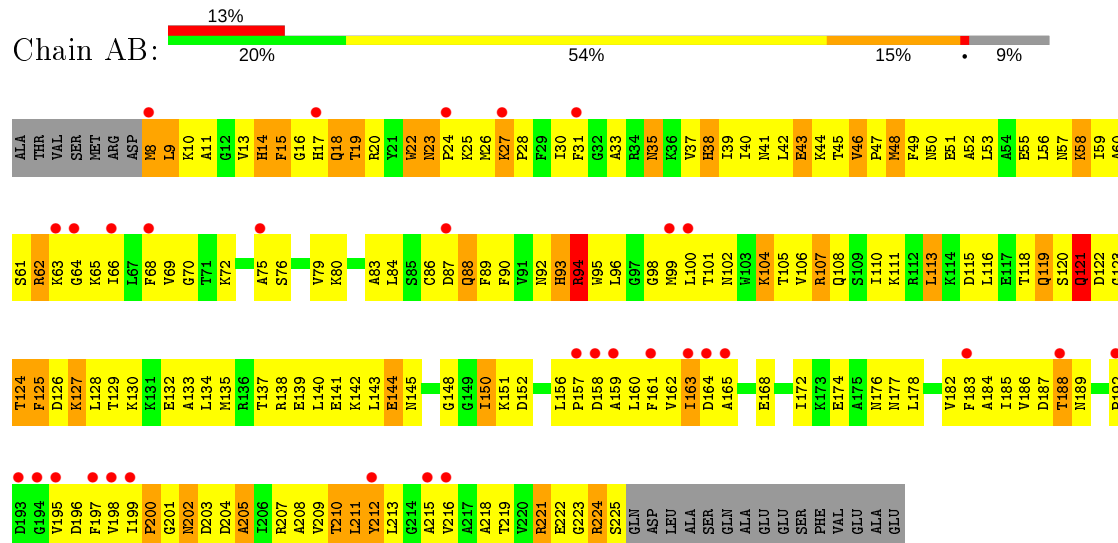


• Molecule 17: 30S ribosomal protein S18

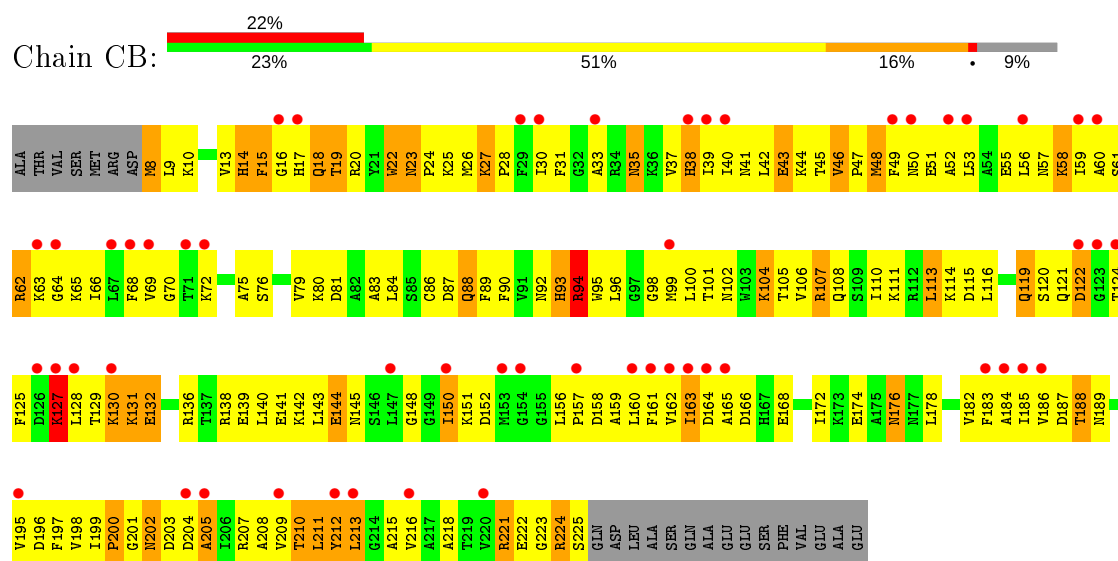


• Molecule 17: 30S ribosomal protein S18

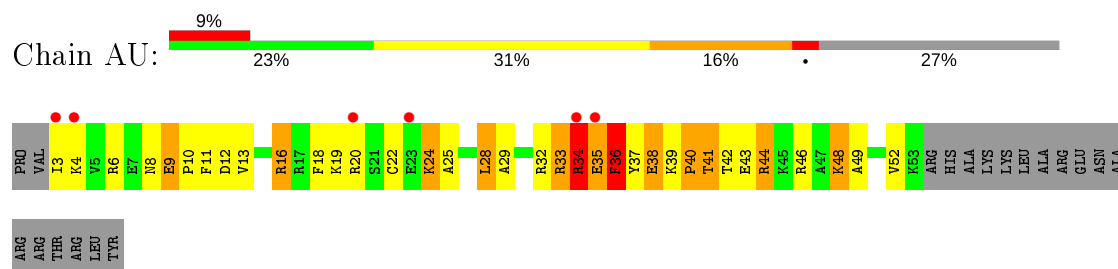
- Molecule 20: 30S ribosomal protein S2



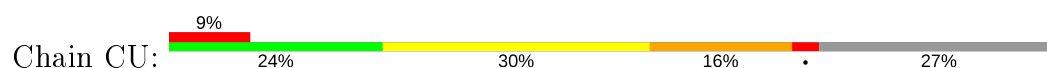
- Molecule 20: 30S ribosomal protein S2

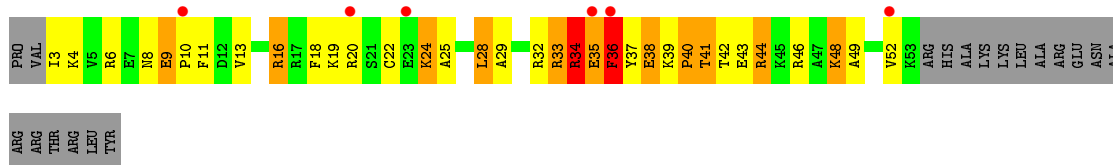


- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

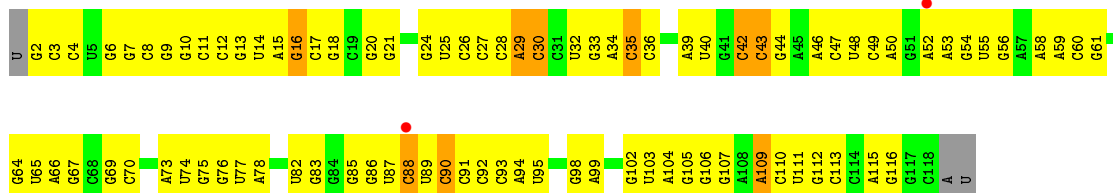




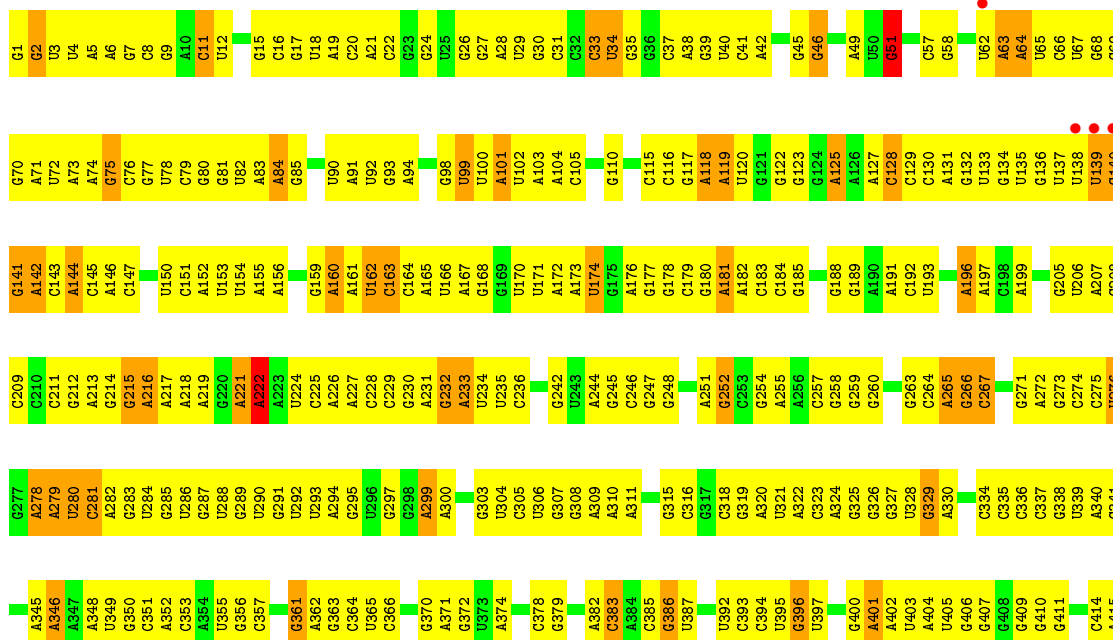
• Molecule 22: 5S rRNA



• Molecule 22: 5S rRNA

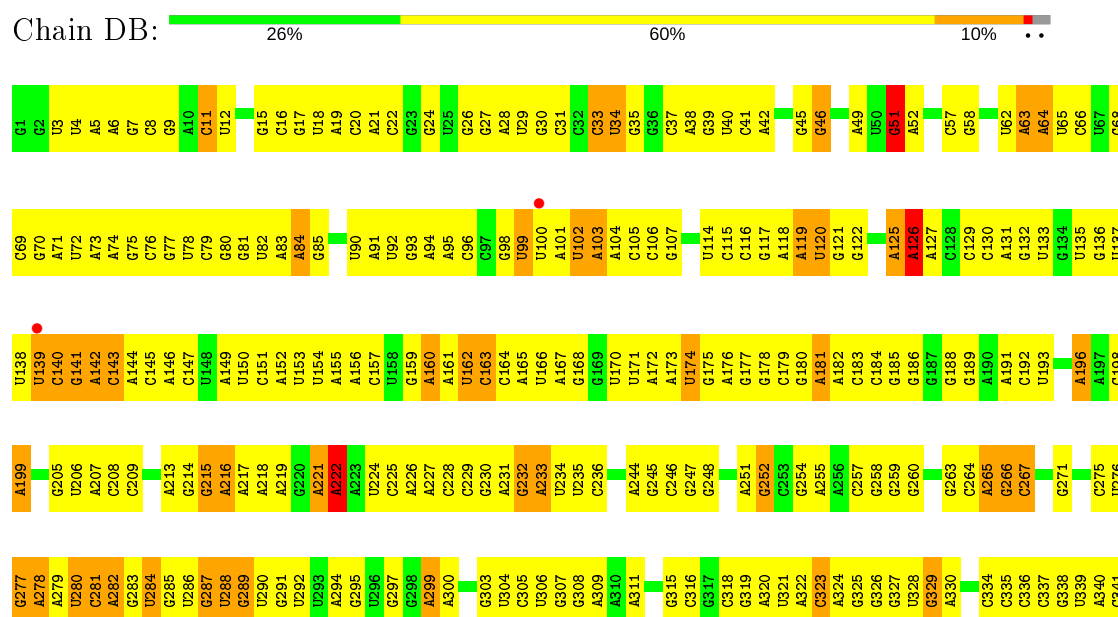
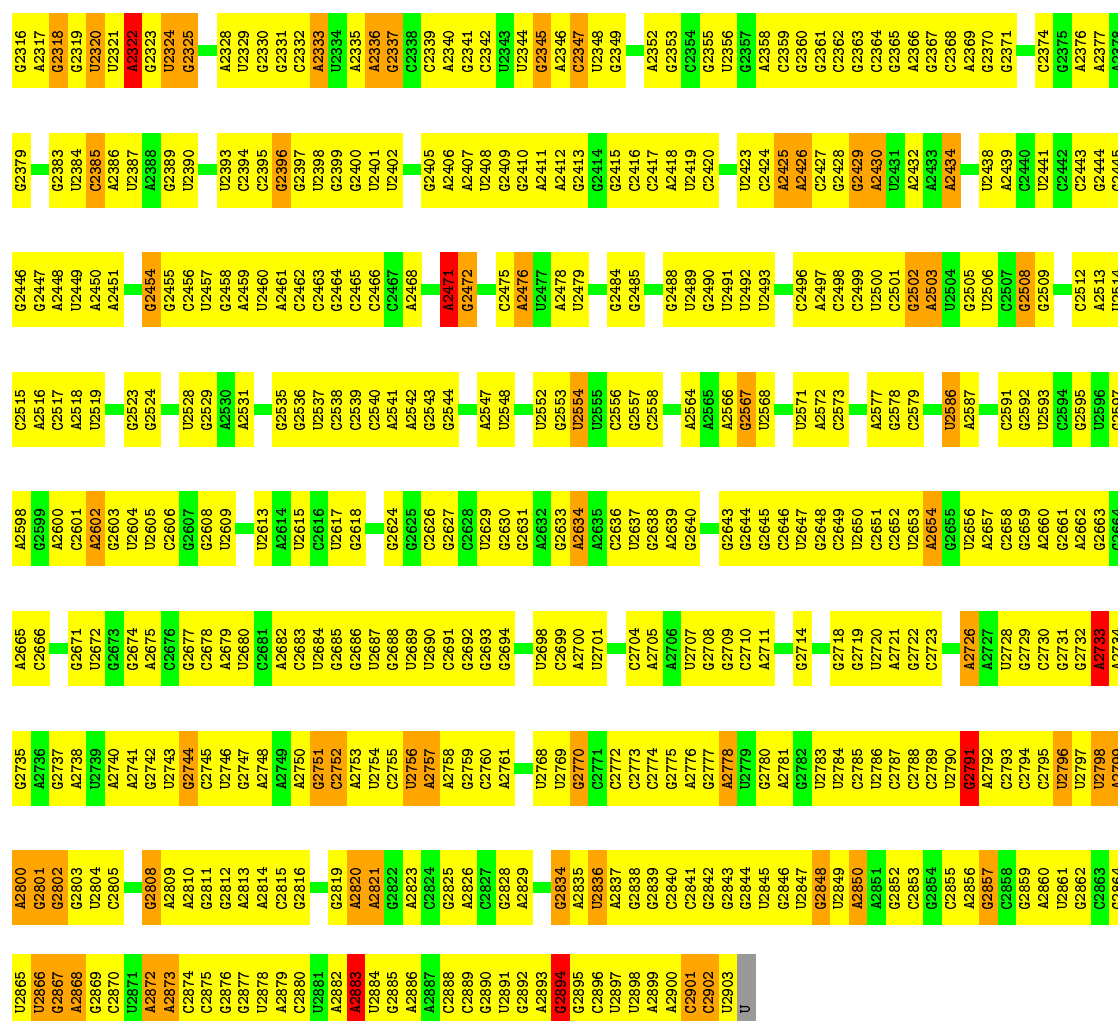


• Molecule 23: 23S rRNA



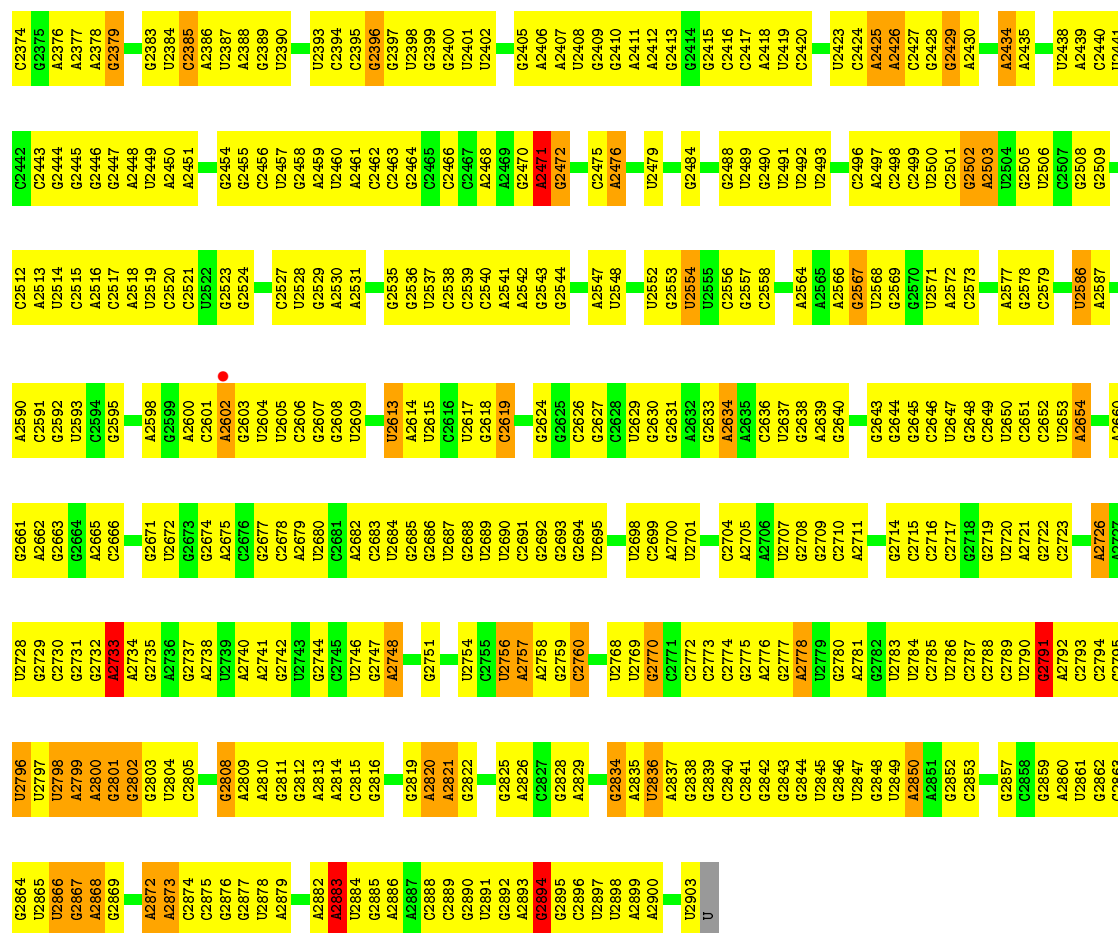


G2250	U2189	G2065	U1991	U1911	C1844	C1771	C1704	U1624	A1553	U1486	A1420	G1355
G2257	G2190	C2066	G1992	A1912	G1845	A1772	A1705	U1629	U1554	U1487	G1421	G1356
C2258	A2191	G2067	U1993	A1913	A1847	A1773	C1706	U1629	C1555	C1488	C1357	C1358
U2192	U2192	U2068	C1997	C1914	A1846	C1774	G1707	G1633	C1556	G1425	G1426	G1361
C2193	G2193	C2069	A1998	A1915	A1848	G1775	U1709	A1634	C1557	A1490	A1427	C1362
C2260	U2194	A2070	C1999	A1917	G1849	G1776	G1710	A1635	U1559	G1492	G1428	A1365
C2261	A2071	A2071	C2001	A1918	G1850	U1777	U1711	U1636	G1560	C1493	A1429	G1368
U2262	C2072	C2072	C2001	A1919	A1853	U1778	U1712	A1637	U1561	A1494	A1430	G1369
A2134	A2135	U2074	U2007	G1922	U1855	A1783	U1713	C1638	U1562	A1495	A1431	G1370
A2135	A2136	U2075	C2008	U1923	U1856	A1784	U1714	A1640	U1563	G1432	A1432	G1371
U2137	U2137	U2076	A2009	C1924	U1857	A1785	U1715	A1641	C1564	A1433	A1433	G1372
G2138	G2138	A2077	G2012	A1927	A1858	A1786	A1717	G1642	C1565	A1434	A1434	G1373
U2139	U2139	C2078	G2012	A1928	U1859	A1787	G1718	G1643	U1567	G1437	A1437	U1372
G2140	G2140	U2079	A2015	A1928	G1860	C1788	G1719	G1643	C1568	A1503	A1503	A1373
C2143	C2143	A2080	A2016	G1929	G1861	C1789	A1722	U1647	A1571	A1504	A1504	A1374
G2144	G2144	U2081	U2017	G1930	G1862	C1790	G1723	G1648	A1572	A1505	A1505	U1375
C2145	C2145	U2085	G2018	U1931	G1863	A1791	G1723	G1649	A1573	U1506	U1440	C1376
C2146	C2146	U2086	G2018	A1932	U1864	G1792	G1725	G1650	A1574	A1507	G1441	G1377
A2147	A2147	U2087	A2019	G1933	U1865	C1793	U1726	G1651	U1575	A1508	G1442	A1378
G2148	G2148	A2088	A2020	G1934	A1866	A1794	C1726	A1652	C1574	A1509	U1443	U1379
C2149	C2149	C2089	C2021	G1935	G1867	C1795	G1727	G1653	C1575	G1511	G1444	G1380
C2150	C2150	A2090	A2022	A1936	G1868	U1796	C1728	A1654	U1576	G1512	G1445	G1381
U2151	U2151	C2091	C2023	A1937	G1869	G1797	U1729	A1655	C1577	U1513	C1446	G1382
G2152	G2152	U2092	G2024	A1938	C1870	U1798	C1730	C1656	U1578	G1514	C1447	A1383
C2153	C2153	G2093	G2025	A1939	A1871	G1799	G1731	U1657	A1579	A1515	G1448	A1384
G2154	G2154	A2094	U2026	U1940	A1872	C1800	C1732	C1658	A1580	A1516	G1449	A1385
U2155	U2155	A2095	G2027	G1941	G1873	A1801	G1733	G1659	G1581	G1517	G1450	C1386
G2156	G2156	C2096	A2028	U1942	C1874	A1802	G1734	G1662	G1451	G1452	C1451	A1387
C2157	C2157	A2097	G2029	U1943	G1875	A1803	A1735	U1663	G1453	G1453	C1389	G1388
A	A	U2098	A2030	G1944	A1876	C1804	U1736	G1664	U1584	A1524	A1453	C1389
G	G	U2099	A2031	U1946	A1877	G1737	G1737	A1664	C1585	A1525	C1454	U1390
C	C	G2100	G2032	C1947	G1878	A1810	G1738	A1666	A1586	G1455	G1456	U1391
G	G	A2101	A2033	G1948	C1879	U1812	G1740	G1667	A1591	C1527	U1457	A1393
A	A	G2102	A2033	G1948	C1879	U1812	G1740	A1668	G1529	U1458	U1458	U1394
C	C	G2103	A2037	U1955	U1880	G1813	G1741	A1669	C1592	G1459	G1459	A1395
C2104	C2104	C2104	G2038	U1956	U1881	A1821	U1742	C1670	C1593	U1460	C1461	U1396
U2105	U2105	U2105	G2039	C1957	U1882	G1816	G1743	G1674	A1594	C1462	C1462	U1397
U2106	U2106	G2040	G2040	C1958	U1883	G1817	A1744	G1675	C1595	C1463	G1463	U1400
G2107	G2107	U2041	U2041	G1959	G1884	A1818	A1745	G1676	U1534	G1464	G1464	G1401
A2108	A2108	A2042	A2042	U1986	U1885	U1819	A1746	A1677	A1535	G1465	U1402	U1402
U2109	U2109	C2043	C2043	C1887	C1887	U1820	U1747	A1678	C1536	U1466	A1403	A1403
G2110	G2110	G2046	G2046	G1888	G1888	A1821	U1751	A1679	U1537	U1466	C1404	C1404
U	U	C2047	C2047	A1889	A1889	G1824	G1751	U1679	A1603	A1469	U1405	U1405
G	G	G2048	G2048	G1968	A1890	U1825	G1756	U1680	G1539	A1470	U1406	U1406
C	C	G2049	G2049	A1969	C1893	G1826	A1757	G1681	G1540	G1471	G1407	G1407
A	A	G2050	G2050	U1971	C1894	U1827	G1757	U1683	U1542	A1471	G1408	G1408
G	G	A2052	A2052	G1972	G1898	G1828	C1760	G1684	G1543	G1475	U1409	U1409
C	C	G2053	G2053	G1973	U1898	A1829	C1761	G1685	A1544	U1476	G1410	G1410
A	A	A2054	A2054	C1974	A1901	C1830	C1762	G1685	A1545	A1477	U1411	U1411
U	U	C2055	C2055	U1979	C1902	G1831	G1763	G1691	G1546	G1478	U1412	U1412
G	G	G2056	G2056	G1980	C1902	C1832	C1764	U1692	C1547	G1479	A1413	A1413
U	U	A2060	A2060	A1981	G1906	C1838	U1765	U1692	A1548	G1482	G1416	G1416
G	G	G2061	G2061	A1987	G1907	U1841	G1766	U1693	A1549	G1483	C1417	C1417
U	U	A2062	A2062	C1908	G1908	G1842	C1767	U1693	C1550	U1484	U1484	U1484
G	G	C2063	C2063	G1988	G1910	C1843	G1768	A1700	A1552	U1485	A1419	A1419

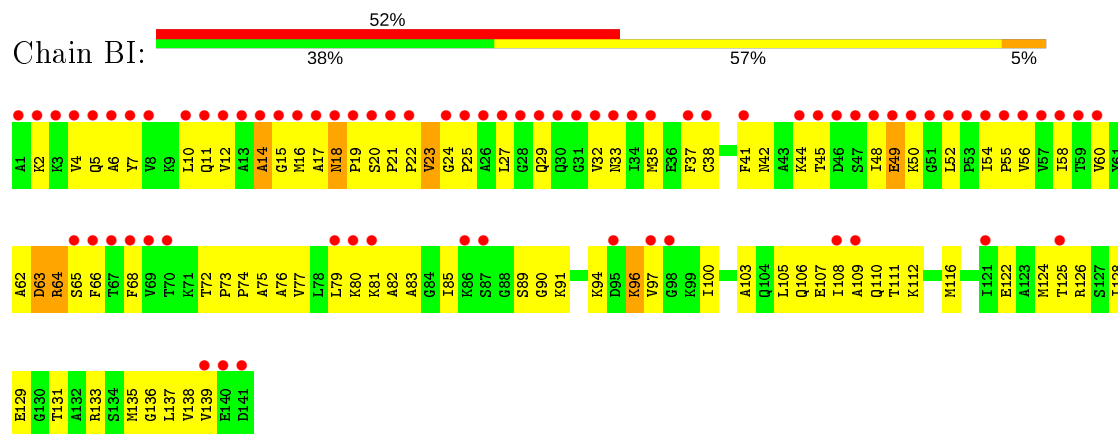


G1292	G1293	U1222	G1223	U1224	U1159	G1087	G1016	G950	C	A820	U741	6674	C610	C544	A480	G410	G411	A345
G1296	G1297	G1223	G1223	U1224	G1160	A1088	G1017	C951	A	A821	A742	A675	6611	U545	G481	G411	G411	A346
G1298	G1299	U1224	U1018	U1019	G1161	A1089	U1018	G952	U	G922	A743	A676	6612	U546	A482	C414	C414	A347
G1300	G1301	G1228	U1019	U1020	G1162	G1091	A1020	G953	C	C923	U744	A677	A613	A547	A483	C414	C414	A348
G1302	G1303	G1229	G1092	G1093	G1163	G1092	A1021	G954	C	U824	G745	A678	A614	U548	A484	U416	U416	U349
G1304	G1305	A1230	G1093	U1094	G1164	G1093	G1022	G955	C	A825	U746	C679	U615	U549	C485	C417	C417	U350
G1306	G1307	U1231	U1023	U1024	A1165	G956	G1023	G956	G	U826	U747	C680	A616	C550	C486	C418	C418	C351
G1308	G1309	G1235	G1024	G1025	G1166	C957	U1024	C957	C	U827	A753	G682	6617	G551	G491	U419	U419	A352
G1310	G1311	G1236	G1025	G1026	G1167	U958	G1026	U958	U	U828	U754	U683	6620	U554	A492	C420	C420	C353
G1312	C1315	G1237	G1026	A1027	G1168	A959	G1027	A959	U	G831	U755	U683	6621	U555	A493	C420	C420	A354
C1316	C1317	A1237	A1028	A1029	G1169	C961	A1028	C961	A	U832	A756	U686	6622	U556	G494	A423	A423	U355
C1318	C1319	G1238	U1029	G1030	C1170	G962	A1029	G962	C	A833	C757	C687	6623	C557	G495	G424	G424	U356
C1320	C1321	G1239	G1031	U1032	G1171	G963	G1031	G963	C958	G834	C758	U688	6624	U558	G496	G425	G425	C357
C1322	C1323	U1240	G1032	U1033	C1172	G964	G1032	G964	A899	C935	C759	U689	6625	U559	A497	G426	G426	U358
C1324	C1325	G1241	U1033	U1034	U1173	U967	U1033	U967	A899	G836	C760	U690	6626	C560	G498	U427	U427	G359
C1326	C1327	U1242	U1034	U1035	U1174	C968	U1034	C968	C908	C937	C761	C692	6627	C561	U499	A428	A428	U360
C1328	C1329	U1243	U1035	U1036	U1175	C969	U1035	C969	C903	C938	C762	C693	6628	U562	G500	U431	U431	G361
C1330	C1331	A1244	U1036	U1037	U1176	U970	U1036	U970	G904	U839	C763	C694	6629	U563	A501	U432	U432	A362
C1332	C1333	G1245	G1037	G1038	C1177	G971	G1037	G971	A905	C840	C770	U694	6630	C564	A502	A432	A432	G363
C1334	C1335	G1246	G1038	G1039	U1178	A972	G1038	A972	U906	G841	C771	U695	6631	C565	A503	C433	C433	C364
C1336	C1337	U1247	U1039	U1040	U1179	A973	U1039	A973	C907	U842	C772	U696	6632	U566	A504	U434	U434	U365
C1338	C1339	G1248	U1040	U1041	U1180	C974	U1040	C974	C908	U843	C773	U697	6633	U567	A505	C435	C435	C366
C1340	C1341	U1249	U1041	U1042	U1181	G975	U1041	G975	C909	U844	C774	U698	6634	G570	G506	C436	C436	G367
C1342	C1343	G1250	U1042	U1043	U1182	G976	U1042	G976	A910	U845	C775	U699	6635	U571	A507	U437	U437	A368
C1344	C1345	G1251	U1043	U1044	U1183	G977	U1043	G977	A911	U846	C776	U700	6636	U572	A508	G438	G438	U369
C1346	C1347	U1252	U1044	U1045	U1184	G978	U1044	G978	U913	C848	C777	U701	6637	U573	C509	A439	A439	G370
C1348	C1349	G1253	U1045	U1046	U1185	A979	U1045	A979	U913	U849	C778	U702	6638	U574	C510	G440	G440	A371
C1350	C1351	U1254	U1046	U1047	U1186	G980	U1046	G980	A917	C850	C779	U703	6639	U575	U511	U441	U441	G372
C1352	C1353	G1255	U1047	U1048	U1187	A981	U1047	A981	A918	C851	C780	U704	6640	U576	G512	G442	G442	U373
C1354	C1355	U1256	U1048	U1049	U1188	C982	U1048	C982	A919	C852	C781	U705	6641	U577	A513	A443	A443	A374
C1356	C1357	G1256	U1049	U1050	U1189	A983	U1049	A983	U919	C853	C782	U706	6642	U578	A514	C444	C444	A375
C1358	C1359	U1257	U1050	U1051	U1190	C984	U1050	C984	A920	C854	C783	U707	6643	U579	A515	C445	C445	C378
C1360	C1361	G1258	U1051	U1052	U1191	A984	U1051	A984	C921	C855	C784	U708	6644	U580	C516	G446	G446	G379
C1362	C1363	U1259	U1052	U1053	U1192	C985	U1052	C985	C922	C856	C785	U709	6645	U581	C517	G447	G447	G380
C1364	C1365	G1259	U1053	U1054	U1193	G986	U1053	G986	C923	C857	C786	U710	6646	U582	G518	U451	U451	G381
C1366	C1367	U1260	U1054	U1055	U1194	A988	U1054	A988	G924	C858	C787	U711	6647	U583	U519	A454	A454	A382
C1368	C1369	G1261	U1055	U1056	U1195	G989	U1055	G989	A925	C859	C788	U712	6648	U584	A522	C454	C454	C383
C1370	C1371	U1262	U1056	U1057	U1196	A990	U1056	A990	A926	A863	C789	U713	6649	U585	A523	C455	C455	A384
C1372	C1373	G1263	U1057	U1058	U1197	G991	U1057	G991	A927	C864	C790	U714	6650	U586	C523	C456	C456	G385
C1374	C1375	U1264	U1058	U1059	U1198	C992	U1058	C992	A928	C865	C791	U715	6651	U587	G524	A457	A457	G386
C1376	C1377	G1265	U1059	U1060	U1199	G993	U1059	G993	A929	C866	C792	U716	6652	U588	U525	G458	G458	U387
C1378	C1379	U1266	U1060	U1061	U1200	C994	U1060	C994	G930	A866	C793	U717	6653	U589	A526	U459	U459	U388
C1380	C1381	G1267	U1061	U1062	U1201	G995	U1061	G995	U931	G869	C794	U718	6654	U590	A527	C460	C460	U389
C1382	C1383	U1268	U1062	U1063	U1202	C996	U1062	C996	U932	C870	C795	U719	6655	U591	A528	C461	C461	U390
C1384	C1385	G1269	U1063	U1064	U1203	G997	U1063	G997	U933	C871	C796	U720	6656	U592	A529	G462	G462	U391
C1386	C1387	U1270	U1064	U1065	U1204	C998	U1064	C998	A933	C872	C797	U721	6657	U593	A530	U463	U463	C394
C1388	C1389	G1271	U1065	U1066	U1205	G999	U1065	G999	A934	C873	C798	U722	6658	U594	C531	G464	G464	U395
C1390	C1391	U1272	U1066	U1067	U1206	A990	U1066	A990	U934	C874	C799	U723	6659	U595	A532	G465	G465	U396
C1392	C1393	G1273	U1067	U1068	U1207	C999	U1067	C999	A935	C875	C800	C723	6660	U596	C532	A466	A466	G397
C1394	C1395	U1274	U1068	U1069	U1208	G999	U1068	G999	A936	C876	C801	C724	6661	U597	A533	G467	G467	U398
C1396	C1397	G1275	U1069	U1070	U1209	A999	U1069	A999	A937	C877	C802	C725	6662	U598	G533	G468	G468	G400
C1398	C1399	U1276	U1070	U1071	U1210	C999	U1070	C999	A938	C878	C803	C726	6663	U599	U534	G469	G469	A401
C1400	C1401	G1277	U1071	U1072	U1211	A1000	U1071	A1000	A939	C879	C804	C727	6664	U600	G535	G470	G470	A402
C1402	C1403	U1278	U1072	U1073	U1212	C1001	U1072	C1001	A940	C880	C805	C728	6665	U601	G536	G471	G471	U403
C1404	C1405	G1279	U1073	U1074	U1213	A1001	U1073	A1001	A941	C881	C806	C729	6666	U602	G537	G472	G472	A404
C1406	C1407	U1280	U1074	U1075	U1214	C1002	U1074	C1002	A942	C882	C807	C730	6667	U603	A538	G473	G473	U405
C1408	C1409	G1281	U1075	U1076	U1215	A1002	U1075	A1002	A943	C883	C808	C731	6668	U604	C539	G474	G474	U406
C1410	C1411	U1282	U1076	U1077	U1216	C1003	U1076	C1003	A944	C884	C809	C732	6669	U605	C540	G475	G475	G407
C1412	C1413	G1283	U1077	U1078	U1217	A1003	U1077	A1003	A945	C885	C810	C733	6670	U606	G541	G476	G476	A408
C1414	C1415	U1284	U1078	U1079	U1218	C1004	U1078	C1004	A946	C886	C811	C734	6671	U607	A542	G477	G477	G409
C1416	C1417	G1285	U1079	U1080	U1219	A1004	U1079	A1004	A947	C887	C812	C735	6672	U608	G543	G478	G478	
C1418	C1419	U1286	U1080	U1081	U1220	C1005	U1080	C1005	A948	C888	C813	C736	6673	U609		G479	G479	
C1420	C1421	G1287	U1081	U1082	U1221	A1005	U1081	A1005	A949	C889	C814	C737	6674	U610				
C1422	C1423	U1288	U1082	U1083	U1222	C1006	U1082	C1006	A950	C890	C815	C738	6675	U611				
C1424	C1425	G1289	U1083	U1084	U1223	A1006	U1083	A1006	A951	C891	C816	C739	6676	U612				
C1426	C1427	U1290	U1084	U1085	U1224	C1007	U1084	C1007	A952	C892	C817	C740	6677	U613				
C1428	C1429	G1291	U1085	U1086	U1225	A1007	U1085	A1007	A953	C893	C818	C741	6678	U614				
C1430	C1431	U1292	U1086	U1087	U1226	C1008	U1086	C1008	A954	C894	C819	C742	6679	U615				
C1432	C1433	G1293	U1087	U1088	U1227	A1008	U1087	A1008	A955	C895	C820	C743	6680	U616				
C1434	C1435	U1294	U1088	U1089	U1228	C1009	U1088	C1009	A956	C896	C821	C744	6681	U617				
C1436	C1437	G1295	U1089	U1090	U1229	A1009	U1089	A1009	A957	C897	C822	C745	6682	U618				
C1438	C1439	U1296	U1090	U1091	U1230	C1010	U1090	C1010	A958	C898	C823	C746	6683	U619				
C1440	C1441	G1297	U1091	U1092	U1231	A1010	U1091	A1010	A959	C899	C824	C747	6684	U620				
C1																		

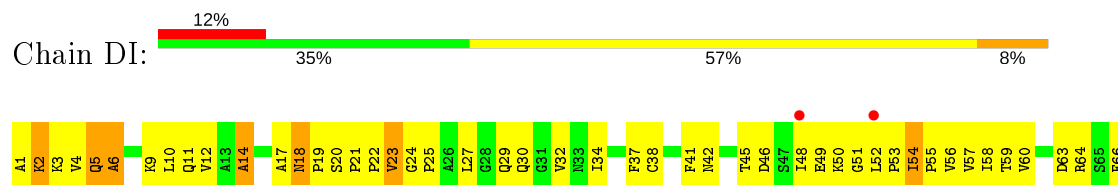


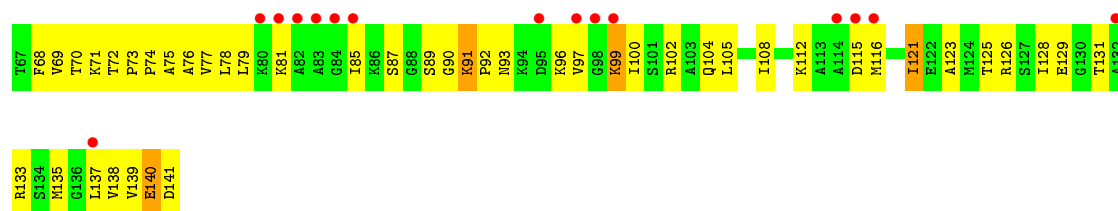


• Molecule 24: 50S ribosomal protein L11

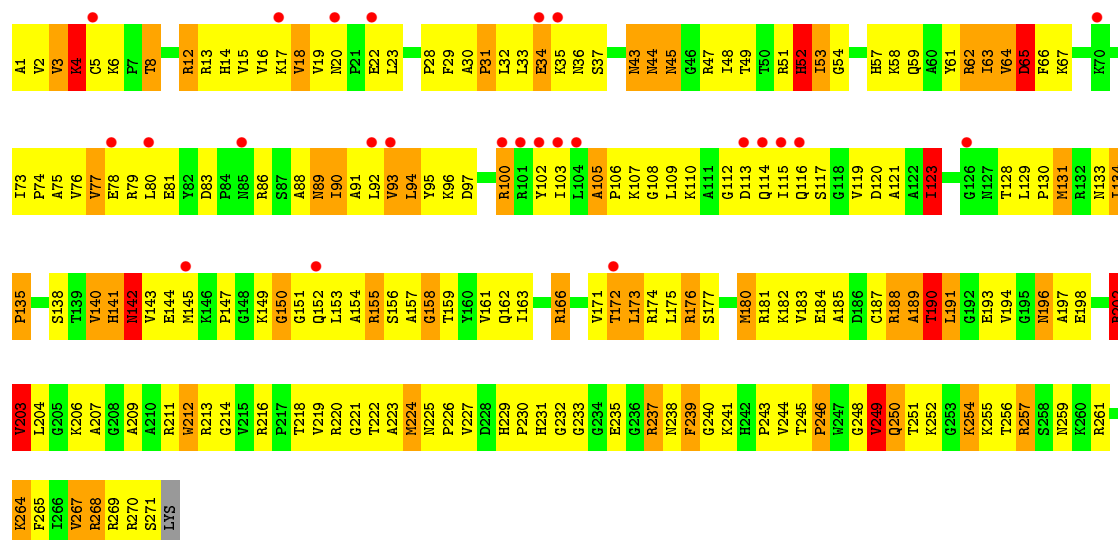


• Molecule 24: 50S ribosomal protein L11

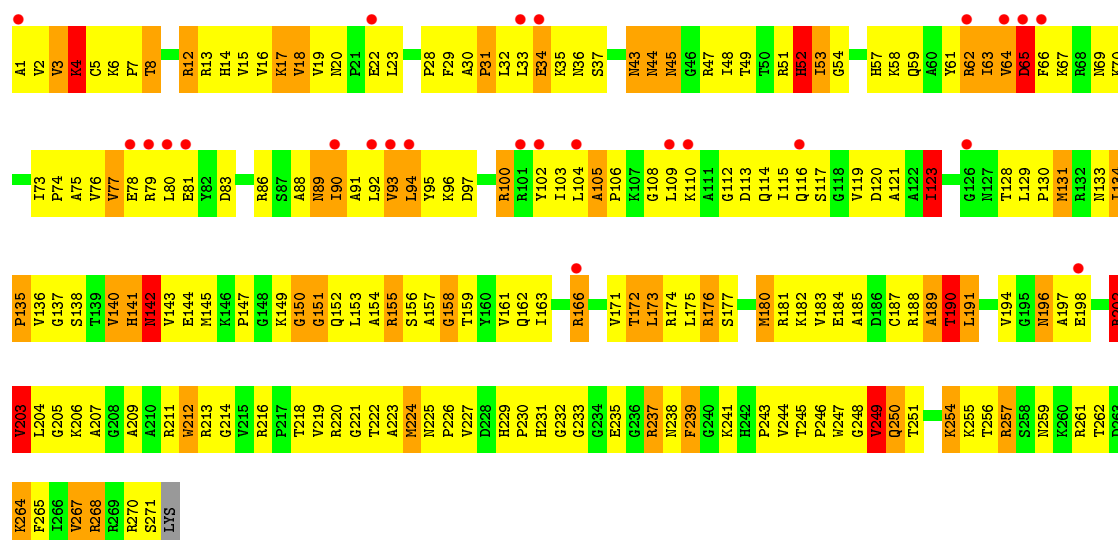
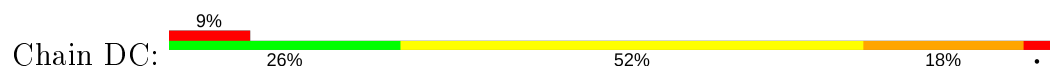




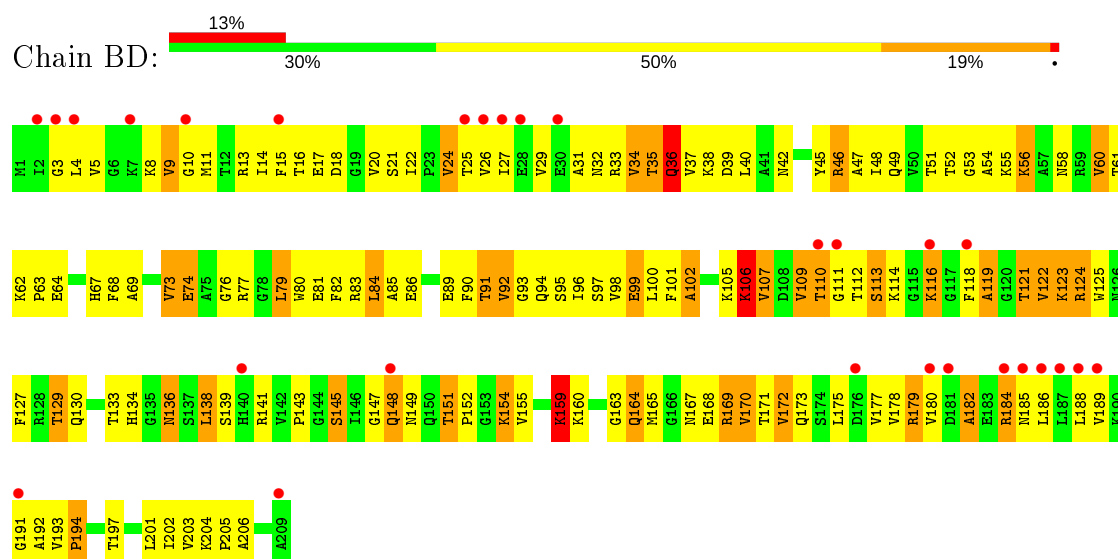
• Molecule 25: 50S ribosomal protein L2

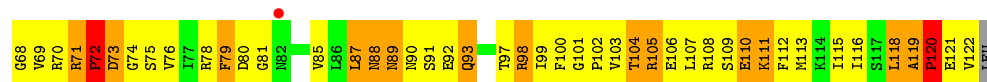
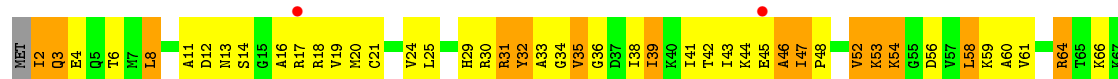


• Molecule 25: 50S ribosomal protein L2

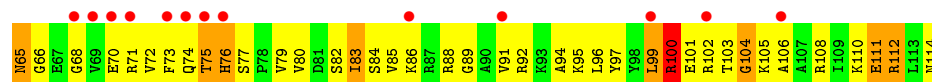


• Molecule 26: 50S ribosomal protein L3

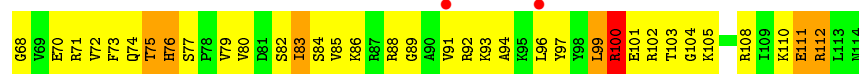
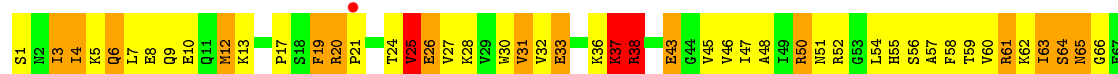




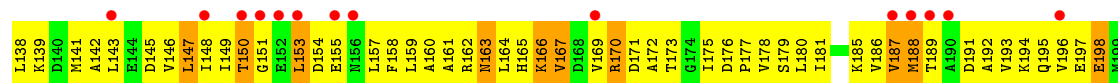
• Molecule 28: 50S ribosomal protein L19



• Molecule 28: 50S ribosomal protein L19

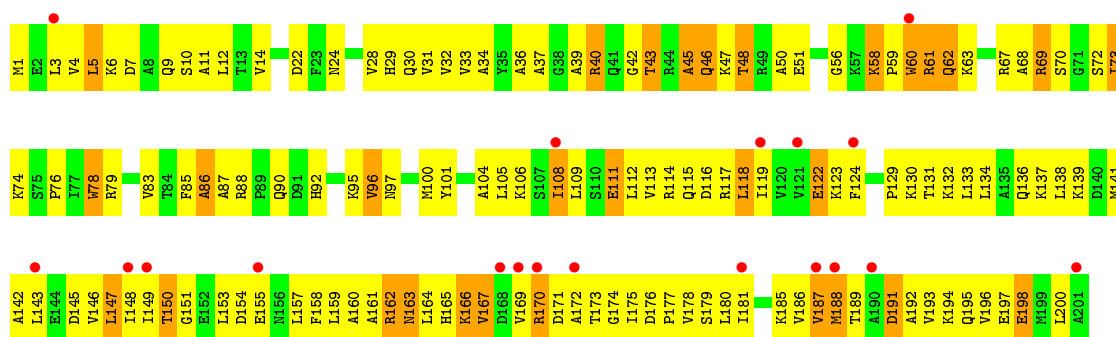


• Molecule 29: 50S ribosomal protein L4

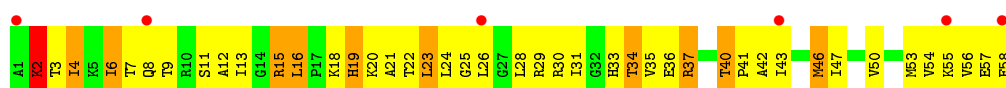


• Molecule 29: 50S ribosomal protein L4





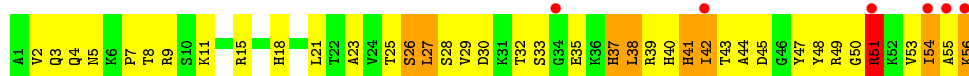
• Molecule 30: 50S ribosomal protein L30



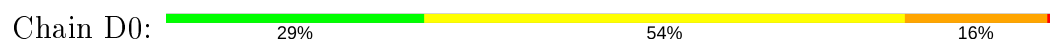
• Molecule 30: 50S ribosomal protein L30



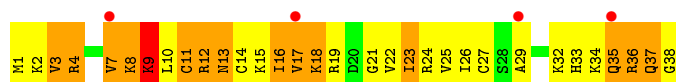
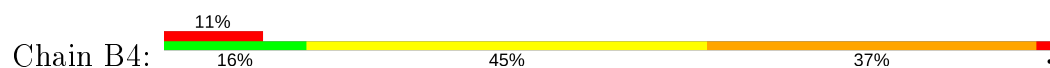
• Molecule 31: 50S ribosomal protein L32



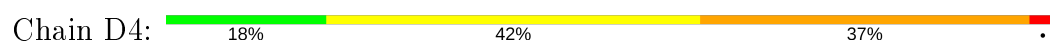
• Molecule 31: 50S ribosomal protein L32



• Molecule 32: 50S ribosomal protein L36

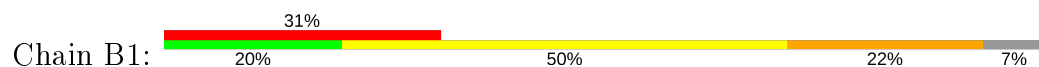


• Molecule 32: 50S ribosomal protein L36





- 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



- Molecule 35: 50S ribosomal protein L25

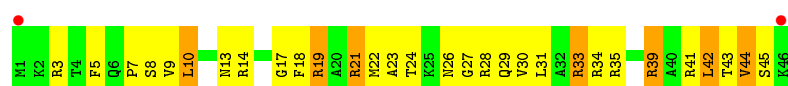




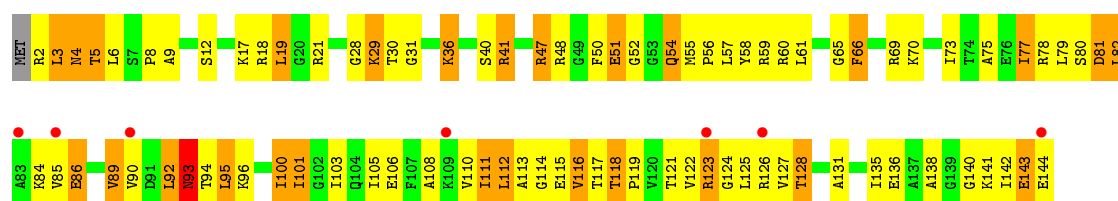
- Molecule 36: 50S ribosomal protein L34



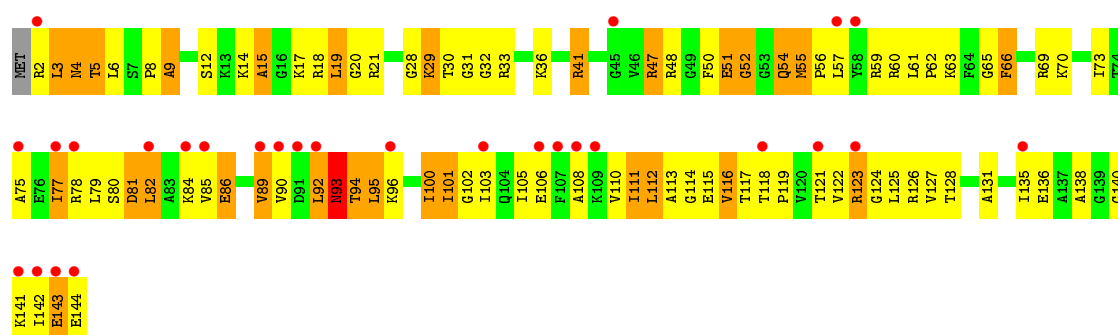
- Molecule 36: 50S ribosomal protein L34



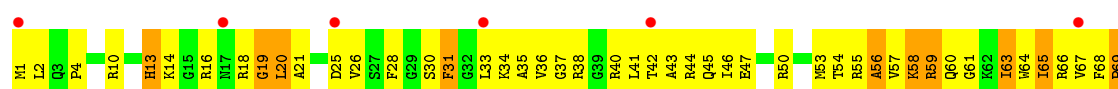
- Molecule 37: 50S ribosomal protein L15

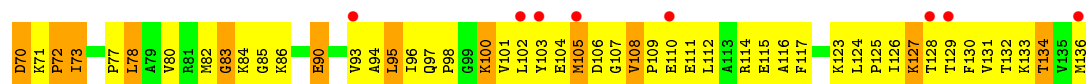


- Molecule 37: 50S ribosomal protein L15

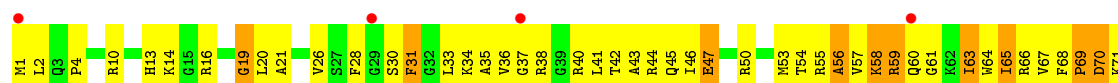


- Molecule 38: 50S ribosomal protein L16





• Molecule 38: 50S ribosomal protein L16



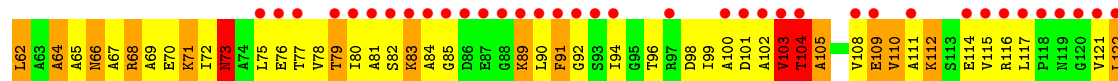
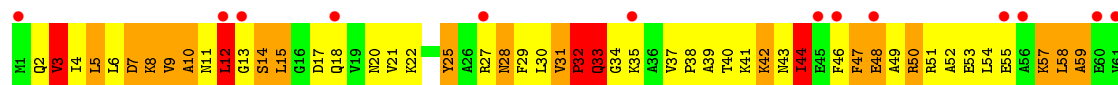
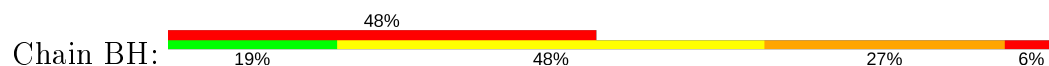
• Molecule 39: 50S ribosomal protein L29



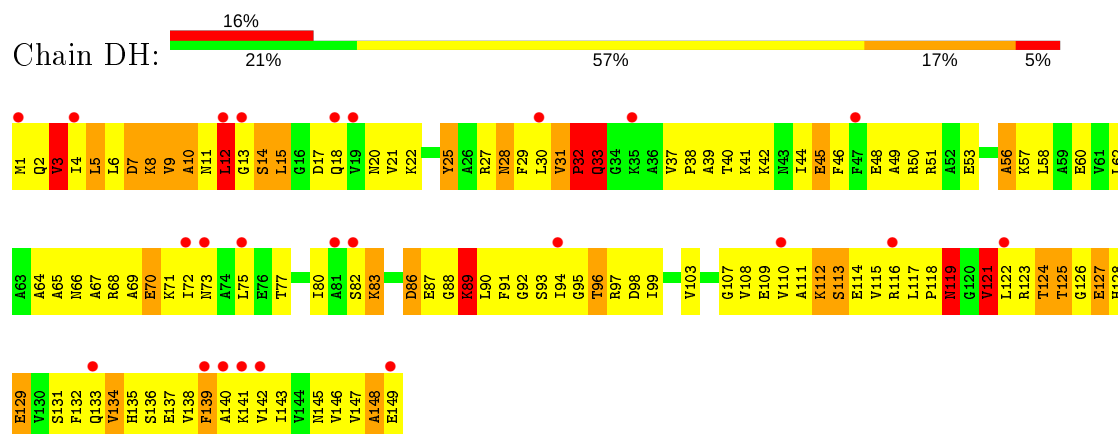
• Molecule 39: 50S ribosomal protein L29



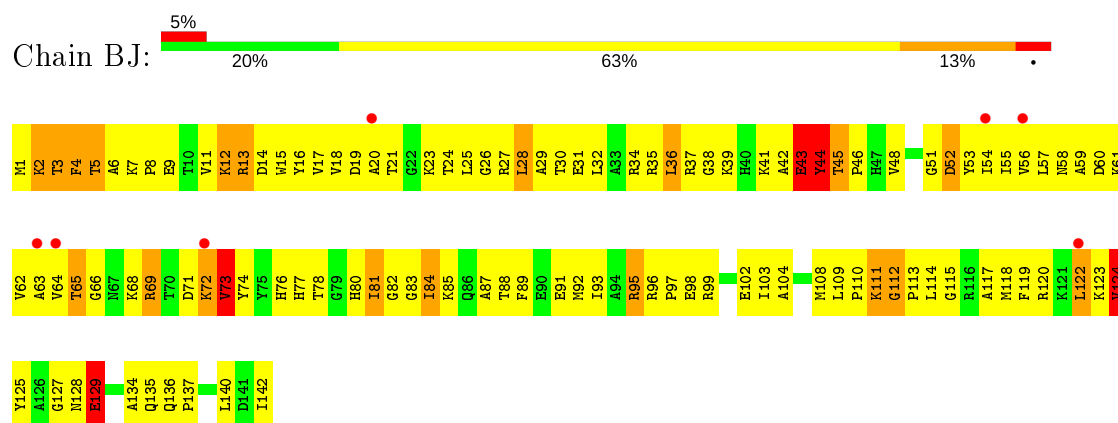
• Molecule 40: 50S ribosomal protein L9



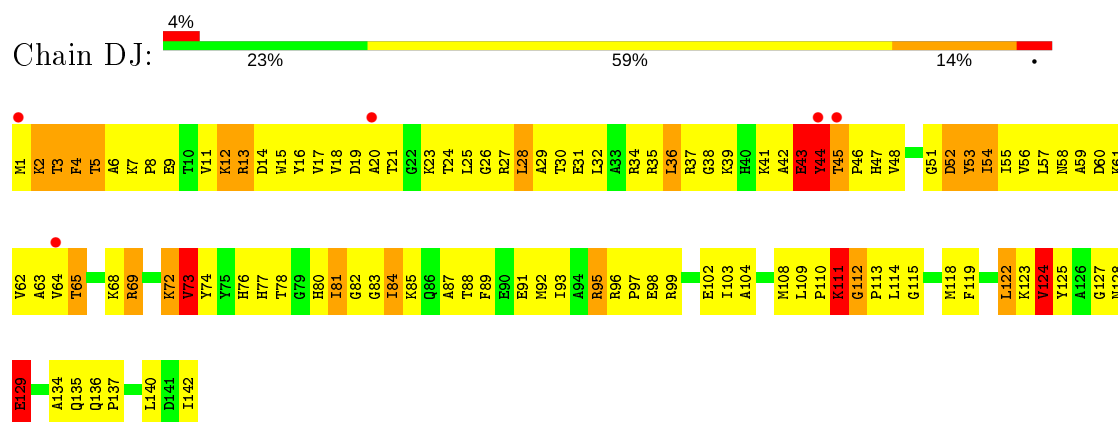
- Molecule 40: 50S ribosomal protein L9



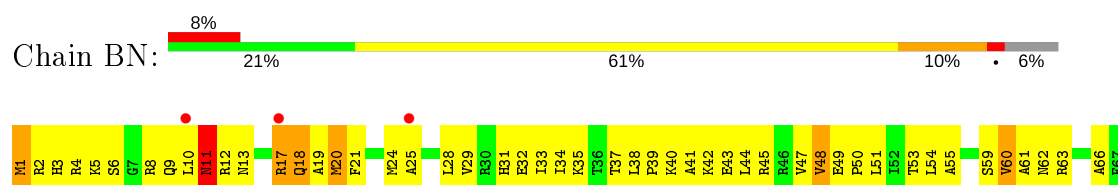
- Molecule 41: 50S ribosomal protein L13

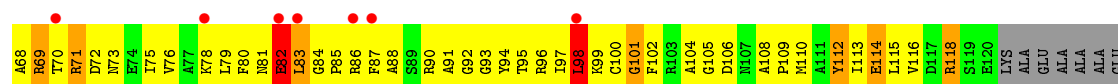


- Molecule 41: 50S ribosomal protein L13

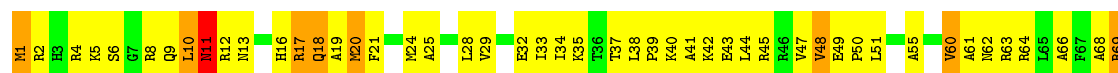


- Molecule 42: 50S ribosomal protein L17

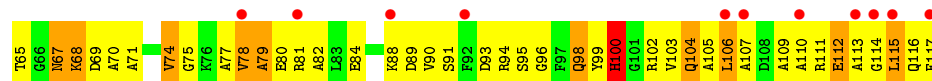
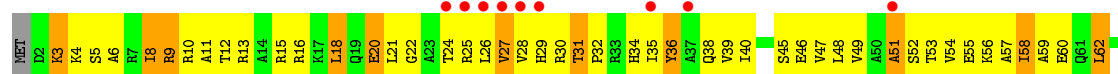




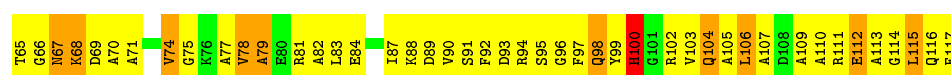
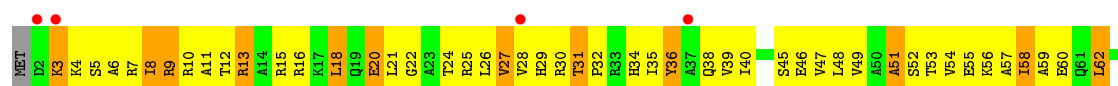
- Molecule 42: 50S ribosomal protein L17



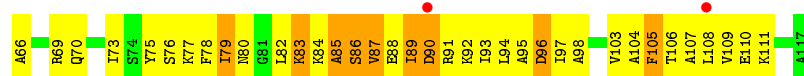
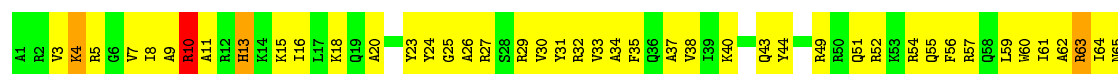
- Molecule 43: 50S ribosomal protein L18



- Molecule 43: 50S ribosomal protein L18

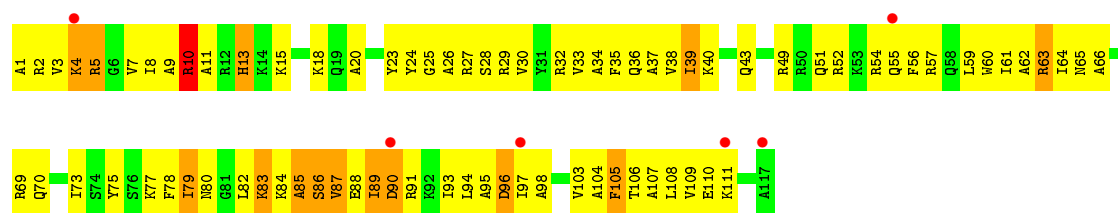


- Molecule 44: 50S ribosomal protein L20

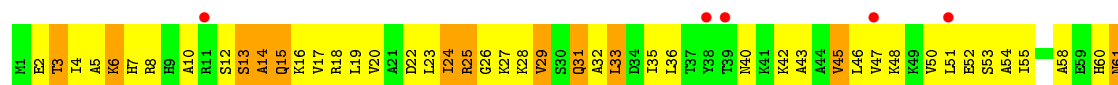


- Molecule 44: 50S ribosomal protein L20

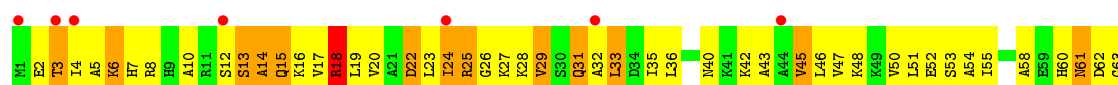




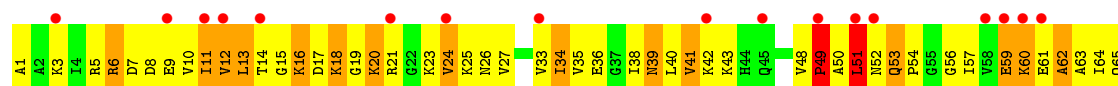
• Molecule 45: 50S ribosomal protein L22



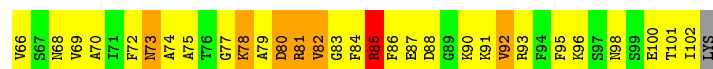
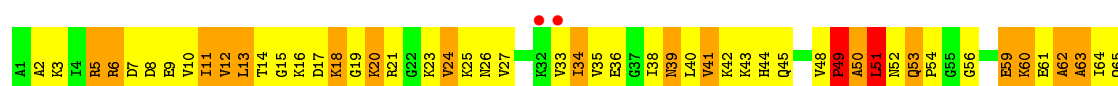
• Molecule 45: 50S ribosomal protein L22



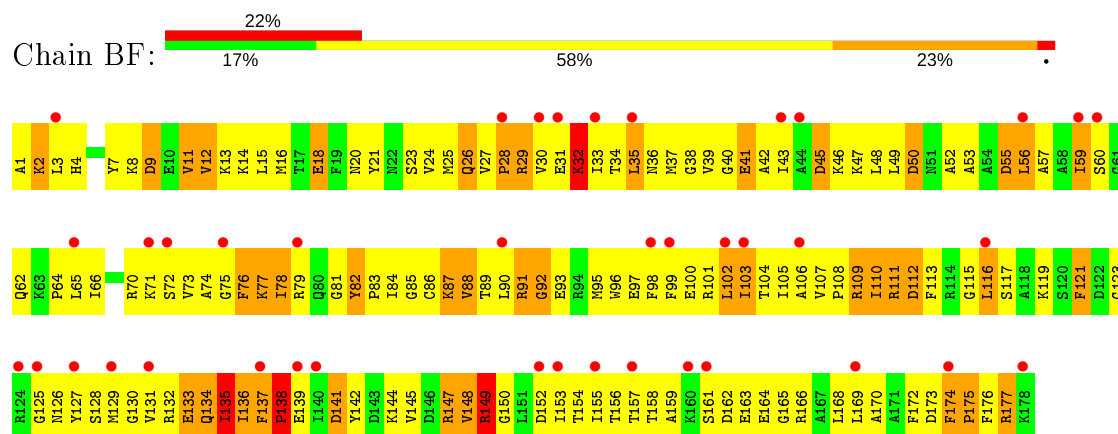
• Molecule 46: 50S ribosomal protein L24



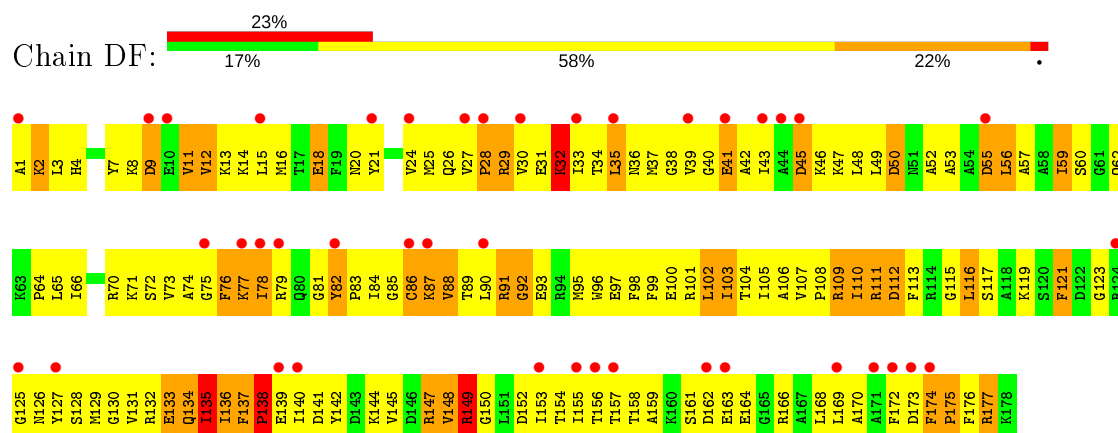
• Molecule 46: 50S ribosomal protein L24



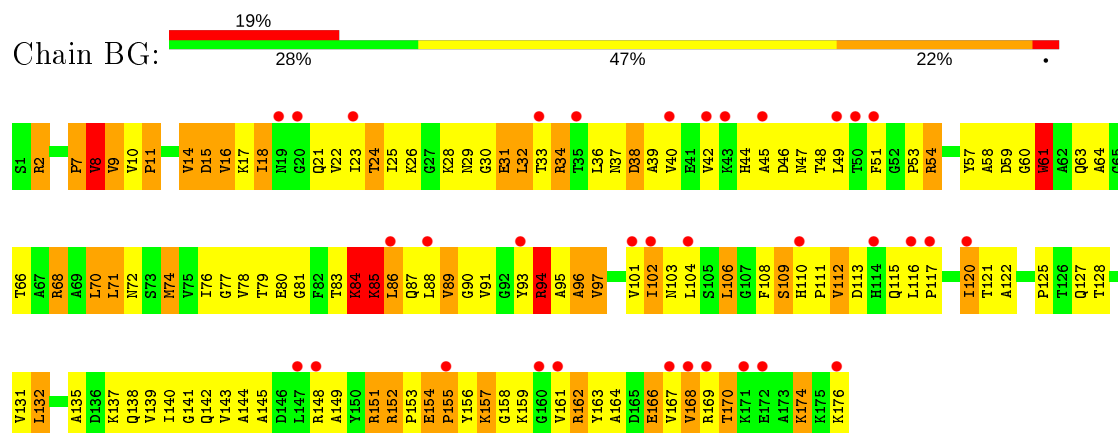
- Molecule 47: 50S ribosomal protein L5



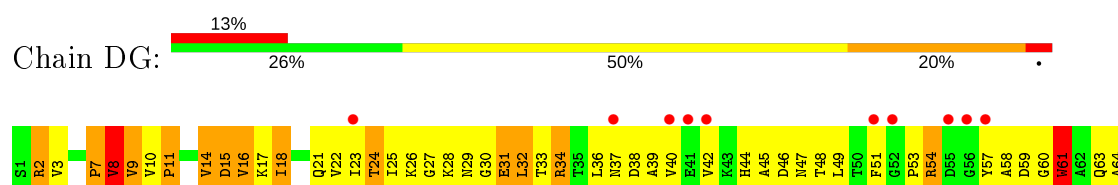
- Molecule 47: 50S ribosomal protein L5

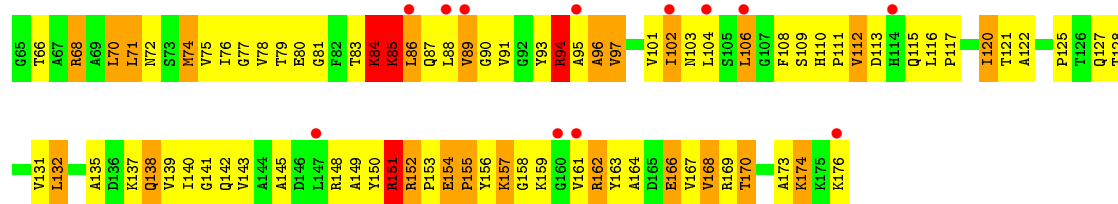


- Molecule 48: 50S ribosomal protein L6

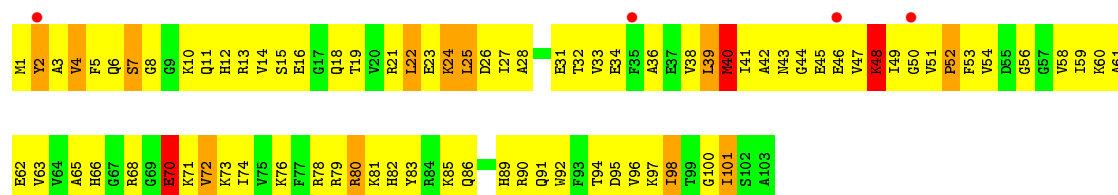


- Molecule 48: 50S ribosomal protein L6

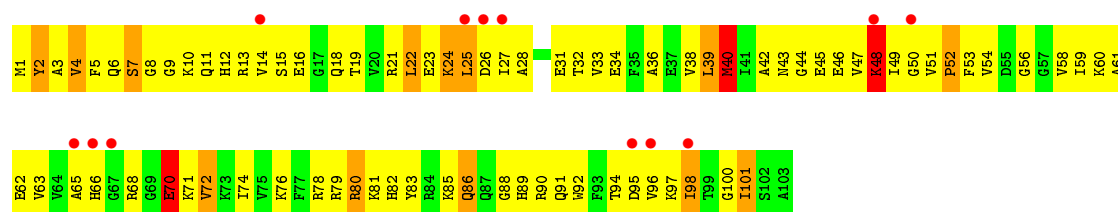




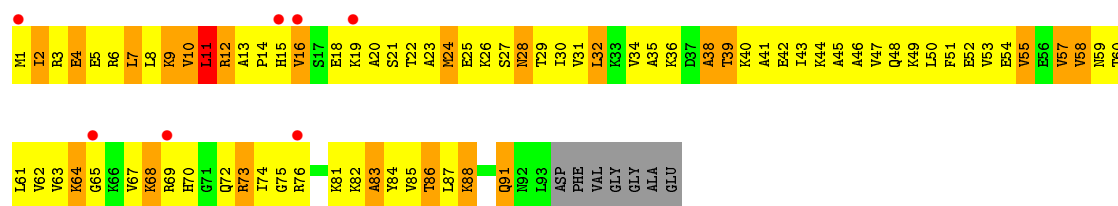
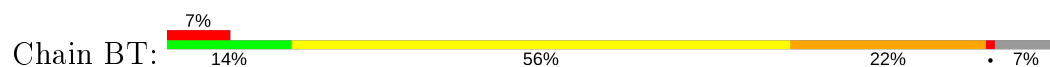
• Molecule 49: 50S ribosomal protein L21



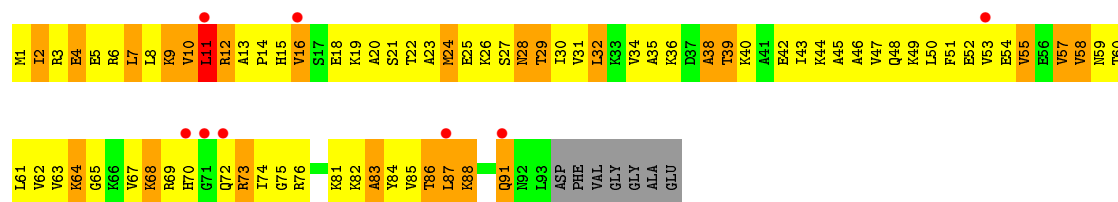
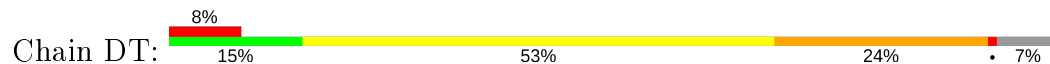
• Molecule 49: 50S ribosomal protein L21



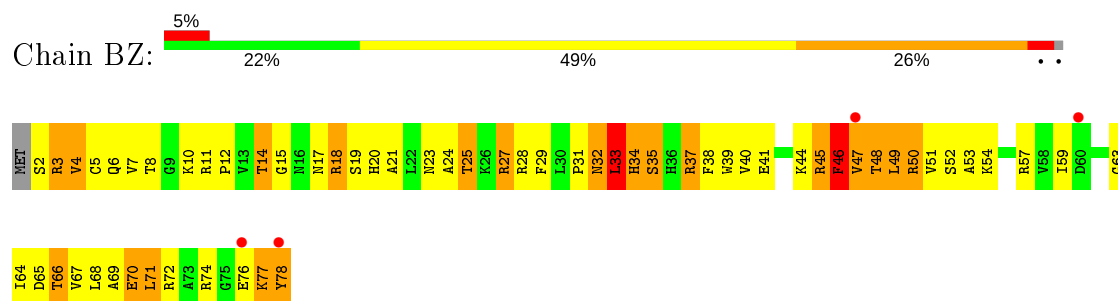
• Molecule 50: 50S ribosomal protein L23



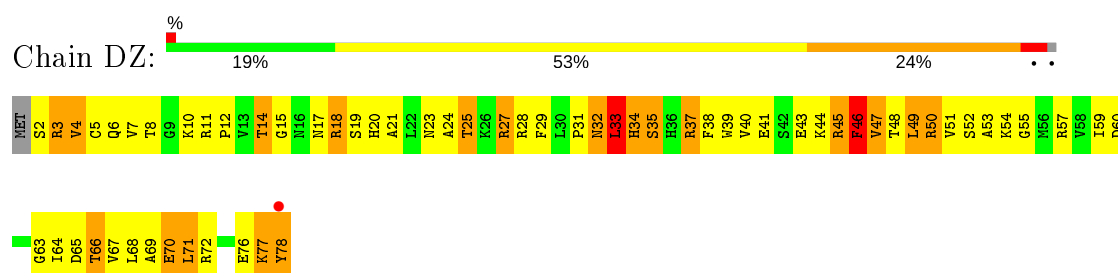
• Molecule 50: 50S ribosomal protein L23



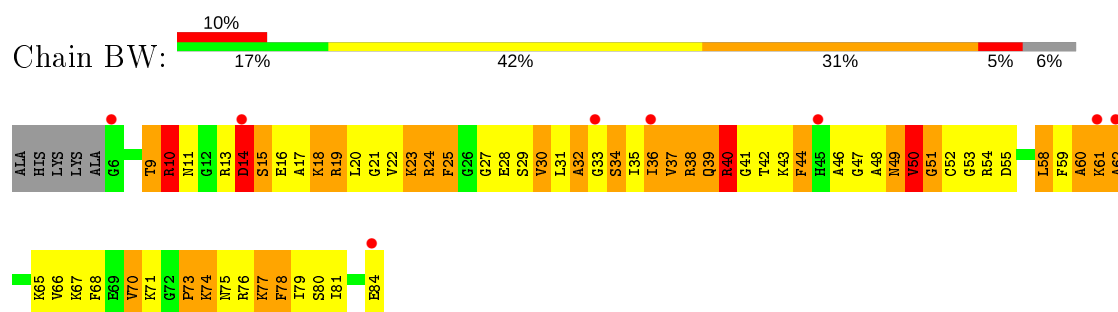
- Molecule 51: 50S ribosomal protein L28



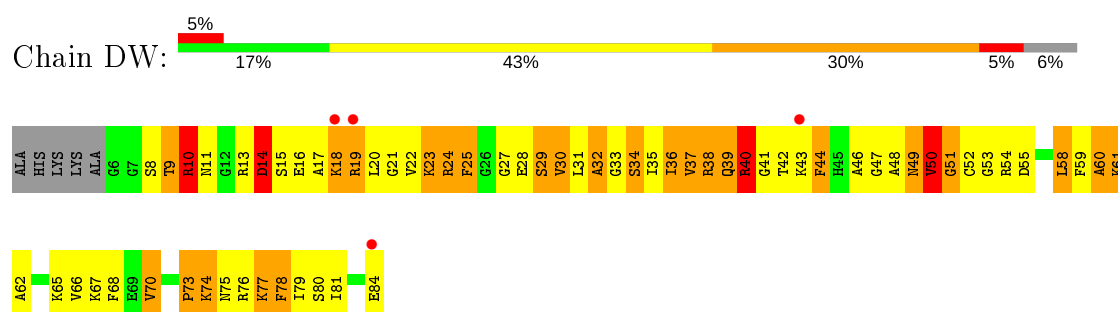
- Molecule 51: 50S ribosomal protein L28



- Molecule 52: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L27



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.54 138.41 – 3.55	Depositor EDS
% Data completeness (in resolution range)	88.8 (70.00-3.54) 89.9 (138.41-3.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.281 , 0.320 0.246 , 0.278	Depositor DCC
R_{free} test set	30217 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	125.1	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284252	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.26	2/36762 (0.0%)	0.76	22/57350 (0.0%)
1	CA	0.26	3/36762 (0.0%)	0.76	23/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	0/2227
4	AE	0.23	0/1118	0.45	0/1504
4	CE	0.23	0/1118	0.45	0/1504
5	AF	0.24	0/835	0.44	0/1128
5	CF	0.24	0/835	0.45	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.44	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.46	0/1375
8	CI	0.24	0/1034	0.46	0/1375
9	AJ	0.22	0/796	0.48	0/1077
9	CJ	0.22	0/796	0.47	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.48	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.45	0/1043
13	CN	0.24	0/785	0.45	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.22	0/722	0.47	0/964
15	AP	0.25	0/659	0.46	0/884
15	CP	0.25	0/648	0.46	0/870
16	AQ	0.24	0/657	0.46	0/881
16	CQ	0.24	0/666	0.46	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.46	0/621
17	CR	0.23	0/462	0.46	0/621
18	AS	0.25	0/652	0.46	0/877
18	CS	0.25	0/660	0.48	0/888
19	AT	0.24	0/671	0.39	0/888
19	CT	0.24	0/671	0.39	0/888
20	AB	0.25	0/1735	0.45	0/2338
20	CB	0.25	0/1735	0.45	0/2338
21	AU	0.26	0/430	0.47	0/570
21	CU	0.26	0/430	0.47	0/570
22	BA	0.23	0/2803	0.74	0/4371
22	DA	0.23	0/2803	0.74	0/4371
23	BB	0.29	10/68314 (0.0%)	0.77	47/106569 (0.0%)
23	DB	0.28	9/68314 (0.0%)	0.78	58/106569 (0.1%)
24	BI	0.24	0/1046	0.46	0/1410
24	DI	0.25	0/1046	0.48	0/1410
25	BC	0.22	0/2121	0.48	0/2852
25	DC	0.22	0/2121	0.48	0/2852
26	BD	0.24	0/1586	0.48	0/2134
26	DD	0.24	0/1586	0.48	0/2134
27	BK	0.24	0/939	0.53	0/1258
27	DK	0.24	0/939	0.53	0/1258
28	BP	0.24	0/929	0.50	0/1242
28	DP	0.24	0/929	0.50	0/1242
29	BE	0.24	0/1571	0.50	0/2113
29	DE	0.24	0/1571	0.50	0/2113
30	BY	0.23	0/453	0.48	0/605
30	DY	0.23	0/453	0.48	0/605
31	B0	0.22	0/450	0.53	0/599
31	D0	0.22	0/450	0.53	0/599
32	B4	0.23	0/303	0.46	0/397
32	D4	0.23	0/303	0.46	0/397
33	B1	0.27	0/416	0.48	0/554
33	D1	0.27	0/416	0.48	0/554
34	B3	0.24	0/513	0.47	0/676
34	D3	0.24	0/513	0.47	0/676
35	BV	0.25	0/766	0.42	0/1025
35	DV	0.25	0/766	0.42	0/1025
36	B2	0.25	0/380	0.45	0/498
36	D2	0.25	0/380	0.45	0/498
37	BL	0.23	0/1054	0.47	0/1403
37	DL	0.24	0/1054	0.47	0/1403
38	BM	0.25	0/1093	0.47	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.47	0/1460
39	BX	0.24	0/510	0.52	0/677
39	DX	0.24	0/510	0.52	0/677
40	BH	0.25	0/1122	0.47	0/1515
40	DH	0.25	0/1122	0.47	0/1515
41	BJ	0.23	0/1152	0.48	0/1551
41	DJ	0.23	0/1152	0.48	0/1551
42	BN	0.24	0/973	0.51	0/1301
42	DN	0.24	0/973	0.51	0/1301
43	BO	0.23	0/902	0.48	0/1209
43	DO	0.23	0/902	0.48	0/1209
44	BQ	0.25	0/960	0.47	0/1278
44	DQ	0.25	0/960	0.47	0/1278
45	BS	0.22	0/864	0.51	0/1156
45	DS	0.22	0/864	0.51	0/1156
46	BU	0.25	0/787	0.46	0/1051
46	DU	0.26	0/787	0.46	0/1051
47	BF	0.26	0/1444	0.50	0/1937
47	DF	0.26	0/1444	0.50	0/1937
48	BG	0.23	0/1343	0.47	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.25	0/829	0.48	0/1107
49	DR	0.25	0/829	0.48	0/1107
50	BT	0.22	0/744	0.53	0/994
50	DT	0.22	0/744	0.54	0/994
51	BZ	0.25	0/635	0.50	0/848
51	DZ	0.25	0/635	0.50	0/848
52	BW	0.28	0/603	0.48	0/797
52	DW	0.28	0/603	0.48	0/797
All	All	0.26	24/306360 (0.0%)	0.70	150/457969 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	15
1	CA	1	15
23	BB	0	41
23	DB	0	40
All	All	1	111

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-16.49	1.26	1.41
23	DB	1086	A	C5-C6	-16.38	1.26	1.41
23	BB	2322	A	O3'-P	14.51	1.78	1.61
23	BB	2318	G	O3'-P	-12.62	1.46	1.61
23	DB	1088	A	C6-N1	-10.61	1.28	1.35

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1213	A	O5'-P-OP1	-32.89	71.23	110.70
23	DB	2204	G	O5'-P-OP1	-29.68	75.08	110.70
1	AA	1213	A	O5'-P-OP2	-28.32	76.72	110.70
23	BB	2204	G	O5'-P-OP2	-28.25	76.80	110.70
23	BB	2791	G	O5'-P-OP1	-28.20	76.86	110.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	CA	366	A	C3'

5 of 111 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	1241	0
1	CA	32831	0	16521	1247	0
2	AC	1624	0	1699	150	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CC	1624	0	1699	150	0
3	AD	1643	0	1710	174	0
3	CD	1643	0	1710	174	0
4	AE	1105	0	1148	94	0
4	CE	1105	0	1148	93	0
5	AF	817	0	808	99	0
5	CF	817	0	808	93	0
6	AG	1174	0	1230	105	0
6	CG	1196	0	1246	98	0
7	AH	979	0	1034	82	0
7	CH	979	0	1034	79	0
8	AI	1022	0	1070	133	0
8	CI	1022	0	1070	132	0
9	AJ	786	0	828	81	0
9	CJ	786	0	828	87	0
10	AK	877	0	887	106	0
10	CK	877	0	887	104	0
11	AL	955	0	1019	95	0
11	CL	955	0	1019	95	0
12	AM	883	0	944	107	0
12	CM	876	0	937	111	0
13	AN	774	0	827	108	0
13	CN	774	0	827	110	0
14	AO	714	0	734	47	0
14	CO	714	0	734	41	0
15	AP	649	0	666	65	0
15	CP	638	0	656	66	0
16	AQ	648	0	691	76	0
16	CQ	657	0	702	67	0
17	AR	455	0	478	48	0
17	CR	455	0	478	44	0
18	AS	637	0	665	87	0
18	CS	644	0	675	93	0
19	AT	665	0	714	56	0
19	CT	665	0	714	55	0
20	AB	1704	0	1732	218	0
20	CB	1704	0	1732	205	0
21	AU	425	0	449	75	0
21	CU	425	0	449	69	0
22	BA	2507	0	1270	101	0
22	DA	2507	0	1270	96	0
23	BB	60995	0	30678	2199	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	DB	60995	0	30677	2300	0
24	BI	1032	0	1088	106	0
24	DI	1032	0	1088	176	0
25	BC	2082	0	2157	243	0
25	DC	2082	0	2157	245	0
26	BD	1565	0	1616	196	0
26	DD	1565	0	1616	186	0
27	BK	930	0	1000	110	0
27	DK	930	0	1000	108	0
28	BP	917	0	965	111	0
28	DP	917	0	965	109	0
29	BE	1552	0	1619	165	0
29	DE	1552	0	1619	153	0
30	BY	449	0	491	54	0
30	DY	449	0	491	59	0
31	B0	444	0	461	41	0
31	D0	444	0	461	45	0
32	B4	302	0	340	40	0
32	D4	302	0	340	42	0
33	B1	409	0	440	52	0
33	D1	409	0	440	47	0
34	B3	504	0	574	53	0
34	D3	504	0	574	45	0
35	BV	753	0	780	89	0
35	DV	753	0	780	97	0
36	B2	377	0	418	31	0
36	D2	377	0	418	34	0
37	BL	1045	0	1117	132	0
37	DL	1045	0	1117	153	0
38	BM	1074	0	1157	117	0
38	DM	1074	0	1157	119	0
39	BX	509	0	543	71	0
39	DX	509	0	543	72	0
40	BH	1111	0	1148	197	0
40	DH	1111	0	1148	150	0
41	BJ	1129	0	1162	143	0
41	DJ	1129	0	1162	144	0
42	BN	960	0	1000	118	0
42	DN	960	0	1000	118	0
43	BO	892	0	923	88	0
43	DO	892	0	923	103	0
44	BQ	947	0	1022	144	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DQ	947	0	1022	141	0
45	BS	857	0	922	83	0
45	DS	857	0	922	87	0
46	BU	779	0	834	113	0
46	DU	779	0	834	114	0
47	BF	1420	0	1460	225	0
47	DF	1420	0	1460	228	0
48	BG	1323	0	1374	189	0
48	DG	1323	0	1374	191	0
49	BR	816	0	839	109	0
49	DR	816	0	839	112	0
50	BT	738	0	807	124	0
50	DT	738	0	807	128	0
51	BZ	625	0	652	80	0
51	DZ	625	0	652	77	0
52	BW	596	0	610	128	0
52	DW	596	0	610	131	0
53	AA	60	0	0	0	0
53	BB	110	0	0	0	0
53	CA	61	0	0	0	0
53	CN	1	0	0	0	0
53	DB	111	0	0	0	0
54	AA	93	0	117	6	0
54	BB	31	0	39	1	0
54	CA	93	0	117	5	0
54	DB	31	0	39	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	292	0	0	1	0
56	AE	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	2	0	0	0	0
56	AN	2	0	0	0	0
56	AT	2	0	0	0	0
56	B2	1	0	0	0	0
56	BB	492	0	0	7	0
56	BC	7	0	0	0	0
56	BE	3	0	0	0	0
56	BH	1	0	0	0	0
56	BL	3	0	0	0	0
56	CA	297	0	0	2	0
56	CE	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CK	1	0	0	0	0
56	CL	2	0	0	0	0
56	CN	4	0	0	0	0
56	CT	2	0	0	0	0
56	DB	502	0	0	8	0
56	DC	4	0	0	0	0
56	DE	2	0	0	0	0
56	DL	4	0	0	0	0
All	All	284252	0	190973	16353	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 35.

The worst 5 of 16353 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	1.42	1.17
23:DB:855:G:H21	52:DW:23:LYS:HG2	1.12	1.14
26:BD:106:LYS:HB3	26:BD:206:ALA:H	1.13	1.11
26:DD:106:LYS:HB3	26:DD:206:ALA:H	1.13	1.09
37:BL:143:GLU:HG2	37:BL:144:GLU:H	1.18	1.08

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%)	157 (77%)	34 (17%)	13 (6%)	1	16
2	CC	204/232 (88%)	156 (76%)	35 (17%)	13 (6%)	1	16
3	AD	203/205 (99%)	144 (71%)	45 (22%)	14 (7%)	1	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CD	203/205 (99%)	143 (70%)	45 (22%)	15 (7%)	1	13
4	AE	148/166 (89%)	114 (77%)	30 (20%)	4 (3%)	5	35
4	CE	148/166 (89%)	115 (78%)	29 (20%)	4 (3%)	5	35
5	AF	98/135 (73%)	71 (72%)	17 (17%)	10 (10%)	0	7
5	CF	98/135 (73%)	70 (71%)	19 (19%)	9 (9%)	1	8
6	AG	148/178 (83%)	117 (79%)	22 (15%)	9 (6%)	1	17
6	CG	150/178 (84%)	121 (81%)	18 (12%)	11 (7%)	1	13
7	AH	127/129 (98%)	99 (78%)	24 (19%)	4 (3%)	4	32
7	CH	127/129 (98%)	99 (78%)	23 (18%)	5 (4%)	3	26
8	AI	125/129 (97%)	88 (70%)	28 (22%)	9 (7%)	1	14
8	CI	125/129 (97%)	86 (69%)	29 (23%)	10 (8%)	1	11
9	AJ	96/103 (93%)	71 (74%)	15 (16%)	10 (10%)	0	7
9	CJ	96/103 (93%)	70 (73%)	15 (16%)	11 (12%)	0	6
10	AK	115/128 (90%)	83 (72%)	26 (23%)	6 (5%)	2	20
10	CK	115/128 (90%)	84 (73%)	25 (22%)	6 (5%)	2	20
11	AL	121/123 (98%)	79 (65%)	34 (28%)	8 (7%)	1	16
11	CL	121/123 (98%)	79 (65%)	34 (28%)	8 (7%)	1	16
12	AM	112/117 (96%)	76 (68%)	28 (25%)	8 (7%)	1	14
12	CM	111/117 (95%)	77 (69%)	26 (23%)	8 (7%)	1	14
13	AN	92/100 (92%)	61 (66%)	21 (23%)	10 (11%)	0	6
13	CN	92/100 (92%)	58 (63%)	24 (26%)	10 (11%)	0	6
14	AO	86/89 (97%)	63 (73%)	19 (22%)	4 (5%)	2	22
14	CO	86/89 (97%)	64 (74%)	19 (22%)	3 (4%)	3	30
15	AP	80/82 (98%)	57 (71%)	19 (24%)	4 (5%)	2	21
15	CP	78/82 (95%)	55 (70%)	18 (23%)	5 (6%)	1	16
16	AQ	78/83 (94%)	56 (72%)	16 (20%)	6 (8%)	1	11
16	CQ	79/83 (95%)	56 (71%)	17 (22%)	6 (8%)	1	12
17	AR	53/74 (72%)	39 (74%)	11 (21%)	3 (6%)	1	18
17	CR	53/74 (72%)	40 (76%)	10 (19%)	3 (6%)	1	18
18	AS	77/91 (85%)	60 (78%)	11 (14%)	6 (8%)	1	11
18	CS	78/91 (86%)	61 (78%)	11 (14%)	6 (8%)	1	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AT	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	1	17
19	CT	83/86 (96%)	64 (77%)	14 (17%)	5 (6%)	1	17
20	AB	216/240 (90%)	149 (69%)	52 (24%)	15 (7%)	1	14
20	CB	216/240 (90%)	149 (69%)	51 (24%)	16 (7%)	1	13
21	AU	49/70 (70%)	28 (57%)	14 (29%)	7 (14%)	0	3
21	CU	49/70 (70%)	27 (55%)	15 (31%)	7 (14%)	0	3
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	3	29
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	3	29
25	BC	269/272 (99%)	168 (62%)	58 (22%)	43 (16%)	0	3
25	DC	269/272 (99%)	167 (62%)	59 (22%)	43 (16%)	0	3
26	BD	207/209 (99%)	119 (58%)	59 (28%)	29 (14%)	0	4
26	DD	207/209 (99%)	119 (58%)	59 (28%)	29 (14%)	0	4
27	BK	119/123 (97%)	79 (66%)	22 (18%)	18 (15%)	0	3
27	DK	119/123 (97%)	78 (66%)	23 (19%)	18 (15%)	0	3
28	BP	112/114 (98%)	61 (54%)	36 (32%)	15 (13%)	0	4
28	DP	112/114 (98%)	60 (54%)	37 (33%)	15 (13%)	0	4
29	BE	199/201 (99%)	126 (63%)	48 (24%)	25 (13%)	0	5
29	DE	199/201 (99%)	127 (64%)	46 (23%)	26 (13%)	0	4
30	BY	56/58 (97%)	40 (71%)	13 (23%)	3 (5%)	2	19
30	DY	56/58 (97%)	40 (71%)	13 (23%)	3 (5%)	2	19
31	B0	54/56 (96%)	43 (80%)	6 (11%)	5 (9%)	0	8
31	D0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	0	8
32	B4	36/38 (95%)	18 (50%)	7 (19%)	11 (31%)	0	0
32	D4	36/38 (95%)	18 (50%)	7 (19%)	11 (31%)	0	0
33	B1	48/54 (89%)	31 (65%)	12 (25%)	5 (10%)	0	7
33	D1	48/54 (89%)	33 (69%)	10 (21%)	5 (10%)	0	7
34	B3	62/64 (97%)	41 (66%)	16 (26%)	5 (8%)	1	10
34	D3	62/64 (97%)	41 (66%)	16 (26%)	5 (8%)	1	10
35	BV	92/94 (98%)	67 (73%)	20 (22%)	5 (5%)	2	19
35	DV	92/94 (98%)	67 (73%)	21 (23%)	4 (4%)	2	24
36	B2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	1	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	D2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	1	15
37	BL	141/144 (98%)	90 (64%)	29 (21%)	22 (16%)	0	3
37	DL	141/144 (98%)	90 (64%)	27 (19%)	24 (17%)	0	2
38	BM	134/136 (98%)	80 (60%)	40 (30%)	14 (10%)	0	7
38	DM	134/136 (98%)	81 (60%)	39 (29%)	14 (10%)	0	7
39	BX	61/63 (97%)	38 (62%)	16 (26%)	7 (12%)	0	6
39	DX	61/63 (97%)	37 (61%)	17 (28%)	7 (12%)	0	6
40	BH	147/149 (99%)	83 (56%)	27 (18%)	37 (25%)	0	0
40	DH	147/149 (99%)	89 (60%)	30 (20%)	28 (19%)	0	2
41	BJ	140/142 (99%)	86 (61%)	36 (26%)	18 (13%)	0	4
41	DJ	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	4
42	BN	118/127 (93%)	77 (65%)	30 (25%)	11 (9%)	0	8
42	DN	118/127 (93%)	76 (64%)	30 (25%)	12 (10%)	0	7
43	BO	114/117 (97%)	79 (69%)	24 (21%)	11 (10%)	0	8
43	DO	114/117 (97%)	80 (70%)	23 (20%)	11 (10%)	0	8
44	BQ	115/117 (98%)	75 (65%)	33 (29%)	7 (6%)	1	17
44	DQ	115/117 (98%)	77 (67%)	30 (26%)	8 (7%)	1	14
45	BS	108/110 (98%)	67 (62%)	29 (27%)	12 (11%)	0	6
45	DS	108/110 (98%)	66 (61%)	29 (27%)	13 (12%)	0	5
46	BU	100/103 (97%)	58 (58%)	25 (25%)	17 (17%)	0	2
46	DU	100/103 (97%)	59 (59%)	23 (23%)	18 (18%)	0	2
47	BF	176/178 (99%)	101 (57%)	49 (28%)	26 (15%)	0	3
47	DF	176/178 (99%)	102 (58%)	49 (28%)	25 (14%)	0	3
48	BG	174/176 (99%)	95 (55%)	48 (28%)	31 (18%)	0	2
48	DG	174/176 (99%)	94 (54%)	50 (29%)	30 (17%)	0	2
49	BR	101/103 (98%)	62 (61%)	26 (26%)	13 (13%)	0	4
49	DR	101/103 (98%)	62 (61%)	26 (26%)	13 (13%)	0	4
50	BT	91/100 (91%)	52 (57%)	23 (25%)	16 (18%)	0	2
50	DT	91/100 (91%)	51 (56%)	23 (25%)	17 (19%)	0	2
51	BZ	75/78 (96%)	51 (68%)	14 (19%)	10 (13%)	0	4
51	DZ	75/78 (96%)	50 (67%)	15 (20%)	10 (13%)	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	BW	77/84 (92%)	32 (42%)	22 (29%)	23 (30%)	0	0
52	DW	77/84 (92%)	30 (39%)	24 (31%)	23 (30%)	0	0
All	All	11241/11914 (94%)	7497 (67%)	2537 (23%)	1207 (11%)	0	7

5 of 1207 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	192	ALA

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%)	145 (85%)	25 (15%)	3	19
2	CC	170/189 (90%)	145 (85%)	25 (15%)	3	19
3	AD	172/172 (100%)	148 (86%)	24 (14%)	3	21
3	CD	172/172 (100%)	148 (86%)	24 (14%)	3	21
4	AE	113/125 (90%)	102 (90%)	11 (10%)	8	35
4	CE	113/125 (90%)	102 (90%)	11 (10%)	8	35
5	AF	87/116 (75%)	70 (80%)	17 (20%)	1	8
5	CF	87/116 (75%)	70 (80%)	17 (20%)	1	8
6	AG	123/146 (84%)	109 (89%)	14 (11%)	5	29
6	CG	125/146 (86%)	114 (91%)	11 (9%)	10	39
7	AH	104/104 (100%)	97 (93%)	7 (7%)	16	49
7	CH	104/104 (100%)	97 (93%)	7 (7%)	16	49
8	AI	105/106 (99%)	89 (85%)	16 (15%)	3	18
8	CI	105/106 (99%)	89 (85%)	16 (15%)	3	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	3	21
9	CJ	86/90 (96%)	75 (87%)	11 (13%)	4	24
10	AK	90/98 (92%)	76 (84%)	14 (16%)	2	17
10	CK	90/98 (92%)	77 (86%)	13 (14%)	3	20
11	AL	103/103 (100%)	92 (89%)	11 (11%)	6	32
11	CL	103/103 (100%)	92 (89%)	11 (11%)	6	32
12	AM	92/95 (97%)	79 (86%)	13 (14%)	3	21
12	CM	91/95 (96%)	79 (87%)	12 (13%)	4	23
13	AN	79/83 (95%)	64 (81%)	15 (19%)	1	9
13	CN	79/83 (95%)	64 (81%)	15 (19%)	1	9
14	AO	76/77 (99%)	69 (91%)	7 (9%)	9	38
14	CO	76/77 (99%)	69 (91%)	7 (9%)	9	38
15	AP	65/65 (100%)	59 (91%)	6 (9%)	9	38
15	CP	65/65 (100%)	58 (89%)	7 (11%)	6	31
16	AQ	74/77 (96%)	59 (80%)	15 (20%)	1	7
16	CQ	75/77 (97%)	62 (83%)	13 (17%)	2	12
17	AR	48/64 (75%)	41 (85%)	7 (15%)	3	19
17	CR	48/64 (75%)	41 (85%)	7 (15%)	3	19
18	AS	70/78 (90%)	56 (80%)	14 (20%)	1	8
18	CS	71/78 (91%)	56 (79%)	15 (21%)	1	7
19	AT	65/65 (100%)	58 (89%)	7 (11%)	6	31
19	CT	65/65 (100%)	58 (89%)	7 (11%)	6	31
20	AB	180/198 (91%)	149 (83%)	31 (17%)	2	12
20	CB	180/198 (91%)	147 (82%)	33 (18%)	1	9
21	AU	44/60 (73%)	33 (75%)	11 (25%)	0	4
21	CU	44/60 (73%)	33 (75%)	11 (25%)	0	4
24	BI	109/109 (100%)	107 (98%)	2 (2%)	59	81
24	DI	109/109 (100%)	103 (94%)	6 (6%)	21	56
25	BC	216/217 (100%)	182 (84%)	34 (16%)	2	17
25	DC	216/217 (100%)	183 (85%)	33 (15%)	2	18
26	BD	164/164 (100%)	139 (85%)	25 (15%)	3	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	DD	164/164 (100%)	138 (84%)	26 (16%)	2	15
27	BK	102/104 (98%)	77 (76%)	25 (24%)	0	4
27	DK	102/104 (98%)	77 (76%)	25 (24%)	0	4
28	BP	99/99 (100%)	81 (82%)	18 (18%)	1	10
28	DP	99/99 (100%)	81 (82%)	18 (18%)	1	10
29	BE	165/165 (100%)	144 (87%)	21 (13%)	4	24
29	DE	165/165 (100%)	144 (87%)	21 (13%)	4	24
30	BY	48/48 (100%)	37 (77%)	11 (23%)	1	5
30	DY	48/48 (100%)	37 (77%)	11 (23%)	1	5
31	B0	47/47 (100%)	38 (81%)	9 (19%)	1	8
31	D0	47/47 (100%)	38 (81%)	9 (19%)	1	8
32	B4	34/34 (100%)	28 (82%)	6 (18%)	2	11
32	D4	34/34 (100%)	28 (82%)	6 (18%)	2	11
33	B1	45/48 (94%)	36 (80%)	9 (20%)	1	8
33	D1	45/48 (94%)	37 (82%)	8 (18%)	2	10
34	B3	51/51 (100%)	46 (90%)	5 (10%)	8	35
34	D3	51/51 (100%)	46 (90%)	5 (10%)	8	35
35	BV	78/78 (100%)	63 (81%)	15 (19%)	1	8
35	DV	78/78 (100%)	63 (81%)	15 (19%)	1	8
36	B2	38/38 (100%)	31 (82%)	7 (18%)	1	9
36	D2	38/38 (100%)	31 (82%)	7 (18%)	1	9
37	BL	102/103 (99%)	91 (89%)	11 (11%)	6	31
37	DL	102/103 (99%)	91 (89%)	11 (11%)	6	31
38	BM	109/109 (100%)	92 (84%)	17 (16%)	2	17
38	DM	109/109 (100%)	93 (85%)	16 (15%)	3	19
39	BX	55/55 (100%)	49 (89%)	6 (11%)	6	31
39	DX	55/55 (100%)	49 (89%)	6 (11%)	6	31
40	BH	114/114 (100%)	86 (75%)	28 (25%)	0	4
40	DH	114/114 (100%)	91 (80%)	23 (20%)	1	7
41	BJ	116/116 (100%)	98 (84%)	18 (16%)	2	17
41	DJ	116/116 (100%)	98 (84%)	18 (16%)	2	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BN	100/103 (97%)	85 (85%)	15 (15%)	3	19
42	DN	100/103 (97%)	86 (86%)	14 (14%)	3	21
43	BO	86/87 (99%)	68 (79%)	18 (21%)	1	7
43	DO	86/87 (99%)	68 (79%)	18 (21%)	1	7
44	BQ	89/89 (100%)	81 (91%)	8 (9%)	9	38
44	DQ	89/89 (100%)	80 (90%)	9 (10%)	7	34
45	BS	93/93 (100%)	78 (84%)	15 (16%)	2	15
45	DS	93/93 (100%)	76 (82%)	17 (18%)	1	9
46	BU	83/84 (99%)	68 (82%)	15 (18%)	1	10
46	DU	83/84 (99%)	68 (82%)	15 (18%)	1	10
47	BF	149/149 (100%)	117 (78%)	32 (22%)	1	6
47	DF	149/149 (100%)	116 (78%)	33 (22%)	1	6
48	BG	137/137 (100%)	113 (82%)	24 (18%)	2	11
48	DG	137/137 (100%)	113 (82%)	24 (18%)	2	11
49	BR	84/84 (100%)	71 (84%)	13 (16%)	2	17
49	DR	84/84 (100%)	71 (84%)	13 (16%)	2	17
50	BT	80/84 (95%)	69 (86%)	11 (14%)	3	21
50	DT	80/84 (95%)	68 (85%)	12 (15%)	3	19
51	BZ	67/68 (98%)	53 (79%)	14 (21%)	1	7
51	DZ	67/68 (98%)	54 (81%)	13 (19%)	1	8
52	BW	59/62 (95%)	44 (75%)	15 (25%)	0	4
52	DW	59/62 (95%)	44 (75%)	15 (25%)	0	4
All	All	9333/9700 (96%)	7889 (84%)	1444 (16%)	2	17

5 of 1444 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BG	54	ARG
6	CG	109	LYS
47	DF	2	LYS
49	BR	4	VAL
2	CC	41	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 326 such sidechains are listed below:

Mol	Chain	Res	Type
47	BF	126	ASN
7	CH	3	GLN
45	DS	40	ASN
48	BG	63	GLN
2	CC	31	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	246 (16%)	21 (1%)
1	CA	1529/1542 (99%)	231 (15%)	19 (1%)
22	BA	116/120 (96%)	16 (13%)	0
22	DA	116/120 (96%)	14 (12%)	0
23	BB	2837/2904 (97%)	424 (14%)	20 (0%)
23	DB	2837/2904 (97%)	424 (14%)	21 (0%)
All	All	8964/9132 (98%)	1355 (15%)	81 (0%)

5 of 1355 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 81 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2756	U
1	CA	279	A
23	DB	2336	A
23	BB	2798	U
1	CA	51	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 353 ligands modelled in this entry, 345 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	LLL	AA	2063	-	29,33,33	2.37	12 (41%)	34,49,49	1.34	3 (8%)
54	LLL	BB	3111	-	29,33,33	2.37	12 (41%)	34,49,49	1.22	4 (11%)
54	LLL	AA	2062	-	29,33,33	2.41	15 (51%)	34,49,49	1.27	4 (11%)
54	LLL	CA	2063	-	29,33,33	2.42	13 (44%)	34,49,49	1.24	3 (8%)
54	LLL	AA	2061	-	29,33,33	2.32	10 (34%)	34,49,49	1.28	4 (11%)
54	LLL	CA	2064	-	29,33,33	2.28	11 (37%)	34,49,49	1.20	3 (8%)
54	LLL	DB	3112	-	29,33,33	2.37	12 (41%)	34,49,49	1.19	3 (8%)
54	LLL	CA	2062	-	29,33,33	2.34	12 (41%)	34,49,49	1.20	3 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	LLL	AA	2063	-	-	2/11/65/65	0/3/3/3
54	LLL	BB	3111	-	-	2/11/65/65	0/3/3/3
54	LLL	AA	2062	-	-	2/11/65/65	0/3/3/3
54	LLL	CA	2063	-	-	4/11/65/65	0/3/3/3
54	LLL	AA	2061	-	-	1/11/65/65	0/3/3/3
54	LLL	CA	2064	-	-	1/11/65/65	0/3/3/3
54	LLL	DB	3112	-	-	1/11/65/65	0/3/3/3
54	LLL	CA	2062	-	-	1/11/65/65	0/3/3/3

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CA	2063	LLL	O53-C53	6.49	1.52	1.43
54	AA	2062	LLL	O53-C53	6.38	1.52	1.43
54	DB	3112	LLL	O53-C53	6.35	1.52	1.43
54	BB	3111	LLL	O53-C53	6.33	1.52	1.43
54	AA	2061	LLL	O53-C53	6.28	1.52	1.43

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AA	2063	LLL	C53-O53-C13	4.34	118.52	111.53
54	CA	2063	LLL	C53-O53-C13	4.05	118.06	111.53
54	AA	2062	LLL	C53-O53-C13	3.95	117.90	111.53
54	CA	2062	LLL	C53-O53-C13	3.92	117.85	111.53
54	BB	3111	LLL	C53-O53-C13	3.87	117.76	111.53

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	AA	2063	LLL	C23-C33-N33-C93
54	DB	3112	LLL	C23-C33-N33-C93
54	AA	2061	LLL	C23-C33-N33-C93
54	CA	2062	LLL	C23-C33-N33-C93
54	AA	2062	LLL	C23-C33-N33-C93

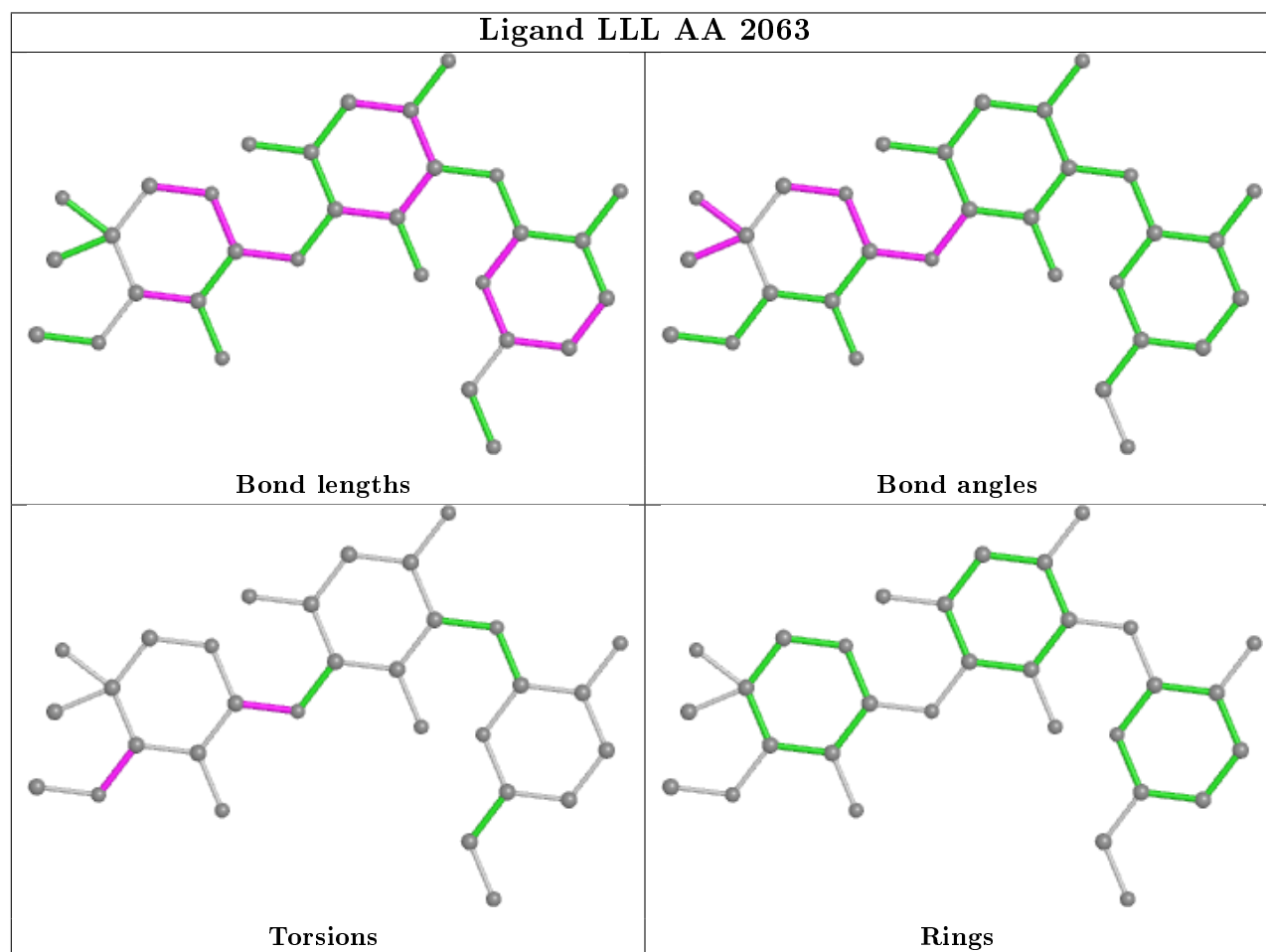
There are no ring outliers.

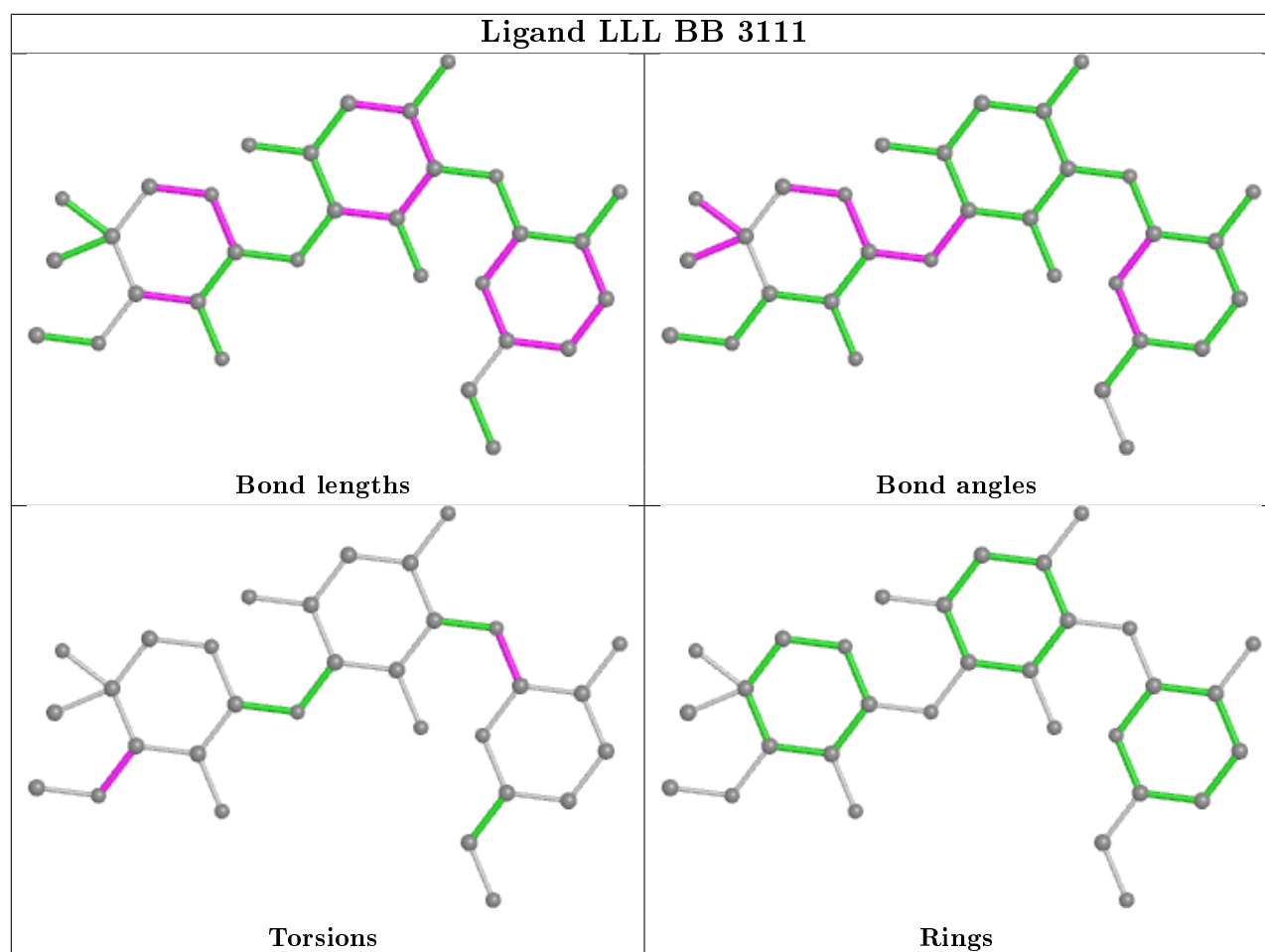
5 monomers are involved in 12 short contacts:

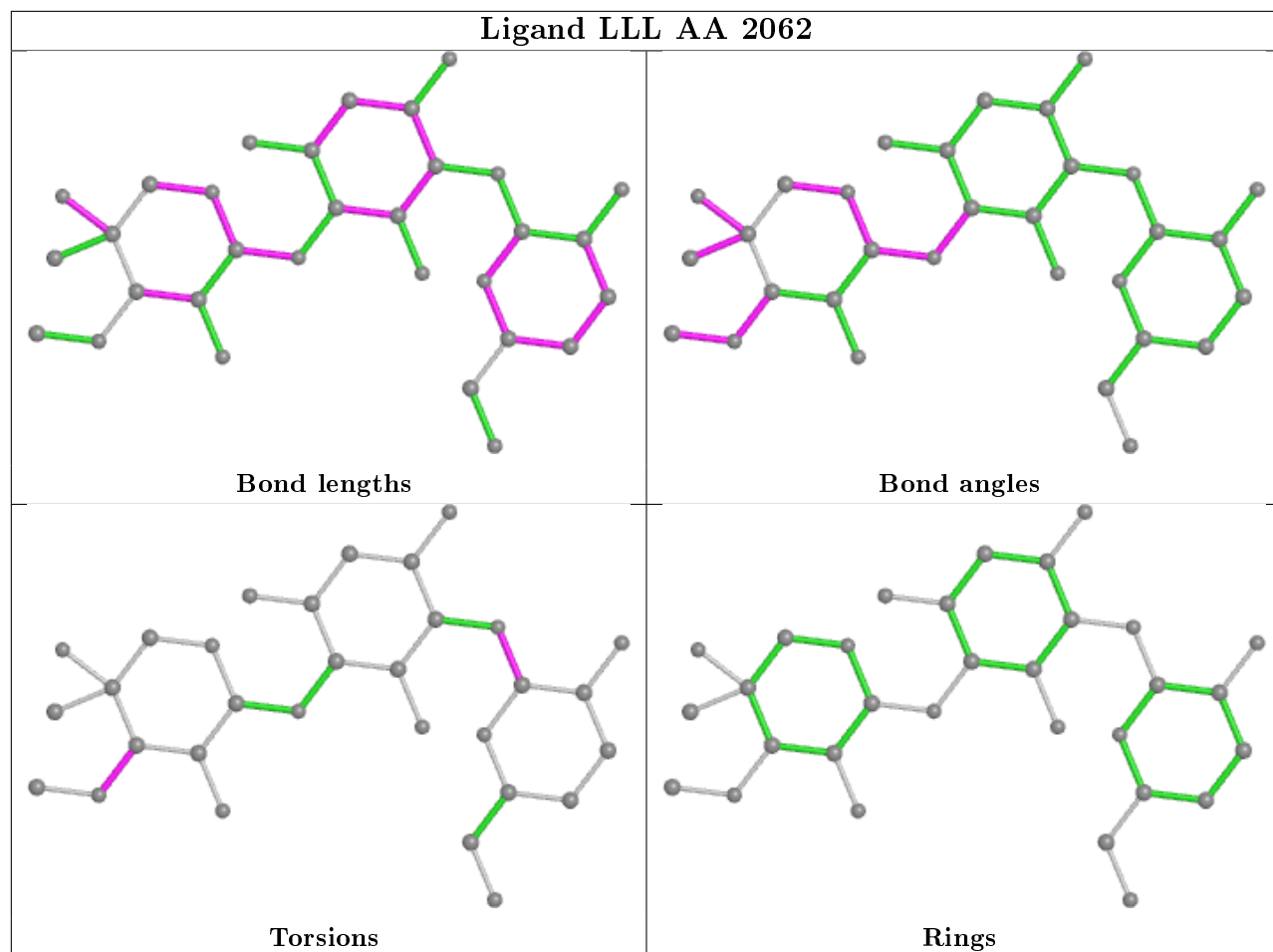
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	AA	2063	LLL	3	0
54	BB	3111	LLL	1	0
54	AA	2062	LLL	2	0
54	AA	2061	LLL	1	0
54	CA	2062	LLL	5	0

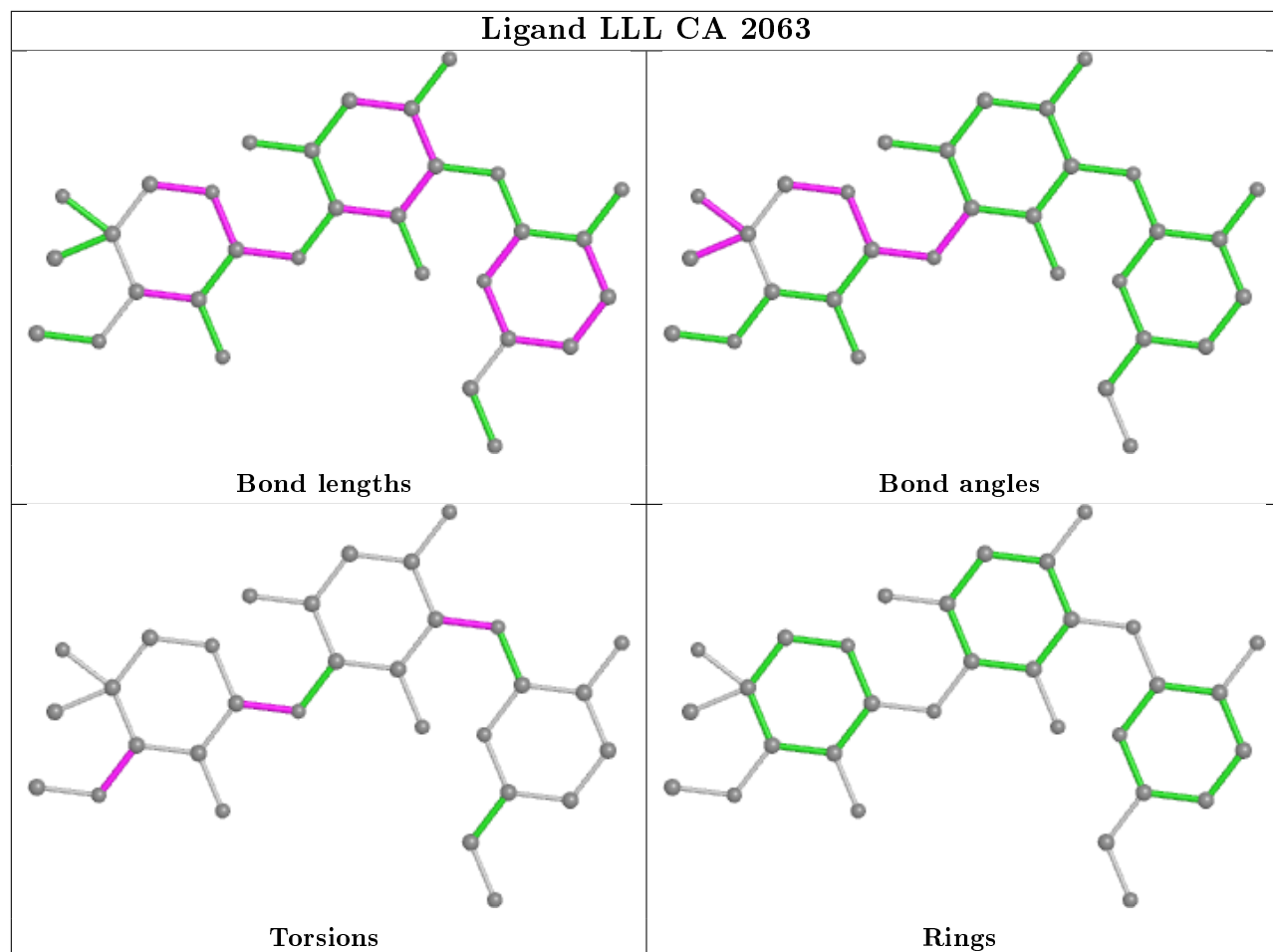
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

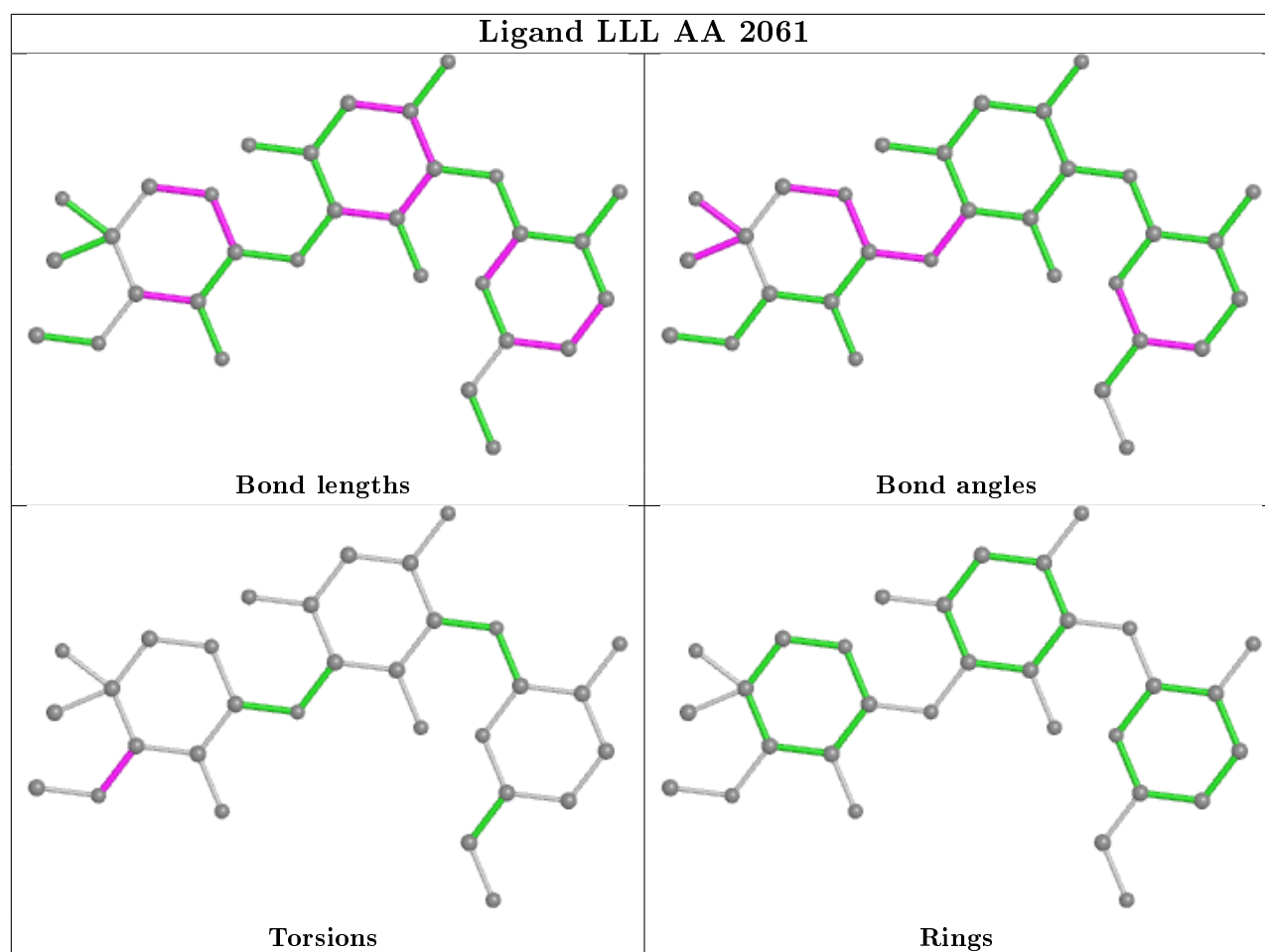
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

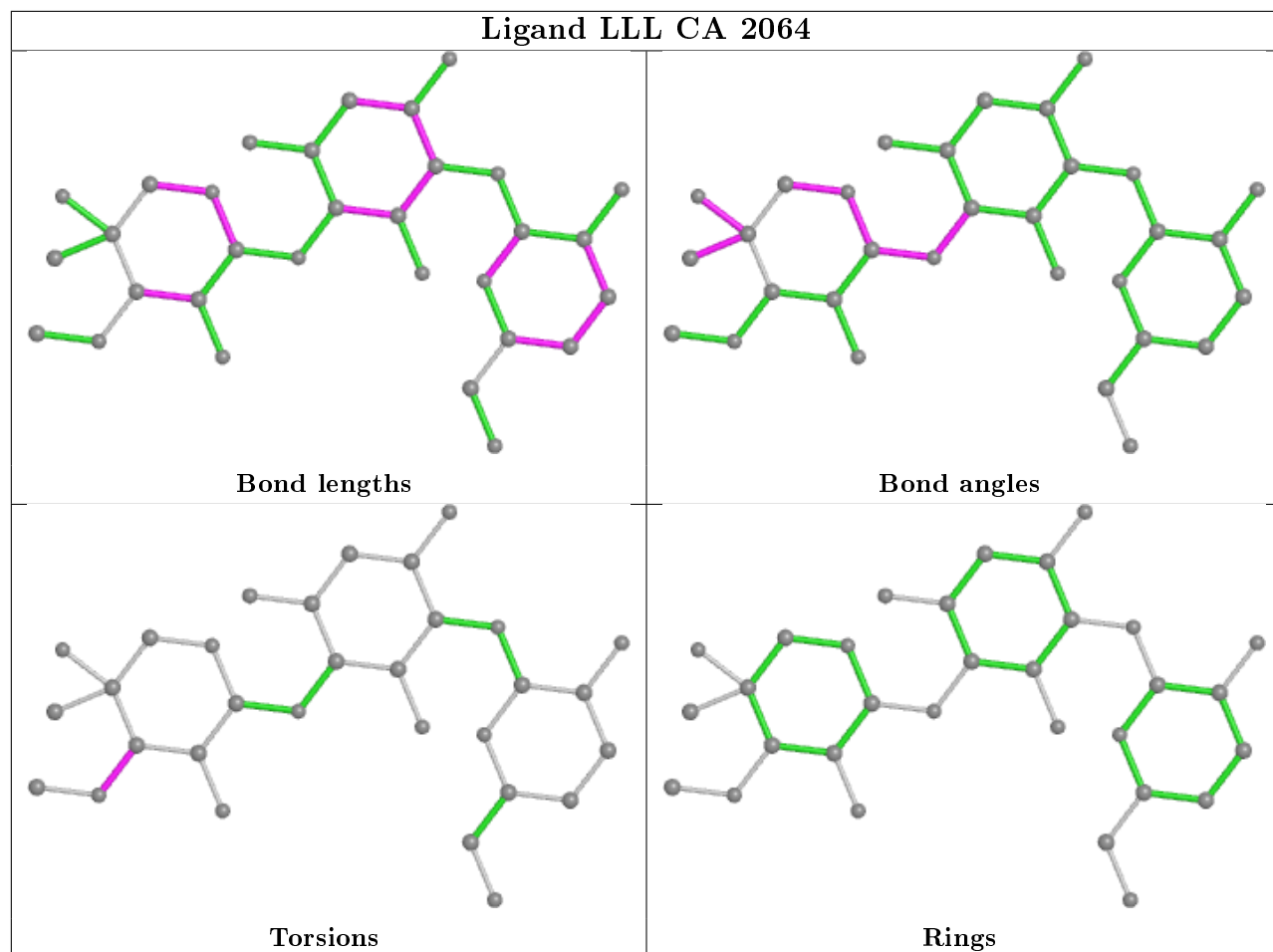


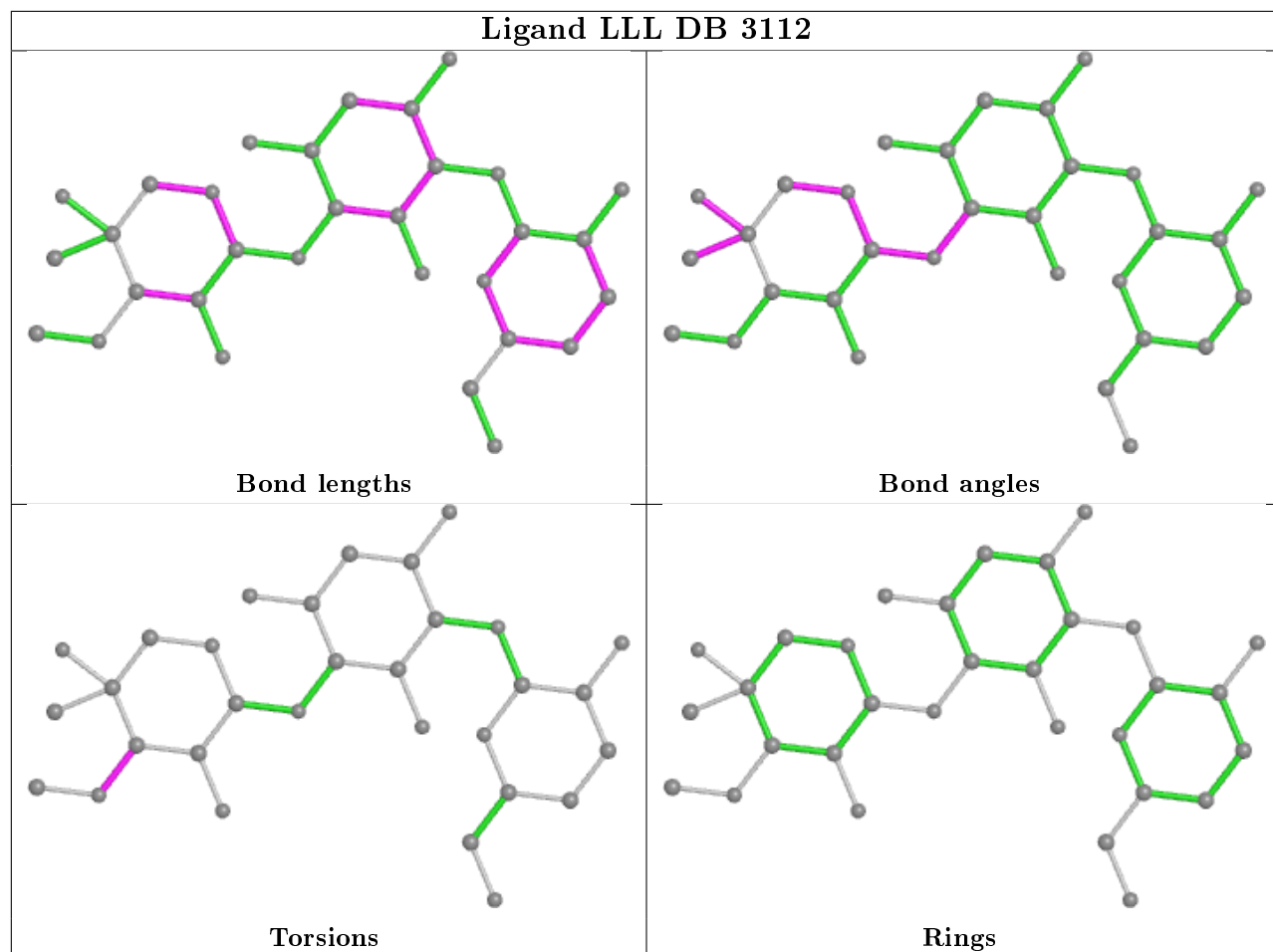


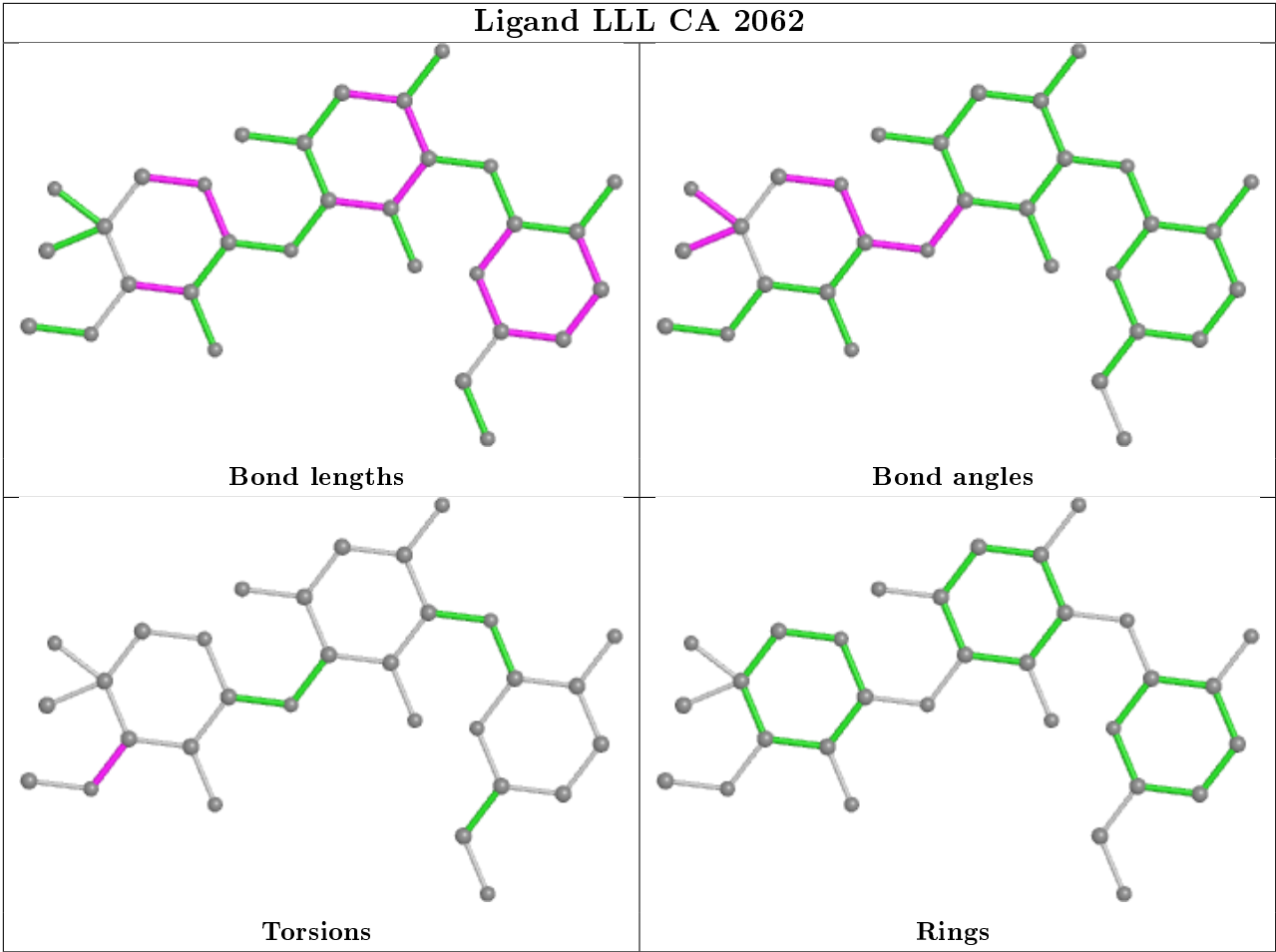












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	BB	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BB	2322:A	O3'	2323:G	P	1.78

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%)	-0.59	8 (0%)	91 84	22, 85, 131, 156	0
1	CA	1530/1542 (99%)	-0.60	3 (0%)	95 91	5, 60, 120, 167	0
2	AC	206/232 (88%)	0.03	3 (1%)	73 61	14, 72, 111, 136	0
2	CC	206/232 (88%)	0.14	13 (6%)	20 14	5, 74, 103, 160	0
3	AD	205/205 (100%)	0.97	40 (19%)	1 1	21, 87, 115, 135	0
3	CD	205/205 (100%)	0.31	13 (6%)	20 14	8, 65, 107, 121	0
4	AE	150/166 (90%)	0.35	11 (7%)	15 11	6, 74, 105, 134	0
4	CE	150/166 (90%)	0.86	24 (16%)	1 2	5, 59, 96, 125	0
5	AF	100/135 (74%)	1.71	46 (46%)	0 0	22, 72, 115, 148	0
5	CF	100/135 (74%)	1.13	20 (20%)	1 0	12, 72, 109, 123	0
6	AG	150/178 (84%)	0.28	20 (13%)	3 3	47, 89, 116, 152	0
6	CG	152/178 (85%)	-0.13	3 (1%)	65 52	29, 80, 115, 134	0
7	AH	129/129 (100%)	0.50	18 (13%)	2 3	31, 80, 112, 136	0
7	CH	129/129 (100%)	0.42	13 (10%)	7 6	5, 56, 91, 112	0
8	AI	127/129 (98%)	0.49	20 (15%)	2 2	31, 83, 118, 143	0
8	CI	127/129 (98%)	0.01	2 (1%)	72 59	35, 84, 118, 157	0
9	AJ	98/103 (95%)	0.43	6 (6%)	21 15	22, 87, 121, 135	0
9	CJ	98/103 (95%)	0.40	12 (12%)	4 4	33, 84, 110, 125	0
10	AK	117/128 (91%)	0.47	7 (5%)	21 15	5, 67, 102, 117	0
10	CK	117/128 (91%)	-0.06	4 (3%)	45 33	5, 56, 101, 119	0
11	AL	123/123 (100%)	0.52	15 (12%)	4 4	22, 75, 110, 146	0
11	CL	123/123 (100%)	0.31	4 (3%)	46 34	5, 47, 103, 123	0
12	AM	114/117 (97%)	0.15	3 (2%)	56 42	58, 96, 124, 147	0
12	CM	113/117 (96%)	0.22	8 (7%)	16 12	48, 89, 116, 135	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%)	0.05	2 (2%) 63 50	27, 85, 121, 154	0
13	CN	96/100 (96%)	0.08	6 (6%) 20 14	40, 87, 114, 142	0
14	AO	88/89 (98%)	0.52	6 (6%) 17 13	38, 80, 109, 133	0
14	CO	88/89 (98%)	0.32	4 (4%) 33 24	5, 56, 107, 128	0
15	AP	82/82 (100%)	0.75	9 (10%) 5 5	48, 88, 121, 135	0
15	CP	80/82 (97%)	0.18	5 (6%) 20 14	11, 59, 109, 147	0
16	AQ	80/83 (96%)	0.72	11 (13%) 2 3	31, 87, 117, 124	0
16	CQ	81/83 (97%)	0.07	0 100 100	9, 58, 99, 121	0
17	AR	55/74 (74%)	0.79	6 (10%) 5 5	19, 76, 118, 138	0
17	CR	55/74 (74%)	0.91	10 (18%) 1 1	19, 68, 119, 131	0
18	AS	79/91 (86%)	0.82	12 (15%) 2 2	68, 100, 124, 136	0
18	CS	80/91 (87%)	0.14	5 (6%) 20 14	48, 94, 127, 153	0
19	AT	85/86 (98%)	0.20	2 (2%) 59 45	39, 92, 123, 144	0
19	CT	85/86 (98%)	0.04	3 (3%) 44 32	19, 61, 106, 125	0
20	AB	218/240 (90%)	0.79	32 (14%) 2 2	20, 87, 113, 132	0
20	CB	218/240 (90%)	1.16	53 (24%) 0 0	29, 89, 118, 144	0
21	AU	51/70 (72%)	0.74	6 (11%) 4 4	36, 89, 126, 134	0
21	CU	51/70 (72%)	0.32	6 (11%) 4 4	46, 78, 116, 132	0
22	BA	117/120 (97%)	-0.65	2 (1%) 70 57	47, 78, 117, 140	0
22	DA	117/120 (97%)	-0.55	2 (1%) 70 57	30, 80, 115, 155	0
23	BB	2841/2904 (97%)	-0.30	34 (1%) 79 67	9, 58, 127, 165	0
23	DB	2841/2904 (97%)	-0.31	14 (0%) 91 84	5, 45, 124, 163	0
24	BI	141/141 (100%)	2.36	74 (52%) 0 0	59, 117, 149, 158	0
24	DI	141/141 (100%)	0.89	17 (12%) 4 4	70, 117, 148, 160	0
25	BC	271/272 (99%)	0.73	25 (9%) 9 7	5, 47, 88, 105	0
25	DC	271/272 (99%)	0.70	25 (9%) 9 7	5, 32, 80, 112	0
26	BD	209/209 (100%)	0.65	28 (13%) 3 3	12, 71, 107, 141	0
26	DD	209/209 (100%)	0.57	27 (12%) 3 3	5, 49, 98, 135	0
27	BK	121/123 (98%)	1.37	32 (26%) 0 0	16, 67, 106, 134	0
27	DK	121/123 (98%)	0.54	3 (2%) 57 43	5, 37, 90, 130	0
28	BP	114/114 (100%)	1.20	30 (26%) 0 0	25, 81, 113, 131	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%)	0.33	3 (2%) 56 42	7, 49, 94, 112	0
29	BE	201/201 (100%)	0.78	32 (15%) 1 2	5, 65, 104, 147	0
29	DE	201/201 (100%)	0.42	19 (9%) 8 6	5, 62, 107, 138	0
30	BY	58/58 (100%)	0.59	6 (10%) 6 6	26, 69, 107, 137	0
30	DY	58/58 (100%)	0.12	3 (5%) 27 20	6, 64, 110, 117	0
31	B0	56/56 (100%)	0.57	6 (10%) 6 5	5, 71, 113, 136	0
31	D0	56/56 (100%)	0.06	0 100 100	10, 43, 99, 104	0
32	B4	38/38 (100%)	0.71	4 (10%) 6 6	33, 76, 108, 125	0
32	D4	38/38 (100%)	-0.26	0 100 100	15, 65, 94, 105	0
33	B1	50/54 (92%)	1.84	17 (34%) 0 0	50, 75, 102, 115	0
33	D1	50/54 (92%)	1.26	9 (18%) 1 1	27, 74, 105, 118	0
34	B3	64/64 (100%)	0.55	6 (9%) 8 6	9, 55, 82, 106	0
34	D3	64/64 (100%)	0.57	8 (12%) 3 4	5, 39, 84, 101	0
35	BV	94/94 (100%)	0.20	7 (7%) 14 11	31, 86, 115, 129	0
35	DV	94/94 (100%)	0.43	8 (8%) 10 9	8, 79, 108, 125	0
36	B2	46/46 (100%)	0.39	3 (6%) 18 13	8, 40, 81, 113	0
36	D2	46/46 (100%)	0.12	2 (4%) 35 25	5, 28, 69, 113	0
37	BL	143/144 (99%)	0.38	7 (4%) 29 21	9, 63, 99, 134	0
37	DL	143/144 (99%)	0.81	28 (19%) 1 1	5, 55, 95, 123	0
38	BM	136/136 (100%)	0.75	14 (10%) 6 6	5, 65, 100, 131	0
38	DM	136/136 (100%)	0.39	7 (5%) 28 20	5, 55, 94, 134	0
39	BX	63/63 (100%)	1.04	14 (22%) 0 0	18, 76, 110, 123	0
39	DX	63/63 (100%)	0.09	2 (3%) 47 35	36, 82, 107, 142	0
40	BH	149/149 (100%)	2.55	71 (47%) 0 0	25, 98, 122, 146	0
40	DH	149/149 (100%)	1.00	24 (16%) 1 1	18, 88, 112, 141	0
41	BJ	142/142 (100%)	0.29	7 (4%) 29 21	16, 70, 106, 118	0
41	DJ	142/142 (100%)	0.28	5 (3%) 44 32	5, 60, 101, 131	0
42	BN	120/127 (94%)	0.47	10 (8%) 11 9	14, 65, 101, 145	0
42	DN	120/127 (94%)	0.09	2 (1%) 70 57	5, 42, 75, 118	0
43	BO	116/117 (99%)	0.73	20 (17%) 1 1	40, 78, 104, 128	0
43	DO	116/117 (99%)	-0.04	4 (3%) 45 33	5, 73, 106, 157	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%)	-0.24	2 (1%) 70 57	5, 60, 95, 109	0
44	DQ	117/117 (100%)	0.44	6 (5%) 28 20	5, 50, 92, 120	0
45	BS	110/110 (100%)	0.81	14 (12%) 3 4	6, 56, 98, 118	0
45	DS	110/110 (100%)	1.14	18 (16%) 1 1	5, 48, 95, 128	0
46	BU	102/103 (99%)	1.45	33 (32%) 0 0	9, 71, 105, 123	0
46	DU	102/103 (99%)	0.25	2 (1%) 65 52	34, 80, 112, 130	0
47	BF	178/178 (100%)	1.11	40 (22%) 0 0	40, 95, 125, 140	0
47	DF	178/178 (100%)	1.25	41 (23%) 0 0	38, 85, 125, 138	0
48	BG	176/176 (100%)	0.92	34 (19%) 1 1	37, 88, 114, 146	0
48	DG	176/176 (100%)	0.55	22 (12%) 3 4	17, 82, 110, 133	0
49	BR	103/103 (100%)	0.05	4 (3%) 39 28	13, 78, 112, 120	0
49	DR	103/103 (100%)	0.52	12 (11%) 4 4	15, 72, 111, 128	0
50	BT	93/100 (93%)	0.43	7 (7%) 14 11	14, 70, 112, 124	0
50	DT	93/100 (93%)	0.47	8 (8%) 10 8	8, 66, 108, 120	0
51	BZ	77/78 (98%)	0.56	4 (5%) 27 20	5, 54, 93, 115	0
51	DZ	77/78 (98%)	0.08	1 (1%) 77 65	5, 43, 87, 114	0
52	BW	79/84 (94%)	0.65	8 (10%) 7 6	8, 75, 111, 136	0
52	DW	79/84 (94%)	0.07	4 (5%) 28 20	12, 65, 103, 122	0
All	All	20417/21046 (97%)	0.15	1415 (6%) 16 13	5, 68, 120, 167	0

The worst 5 of 1415 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
40	BH	86	ASP	9.9
40	BH	93	SER	9.3
40	BH	45	GLU	9.2
40	BH	85	GLY	9.1
40	BH	142	VAL	8.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
53	MG	AA	2035	1/1	0.41	0.08	71,71,71,71	0
53	MG	DB	3059	1/1	0.43	0.47	100,100,100,100	0
53	MG	AA	2039	1/1	0.46	0.35	92,92,92,92	0
53	MG	BB	3100	1/1	0.49	0.20	105,105,105,105	0
53	MG	BB	3057	1/1	0.50	0.31	72,72,72,72	0
53	MG	AA	2056	1/1	0.55	0.23	103,103,103,103	0
53	MG	AA	2005	1/1	0.61	0.10	72,72,72,72	0
53	MG	AA	2023	1/1	0.63	0.51	44,44,44,44	1
53	MG	AA	2025	1/1	0.66	0.26	50,50,50,50	1
53	MG	BB	3042	1/1	0.67	0.08	96,96,96,96	0
53	MG	AA	2022	1/1	0.69	0.32	100,100,100,100	0
53	MG	DB	3095	1/1	0.70	0.13	96,96,96,96	0
53	MG	AA	2057	1/1	0.71	0.24	80,80,80,80	0
53	MG	CA	2026	1/1	0.74	0.38	40,40,40,40	1
53	MG	AA	2059	1/1	0.74	0.32	102,102,102,102	0
53	MG	AA	2030	1/1	0.74	0.07	88,88,88,88	0
53	MG	CA	2027	1/1	0.74	0.16	55,55,55,55	1
53	MG	BB	3043	1/1	0.76	0.20	86,86,86,86	0
53	MG	BB	3081	1/1	0.78	0.23	40,40,40,40	0
53	MG	AA	2037	1/1	0.78	0.55	87,87,87,87	0
54	LLL	AA	2062	31/31	0.78	0.37	73,73,73,73	31
53	MG	CA	2018	1/1	0.78	0.15	60,60,60,60	0
53	MG	AA	2014	1/1	0.79	0.07	72,72,72,72	0
53	MG	CA	2036	1/1	0.79	0.06	74,74,74,74	0
53	MG	DB	3013	1/1	0.79	0.18	37,37,37,37	0
54	LLL	AA	2063	31/31	0.80	0.39	62,62,62,62	31
53	MG	AA	2012	1/1	0.80	0.07	70,70,70,70	0
53	MG	DB	3030	1/1	0.80	0.28	26,26,26,26	0
53	MG	DB	3060	1/1	0.80	0.11	79,79,79,79	0
53	MG	AA	2049	1/1	0.80	0.07	93,93,93,93	0
53	MG	AA	2055	1/1	0.81	0.06	57,57,57,57	0
53	MG	AA	2019	1/1	0.82	0.16	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	CA	2043	1/1	0.83	0.07	31,31,31,31	0
53	MG	CA	2035	1/1	0.83	0.08	85,85,85,85	0
53	MG	CA	2022	1/1	0.84	0.05	105,105,105,105	0
53	MG	BB	3010	1/1	0.84	0.11	73,73,73,73	0
53	MG	BB	3097	1/1	0.84	0.12	56,56,56,56	0
54	LLL	BB	3111	31/31	0.85	0.33	67,67,67,67	31
53	MG	DB	3057	1/1	0.85	0.08	53,53,53,53	0
53	MG	BB	3023	1/1	0.85	0.13	11,11,11,11	0
53	MG	BB	3078	1/1	0.85	0.30	67,67,67,67	0
53	MG	BB	3077	1/1	0.86	0.10	44,44,44,44	0
53	MG	AA	2015	1/1	0.86	0.20	78,78,78,78	0
53	MG	BB	3095	1/1	0.86	0.14	59,59,59,59	0
53	MG	BB	3038	1/1	0.86	0.12	77,77,77,77	0
53	MG	AA	2047	1/1	0.86	0.46	73,73,73,73	0
53	MG	DB	3092	1/1	0.87	0.14	76,76,76,76	0
53	MG	CA	2052	1/1	0.87	0.10	66,66,66,66	0
54	LLL	DB	3112	31/31	0.87	0.36	54,54,54,54	0
53	MG	DB	3111	1/1	0.87	0.20	43,43,43,43	0
53	MG	AA	2017	1/1	0.87	0.07	76,76,76,76	0
53	MG	DB	3058	1/1	0.87	0.79	96,96,96,96	0
53	MG	CA	2008	1/1	0.87	0.07	86,86,86,86	0
53	MG	AA	2032	1/1	0.88	0.12	67,67,67,67	0
53	MG	BB	3033	1/1	0.88	0.55	90,90,90,90	0
53	MG	AA	2042	1/1	0.88	0.08	28,28,28,28	0
53	MG	AA	2036	1/1	0.88	0.06	62,62,62,62	0
54	LLL	CA	2063	31/31	0.88	0.24	70,70,70,70	0
53	MG	AA	2024	1/1	0.88	0.13	73,73,73,73	0
54	LLL	CA	2064	31/31	0.88	0.28	41,41,41,41	31
53	MG	BB	3093	1/1	0.88	0.30	80,80,80,80	0
53	MG	AA	2002	1/1	0.89	0.32	100,100,100,100	0
53	MG	CA	2014	1/1	0.89	0.05	72,72,72,72	0
53	MG	DB	3034	1/1	0.89	0.20	74,74,74,74	0
53	MG	BB	3094	1/1	0.89	0.12	69,69,69,69	0
53	MG	AA	2034	1/1	0.89	0.06	42,42,42,42	0
53	MG	AA	2046	1/1	0.89	0.11	95,95,95,95	0
53	MG	DB	3023	1/1	0.89	0.06	13,13,13,13	0
53	MG	AA	2013	1/1	0.89	0.04	70,70,70,70	0
53	MG	AA	2053	1/1	0.89	0.16	58,58,58,58	0
53	MG	AA	2031	1/1	0.89	0.13	49,49,49,49	0
53	MG	BB	3024	1/1	0.89	0.05	21,21,21,21	0
53	MG	BB	3027	1/1	0.89	0.10	24,24,24,24	0
53	MG	CA	2015	1/1	0.90	0.06	108,108,108,108	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	CA	2009	1/1	0.90	0.05	84,84,84,84	0
53	MG	DB	3097	1/1	0.90	0.19	42,42,42,42	0
53	MG	CA	2042	1/1	0.90	0.09	66,66,66,66	0
53	MG	AA	2050	1/1	0.90	0.05	103,103,103,103	0
53	MG	BB	3004	1/1	0.90	0.05	43,43,43,43	0
53	MG	AA	2011	1/1	0.90	0.08	41,41,41,41	0
55	ZN	B4	101	1/1	0.90	0.08	82,82,82,82	0
53	MG	BB	3099	1/1	0.90	0.10	56,56,56,56	0
53	MG	DB	3032	1/1	0.90	0.10	45,45,45,45	0
53	MG	AA	2051	1/1	0.90	0.22	66,66,66,66	0
53	MG	BB	3079	1/1	0.90	0.14	52,52,52,52	0
53	MG	AA	2007	1/1	0.90	0.09	70,70,70,70	0
53	MG	BB	3061	1/1	0.90	0.06	45,45,45,45	0
53	MG	DB	3009	1/1	0.90	0.08	5,5,5,5	0
53	MG	BB	3052	1/1	0.90	0.09	26,26,26,26	0
53	MG	AA	2058	1/1	0.90	0.07	94,94,94,94	0
53	MG	CA	2037	1/1	0.91	0.08	69,69,69,69	0
53	MG	BB	3107	1/1	0.91	0.12	41,41,41,41	0
53	MG	CA	2057	1/1	0.91	0.05	61,61,61,61	0
53	MG	BB	3030	1/1	0.91	0.05	53,53,53,53	0
53	MG	DB	3107	1/1	0.91	0.08	15,15,15,15	0
53	MG	DB	3022	1/1	0.91	0.07	23,23,23,23	0
53	MG	DB	3066	1/1	0.91	0.31	100,100,100,100	0
53	MG	DB	3045	1/1	0.91	0.08	66,66,66,66	0
53	MG	DB	3015	1/1	0.91	0.10	50,50,50,50	0
53	MG	DB	3052	1/1	0.91	0.17	62,62,62,62	0
53	MG	CA	2011	1/1	0.92	0.08	82,82,82,82	0
53	MG	DB	3099	1/1	0.92	0.18	5,5,5,5	0
53	MG	BB	3088	1/1	0.92	0.08	26,26,26,26	0
53	MG	BB	3063	1/1	0.92	0.18	51,51,51,51	0
53	MG	DB	3087	1/1	0.92	0.23	63,63,63,63	0
53	MG	CA	2020	1/1	0.92	0.52	85,85,85,85	0
53	MG	BB	3036	1/1	0.92	0.14	57,57,57,57	0
53	MG	BB	3022	1/1	0.92	0.19	44,44,44,44	0
53	MG	CA	2056	1/1	0.92	0.09	32,32,32,32	0
53	MG	DB	3055	1/1	0.92	0.18	11,11,11,11	0
53	MG	DB	3004	1/1	0.92	0.20	21,21,21,21	0
53	MG	AA	2026	1/1	0.92	0.13	51,51,51,51	1
53	MG	BB	3013	1/1	0.93	0.12	41,41,41,41	0
53	MG	BB	3032	1/1	0.93	0.14	36,36,36,36	0
53	MG	AA	2060	1/1	0.93	0.11	46,46,46,46	0
53	MG	BB	3062	1/1	0.93	0.18	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	BB	3110	1/1	0.93	0.14	74,74,74,74	0
53	MG	CA	2029	1/1	0.93	0.17	57,57,57,57	1
53	MG	DB	3033	1/1	0.93	0.11	18,18,18,18	0
53	MG	DB	3110	1/1	0.93	0.18	29,29,29,29	0
53	MG	BB	3026	1/1	0.93	0.10	24,24,24,24	0
53	MG	CA	2053	1/1	0.93	0.09	51,51,51,51	0
53	MG	AA	2018	1/1	0.93	0.10	76,76,76,76	0
53	MG	DB	3061	1/1	0.93	0.14	58,58,58,58	0
53	MG	BB	3051	1/1	0.93	0.12	43,43,43,43	0
53	MG	CA	2038	1/1	0.93	0.17	77,77,77,77	0
53	MG	DB	3074	1/1	0.93	0.11	5,5,5,5	0
53	MG	CA	2023	1/1	0.93	0.06	54,54,54,54	0
53	MG	DB	3072	1/1	0.93	0.07	25,25,25,25	0
53	MG	BB	3034	1/1	0.93	0.10	52,52,52,52	0
53	MG	BB	3082	1/1	0.93	0.16	5,5,5,5	0
53	MG	CA	2060	1/1	0.93	0.05	55,55,55,55	0
53	MG	DB	3042	1/1	0.93	0.13	22,22,22,22	0
53	MG	BB	3080	1/1	0.93	0.21	56,56,56,56	0
53	MG	BB	3102	1/1	0.93	0.10	16,16,16,16	0
53	MG	BB	3054	1/1	0.93	0.06	39,39,39,39	0
53	MG	BB	3085	1/1	0.93	0.19	59,59,59,59	0
53	MG	CA	2047	1/1	0.93	0.11	74,74,74,74	0
53	MG	DB	3029	1/1	0.94	0.06	66,66,66,66	0
53	MG	DB	3084	1/1	0.94	0.18	25,25,25,25	0
53	MG	AA	2054	1/1	0.94	0.06	66,66,66,66	0
53	MG	CA	2019	1/1	0.94	0.11	63,63,63,63	0
53	MG	DB	3010	1/1	0.94	0.10	14,14,14,14	0
53	MG	BB	3053	1/1	0.94	0.06	59,59,59,59	0
53	MG	BB	3065	1/1	0.94	0.11	44,44,44,44	0
53	MG	DB	3036	1/1	0.94	0.09	26,26,26,26	0
53	MG	DB	3037	1/1	0.94	0.21	5,5,5,5	0
53	MG	AA	2008	1/1	0.94	0.13	81,81,81,81	0
53	MG	DB	3090	1/1	0.94	0.18	57,57,57,57	0
53	MG	DB	3039	1/1	0.94	0.06	36,36,36,36	0
53	MG	BB	3098	1/1	0.94	0.18	43,43,43,43	0
53	MG	AA	2021	1/1	0.94	0.10	23,23,23,23	0
53	MG	BB	3005	1/1	0.94	0.15	5,5,5,5	0
53	MG	BB	3008	1/1	0.94	0.07	80,80,80,80	0
53	MG	DB	3006	1/1	0.94	0.10	5,5,5,5	0
53	MG	CA	2059	1/1	0.94	0.17	51,51,51,51	0
53	MG	BB	3055	1/1	0.94	0.17	40,40,40,40	0
53	MG	BB	3035	1/1	0.94	0.08	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	DB	3035	1/1	0.94	0.08	54,54,54,54	0
54	LLL	AA	2061	31/31	0.94	0.29	20,20,20,20	0
53	MG	DB	3043	1/1	0.95	0.12	5,5,5,5	0
53	MG	BB	3104	1/1	0.95	0.15	18,18,18,18	0
53	MG	DB	3018	1/1	0.95	0.14	48,48,48,48	0
53	MG	BB	3089	1/1	0.95	0.17	63,63,63,63	0
53	MG	BB	3064	1/1	0.95	0.07	37,37,37,37	0
53	MG	BB	3029	1/1	0.95	0.07	5,5,5,5	0
53	MG	BB	3003	1/1	0.95	0.09	17,17,17,17	0
53	MG	CA	2028	1/1	0.95	0.05	77,77,77,77	0
53	MG	CA	2048	1/1	0.95	0.23	65,65,65,65	0
53	MG	BB	3068	1/1	0.95	0.07	37,37,37,37	0
53	MG	DB	3105	1/1	0.95	0.11	30,30,30,30	0
53	MG	DB	3053	1/1	0.95	0.06	66,66,66,66	0
53	MG	CA	2049	1/1	0.95	0.16	63,63,63,63	0
53	MG	BB	3037	1/1	0.95	0.10	29,29,29,29	0
53	MG	CA	2025	1/1	0.95	0.11	72,72,72,72	0
53	MG	CA	2054	1/1	0.95	0.08	91,91,91,91	0
53	MG	AA	2020	1/1	0.95	0.04	91,91,91,91	0
53	MG	BB	3066	1/1	0.95	0.10	37,37,37,37	0
54	LLL	CA	2062	31/31	0.95	0.21	9,9,9,9	0
53	MG	BB	3021	1/1	0.95	0.12	22,22,22,22	0
53	MG	AA	2041	1/1	0.95	0.10	57,57,57,57	0
53	MG	CA	2030	1/1	0.95	0.08	31,31,31,31	0
53	MG	AA	2045	1/1	0.95	0.10	48,48,48,48	0
53	MG	DB	3028	1/1	0.95	0.09	37,37,37,37	0
53	MG	DB	3050	1/1	0.95	0.07	73,73,73,73	0
53	MG	CA	2058	1/1	0.95	0.21	63,63,63,63	0
53	MG	DB	3108	1/1	0.95	0.08	5,5,5,5	0
53	MG	BB	3019	1/1	0.95	0.08	49,49,49,49	0
53	MG	AA	2048	1/1	0.95	0.11	48,48,48,48	0
53	MG	BB	3072	1/1	0.95	0.14	57,57,57,57	0
53	MG	BB	3101	1/1	0.95	0.09	11,11,11,11	0
53	MG	BB	3074	1/1	0.95	0.09	9,9,9,9	0
53	MG	CA	2021	1/1	0.95	0.11	70,70,70,70	0
53	MG	AA	2003	1/1	0.95	0.13	29,29,29,29	0
53	MG	AA	2027	1/1	0.95	0.18	56,56,56,56	0
53	MG	BB	3047	1/1	0.95	0.08	77,77,77,77	0
55	ZN	D4	101	1/1	0.95	0.08	45,45,45,45	0
53	MG	BB	3049	1/1	0.95	0.10	20,20,20,20	0
53	MG	BB	3096	1/1	0.95	0.12	44,44,44,44	0
53	MG	DB	3027	1/1	0.95	0.13	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	DB	3003	1/1	0.95	0.12	17,17,17,17	0
53	MG	CN	201	1/1	0.95	0.07	50,50,50,50	0
53	MG	BB	3091	1/1	0.95	0.15	34,34,34,34	0
53	MG	BB	3071	1/1	0.96	0.09	63,63,63,63	0
53	MG	DB	3005	1/1	0.96	0.17	6,6,6,6	0
53	MG	DB	3024	1/1	0.96	0.17	53,53,53,53	0
53	MG	DB	3083	1/1	0.96	0.17	56,56,56,56	0
53	MG	BB	3044	1/1	0.96	0.14	55,55,55,55	0
53	MG	CA	2007	1/1	0.96	0.11	47,47,47,47	0
53	MG	BB	3050	1/1	0.96	0.08	18,18,18,18	0
53	MG	BB	3067	1/1	0.96	0.07	40,40,40,40	0
53	MG	BB	3046	1/1	0.96	0.13	50,50,50,50	0
53	MG	DB	3048	1/1	0.96	0.07	36,36,36,36	0
53	MG	DB	3085	1/1	0.96	0.13	5,5,5,5	0
53	MG	DB	3021	1/1	0.96	0.16	5,5,5,5	0
53	MG	DB	3062	1/1	0.96	0.08	43,43,43,43	0
53	MG	BB	3108	1/1	0.96	0.10	12,12,12,12	0
53	MG	BB	3090	1/1	0.96	0.09	60,60,60,60	0
53	MG	CA	2061	1/1	0.96	0.06	25,25,25,25	0
53	MG	BB	3009	1/1	0.96	0.07	70,70,70,70	0
53	MG	AA	2001	1/1	0.96	0.08	27,27,27,27	0
53	MG	BB	3058	1/1	0.96	0.10	32,32,32,32	0
53	MG	DB	3051	1/1	0.96	0.18	57,57,57,57	0
53	MG	AA	2016	1/1	0.96	0.10	36,36,36,36	0
53	MG	DB	3068	1/1	0.96	0.13	5,5,5,5	0
53	MG	DB	3020	1/1	0.96	0.20	5,5,5,5	0
53	MG	BB	3073	1/1	0.96	0.21	33,33,33,33	0
53	MG	DB	3064	1/1	0.96	0.04	11,11,11,11	0
53	MG	DB	3016	1/1	0.96	0.07	17,17,17,17	0
53	MG	DB	3102	1/1	0.96	0.15	16,16,16,16	0
53	MG	DB	3101	1/1	0.96	0.26	26,26,26,26	0
53	MG	CA	2034	1/1	0.96	0.13	15,15,15,15	0
53	MG	BB	3087	1/1	0.96	0.24	73,73,73,73	0
53	MG	CA	2041	1/1	0.96	0.09	69,69,69,69	0
53	MG	DB	3080	1/1	0.96	0.09	5,5,5,5	0
53	MG	BB	3020	1/1	0.96	0.11	13,13,13,13	0
53	MG	DB	3071	1/1	0.96	0.10	34,34,34,34	0
53	MG	DB	3026	1/1	0.96	0.10	33,33,33,33	0
53	MG	DB	3089	1/1	0.97	0.29	52,52,52,52	0
53	MG	AA	2038	1/1	0.97	0.08	45,45,45,45	0
53	MG	BB	3006	1/1	0.97	0.09	19,19,19,19	0
53	MG	DB	3019	1/1	0.97	0.05	6,6,6,6	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	CA	2024	1/1	0.97	0.07	23,23,23,23	0
53	MG	BB	3069	1/1	0.97	0.07	5,5,5,5	0
53	MG	DB	3038	1/1	0.97	0.14	17,17,17,17	0
53	MG	DB	3054	1/1	0.97	0.08	13,13,13,13	0
53	MG	BB	3031	1/1	0.97	0.06	32,32,32,32	0
53	MG	BB	3040	1/1	0.97	0.20	40,40,40,40	0
53	MG	DB	3082	1/1	0.97	0.07	42,42,42,42	0
53	MG	CA	2010	1/1	0.97	0.07	59,59,59,59	0
53	MG	BB	3001	1/1	0.97	0.07	8,8,8,8	0
53	MG	DB	3078	1/1	0.97	0.09	48,48,48,48	0
53	MG	BB	3056	1/1	0.97	0.07	22,22,22,22	0
53	MG	CA	2016	1/1	0.97	0.12	10,10,10,10	0
53	MG	DB	3104	1/1	0.97	0.17	55,55,55,55	0
53	MG	DB	3086	1/1	0.97	0.19	24,24,24,24	0
53	MG	AA	2052	1/1	0.97	0.10	69,69,69,69	0
53	MG	DB	3056	1/1	0.97	0.11	5,5,5,5	0
53	MG	DB	3031	1/1	0.97	0.18	8,8,8,8	0
53	MG	CA	2031	1/1	0.97	0.10	37,37,37,37	0
53	MG	DB	3063	1/1	0.97	0.09	21,21,21,21	0
53	MG	BB	3017	1/1	0.97	0.06	16,16,16,16	0
53	MG	AA	2044	1/1	0.97	0.05	48,48,48,48	0
53	MG	DB	3070	1/1	0.97	0.09	43,43,43,43	0
53	MG	CA	2017	1/1	0.97	0.04	5,5,5,5	0
53	MG	BB	3011	1/1	0.97	0.23	21,21,21,21	0
53	MG	BB	3014	1/1	0.97	0.06	39,39,39,39	0
53	MG	BB	3039	1/1	0.97	0.14	35,35,35,35	0
53	MG	DB	3017	1/1	0.97	0.15	5,5,5,5	0
53	MG	BB	3075	1/1	0.97	0.19	33,33,33,33	0
53	MG	DB	3077	1/1	0.97	0.15	50,50,50,50	0
53	MG	BB	3070	1/1	0.97	0.15	24,24,24,24	0
53	MG	BB	3105	1/1	0.97	0.12	34,34,34,34	0
53	MG	AA	2006	1/1	0.97	0.05	57,57,57,57	0
53	MG	CA	2044	1/1	0.97	0.07	67,67,67,67	0
53	MG	BB	3002	1/1	0.98	0.07	5,5,5,5	0
53	MG	BB	3084	1/1	0.98	0.30	67,67,67,67	0
53	MG	AA	2029	1/1	0.98	0.14	50,50,50,50	0
53	MG	BB	3012	1/1	0.98	0.07	31,31,31,31	0
53	MG	AA	2033	1/1	0.98	0.04	69,69,69,69	0
53	MG	CA	2006	1/1	0.98	0.15	73,73,73,73	0
53	MG	CA	2001	1/1	0.98	0.05	5,5,5,5	0
53	MG	DB	3081	1/1	0.98	0.12	5,5,5,5	0
53	MG	BB	3059	1/1	0.98	0.09	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	DB	3069	1/1	0.98	0.19	21,21,21,21	0
53	MG	DB	3007	1/1	0.98	0.16	18,18,18,18	0
53	MG	DB	3012	1/1	0.98	0.17	14,14,14,14	0
53	MG	AA	2040	1/1	0.98	0.15	65,65,65,65	0
53	MG	BB	3083	1/1	0.98	0.18	33,33,33,33	0
53	MG	BB	3092	1/1	0.98	0.09	40,40,40,40	0
53	MG	DB	3046	1/1	0.98	0.10	5,5,5,5	0
53	MG	BB	3076	1/1	0.98	0.09	23,23,23,23	0
53	MG	DB	3091	1/1	0.98	0.26	45,45,45,45	0
53	MG	DB	3100	1/1	0.98	0.09	5,5,5,5	0
53	MG	DB	3065	1/1	0.98	0.16	16,16,16,16	0
53	MG	DB	3049	1/1	0.98	0.08	5,5,5,5	0
53	MG	DB	3094	1/1	0.98	0.04	14,14,14,14	0
53	MG	CA	2046	1/1	0.98	0.07	70,70,70,70	0
53	MG	CA	2013	1/1	0.98	0.13	48,48,48,48	0
53	MG	BB	3016	1/1	0.98	0.18	43,43,43,43	0
53	MG	DB	3073	1/1	0.98	0.10	33,33,33,33	0
53	MG	DB	3014	1/1	0.98	0.08	13,13,13,13	0
53	MG	DB	3011	1/1	0.98	0.21	35,35,35,35	0
53	MG	DB	3079	1/1	0.98	0.14	43,43,43,43	0
53	MG	DB	3106	1/1	0.98	0.17	37,37,37,37	0
53	MG	CA	2040	1/1	0.98	0.08	12,12,12,12	0
53	MG	CA	2039	1/1	0.98	0.14	19,19,19,19	0
53	MG	DB	3041	1/1	0.98	0.14	41,41,41,41	0
53	MG	DB	3096	1/1	0.98	0.17	5,5,5,5	0
53	MG	DB	3025	1/1	0.98	0.13	5,5,5,5	0
53	MG	DB	3093	1/1	0.98	0.19	7,7,7,7	0
53	MG	BB	3018	1/1	0.98	0.23	54,54,54,54	0
53	MG	DB	3040	1/1	0.98	0.13	5,5,5,5	0
53	MG	AA	2010	1/1	0.98	0.06	45,45,45,45	0
53	MG	AA	2028	1/1	0.98	0.08	53,53,53,53	0
53	MG	BB	3106	1/1	0.98	0.08	31,31,31,31	0
53	MG	BB	3041	1/1	0.98	0.12	18,18,18,18	0
53	MG	AA	2004	1/1	0.98	0.15	35,35,35,35	0
53	MG	CA	2055	1/1	0.98	0.09	31,31,31,31	0
53	MG	BB	3109	1/1	0.98	0.12	37,37,37,37	0
53	MG	AA	2043	1/1	0.98	0.09	44,44,44,44	0
53	MG	CA	2032	1/1	0.98	0.15	22,22,22,22	0
53	MG	CA	2051	1/1	0.98	0.07	38,38,38,38	0
53	MG	CA	2050	1/1	0.98	0.16	5,5,5,5	0
53	MG	BB	3045	1/1	0.98	0.07	19,19,19,19	0
53	MG	DB	3008	1/1	0.98	0.12	8,8,8,8	0

Continued on next page...

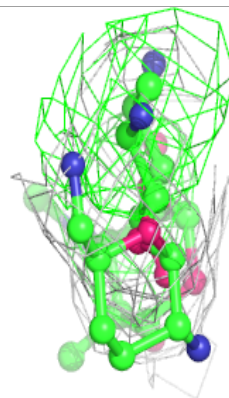
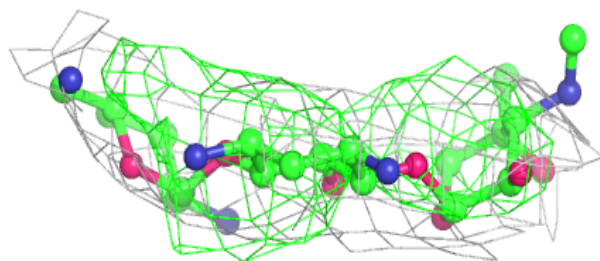
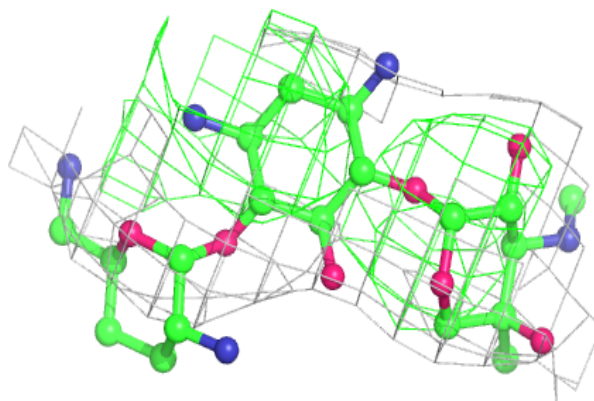
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	BB	3103	1/1	0.98	0.11	5,5,5,5	0
53	MG	DB	3044	1/1	0.98	0.06	18,18,18,18	0
53	MG	CA	2033	1/1	0.99	0.17	57,57,57,57	0
53	MG	DB	3098	1/1	0.99	0.22	23,23,23,23	0
53	MG	DB	3047	1/1	0.99	0.20	5,5,5,5	0
53	MG	CA	2002	1/1	0.99	0.12	27,27,27,27	0
53	MG	DB	3076	1/1	0.99	0.12	43,43,43,43	0
53	MG	DB	3075	1/1	0.99	0.08	41,41,41,41	0
53	MG	BB	3086	1/1	0.99	0.19	5,5,5,5	0
53	MG	CA	2045	1/1	0.99	0.16	77,77,77,77	0
53	MG	CA	2005	1/1	0.99	0.10	10,10,10,10	0
53	MG	CA	2012	1/1	0.99	0.08	49,49,49,49	0
53	MG	AA	2009	1/1	0.99	0.14	27,27,27,27	0
53	MG	CA	2003	1/1	0.99	0.08	44,44,44,44	0
53	MG	DB	3001	1/1	0.99	0.12	5,5,5,5	0
53	MG	BB	3060	1/1	0.99	0.19	59,59,59,59	0
53	MG	BB	3025	1/1	0.99	0.09	51,51,51,51	0
53	MG	CA	2004	1/1	0.99	0.05	13,13,13,13	0
53	MG	DB	3067	1/1	0.99	0.11	5,5,5,5	0
53	MG	BB	3048	1/1	0.99	0.04	22,22,22,22	0
53	MG	BB	3028	1/1	0.99	0.15	16,16,16,16	0
53	MG	DB	3103	1/1	0.99	0.08	7,7,7,7	0
53	MG	DB	3088	1/1	0.99	0.27	18,18,18,18	0
53	MG	DB	3109	1/1	0.99	0.10	28,28,28,28	0
53	MG	BB	3007	1/1	0.99	0.06	60,60,60,60	0
53	MG	DB	3002	1/1	0.99	0.13	12,12,12,12	0
53	MG	BB	3015	1/1	1.00	0.06	5,5,5,5	0

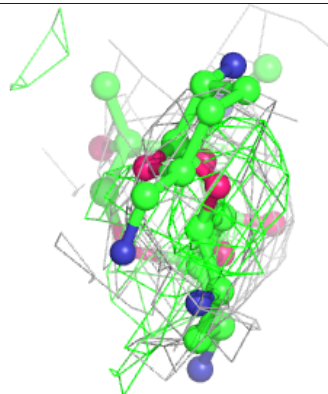
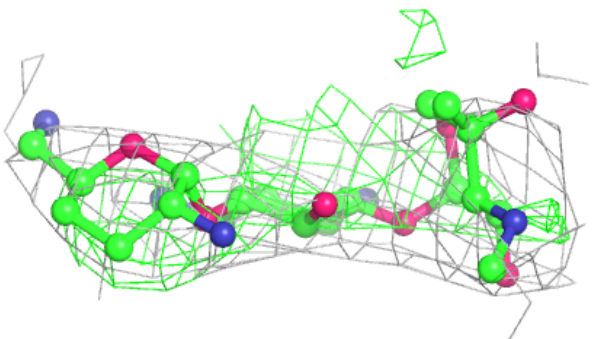
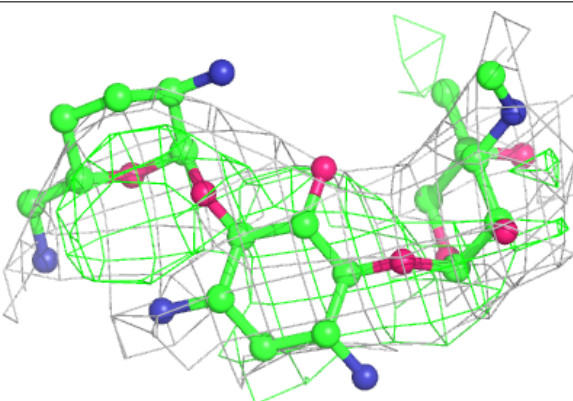
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LLL AA 2062:

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

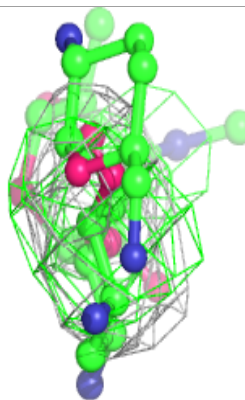
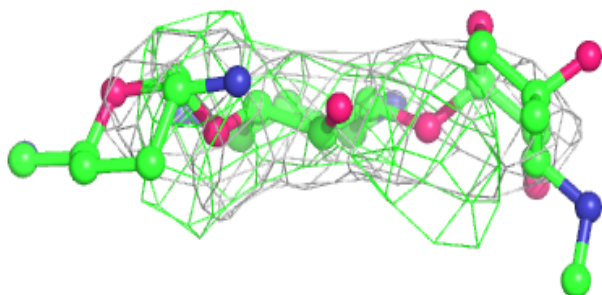
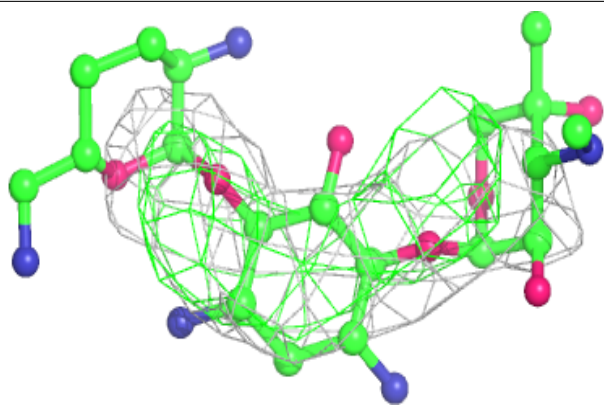
**Electron density around LLL AA 2063:**

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

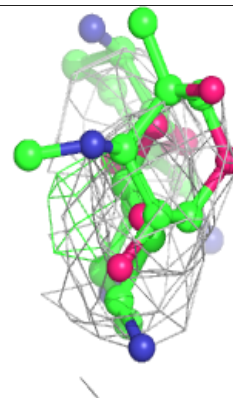
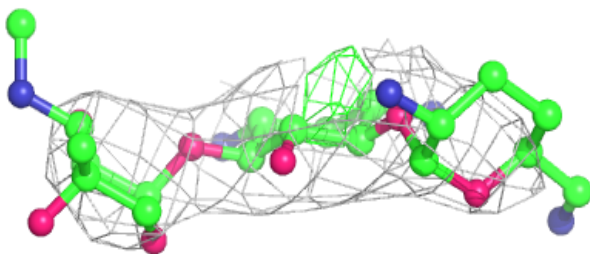
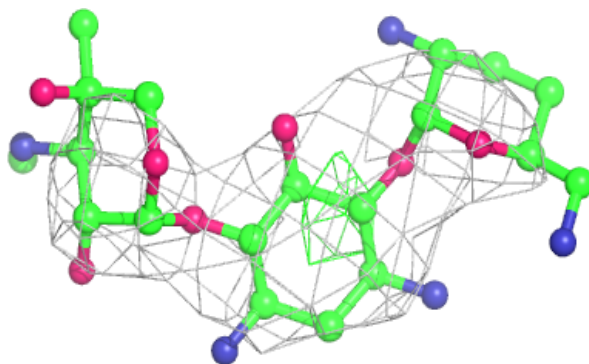


Electron density around LLL BB 3111:

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

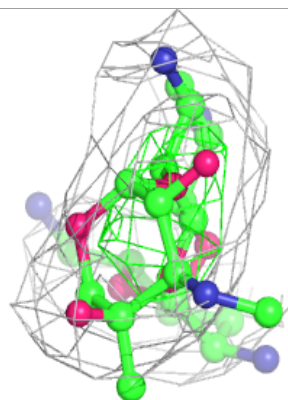
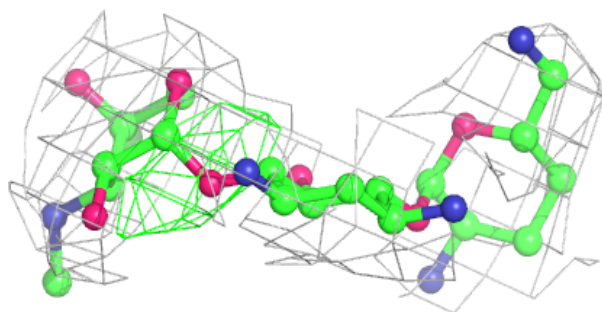
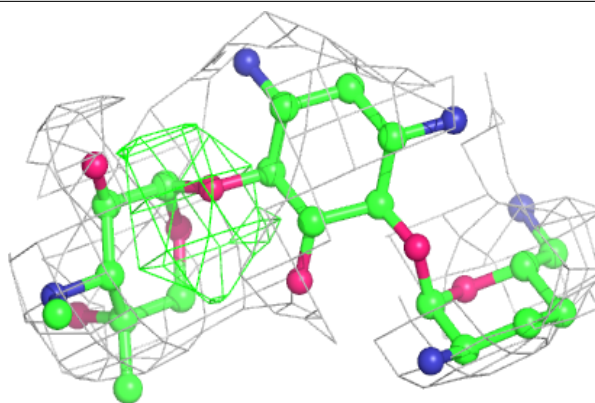
**Electron density around LLL DB 3112:**

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

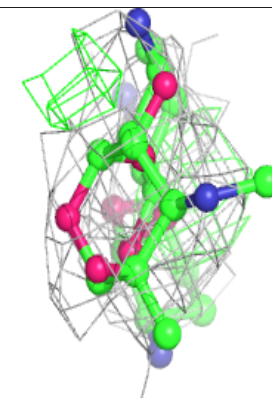
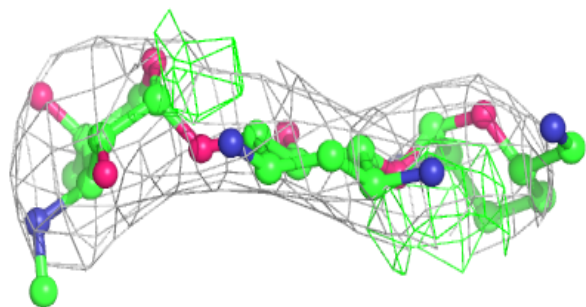
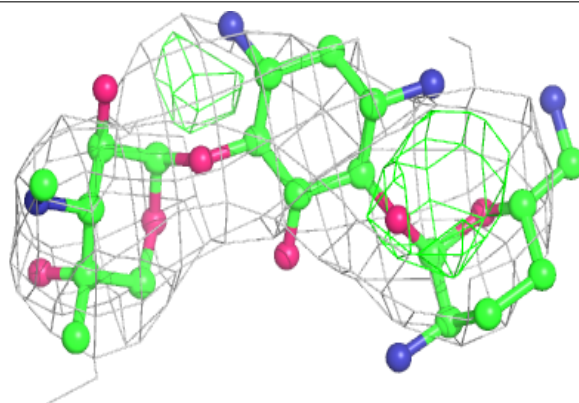


Electron density around LLL CA 2063:

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

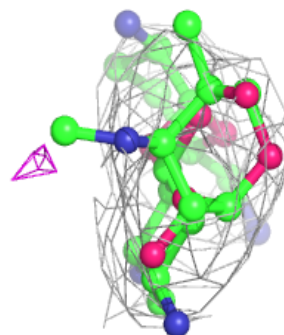
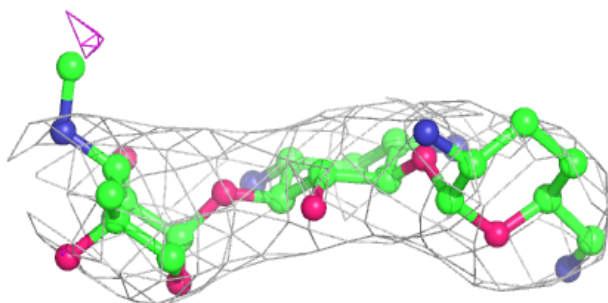
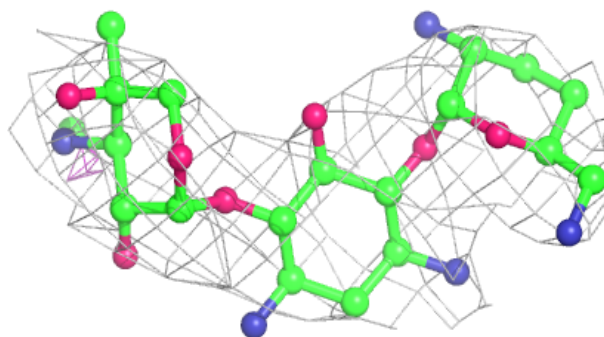
**Electron density around LLL CA 2064:**

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

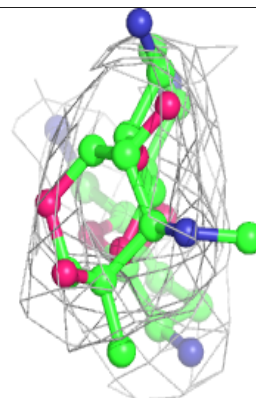
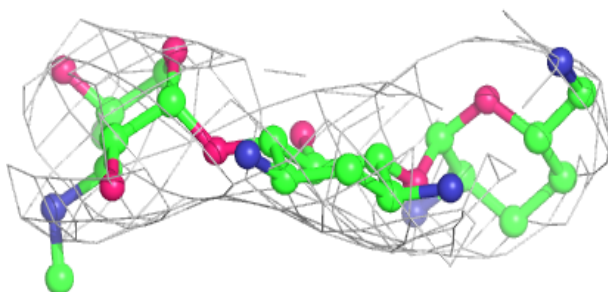
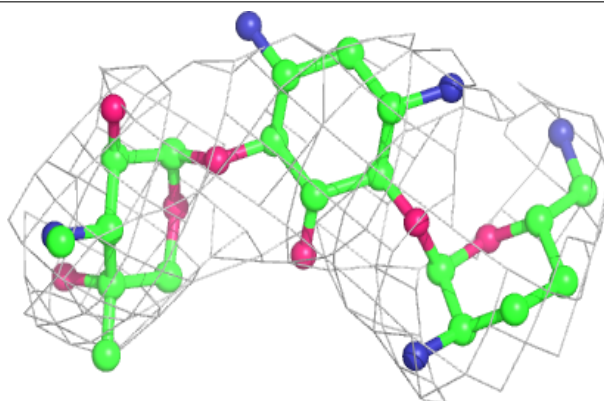


Electron density around LLL AA 2061:

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

**Electron density around LLL CA 2062:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.