



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 09:03 PM UTC

PDB ID : 4V52 / pdb_00004v52
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with neomycin.
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 : 2007-06-15
Resolution : 3.21 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

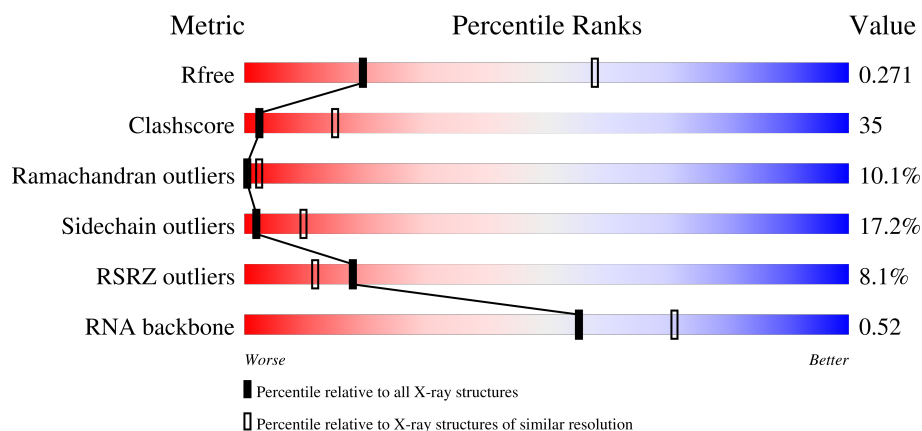
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)
RNA backbone	3983	1055 (3.50-2.94)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	3% 27% 59% 12% ..
1	CA	1542	3% 28% 59% 11% ..
2	AC	232	9% 31% 46% 12% 11%

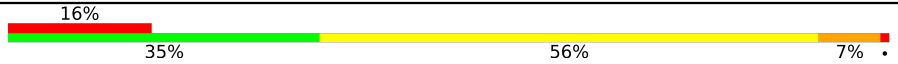
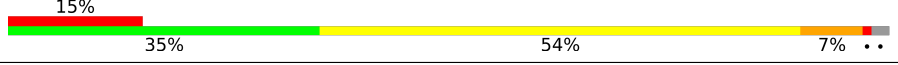
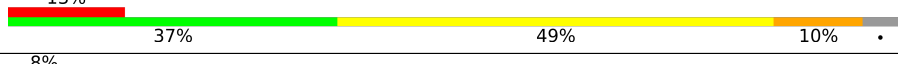
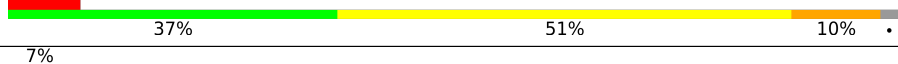
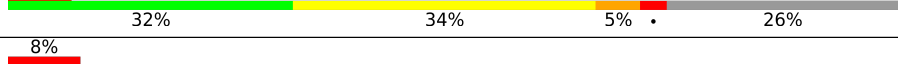
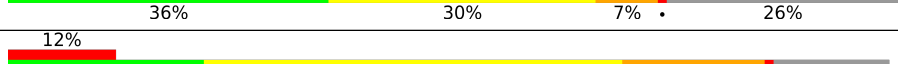
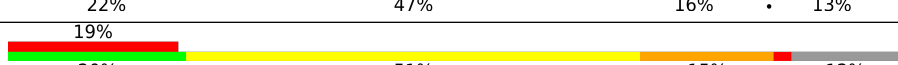
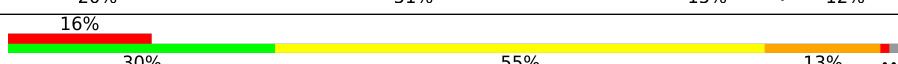
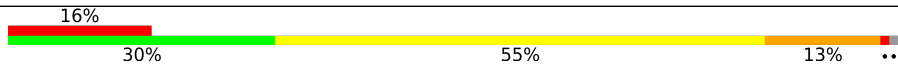
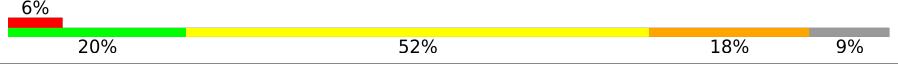
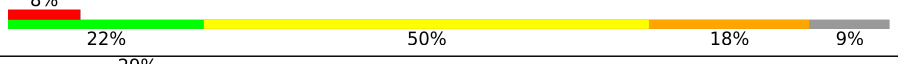
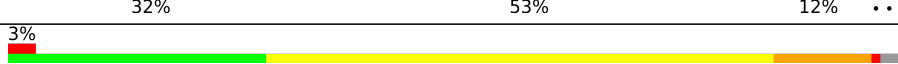
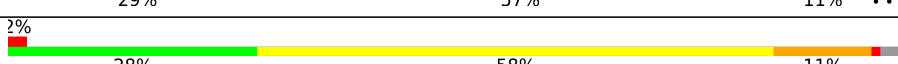
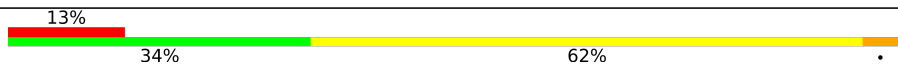
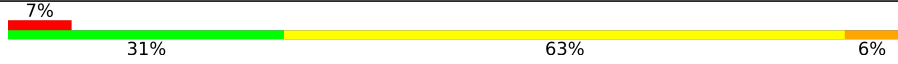
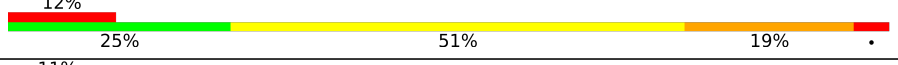
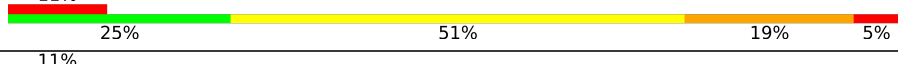
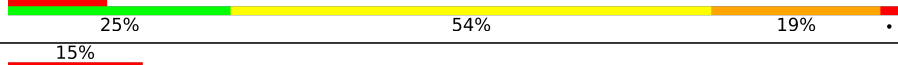
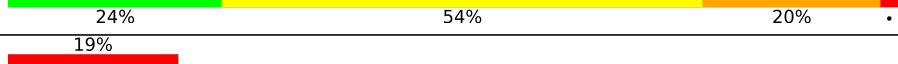
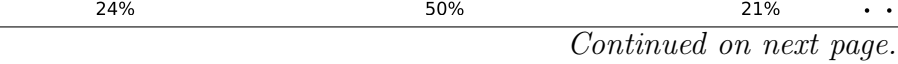
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Mol	Chain	Length	Quality of chain
2	CC	232	
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	

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Mol	Chain	Length	Quality of chain
15	AP	82	
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	70	
21	CU	70	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	

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

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

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Mol	Chain	Length	Quality of chain
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
54	MG	AA	1660	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284172 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			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0	0
			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			

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

- Molecule 27 is a protein called 50S ribosomal protein 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			

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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			

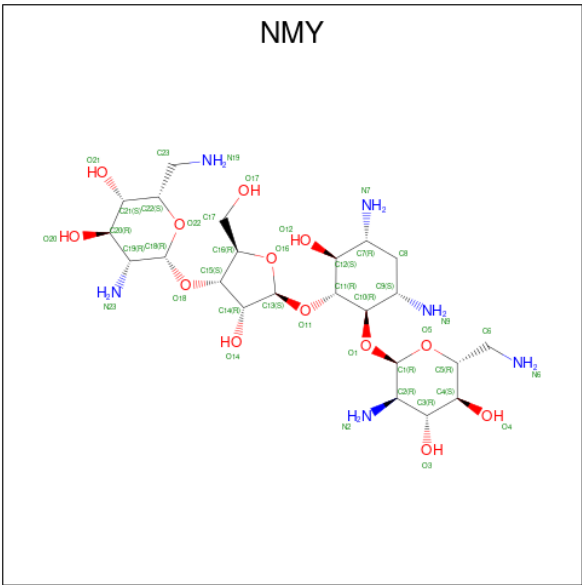
- Molecule 51 is a protein called 50S ribosomal protein L28.

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 NEOMYCIN (CCD ID: NMY) (formula: C₂₃H₄₆N₆O₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
53	AA	1	Total	C	N	O	0	0
			42	23	6	13		
53	BB	1	Total	C	N	O	0	0
			42	23	6	13		
53	CA	1	Total	C	N	O	0	0
			42	23	6	13		
53	DB	1	Total	C	N	O	0	0
			42	23	6	13		

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

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

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	291	Total 291	O 291	0	0
56	AL	4	Total 4	O 4	0	0
56	AN	4	Total 4	O 4	0	0
56	AT	1	Total 1	O 1	0	0
56	BB	497	Total 497	O 497	0	0
56	BC	5	Total 5	O 5	0	0
56	BE	1	Total 1	O 1	0	0
56	BL	1	Total 1	O 1	0	0
56	BN	1	Total 1	O 1	0	0
56	BR	1	Total 1	O 1	0	0
56	CA	298	Total 298	O 298	0	0
56	CE	3	Total 3	O 3	0	0
56	CL	2	Total 2	O 2	0	0
56	CN	4	Total 4	O 4	0	0
56	CP	1	Total 1	O 1	0	0
56	CT	1	Total 1	O 1	0	0
56	DB	502	Total 502	O 502	0	0
56	DC	6	Total 6	O 6	0	0

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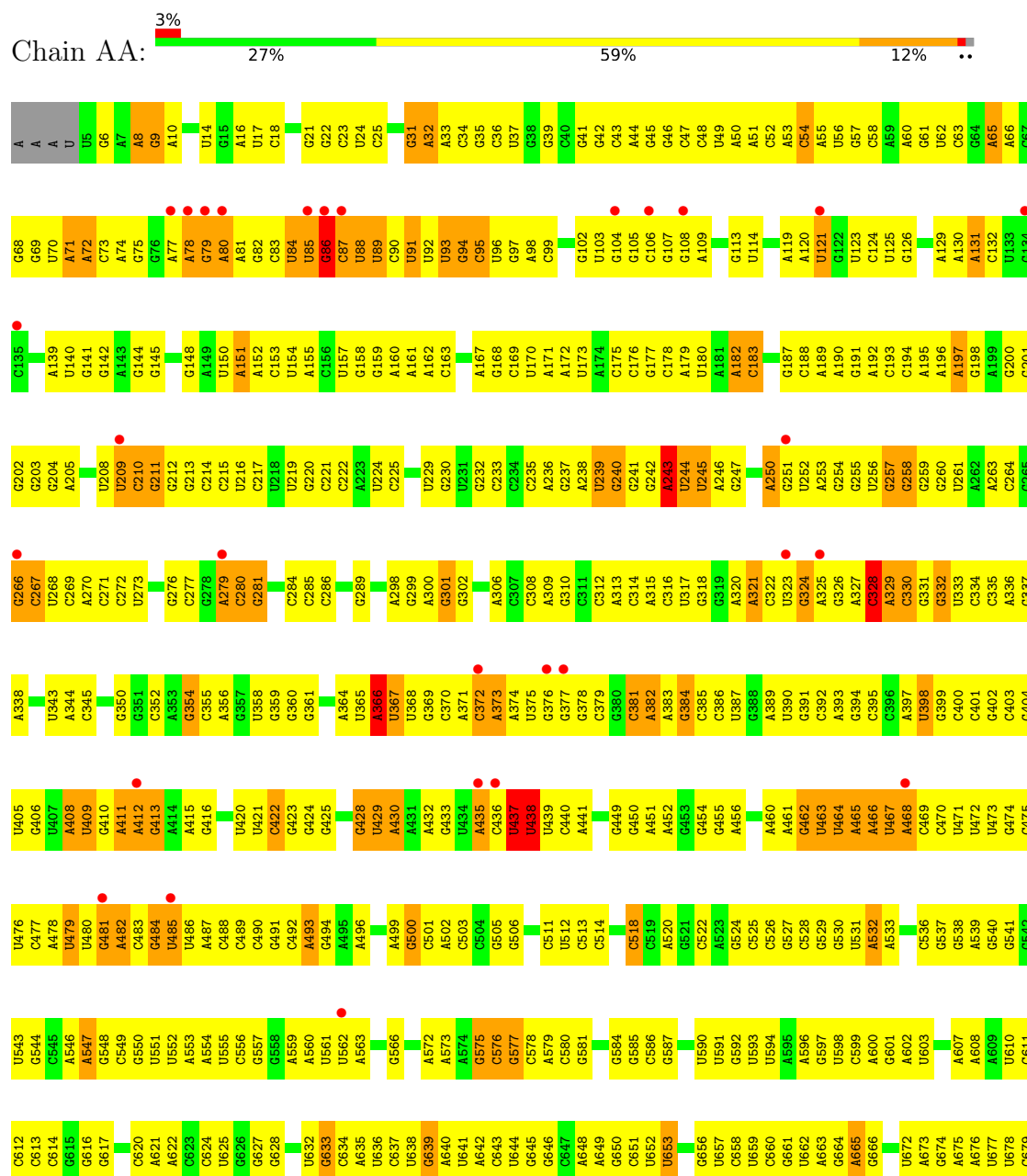
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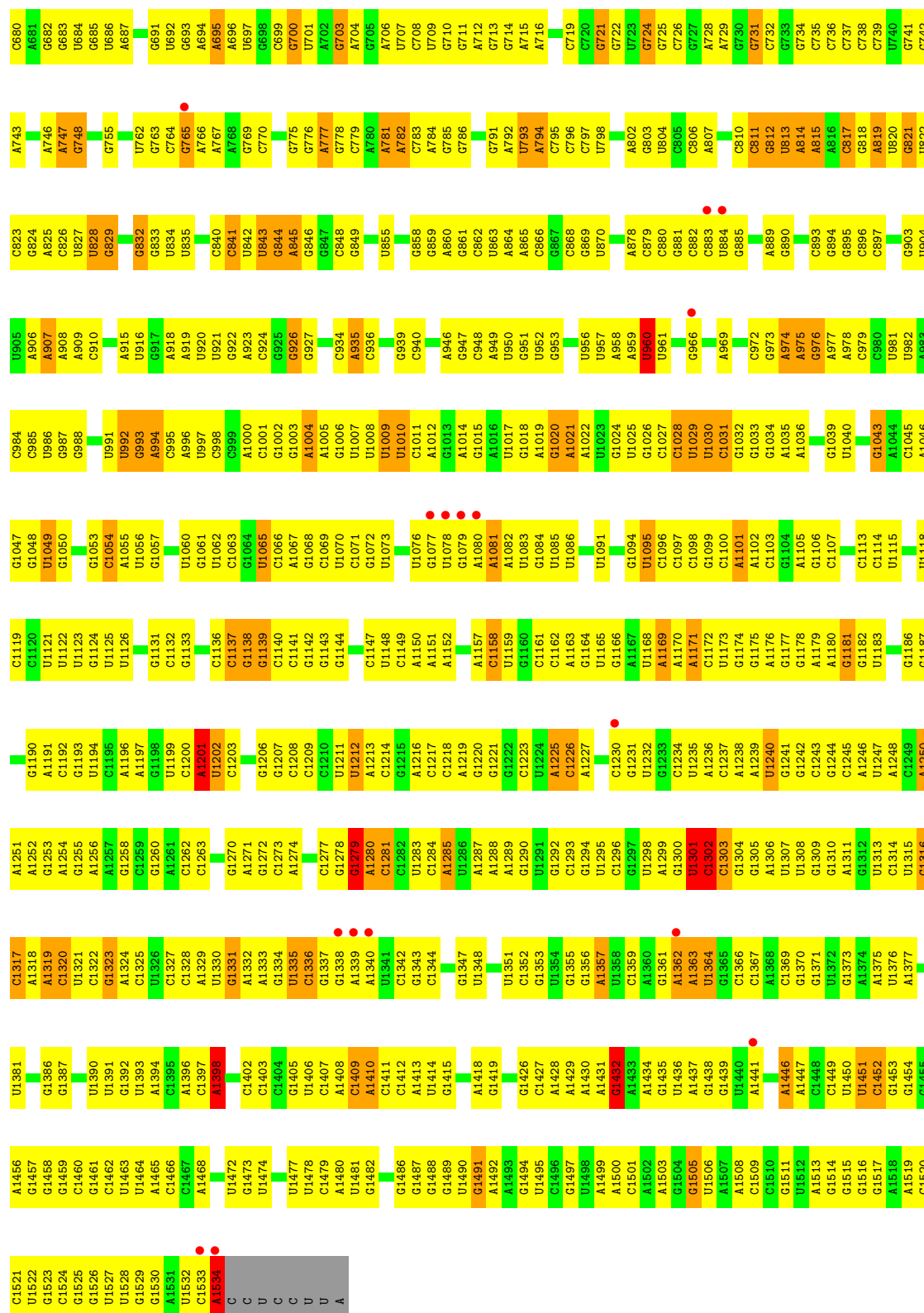
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DE	1	Total	O	0	0
			1	1		
56	DL	2	Total	O	0	0
			2	2		
56	DR	1	Total	O	0	0
			1	1		

3 Residue-property plots

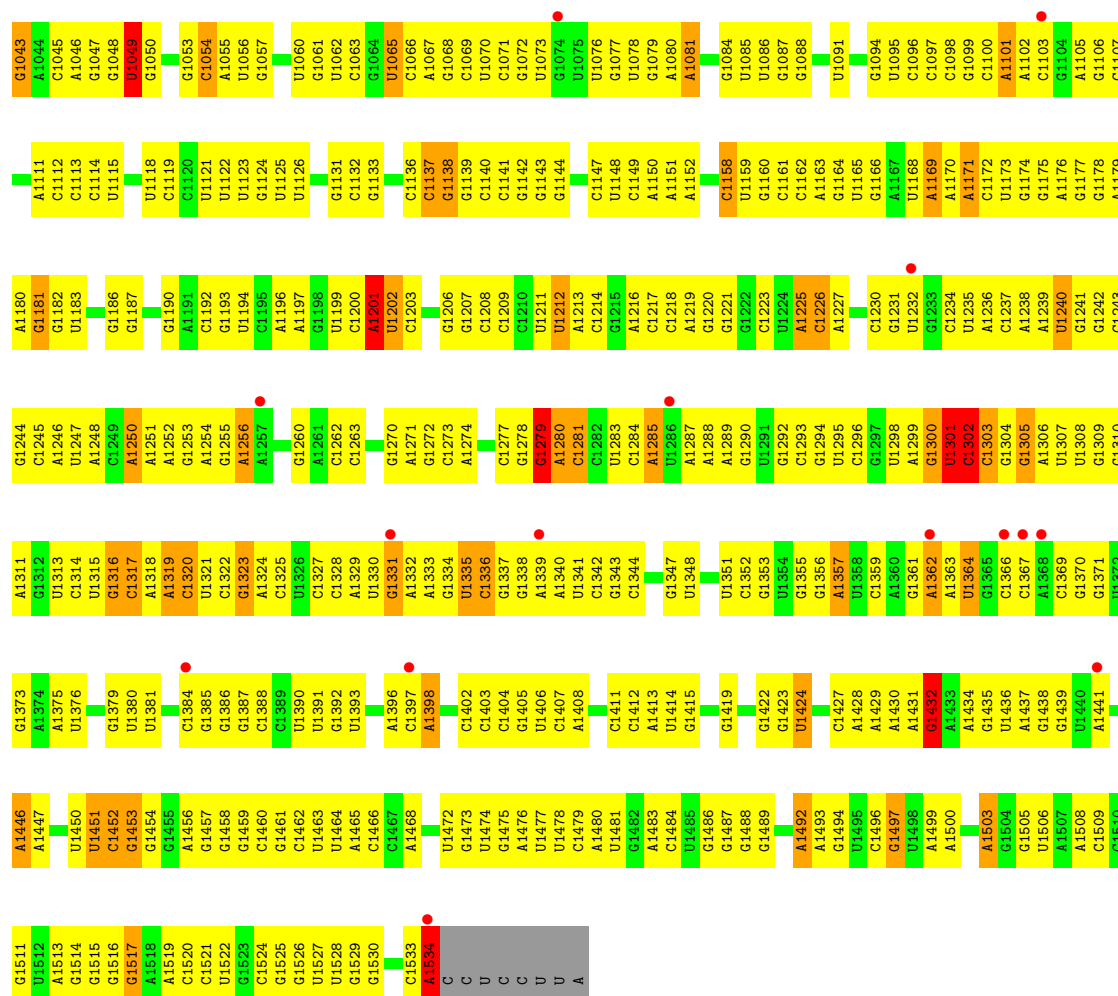
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

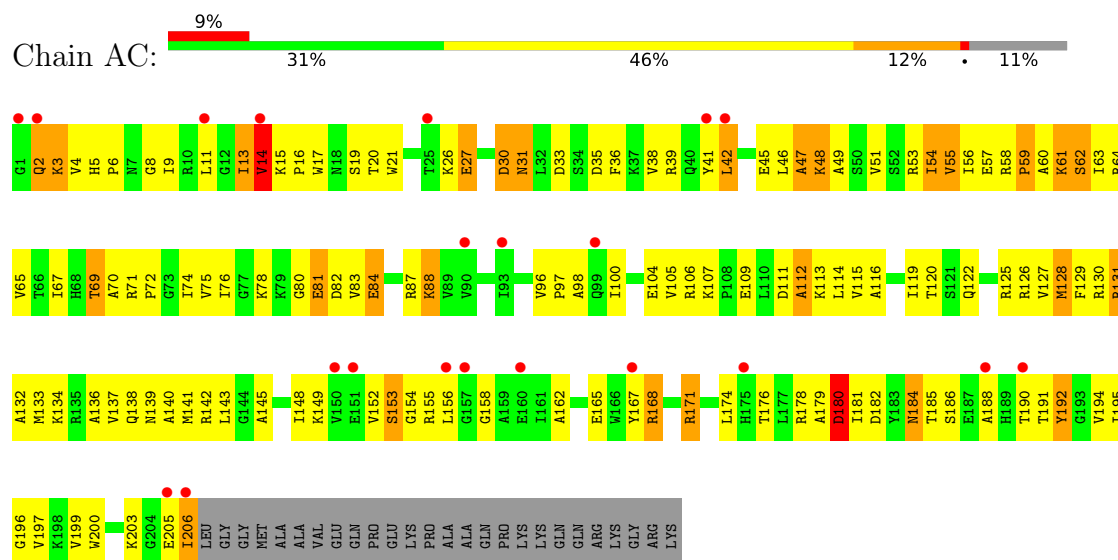




A	A	A	U	U5	G6	A7	A8	G9	A10	U14	G15	A16	U17	C18	G21	G22	G23	U24	C25	G31	A32	A33	C34	G35	C36	U37	G38	G39	C40	G41	G42	C43	A44	G45	G46	C47	C48	U49	A50	A51	C52	A53	C54	A55	U56	G57	C58	A59	G60	G61	U62	C63	G64	A65	G69				
U70	A71	A72	A77	A78	A79	A80	A81	G82	C83	U84	U85	G86	C87	U88	U89	C90	U91	U92	U93	C94	C95	U96	G97	A98	C99	G102	U103	G104	G105	C106	G107	G108	A109	G113	U114	A119	A120	U121	G122	U123	C124	U125	G126	A129	A130	A131	C132	G139	U140	G141	G142	A143	G144						
G145	G148	A149	U150	A151	A152	C153	U154	A155	C156	U157	G158	G159	A160	U161	A162	C163	A167	G168	C169	U170	A171	A172	U173	A174	C175	C176	G177	C178	A179	U180	A181	A182	C183	G187	C188	A189	A190	G191	A192	G193	C194	A195	A196	A197	G198	A199	G200	G201	G202	G203	G204	A205	U208	U209	A271	C210			
G211	G212	C213	G214	C215	U216	C217	U218	U219	C220	A221	C222	U223	U224	C225	G226	U229	G230	U231	G232	C233	C234	C235	A306	C307	C308	A309	G310	C311	C312	A313	C314	A315	C316	U317	A246	G247	A250	G251	U252	A253	G254	G255	U256	G257	C328	A329	C330	U331	G332	U333	C334	C335	A336	G337	A338	C345	G348		
A349	G350	C351	G352	A353	G354	C355	A356	G357	U358	U359	A360	A361	A362	A363	A364	U365	A366	U367	C370	A371	C372	A373	A374	U375	G376	G377	G378	C379	G380	C381	A382	A383	G384	C385	C386	U387	G388	A389	U390	U391	U392	C392	G393	A394	G395	C396	A397	U398	C400	C401	G402	C403	G404	U405	U406	A407	A408	U409	G410
A411	A412	G413	G414	A415	G416	U420	U421	C422	G423	G424	G425	U428	U429	A430	A431	A432	G433	U434	A435	C436	U437	U438	U439	C440	A441	G449	G450	A451	A452	G453	C454	G455	A456	A460	A461	G462	U463	U464	A465	A466	U467	A468	C469	C470	U471	U472	U473	G474	C475	U476	C477	A478	U479	U480	G481				
A482	C483	G484	U485	U486	A487	C488	G489	C490	G491	C492	G493	G494	A495	A496	A499	G500	C501	A502	C503	G504	C505	G506	A509	A510	C511	U512	C513	C514	G515	U516	C517	C518	C519	A520	G521	C522	A523	G524	C525	U526	G527	C528	G529	C530	U531	A532	C536	G537	G538	A539	G540	U541	G542	U543	G544	C545			
A546	A547	G548	C549	U550	U551	U552	A553	A554	U555	C556	G557	G558	A559	A560	U561	A562	A563	G566	A572	C573	A574	G575	C576	G577	C578	A579	C580	G581	G584	G585	C586	G587	U590	U591	G592	U593	U594	A595	A596	G597	U598	C599	A600	G601	A602	U603	A607	G608	U609	U610	C611	G612	C613	G614					
G615	G616	G617	U618	G619	A621	G622	A623	G624	U625	G626	G627	G628	U632	G633	A634	A635	G636	C637	U638	G639	A640	U641	A642	G643	A648	A649	G650	C651	G652	U653	G656	U657	C658	U659	C660	G661	U662	A663	A664	A665	G666	G667	U672	A673	G674	A675	A676	U677	U678	G679	C680	A681	G682	G683					
U684	G685	U686	A687	G691	U692	G693	A694	A695	U696	G697	G698	C699	G700	U701	A702	G703	A704	G705	A706	U707	G708	U709	G710	G711	A712	U713	G714	A715	G716	C719	U720	G721	G722	U723	G724	G725	C726	G727	A728	U729	A730	G731	C732	G733	G734	C735	U736	C737	U738	C739	U740	G741	G742	A743	G744	U745	A746		
A747	G748	G755	U762	G763	C764	G765	A766	A767	U768	G769	G770	G775	G776	A777	G778	C779	A780	U781	A782	C783	U784	G785	A792	U793	U794	A795	C796	C797	U798	A802	G803	U804	C805	C806	A807	C810	G811	G812	U813	A814	A815	C816	C817	G818	A819	U820	G821	U822	C823	G824	A825	C826	U827						
U828	G829	G832	G833	U834	U835	C840	U841	U842	U843	U844	G845	A846	G847	C848	G849	U855	G858	A859	C860	G861	C862	U863	A864	C865	C866	G867	C868	G869	A872	A873	G874	A878	C879	C880	G881	C882	C883	U884	G885	C893	G894	G895	C896	C897	A901	G902	G903	U904	U905	A906	A907								
A908	A909	C910	A915	U916	G917	A918	A919	U920	U921	U922	A923	C924	G925	C926	G927	G928	G929	C932	G933	C934	A935	C936	G939	C940	G941	A946	C947	C948	U949	U950	G951	U952	G953	U956	U957	A958	A959	U960	U961	U965	G966	C967	U968	A969	C970	G971	C972	G973	A1035	A1036	U1039	U1040	A978						
C979	C980	U981	U982	C983	C984	C985	U986	G987	G988	U991	G992	G993	A994	C995	A996	U997	C998	C999	A1000	G1001	G1002	G1003	A1004	A1005	G1006	U1007	U1008	U1009	U1010	C1011	A1012	G1013	G1014	G1015	A1016	U1017	G1018	A1019	G1020	A1021	A1022	U1025	G1026	C1027	U1028	U1029	U1030	C1031	G1032	G1033	G1034	A1035	A1036	U1039	U1040	A978			

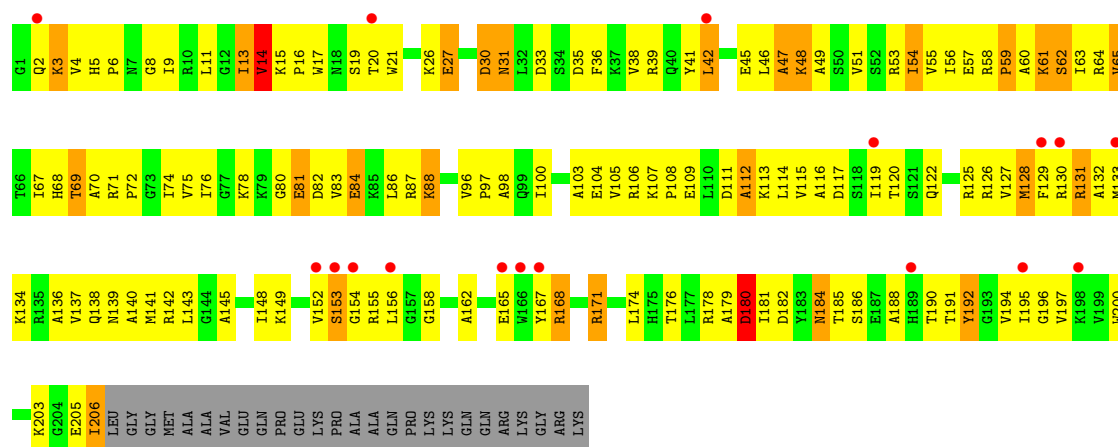


• Molecule 2: 30S ribosomal protein S3

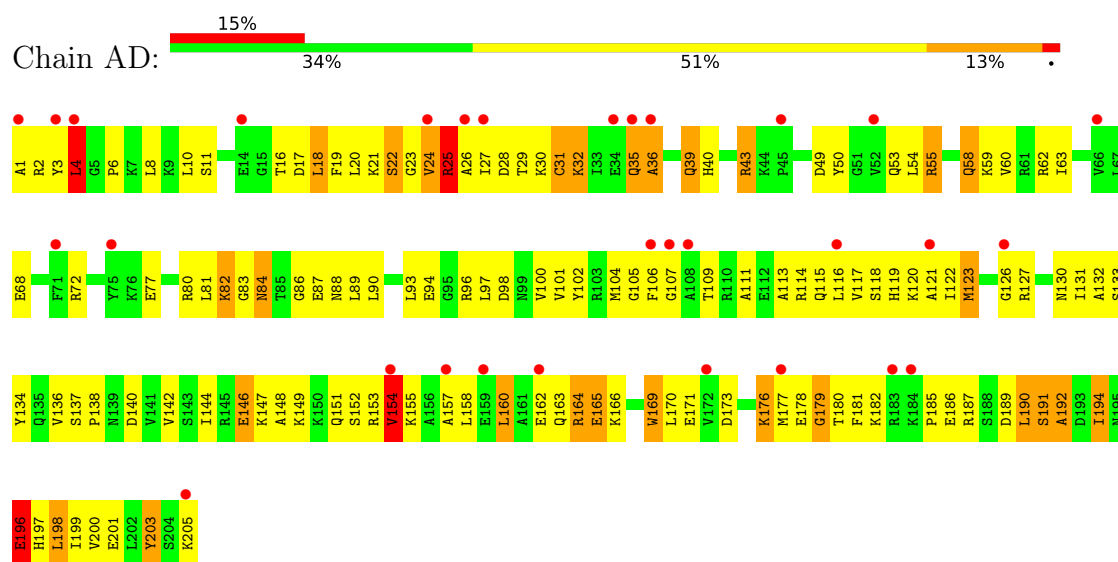


• Molecule 2: 30S ribosomal protein S3

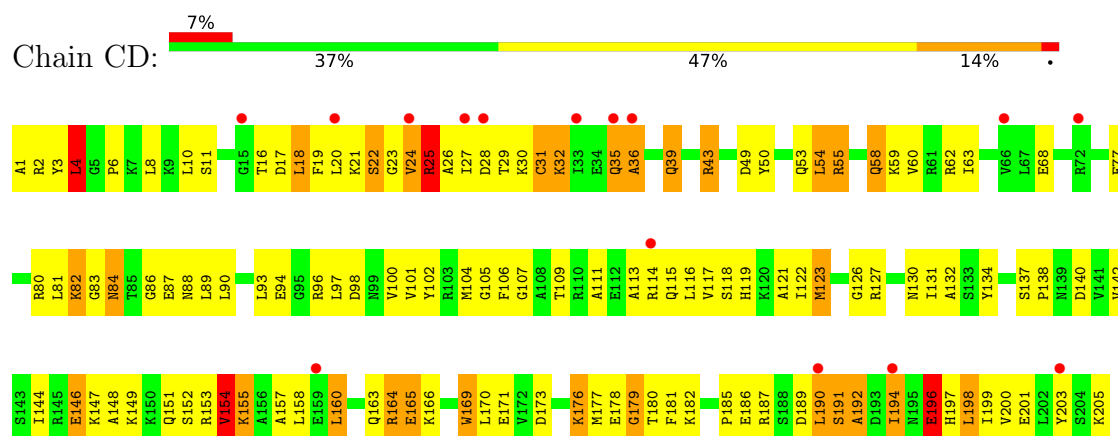




• Molecule 3: 30S ribosomal protein S4

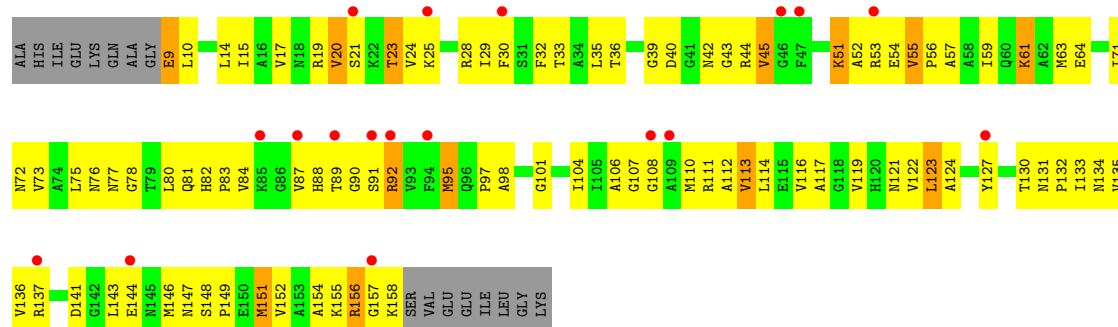


• Molecule 3: 30S ribosomal protein S4

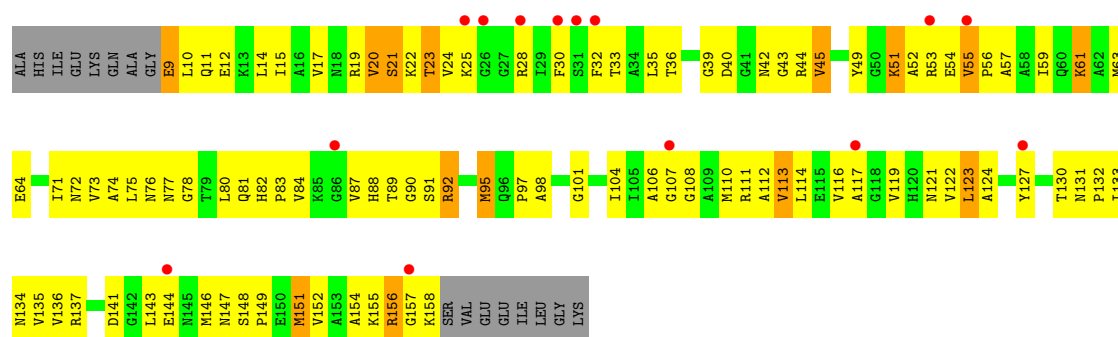


• Molecule 4: 30S ribosomal protein S5

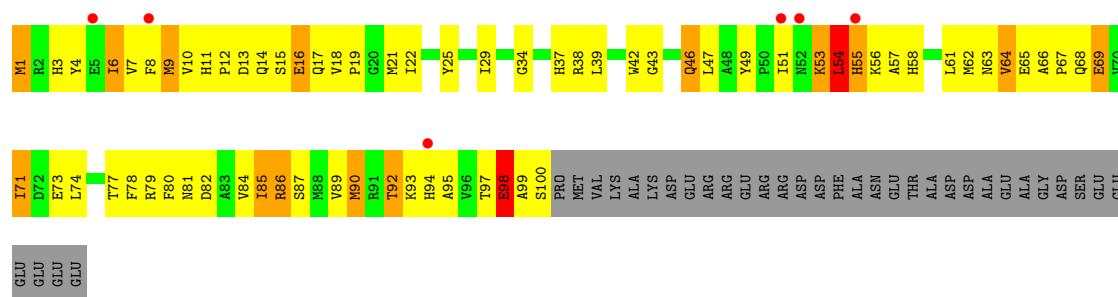
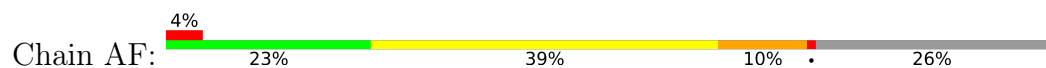




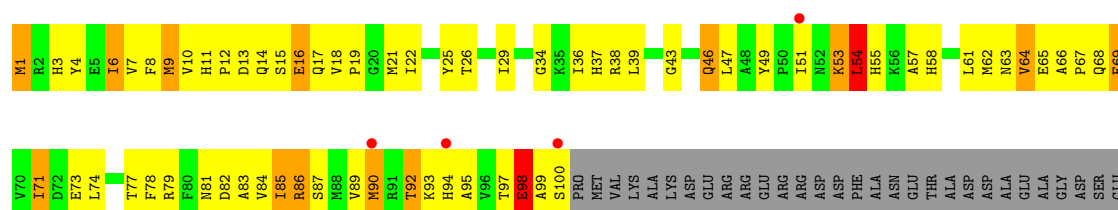
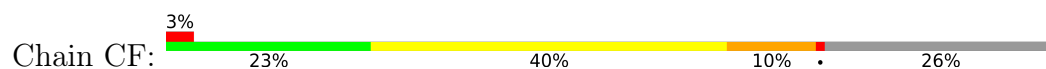
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6

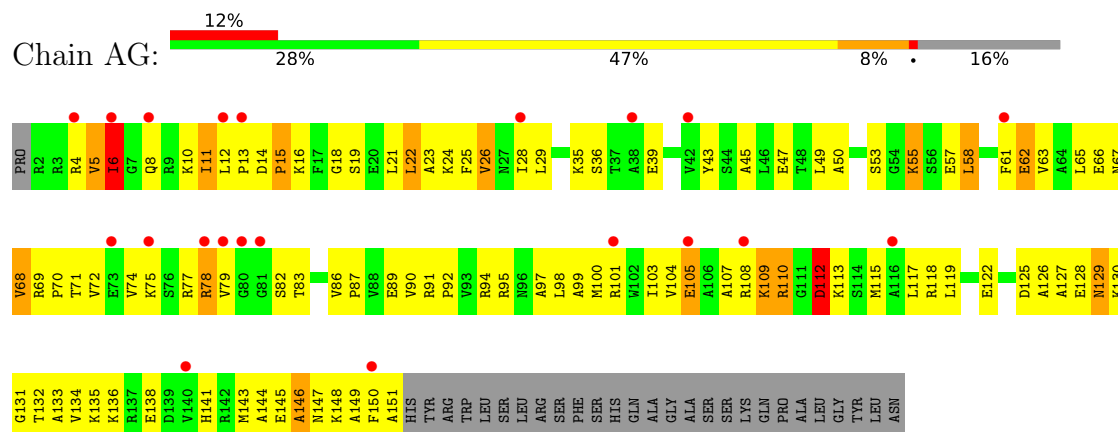


• Molecule 5: 30S ribosomal protein S6

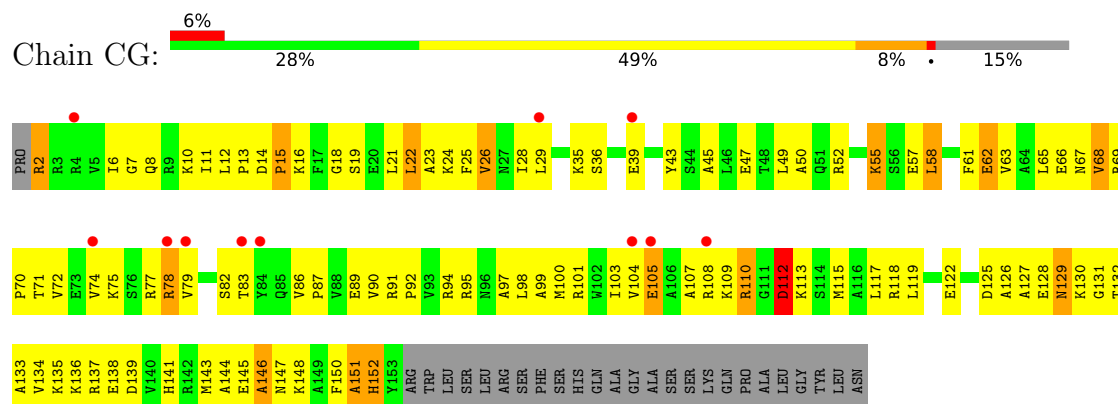


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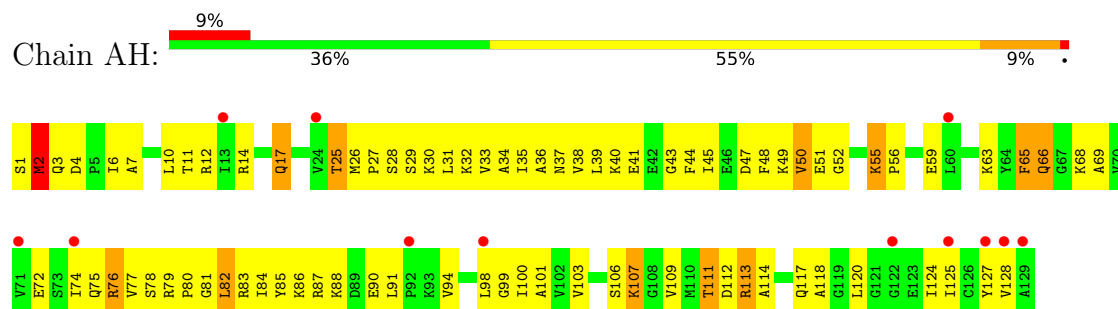
• Molecule 6: 30S ribosomal protein S7



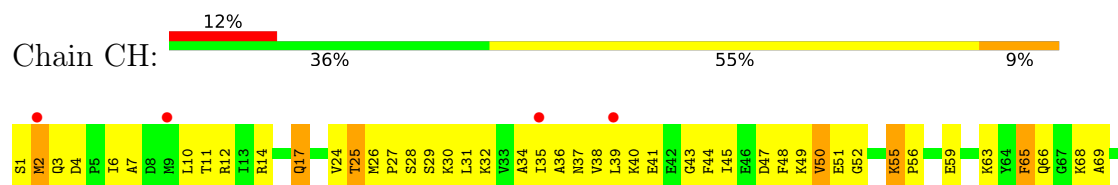
• Molecule 6: 30S ribosomal protein S7

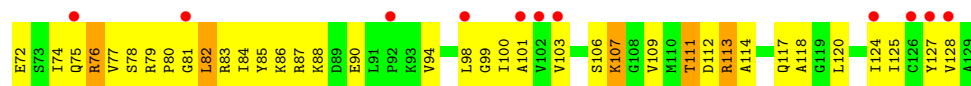


• Molecule 7: 30S ribosomal protein S8

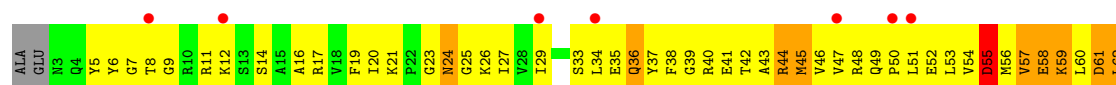


• Molecule 7: 30S ribosomal protein S8

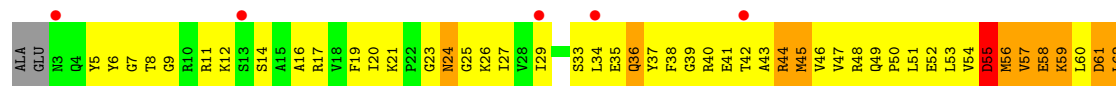




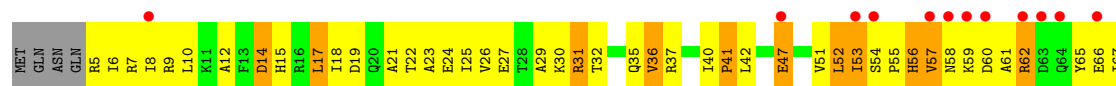
• Molecule 8: 30S ribosomal protein S9



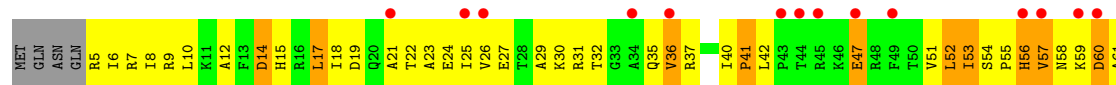
• Molecule 8: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S10

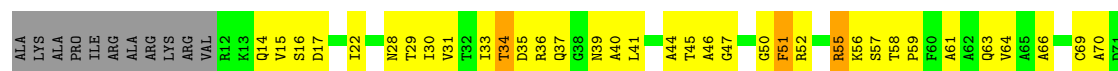


• Molecule 9: 30S ribosomal protein S10

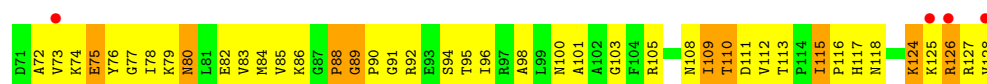
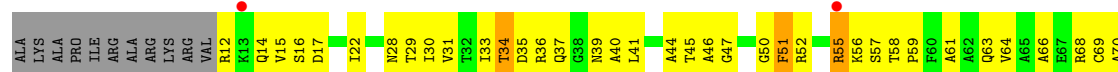


• Molecule 10: 30S ribosomal protein S11

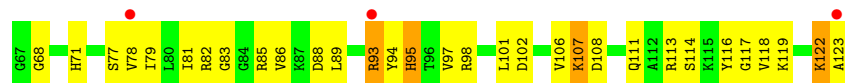




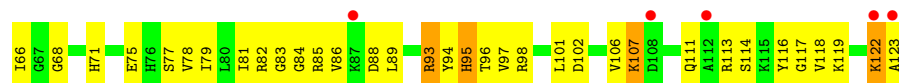
• Molecule 10: 30S ribosomal protein S11



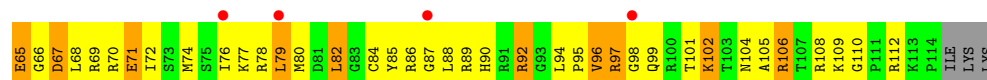
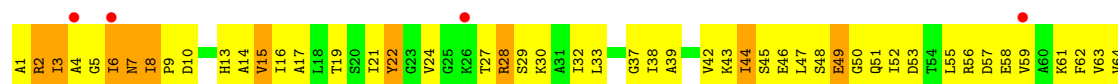
• Molecule 11: 30S ribosomal protein S12



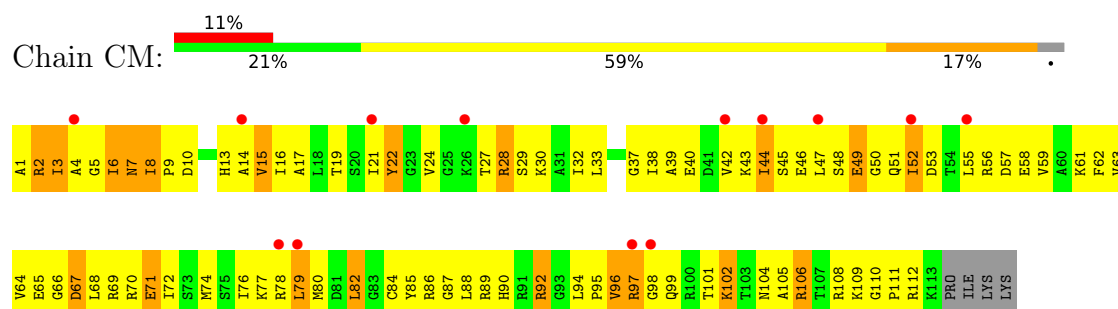
• Molecule 11: 30S ribosomal protein S12



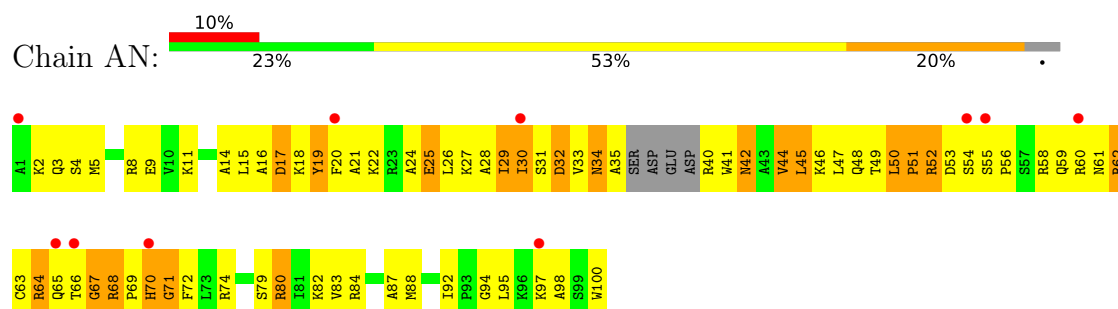
• Molecule 12: 30S ribosomal protein S13



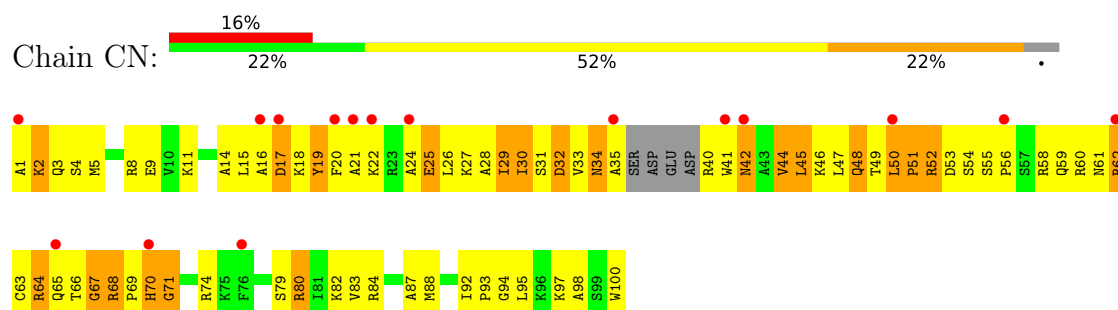
- Molecule 12: 30S ribosomal protein S13



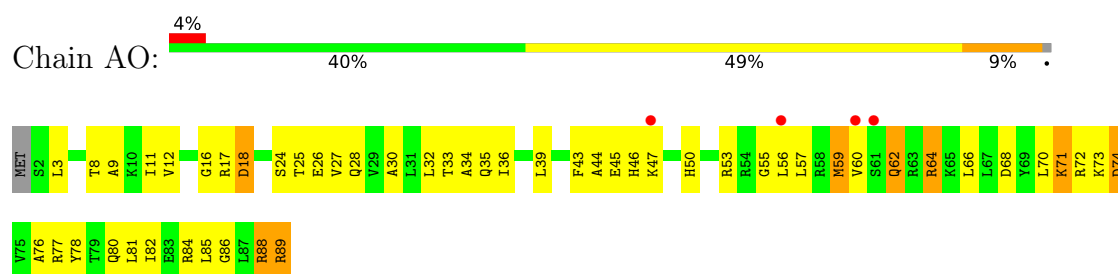
- Molecule 13: 30S ribosomal protein S14



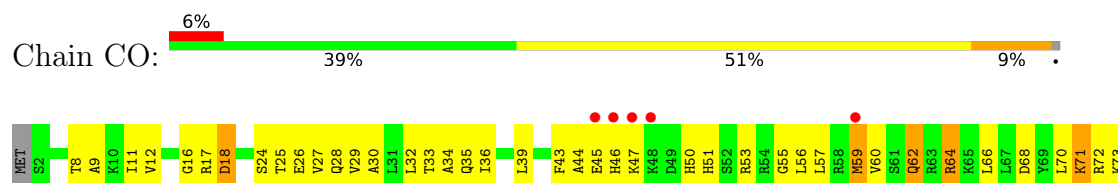
- Molecule 13: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S15

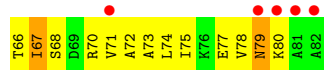
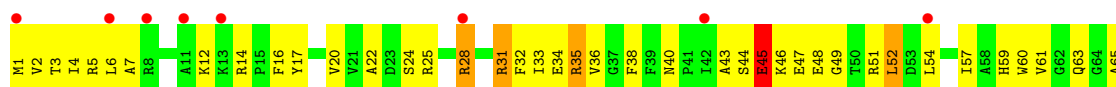


- Molecule 14: 30S ribosomal protein S15

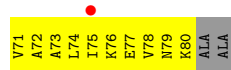
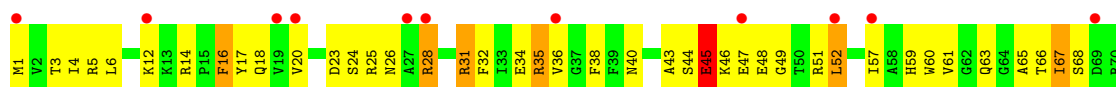




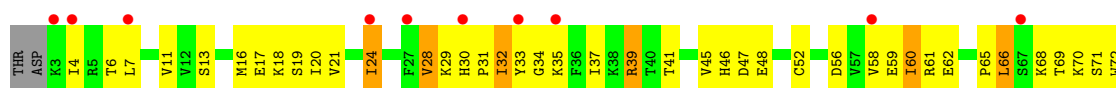
• Molecule 15: 30S ribosomal protein S16



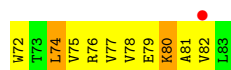
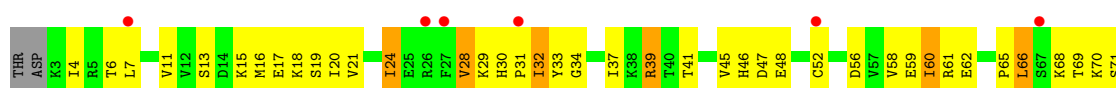
• Molecule 15: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S17

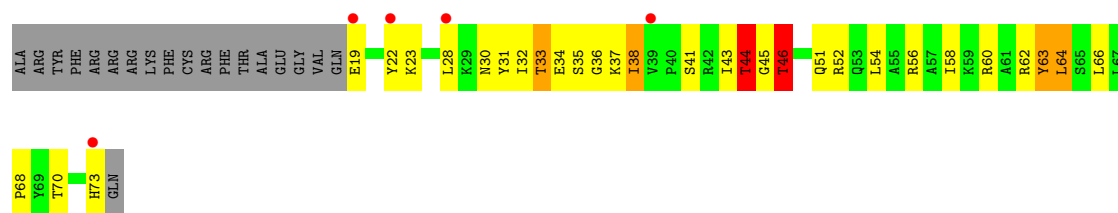


• Molecule 16: 30S ribosomal protein S17

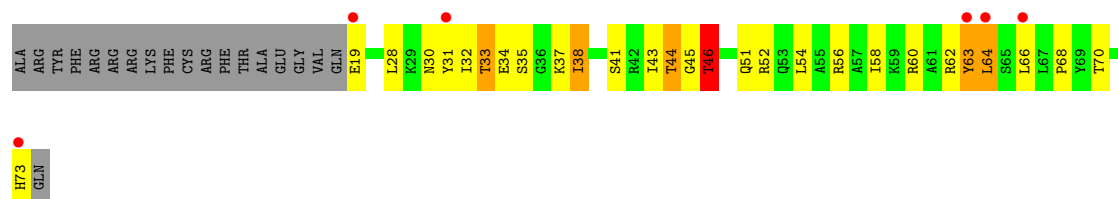


• Molecule 17: 30S ribosomal protein S18

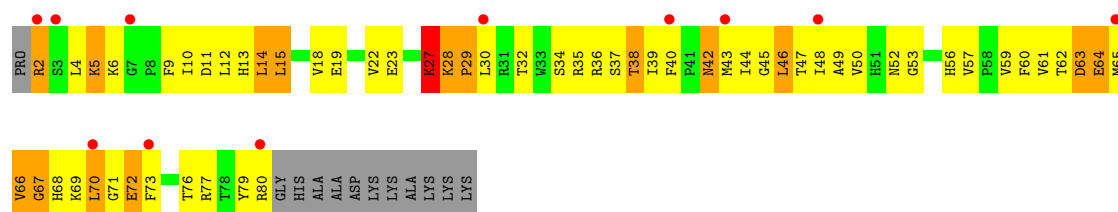
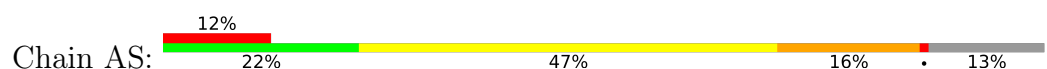




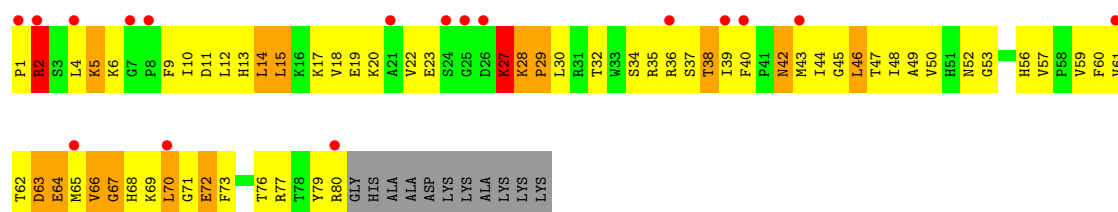
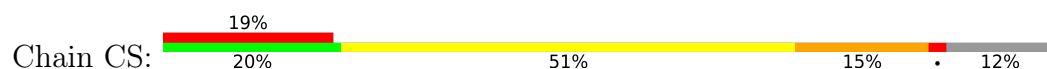
• Molecule 17: 30S ribosomal protein S18



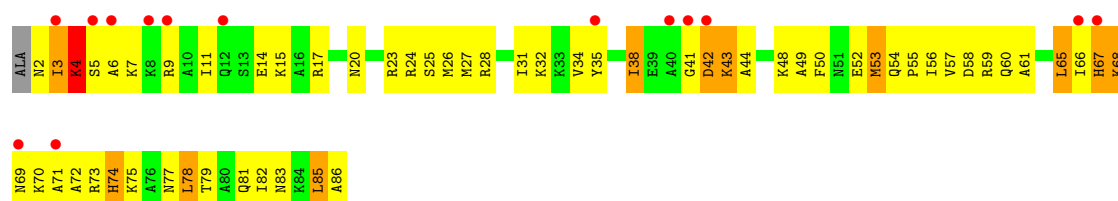
• Molecule 18: 30S ribosomal protein S19



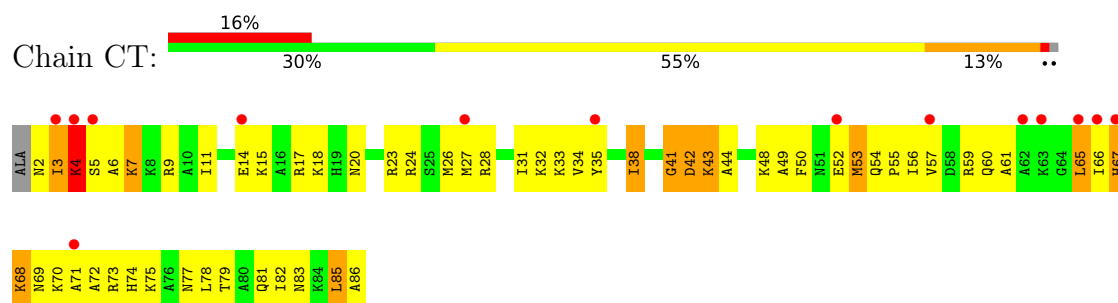
• Molecule 18: 30S ribosomal protein S19



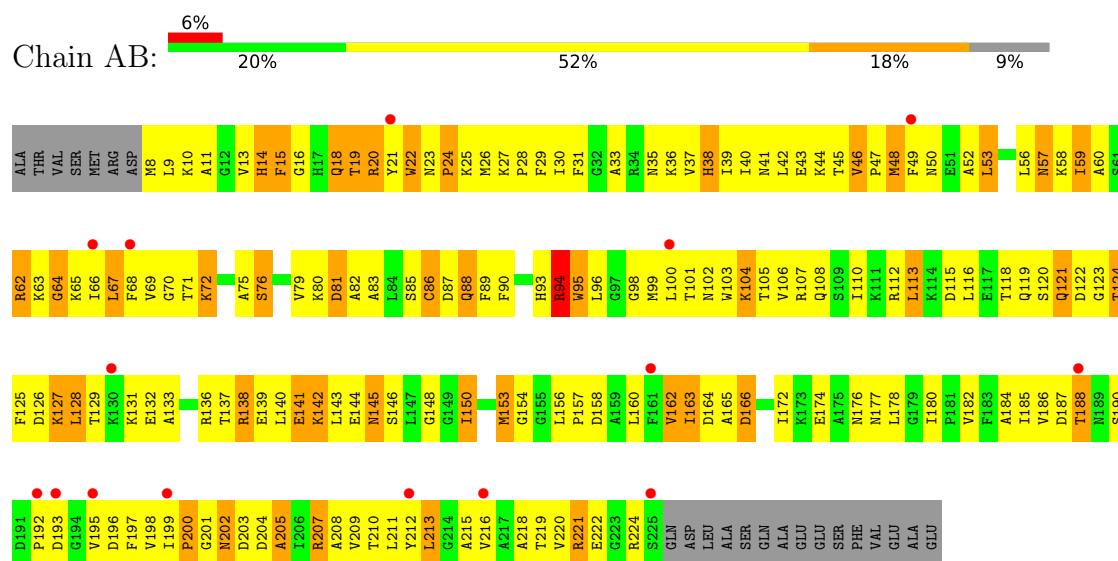
• Molecule 19: 30S ribosomal protein S20



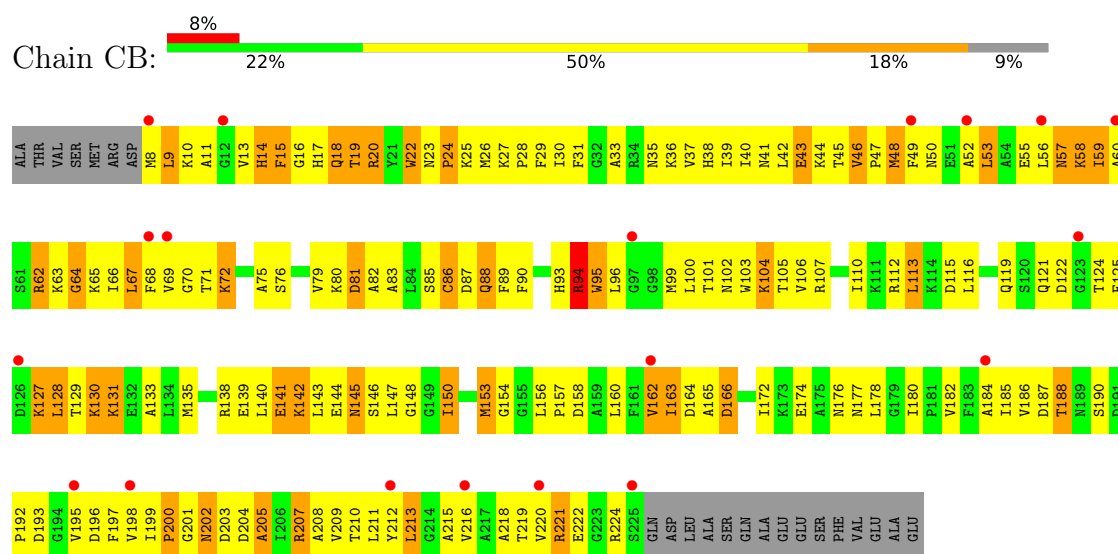
- Molecule 19: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S2

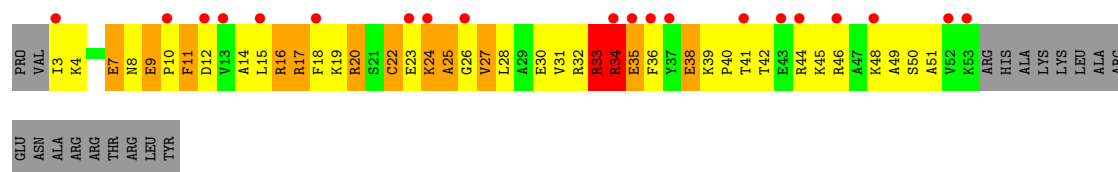


- Molecule 20: 30S ribosomal protein S2

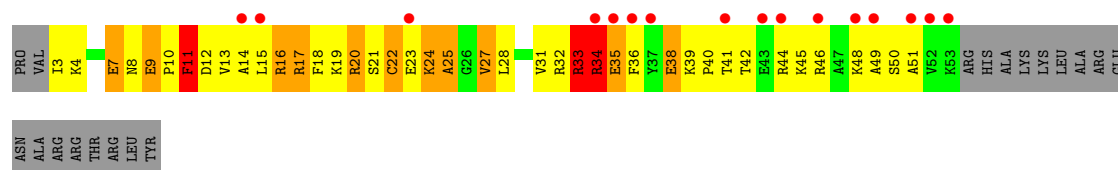


- Molecule 21: 30S ribosomal protein S21

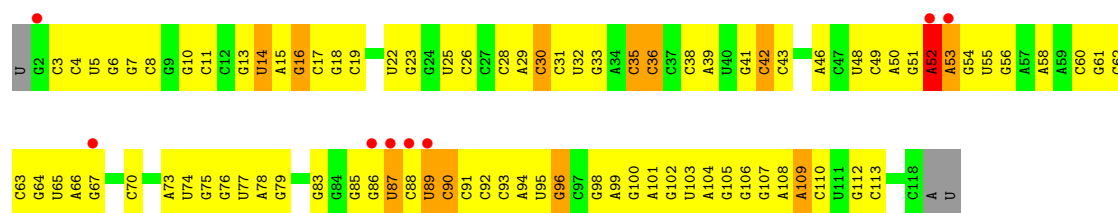




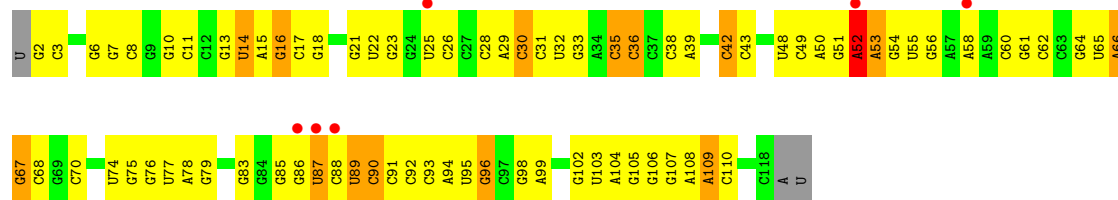
- Molecule 21: 30S ribosomal protein S21



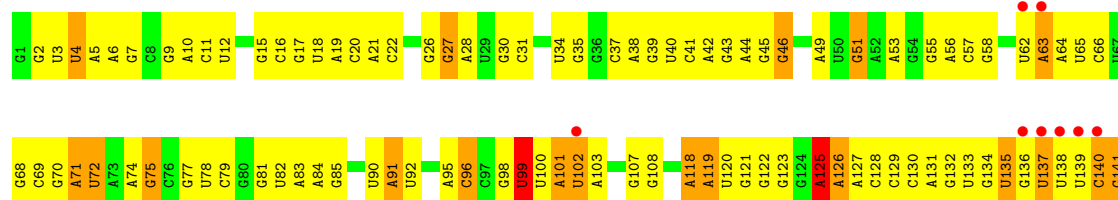
- Molecule 22: 5S rRNA



- Molecule 22: 5S rRNA

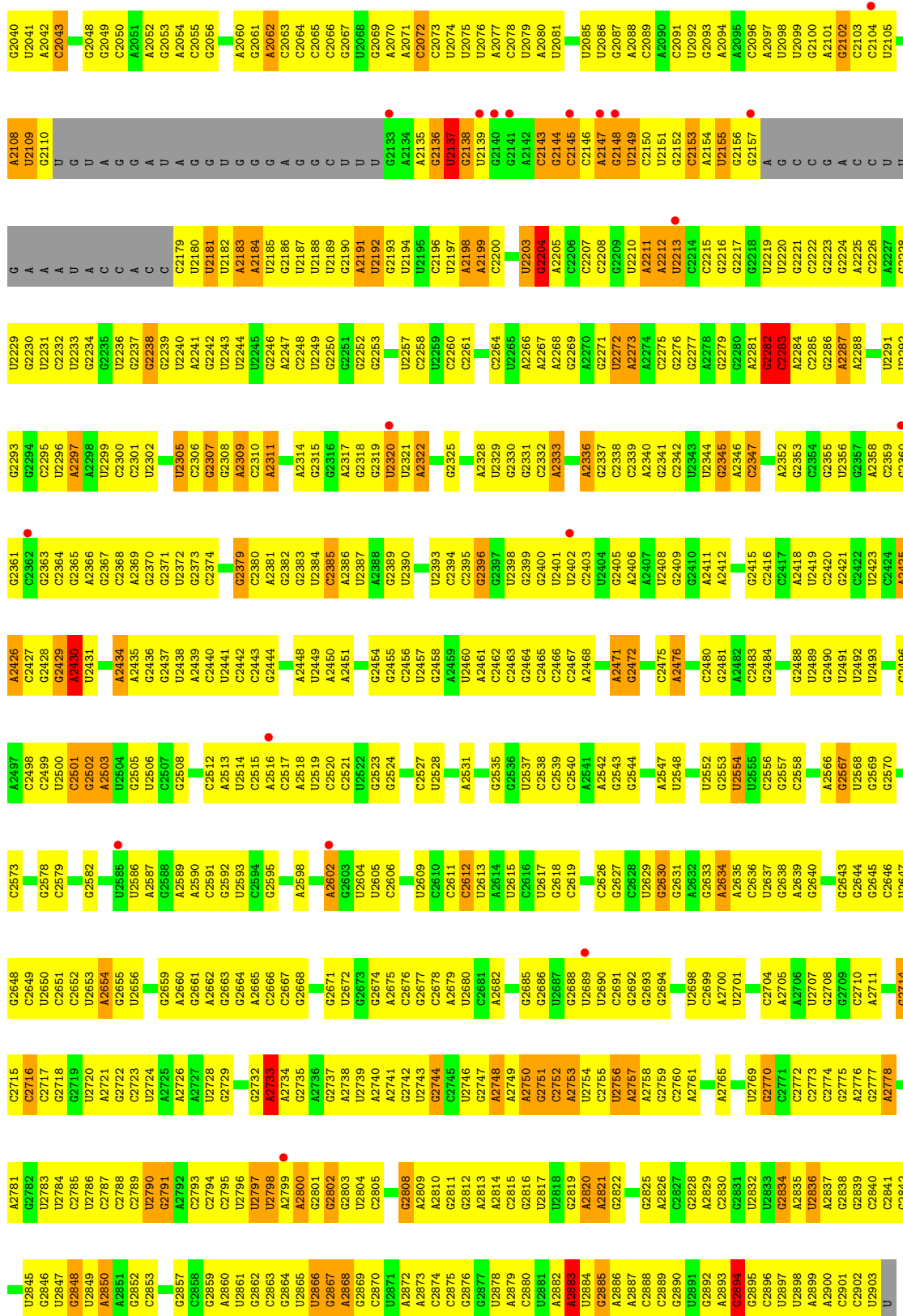


- Molecule 23: 23S rRNA



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A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042																																																																																																																																																																																																																							
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U2060	U2061	U2062	U2063	U2064	U2065	U2066	U2067	U2068	U2069	U2070	U2071	U2072	U2073	U2074	U2075	U2076	U2077	U2078	U2079	U2080	U2081	U2082	U2083	U2084	U2085	U2086	U2087	U2088	U2089	U2090	U2091	U2092	U2093	U2094	U2095	U2096	U2097	U2098	U2099	U2100	U2101	U2102	U2103	U2104	U2105	U2106	U2107	U2108	U2109	U2110	U2111	U2112	U2113	U2114	U2115	U2116	U2117	U2118	U2119	U2120	U2121	U2122	U2123	U2124	U2125	U2126	U2127	U2128	U2129	U2130	U2131	U2132	U2133	U2134	U2135	U2136	U2137	U2138	U2139	U2140	U2141	U2142	U2143	U2144	U2145	U2146	U2147	U2148	U2149	U2150	U2151	U2152	U2153	U2154	U2155	U2156	U2157	U2158	U2159	U2160	U2161	U2162	U2163	U2164	U2165	U2166	U2167	U2168	U2169	U2170	U2171	U2172	U2173	U2174	U2175	U2176	U2177	U2178	U2179	U2180	U2181	U2182	U2183	U2184	U2185	U2186	U2187	U2188	U2189	U2190	U2191	U2192	U2193	U2194	U2195	U2196	U2197	U2198	U2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	U2230	U2231	U2232	U2233	U2234	U2235	U2236	U2237	U2238	U2239	U2240	U2241	U2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	U2250	U2251	U2252	U2253	U2254	U2255	U2256	U2257	U2258	U2259																																																																																																																																																																																																																																																																																																																																																																																																																							
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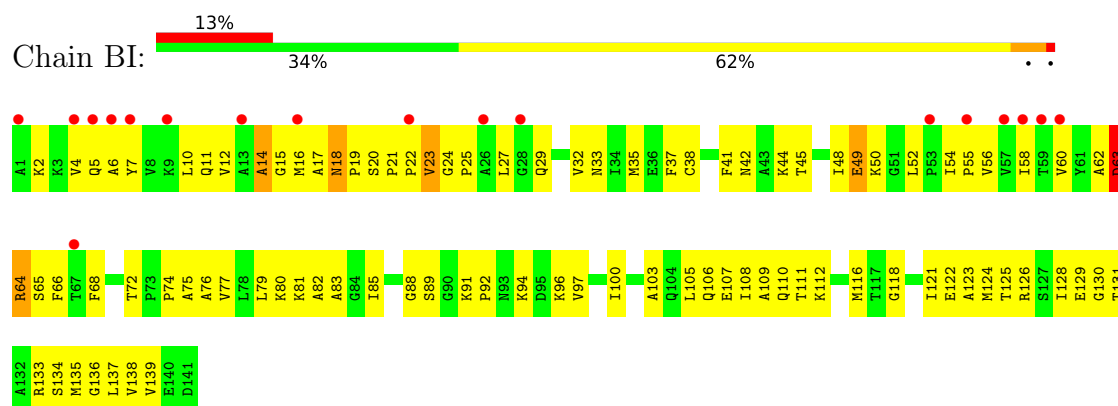
• Molecule 23: 23S rRNA

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U824	A752	C678	A613	U545	A503	A330	C269	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193	G132	U193

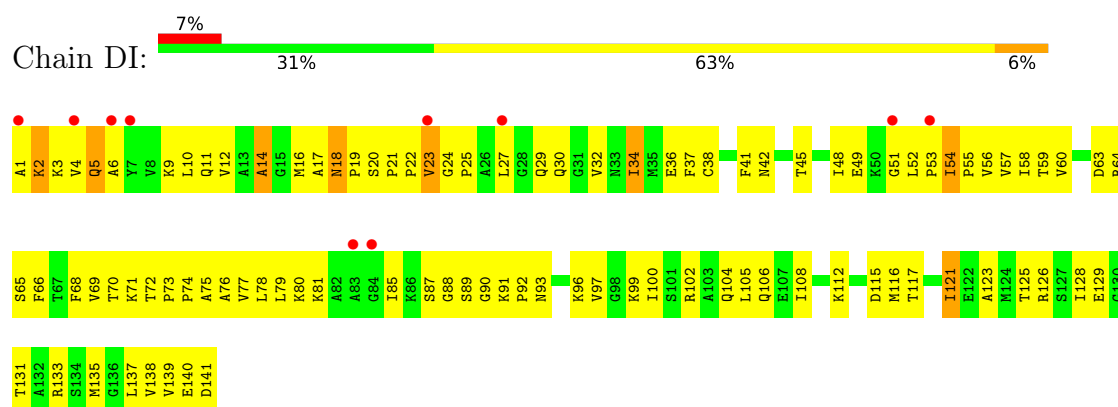




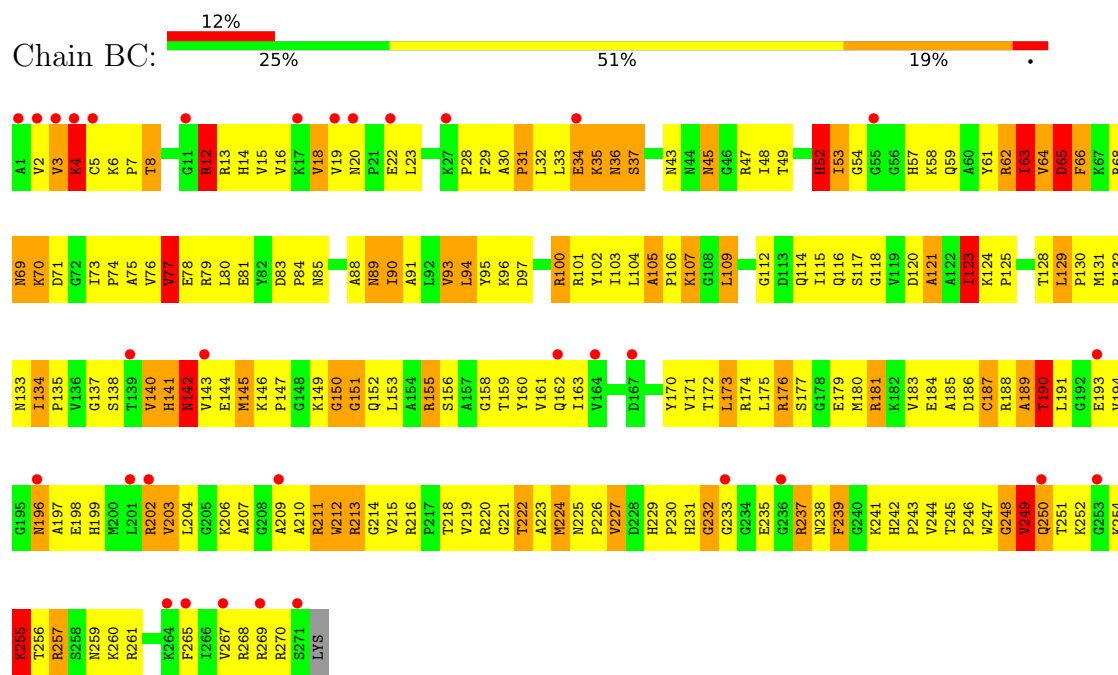
- Molecule 24: 50S ribosomal protein L11



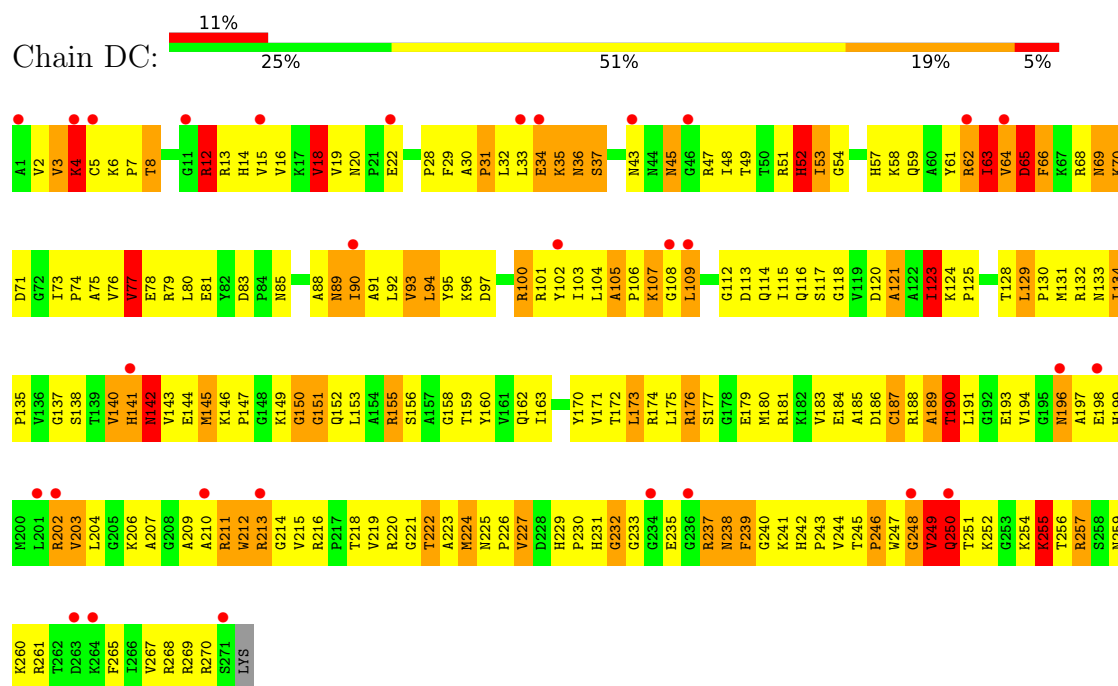
- Molecule 24: 50S ribosomal protein L11



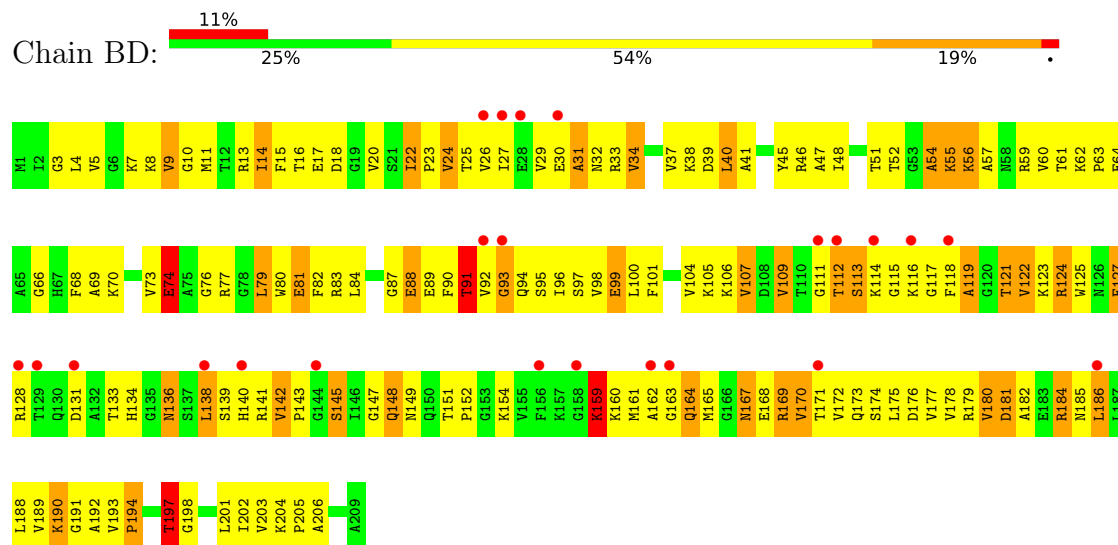
- Molecule 25: 50S ribosomal protein L2



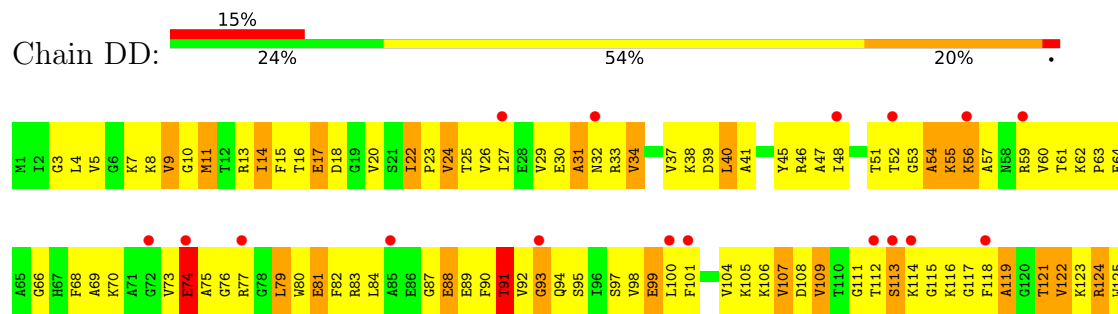
- Molecule 25: 50S ribosomal protein L2

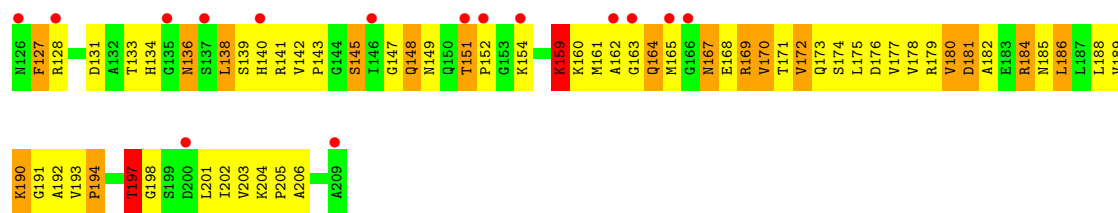


• Molecule 26: 50S ribosomal protein L3

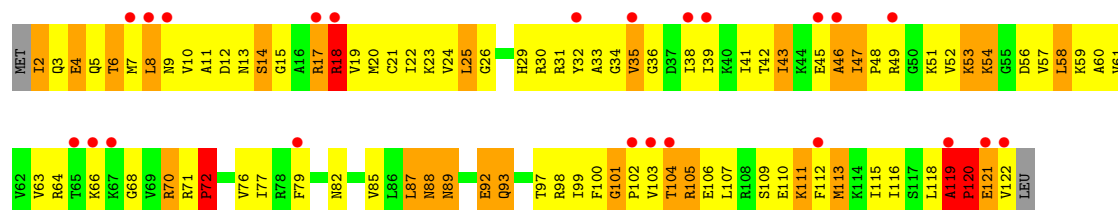


• Molecule 26: 50S ribosomal protein L3

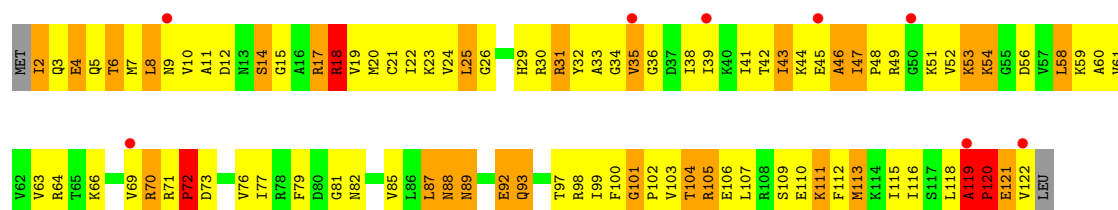




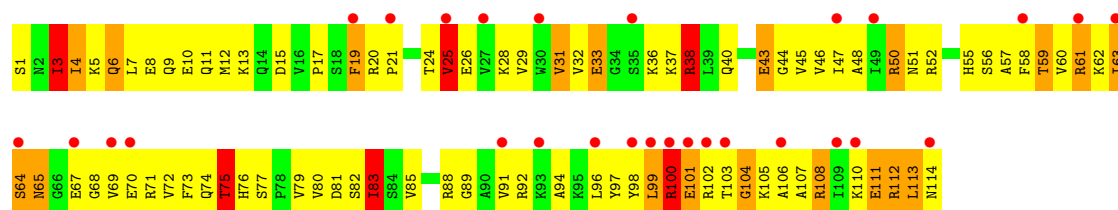
• Molecule 27: 50S ribosomal protein L14



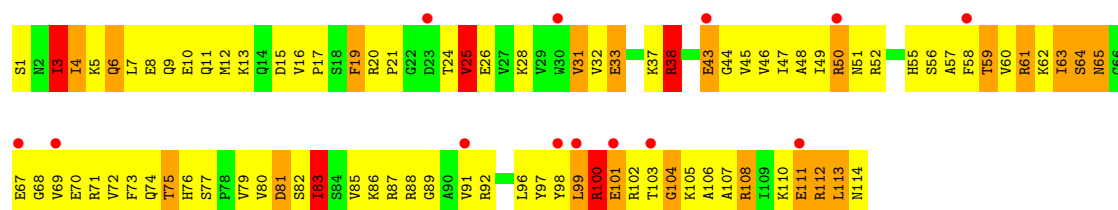
• Molecule 27: 50S ribosomal protein L14



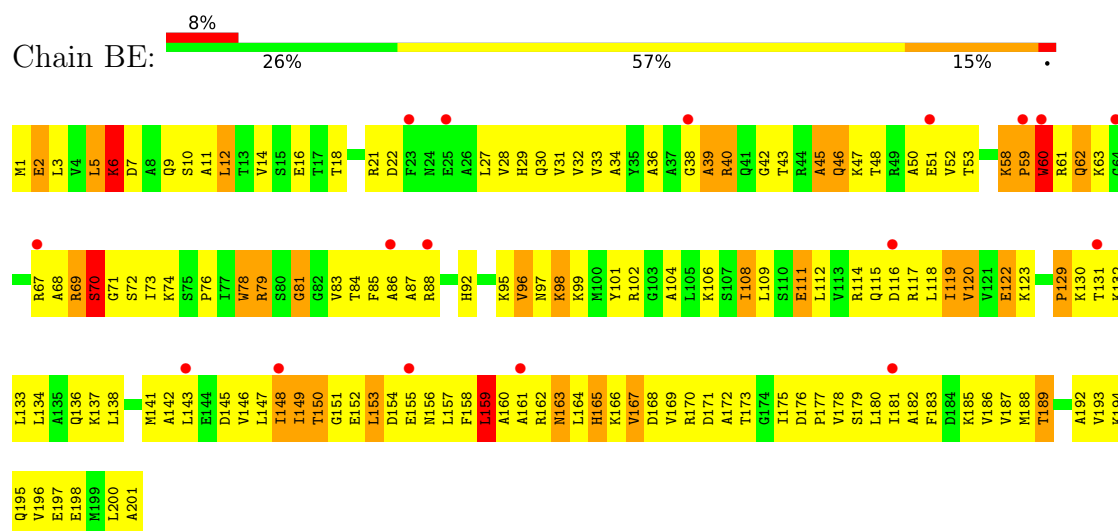
• Molecule 28: 50S ribosomal protein L19



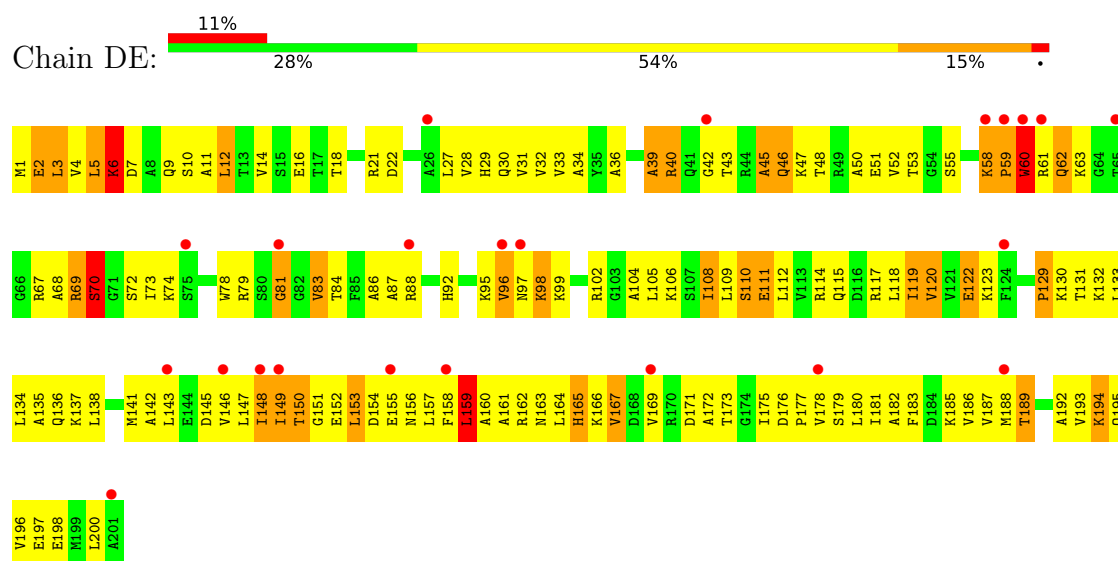
• Molecule 28: 50S ribosomal protein L19



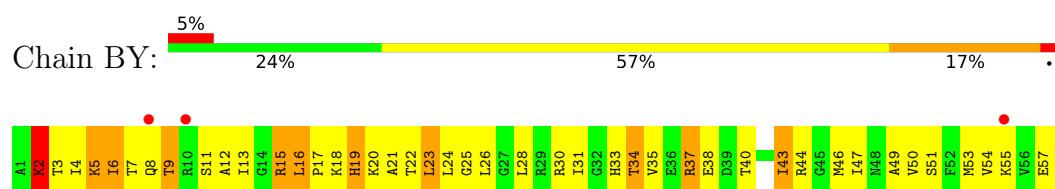
- Molecule 29: 50S ribosomal protein L4



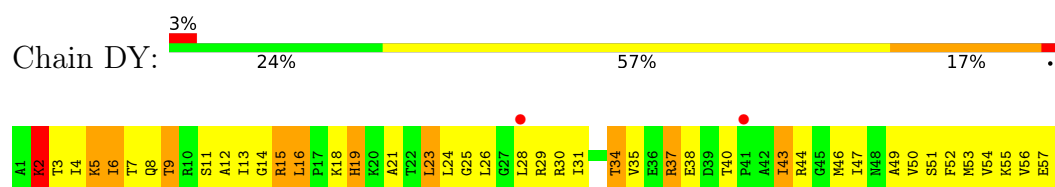
- Molecule 29: 50S ribosomal protein L4



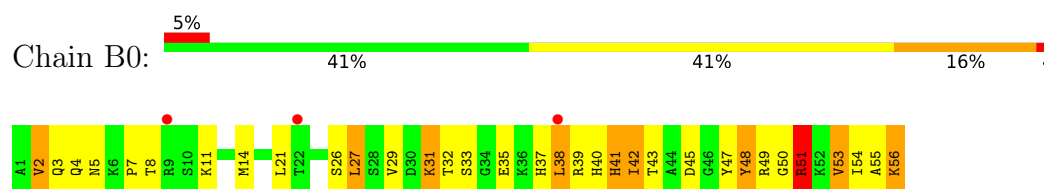
- Molecule 30: 50S ribosomal protein L30



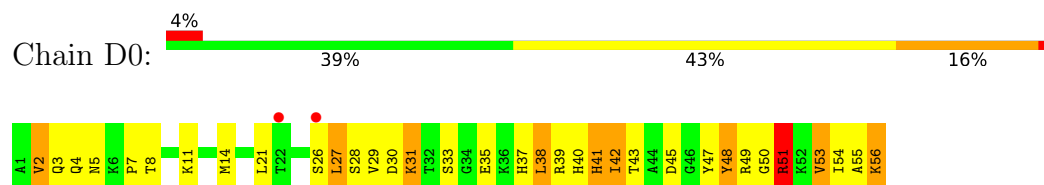
- Molecule 30: 50S ribosomal protein L30



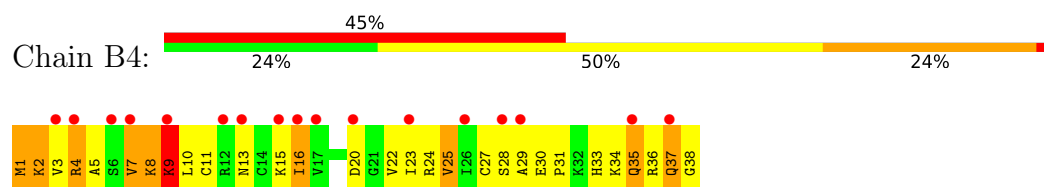
- Molecule 31: 50S ribosomal protein L32



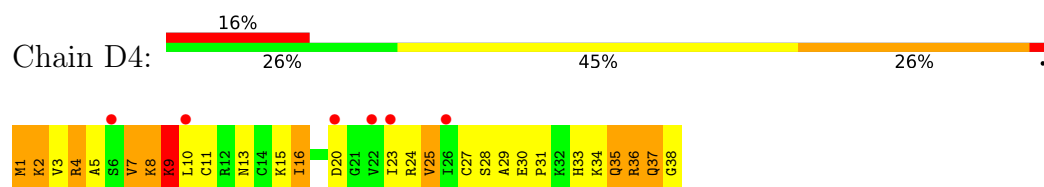
- Molecule 31: 50S ribosomal protein L32



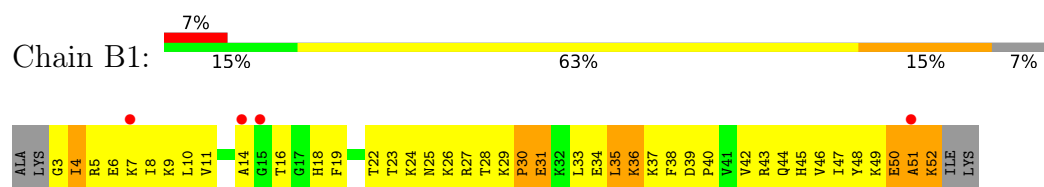
- Molecule 32: 50S ribosomal protein L36



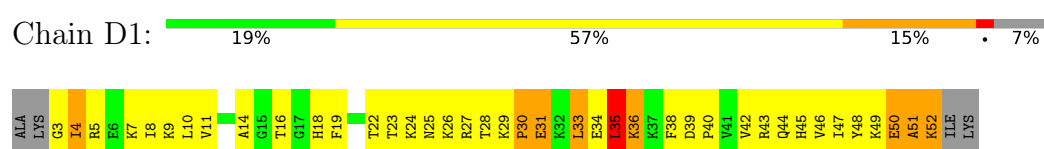
- Molecule 32: 50S ribosomal protein L36



- Molecule 33: 50S ribosomal protein L33

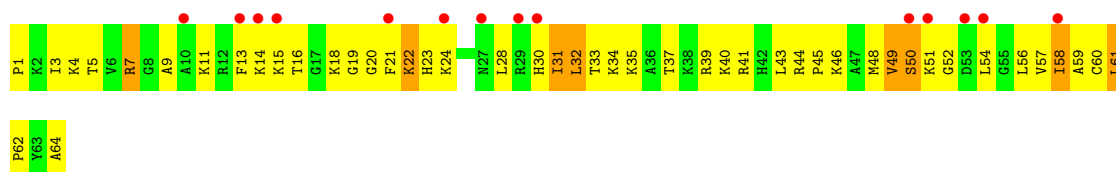


- Molecule 33: 50S ribosomal protein L33

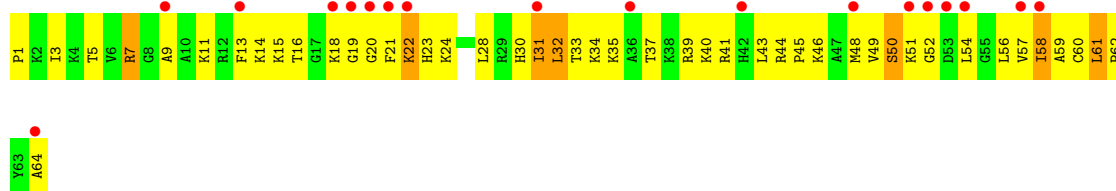


- Molecule 34: 50S ribosomal protein L35

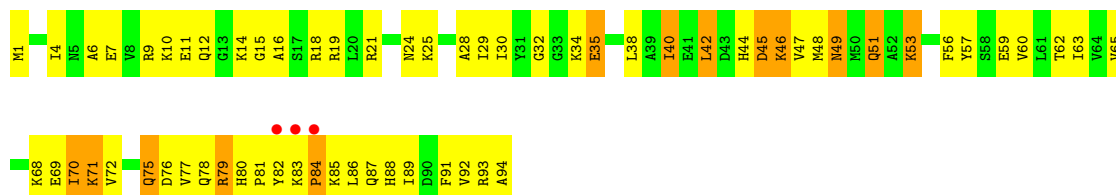




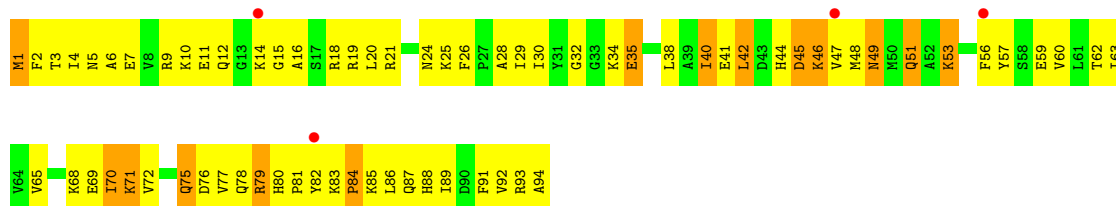
- Molecule 34: 50S ribosomal protein L35



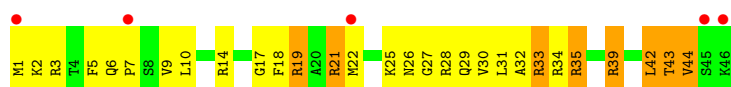
- Molecule 35: 50S ribosomal protein L25



- Molecule 35: 50S ribosomal protein L25



- Molecule 36: 50S ribosomal protein L34

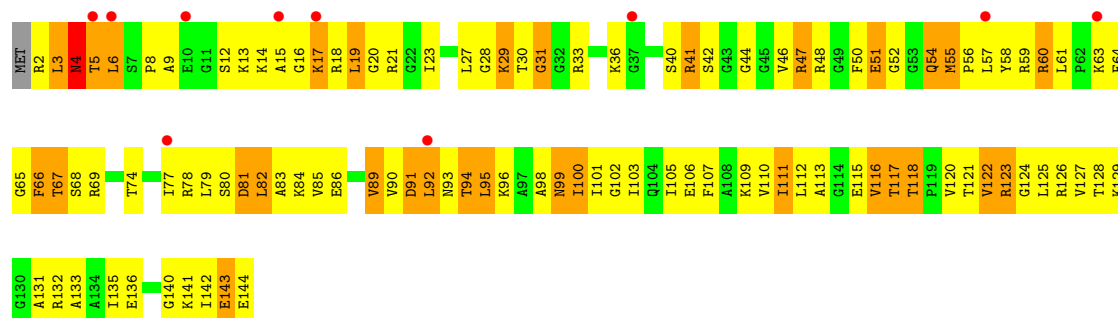


- Molecule 36: 50S ribosomal protein L34

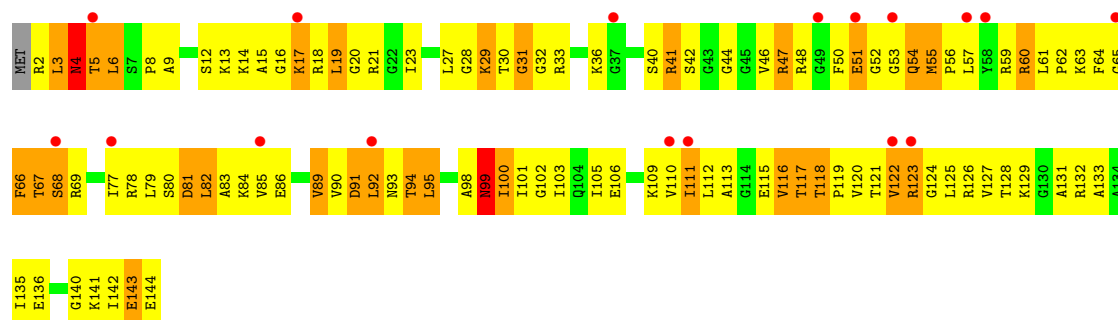




• Molecule 37: 50S ribosomal protein L15



• Molecule 37: 50S ribosomal protein L15



• Molecule 38: 50S ribosomal protein L16

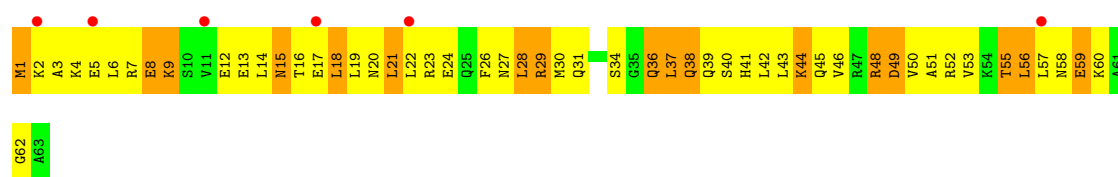
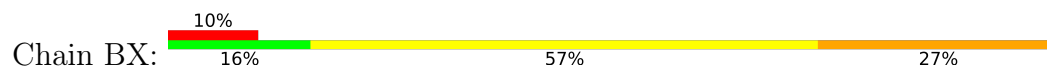


• Molecule 38: 50S ribosomal protein L16

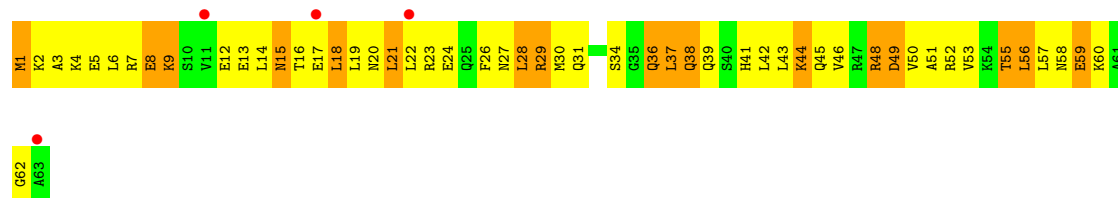
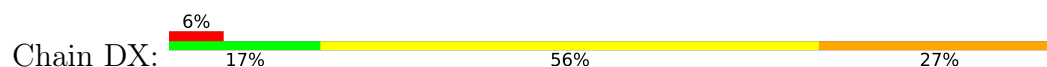




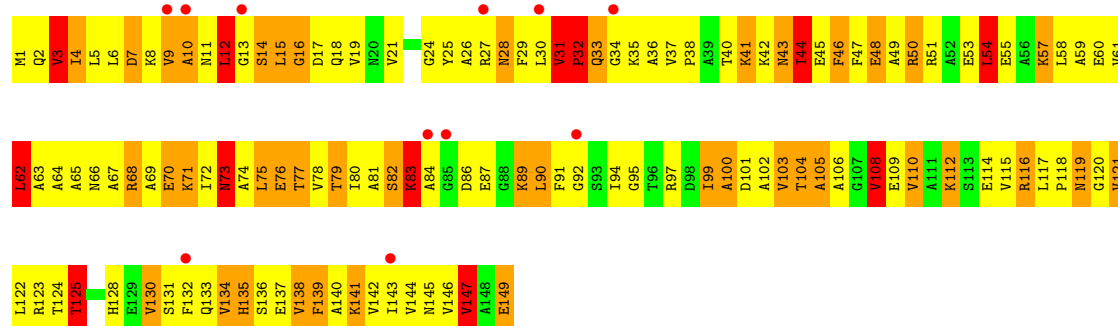
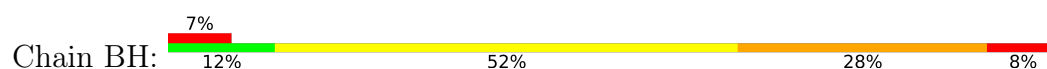
• Molecule 39: 50S ribosomal protein L29



• Molecule 39: 50S ribosomal protein L29

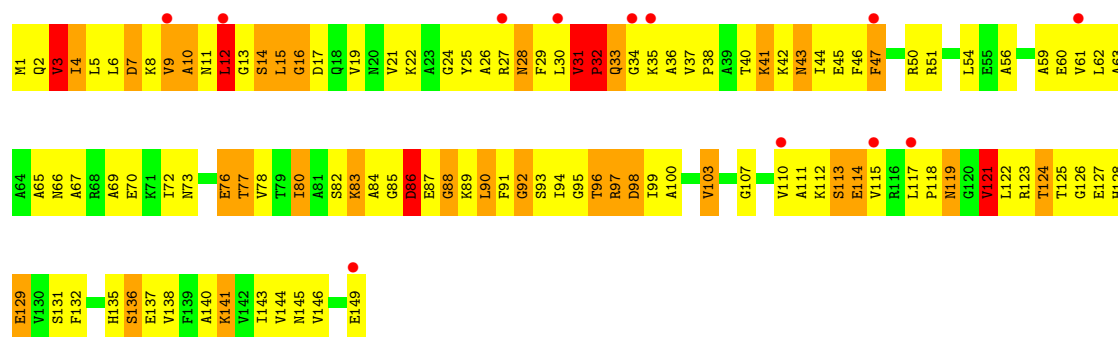


• Molecule 40: 50S ribosomal protein L9

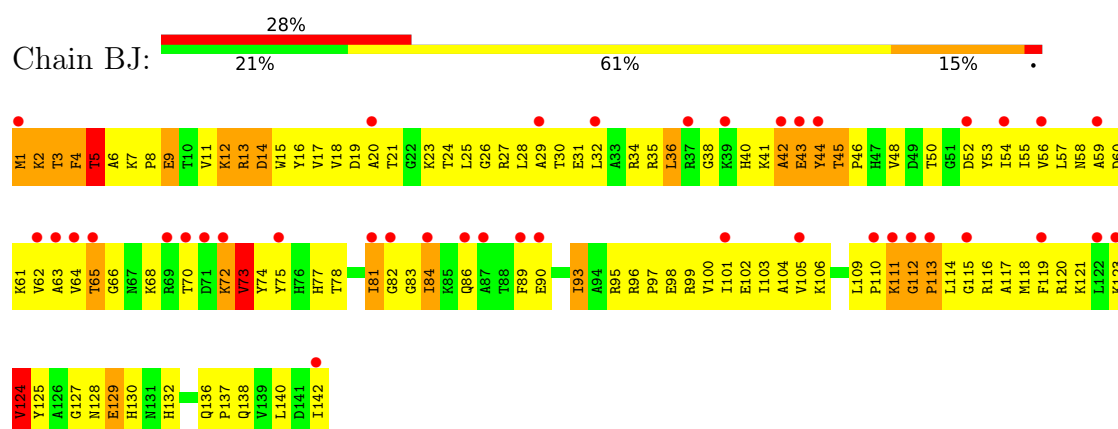


• Molecule 40: 50S ribosomal protein L9

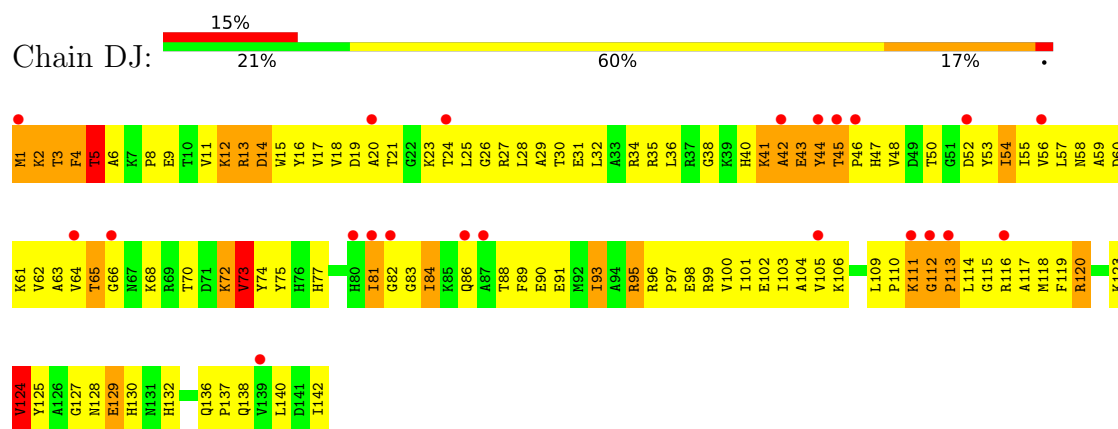




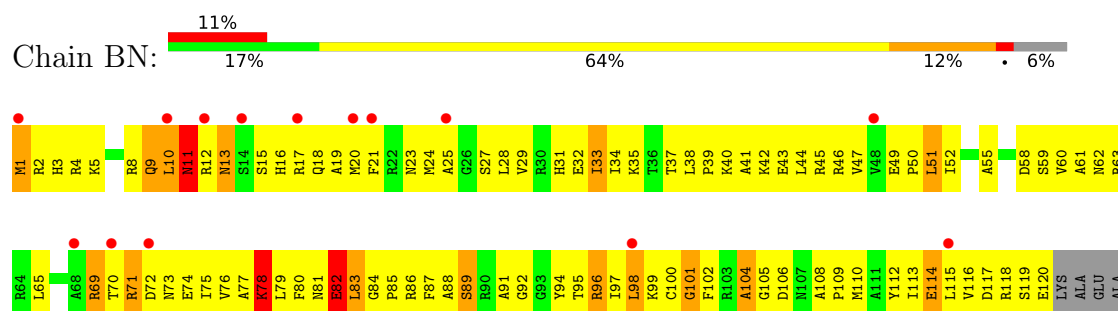
• Molecule 41: 50S ribosomal protein L13



• Molecule 41: 50S ribosomal protein L13

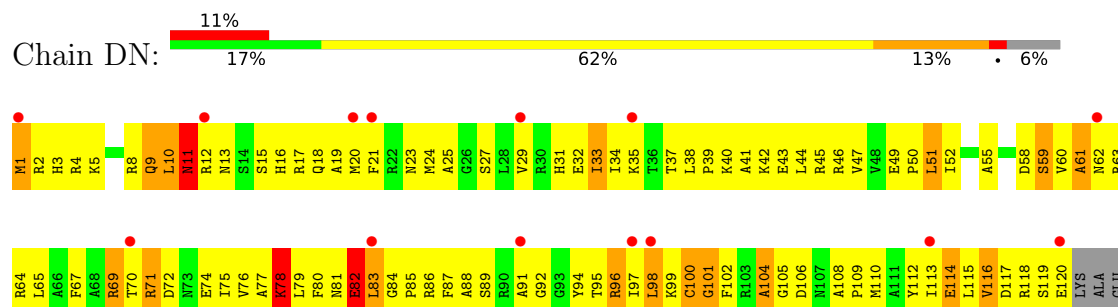


• Molecule 42: 50S ribosomal protein L17



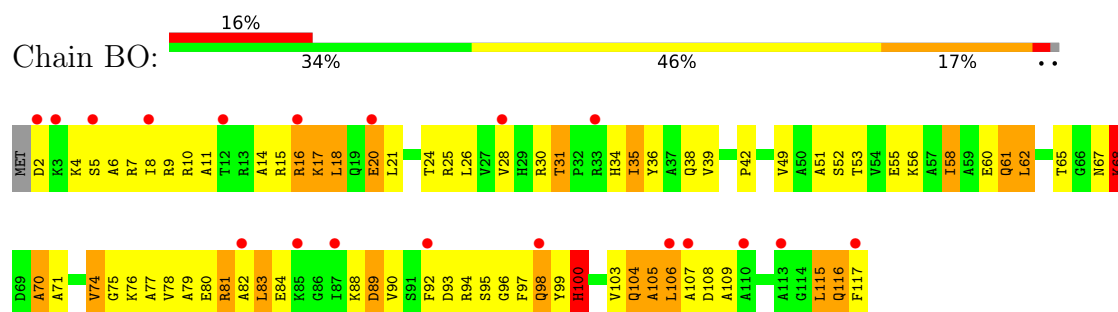
ALA
ALA
GLU

• Molecule 42: 50S ribosomal protein L17

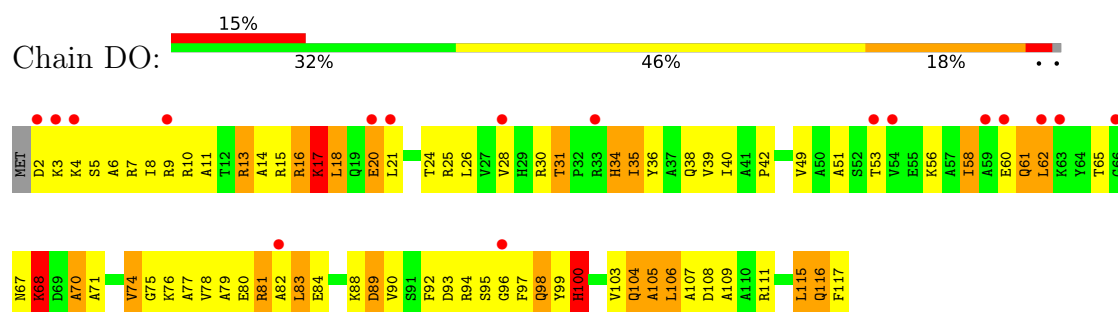


ALA
ALA
GLU

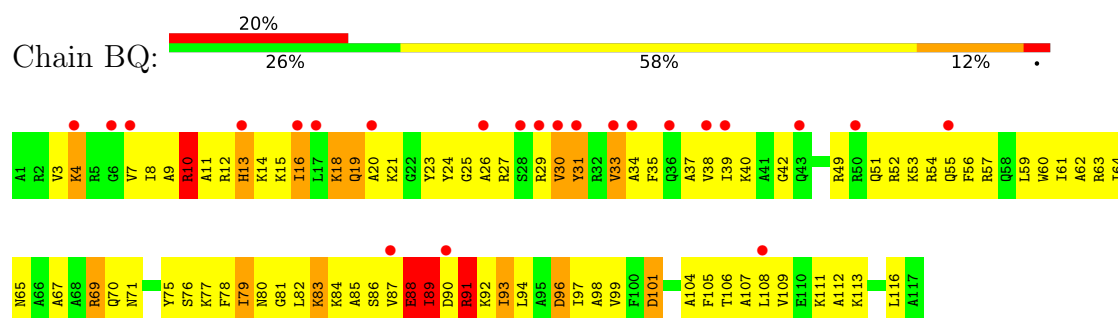
• Molecule 43: 50S ribosomal protein L18



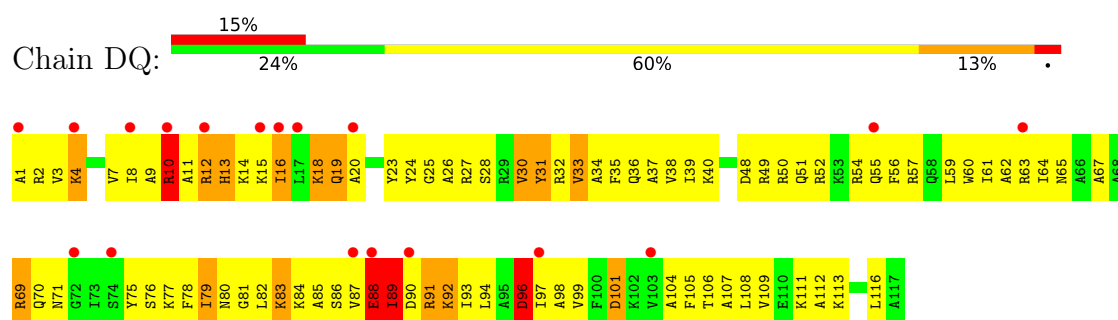
• Molecule 43: 50S ribosomal protein L18



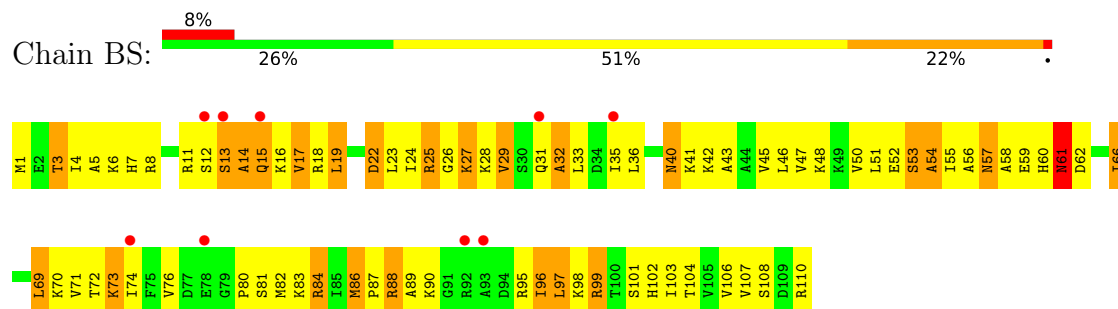
• Molecule 44: 50S ribosomal protein L20



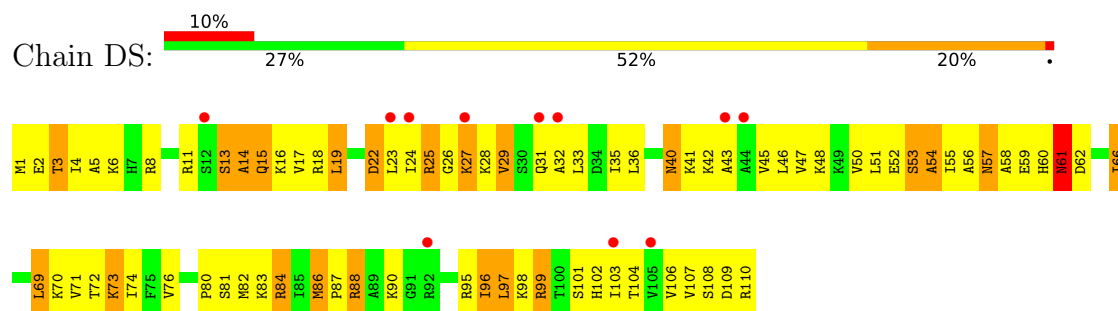
• Molecule 44: 50S ribosomal protein L20



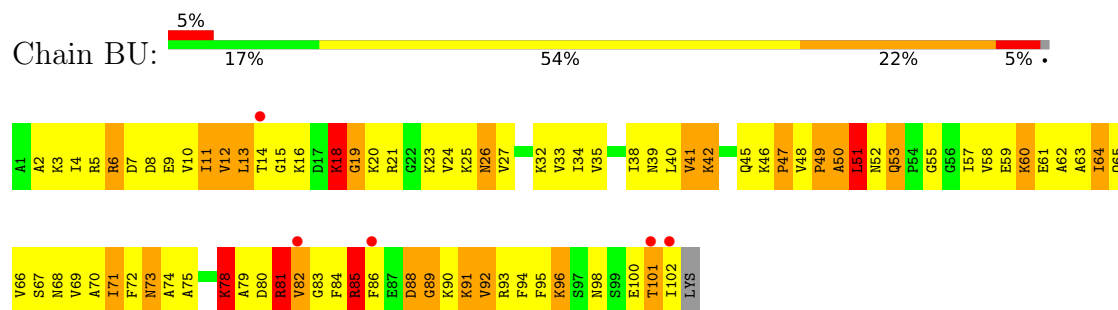
• Molecule 45: 50S ribosomal protein L22



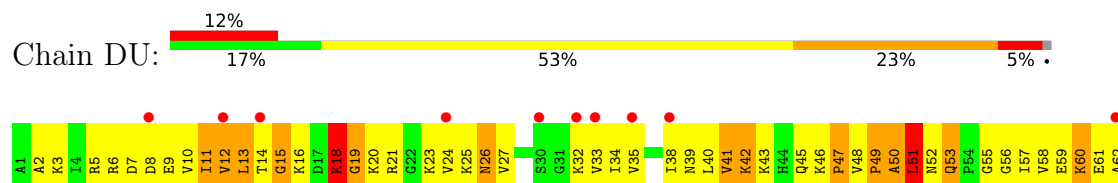
• Molecule 45: 50S ribosomal protein L22

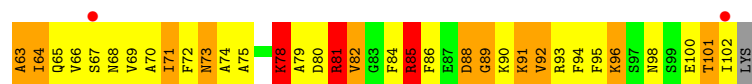


• Molecule 46: 50S ribosomal protein L24

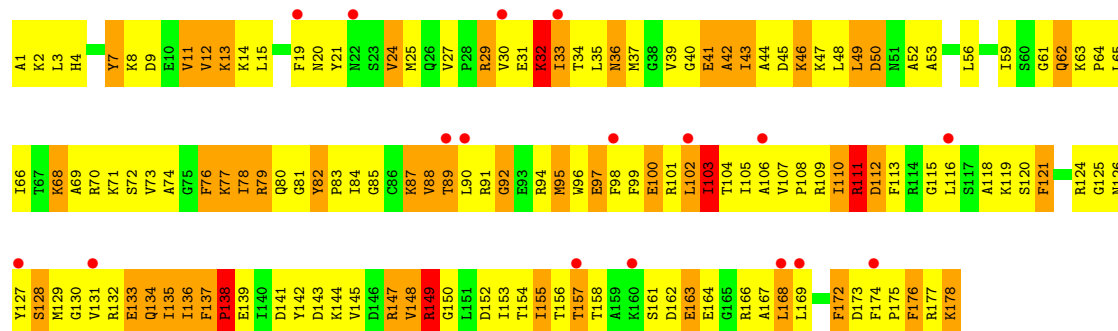
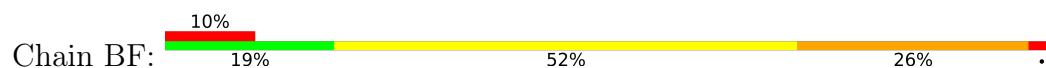


• Molecule 46: 50S ribosomal protein L24

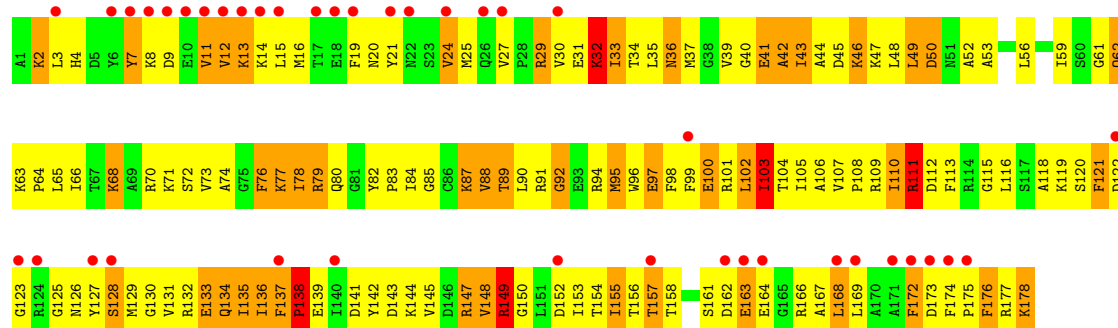
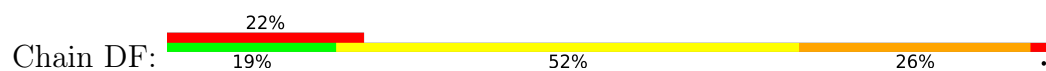




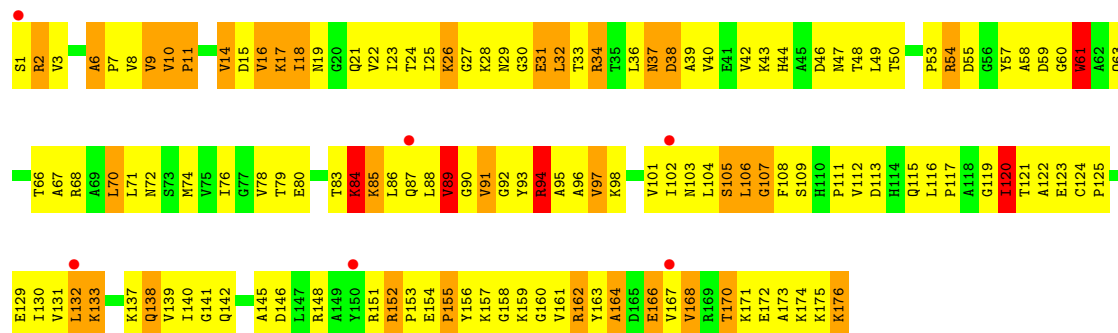
• Molecule 47: 50S ribosomal protein L5



• Molecule 47: 50S ribosomal protein L5

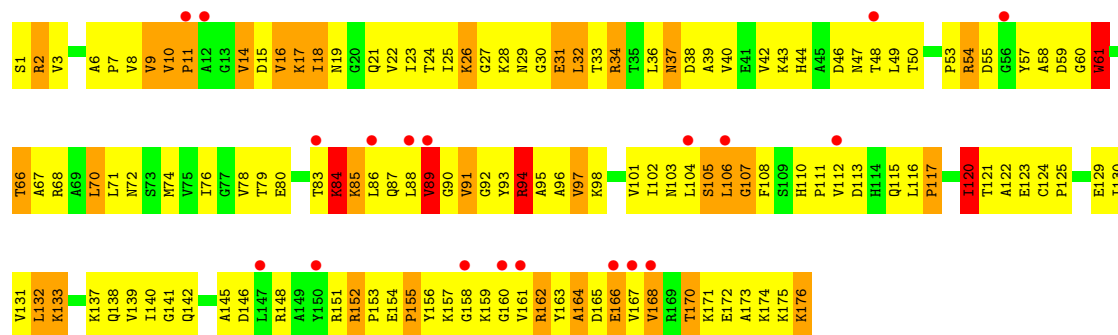


• Molecule 48: 50S ribosomal protein L6

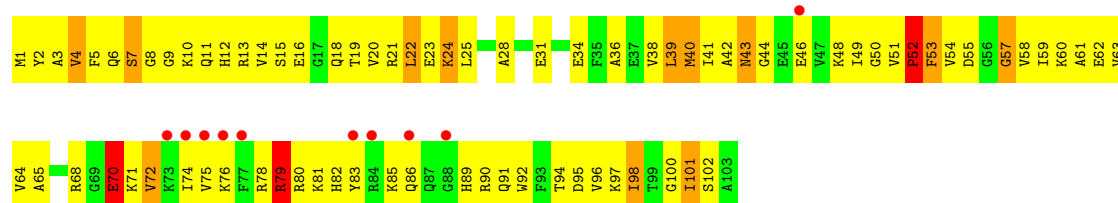


• Molecule 48: 50S ribosomal protein L6

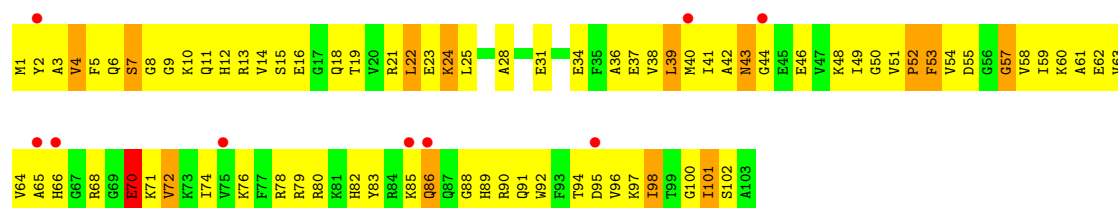




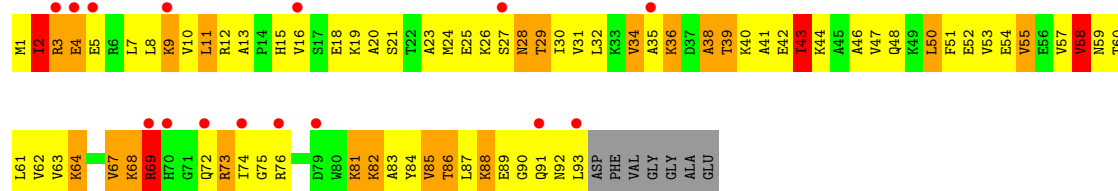
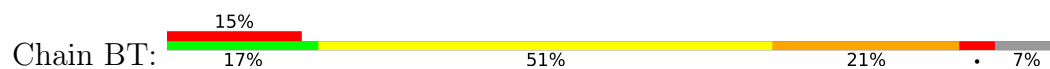
• Molecule 49: 50S ribosomal protein L21



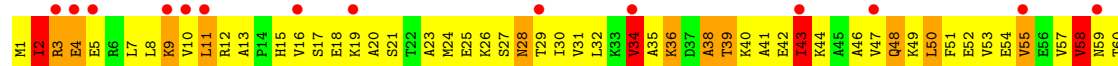
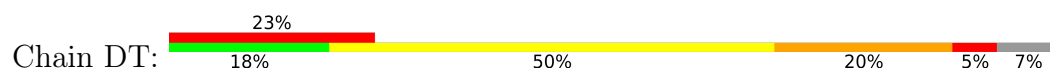
• Molecule 49: 50S ribosomal protein L21

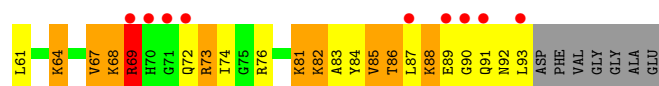


• Molecule 50: 50S ribosomal protein L23

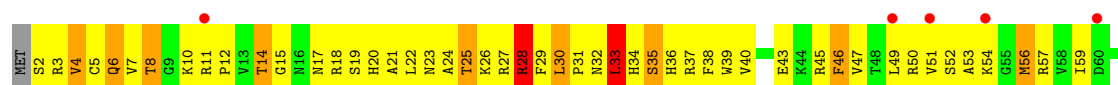


• Molecule 50: 50S ribosomal protein L23

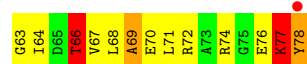
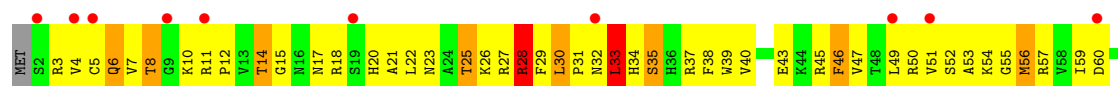




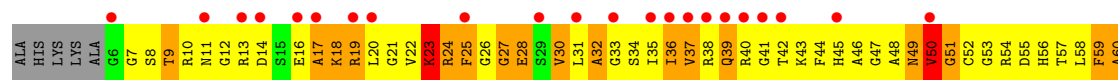
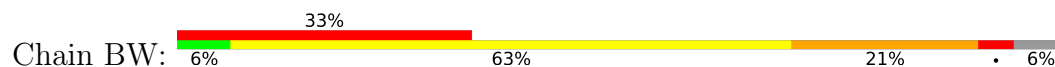
- Molecule 51: 50S ribosomal protein L28



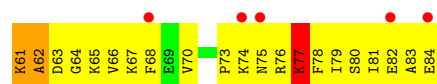
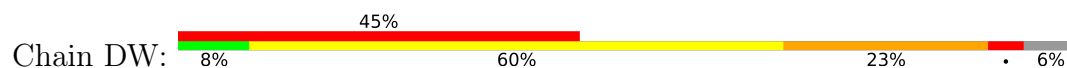
- Molecule 51: 50S ribosomal protein L28



- 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 – 3.21 70.00 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.21) 66.6 (70.00-3.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.274 , 0.309 0.239 , 0.271	Depositor DCC
R_{free} test set	30053 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	284172	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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: NMY, ZN, MG

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	0/36762	0.62	35/57350 (0.1%)
1	CA	0.27	0/36762	0.62	39/57350 (0.1%)
2	AC	0.27	0/1651	0.69	0/2225
2	CC	0.28	0/1651	0.69	0/2225
3	AD	0.26	0/1665	0.70	1/2227 (0.0%)
3	CD	0.26	0/1665	0.69	1/2227 (0.0%)
4	AE	0.29	0/1118	0.79	0/1504
4	CE	0.29	0/1118	0.78	0/1504
5	AF	0.28	0/835	0.70	0/1128
5	CF	0.27	0/835	0.70	0/1128
6	AG	0.28	0/1187	0.79	2/1591 (0.1%)
6	CG	0.28	0/1211	0.80	3/1624 (0.2%)
7	AH	0.28	0/989	0.72	0/1326
7	CH	0.28	0/989	0.74	0/1326
8	AI	0.27	0/1034	0.67	0/1375
8	CI	0.27	0/1034	0.68	0/1375
9	AJ	0.29	0/796	0.77	0/1077
9	CJ	0.29	0/796	0.77	0/1077
10	AK	0.30	0/893	0.76	0/1205
10	CK	0.30	0/893	0.76	0/1205
11	AL	0.28	0/969	0.76	0/1300
11	CL	0.28	0/969	0.75	0/1300
12	AM	0.27	0/892	0.71	0/1193
12	CM	0.28	0/884	0.74	1/1181 (0.1%)
13	AN	0.27	0/785	0.75	1/1043 (0.1%)
13	CN	0.27	0/785	0.75	1/1043 (0.1%)
14	AO	0.27	0/722	0.79	3/964 (0.3%)
14	CO	0.26	0/722	0.78	3/964 (0.3%)
15	AP	0.29	0/659	0.77	1/884 (0.1%)
15	CP	0.28	0/648	0.79	1/870 (0.1%)
16	AQ	0.25	0/657	0.70	0/881
16	CQ	0.25	0/666	0.71	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.29	0/462	0.71	0/621
17	CR	0.29	0/462	0.72	0/621
18	AS	0.27	0/652	0.69	0/877
18	CS	0.28	0/660	0.71	0/888
19	AT	0.29	0/671	0.72	0/888
19	CT	0.28	0/671	0.71	0/888
20	AB	0.29	0/1735	0.74	0/2338
20	CB	0.29	0/1735	0.75	0/2338
21	AU	0.29	0/430	0.90	1/570 (0.2%)
21	CU	0.29	0/430	0.90	1/570 (0.2%)
22	BA	0.27	0/2803	0.64	3/4371 (0.1%)
22	DA	0.27	0/2803	0.65	4/4371 (0.1%)
23	BB	0.27	1/68314 (0.0%)	0.64	70/106569 (0.1%)
23	DB	0.27	3/68314 (0.0%)	0.64	77/106569 (0.1%)
24	BI	0.32	0/1046	0.82	1/1410 (0.1%)
24	DI	0.36	0/1046	0.86	0/1410
25	BC	0.27	0/2121	0.77	2/2852 (0.1%)
25	DC	0.27	0/2121	0.77	2/2852 (0.1%)
26	BD	0.27	0/1586	0.73	1/2134 (0.0%)
26	DD	0.27	0/1586	0.74	1/2134 (0.0%)
27	BK	0.30	0/939	0.87	3/1258 (0.2%)
27	DK	0.30	0/939	0.86	3/1258 (0.2%)
28	BP	0.28	0/929	0.83	3/1242 (0.2%)
28	DP	0.28	0/929	0.85	4/1242 (0.3%)
29	BE	0.27	0/1571	0.85	6/2113 (0.3%)
29	DE	0.27	0/1571	0.85	6/2113 (0.3%)
30	BY	0.30	0/453	0.78	0/605
30	DY	0.30	0/453	0.79	0/605
31	B0	0.27	0/450	0.83	2/599 (0.3%)
31	D0	0.27	0/450	0.83	2/599 (0.3%)
32	B4	0.26	0/303	0.74	1/397 (0.3%)
32	D4	0.27	0/303	0.75	1/397 (0.3%)
33	B1	0.28	0/416	0.73	0/554
33	D1	0.28	0/416	0.72	0/554
34	B3	0.28	0/513	0.73	0/676
34	D3	0.28	0/513	0.73	0/676
35	BV	0.27	0/766	0.72	0/1025
35	DV	0.27	0/766	0.72	0/1025
36	B2	0.29	0/380	0.86	0/498
36	D2	0.29	0/380	0.85	0/498
37	BL	0.29	0/1054	0.82	0/1403
37	DL	0.28	0/1054	0.82	0/1403
38	BM	0.28	0/1093	0.79	1/1460 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.29	0/1093	0.80	1/1460 (0.1%)
39	BX	0.26	0/510	0.87	3/677 (0.4%)
39	DX	0.26	0/510	0.87	3/677 (0.4%)
40	BH	0.29	0/1122	0.75	0/1515
40	DH	0.29	0/1122	0.77	1/1515 (0.1%)
41	BJ	0.28	0/1152	0.76	1/1551 (0.1%)
41	DJ	0.28	0/1152	0.76	1/1551 (0.1%)
42	BN	0.27	0/973	0.85	2/1301 (0.2%)
42	DN	0.27	0/973	0.85	2/1301 (0.2%)
43	BO	0.26	0/902	0.87	6/1209 (0.5%)
43	DO	0.26	0/902	0.87	7/1209 (0.6%)
44	BQ	0.28	0/960	0.93	6/1278 (0.5%)
44	DQ	0.28	0/960	0.93	6/1278 (0.5%)
45	BS	0.28	0/864	0.86	3/1156 (0.3%)
45	DS	0.28	0/864	0.87	3/1156 (0.3%)
46	BU	0.27	0/787	0.75	1/1051 (0.1%)
46	DU	0.27	0/787	0.75	1/1051 (0.1%)
47	BF	0.28	0/1444	0.87	4/1937 (0.2%)
47	DF	0.28	0/1444	0.88	4/1937 (0.2%)
48	BG	0.28	0/1343	0.75	4/1816 (0.2%)
48	DG	0.28	0/1343	0.75	2/1816 (0.1%)
49	BR	0.27	0/829	0.71	0/1107
49	DR	0.26	0/829	0.70	0/1107
50	BT	0.27	0/744	0.96	4/994 (0.4%)
50	DT	0.28	0/744	0.98	5/994 (0.5%)
51	BZ	0.28	0/635	0.88	2/848 (0.2%)
51	DZ	0.28	0/635	0.88	2/848 (0.2%)
52	BW	0.29	0/603	0.83	1/797 (0.1%)
52	DW	0.29	0/603	0.83	1/797 (0.1%)
All	All	0.27	4/306360 (0.0%)	0.68	363/457969 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	13
1	CA	0	11
23	BB	0	43
23	DB	0	42
All	All	0	109

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	2323	G	O3'-P	7.79	1.72	1.61
23	DB	1086	A	C5-C6	-7.32	1.26	1.41
23	BB	1086	A	C5-C6	-7.28	1.26	1.41
23	DB	2318	G	O3'-P	-5.83	1.52	1.61

The worst 5 of 363 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-10.95	75.14	108.00
23	DB	508	A	C4'-C3'-O3'	-10.89	96.67	113.00
23	BB	2204	G	O5'-P-OP2	-10.38	76.86	108.00
23	BB	2791	G	O5'-P-OP1	-10.16	77.53	108.00
23	BB	2790	U	OP1-P-O3'	9.95	137.84	108.00

There are no chirality outliers.

5 of 109 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	78	A	Sidechain
1	AA	86	G	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1154	0
1	CA	32831	0	16521	1153	0
2	AC	1624	0	1699	137	0
2	CC	1624	0	1699	139	0
3	AD	1643	0	1710	168	0
3	CD	1643	0	1710	161	0
4	AE	1105	0	1148	93	0
4	CE	1105	0	1148	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AF	817	0	808	86	0
5	CF	817	0	808	85	0
6	AG	1174	0	1230	99	0
6	CG	1196	0	1246	96	0
7	AH	979	0	1034	91	0
7	CH	979	0	1034	86	0
8	AI	1022	0	1070	130	0
8	CI	1022	0	1070	126	0
9	AJ	786	0	828	88	0
9	CJ	786	0	828	90	0
10	AK	877	0	887	99	0
10	CK	877	0	887	100	0
11	AL	955	0	1019	80	0
11	CL	955	0	1019	79	0
12	AM	883	0	944	123	0
12	CM	876	0	937	120	0
13	AN	774	0	827	114	0
13	CN	774	0	827	114	0
14	AO	714	0	734	59	0
14	CO	714	0	734	53	0
15	AP	649	0	666	56	0
15	CP	638	0	656	53	0
16	AQ	648	0	691	48	0
16	CQ	657	0	702	49	0
17	AR	455	0	478	32	0
17	CR	455	0	478	30	0
18	AS	637	0	665	88	0
18	CS	644	0	675	92	0
19	AT	665	0	714	59	0
19	CT	665	0	714	58	0
20	AB	1704	0	1732	209	0
20	CB	1704	0	1732	210	0
21	AU	425	0	449	62	0
21	CU	425	0	449	62	0
22	BA	2507	0	1270	97	0
22	DA	2507	0	1270	90	0
23	BB	60995	0	30678	2153	0
23	DB	60995	0	30677	2257	0
24	BI	1032	0	1088	118	0
24	DI	1032	0	1088	202	0
25	BC	2082	0	2157	275	0
25	DC	2082	0	2157	259	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	BD	1565	0	1616	219	0
26	DD	1565	0	1616	227	0
27	BK	930	0	1000	121	0
27	DK	930	0	1000	126	0
28	BP	917	0	965	124	0
28	DP	917	0	965	119	0
29	BE	1552	0	1619	194	0
29	DE	1552	0	1619	178	0
30	BY	449	0	491	55	0
30	DY	449	0	491	50	0
31	B0	444	0	461	48	0
31	D0	444	0	461	46	0
32	B4	302	0	340	31	0
32	D4	302	0	341	29	0
33	B1	409	0	440	55	0
33	D1	409	0	440	45	0
34	B3	504	0	574	60	0
34	D3	504	0	574	57	0
35	BV	753	0	780	84	0
35	DV	753	0	780	88	0
36	B2	377	0	418	47	0
36	D2	377	0	418	49	0
37	BL	1045	0	1117	152	0
37	DL	1045	0	1117	160	0
38	BM	1074	0	1157	124	0
38	DM	1074	0	1157	125	0
39	BX	509	0	543	68	0
39	DX	509	0	543	61	0
40	BH	1111	0	1148	206	0
40	DH	1111	0	1148	160	0
41	BJ	1129	0	1162	149	0
41	DJ	1129	0	1162	151	0
42	BN	960	0	1000	127	0
42	DN	960	0	1000	129	0
43	BO	892	0	923	80	0
43	DO	892	0	923	97	0
44	BQ	947	0	1022	147	0
44	DQ	947	0	1022	152	0
45	BS	857	0	922	109	0
45	DS	857	0	922	106	0
46	BU	779	0	834	128	0
46	DU	779	0	834	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BF	1420	0	1460	250	0
47	DF	1420	0	1460	251	0
48	BG	1323	0	1374	193	0
48	DG	1323	0	1374	192	0
49	BR	816	0	839	99	0
49	DR	816	0	839	104	0
50	BT	738	0	807	136	0
50	DT	738	0	807	127	0
51	BZ	625	0	652	85	0
51	DZ	625	0	652	84	0
52	BW	596	0	610	136	0
52	DW	596	0	610	143	0
53	AA	42	0	46	2	0
53	BB	42	0	46	0	0
53	CA	42	0	46	0	0
53	DB	42	0	46	1	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	60	0	0	0	0
54	CE	1	0	0	0	0
54	CN	1	0	0	0	0
54	DB	111	0	0	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	291	0	0	2	0
56	AL	4	0	0	0	0
56	AN	4	0	0	0	0
56	AT	1	0	0	0	0
56	BB	497	0	0	8	0
56	BC	5	0	0	0	0
56	BE	1	0	0	0	0
56	BL	1	0	0	0	0
56	BN	1	0	0	0	0
56	BR	1	0	0	0	0
56	CA	298	0	0	1	0
56	CE	3	0	0	0	0
56	CL	2	0	0	0	0
56	CN	4	0	0	0	0
56	CP	1	0	0	0	0
56	CT	1	0	0	0	0
56	DB	502	0	0	10	0
56	DC	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DE	1	0	0	0	0
56	DL	2	0	0	0	0
56	DR	1	0	0	0	0
All	All	284172	0	190846	16549	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 16549 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	1.38	1.21
21:CU:36:PHE:HB3	21:CU:40:PRO:HD3	1.32	1.11
40:DH:31:VAL:HB	40:DH:32:PRO:HD2	1.30	1.11
6:CG:2:ARG:HH11	6:CG:2:ARG:HB3	1.10	1.11
40:BH:31:VAL:HB	40:BH:32:PRO:HD2	1.29	1.10

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%)	155 (76%)	35 (17%)	14 (7%)	1	6
2	CC	204/232 (88%)	155 (76%)	36 (18%)	13 (6%)	1	7
3	AD	203/205 (99%)	154 (76%)	34 (17%)	15 (7%)	1	5
3	CD	203/205 (99%)	151 (74%)	37 (18%)	15 (7%)	1	5
4	AE	148/166 (89%)	120 (81%)	25 (17%)	3 (2%)	6	30
4	CE	148/166 (89%)	120 (81%)	24 (16%)	4 (3%)	4	24
5	AF	98/135 (73%)	67 (68%)	26 (26%)	5 (5%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CF	98/135 (73%)	65 (66%)	28 (29%)	5 (5%)	1	12
6	AG	148/178 (83%)	124 (84%)	18 (12%)	6 (4%)	2	16
6	CG	150/178 (84%)	127 (85%)	18 (12%)	5 (3%)	3	20
7	AH	127/129 (98%)	98 (77%)	25 (20%)	4 (3%)	3	21
7	CH	127/129 (98%)	97 (76%)	27 (21%)	3 (2%)	4	26
8	AI	125/129 (97%)	95 (76%)	20 (16%)	10 (8%)	1	4
8	CI	125/129 (97%)	97 (78%)	19 (15%)	9 (7%)	1	6
9	AJ	96/103 (93%)	73 (76%)	15 (16%)	8 (8%)	0	4
9	CJ	96/103 (93%)	74 (77%)	13 (14%)	9 (9%)	0	3
10	AK	115/128 (90%)	88 (76%)	22 (19%)	5 (4%)	2	15
10	CK	115/128 (90%)	85 (74%)	25 (22%)	5 (4%)	2	15
11	AL	121/123 (98%)	79 (65%)	33 (27%)	9 (7%)	1	5
11	CL	121/123 (98%)	80 (66%)	32 (26%)	9 (7%)	1	5
12	AM	112/117 (96%)	76 (68%)	27 (24%)	9 (8%)	1	4
12	CM	111/117 (95%)	77 (69%)	26 (23%)	8 (7%)	1	6
13	AN	92/100 (92%)	58 (63%)	24 (26%)	10 (11%)	0	2
13	CN	92/100 (92%)	58 (63%)	23 (25%)	11 (12%)	0	1
14	AO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	3	19
14	CO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	3	19
15	AP	80/82 (98%)	60 (75%)	14 (18%)	6 (8%)	1	5
15	CP	78/82 (95%)	58 (74%)	14 (18%)	6 (8%)	1	5
16	AQ	78/83 (94%)	58 (74%)	16 (20%)	4 (5%)	1	12
16	CQ	79/83 (95%)	59 (75%)	16 (20%)	4 (5%)	1	12
17	AR	53/74 (72%)	43 (81%)	8 (15%)	2 (4%)	2	17
17	CR	53/74 (72%)	43 (81%)	9 (17%)	1 (2%)	6	31
18	AS	77/91 (85%)	54 (70%)	17 (22%)	6 (8%)	1	5
18	CS	78/91 (86%)	54 (69%)	17 (22%)	7 (9%)	0	3
19	AT	83/86 (96%)	65 (78%)	12 (14%)	6 (7%)	1	6
19	CT	83/86 (96%)	66 (80%)	11 (13%)	6 (7%)	1	6
20	AB	216/240 (90%)	150 (69%)	44 (20%)	22 (10%)	0	2
20	CB	216/240 (90%)	147 (68%)	48 (22%)	21 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	AU	49/70 (70%)	28 (57%)	11 (22%)	10 (20%)	0	0
21	CU	49/70 (70%)	28 (57%)	10 (20%)	11 (22%)	0	0
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	2	18
24	DI	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	2	18
25	BC	269/272 (99%)	174 (65%)	49 (18%)	46 (17%)	0	0
25	DC	269/272 (99%)	174 (65%)	47 (18%)	48 (18%)	0	0
26	BD	207/209 (99%)	112 (54%)	63 (30%)	32 (16%)	0	0
26	DD	207/209 (99%)	114 (55%)	58 (28%)	35 (17%)	0	0
27	BK	119/123 (97%)	75 (63%)	28 (24%)	16 (13%)	0	1
27	DK	119/123 (97%)	75 (63%)	27 (23%)	17 (14%)	0	1
28	BP	112/114 (98%)	62 (55%)	35 (31%)	15 (13%)	0	1
28	DP	112/114 (98%)	63 (56%)	34 (30%)	15 (13%)	0	1
29	BE	199/201 (99%)	131 (66%)	51 (26%)	17 (8%)	0	3
29	DE	199/201 (99%)	130 (65%)	53 (27%)	16 (8%)	1	4
30	BY	56/58 (97%)	36 (64%)	14 (25%)	6 (11%)	0	2
30	DY	56/58 (97%)	37 (66%)	13 (23%)	6 (11%)	0	2
31	B0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	0	3
31	D0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	0	3
32	B4	36/38 (95%)	21 (58%)	7 (19%)	8 (22%)	0	0
32	D4	36/38 (95%)	20 (56%)	7 (19%)	9 (25%)	0	0
33	B1	48/54 (89%)	37 (77%)	5 (10%)	6 (12%)	0	1
33	D1	48/54 (89%)	37 (77%)	5 (10%)	6 (12%)	0	1
34	B3	62/64 (97%)	44 (71%)	13 (21%)	5 (8%)	1	4
34	D3	62/64 (97%)	44 (71%)	13 (21%)	5 (8%)	1	4
35	BV	92/94 (98%)	65 (71%)	23 (25%)	4 (4%)	2	15
35	DV	92/94 (98%)	65 (71%)	23 (25%)	4 (4%)	2	15
36	B2	44/46 (96%)	29 (66%)	14 (32%)	1 (2%)	5	27
36	D2	44/46 (96%)	28 (64%)	15 (34%)	1 (2%)	5	27
37	BL	141/144 (98%)	88 (62%)	30 (21%)	23 (16%)	0	0
37	DL	141/144 (98%)	88 (62%)	29 (21%)	24 (17%)	0	0
38	BM	134/136 (98%)	86 (64%)	31 (23%)	17 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DM	134/136 (98%)	86 (64%)	32 (24%)	16 (12%)	0	1
39	BX	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	0	4
39	DX	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	0	4
40	BH	147/149 (99%)	77 (52%)	41 (28%)	29 (20%)	0	0
40	DH	147/149 (99%)	85 (58%)	39 (26%)	23 (16%)	0	0
41	BJ	140/142 (99%)	88 (63%)	36 (26%)	16 (11%)	0	2
41	DJ	140/142 (99%)	89 (64%)	33 (24%)	18 (13%)	0	1
42	BN	118/127 (93%)	72 (61%)	34 (29%)	12 (10%)	0	2
42	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	0	2
43	BO	114/117 (97%)	84 (74%)	25 (22%)	5 (4%)	2	14
43	DO	114/117 (97%)	83 (73%)	25 (22%)	6 (5%)	1	11
44	BQ	115/117 (98%)	73 (64%)	34 (30%)	8 (7%)	1	6
44	DQ	115/117 (98%)	70 (61%)	38 (33%)	7 (6%)	1	9
45	BS	108/110 (98%)	69 (64%)	28 (26%)	11 (10%)	0	2
45	DS	108/110 (98%)	69 (64%)	29 (27%)	10 (9%)	0	3
46	BU	100/103 (97%)	53 (53%)	25 (25%)	22 (22%)	0	0
46	DU	100/103 (97%)	54 (54%)	23 (23%)	23 (23%)	0	0
47	BF	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0	1
47	DF	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0	1
48	BG	174/176 (99%)	100 (58%)	48 (28%)	26 (15%)	0	1
48	DG	174/176 (99%)	101 (58%)	48 (28%)	25 (14%)	0	1
49	BR	101/103 (98%)	65 (64%)	25 (25%)	11 (11%)	0	2
49	DR	101/103 (98%)	64 (63%)	28 (28%)	9 (9%)	0	3
50	BT	91/100 (91%)	50 (55%)	31 (34%)	10 (11%)	0	2
50	DT	91/100 (91%)	51 (56%)	30 (33%)	10 (11%)	0	2
51	BZ	75/78 (96%)	53 (71%)	18 (24%)	4 (5%)	1	11
51	DZ	75/78 (96%)	50 (67%)	21 (28%)	4 (5%)	1	11
52	BW	77/84 (92%)	29 (38%)	27 (35%)	21 (27%)	0	0
52	DW	77/84 (92%)	29 (38%)	26 (34%)	22 (29%)	0	0
All	All	11241/11914 (94%)	7579 (67%)	2528 (22%)	1134 (10%)	0	2

5 of 1134 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	54	ILE
2	AC	153	SER
2	AC	205	GLU
5	AF	92	THR

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%)	139 (82%)	31 (18%)	2	8
2	CC	170/189 (90%)	139 (82%)	31 (18%)	2	8
3	AD	172/172 (100%)	147 (86%)	25 (14%)	3	15
3	CD	172/172 (100%)	145 (84%)	27 (16%)	2	12
4	AE	113/125 (90%)	93 (82%)	20 (18%)	2	9
4	CE	113/125 (90%)	93 (82%)	20 (18%)	2	9
5	AF	87/116 (75%)	69 (79%)	18 (21%)	1	6
5	CF	87/116 (75%)	69 (79%)	18 (21%)	1	6
6	AG	123/146 (84%)	103 (84%)	20 (16%)	2	11
6	CG	125/146 (86%)	105 (84%)	20 (16%)	2	12
7	AH	104/104 (100%)	94 (90%)	10 (10%)	8	31
7	CH	104/104 (100%)	94 (90%)	10 (10%)	8	31
8	AI	105/106 (99%)	88 (84%)	17 (16%)	2	11
8	CI	105/106 (99%)	86 (82%)	19 (18%)	2	8
9	AJ	86/90 (96%)	71 (83%)	15 (17%)	2	9
9	CJ	86/90 (96%)	72 (84%)	14 (16%)	2	11
10	AK	90/98 (92%)	79 (88%)	11 (12%)	5	21
10	CK	90/98 (92%)	79 (88%)	11 (12%)	5	21
11	AL	103/103 (100%)	91 (88%)	12 (12%)	5	23
11	CL	103/103 (100%)	91 (88%)	12 (12%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AM	92/95 (97%)	77 (84%)	15 (16%)	2	11
12	CM	91/95 (96%)	76 (84%)	15 (16%)	2	10
13	AN	79/83 (95%)	64 (81%)	15 (19%)	1	8
13	CN	79/83 (95%)	64 (81%)	15 (19%)	1	8
14	AO	76/77 (99%)	70 (92%)	6 (8%)	11	39
14	CO	76/77 (99%)	70 (92%)	6 (8%)	11	39
15	AP	65/65 (100%)	59 (91%)	6 (9%)	8	32
15	CP	65/65 (100%)	59 (91%)	6 (9%)	8	32
16	AQ	74/77 (96%)	64 (86%)	10 (14%)	4	18
16	CQ	75/77 (97%)	65 (87%)	10 (13%)	4	18
17	AR	48/64 (75%)	41 (85%)	7 (15%)	3	15
17	CR	48/64 (75%)	41 (85%)	7 (15%)	3	15
18	AS	70/78 (90%)	55 (79%)	15 (21%)	1	6
18	CS	71/78 (91%)	55 (78%)	16 (22%)	1	5
19	AT	65/65 (100%)	54 (83%)	11 (17%)	2	10
19	CT	65/65 (100%)	53 (82%)	12 (18%)	1	8
20	AB	180/198 (91%)	146 (81%)	34 (19%)	1	8
20	CB	180/198 (91%)	146 (81%)	34 (19%)	1	8
21	AU	44/60 (73%)	31 (70%)	13 (30%)	0	1
21	CU	44/60 (73%)	31 (70%)	13 (30%)	0	1
24	BI	109/109 (100%)	108 (99%)	1 (1%)	70	79
24	DI	109/109 (100%)	105 (96%)	4 (4%)	30	60
25	BC	216/217 (100%)	177 (82%)	39 (18%)	2	8
25	DC	216/217 (100%)	177 (82%)	39 (18%)	2	8
26	BD	164/164 (100%)	138 (84%)	26 (16%)	2	12
26	DD	164/164 (100%)	138 (84%)	26 (16%)	2	12
27	BK	102/104 (98%)	81 (79%)	21 (21%)	1	6
27	DK	102/104 (98%)	81 (79%)	21 (21%)	1	6
28	BP	99/99 (100%)	79 (80%)	20 (20%)	1	7
28	DP	99/99 (100%)	80 (81%)	19 (19%)	1	8
29	BE	165/165 (100%)	139 (84%)	26 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DE	165/165 (100%)	138 (84%)	27 (16%)	2	11
30	BY	48/48 (100%)	38 (79%)	10 (21%)	1	6
30	DY	48/48 (100%)	37 (77%)	11 (23%)	1	4
31	B0	47/47 (100%)	37 (79%)	10 (21%)	1	6
31	D0	47/47 (100%)	37 (79%)	10 (21%)	1	6
32	B4	34/34 (100%)	27 (79%)	7 (21%)	1	6
32	D4	34/34 (100%)	28 (82%)	6 (18%)	2	9
33	B1	45/48 (94%)	41 (91%)	4 (9%)	9	33
33	D1	45/48 (94%)	39 (87%)	6 (13%)	4	18
34	B3	51/51 (100%)	47 (92%)	4 (8%)	11	39
34	D3	51/51 (100%)	48 (94%)	3 (6%)	18	48
35	BV	78/78 (100%)	63 (81%)	15 (19%)	1	8
35	DV	78/78 (100%)	62 (80%)	16 (20%)	1	6
36	B2	38/38 (100%)	31 (82%)	7 (18%)	1	8
36	D2	38/38 (100%)	31 (82%)	7 (18%)	1	8
37	BL	102/103 (99%)	86 (84%)	16 (16%)	2	12
37	DL	102/103 (99%)	86 (84%)	16 (16%)	2	12
38	BM	109/109 (100%)	89 (82%)	20 (18%)	2	8
38	DM	109/109 (100%)	88 (81%)	21 (19%)	1	7
39	BX	55/55 (100%)	41 (74%)	14 (26%)	0	3
39	DX	55/55 (100%)	41 (74%)	14 (26%)	0	3
40	BH	114/114 (100%)	65 (57%)	49 (43%)	0	0
40	DH	114/114 (100%)	90 (79%)	24 (21%)	1	6
41	BJ	116/116 (100%)	101 (87%)	15 (13%)	4	19
41	DJ	116/116 (100%)	101 (87%)	15 (13%)	4	19
42	BN	100/103 (97%)	85 (85%)	15 (15%)	3	14
42	DN	100/103 (97%)	84 (84%)	16 (16%)	2	12
43	BO	86/87 (99%)	68 (79%)	18 (21%)	1	6
43	DO	86/87 (99%)	68 (79%)	18 (21%)	1	6
44	BQ	89/89 (100%)	75 (84%)	14 (16%)	2	12
44	DQ	89/89 (100%)	75 (84%)	14 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BS	93/93 (100%)	79 (85%)	14 (15%)	3	13
45	DS	93/93 (100%)	81 (87%)	12 (13%)	4	19
46	BU	83/84 (99%)	66 (80%)	17 (20%)	1	6
46	DU	83/84 (99%)	66 (80%)	17 (20%)	1	6
47	BF	149/149 (100%)	115 (77%)	34 (23%)	1	4
47	DF	149/149 (100%)	115 (77%)	34 (23%)	1	4
48	BG	137/137 (100%)	113 (82%)	24 (18%)	2	9
48	DG	137/137 (100%)	113 (82%)	24 (18%)	2	9
49	BR	84/84 (100%)	71 (84%)	13 (16%)	2	13
49	DR	84/84 (100%)	73 (87%)	11 (13%)	4	19
50	BT	80/84 (95%)	61 (76%)	19 (24%)	1	4
50	DT	80/84 (95%)	61 (76%)	19 (24%)	1	4
51	BZ	67/68 (98%)	51 (76%)	16 (24%)	1	4
51	DZ	67/68 (98%)	52 (78%)	15 (22%)	1	5
52	BW	59/62 (95%)	47 (80%)	12 (20%)	1	6
52	DW	59/62 (95%)	47 (80%)	12 (20%)	1	6
All	All	9333/9700 (96%)	7729 (83%)	1604 (17%)	2	10

5 of 1604 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	CG	152	HIS
25	DC	100	ARG
52	DW	49	ASN
8	CI	110	VAL
6	CG	129	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 392 such sidechains are listed below:

Mol	Chain	Res	Type
8	CI	36	GLN
25	DC	114	GLN
10	CK	39	ASN
18	CS	13	HIS
27	DK	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	239 (15%)	16 (1%)
1	CA	1529/1542 (99%)	229 (14%)	17 (1%)
22	BA	116/120 (96%)	17 (14%)	1 (0%)
22	DA	116/120 (96%)	17 (14%)	1 (0%)
23	BB	2837/2904 (97%)	435 (15%)	18 (0%)
23	DB	2837/2904 (97%)	434 (15%)	20 (0%)
All	All	8964/9132 (98%)	1371 (15%)	73 (0%)

5 of 1371 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	31	G
1	AA	32	A

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	DB	546	U
23	DB	2832	U
23	DB	858	G
23	DB	2213	U
23	BB	1419	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	NMY	AA	1601	-	43,45,45	1.85	11 (25%)	62,67,67	1.18	5 (8%)
53	NMY	CA	1601	-	43,45,45	1.85	11 (25%)	62,67,67	1.28	7 (11%)
53	NMY	BB	3001	-	43,45,45	1.85	11 (25%)	62,67,67	1.19	6 (9%)
53	NMY	DB	3001	-	43,45,45	1.91	11 (25%)	62,67,67	1.31	6 (9%)

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
53	NMY	AA	1601	-	-	3/18/94/94	0/4/4/4
53	NMY	CA	1601	-	-	5/18/94/94	0/4/4/4
53	NMY	BB	3001	-	-	4/18/94/94	0/4/4/4
53	NMY	DB	3001	-	-	4/18/94/94	0/4/4/4

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	CA	1601	NMY	O22-C18	4.73	1.54	1.41
53	BB	3001	NMY	C3-C2	4.72	1.59	1.53
53	DB	3001	NMY	C3-C2	4.71	1.59	1.53
53	AA	1601	NMY	C3-C2	4.68	1.59	1.53
53	AA	1601	NMY	O22-C18	4.66	1.53	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DB	3001	NMY	O11-C13-O16	4.94	116.41	111.37
53	DB	3001	NMY	O18-C18-C19	4.31	115.12	108.08
53	CA	1601	NMY	O18-C18-C19	4.03	114.67	108.08
53	BB	3001	NMY	O18-C18-C19	3.90	114.46	108.08
53	AA	1601	NMY	O18-C18-C19	3.76	114.24	108.08

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

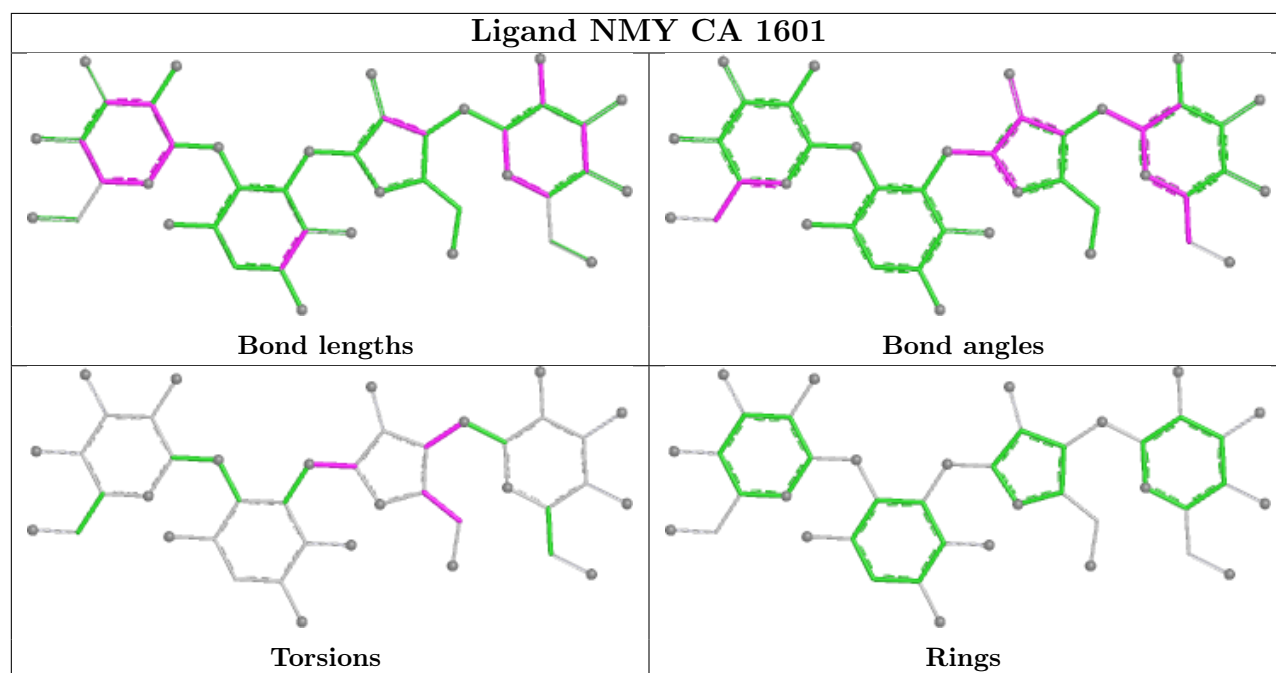
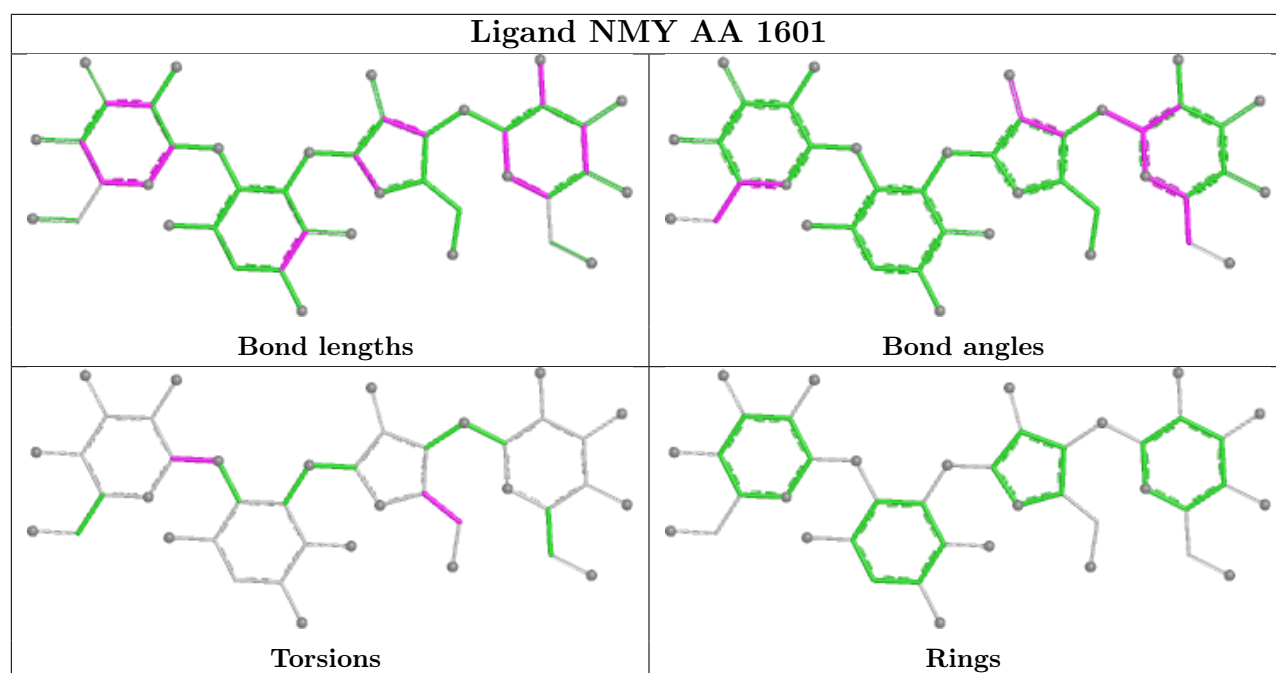
Mol	Chain	Res	Type	Atoms
53	AA	1601	NMY	O16-C16-C17-O17
53	BB	3001	NMY	C19-C18-O18-C15
53	CA	1601	NMY	C14-C13-O11-C11
53	DB	3001	NMY	C19-C18-O18-C15
53	CA	1601	NMY	O16-C16-C17-O17

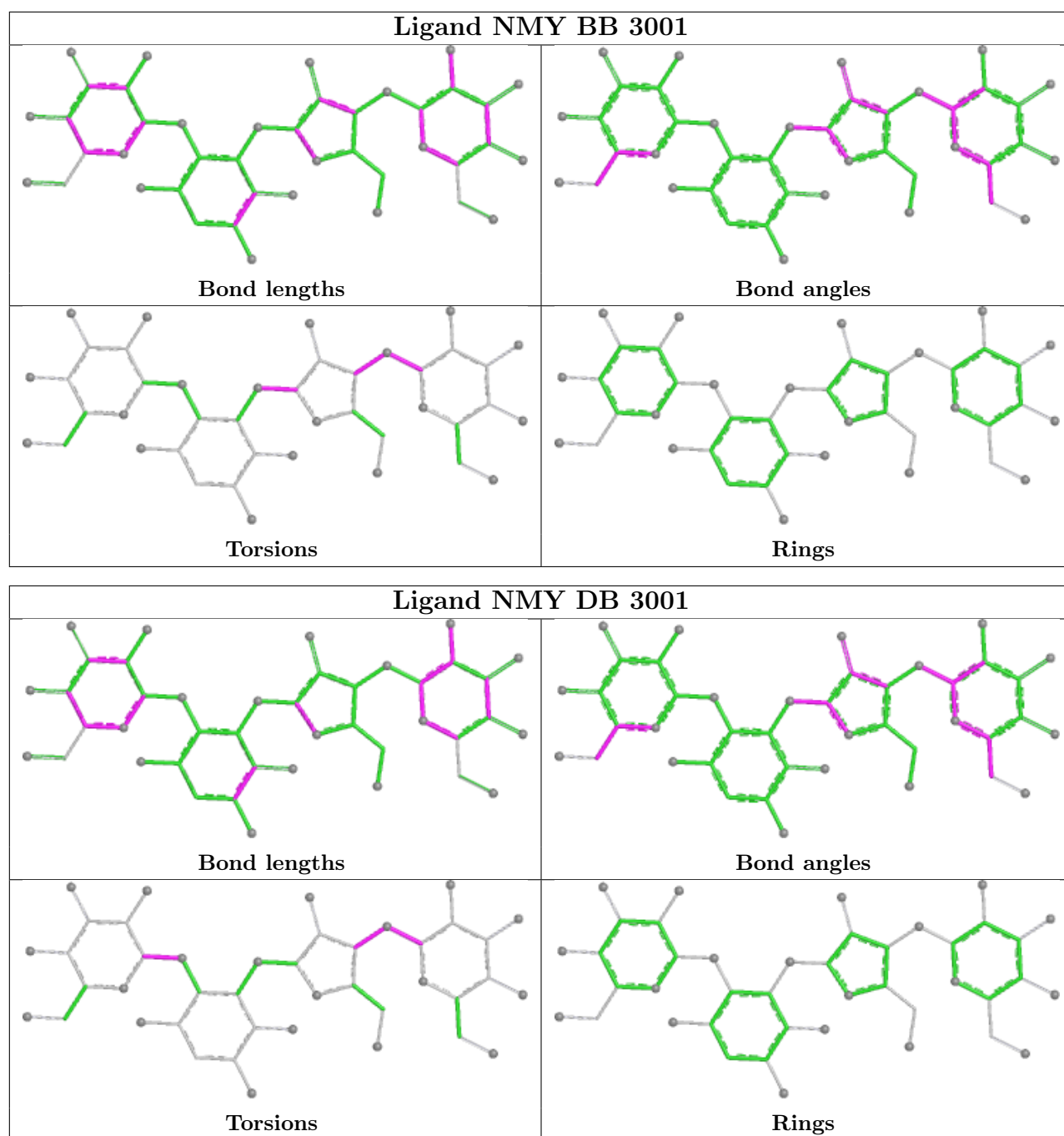
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	AA	1601	NMY	2	0
53	DB	3001	NMY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.04	45 (2%)	53	35	22, 76, 152, 180	0
1	CA	1530/1542 (99%)	-0.08	46 (3%)	52	34	12, 57, 136, 180	0
2	AC	206/232 (88%)	0.46	21 (10%)	12	8	16, 66, 135, 180	0
2	CC	206/232 (88%)	0.44	17 (8%)	17	11	14, 74, 124, 180	0
3	AD	205/205 (100%)	0.90	30 (14%)	6	4	8, 84, 155, 180	0
3	CD	205/205 (100%)	0.52	15 (7%)	21	13	15, 62, 135, 180	0
4	AE	150/166 (90%)	0.68	18 (12%)	9	6	7, 67, 122, 158	0
4	CE	150/166 (90%)	0.55	14 (9%)	14	10	10, 59, 122, 180	0
5	AF	100/135 (74%)	0.50	6 (6%)	27	17	32, 80, 148, 180	0
5	CF	100/135 (74%)	0.31	4 (4%)	42	26	23, 69, 138, 180	0
6	AG	150/178 (84%)	0.68	21 (14%)	6	5	39, 105, 151, 180	0
6	CG	152/178 (85%)	0.46	11 (7%)	21	14	32, 89, 152, 180	0
7	AH	129/129 (100%)	0.59	12 (9%)	14	10	29, 79, 133, 180	0
7	CH	129/129 (100%)	0.51	15 (11%)	9	7	7, 55, 120, 148	0
8	AI	127/129 (98%)	0.91	16 (12%)	8	6	37, 90, 164, 180	0
8	CI	127/129 (98%)	1.05	20 (15%)	5	4	32, 95, 162, 180	0
9	AJ	98/103 (95%)	0.87	16 (16%)	4	3	17, 85, 158, 180	0
9	CJ	98/103 (95%)	1.29	23 (23%)	2	2	22, 89, 150, 180	0
10	AK	117/128 (91%)	0.31	4 (3%)	48	30	17, 63, 128, 162	0
10	CK	117/128 (91%)	0.20	6 (5%)	33	21	10, 51, 116, 164	0
11	AL	123/123 (100%)	1.04	25 (20%)	3	2	19, 74, 135, 180	0
11	CL	123/123 (100%)	0.72	19 (15%)	5	4	6, 50, 127, 180	0
12	AM	114/117 (97%)	0.63	8 (7%)	22	14	52, 119, 180, 180	0
12	CM	113/117 (96%)	0.73	13 (11%)	9	7	53, 105, 167, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.88	10 (10%) 11 8	24, 79, 118, 152	0
13	CN	96/100 (96%)	1.18	16 (16%) 4 3	26, 82, 119, 139	0
14	AO	88/89 (98%)	0.21	4 (4%) 38 24	39, 76, 123, 180	0
14	CO	88/89 (98%)	0.22	5 (5%) 29 19	15, 55, 123, 154	0
15	AP	82/82 (100%)	1.05	13 (15%) 5 4	30, 86, 150, 180	0
15	CP	80/82 (97%)	0.99	12 (15%) 5 4	8, 56, 135, 180	0
16	AQ	80/83 (96%)	0.88	11 (13%) 6 5	49, 96, 155, 180	0
16	CQ	81/83 (97%)	0.36	7 (8%) 16 11	25, 66, 128, 180	0
17	AR	55/74 (74%)	0.70	5 (9%) 15 10	15, 74, 125, 165	0
17	CR	55/74 (74%)	0.43	6 (10%) 10 7	19, 63, 119, 170	0
18	AS	79/91 (86%)	0.95	11 (13%) 6 5	73, 121, 176, 180	0
18	CS	80/91 (87%)	0.96	17 (21%) 2 2	58, 109, 168, 180	0
19	AT	85/86 (98%)	0.91	14 (16%) 4 3	52, 104, 164, 180	0
19	CT	85/86 (98%)	0.67	14 (16%) 4 3	22, 62, 125, 179	0
20	AB	218/240 (90%)	0.42	15 (6%) 23 15	29, 99, 155, 180	0
20	CB	218/240 (90%)	0.50	19 (8%) 16 11	31, 102, 160, 180	0
21	AU	51/70 (72%)	1.58	20 (39%) 1 1	43, 92, 146, 180	0
21	CU	51/70 (72%)	1.55	16 (31%) 1 1	40, 85, 133, 166	0
22	BA	117/120 (97%)	0.20	8 (6%) 23 15	49, 83, 138, 174	0
22	DA	117/120 (97%)	0.38	6 (5%) 33 21	36, 75, 124, 180	0
23	BB	2841/2904 (97%)	-0.05	73 (2%) 57 38	16, 60, 154, 180	0
23	DB	2841/2904 (97%)	-0.21	67 (2%) 59 40	6, 47, 151, 180	0
24	BI	141/141 (100%)	0.97	18 (12%) 7 6	93, 176, 180, 180	0
24	DI	141/141 (100%)	0.59	10 (7%) 22 14	101, 177, 180, 180	0
25	BC	271/272 (99%)	0.72	32 (11%) 9 7	9, 50, 104, 180	0
25	DC	271/272 (99%)	0.64	30 (11%) 10 7	5, 35, 87, 135	0
26	BD	209/209 (100%)	0.85	23 (11%) 10 7	20, 76, 135, 180	0
26	DD	209/209 (100%)	0.77	32 (15%) 5 4	5, 50, 126, 180	0
27	BK	121/123 (98%)	0.87	23 (19%) 3 2	14, 72, 133, 180	0
27	DK	121/123 (98%)	0.37	8 (6%) 24 15	6, 43, 104, 164	0
28	BP	114/114 (100%)	1.27	28 (24%) 2 2	35, 86, 151, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.55	13 (11%) 10 7	6, 49, 113, 160	0
29	BE	201/201 (100%)	0.43	17 (8%) 16 11	10, 67, 144, 180	0
29	DE	201/201 (100%)	0.50	23 (11%) 10 7	5, 72, 137, 180	0
30	BY	58/58 (100%)	0.46	3 (5%) 33 21	34, 74, 139, 180	0
30	DY	58/58 (100%)	0.43	2 (3%) 48 30	21, 60, 141, 177	0
31	B0	56/56 (100%)	0.50	3 (5%) 31 20	15, 74, 151, 180	0
31	D0	56/56 (100%)	0.57	2 (3%) 46 29	9, 49, 124, 180	0
32	B4	38/38 (100%)	2.02	17 (44%) 0 1	35, 91, 145, 151	0
32	D4	38/38 (100%)	1.07	6 (15%) 5 4	18, 68, 129, 150	0
33	B1	50/54 (92%)	0.66	4 (8%) 18 12	52, 90, 134, 174	0
33	D1	50/54 (92%)	0.15	0 100 100	14, 76, 127, 175	0
34	B3	64/64 (100%)	1.11	14 (21%) 2 2	26, 59, 87, 158	0
34	D3	64/64 (100%)	1.40	18 (28%) 1 1	9, 49, 112, 156	0
35	BV	94/94 (100%)	0.30	3 (3%) 50 32	29, 97, 155, 178	0
35	DV	94/94 (100%)	0.36	4 (4%) 40 25	21, 89, 153, 167	0
36	B2	46/46 (100%)	0.90	5 (10%) 10 7	14, 50, 83, 144	0
36	D2	46/46 (100%)	0.67	5 (10%) 10 7	5, 38, 76, 180	0
37	BL	143/144 (99%)	0.62	10 (6%) 22 14	25, 70, 133, 180	0
37	DL	143/144 (99%)	0.77	17 (11%) 9 6	9, 59, 117, 147	0
38	BM	136/136 (100%)	0.72	17 (12%) 8 6	21, 68, 136, 180	0
38	DM	136/136 (100%)	0.70	14 (10%) 12 8	13, 54, 118, 167	0
39	BX	63/63 (100%)	0.60	6 (9%) 14 9	21, 81, 149, 175	0
39	DX	63/63 (100%)	0.39	4 (6%) 26 16	38, 97, 156, 180	0
40	BH	149/149 (100%)	0.70	11 (7%) 20 13	31, 134, 180, 180	0
40	DH	149/149 (100%)	0.44	12 (8%) 18 12	32, 110, 160, 180	0
41	BJ	142/142 (100%)	1.36	40 (28%) 1 1	23, 82, 140, 169	0
41	DJ	142/142 (100%)	0.87	22 (15%) 5 4	17, 61, 126, 180	0
42	BN	120/127 (94%)	0.83	14 (11%) 9 7	24, 71, 139, 180	0
42	DN	120/127 (94%)	0.69	14 (11%) 9 7	7, 43, 91, 172	0
43	BO	116/117 (99%)	0.95	19 (16%) 4 3	35, 83, 145, 180	0
43	DO	116/117 (99%)	0.79	17 (14%) 6 4	19, 73, 135, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	1.02	23 (19%) 3 2	10, 66, 129, 167	0
44	DQ	117/117 (100%)	0.77	18 (15%) 5 4	8, 50, 104, 180	0
45	BS	110/110 (100%)	0.66	9 (8%) 17 11	6, 62, 123, 152	0
45	DS	110/110 (100%)	0.61	11 (10%) 12 8	12, 48, 129, 180	0
46	BU	102/103 (99%)	0.61	5 (4%) 35 22	21, 77, 140, 180	0
46	DU	102/103 (99%)	0.79	12 (11%) 9 7	22, 94, 154, 180	0
47	BF	178/178 (100%)	0.64	17 (9%) 13 9	56, 128, 177, 180	0
47	DF	178/178 (100%)	1.29	40 (22%) 2 2	30, 107, 168, 180	0
48	BG	176/176 (100%)	0.52	6 (3%) 48 30	49, 112, 163, 180	0
48	DG	176/176 (100%)	0.68	19 (10%) 11 7	35, 97, 161, 180	0
49	BR	103/103 (100%)	0.57	10 (9%) 13 9	25, 87, 151, 176	0
49	DR	103/103 (100%)	0.61	9 (8%) 16 11	23, 76, 139, 161	0
50	BT	93/100 (93%)	0.74	15 (16%) 4 3	22, 77, 159, 180	0
50	DT	93/100 (93%)	1.21	23 (24%) 2 2	24, 64, 156, 179	0
51	BZ	77/78 (98%)	0.73	8 (10%) 11 8	12, 51, 112, 143	0
51	DZ	77/78 (98%)	0.74	11 (14%) 6 5	9, 48, 94, 128	0
52	BW	79/84 (94%)	1.89	28 (35%) 1 1	18, 85, 141, 159	0
52	DW	79/84 (94%)	2.14	38 (48%) 0 1	20, 71, 134, 180	0
All	All	20417/21046 (97%)	0.37	1656 (8%) 18 12	5, 69, 156, 180	0

The worst 5 of 1656 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	DA	88	C	21.7
8	CI	129	ARG	17.2
22	BA	88	C	15.8
8	CI	128	LYS	11.9
11	CL	123	ALA	11.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	AA	1626	1/1	-0.05	0.19	64,64,64,64	1
54	MG	AA	1660	1/1	0.26	0.52	163,163,163,163	0
54	MG	DB	3067	1/1	0.29	0.16	178,178,178,178	0
54	MG	AA	1623	1/1	0.64	0.14	129,129,129,129	0
54	MG	AA	1603	1/1	0.67	0.12	133,133,133,133	0
54	MG	AA	1638	1/1	0.70	0.16	147,147,147,147	0
54	MG	CA	1609	1/1	0.76	0.13	121,121,121,121	0
53	NMY	DB	3001	42/42	0.76	0.37	88,88,88,88	42
54	MG	AA	1624	1/1	0.77	0.33	32,32,32,32	1
53	NMY	AA	1601	42/42	0.78	0.14	71,71,71,71	0
54	MG	AA	1648	1/1	0.79	0.22	94,94,94,94	0
54	MG	CA	1629	1/1	0.79	0.19	46,46,46,46	1
54	MG	AA	1640	1/1	0.79	0.21	104,104,104,104	0
54	MG	DB	3059	1/1	0.80	0.40	180,180,180,180	0
54	MG	AA	1620	1/1	0.81	0.13	130,130,130,130	0
54	MG	BB	3034	1/1	0.82	0.08	136,136,136,136	0
54	MG	BB	3043	1/1	0.82	0.12	170,170,170,170	0
53	NMY	CA	1601	42/42	0.82	0.17	71,71,71,71	0
54	MG	CA	1616	1/1	0.83	0.13	167,167,167,167	0
53	NMY	BB	3001	42/42	0.84	0.85	100,100,100,100	42
54	MG	AA	1658	1/1	0.84	0.11	115,115,115,115	0
54	MG	CA	1657	1/1	0.84	0.15	91,91,91,91	0
54	MG	BB	3101	1/1	0.84	0.10	138,138,138,138	0
54	MG	AA	1609	1/1	0.84	0.09	127,127,127,127	0
54	MG	CA	1638	1/1	0.86	0.21	142,142,142,142	0
54	MG	CA	1621	1/1	0.88	0.23	118,118,118,118	0
54	MG	BB	3082	1/1	0.88	0.15	59,59,59,59	0
54	MG	BB	3048	1/1	0.88	0.14	128,128,128,128	0
54	MG	AA	1615	1/1	0.89	0.08	110,110,110,110	0
54	MG	CA	1627	1/1	0.89	0.19	29,29,29,29	1
54	MG	DB	3031	1/1	0.89	0.12	32,32,32,32	0
54	MG	DB	3035	1/1	0.89	0.21	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3058	1/1	0.89	0.09	76,76,76,76	0
54	MG	CA	1635	1/1	0.89	0.11	96,96,96,96	0
54	MG	DB	3084	1/1	0.89	0.12	92,92,92,92	0
54	MG	DB	3096	1/1	0.89	0.13	127,127,127,127	0
54	MG	BB	3011	1/1	0.90	0.08	66,66,66,66	0
54	MG	AA	1647	1/1	0.90	0.08	87,87,87,87	0
54	MG	DB	3061	1/1	0.90	0.15	115,115,115,115	0
54	MG	BB	3039	1/1	0.91	0.06	131,131,131,131	0
54	MG	BB	3094	1/1	0.91	0.08	93,93,93,93	0
54	MG	AA	1635	1/1	0.91	0.08	45,45,45,45	0
54	MG	DB	3053	1/1	0.92	0.07	102,102,102,102	0
54	MG	CA	1623	1/1	0.92	0.07	131,131,131,131	0
54	MG	CA	1612	1/1	0.92	0.07	84,84,84,84	0
54	MG	DB	3014	1/1	0.92	0.10	48,48,48,48	0
54	MG	AA	1628	1/1	0.92	0.09	57,57,57,57	0
54	MG	BB	3098	1/1	0.92	0.12	80,80,80,80	0
55	ZN	D4	101	1/1	0.92	0.10	57,57,57,57	0
54	MG	BB	3044	1/1	0.93	0.06	108,108,108,108	0
54	MG	CA	1607	1/1	0.93	0.08	100,100,100,100	0
54	MG	AA	1631	1/1	0.93	0.08	107,107,107,107	0
54	MG	CA	1641	1/1	0.93	0.11	63,63,63,63	0
54	MG	AA	1653	1/1	0.93	0.10	79,79,79,79	0
54	MG	BB	3081	1/1	0.94	0.14	52,52,52,52	0
54	MG	AA	1656	1/1	0.94	0.12	60,60,60,60	0
54	MG	CA	1636	1/1	0.94	0.09	56,56,56,56	0
54	MG	DB	3034	1/1	0.94	0.06	43,43,43,43	0
54	MG	AA	1651	1/1	0.94	0.07	109,109,109,109	0
54	MG	BB	3073	1/1	0.94	0.08	67,67,67,67	0
54	MG	DB	3051	1/1	0.95	0.06	87,87,87,87	0
54	MG	AA	1650	1/1	0.95	0.07	114,114,114,114	0
54	MG	CA	1652	1/1	0.95	0.11	77,77,77,77	0
54	MG	DB	3060	1/1	0.95	0.07	124,124,124,124	0
54	MG	BB	3079	1/1	0.95	0.13	75,75,75,75	0
54	MG	AA	1636	1/1	0.95	0.15	88,88,88,88	0
54	MG	BB	3010	1/1	0.95	0.06	82,82,82,82	0
54	MG	DB	3093	1/1	0.95	0.05	67,67,67,67	0
54	MG	AA	1637	1/1	0.95	0.10	89,89,89,89	0
55	ZN	B4	101	1/1	0.95	0.09	72,72,72,72	0
54	MG	AA	1621	1/1	0.95	0.10	85,85,85,85	0
54	MG	DB	3019	1/1	0.96	0.10	48,48,48,48	0
54	MG	DB	3029	1/1	0.96	0.06	33,33,33,33	0
54	MG	CA	1619	1/1	0.96	0.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3092	1/1	0.96	0.05	32,32,32,32	0
54	MG	CA	1622	1/1	0.96	0.06	75,75,75,75	0
54	MG	AA	1619	1/1	0.96	0.12	85,85,85,85	0
54	MG	BB	3095	1/1	0.96	0.06	46,46,46,46	0
54	MG	BB	3052	1/1	0.96	0.07	59,59,59,59	0
54	MG	BB	3100	1/1	0.96	0.10	68,68,68,68	0
54	MG	AA	1657	1/1	0.96	0.07	69,69,69,69	0
54	MG	AA	1616	1/1	0.96	0.08	77,77,77,77	0
54	MG	BB	3040	1/1	0.96	0.06	28,28,28,28	0
54	MG	CA	1642	1/1	0.96	0.05	94,94,94,94	0
54	MG	CA	1611	1/1	0.96	0.05	60,60,60,60	0
54	MG	AA	1625	1/1	0.96	0.15	72,72,72,72	0
54	MG	AA	1618	1/1	0.96	0.06	79,79,79,79	0
54	MG	CA	1643	1/1	0.97	0.04	43,43,43,43	0
54	MG	CA	1647	1/1	0.97	0.05	90,90,90,90	0
54	MG	CA	1648	1/1	0.97	0.11	55,55,55,55	0
54	MG	CA	1649	1/1	0.97	0.06	73,73,73,73	0
54	MG	BB	3111	1/1	0.97	0.11	81,81,81,81	0
54	MG	AA	1654	1/1	0.97	0.04	51,51,51,51	0
54	MG	DB	3005	1/1	0.97	0.09	30,30,30,30	0
54	MG	BB	3018	1/1	0.97	0.06	43,43,43,43	0
54	MG	DB	3016	1/1	0.97	0.05	49,49,49,49	0
54	MG	BB	3019	1/1	0.97	0.06	45,45,45,45	0
54	MG	BB	3072	1/1	0.97	0.05	52,52,52,52	0
54	MG	BB	3029	1/1	0.97	0.12	32,32,32,32	0
54	MG	BB	3032	1/1	0.97	0.07	45,45,45,45	0
54	MG	AA	1613	1/1	0.97	0.04	65,65,65,65	0
54	MG	BB	3035	1/1	0.97	0.12	32,32,32,32	0
54	MG	BB	3088	1/1	0.97	0.11	57,57,57,57	0
54	MG	DB	3054	1/1	0.97	0.06	65,65,65,65	0
54	MG	BB	3091	1/1	0.97	0.06	75,75,75,75	0
54	MG	CA	1628	1/1	0.97	0.04	61,61,61,61	0
54	MG	BB	3038	1/1	0.97	0.04	50,50,50,50	0
54	MG	AA	1629	1/1	0.97	0.05	70,70,70,70	0
54	MG	AA	1641	1/1	0.97	0.10	56,56,56,56	0
54	MG	DB	3091	1/1	0.97	0.07	47,47,47,47	0
54	MG	CA	1637	1/1	0.97	0.04	79,79,79,79	0
54	MG	AA	1652	1/1	0.97	0.05	73,73,73,73	0
54	MG	DB	3105	1/1	0.97	0.05	40,40,40,40	0
54	MG	DB	3107	1/1	0.97	0.05	27,27,27,27	0
54	MG	DB	3111	1/1	0.97	0.10	28,28,28,28	0
54	MG	AA	1627	1/1	0.97	0.04	15,15,15,15	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3045	1/1	0.97	0.07	67,67,67,67	0
54	MG	BB	3033	1/1	0.98	0.04	55,55,55,55	0
54	MG	BB	3059	1/1	0.98	0.04	30,30,30,30	0
54	MG	BB	3107	1/1	0.98	0.04	54,54,54,54	0
54	MG	BB	3065	1/1	0.98	0.05	24,24,24,24	0
54	MG	CA	1654	1/1	0.98	0.04	78,78,78,78	0
54	MG	BB	3068	1/1	0.98	0.04	55,55,55,55	0
54	MG	CA	1659	1/1	0.98	0.04	62,62,62,62	0
54	MG	CA	1661	1/1	0.98	0.05	61,61,61,61	0
54	MG	CE	201	1/1	0.98	0.07	97,97,97,97	0
54	MG	CN	201	1/1	0.98	0.04	48,48,48,48	0
54	MG	AA	1661	1/1	0.98	0.05	79,79,79,79	0
54	MG	DB	3008	1/1	0.98	0.04	16,16,16,16	0
54	MG	CA	1610	1/1	0.98	0.04	79,79,79,79	0
54	MG	BB	3004	1/1	0.98	0.11	38,38,38,38	0
54	MG	BB	3074	1/1	0.98	0.04	31,31,31,31	0
54	MG	CA	1615	1/1	0.98	0.10	41,41,41,41	0
54	MG	DB	3030	1/1	0.98	0.04	74,74,74,74	0
54	MG	BB	3076	1/1	0.98	0.10	60,60,60,60	0
54	MG	BB	3078	1/1	0.98	0.04	32,32,32,32	0
54	MG	AA	1605	1/1	0.98	0.06	48,48,48,48	0
54	MG	DB	3046	1/1	0.98	0.08	55,55,55,55	0
54	MG	AA	1633	1/1	0.98	0.11	51,51,51,51	0
54	MG	BB	3014	1/1	0.98	0.04	42,42,42,42	0
54	MG	CA	1626	1/1	0.98	0.07	8,8,8,8	1
54	MG	DB	3055	1/1	0.98	0.04	42,42,42,42	0
54	MG	BB	3085	1/1	0.98	0.04	44,44,44,44	0
54	MG	AA	1643	1/1	0.98	0.04	53,53,53,53	0
54	MG	BB	3090	1/1	0.98	0.04	49,49,49,49	0
54	MG	DB	3063	1/1	0.98	0.05	71,71,71,71	0
54	MG	CA	1633	1/1	0.98	0.09	73,73,73,73	0
54	MG	DB	3071	1/1	0.98	0.04	61,61,61,61	0
54	MG	DB	3078	1/1	0.98	0.04	46,46,46,46	0
54	MG	AA	1646	1/1	0.98	0.04	94,94,94,94	0
54	MG	BB	3023	1/1	0.98	0.10	41,41,41,41	0
54	MG	AA	1659	1/1	0.98	0.11	112,112,112,112	0
54	MG	AA	1639	1/1	0.98	0.04	57,57,57,57	0
54	MG	DB	3097	1/1	0.98	0.11	33,33,33,33	0
54	MG	BB	3096	1/1	0.98	0.04	42,42,42,42	0
54	MG	BB	3056	1/1	0.98	0.06	34,34,34,34	0
54	MG	BB	3099	1/1	0.98	0.07	41,41,41,41	0
54	MG	CA	1644	1/1	0.98	0.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1646	1/1	0.98	0.03	72,72,72,72	0
54	MG	AA	1630	1/1	0.99	0.02	35,35,35,35	0
54	MG	AA	1611	1/1	0.99	0.03	28,28,28,28	0
54	MG	BB	3012	1/1	0.99	0.05	25,25,25,25	0
54	MG	BB	3060	1/1	0.99	0.04	30,30,30,30	0
54	MG	BB	3061	1/1	0.99	0.02	41,41,41,41	0
54	MG	BB	3063	1/1	0.99	0.07	31,31,31,31	0
54	MG	CA	1630	1/1	0.99	0.07	40,40,40,40	0
54	MG	CA	1631	1/1	0.99	0.03	34,34,34,34	0
54	MG	CA	1632	1/1	0.99	0.10	47,47,47,47	0
54	MG	BB	3064	1/1	0.99	0.03	26,26,26,26	0
54	MG	BB	3013	1/1	0.99	0.04	41,41,41,41	0
54	MG	BB	3066	1/1	0.99	0.03	44,44,44,44	0
54	MG	BB	3067	1/1	0.99	0.03	34,34,34,34	0
54	MG	AA	1632	1/1	0.99	0.06	37,37,37,37	0
54	MG	CA	1640	1/1	0.99	0.08	57,57,57,57	0
54	MG	BB	3069	1/1	0.99	0.12	32,32,32,32	0
54	MG	BB	3015	1/1	0.99	0.07	27,27,27,27	0
54	MG	AA	1612	1/1	0.99	0.02	37,37,37,37	0
54	MG	AA	1634	1/1	0.99	0.03	52,52,52,52	0
54	MG	BB	3075	1/1	0.99	0.03	13,13,13,13	0
54	MG	BB	3020	1/1	0.99	0.04	45,45,45,45	0
54	MG	BB	3021	1/1	0.99	0.07	22,22,22,22	0
54	MG	BB	3022	1/1	0.99	0.03	22,22,22,22	0
54	MG	BB	3080	1/1	0.99	0.03	37,37,37,37	0
54	MG	AA	1622	1/1	0.99	0.08	27,27,27,27	0
54	MG	CA	1655	1/1	0.99	0.03	69,69,69,69	0
54	MG	CA	1656	1/1	0.99	0.03	27,27,27,27	0
54	MG	BB	3025	1/1	0.99	0.07	14,14,14,14	0
54	MG	CA	1658	1/1	0.99	0.07	52,52,52,52	0
54	MG	BB	3083	1/1	0.99	0.03	5,5,5,5	0
54	MG	CA	1660	1/1	0.99	0.04	69,69,69,69	0
54	MG	BB	3026	1/1	0.99	0.06	54,54,54,54	0
54	MG	BB	3086	1/1	0.99	0.05	66,66,66,66	0
54	MG	AA	1602	1/1	0.99	0.07	29,29,29,29	0
54	MG	BB	3089	1/1	0.99	0.04	45,45,45,45	0
54	MG	BB	3031	1/1	0.99	0.03	47,47,47,47	0
54	MG	DB	3009	1/1	0.99	0.03	19,19,19,19	0
54	MG	DB	3012	1/1	0.99	0.08	37,37,37,37	0
54	MG	AA	1614	1/1	0.99	0.04	64,64,64,64	0
54	MG	DB	3015	1/1	0.99	0.03	22,22,22,22	0
54	MG	AA	1606	1/1	0.99	0.06	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3017	1/1	0.99	0.05	6,6,6,6	0
54	MG	BB	3093	1/1	0.99	0.03	36,36,36,36	0
54	MG	DB	3021	1/1	0.99	0.08	9,9,9,9	0
54	MG	DB	3023	1/1	0.99	0.04	29,29,29,29	0
54	MG	DB	3024	1/1	0.99	0.05	55,55,55,55	0
54	MG	DB	3025	1/1	0.99	0.03	44,44,44,44	0
54	MG	DB	3026	1/1	0.99	0.04	15,15,15,15	0
54	MG	DB	3027	1/1	0.99	0.04	36,36,36,36	0
54	MG	AA	1607	1/1	0.99	0.04	64,64,64,64	0
54	MG	AA	1617	1/1	0.99	0.04	45,45,45,45	0
54	MG	BB	3036	1/1	0.99	0.03	36,36,36,36	0
54	MG	DB	3032	1/1	0.99	0.03	18,18,18,18	0
54	MG	DB	3033	1/1	0.99	0.04	62,62,62,62	0
54	MG	BB	3097	1/1	0.99	0.04	32,32,32,32	0
54	MG	BB	3037	1/1	0.99	0.02	42,42,42,42	0
54	MG	DB	3036	1/1	0.99	0.06	40,40,40,40	0
54	MG	DB	3037	1/1	0.99	0.05	15,15,15,15	0
54	MG	DB	3038	1/1	0.99	0.06	17,17,17,17	0
54	MG	DB	3040	1/1	0.99	0.06	58,58,58,58	0
54	MG	DB	3045	1/1	0.99	0.04	22,22,22,22	0
54	MG	AA	1608	1/1	0.99	0.03	54,54,54,54	0
54	MG	DB	3048	1/1	0.99	0.12	23,23,23,23	0
54	MG	DB	3049	1/1	0.99	0.03	46,46,46,46	0
54	MG	AA	1642	1/1	0.99	0.03	59,59,59,59	0
54	MG	DB	3052	1/1	0.99	0.09	32,32,32,32	0
54	MG	AA	1604	1/1	0.99	0.03	36,36,36,36	0
54	MG	BB	3106	1/1	0.99	0.07	33,33,33,33	0
54	MG	BB	3002	1/1	0.99	0.04	24,24,24,24	0
54	MG	DB	3056	1/1	0.99	0.03	12,12,12,12	0
54	MG	DB	3058	1/1	0.99	0.03	43,43,43,43	0
54	MG	BB	3109	1/1	0.99	0.03	32,32,32,32	0
54	MG	BB	3110	1/1	0.99	0.04	30,30,30,30	0
54	MG	BB	3003	1/1	0.99	0.03	24,24,24,24	0
54	MG	DB	3062	1/1	0.99	0.07	47,47,47,47	0
54	MG	CA	1602	1/1	0.99	0.10	6,6,6,6	0
54	MG	DB	3064	1/1	0.99	0.05	33,33,33,33	0
54	MG	DB	3065	1/1	0.99	0.10	16,16,16,16	0
54	MG	DB	3066	1/1	0.99	0.06	29,29,29,29	0
54	MG	CA	1605	1/1	0.99	0.05	16,16,16,16	0
54	MG	DB	3068	1/1	0.99	0.04	19,19,19,19	0
54	MG	AA	1645	1/1	0.99	0.05	60,60,60,60	0
54	MG	DB	3072	1/1	0.99	0.04	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3073	1/1	0.99	0.03	33,33,33,33	0
54	MG	BB	3046	1/1	0.99	0.04	46,46,46,46	0
54	MG	DB	3079	1/1	0.99	0.04	43,43,43,43	0
54	MG	DB	3081	1/1	0.99	0.05	18,18,18,18	0
54	MG	DB	3083	1/1	0.99	0.03	24,24,24,24	0
54	MG	BB	3047	1/1	0.99	0.04	46,46,46,46	0
54	MG	DB	3085	1/1	0.99	0.08	25,25,25,25	0
54	MG	DB	3086	1/1	0.99	0.03	18,18,18,18	0
54	MG	DB	3090	1/1	0.99	0.06	34,34,34,34	0
54	MG	BB	3005	1/1	0.99	0.07	39,39,39,39	0
54	MG	DB	3092	1/1	0.99	0.05	46,46,46,46	0
54	MG	BB	3051	1/1	0.99	0.03	41,41,41,41	0
54	MG	DB	3094	1/1	0.99	0.04	21,21,21,21	0
54	MG	CA	1613	1/1	0.99	0.05	77,77,77,77	0
54	MG	CA	1614	1/1	0.99	0.03	58,58,58,58	0
54	MG	DB	3098	1/1	0.99	0.07	36,36,36,36	0
54	MG	DB	3100	1/1	0.99	0.06	9,9,9,9	0
54	MG	DB	3104	1/1	0.99	0.04	21,21,21,21	0
54	MG	BB	3009	1/1	0.99	0.07	64,64,64,64	0
54	MG	BB	3053	1/1	0.99	0.12	25,25,25,25	0
54	MG	DB	3108	1/1	0.99	0.02	21,21,21,21	0
54	MG	DB	3109	1/1	0.99	0.04	10,10,10,10	0
54	MG	DB	3110	1/1	0.99	0.03	19,19,19,19	0
54	MG	BB	3054	1/1	0.99	0.04	46,46,46,46	0
54	MG	DB	3112	1/1	0.99	0.08	37,37,37,37	0
54	MG	CA	1620	1/1	0.99	0.14	70,70,70,70	0
54	MG	BB	3055	1/1	0.99	0.03	58,58,58,58	0
54	MG	CA	1603	1/1	1.00	0.06	30,30,30,30	0
54	MG	CA	1604	1/1	1.00	0.02	52,52,52,52	0
54	MG	BB	3084	1/1	1.00	0.02	21,21,21,21	0
54	MG	CA	1645	1/1	1.00	0.10	45,45,45,45	0
54	MG	DB	3039	1/1	1.00	0.02	19,19,19,19	0
54	MG	CA	1606	1/1	1.00	0.02	19,19,19,19	0
54	MG	DB	3041	1/1	1.00	0.03	15,15,15,15	0
54	MG	DB	3042	1/1	1.00	0.03	7,7,7,7	0
54	MG	DB	3043	1/1	1.00	0.03	15,15,15,15	0
54	MG	DB	3044	1/1	1.00	0.07	12,12,12,12	0
54	MG	BB	3062	1/1	1.00	0.02	29,29,29,29	0
54	MG	CA	1608	1/1	1.00	0.04	40,40,40,40	0
54	MG	DB	3047	1/1	1.00	0.04	24,24,24,24	0
54	MG	BB	3017	1/1	1.00	0.03	28,28,28,28	0
54	MG	CA	1650	1/1	1.00	0.02	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3050	1/1	1.00	0.07	32,32,32,32	0
54	MG	CA	1651	1/1	1.00	0.02	40,40,40,40	0
54	MG	BB	3087	1/1	1.00	0.09	41,41,41,41	0
54	MG	CA	1653	1/1	1.00	0.08	33,33,33,33	0
54	MG	BB	3030	1/1	1.00	0.04	36,36,36,36	0
54	MG	AA	1644	1/1	1.00	0.02	24,24,24,24	0
54	MG	AA	1655	1/1	1.00	0.01	38,38,38,38	0
54	MG	DB	3057	1/1	1.00	0.03	5,5,5,5	0
54	MG	AA	1649	1/1	1.00	0.01	19,19,19,19	0
54	MG	BB	3049	1/1	1.00	0.05	14,14,14,14	0
54	MG	BB	3050	1/1	1.00	0.02	18,18,18,18	0
54	MG	CA	1617	1/1	1.00	0.03	9,9,9,9	0
54	MG	CA	1618	1/1	1.00	0.07	8,8,8,8	0
54	MG	BB	3070	1/1	1.00	0.03	15,15,15,15	0
54	MG	BB	3071	1/1	1.00	0.02	29,29,29,29	0
54	MG	DB	3002	1/1	1.00	0.02	5,5,5,5	0
54	MG	DB	3003	1/1	1.00	0.04	9,9,9,9	0
54	MG	DB	3004	1/1	1.00	0.02	14,14,14,14	0
54	MG	AA	1610	1/1	1.00	0.01	10,10,10,10	0
54	MG	DB	3069	1/1	1.00	0.02	6,6,6,6	0
54	MG	DB	3070	1/1	1.00	0.08	23,23,23,23	0
54	MG	DB	3006	1/1	1.00	0.03	20,20,20,20	0
54	MG	DB	3007	1/1	1.00	0.03	12,12,12,12	0
54	MG	BB	3006	1/1	1.00	0.02	5,5,5,5	0
54	MG	DB	3074	1/1	1.00	0.02	28,28,28,28	0
54	MG	DB	3075	1/1	1.00	0.02	7,7,7,7	0
54	MG	DB	3076	1/1	1.00	0.05	26,26,26,26	0
54	MG	DB	3077	1/1	1.00	0.04	47,47,47,47	0
54	MG	BB	3007	1/1	1.00	0.01	5,5,5,5	0
54	MG	DB	3010	1/1	1.00	0.04	5,5,5,5	0
54	MG	DB	3080	1/1	1.00	0.05	39,39,39,39	0
54	MG	DB	3011	1/1	1.00	0.02	7,7,7,7	0
54	MG	DB	3082	1/1	1.00	0.01	6,6,6,6	0
54	MG	CA	1624	1/1	1.00	0.02	34,34,34,34	0
54	MG	DB	3013	1/1	1.00	0.06	21,21,21,21	0
54	MG	CA	1625	1/1	1.00	0.04	34,34,34,34	0
54	MG	BB	3024	1/1	1.00	0.01	7,7,7,7	0
54	MG	DB	3087	1/1	1.00	0.09	25,25,25,25	0
54	MG	DB	3088	1/1	1.00	0.03	48,48,48,48	0
54	MG	DB	3089	1/1	1.00	0.03	10,10,10,10	0
54	MG	BB	3008	1/1	1.00	0.04	64,64,64,64	0
54	MG	BB	3077	1/1	1.00	0.01	37,37,37,37	0

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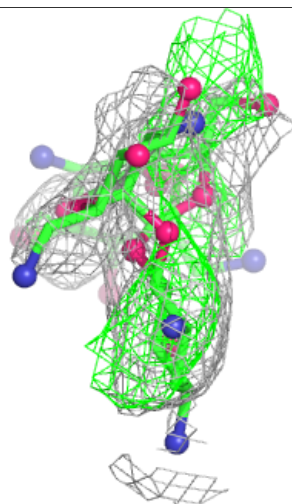
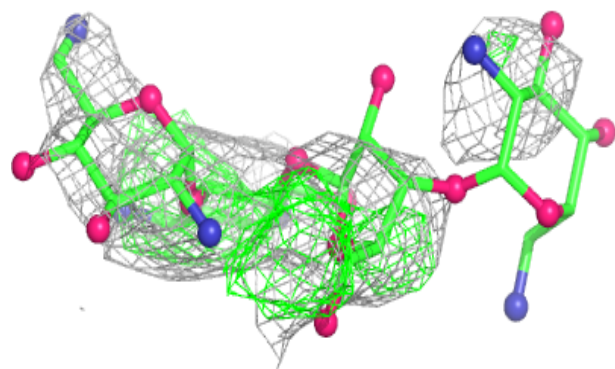
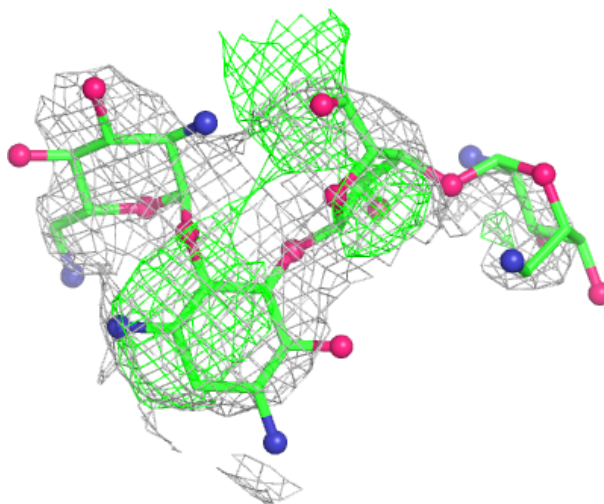
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3018	1/1	1.00	0.05	8,8,8,8	0
54	MG	BB	3102	1/1	1.00	0.04	28,28,28,28	0
54	MG	DB	3020	1/1	1.00	0.05	5,5,5,5	0
54	MG	DB	3095	1/1	1.00	0.02	39,39,39,39	0
54	MG	BB	3103	1/1	1.00	0.03	37,37,37,37	0
54	MG	DB	3022	1/1	1.00	0.01	5,5,5,5	0
54	MG	BB	3104	1/1	1.00	0.06	8,8,8,8	0
54	MG	DB	3099	1/1	1.00	0.07	29,29,29,29	0
54	MG	BB	3105	1/1	1.00	0.04	21,21,21,21	0
54	MG	DB	3101	1/1	1.00	0.02	5,5,5,5	0
54	MG	DB	3102	1/1	1.00	0.04	14,14,14,14	0
54	MG	DB	3103	1/1	1.00	0.02	16,16,16,16	0
54	MG	BB	3016	1/1	1.00	0.01	18,18,18,18	0
54	MG	CA	1634	1/1	1.00	0.03	8,8,8,8	0
54	MG	DB	3106	1/1	1.00	0.05	39,39,39,39	0
54	MG	BB	3057	1/1	1.00	0.03	20,20,20,20	0
54	MG	DB	3028	1/1	1.00	0.01	8,8,8,8	0
54	MG	BB	3108	1/1	1.00	0.02	25,25,25,25	0
54	MG	BB	3027	1/1	1.00	0.02	34,34,34,34	0
54	MG	BB	3041	1/1	1.00	0.06	28,28,28,28	0
54	MG	CA	1639	1/1	1.00	0.02	14,14,14,14	0
54	MG	BB	3042	1/1	1.00	0.05	8,8,8,8	0
54	MG	BB	3028	1/1	1.00	0.02	32,32,32,32	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.

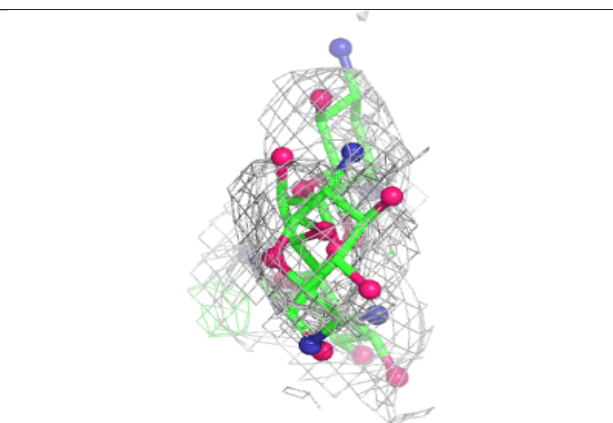
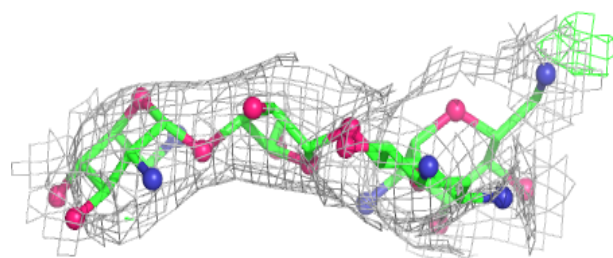
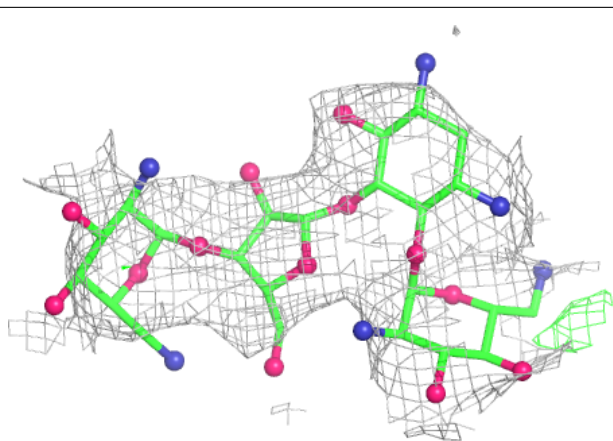
Electron density around NMY DB 3001:

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

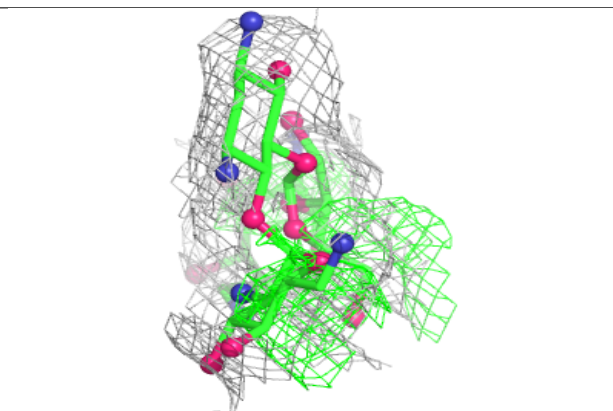
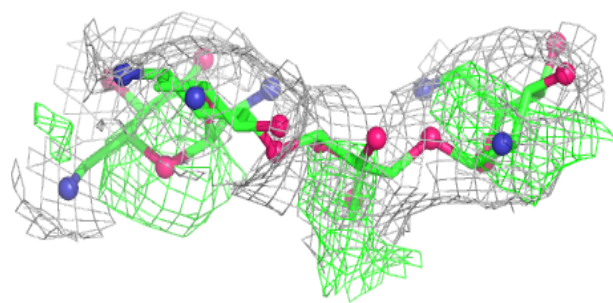
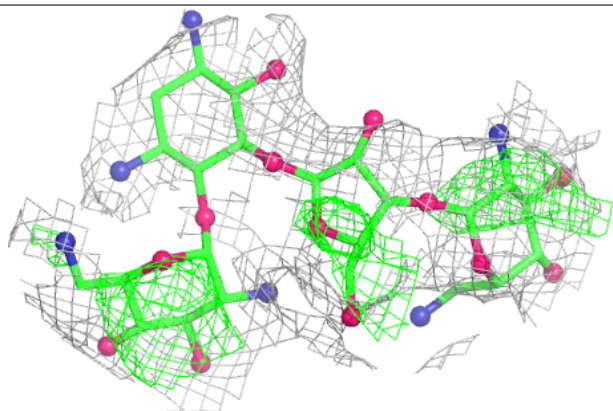


Electron density around NMY AA 1601:

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

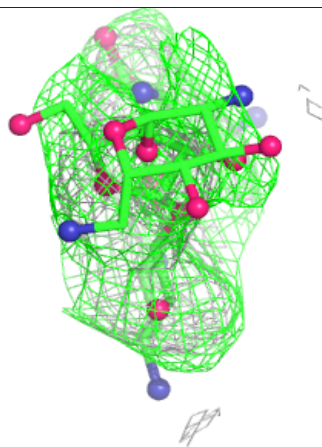
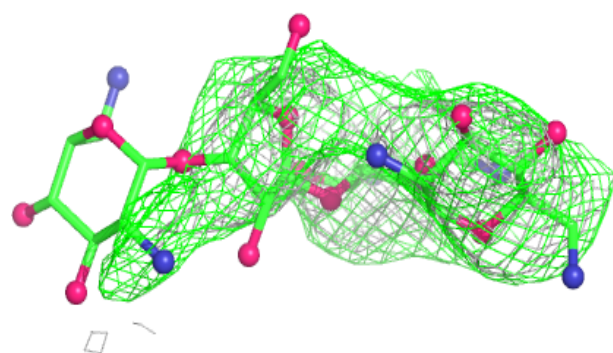
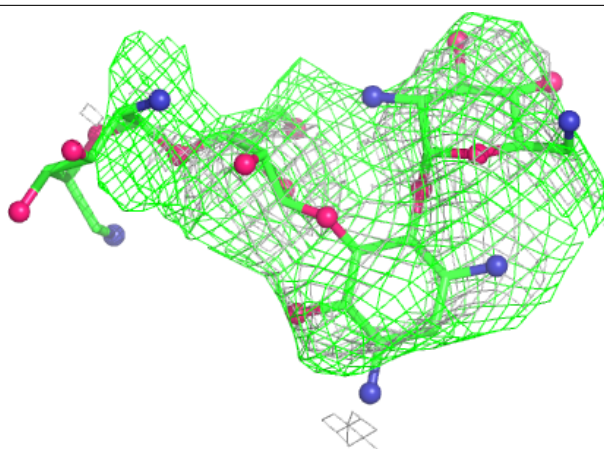
**Electron density around NMY CA 1601:**

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



Electron density around NMY BB 3001:

$2mF_o - DF_c$ (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.