



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 09:05 AM UTC

PDB ID : 4V64 / pdb_00004v64
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with hygromycin B.
Authors : Borovinskaya, M.A.; Shoji, S.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2008-06-11
Resolution : 3.50 Å(reported)

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

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

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

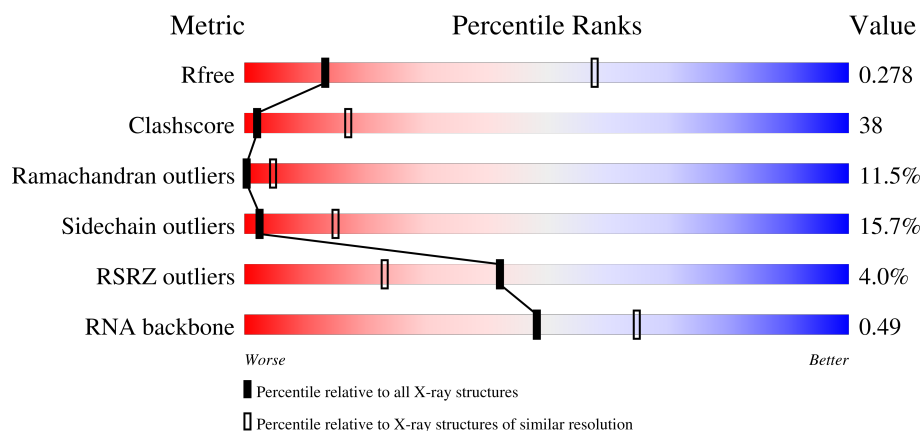
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

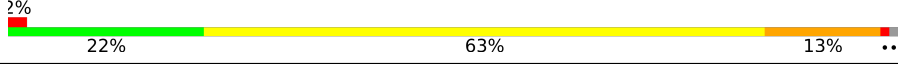
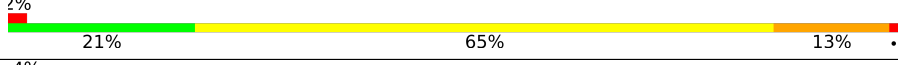
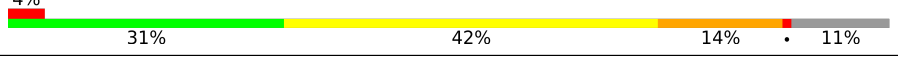
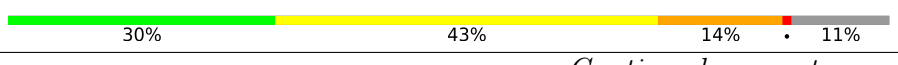
The reported resolution of this entry is 3.50 Å.

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



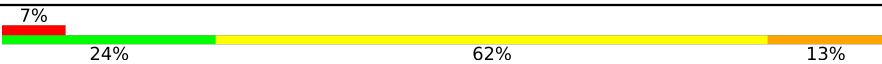
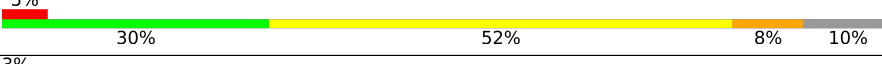
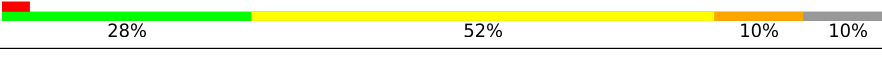
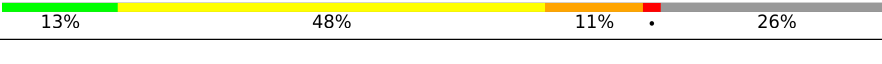
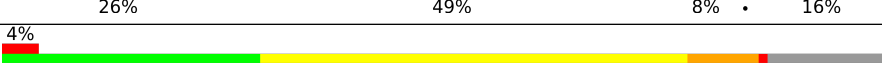
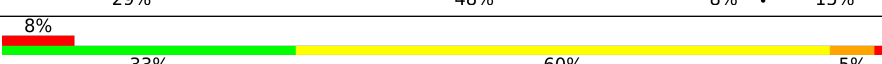
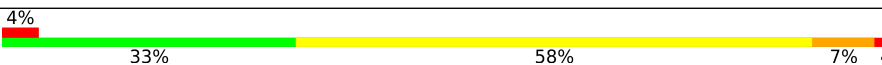
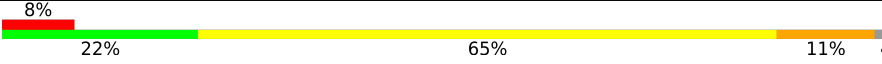
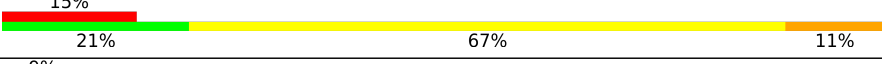
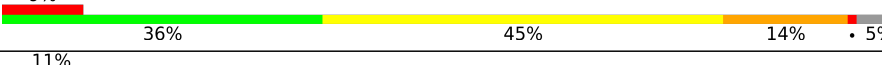
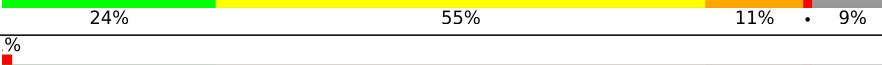
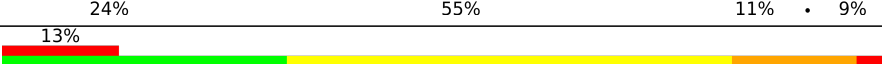
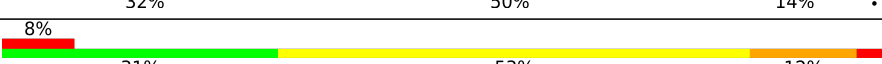
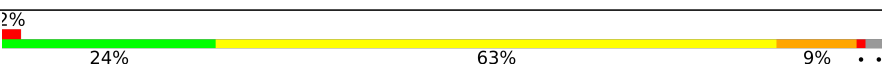
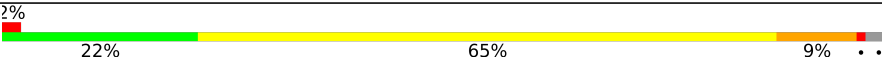
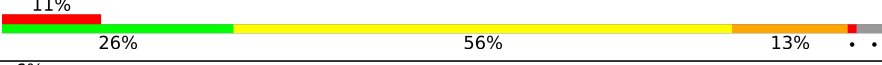
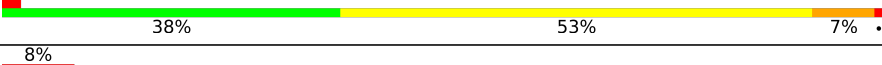
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	
1	CA	1542	
2	AC	232	
2	CC	232	

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

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	71	
21	CU	71	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BV	94	
24	DV	94	
25	BC	273	
25	DC	273	
26	BD	209	
26	DD	209	
27	BE	201	
27	DE	201	

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Mol	Chain	Length	Quality of chain
28	BF	178	
28	DF	178	
29	BG	176	
29	DG	176	
30	BH	149	
30	DH	149	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	

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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	100	
41	DT	100	
42	BU	103	
42	DU	103	
43	BW	84	
43	DW	84	
44	BX	63	
44	DX	63	
45	BY	58	
45	DY	58	
46	BZ	78	
46	DZ	78	
47	B0	56	
47	D0	56	
48	B1	54	
48	D1	54	
49	B2	46	
49	D2	46	
50	B3	64	
50	D3	64	
51	B4	38	
51	D4	38	
52	BI	141	
52	DI	141	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284077 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

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

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

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

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

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

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

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
5	CF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
7	CH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
8	CI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
16	CQ	81	Total	C	N	O	S	0	0	0
			656	417	122	114	3			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
17	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
18	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
19	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
20	CB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
21	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
22	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 23 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
23	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
25	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 49 is a protein called 50S ribosomal protein L34.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L36.

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

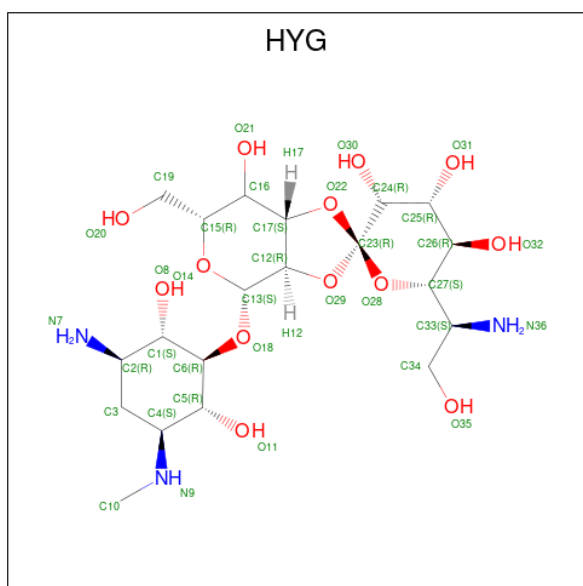
- Molecule 52 is a protein called 50S ribosomal protein L11.

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

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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



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

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

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

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

- Molecule 56 is water.

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

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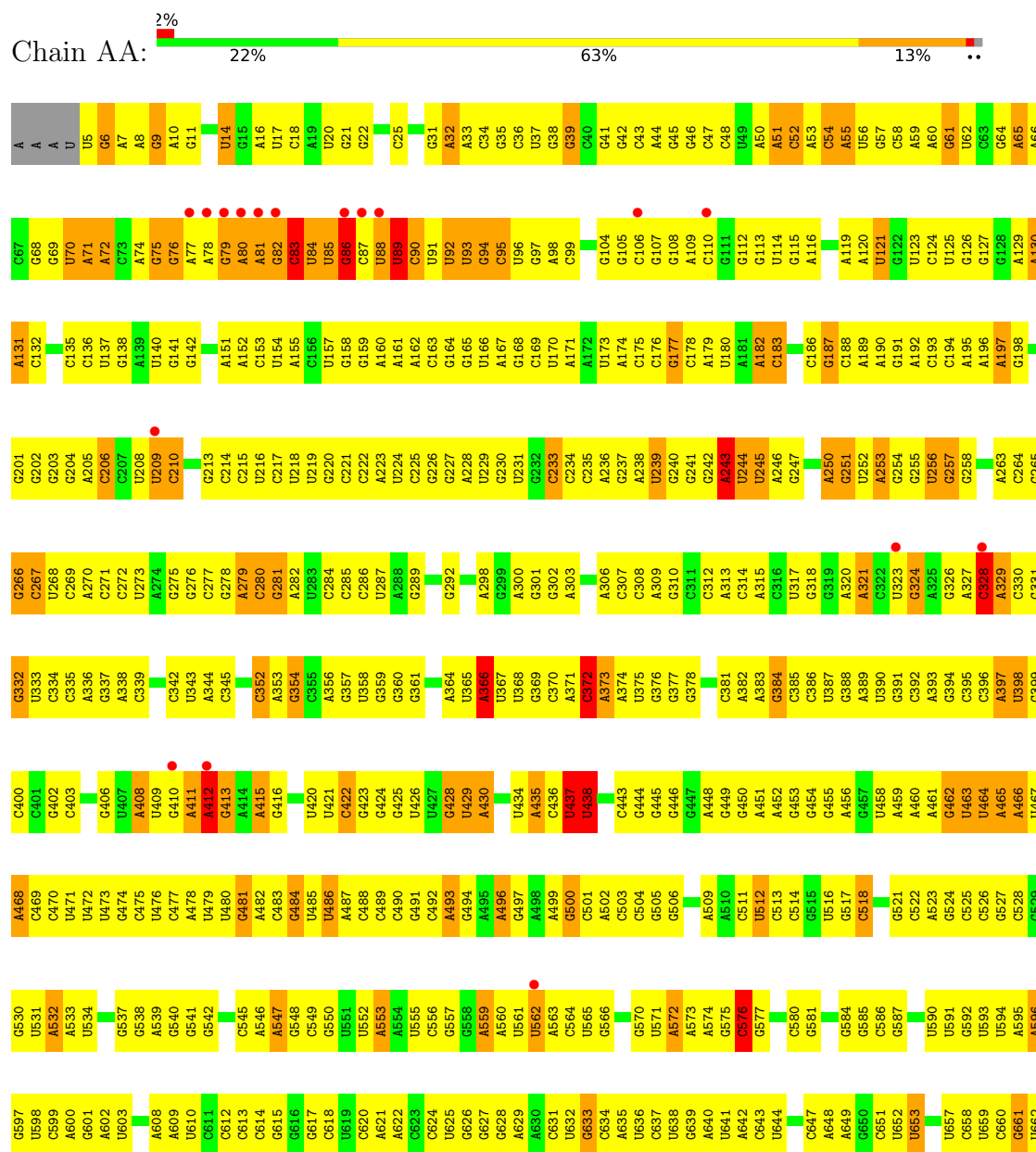
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CN	3	Total 3	O 3	0	0
56	CT	1	Total 1	O 1	0	0
56	DB	499	Total 499	O 499	0	0
56	DC	5	Total 5	O 5	0	0
56	DD	1	Total 1	O 1	0	0
56	DE	1	Total 1	O 1	0	0
56	DL	5	Total 5	O 5	0	0
56	DP	1	Total 1	O 1	0	0
56	D2	1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

3 Residue-property plots

These plots are drawn for all protein, RNA, 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 ribosomal RNA



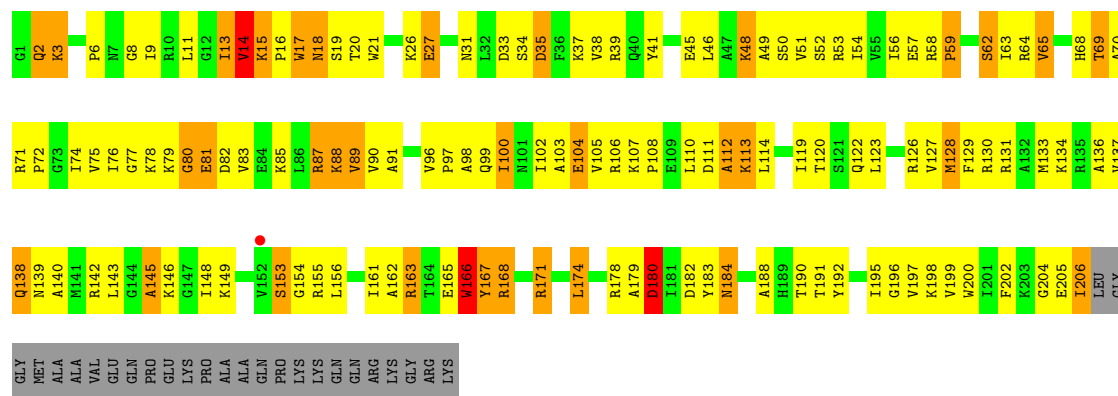
G1515	G1516	G1517	A1518	A1519	C1520	C1521	G1452	G1384	C1259	A1197	C1129	C1063	G1002	A937	A865	C797	G730	A663
G1517	G1518	G1519	G1458	G1459	C1460	G1461	A1456	G1386	G1260	G1196	A1130	G1064	G1003	A938	C866	C798	G731	A664
A1519	G1458	G1459	G1458	G1459	C1460	G1461	A1456	G1386	A1261	G1199	G1131	C1066	A1004	G939	C867	A802	G734	A665
C1520	G1458	G1459	G1458	G1459	C1460	G1461	A1456	G1386	C1262	C1200	C1132	C1066	A1005	C940	C869	G803	C735	G668
C1521	G1459	G1458	G1459	G1458	C1460	G1461	A1456	G1386	C1263	U1201	G1134	A1067	G1006	G941	G875	U804	C736	G669
G1522	G1460	G1461	G1459	G1458	C1460	G1461	A1456	G1386	C1264	U1202	G1135	C1069	U1008	G845	U876	C805	C737	G670
G1523	G1461	G1462	G1459	G1458	C1460	G1461	A1456	G1386	C1265	G1206	C1136	U1070	U1009	A946	U878	C806	C738	G671
G1524	G1462	G1463	G1459	G1458	C1460	G1461	A1456	G1386	C1266	G1207	C1137	C1071	U1010	A947	A879	C807	C739	U672
G1525	G1463	G1464	G1459	G1458	C1460	G1461	A1456	G1386	C1267	C1208	G1138	U1072	A1012	C948	C880	C808	U673	G674
G1526	G1464	G1465	G1459	G1458	C1460	G1461	A1456	G1386	C1268	G1209	G1139	U1073	A1013	A949	C881	C809	G674	U675
G1527	G1465	G1466	G1459	G1458	C1460	G1461	A1456	G1386	C1269	G1210	C1140	G1074	G1014	U950	C882	C810	A743	A676
U1528	G1466	G1467	A1396	A1397	C1468	G1469	A1457	G1387	C1270	U1211	G1142	G1077	G1015	U952	C883	C812	G744	U677
U1529	A1468	C1399	A1396	A1397	C1468	G1469	A1457	G1387	C1271	U1212	G1143	U1078	A1016	G953	U884	U813	G745	U678
G1530	C1400	G1401	A1396	A1397	C1468	G1469	A1457	G1387	C1272	U1213	G1144	U1079	U1017	G954	C885	A814	A747	C679
A1531	G1401	G1402	A1396	A1397	C1468	G1469	A1457	G1387	C1273	U1214	G1145	A1081	G1018	U955	C886	A815	G748	C680
U1532	G1402	G1403	A1396	A1397	C1468	G1469	A1457	G1387	C1274	U1215	A1146	U1082	U1025	U956	A889	A816	A749	A681
C1533	G1403	G1404	A1396	A1397	C1468	G1469	A1457	G1387	C1275	U1216	C1147	A1082	U1026	U957	U890	C817	C750	G682
A1534	G1404	G1405	A1396	A1397	C1468	G1469	A1457	G1387	C1276	U1217	C1148	U1085	U1027	A958	U891	C818	U751	G683
C	G1405	G1406	A1396	A1397	C1468	G1469	A1457	G1387	C1277	U1218	C1149	U1086	U1028	U959	C893	C819	G752	U684
C	G1406	G1407	A1396	A1397	C1468	G1469	A1457	G1387	C1278	U1219	C1150	U1087	U1029	U960	C894	U820	A753	U685
C	G1407	G1408	A1396	A1397	C1468	G1469	A1457	G1387	C1279	U1220	C1151	U1088	U1030	U961	C895	U821	C754	U686
C	G1408	G1409	A1396	A1397	C1468	G1469	A1457	G1387	C1280	U1221	C1152	U1089	U1031	C970	C896	U822	G755	A687
C	G1409	G1410	A1396	A1397	C1468	G1469	A1457	G1387	C1281	U1222	C1153	U1090	U1032	C971	C897	U823		
C	G1410	G1411	A1396	A1397	C1468	G1469	A1457	G1387	C1282	U1223	C1154	U1091	U1033	C972	C898	C824	G761	U682
C	G1411	G1412	A1396	A1397	C1468	G1469	A1457	G1387	C1283	U1224	C1155	U1092	U1034	U965	C899	A825	U762	G693
C	G1412	G1413	A1396	A1397	C1468	G1469	A1457	G1387	C1284	U1225	C1156	U1093	U1035	U966	C900	A826	G763	A694
C	G1413	G1414	A1396	A1397	C1468	G1469	A1457	G1387	C1285	U1226	C1157	U1094	U1036	C967	C901	C827	C764	A695
C	G1414	G1415	A1396	A1397	C1468	G1469	A1457	G1387	C1286	U1227	C1158	U1095	U1037	A968	C902	U827	G765	A696
C	G1415	G1416	A1396	A1397	C1468	G1469	A1457	G1387	C1287	U1228	C1159	U1096	U1038	A969	C903	U828	A766	U697
C	G1416	G1417	A1396	A1397	C1468	G1469	A1457	G1387	C1288	U1229	C1160	U1097	U1039	C970	C904	G829	A767	G698
U1477	G1417	G1418	A1396	A1397	C1468	G1469	A1457	G1387	C1289	U1230	C1161	U1098	U1040	C971	C905	A878	A768	C699
U1478	G1418	G1419	A1396	A1397	C1468	G1469	A1457	G1387	C1290	U1231	C1162	U1099	U1041	C972	C906	A879	C770	G700
C1479	G1419	G1420	A1396	A1397	C1468	G1469	A1457	G1387	C1291	U1232	C1163	U1100	U1042	A973	C907	U830	G771	G703
A1480	G1420	G1421	A1396	A1397	C1468	G1469	A1457	G1387	C1292	U1233	C1164	U1101	U1043	A974	C908	U831	U772	A704
U1481	G1421	G1422	A1396	A1397	C1468	G1469	A1457	G1387	C1293	U1234	C1165	U1102	U1044	A975	C909	U832	U773	A705
A1482	G1422	G1423	A1396	A1397	C1468	G1469	A1457	G1387	C1294	U1235	C1166	U1103	U1045	A976	C910	U833	U774	A706
G1486	G1423	G1424	A1396	A1397	C1468	G1469	A1457	G1387	C1295	U1236	C1167	U1104	U1046	A977	C911	U834	G775	U707
G1487	G1424	G1425	A1396	A1397	C1468	G1469	A1457	G1387	C1296	U1237	C1168	U1105	U1047	A978	C912	U835	G776	C708
G1488	G1425	G1426	A1396	A1397	C1468	G1469	A1457	G1387	C1297	U1238	C1169	U1106	U1048	A979	C913	U836	A777	U709
G1489	G1426	G1427	A1396	A1397	C1468	G1469	A1457	G1387	C1298	U1239	C1170	U1107	U1049	A980	C914	U837	G778	G710
U1490	G1427	G1428	A1396	A1397	C1468	G1469	A1457	G1387	C1299	U1240	C1171	U1108	U1050	A981	C915	U838	G779	G711
G1491	G1428	G1429	A1396	A1397	C1468	G1469	A1457	G1387	C1300	U1241	C1172	U1109	U1051	A982	C916	U839	A780	A712
A1492	G1429	G1430	A1396	A1397	C1468	G1469	A1457	G1387	C1301	U1242	C1173	U1110	U1052	A983	C917	U840	C779	G713
A1493	G1430	G1431	A1396	A1397	C1468	G1469	A1457	G1387	C1302	U1243	C1174	U1111	U1053	A984	C918	U841	A781	G714
A1494	G1431	G1432	A1396	A1397	C1468	G1469	A1457	G1387	C1303	U1244	C1175	U1112	U1054	A985	C919	U842	C783	A715
A1495	G1432	G1433	A1396	A1397	C1468	G1469	A1457	G1387	C1304	U1245	C1176	U1113	U1055	A986	C920	U843	A784	A716
A1496	G1433	G1434	A1396	A1397	C1468	G1469	A1457	G1387	C1305	U1246	C1177	U1114	U1056	A987	C921	U844	G785	C719
A1497	G1434	G1435	A1396	A1397	C1468	G1469	A1457	G1387	C1306	U1247	C1178	U1115	U1057	A988	C922	U845	G786	C720
A1498	G1435	G1436	A1396	A1397	C1468	G1469	A1457	G1387	C1307	U1248	C1179	U1116	U1058	A989	C923	U846	U787	G721
A1499	G1436	G1437	A1396	A1397	C1468	G1469	A1457	G1387	C1308	U1249	C1180	U1117	U1059	A990	C924	U847	U788	G722
A1500	G1437	G1438	A1396	A1397	C1468	G1469	A1457	G1387	C1309	U1250	C1181	U1118	U1060	A991	C925	U848	G789	G723
A1501	G1438	G1439	A1396	A1397	C1468	G1469	A1457	G1387	C1310	U1251	C1182	U1119	U1061	A992	C926	U849	A790	G724
A1502	G1439	G1440	A1396	A1397	C1468	G1469	A1457	G1387	C1311	U1252	C1183	U1120	U1062	A993	C927	U850	A791	G725
A1503	G1440	G1441	A1396	A1397	C1468	G1469	A1457	G1387	C1312	U1253	C1184	U1121	U1063	A994	C928	U851	A792	
A1504	G1441	G1442	A1396	A1397	C1468	G1469	A1457	G1387	C1313	U1254	C1185	U1122	U1064	A995	C929	U852	A793	
G1505	G1442	G1443	A1396	A1397	C1468	G1469	A1457	G1387	C1314	U1255	C1186	U1123	U1065	A996	C930	U853	A794	
U1506	G1443	G1444	A1396	A1397	C1468	G1469	A1457	G1387	C1315	U1256	C1187	U1124	U1066	A997	C931	U854	A795	
A1507	G1444	G1445	A1396	A1397	C1468	G1469	A1457	G1387	C1316	U1257	C1188	U1125	U1067	A998	C932	U855	A796	
A1508	G1445	G1446	A1396	A1397	C1468	G1469	A1457	G1387	C1317	U1258	C1189	U1126	U1068	A999	C933	U856	A797	
C1509	G1446	G1447	A1396	A1397	C1468	G1469	A1457	G1387	C1318	U1259	C1190	U1127	U1069	A1000	C934	U857	A798	
C1510	G1447	G1448	A1396	A1397	C1468	G1469	A1457	G1387	C1319	U1260	C1191	U1128	U1070	A1001	C935	U858	A799	
C1511	G1448	G1449	A1396	A1397	C1468	G1469	A1457	G1387	C1320	U1261	C1192	U1129	U1071	A1002	C936	U859	A800	
C1512	G1449	G1450	A1396	A1397	C1468	G1469	A1457	G1387	C1321	U1262	C1193	U1130	U1072	A1003	C937	U860	A801	
C1513	G1450	G1451	A1396	A1397	C1468	G1469	A1457	G1387	C1322	U1263	C1194	U1131	U1073	A1004	C938	U861	A802	
C1514	G1451	G1452	A1396	A1397	C1468	G1469	A1457	G1387	C1323	U1264	C1195	U1132	U1074	A1005	C939	U862	A803	
C1515	G1452	G1453	A1396	A1397	C1468	G1469	A1457	G1387	C1324	U1265	C1196	U1133	U1075	A1006	C940	U863	A804	
C1516	G1453	G1454	A1396	A1397	C1468	G1469	A1457	G1387	C1325	U1266	C1197	U1134	U1076	A1007	C941	U864	A805	
C1517	G1454	G1455	A1396	A1397	C1468	G1469	A1457	G1387	C1326	U1267	C1198	U1135	U1077	A1008	C942	U865	A806	
C1518	G1455	G1456	A1396	A1397	C1468	G1469	A1457	G1387	C1327	U1268	C1199	U1136	U1078	A1009	C943	U866	A807	
C1519	G1456	G1457	A1396	A1397	C1468	G1469	A1457	G1387	C1328	U1269	C1200	U1137	U1079	A1010	C944	U867	A808	
C1520	G1457	G1458	A1396	A1397	C1468													



LEU
GLY
GLY
MET
ALA
ALA
VAL
GLU
GLN
PRO
GLU
LYS
PRO
ALA
ALA
GLN
PRO
LYS
LYS
LYS
GLN
GLN
ARG
LYS
GLY
ARG
LYS

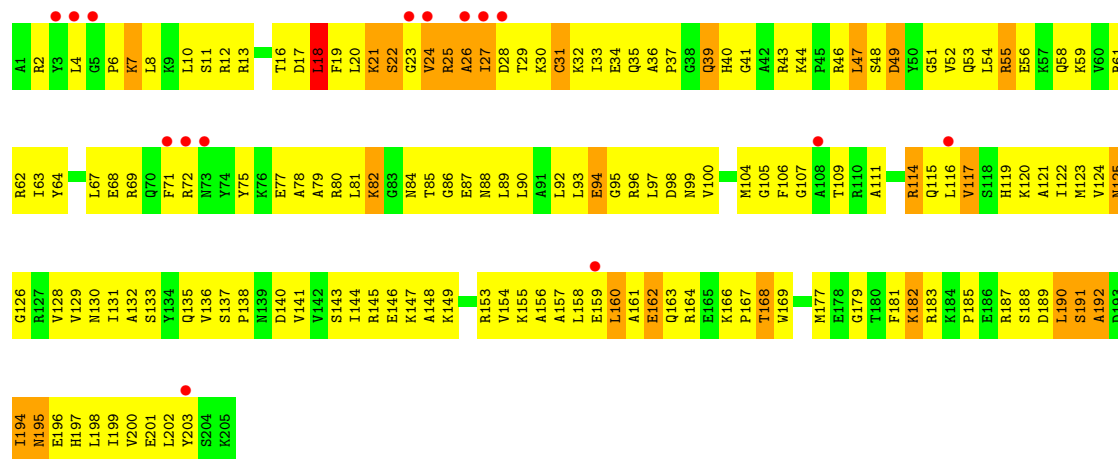
• Molecule 2: 30S ribosomal protein S3

Chain CC: 30% 43% 14% • 11%



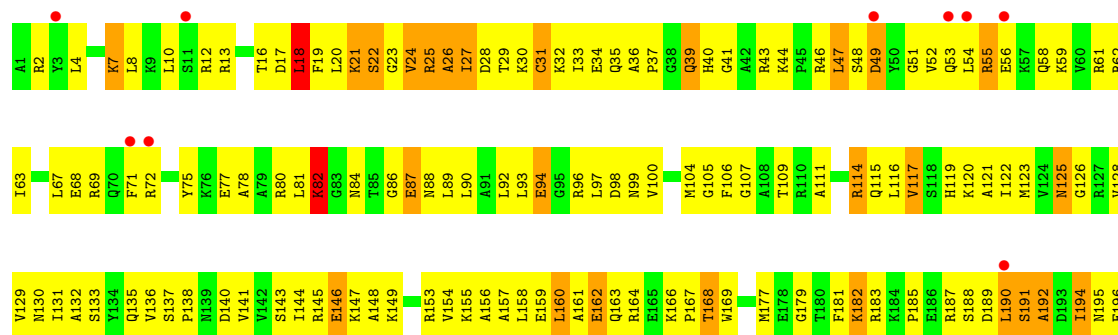
• Molecule 3: 30S ribosomal protein S4

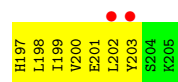
Chain AD: 7% 24% 62% 13%



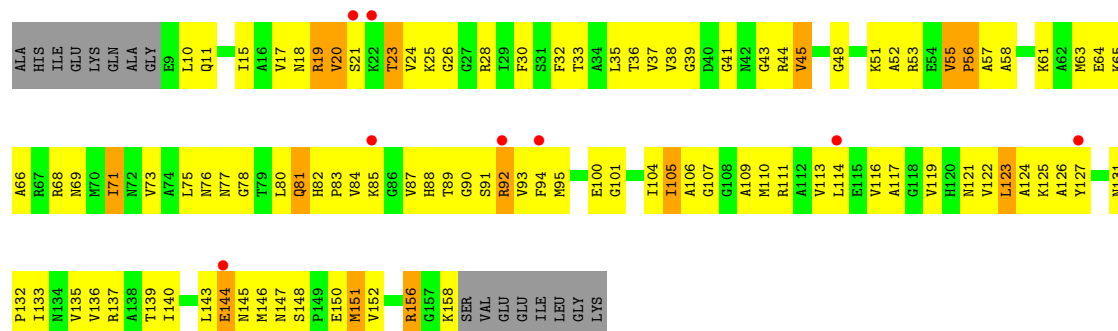
• Molecule 3: 30S ribosomal protein S4

Chain CD: 5% 28% 59% 13% •

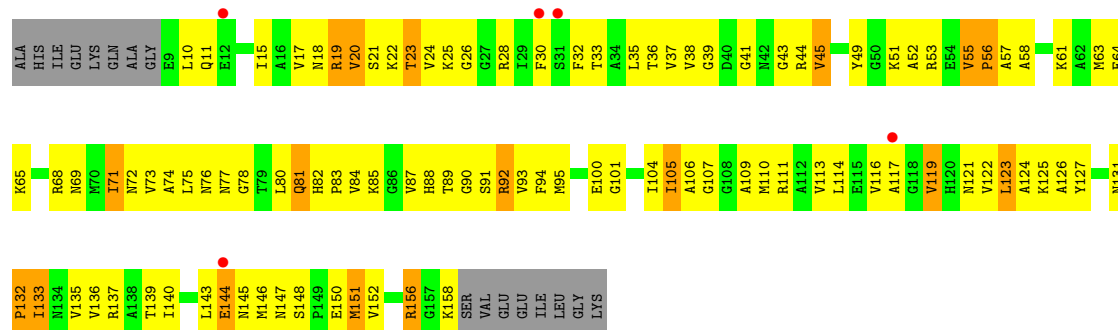




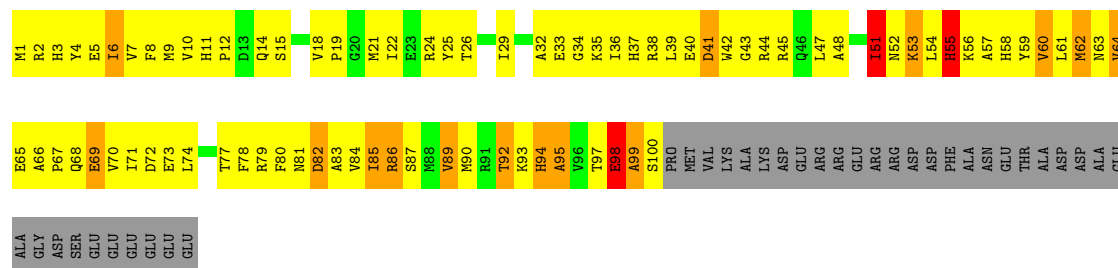
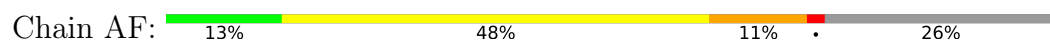
• Molecule 4: 30S ribosomal protein S5



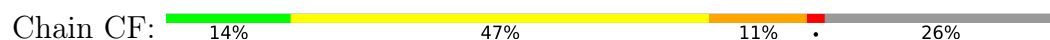
• Molecule 4: 30S ribosomal protein S5

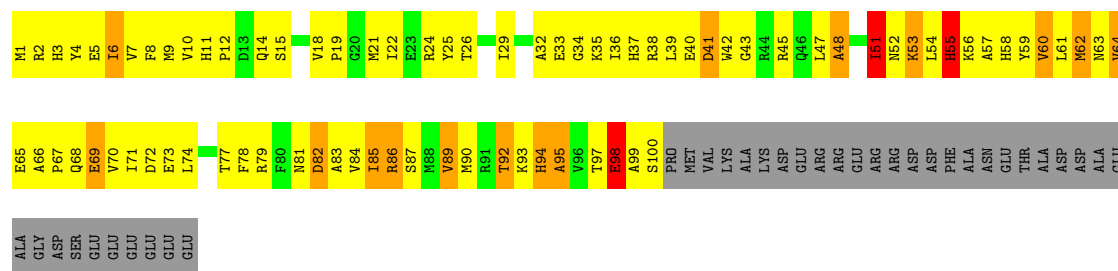


• Molecule 5: 30S ribosomal protein S6

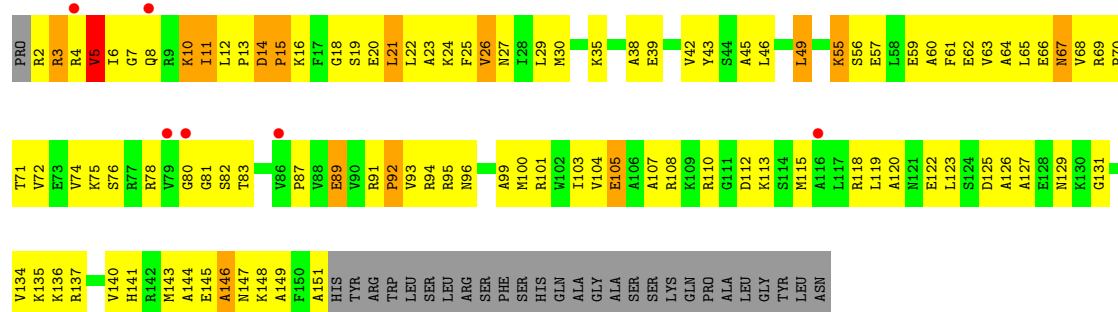


• Molecule 5: 30S ribosomal protein S6

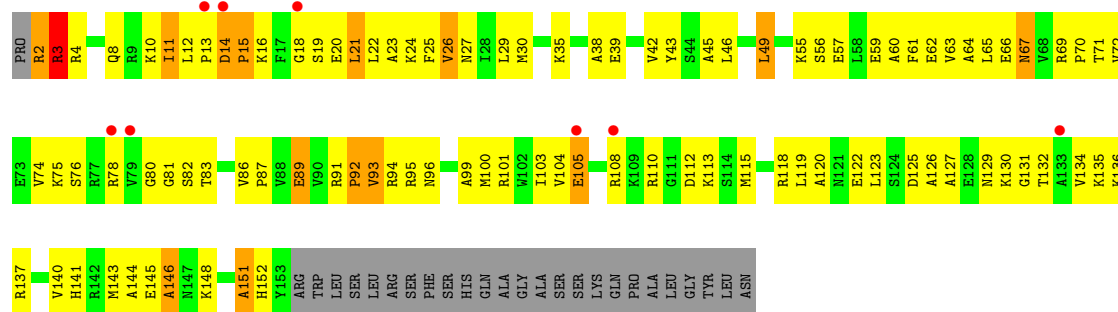




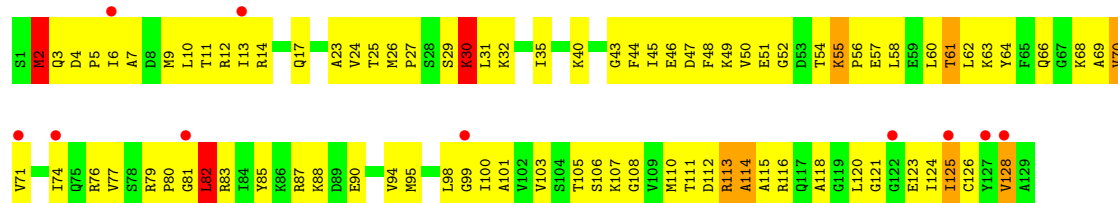
• Molecule 6: 30S ribosomal protein S7



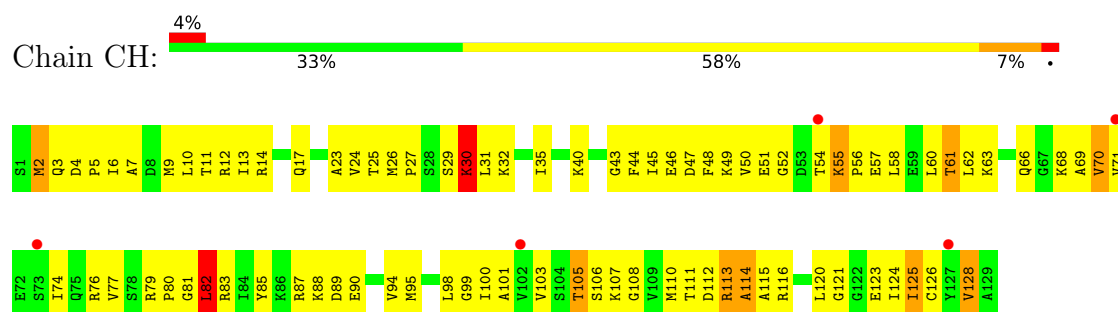
• Molecule 6: 30S ribosomal protein S7



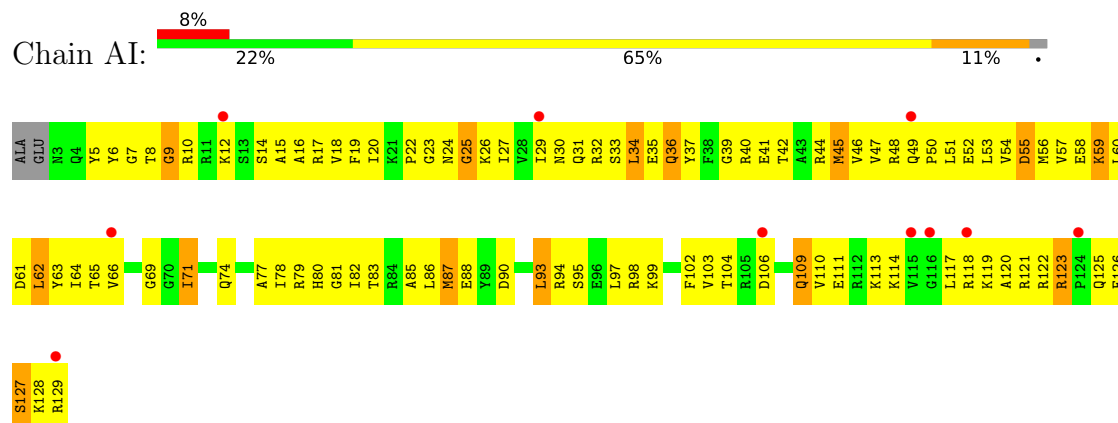
• Molecule 7: 30S ribosomal protein S8



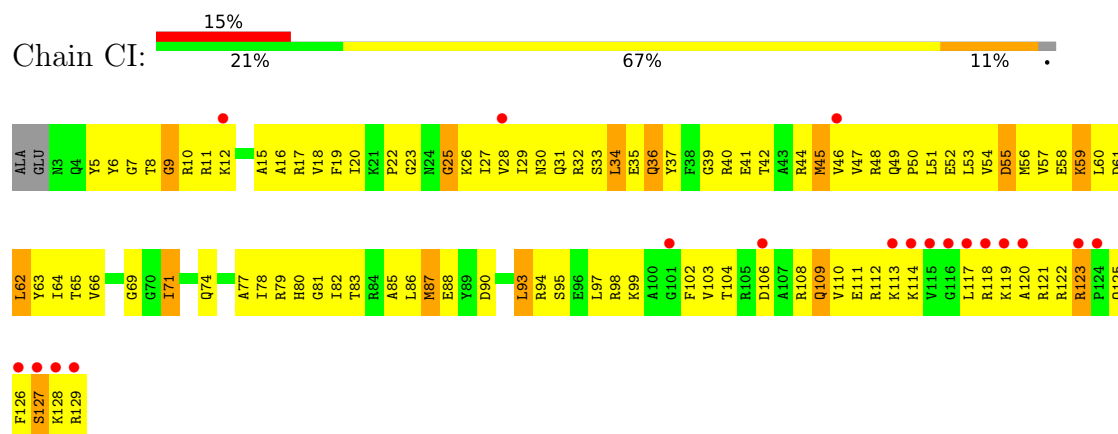
• Molecule 7: 30S ribosomal protein S8



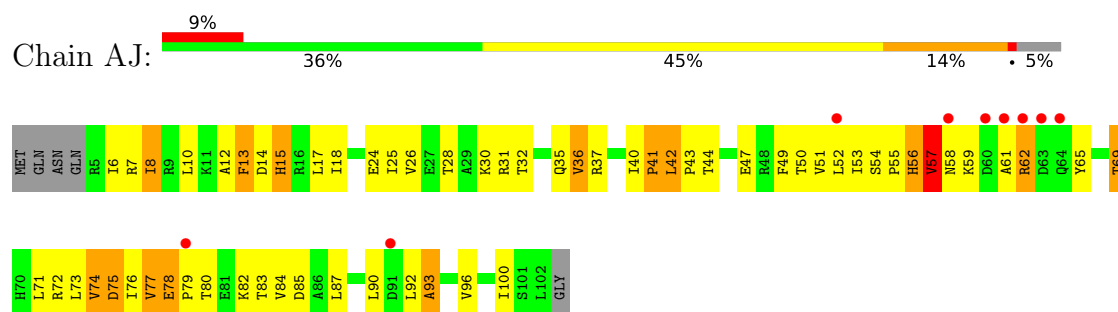
- Molecule 8: 30S ribosomal protein S9



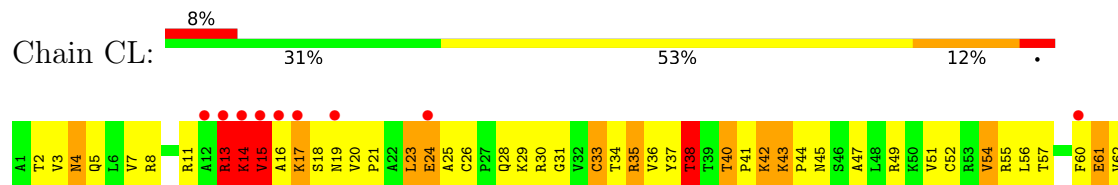
- Molecule 8: 30S ribosomal protein S9

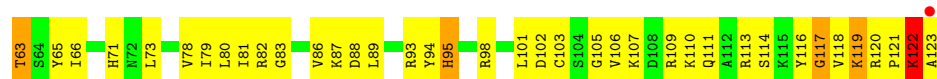


- Molecule 9: 30S ribosomal protein S10



- Molecule 9: 30S ribosomal protein S10





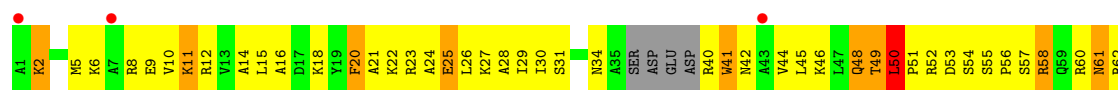
- Molecule 12: 30S ribosomal protein S13



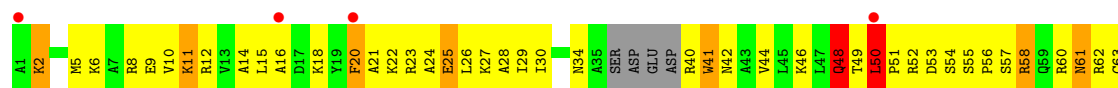
- Molecule 12: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S14

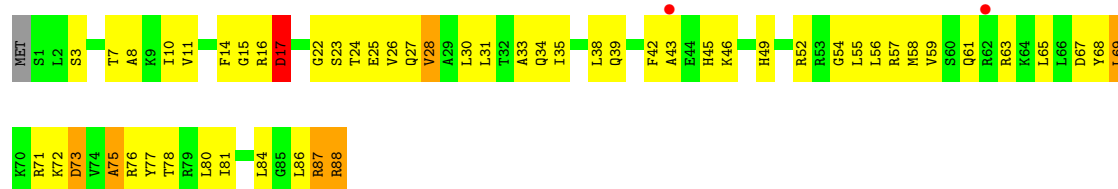


- Molecule 13: 30S ribosomal protein S14

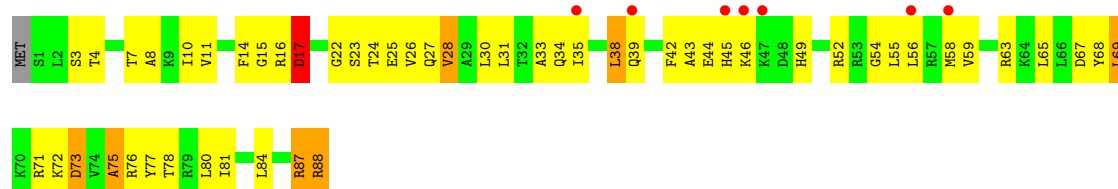
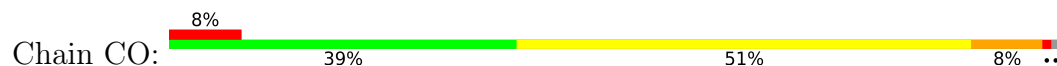


- Molecule 14: 30S ribosomal protein S15

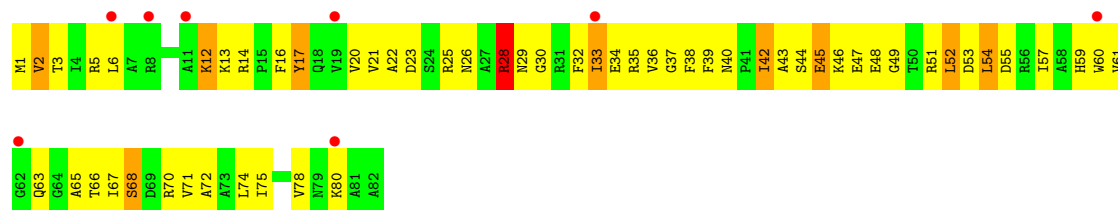




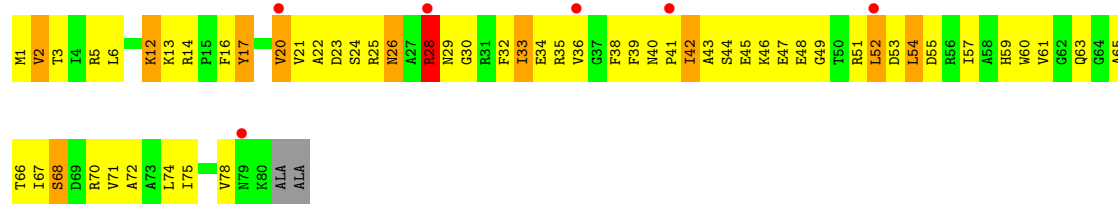
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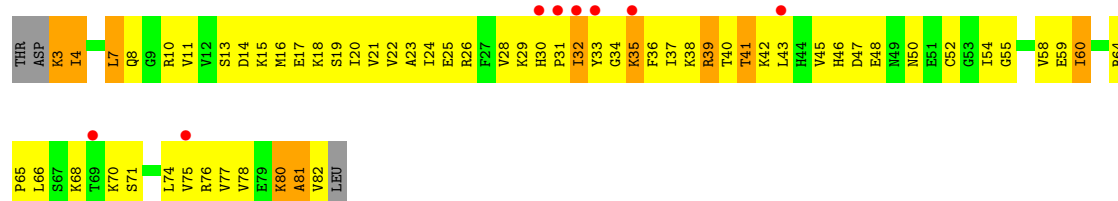
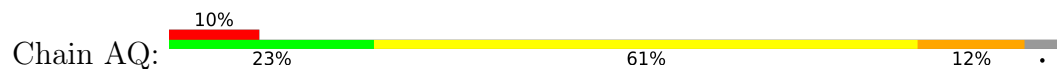
• Molecule 15: 30S ribosomal protein S16



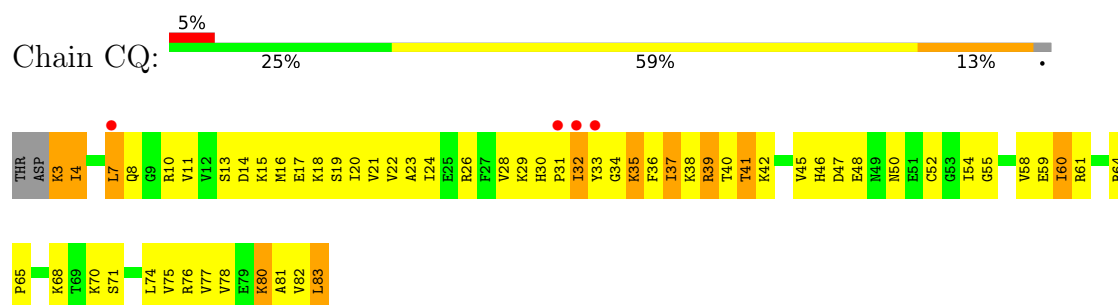
• Molecule 15: 30S ribosomal protein S16



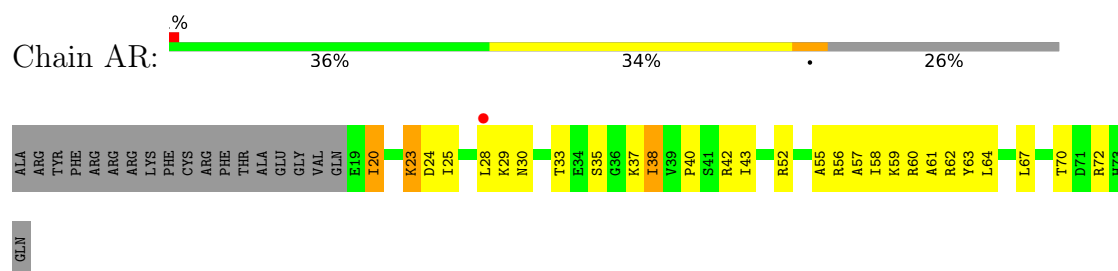
• Molecule 16: 30S ribosomal protein S17



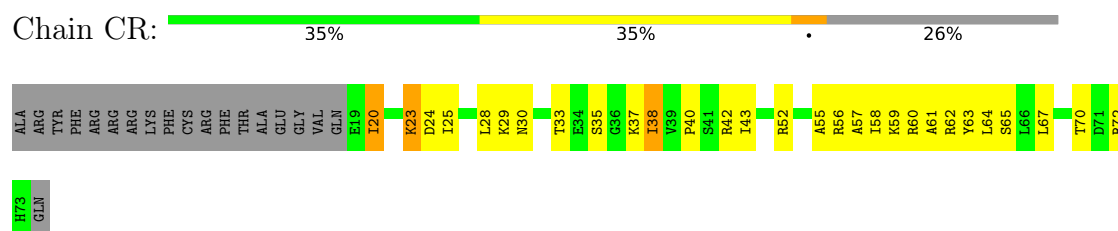
- Molecule 16: 30S ribosomal protein S17



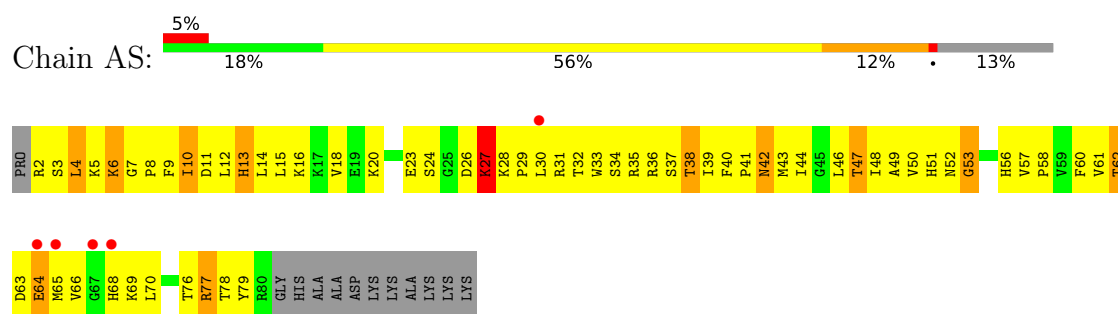
- Molecule 17: 30S ribosomal protein S18



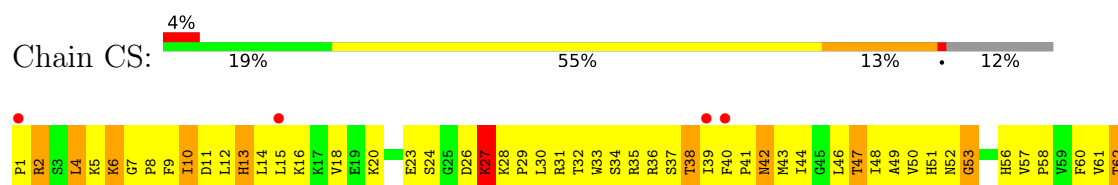
- Molecule 17: 30S ribosomal protein S18

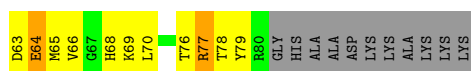


- Molecule 18: 30S ribosomal protein S19

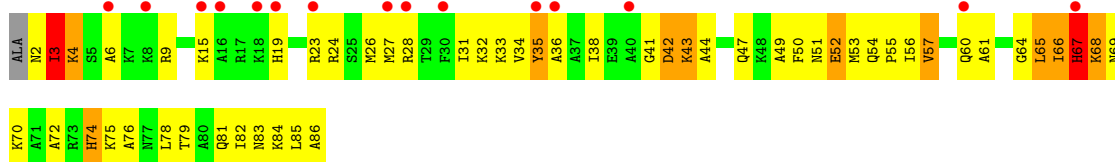


- Molecule 18: 30S ribosomal protein S19

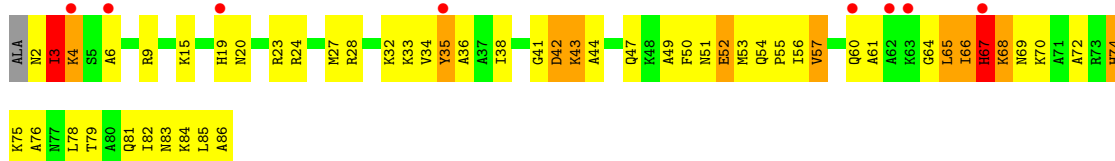




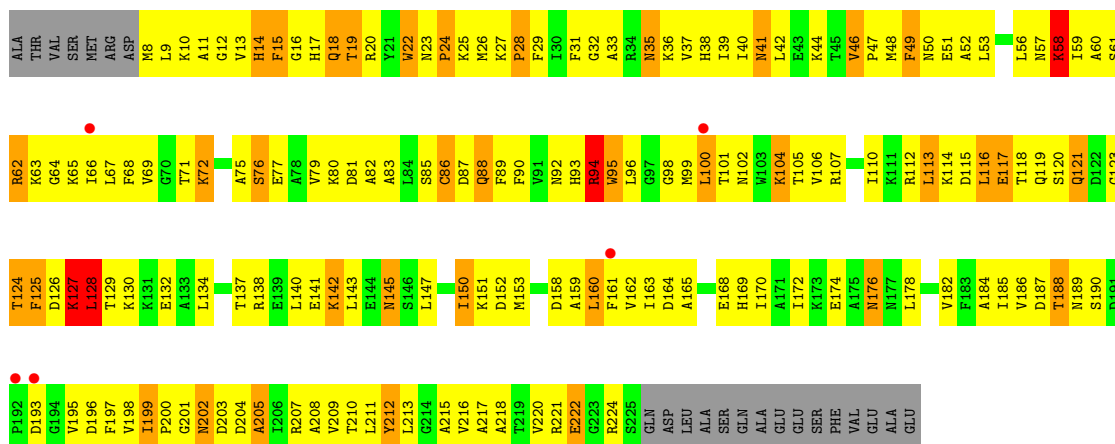
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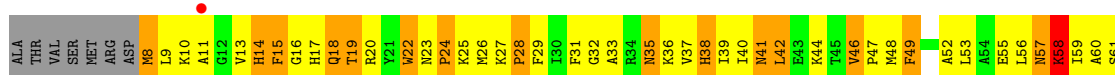
• Molecule 19: 30S ribosomal protein S20

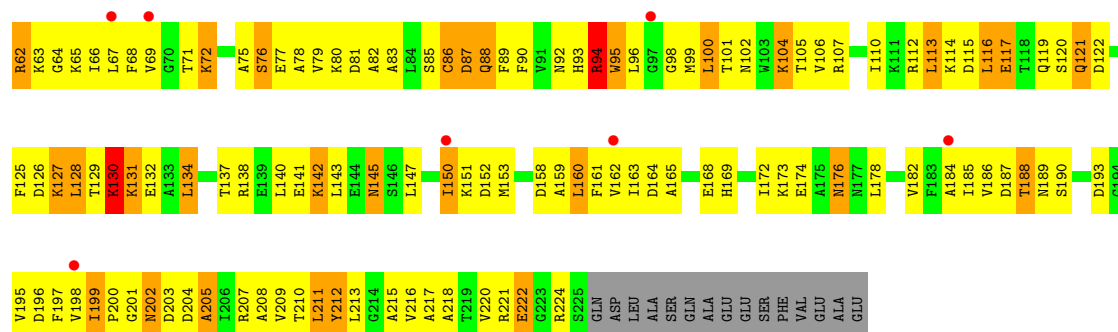


• Molecule 20: 30S ribosomal protein S2

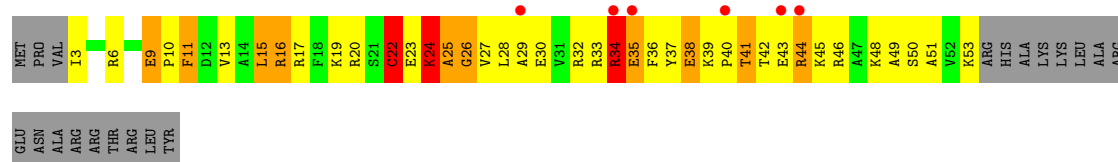
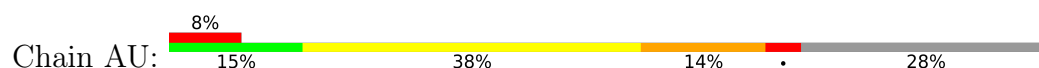


• Molecule 20: 30S ribosomal protein S2

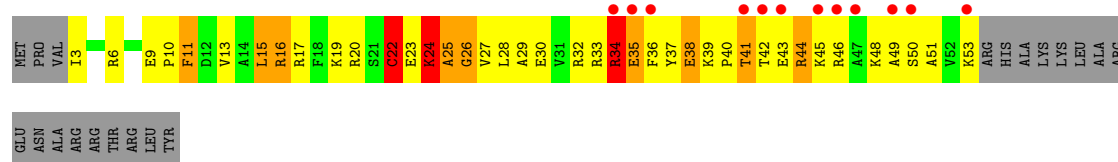
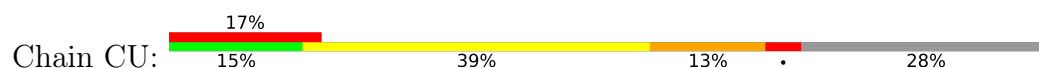




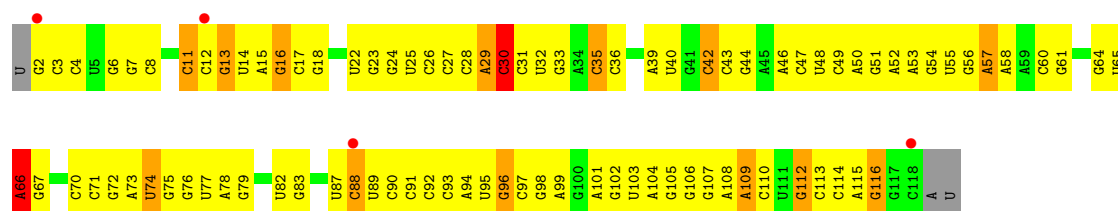
• Molecule 21: 30S ribosomal protein S21



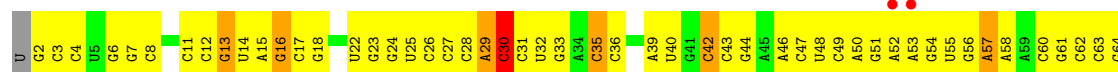
• Molecule 21: 30S ribosomal protein S21



• Molecule 22: 5S ribosomal RNA



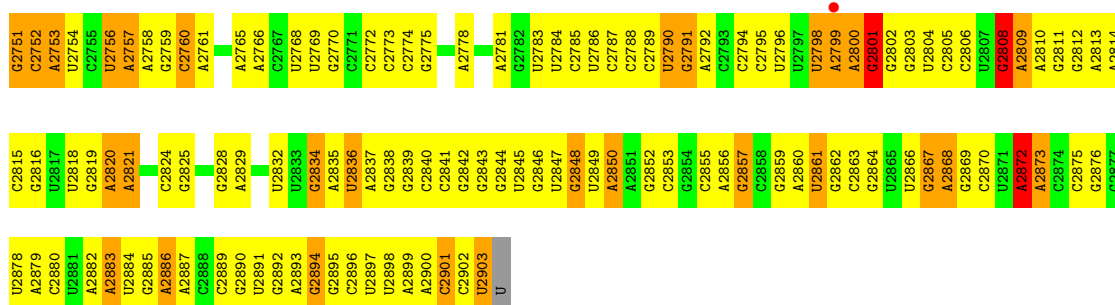
• Molecule 22: 5S ribosomal RNA



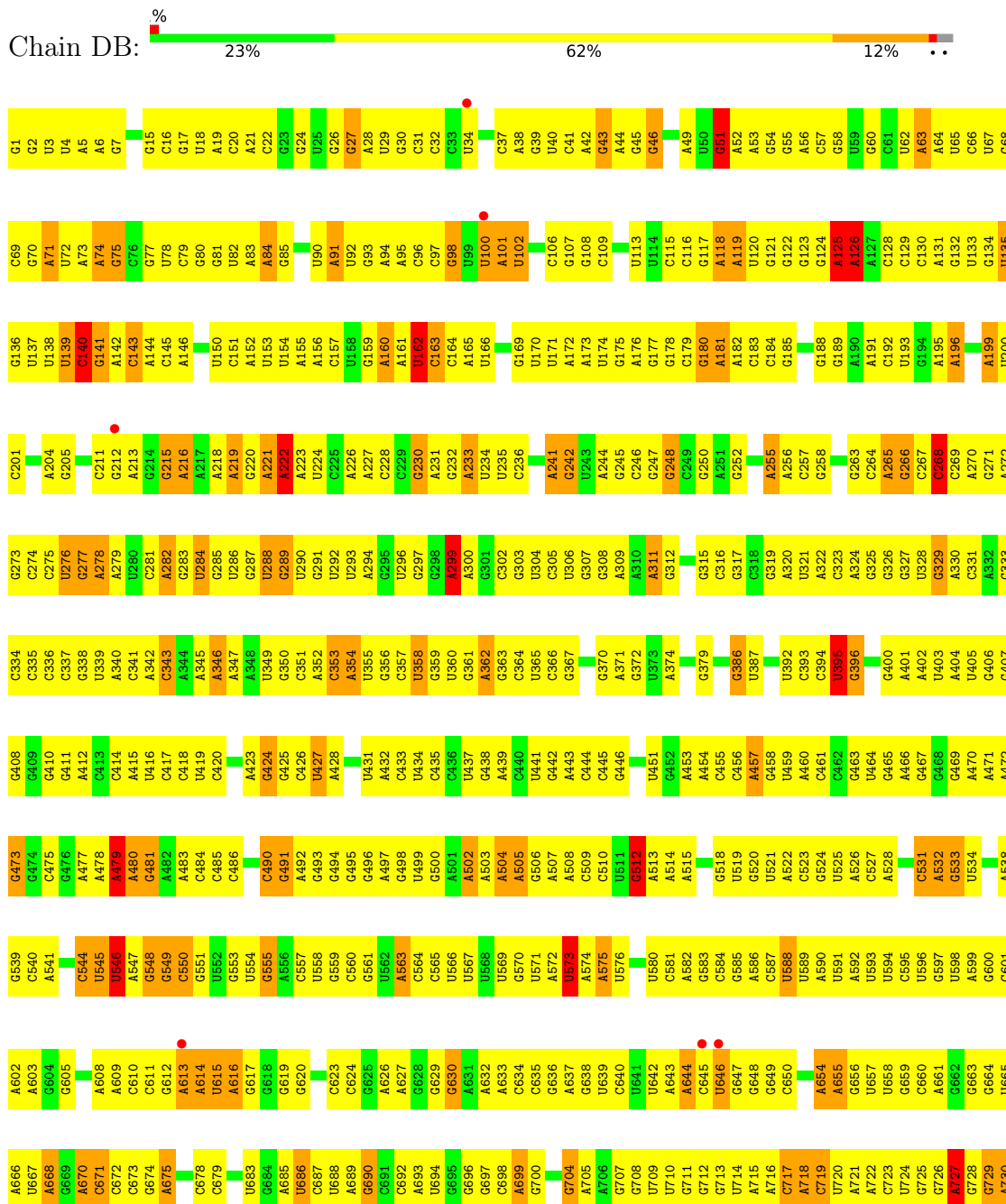






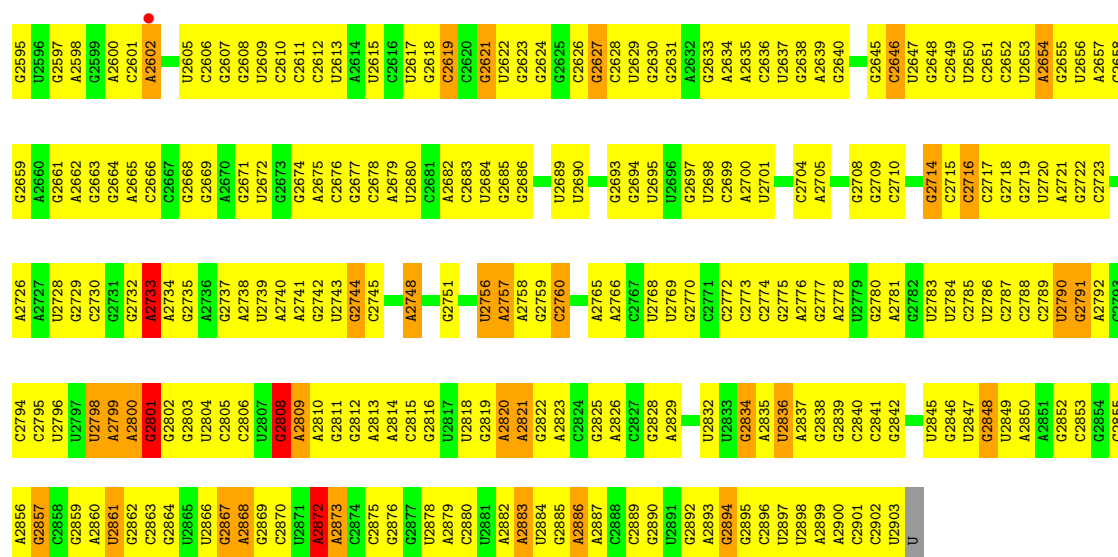


• Molecule 23: 23S ribosomal RNA



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G1601	G1538	G1475	U1412	U1344	A1275	U1209	C1146	U1081	G1002	U934	U871	U810	C740
U1602	U1539	U1476	A1413	C1345	A1276	G1210	G1149	U1082	A1010	C935	C872	C812	U741
G1606	G1540	A1477	G1416	G1346	G1280	G1211	C1150	U1083	U1011	A936	G873	U811	A742
C1607	C1541	G1478	G1417	A1347	G1281	G1212	C1151	U1084	U1012	U937	G874	C814	A743
A1608	U1542	G1479	C1348	C1348	U1282	G1213	A1151	U1085	G1013	G938	G875	C815	U744
A1609	G1543	C1480	G1418	C1349	G1283	A1214	C1152	A1086	C1014	G939	C876	C816	G745
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G1616	G1546	G1483	G1421	A1352	A1286	U1219	A1156	A1089	G1017	A943	G	A819	A750
G1619	G1547	G1484	G1422	U1353	A1287	G1220	U1159	U1090	U1018	C946	G	A820	A751
G1623	A1548	U1485	G1423	A1354	U1288	G1221	G1160	G1091	U1019	A947	G	A821	A752
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G1639	A1552	A1427	G1427	A1366	C1291	U1224	G1163	U1094	A1022	G950	C	U824	U755
A1641	U1553	G1428	G1428	A1367	G1292	G1225	G1165	U1097	U1023	C951	C	U825	A756
G1642	U1554	G1429	G1429	A1367	C1293	G1226	C1166	A1098	G1025	C956	C	U826	G757
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G1644	C1558	C1493	A1431	C1369	C1295	A1230	G1166	C1100	A1027	C958	C	U828	G759
G1645	U1559	A1494	G1432	C1370	G1296	G1231	C1167	U1101	A1028	U959	C	U829	A761
G1646	G1560	A1495	A1433	G1371	C1297	G1232	G1168	C1102	A1029	G960	G	G830	G760
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A1655	C1565	C1498	G1436	A1374	G1236	G1236	U1173	G1107	A1032	A972	U	U833	G775
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A1699	G1673	C1531	U1468	A1405	A1336	U1269	U1201	G1068	C995	A927	C	U861	U803
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A1699	G1675	A1533	G1407	U1407	G1338	C1270	U1203	A1070	C997	U929	C	U863	G805
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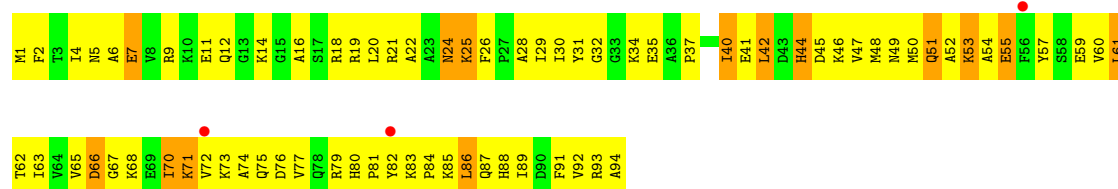




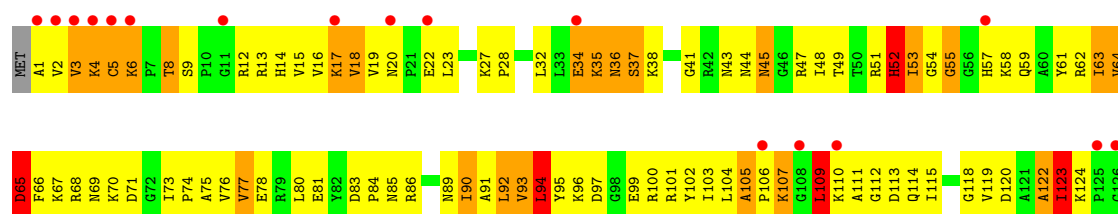
• Molecule 24: 50S ribosomal protein L25

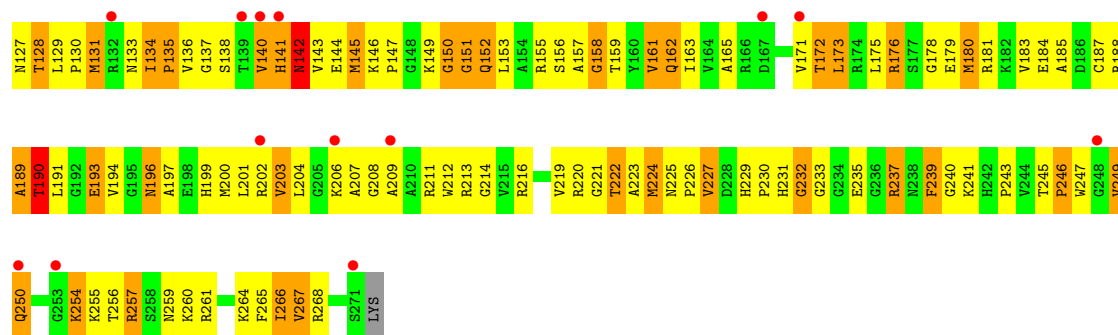


• Molecule 24: 50S ribosomal protein L25

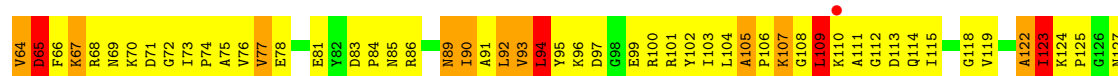
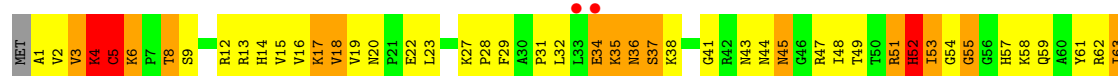


• Molecule 25: 50S ribosomal protein L2





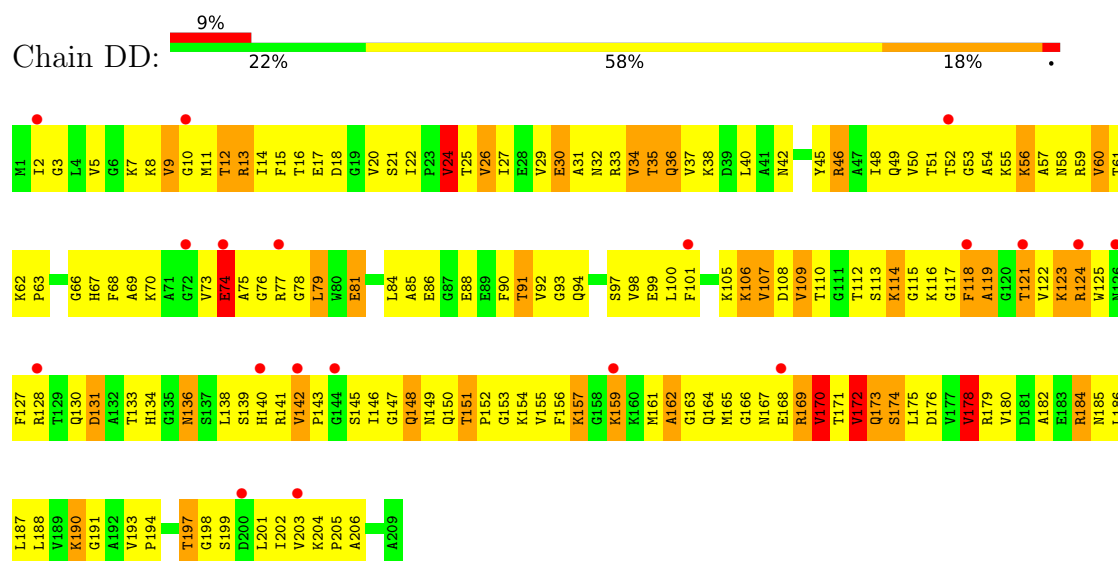
• Molecule 25: 50S ribosomal protein L2



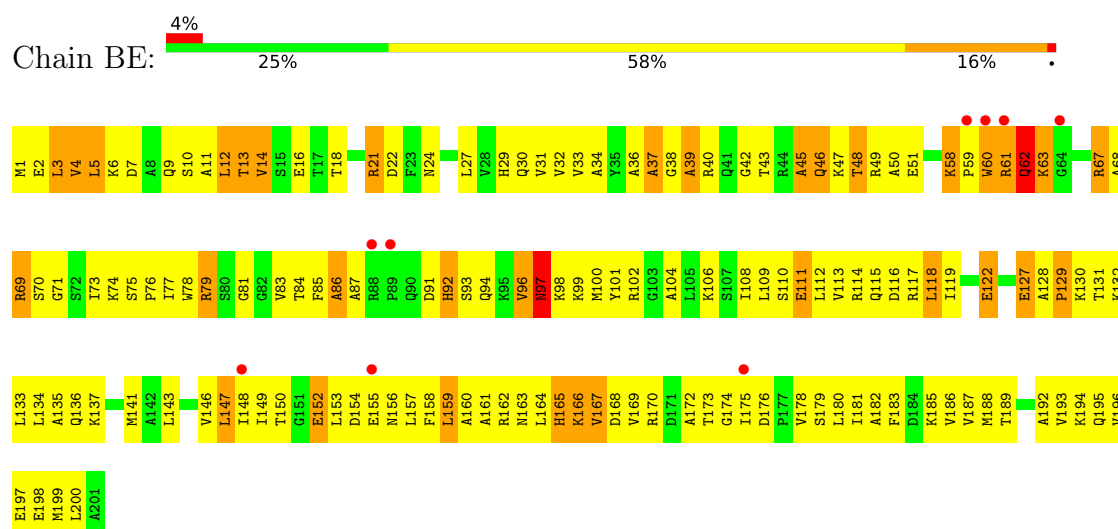
• Molecule 26: 50S ribosomal protein L3



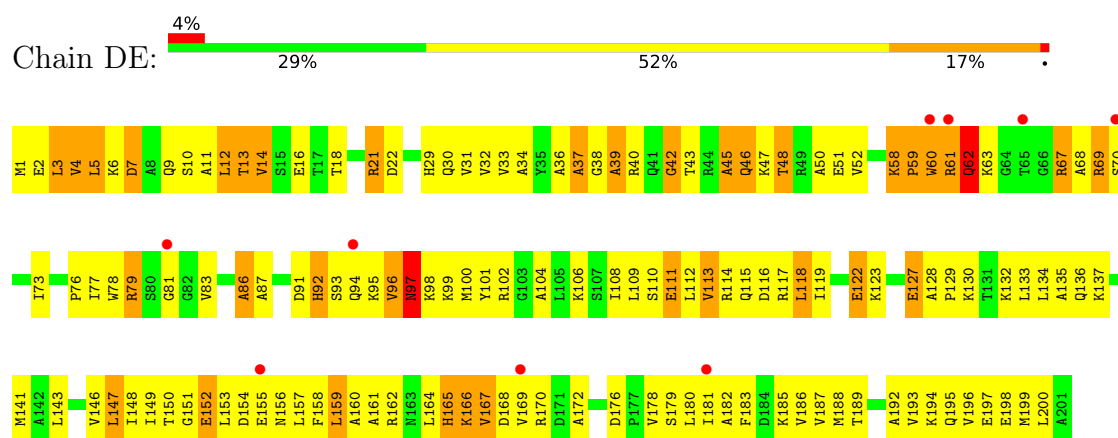
- Molecule 26: 50S ribosomal protein L3



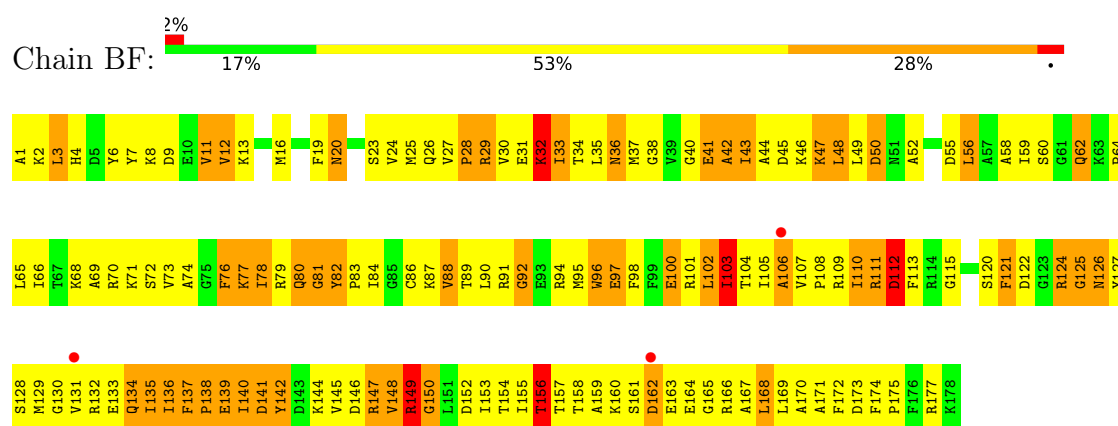
- Molecule 27: 50S ribosomal protein L4



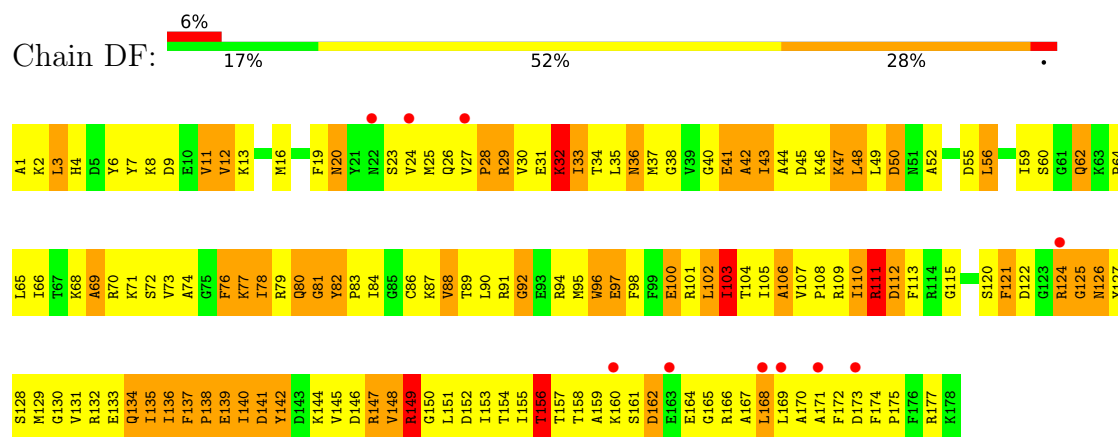
- Molecule 27: 50S ribosomal protein L4



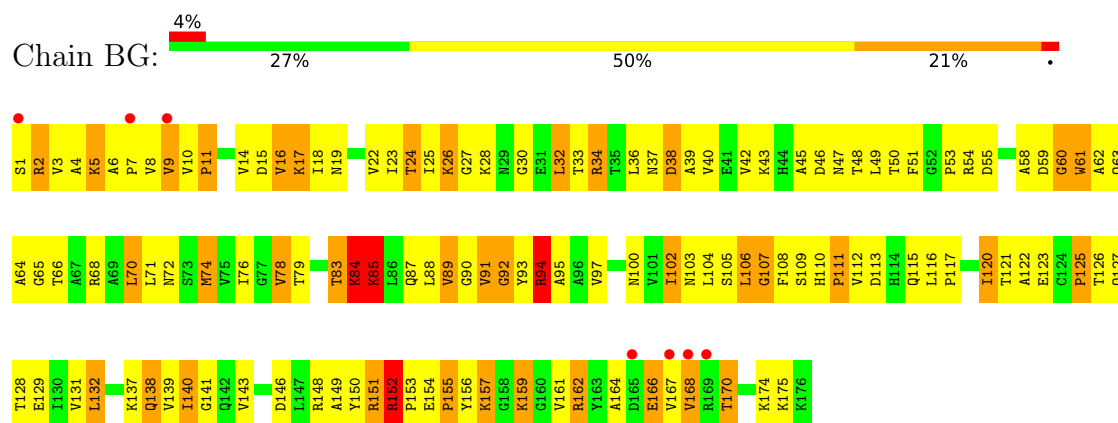
- Molecule 28: 50S ribosomal protein L5



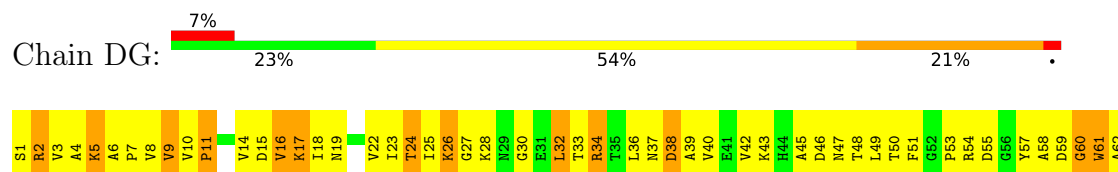
• Molecule 28: 50S ribosomal protein L5

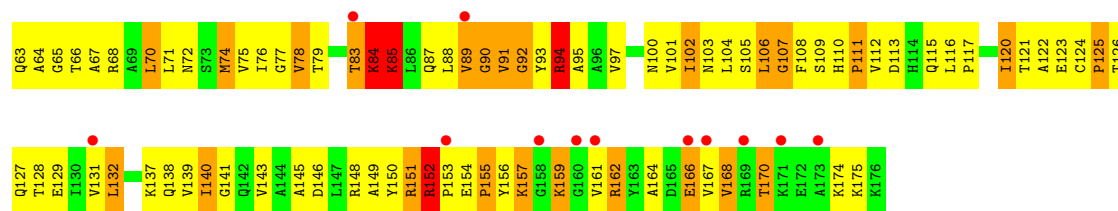


• Molecule 29: 50S ribosomal protein L6

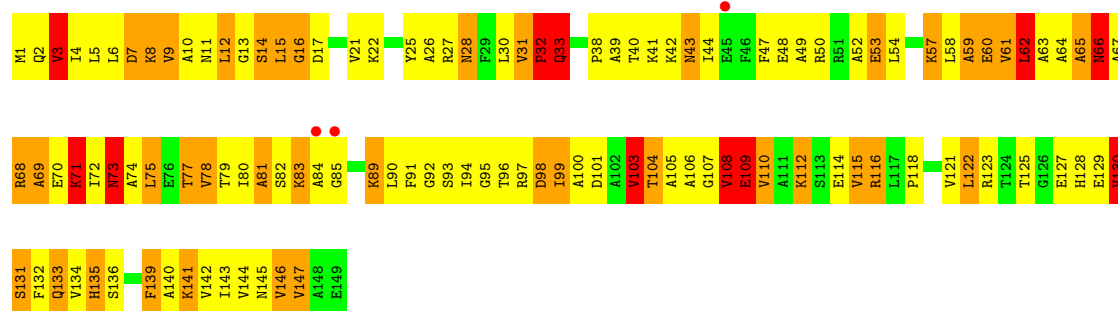
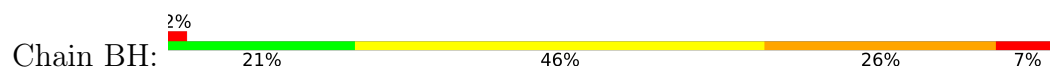


• Molecule 29: 50S ribosomal protein L6

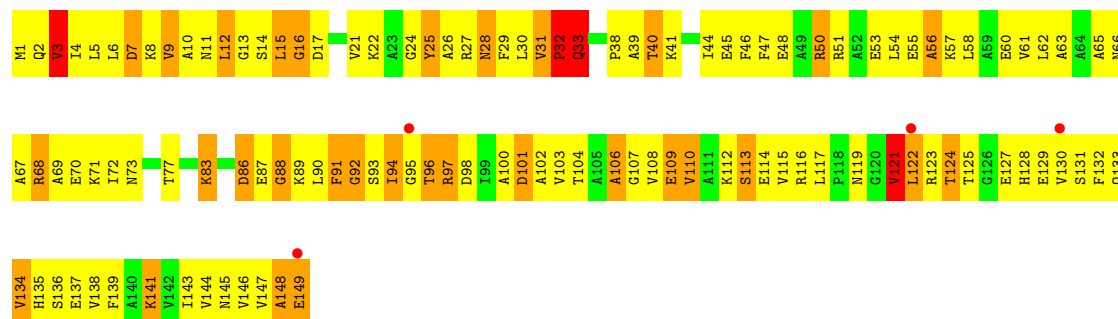




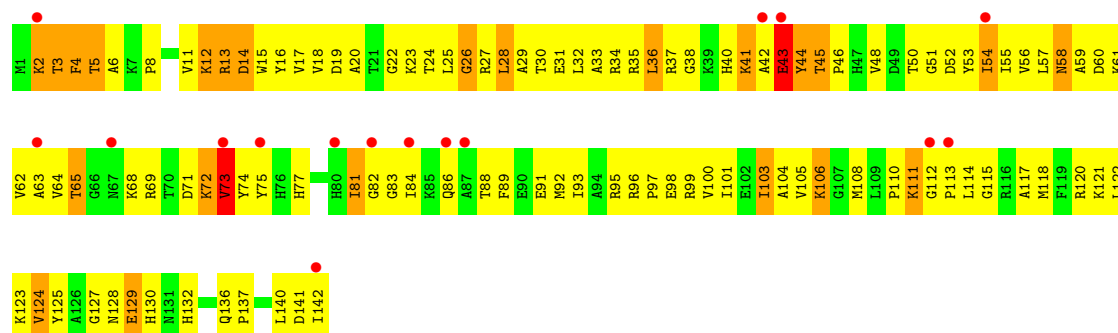
• Molecule 30: 50S ribosomal protein L9



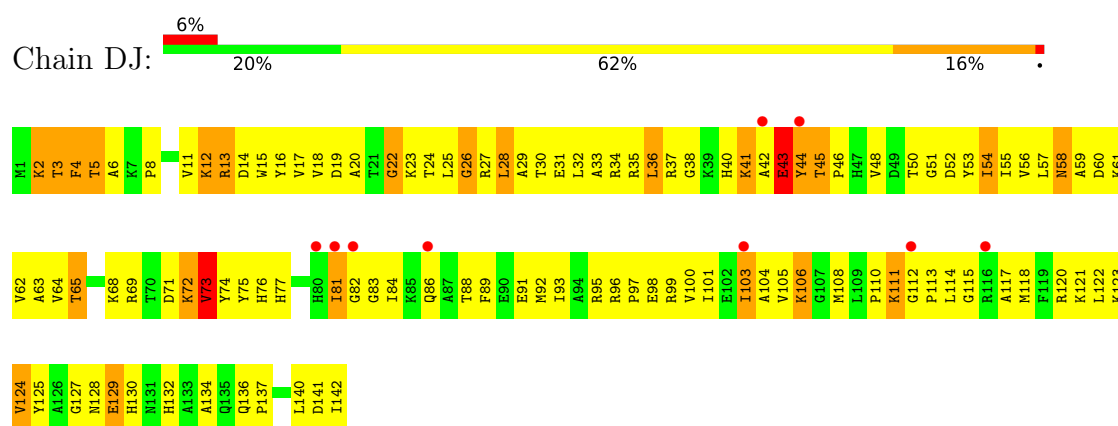
• Molecule 30: 50S ribosomal protein L9



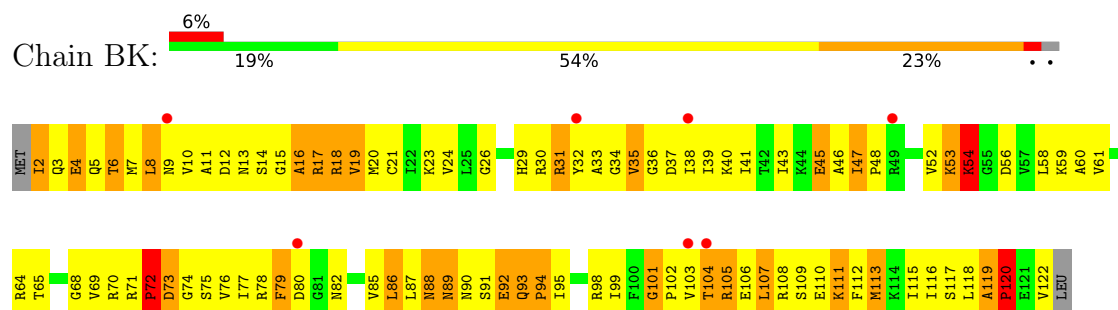
• Molecule 31: 50S ribosomal protein L13



• Molecule 31: 50S ribosomal protein L13



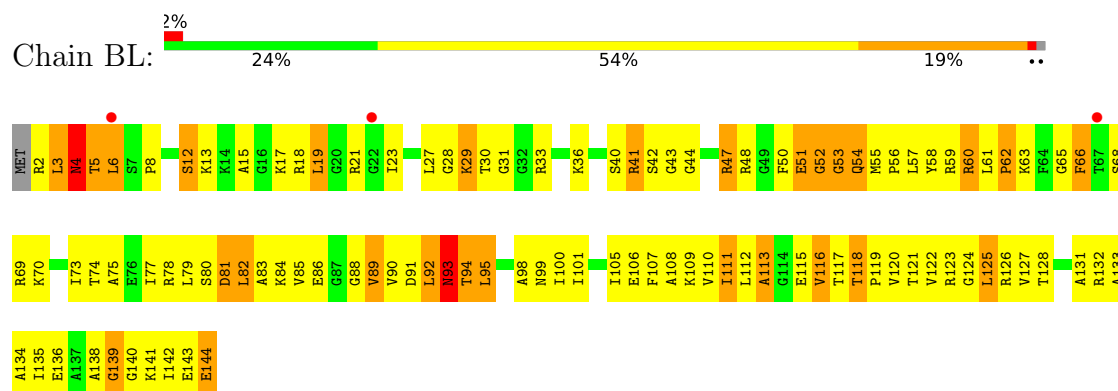
- Molecule 32: 50S ribosomal protein L14



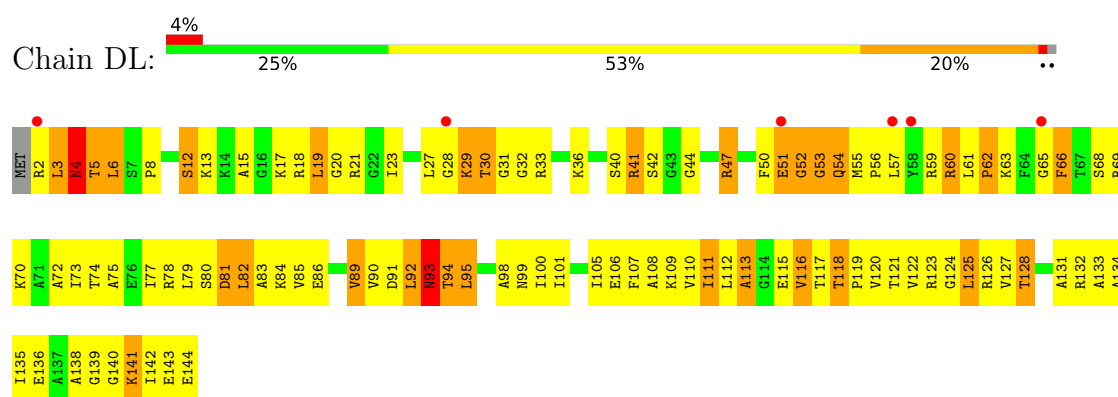
- Molecule 32: 50S ribosomal protein L14



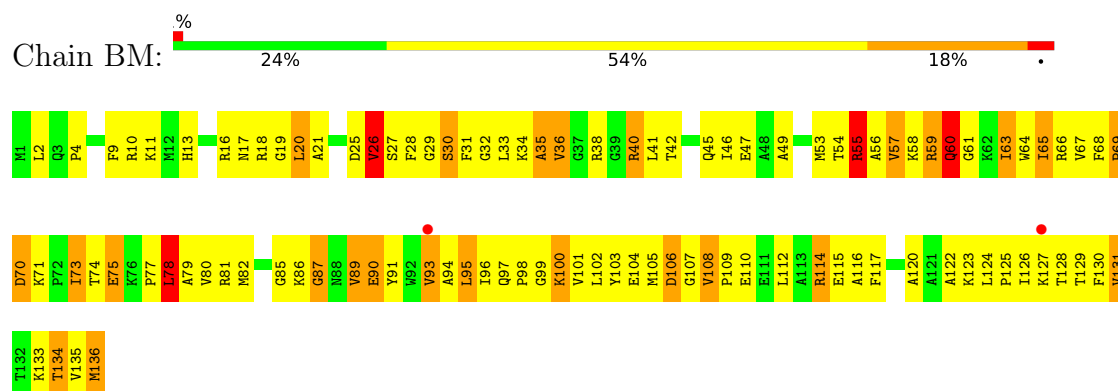
- Molecule 33: 50S ribosomal protein L15



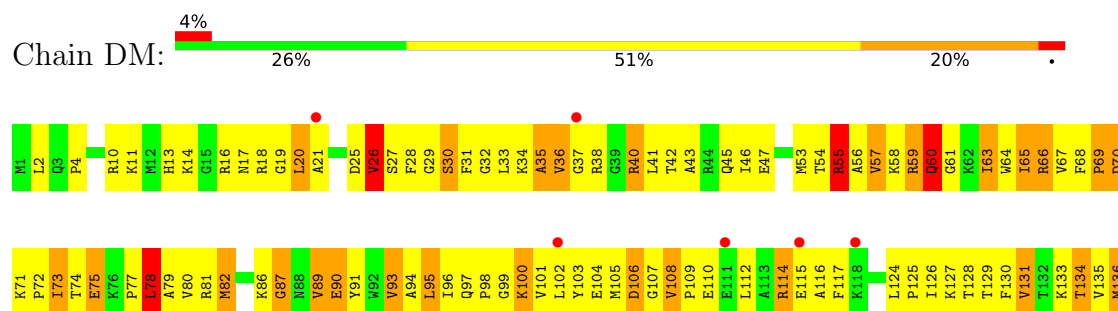
- Molecule 33: 50S ribosomal protein L15



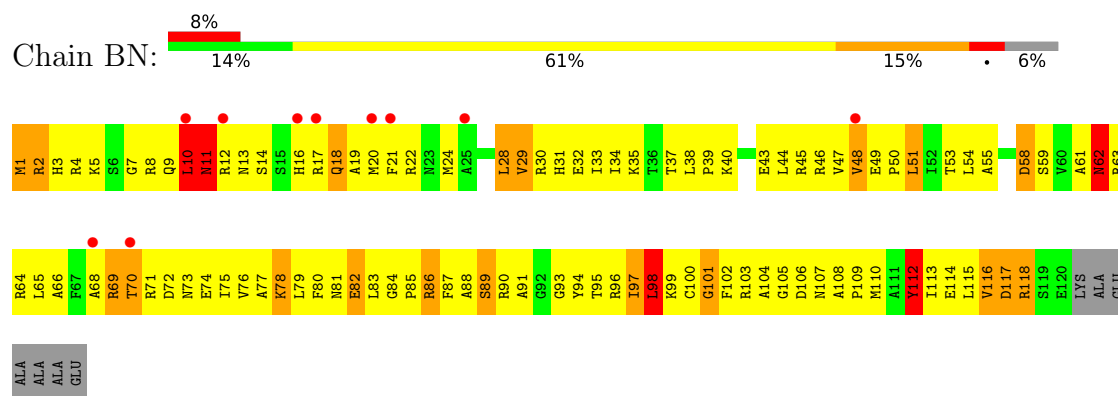
• Molecule 34: 50S ribosomal protein L16



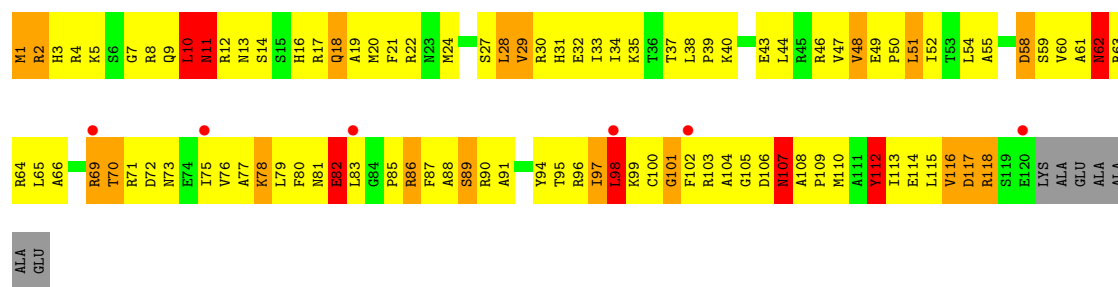
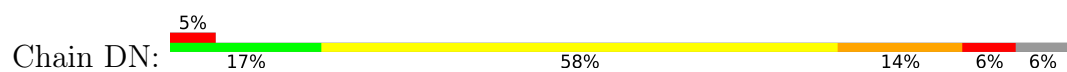
• Molecule 34: 50S ribosomal protein L16



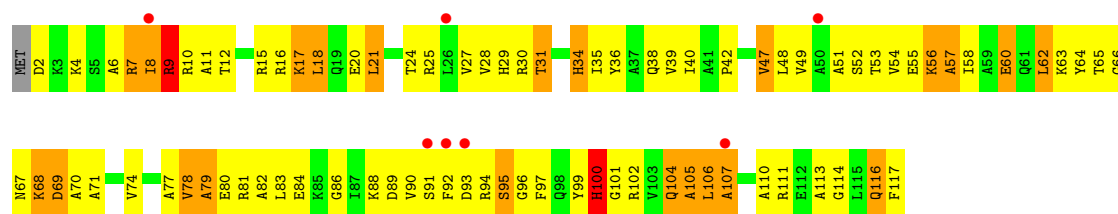
• Molecule 35: 50S ribosomal protein L17



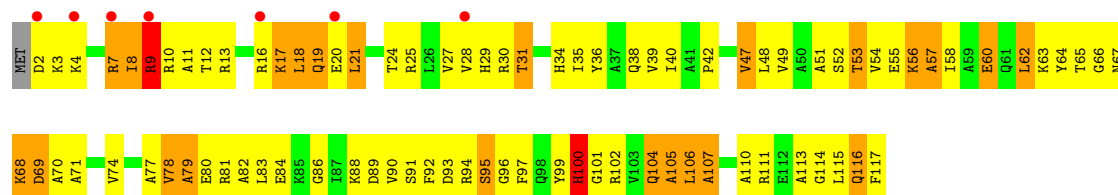
• Molecule 35: 50S ribosomal protein L17



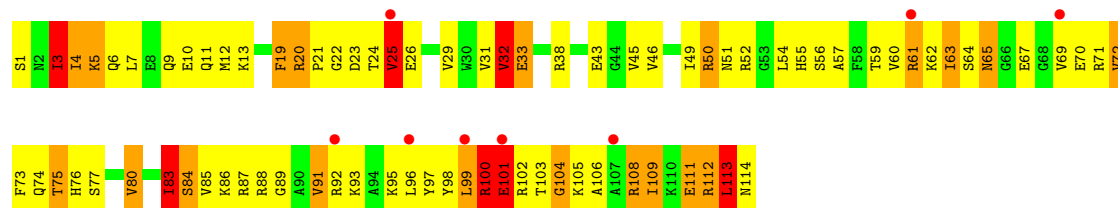
• Molecule 36: 50S ribosomal protein L18



• Molecule 36: 50S ribosomal protein L18



• Molecule 37: 50S ribosomal protein L19

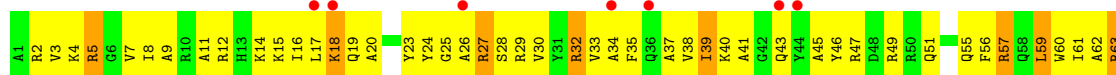


• Molecule 37: 50S ribosomal protein L19





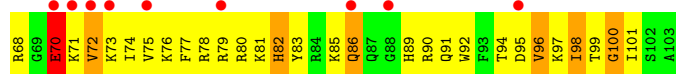
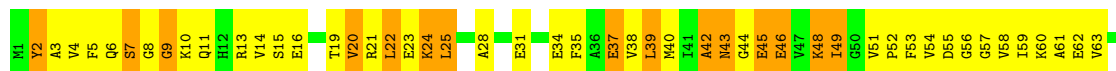
• Molecule 38: 50S ribosomal protein L20



• Molecule 38: 50S ribosomal protein L20



• Molecule 39: 50S ribosomal protein L21

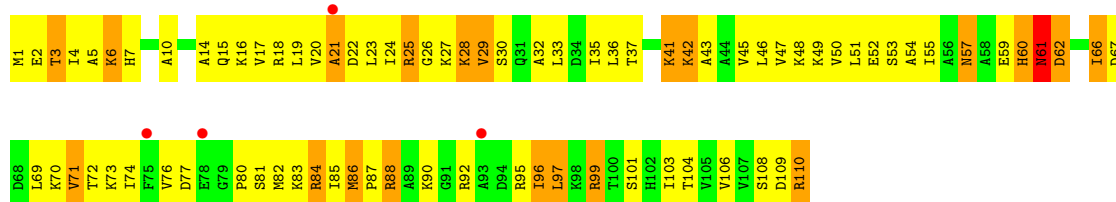


• Molecule 39: 50S ribosomal protein L21

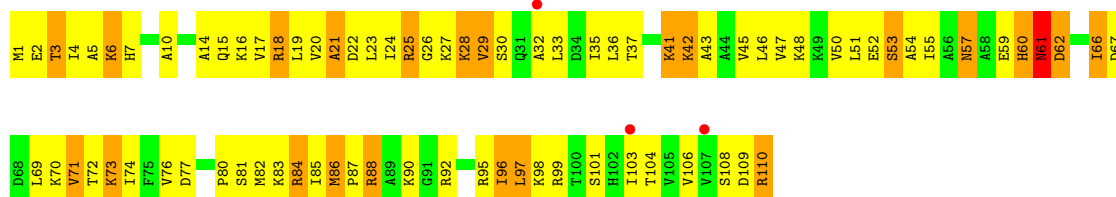


• Molecule 40: 50S ribosomal protein L22

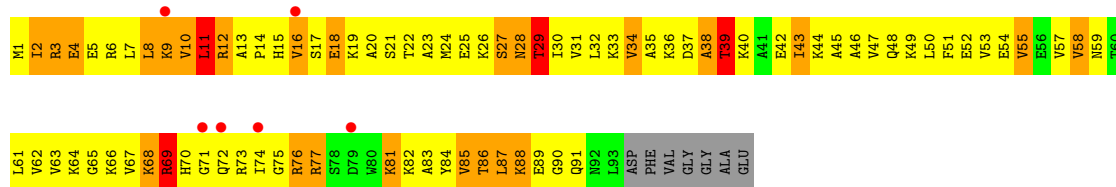
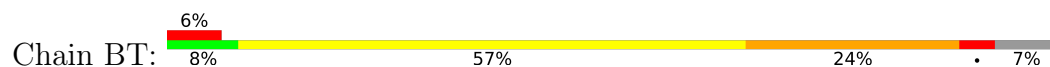




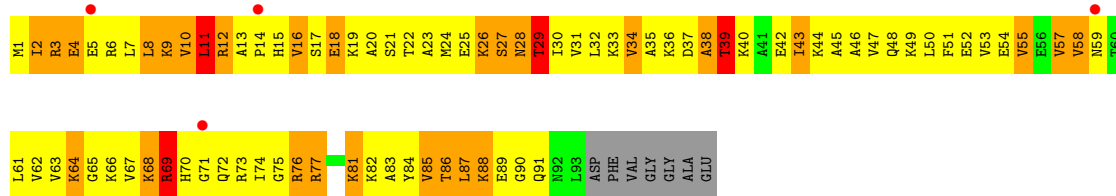
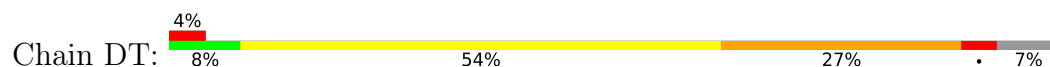
• Molecule 40: 50S ribosomal protein L22



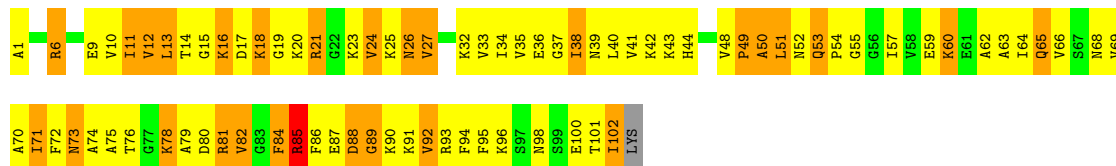
• Molecule 41: 50S ribosomal protein L23



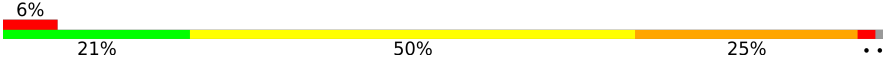
• Molecule 41: 50S ribosomal protein L23

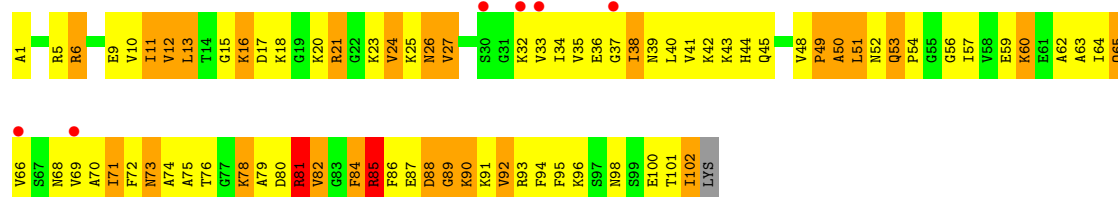


• Molecule 42: 50S ribosomal protein L24



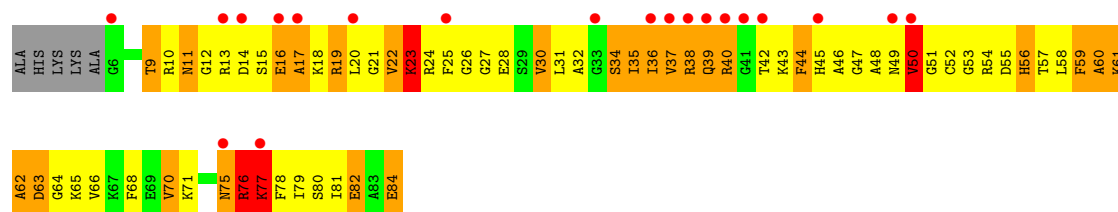
• Molecule 42: 50S ribosomal protein L24

Chain DU: 



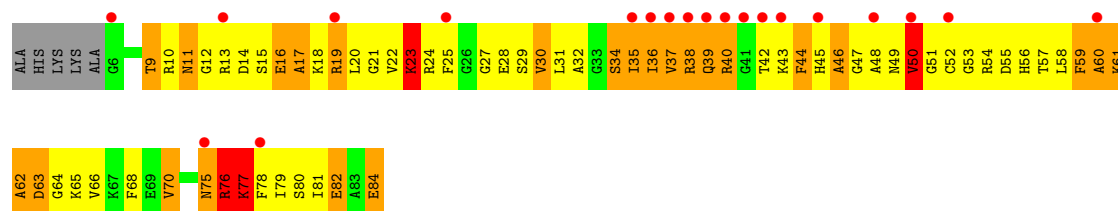
• Molecule 43: 50S ribosomal protein L27

Chain BW: 

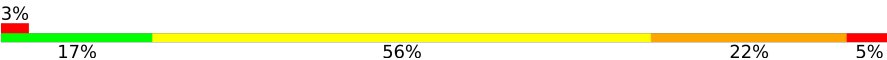


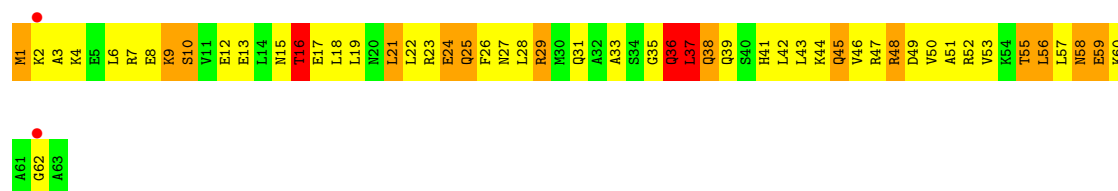
• Molecule 43: 50S ribosomal protein L27

Chain DW: 



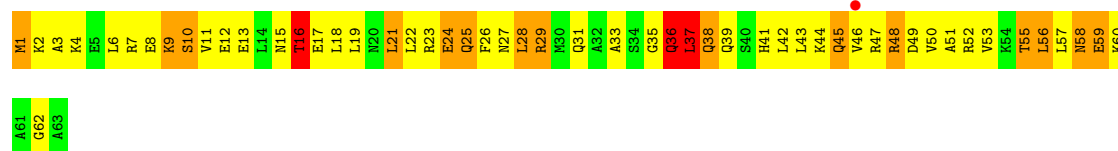
• Molecule 44: 50S ribosomal protein L29

Chain BX: 

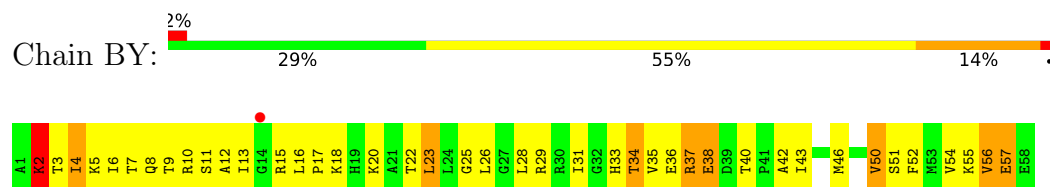


• Molecule 44: 50S ribosomal protein L29

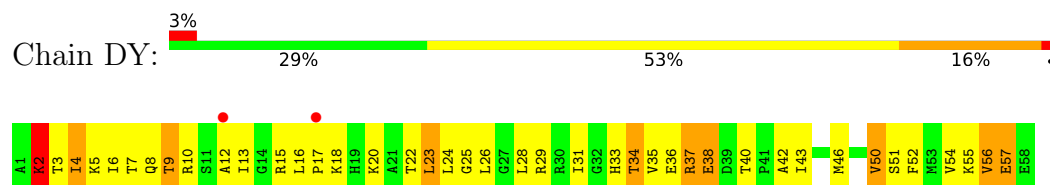
Chain DX: 



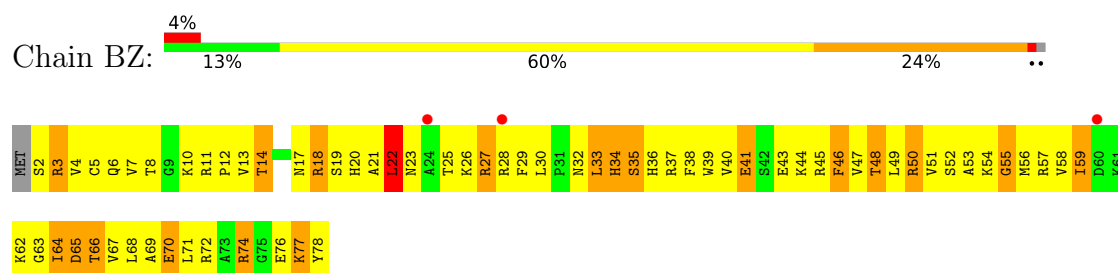
• Molecule 45: 50S ribosomal protein L30



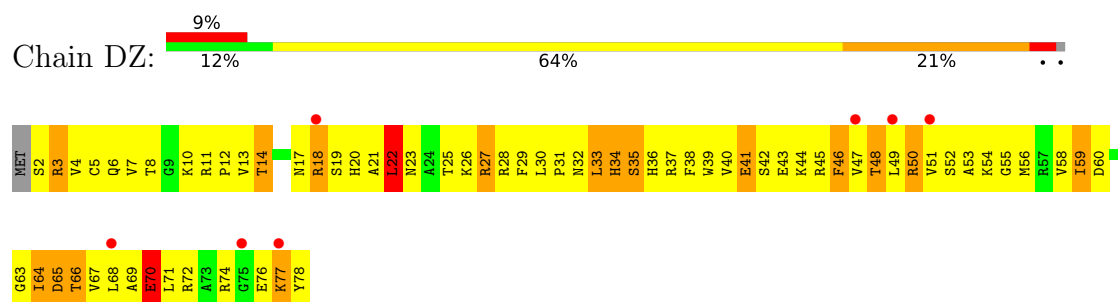
• Molecule 45: 50S ribosomal protein L30



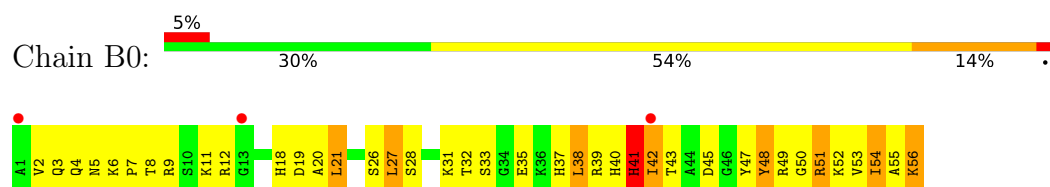
• Molecule 46: 50S ribosomal protein L28



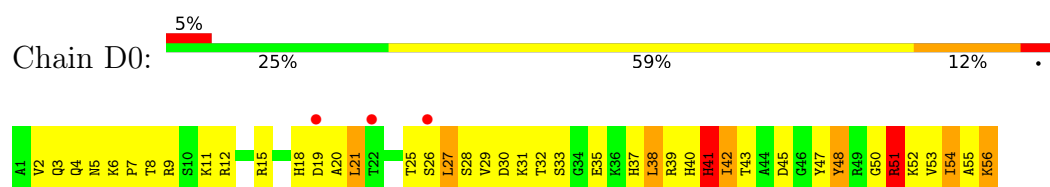
• Molecule 46: 50S ribosomal protein L28



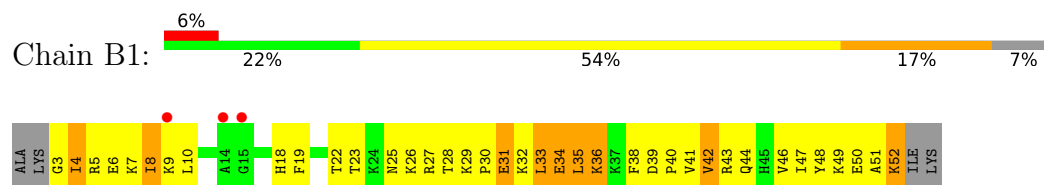
• Molecule 47: 50S ribosomal protein L32



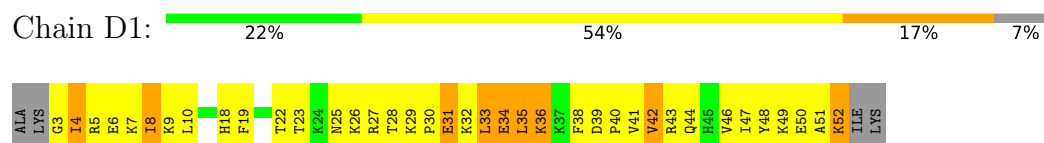
• Molecule 47: 50S ribosomal protein L32



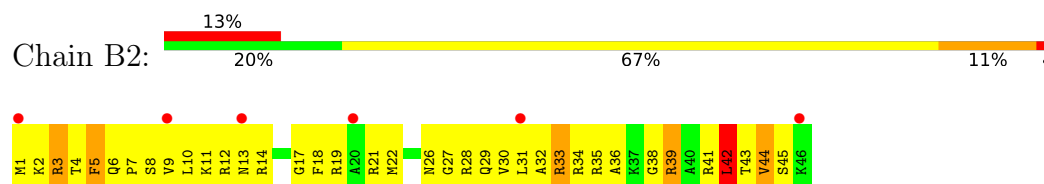
- Molecule 48: 50S ribosomal protein L33



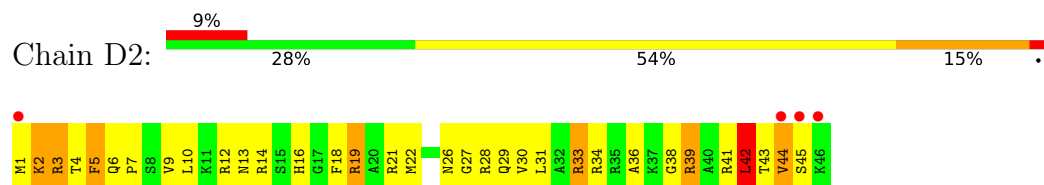
- Molecule 48: 50S ribosomal protein L33



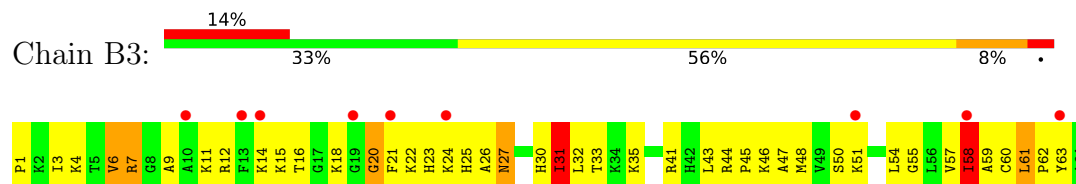
- Molecule 49: 50S ribosomal protein L34



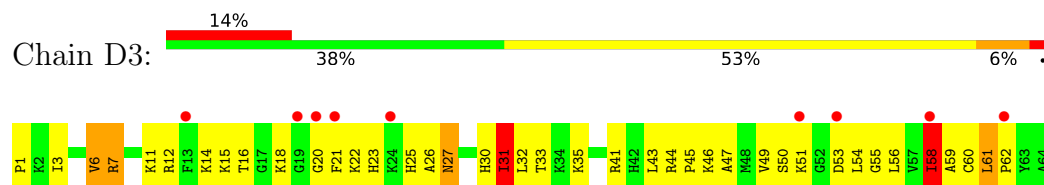
- Molecule 49: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L35



- Molecule 50: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L36

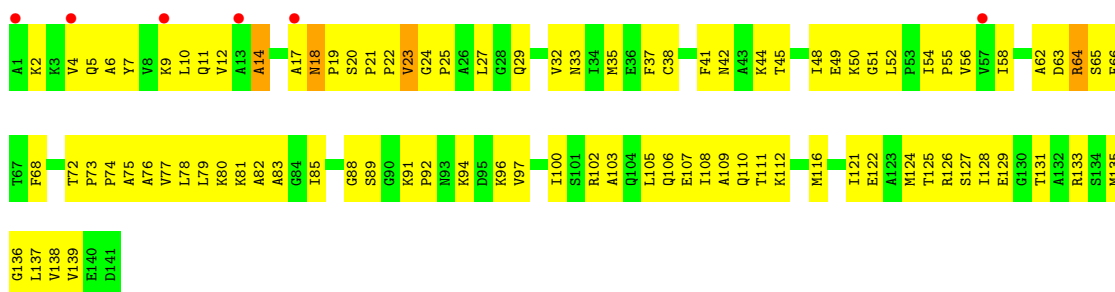




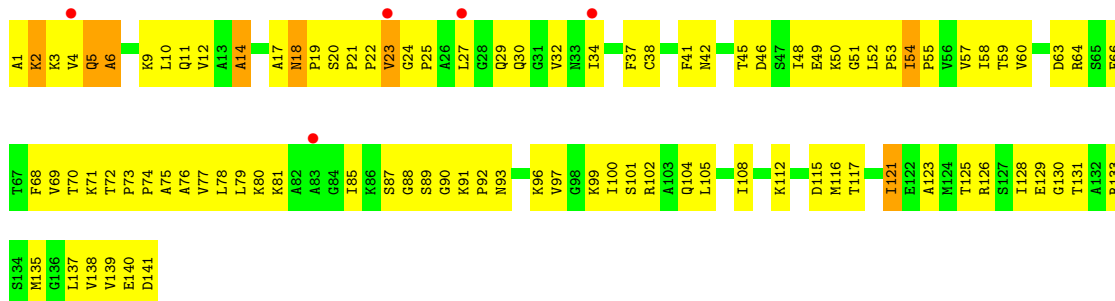
- Molecule 51: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L11



- Molecule 52: 50S ribosomal protein L11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.70Å 379.50Å 739.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.50 70.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	62.1 (70.00-3.50) 62.3 (70.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.269 , 0.318 0.234 , 0.278	Depositor DCC
R_{free} test set	22229 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	117.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	284077	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.27	0/36762	0.63	35/57350 (0.1%)
1	CA	0.27	0/36762	0.64	32/57350 (0.1%)
2	AC	0.27	0/1651	0.69	0/2225
2	CC	0.27	0/1651	0.69	0/2225
3	AD	0.26	0/1665	0.71	0/2227
3	CD	0.26	0/1665	0.71	0/2227
4	AE	0.27	0/1118	0.73	0/1504
4	CE	0.27	0/1118	0.72	0/1504
5	AF	0.28	0/835	0.69	0/1128
5	CF	0.28	0/835	0.69	0/1128
6	AG	0.27	0/1187	0.75	2/1591 (0.1%)
6	CG	0.27	0/1211	0.74	2/1624 (0.1%)
7	AH	0.26	0/989	0.71	0/1326
7	CH	0.27	0/989	0.71	0/1326
8	AI	0.27	0/1034	0.67	0/1375
8	CI	0.27	0/1034	0.67	0/1375
9	AJ	0.29	0/796	0.76	1/1077 (0.1%)
9	CJ	0.29	0/796	0.76	1/1077 (0.1%)
10	AK	0.30	0/893	0.74	0/1205
10	CK	0.30	0/893	0.74	0/1205
11	AL	0.28	0/969	0.75	0/1300
11	CL	0.28	0/969	0.75	0/1300
12	AM	0.26	0/892	0.68	0/1193
12	CM	0.26	0/884	0.68	0/1181
13	AN	0.27	0/785	0.72	0/1043
13	CN	0.27	0/785	0.72	0/1043
14	AO	0.26	0/723	0.69	0/966
14	CO	0.26	0/723	0.69	0/966
15	AP	0.29	0/659	0.73	0/884
15	CP	0.28	0/648	0.71	0/870
16	AQ	0.26	0/657	0.70	0/881
16	CQ	0.26	0/665	0.70	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	0.28	0/462	0.70	0/621
18	AS	0.28	0/652	0.72	0/877
18	CS	0.28	0/660	0.73	0/888
19	AT	0.27	0/671	0.69	0/888
19	CT	0.28	0/671	0.69	0/888
20	AB	0.29	0/1735	0.71	0/2338
20	CB	0.30	0/1735	0.71	0/2338
21	AU	0.29	0/430	0.81	1/570 (0.2%)
21	CU	0.28	0/430	0.80	1/570 (0.2%)
22	BA	0.28	0/2803	0.65	2/4371 (0.0%)
22	DA	0.28	0/2803	0.65	2/4371 (0.0%)
23	BB	0.27	1/68314 (0.0%)	0.64	75/106569 (0.1%)
23	DB	0.27	1/68314 (0.0%)	0.65	86/106569 (0.1%)
24	BV	0.26	0/766	0.68	0/1025
24	DV	0.26	0/766	0.68	0/1025
25	BC	0.28	0/2121	0.74	0/2852
25	DC	0.28	0/2121	0.73	0/2852
26	BD	0.28	0/1586	0.71	2/2134 (0.1%)
26	DD	0.28	0/1586	0.71	2/2134 (0.1%)
27	BE	0.26	0/1571	0.76	1/2113 (0.0%)
27	DE	0.26	0/1571	0.76	1/2113 (0.0%)
28	BF	0.28	0/1444	0.82	1/1937 (0.1%)
28	DF	0.28	0/1444	0.83	2/1937 (0.1%)
29	BG	0.27	0/1343	0.73	0/1816
29	DG	0.27	0/1343	0.72	0/1816
30	BH	0.29	0/1122	0.71	0/1515
30	DH	0.28	0/1122	0.71	1/1515 (0.1%)
31	BJ	0.28	0/1152	0.71	0/1551
31	DJ	0.28	0/1152	0.71	0/1551
32	BK	0.28	0/939	0.81	1/1258 (0.1%)
32	DK	0.28	0/939	0.81	1/1258 (0.1%)
33	BL	0.27	0/1054	0.76	0/1403
33	DL	0.27	0/1054	0.76	0/1403
34	BM	0.27	0/1093	0.73	0/1460
34	DM	0.27	0/1093	0.73	0/1460
35	BN	0.27	0/973	0.84	2/1301 (0.2%)
35	DN	0.27	0/973	0.84	2/1301 (0.2%)
36	BO	0.26	0/902	0.82	3/1209 (0.2%)
36	DO	0.26	0/902	0.82	3/1209 (0.2%)
37	BP	0.28	0/929	0.76	2/1242 (0.2%)
37	DP	0.28	0/929	0.76	2/1242 (0.2%)
38	BQ	0.27	0/960	0.81	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.27	0/960	0.80	0/1278
39	BR	0.25	0/829	0.65	0/1107
39	DR	0.25	0/829	0.65	0/1107
40	BS	0.28	0/864	0.83	1/1156 (0.1%)
40	DS	0.27	0/864	0.83	1/1156 (0.1%)
41	BT	0.26	0/744	0.82	3/994 (0.3%)
41	DT	0.27	0/744	0.83	3/994 (0.3%)
42	BU	0.28	0/787	0.68	0/1051
42	DU	0.28	0/787	0.69	1/1051 (0.1%)
43	BW	0.28	0/603	0.69	0/797
43	DW	0.28	0/603	0.69	0/797
44	BX	0.25	0/510	0.84	3/677 (0.4%)
44	DX	0.25	0/510	0.84	3/677 (0.4%)
45	BY	0.30	0/453	0.87	1/605 (0.2%)
45	DY	0.30	0/453	0.87	1/605 (0.2%)
46	BZ	0.26	0/635	0.83	2/848 (0.2%)
46	DZ	0.27	0/635	0.85	2/848 (0.2%)
47	B0	0.25	0/450	0.76	1/599 (0.2%)
47	D0	0.25	0/450	0.76	1/599 (0.2%)
48	B1	0.29	0/416	0.71	0/554
48	D1	0.28	0/416	0.71	0/554
49	B2	0.29	0/380	0.90	0/498
49	D2	0.29	0/380	0.90	0/498
50	B3	0.29	0/513	0.73	0/676
50	D3	0.30	0/513	0.73	0/676
51	B4	0.27	0/303	0.76	0/397
51	D4	0.27	0/303	0.76	0/397
52	BI	0.32	0/1046	0.80	0/1410
52	DI	0.34	0/1046	0.82	0/1410
All	All	0.27	2/306361 (0.0%)	0.67	289/457973 (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	13
23	BB	0	36
23	DB	0	38
All	All	0	100

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	1086	A	C5-C6	-7.26	1.26	1.41
23	BB	1086	A	C5-C6	-7.25	1.26	1.41

The worst 5 of 289 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	2791	G	O5'-P-OP1	-11.85	72.45	108.00
23	DB	2791	G	O5'-P-OP2	-11.66	73.01	108.00
23	DB	2204	G	O5'-P-OP1	-10.96	75.12	108.00
1	AA	1213	A	O5'-P-OP2	-10.93	75.21	108.00
23	BB	2204	G	O5'-P-OP2	-10.44	76.69	108.00

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	83	C	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1357	0
1	CA	32831	0	16521	1382	0
2	AC	1624	0	1699	143	0
2	CC	1624	0	1699	152	0
3	AD	1643	0	1710	177	0
3	CD	1643	0	1710	171	0
4	AE	1105	0	1148	109	0
4	CE	1105	0	1148	120	0
5	AF	817	0	808	103	0
5	CF	817	0	808	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AG	1174	0	1230	121	0
6	CG	1196	0	1246	112	0
7	AH	979	0	1034	102	0
7	CH	979	0	1034	103	0
8	AI	1022	0	1070	157	0
8	CI	1022	0	1070	154	0
9	AJ	786	0	828	79	0
9	CJ	786	0	828	84	0
10	AK	877	0	887	101	0
10	CK	877	0	887	103	0
11	AL	955	0	1019	93	0
11	CL	955	0	1019	96	0
12	AM	883	0	944	113	0
12	CM	876	0	937	113	0
13	AN	774	0	827	102	0
13	CN	774	0	827	94	0
14	AO	715	0	742	54	0
14	CO	715	0	742	49	0
15	AP	649	0	666	61	0
15	CP	638	0	656	62	0
16	AQ	648	0	691	80	0
16	CQ	656	0	702	79	0
17	AR	455	0	478	37	0
17	CR	455	0	478	38	0
18	AS	637	0	665	103	0
18	CS	644	0	675	100	0
19	AT	665	0	714	54	0
19	CT	665	0	714	54	0
20	AB	1704	0	1732	220	0
20	CB	1704	0	1732	220	0
21	AU	425	0	449	79	0
21	CU	425	0	449	70	0
22	BA	2507	0	1270	110	0
22	DA	2507	0	1270	111	0
23	BB	60995	0	30678	2410	0
23	DB	60995	0	30677	2500	0
24	BV	753	0	780	93	0
24	DV	753	0	780	93	0
25	BC	2082	0	2157	270	0
25	DC	2082	0	2157	283	0
26	BD	1565	0	1616	224	0
26	DD	1565	0	1616	233	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	BE	1552	0	1619	191	0
27	DE	1552	0	1619	180	0
28	BF	1420	0	1460	249	0
28	DF	1420	0	1460	250	0
29	BG	1323	0	1374	172	0
29	DG	1323	0	1374	170	0
30	BH	1111	0	1148	184	0
30	DH	1111	0	1148	156	0
31	BJ	1129	0	1162	158	0
31	DJ	1129	0	1162	160	0
32	BK	930	0	1000	131	0
32	DK	930	0	1000	142	0
33	BL	1045	0	1117	161	0
33	DL	1045	0	1117	163	0
34	BM	1074	0	1157	123	0
34	DM	1074	0	1157	121	0
35	BN	960	0	1000	146	0
35	DN	960	0	1000	138	0
36	BO	892	0	923	102	0
36	DO	892	0	923	108	0
37	BP	917	0	965	116	0
37	DP	917	0	965	118	0
38	BQ	947	0	1022	166	0
38	DQ	947	0	1022	176	0
39	BR	816	0	839	130	0
39	DR	816	0	839	144	0
40	BS	857	0	922	95	0
40	DS	857	0	922	98	0
41	BT	738	0	807	135	0
41	DT	738	0	807	129	0
42	BU	779	0	834	135	0
42	DU	779	0	834	123	0
43	BW	596	0	610	134	0
43	DW	596	0	610	141	0
44	BX	509	0	543	59	0
44	DX	509	0	543	56	0
45	BY	449	0	491	50	0
45	DY	449	0	491	52	0
46	BZ	625	0	652	95	0
46	DZ	625	0	652	97	0
47	B0	444	0	461	43	0
47	D0	444	0	461	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	B1	409	0	440	58	0
48	D1	409	0	440	44	0
49	B2	377	0	418	48	0
49	D2	377	0	418	47	0
50	B3	504	0	574	45	0
50	D3	504	0	574	44	0
51	B4	302	0	340	41	0
51	D4	302	0	340	37	0
52	BI	1032	0	1088	121	0
52	DI	1032	0	1088	189	0
53	AA	58	0	0	0	0
53	AE	1	0	0	0	0
53	AN	1	0	0	0	0
53	BB	110	0	0	0	0
53	CA	61	0	0	0	0
53	CE	1	0	0	0	0
53	DB	111	0	0	0	0
54	AA	36	0	37	2	0
54	CA	36	0	37	1	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	282	0	0	4	0
56	AE	4	0	0	0	0
56	AK	2	0	0	0	0
56	AL	5	0	0	0	0
56	AN	4	0	0	0	0
56	AT	3	0	0	0	0
56	B2	1	0	0	0	0
56	BB	492	0	0	5	0
56	BC	8	0	0	0	0
56	BD	1	0	0	0	0
56	BE	2	0	0	0	0
56	BH	1	0	0	0	0
56	BL	2	0	0	0	0
56	CA	294	0	0	0	0
56	CE	4	0	0	0	0
56	CI	1	0	0	0	0
56	CK	1	0	0	0	0
56	CL	3	0	0	0	0
56	CN	3	0	0	0	0
56	CT	1	0	0	0	0
56	D2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DB	499	0	0	8	0
56	DC	5	0	0	0	0
56	DD	1	0	0	0	0
56	DE	1	0	0	0	0
56	DL	5	0	0	1	0
56	DP	1	0	0	0	0
All	All	284077	0	190751	17785	0

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

The worst 5 of 17785 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:DB:1099:G:H8	52:DI:3:LYS:N	1.38	1.20
23:BB:855:G:H21	43:BW:23:LYS:HG2	1.08	1.15
42:DU:85:ARG:HD3	42:DU:86:PHE:H	1.13	1.14
41:DT:5:GLU:HA	41:DT:8:LEU:HB2	1.25	1.13
42:BU:85:ARG:HD3	42:BU:86:PHE:H	1.11	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	204/232 (88%)	147 (72%)	40 (20%)	17 (8%)	0	7
2	CC	204/232 (88%)	148 (72%)	40 (20%)	16 (8%)	1	8
3	AD	203/205 (99%)	136 (67%)	52 (26%)	15 (7%)	1	9
3	CD	203/205 (99%)	134 (66%)	54 (27%)	15 (7%)	1	9
4	AE	148/166 (89%)	117 (79%)	27 (18%)	4 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CE	148/166 (89%)	117 (79%)	25 (17%)	6 (4%)	2	19
5	AF	98/135 (73%)	66 (67%)	21 (21%)	11 (11%)	0	5
5	CF	98/135 (73%)	67 (68%)	21 (21%)	10 (10%)	0	6
6	AG	148/178 (83%)	122 (82%)	18 (12%)	8 (5%)	1	14
6	CG	150/178 (84%)	124 (83%)	20 (13%)	6 (4%)	2	19
7	AH	127/129 (98%)	92 (72%)	26 (20%)	9 (7%)	1	10
7	CH	127/129 (98%)	90 (71%)	28 (22%)	9 (7%)	1	10
8	AI	125/129 (97%)	88 (70%)	29 (23%)	8 (6%)	1	11
8	CI	125/129 (97%)	88 (70%)	29 (23%)	8 (6%)	1	11
9	AJ	96/103 (93%)	69 (72%)	17 (18%)	10 (10%)	0	5
9	CJ	96/103 (93%)	68 (71%)	18 (19%)	10 (10%)	0	5
10	AK	115/128 (90%)	81 (70%)	26 (23%)	8 (7%)	1	10
10	CK	115/128 (90%)	80 (70%)	27 (24%)	8 (7%)	1	10
11	AL	121/123 (98%)	78 (64%)	29 (24%)	14 (12%)	0	4
11	CL	121/123 (98%)	79 (65%)	28 (23%)	14 (12%)	0	4
12	AM	112/117 (96%)	72 (64%)	36 (32%)	4 (4%)	2	22
12	CM	111/117 (95%)	69 (62%)	38 (34%)	4 (4%)	2	22
13	AN	92/100 (92%)	57 (62%)	25 (27%)	10 (11%)	0	5
13	CN	92/100 (92%)	56 (61%)	26 (28%)	10 (11%)	0	5
14	AO	86/89 (97%)	65 (76%)	16 (19%)	5 (6%)	1	13
14	CO	86/89 (97%)	65 (76%)	16 (19%)	5 (6%)	1	13
15	AP	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	0	5
15	CP	78/82 (95%)	53 (68%)	15 (19%)	10 (13%)	0	3
16	AQ	78/83 (94%)	56 (72%)	17 (22%)	5 (6%)	1	11
16	CQ	79/83 (95%)	56 (71%)	17 (22%)	6 (8%)	1	8
17	AR	53/74 (72%)	41 (77%)	10 (19%)	2 (4%)	2	20
17	CR	53/74 (72%)	41 (77%)	10 (19%)	2 (4%)	2	20
18	AS	77/91 (85%)	58 (75%)	17 (22%)	2 (3%)	4	27
18	CS	78/91 (86%)	58 (74%)	18 (23%)	2 (3%)	4	27
19	AT	83/86 (96%)	59 (71%)	19 (23%)	5 (6%)	1	12
19	CT	83/86 (96%)	59 (71%)	19 (23%)	5 (6%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AB	216/240 (90%)	143 (66%)	53 (24%)	20 (9%)	0	6
20	CB	216/240 (90%)	148 (68%)	46 (21%)	22 (10%)	0	6
21	AU	49/71 (69%)	28 (57%)	14 (29%)	7 (14%)	0	3
21	CU	49/71 (69%)	28 (57%)	14 (29%)	7 (14%)	0	3
24	BV	92/94 (98%)	63 (68%)	23 (25%)	6 (6%)	1	11
24	DV	92/94 (98%)	62 (67%)	24 (26%)	6 (6%)	1	11
25	BC	269/273 (98%)	158 (59%)	65 (24%)	46 (17%)	0	2
25	DC	269/273 (98%)	158 (59%)	65 (24%)	46 (17%)	0	2
26	BD	207/209 (99%)	121 (58%)	56 (27%)	30 (14%)	0	3
26	DD	207/209 (99%)	123 (59%)	52 (25%)	32 (16%)	0	2
27	BE	199/201 (99%)	120 (60%)	56 (28%)	23 (12%)	0	4
27	DE	199/201 (99%)	120 (60%)	56 (28%)	23 (12%)	0	4
28	BF	176/178 (99%)	103 (58%)	39 (22%)	34 (19%)	0	1
28	DF	176/178 (99%)	101 (57%)	41 (23%)	34 (19%)	0	1
29	BG	174/176 (99%)	105 (60%)	37 (21%)	32 (18%)	0	1
29	DG	174/176 (99%)	105 (60%)	36 (21%)	33 (19%)	0	1
30	BH	147/149 (99%)	68 (46%)	43 (29%)	36 (24%)	0	0
30	DH	147/149 (99%)	88 (60%)	32 (22%)	27 (18%)	0	1
31	BJ	140/142 (99%)	85 (61%)	39 (28%)	16 (11%)	0	5
31	DJ	140/142 (99%)	83 (59%)	40 (29%)	17 (12%)	0	4
32	BK	119/123 (97%)	70 (59%)	28 (24%)	21 (18%)	0	1
32	DK	119/123 (97%)	69 (58%)	27 (23%)	23 (19%)	0	1
33	BL	141/144 (98%)	75 (53%)	40 (28%)	26 (18%)	0	1
33	DL	141/144 (98%)	75 (53%)	40 (28%)	26 (18%)	0	1
34	BM	134/136 (98%)	77 (58%)	38 (28%)	19 (14%)	0	3
34	DM	134/136 (98%)	78 (58%)	35 (26%)	21 (16%)	0	2
35	BN	118/127 (93%)	73 (62%)	33 (28%)	12 (10%)	0	6
35	DN	118/127 (93%)	73 (62%)	32 (27%)	13 (11%)	0	5
36	BO	114/117 (97%)	83 (73%)	21 (18%)	10 (9%)	0	7
36	DO	114/117 (97%)	83 (73%)	20 (18%)	11 (10%)	0	6
37	BP	112/114 (98%)	59 (53%)	35 (31%)	18 (16%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	DP	112/114 (98%)	58 (52%)	36 (32%)	18 (16%)	0	2
38	BQ	115/117 (98%)	79 (69%)	27 (24%)	9 (8%)	1	8
38	DQ	115/117 (98%)	75 (65%)	32 (28%)	8 (7%)	1	10
39	BR	101/103 (98%)	60 (59%)	31 (31%)	10 (10%)	0	6
39	DR	101/103 (98%)	61 (60%)	29 (29%)	11 (11%)	0	5
40	BS	108/110 (98%)	75 (69%)	21 (19%)	12 (11%)	0	5
40	DS	108/110 (98%)	75 (69%)	20 (18%)	13 (12%)	0	4
41	BT	91/100 (91%)	47 (52%)	25 (28%)	19 (21%)	0	1
41	DT	91/100 (91%)	47 (52%)	23 (25%)	21 (23%)	0	0
42	BU	100/103 (97%)	53 (53%)	35 (35%)	12 (12%)	0	4
42	DU	100/103 (97%)	51 (51%)	35 (35%)	14 (14%)	0	3
43	BW	77/84 (92%)	29 (38%)	23 (30%)	25 (32%)	0	0
43	DW	77/84 (92%)	29 (38%)	22 (29%)	26 (34%)	0	0
44	BX	61/63 (97%)	37 (61%)	14 (23%)	10 (16%)	0	2
44	DX	61/63 (97%)	37 (61%)	14 (23%)	10 (16%)	0	2
45	BY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	0	7
45	DY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	0	7
46	BZ	75/78 (96%)	47 (63%)	20 (27%)	8 (11%)	0	5
46	DZ	75/78 (96%)	48 (64%)	19 (25%)	8 (11%)	0	5
47	B0	54/56 (96%)	33 (61%)	16 (30%)	5 (9%)	0	6
47	D0	54/56 (96%)	33 (61%)	16 (30%)	5 (9%)	0	6
48	B1	48/54 (89%)	34 (71%)	12 (25%)	2 (4%)	2	19
48	D1	48/54 (89%)	34 (71%)	12 (25%)	2 (4%)	2	19
49	B2	44/46 (96%)	31 (70%)	9 (20%)	4 (9%)	0	7
49	D2	44/46 (96%)	30 (68%)	8 (18%)	6 (14%)	0	3
50	B3	62/64 (97%)	41 (66%)	15 (24%)	6 (10%)	0	6
50	D3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	0	6
51	B4	36/38 (95%)	21 (58%)	10 (28%)	5 (14%)	0	3
51	D4	36/38 (95%)	21 (58%)	9 (25%)	6 (17%)	0	2
52	BI	139/141 (99%)	119 (86%)	16 (12%)	4 (3%)	3	26
52	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11241/11918 (94%)	7279 (65%)	2673 (24%)	1289 (12%)	0 5

5 of 1289 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	112	ALA
2	AC	180	ASP
2	AC	205	GLU
4	AE	20	VAL
5	AF	98	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AC	170/189 (90%)	141 (83%)	29 (17%)	2 12
2	CC	170/189 (90%)	142 (84%)	28 (16%)	2 13
3	AD	172/172 (100%)	146 (85%)	26 (15%)	3 16
3	CD	172/172 (100%)	146 (85%)	26 (15%)	3 16
4	AE	113/125 (90%)	100 (88%)	13 (12%)	5 24
4	CE	113/125 (90%)	99 (88%)	14 (12%)	4 22
5	AF	87/116 (75%)	73 (84%)	14 (16%)	2 14
5	CF	87/116 (75%)	73 (84%)	14 (16%)	2 14
6	AG	123/146 (84%)	109 (89%)	14 (11%)	5 24
6	CG	125/146 (86%)	109 (87%)	16 (13%)	4 21
7	AH	104/104 (100%)	96 (92%)	8 (8%)	12 37
7	CH	104/104 (100%)	96 (92%)	8 (8%)	12 37
8	AI	105/106 (99%)	96 (91%)	9 (9%)	10 33
8	CI	105/106 (99%)	96 (91%)	9 (9%)	10 33
9	AJ	86/90 (96%)	80 (93%)	6 (7%)	14 39
9	CJ	86/90 (96%)	80 (93%)	6 (7%)	14 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AK	90/98 (92%)	78 (87%)	12 (13%)	4	20
10	CK	90/98 (92%)	78 (87%)	12 (13%)	4	20
11	AL	103/103 (100%)	83 (81%)	20 (19%)	1	8
11	CL	103/103 (100%)	84 (82%)	19 (18%)	1	9
12	AM	92/95 (97%)	81 (88%)	11 (12%)	5	23
12	CM	91/95 (96%)	81 (89%)	10 (11%)	6	26
13	AN	79/83 (95%)	69 (87%)	10 (13%)	4	21
13	CN	79/83 (95%)	69 (87%)	10 (13%)	4	21
14	AO	76/77 (99%)	70 (92%)	6 (8%)	11	36
14	CO	76/77 (99%)	70 (92%)	6 (8%)	11	36
15	AP	65/65 (100%)	57 (88%)	8 (12%)	4	22
15	CP	65/65 (100%)	58 (89%)	7 (11%)	6	26
16	AQ	74/77 (96%)	65 (88%)	9 (12%)	5	22
16	CQ	75/77 (97%)	64 (85%)	11 (15%)	3	17
17	AR	48/64 (75%)	45 (94%)	3 (6%)	16	42
17	CR	48/64 (75%)	45 (94%)	3 (6%)	16	42
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%)	53 (82%)	12 (18%)	1	9
19	CT	65/65 (100%)	53 (82%)	12 (18%)	1	9
20	AB	180/198 (91%)	148 (82%)	32 (18%)	2	10
20	CB	180/198 (91%)	146 (81%)	34 (19%)	1	9
21	AU	44/61 (72%)	33 (75%)	11 (25%)	0	4
21	CU	44/61 (72%)	33 (75%)	11 (25%)	0	4
24	BV	78/78 (100%)	64 (82%)	14 (18%)	2	10
24	DV	78/78 (100%)	64 (82%)	14 (18%)	2	10
25	BC	216/218 (99%)	181 (84%)	35 (16%)	2	14
25	DC	216/218 (99%)	179 (83%)	37 (17%)	2	12
26	BD	164/164 (100%)	131 (80%)	33 (20%)	1	7
26	DD	164/164 (100%)	133 (81%)	31 (19%)	1	9
27	BE	165/165 (100%)	146 (88%)	19 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	DE	165/165 (100%)	145 (88%)	20 (12%)	5	22
28	BF	149/149 (100%)	119 (80%)	30 (20%)	1	7
28	DF	149/149 (100%)	119 (80%)	30 (20%)	1	7
29	BG	137/137 (100%)	118 (86%)	19 (14%)	3	19
29	DG	137/137 (100%)	118 (86%)	19 (14%)	3	19
30	BH	114/114 (100%)	79 (69%)	35 (31%)	0	2
30	DH	114/114 (100%)	93 (82%)	21 (18%)	1	9
31	BJ	116/116 (100%)	103 (89%)	13 (11%)	6	25
31	DJ	116/116 (100%)	102 (88%)	14 (12%)	5	22
32	BK	102/104 (98%)	78 (76%)	24 (24%)	1	4
32	DK	102/104 (98%)	79 (78%)	23 (22%)	1	5
33	BL	102/103 (99%)	89 (87%)	13 (13%)	4	21
33	DL	102/103 (99%)	88 (86%)	14 (14%)	3	19
34	BM	109/109 (100%)	85 (78%)	24 (22%)	1	5
34	DM	109/109 (100%)	85 (78%)	24 (22%)	1	5
35	BN	100/103 (97%)	80 (80%)	20 (20%)	1	7
35	DN	100/103 (97%)	80 (80%)	20 (20%)	1	7
36	BO	86/87 (99%)	69 (80%)	17 (20%)	1	7
36	DO	86/87 (99%)	68 (79%)	18 (21%)	1	6
37	BP	99/99 (100%)	81 (82%)	18 (18%)	2	10
37	DP	99/99 (100%)	82 (83%)	17 (17%)	2	12
38	BQ	89/89 (100%)	77 (86%)	12 (14%)	4	20
38	DQ	89/89 (100%)	78 (88%)	11 (12%)	4	22
39	BR	84/84 (100%)	68 (81%)	16 (19%)	1	8
39	DR	84/84 (100%)	69 (82%)	15 (18%)	2	10
40	BS	93/93 (100%)	78 (84%)	15 (16%)	2	14
40	DS	93/93 (100%)	78 (84%)	15 (16%)	2	14
41	BT	80/84 (95%)	61 (76%)	19 (24%)	1	4
41	DT	80/84 (95%)	61 (76%)	19 (24%)	1	4
42	BU	83/84 (99%)	65 (78%)	18 (22%)	1	6
42	DU	83/84 (99%)	65 (78%)	18 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BW	59/62 (95%)	44 (75%)	15 (25%)	0	3
43	DW	59/62 (95%)	44 (75%)	15 (25%)	0	3
44	BX	55/55 (100%)	43 (78%)	12 (22%)	1	6
44	DX	55/55 (100%)	43 (78%)	12 (22%)	1	6
45	BY	48/48 (100%)	43 (90%)	5 (10%)	7	27
45	DY	48/48 (100%)	43 (90%)	5 (10%)	7	27
46	BZ	67/68 (98%)	54 (81%)	13 (19%)	1	8
46	DZ	67/68 (98%)	54 (81%)	13 (19%)	1	8
47	B0	47/47 (100%)	39 (83%)	8 (17%)	2	12
47	D0	47/47 (100%)	39 (83%)	8 (17%)	2	12
48	B1	45/48 (94%)	37 (82%)	8 (18%)	2	10
48	D1	45/48 (94%)	37 (82%)	8 (18%)	2	10
49	B2	38/38 (100%)	33 (87%)	5 (13%)	4	20
49	D2	38/38 (100%)	33 (87%)	5 (13%)	4	20
50	B3	51/51 (100%)	43 (84%)	8 (16%)	2	15
50	D3	51/51 (100%)	45 (88%)	6 (12%)	5	23
51	B4	34/34 (100%)	31 (91%)	3 (9%)	9	32
51	D4	34/34 (100%)	31 (91%)	3 (9%)	9	32
52	BI	109/109 (100%)	109 (100%)	0	100	100
52	DI	109/109 (100%)	106 (97%)	3 (3%)	38	61
All	All	9333/9704 (96%)	7864 (84%)	1469 (16%)	2	15

5 of 1469 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	CQ	7	LEU
29	DG	26	LYS
18	CS	77	ARG
16	CQ	4	ILE
25	DC	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 388 such sidechains are listed below:

Mol	Chain	Res	Type
9	CJ	70	HIS
26	DD	126	ASN
11	CL	45	ASN
19	CT	74	HIS
28	DF	126	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	257 (16%)	27 (1%)
1	CA	1529/1542 (99%)	240 (15%)	27 (1%)
22	BA	116/120 (96%)	22 (18%)	0
22	DA	116/120 (96%)	22 (18%)	0
23	BB	2837/2904 (97%)	461 (16%)	17 (0%)
23	DB	2837/2904 (97%)	462 (16%)	21 (0%)
All	All	8964/9132 (98%)	1464 (16%)	92 (1%)

5 of 1464 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	975	A
23	DB	63	A
1	CA	1049	U
1	CA	1285	A
23	DB	544	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 347 ligands modelled in this entry, 345 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	HYG	AA	2059	-	36,39,39	1.36	6 (16%)	44,60,60	1.48	6 (13%)
54	HYG	CA	2062	-	36,39,39	1.38	6 (16%)	44,60,60	1.48	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	HYG	AA	2059	-	-	9/12/87/87	0/4/4/4
54	HYG	CA	2062	-	-	10/12/87/87	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CA	2062	HYG	O28-C23	2.99	1.44	1.40
54	AA	2059	HYG	O28-C23	2.97	1.44	1.40
54	AA	2059	HYG	C27-C33	2.77	1.56	1.52
54	CA	2062	HYG	C27-C33	2.76	1.56	1.52
54	CA	2062	HYG	O22-C17	-2.43	1.38	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	2062	HYG	O22-C17-C16	4.61	122.21	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AA	2059	HYG	O22-C17-C16	4.55	122.08	111.22
54	CA	2062	HYG	O8-C1-C2	-4.34	101.78	109.90
54	AA	2059	HYG	O8-C1-C2	-4.32	101.81	109.90
54	CA	2062	HYG	O35-C34-C33	-3.51	103.94	111.55

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	AA	2059	HYG	C5-C4-N9-C10
54	AA	2059	HYG	N36-C33-C34-O35
54	CA	2062	HYG	C3-C4-N9-C10
54	CA	2062	HYG	N36-C33-C34-O35
54	CA	2062	HYG	O14-C15-C19-O20

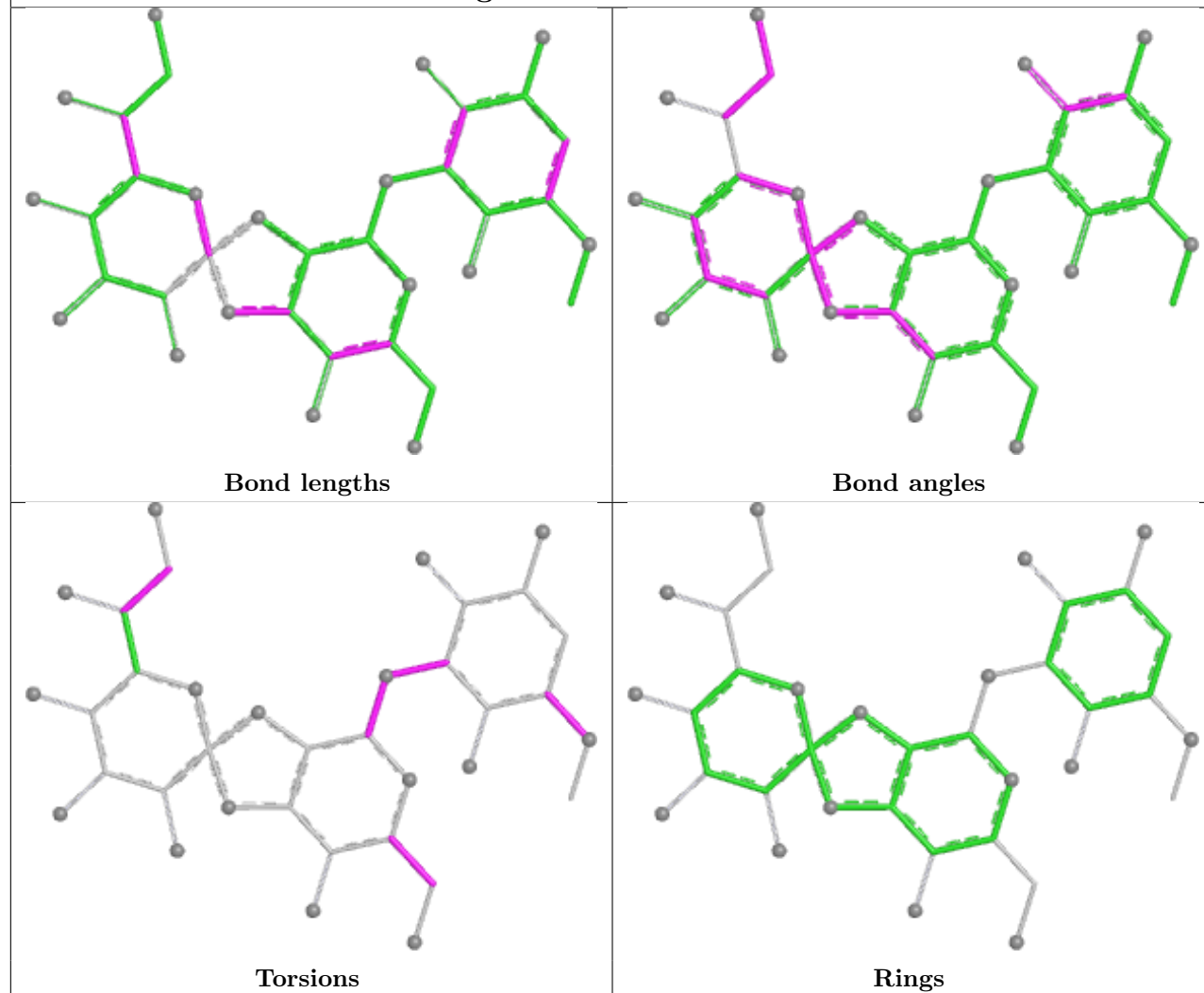
There are no ring outliers.

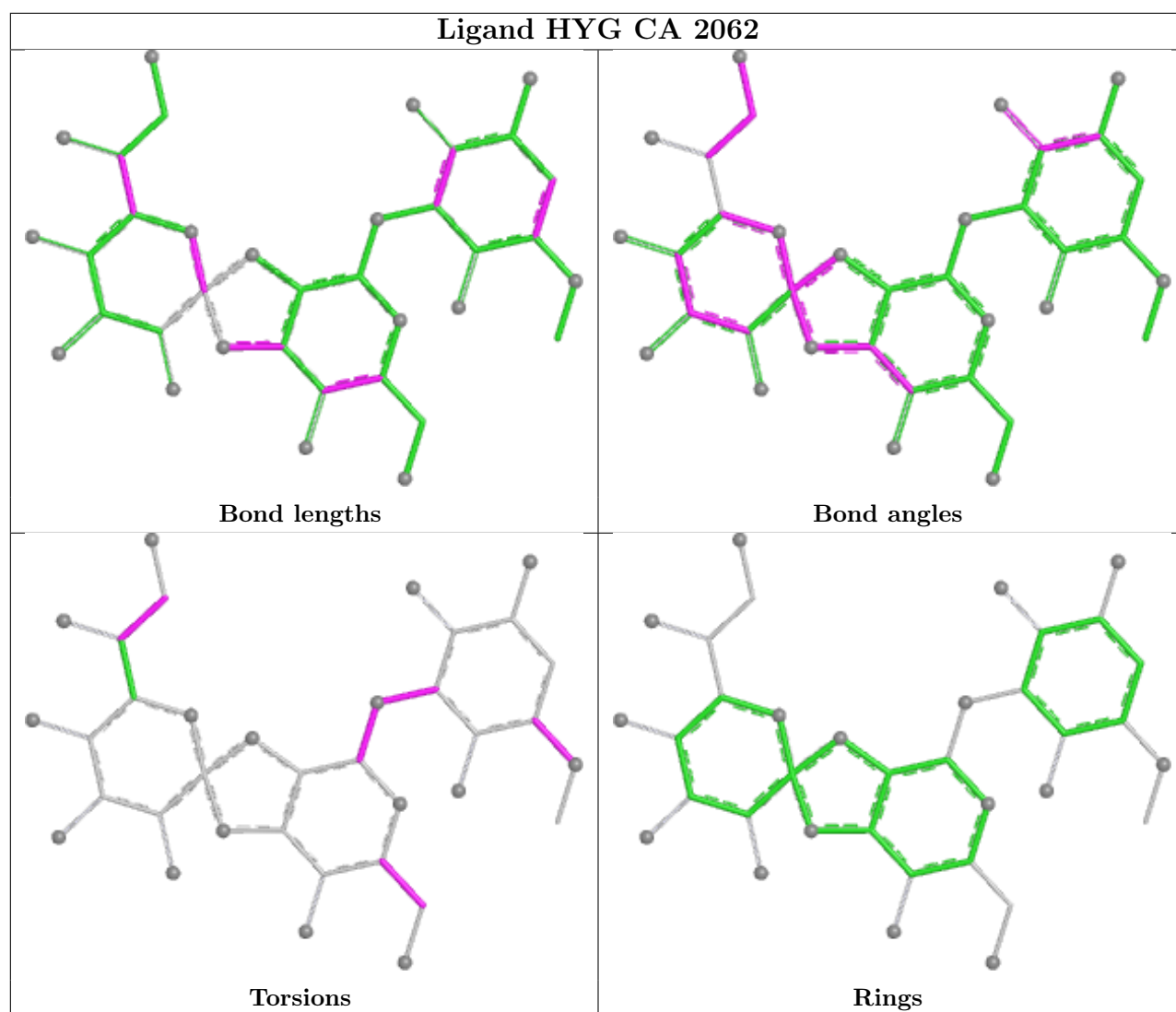
2 monomers are involved in 3 short contacts:

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

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

Ligand HYG AA 2059





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%)	-0.19	26 (1%) 69 43	16, 85, 158, 180	0
1	CA	1530/1542 (99%)	-0.27	34 (2%) 62 37	8, 57, 142, 180	0
2	AC	206/232 (88%)	0.02	9 (4%) 39 21	8, 89, 145, 180	0
2	CC	206/232 (88%)	-0.26	1 (0%) 87 68	15, 81, 138, 180	0
3	AD	205/205 (100%)	0.47	15 (7%) 21 13	19, 97, 160, 180	0
3	CD	205/205 (100%)	0.28	11 (5%) 31 18	5, 63, 135, 180	0
4	AE	150/166 (90%)	0.26	8 (5%) 32 18	5, 76, 136, 167	0
4	CE	150/166 (90%)	0.12	5 (3%) 49 28	5, 62, 135, 175	0
5	AF	100/135 (74%)	-0.15	0 100 100	13, 81, 137, 180	0
5	CF	100/135 (74%)	-0.30	0 100 100	14, 78, 126, 166	0
6	AG	150/178 (84%)	0.10	6 (4%) 42 23	41, 110, 166, 180	0
6	CG	152/178 (85%)	0.03	8 (5%) 32 18	27, 98, 156, 177	0
7	AH	129/129 (100%)	0.38	10 (7%) 19 12	26, 91, 148, 180	0
7	CH	129/129 (100%)	0.08	5 (3%) 43 23	5, 53, 117, 153	0
8	AI	127/129 (98%)	0.29	10 (7%) 18 12	32, 103, 160, 180	0
8	CI	127/129 (98%)	0.60	19 (14%) 5 5	32, 103, 162, 180	0
9	AJ	98/103 (95%)	0.53	9 (9%) 14 9	34, 106, 162, 180	0
9	CJ	98/103 (95%)	0.68	11 (11%) 10 7	42, 107, 156, 180	0
10	AK	117/128 (91%)	-0.17	1 (0%) 81 58	5, 71, 122, 174	0
10	CK	117/128 (91%)	-0.08	1 (0%) 81 58	5, 57, 112, 179	0
11	AL	123/123 (100%)	0.71	16 (13%) 7 6	15, 82, 132, 153	0
11	CL	123/123 (100%)	0.26	10 (8%) 18 12	5, 44, 109, 165	0
12	AM	114/117 (97%)	0.17	2 (1%) 67 42	68, 130, 178, 180	0
12	CM	113/117 (96%)	-0.02	2 (1%) 67 42	32, 108, 156, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.46	11 (11%) 9 6	32, 103, 161, 180	0
13	CN	96/100 (96%)	0.60	6 (6%) 26 15	38, 99, 137, 171	0
14	AO	88/89 (98%)	-0.07	2 (2%) 61 37	35, 83, 132, 180	0
14	CO	88/89 (98%)	0.09	7 (7%) 18 12	8, 54, 111, 165	0
15	AP	82/82 (100%)	0.75	8 (9%) 13 9	43, 99, 163, 180	0
15	CP	80/82 (97%)	0.64	6 (7%) 20 13	5, 51, 143, 164	0
16	AQ	80/83 (96%)	0.30	8 (10%) 12 8	49, 106, 156, 177	0
16	CQ	81/83 (97%)	-0.06	4 (4%) 35 19	5, 51, 121, 157	0
17	AR	55/74 (74%)	-0.08	1 (1%) 67 42	16, 78, 142, 152	0
17	CR	55/74 (74%)	-0.17	0 100 100	13, 69, 132, 149	0
18	AS	79/91 (86%)	0.41	5 (6%) 26 15	67, 128, 175, 180	0
18	CS	80/91 (87%)	0.37	4 (5%) 34 19	49, 113, 171, 180	0
19	AT	85/86 (98%)	0.69	15 (17%) 4 4	43, 100, 153, 175	0
19	CT	85/86 (98%)	0.41	8 (9%) 14 9	14, 58, 121, 177	0
20	AB	218/240 (90%)	-0.06	5 (2%) 61 37	30, 102, 152, 180	0
20	CB	218/240 (90%)	0.01	8 (3%) 45 25	26, 106, 160, 180	0
21	AU	51/71 (71%)	0.62	6 (11%) 9 6	26, 102, 172, 180	0
21	CU	51/71 (71%)	1.17	12 (23%) 2 2	19, 85, 151, 180	0
22	BA	117/120 (97%)	-0.13	4 (3%) 48 27	43, 83, 131, 172	0
22	DA	117/120 (97%)	0.05	5 (4%) 40 21	32, 75, 118, 180	0
23	BB	2841/2904 (97%)	-0.28	36 (1%) 75 50	6, 56, 146, 180	0
23	DB	2841/2904 (97%)	-0.37	30 (1%) 78 54	5, 40, 139, 180	0
24	BV	94/94 (100%)	-0.07	2 (2%) 63 38	11, 96, 146, 176	0
24	DV	94/94 (100%)	-0.12	3 (3%) 50 29	14, 86, 143, 180	0
25	BC	271/273 (99%)	0.46	30 (11%) 10 7	7, 48, 104, 170	0
25	DC	271/273 (99%)	0.22	12 (4%) 39 21	5, 28, 81, 120	0
26	BD	209/209 (100%)	0.57	20 (9%) 13 9	5, 73, 138, 180	0
26	DD	209/209 (100%)	0.38	19 (9%) 15 10	5, 42, 118, 180	0
27	BE	201/201 (100%)	0.12	9 (4%) 38 20	5, 65, 142, 180	0
27	DE	201/201 (100%)	0.15	9 (4%) 38 20	5, 67, 135, 180	0
28	BF	178/178 (100%)	-0.02	3 (1%) 69 43	50, 116, 175, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	178/178 (100%)	0.23	10 (5%) 30 17	7, 101, 172, 180	0
29	BG	176/176 (100%)	0.12	7 (3%) 42 23	23, 102, 155, 180	0
29	DG	176/176 (100%)	0.11	12 (6%) 23 14	24, 90, 161, 180	0
30	BH	149/149 (100%)	0.17	3 (2%) 65 39	14, 117, 177, 180	0
30	DH	149/149 (100%)	-0.01	4 (2%) 56 33	11, 100, 156, 180	0
31	BJ	142/142 (100%)	0.59	16 (11%) 10 7	6, 80, 141, 171	0
31	DJ	142/142 (100%)	0.41	9 (6%) 26 15	5, 60, 119, 164	0
32	BK	121/123 (98%)	0.46	7 (5%) 29 17	5, 73, 135, 180	0
32	DK	121/123 (98%)	0.18	3 (2%) 58 35	5, 35, 102, 145	0
33	BL	143/144 (99%)	0.22	3 (2%) 63 38	10, 64, 128, 180	0
33	DL	143/144 (99%)	0.22	6 (4%) 40 22	5, 54, 118, 162	0
34	BM	136/136 (100%)	0.02	2 (1%) 72 47	8, 70, 129, 172	0
34	DM	136/136 (100%)	0.44	6 (4%) 39 21	5, 51, 114, 168	0
35	BN	120/127 (94%)	0.36	10 (8%) 17 11	7, 66, 132, 163	0
35	DN	120/127 (94%)	0.27	6 (5%) 34 19	5, 42, 86, 145	0
36	BO	116/117 (99%)	0.33	7 (6%) 27 16	27, 87, 135, 156	0
36	DO	116/117 (99%)	0.32	7 (6%) 27 16	17, 78, 142, 180	0
37	BP	114/114 (100%)	0.54	8 (7%) 22 14	20, 85, 149, 178	0
37	DP	114/114 (100%)	0.20	7 (6%) 27 16	5, 48, 107, 159	0
38	BQ	117/117 (100%)	0.34	9 (7%) 19 13	5, 63, 127, 180	0
38	DQ	117/117 (100%)	0.63	11 (9%) 14 9	5, 48, 116, 150	0
39	BR	103/103 (100%)	0.23	9 (8%) 16 10	16, 82, 145, 158	0
39	DR	103/103 (100%)	0.42	9 (8%) 16 10	5, 73, 136, 180	0
40	BS	110/110 (100%)	0.01	4 (3%) 46 25	5, 53, 116, 142	0
40	DS	110/110 (100%)	0.17	3 (2%) 56 33	5, 42, 116, 146	0
41	BT	93/100 (93%)	0.24	6 (6%) 25 15	6, 72, 139, 179	0
41	DT	93/100 (93%)	0.45	4 (4%) 40 21	11, 64, 156, 180	0
42	BU	102/103 (99%)	0.14	0 100 100	5, 78, 144, 178	0
42	DU	102/103 (99%)	0.25	6 (5%) 28 16	10, 90, 154, 180	0
43	BW	79/84 (94%)	1.09	20 (25%) 1 2	10, 79, 157, 163	0
43	DW	79/84 (94%)	1.25	20 (25%) 1 2	5, 75, 131, 174	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	63/63 (100%)	-0.14	2 (3%) 50 29	9, 74, 146, 179	0
44	DX	63/63 (100%)	0.01	1 (1%) 70 45	17, 96, 147, 180	0
45	BY	58/58 (100%)	0.11	1 (1%) 69 43	14, 78, 135, 170	0
45	DY	58/58 (100%)	0.40	2 (3%) 48 27	10, 73, 129, 160	0
46	BZ	77/78 (98%)	0.37	3 (3%) 43 23	5, 49, 121, 160	0
46	DZ	77/78 (98%)	0.45	7 (9%) 15 10	5, 42, 107, 141	0
47	B0	56/56 (100%)	0.21	3 (5%) 31 18	5, 77, 144, 166	0
47	D0	56/56 (100%)	0.42	3 (5%) 31 18	8, 52, 128, 160	0
48	B1	50/54 (92%)	0.13	3 (6%) 27 16	51, 99, 149, 165	0
48	D1	50/54 (92%)	-0.12	0 100 100	43, 93, 138, 171	0
49	B2	46/46 (100%)	0.61	6 (13%) 7 6	7, 49, 103, 135	0
49	D2	46/46 (100%)	0.35	4 (8%) 16 10	5, 28, 99, 180	0
50	B3	64/64 (100%)	1.05	9 (14%) 6 5	16, 56, 110, 137	0
50	D3	64/64 (100%)	0.80	9 (14%) 6 5	5, 43, 112, 152	0
51	B4	38/38 (100%)	1.32	9 (23%) 2 2	33, 92, 143, 146	0
51	D4	38/38 (100%)	0.50	1 (2%) 57 33	5, 68, 112, 150	0
52	BI	141/141 (100%)	0.27	6 (4%) 40 21	67, 169, 180, 180	0
52	DI	141/141 (100%)	0.26	5 (3%) 47 26	91, 160, 180, 180	0
All	All	20417/21050 (96%)	0.02	825 (4%) 42 23	5, 70, 153, 180	0

The worst 5 of 825 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	DA	88	C	15.9
11	AL	13	ARG	11.2
1	AA	79	G	10.0
11	AL	14	LYS	8.5
1	AA	80	A	7.7

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($\text{\AA}^2$)	Q<0.9
53	MG	AA	2023	1/1	0.38	0.12	66,66,66,66	1
53	MG	AA	2037	1/1	0.53	0.21	138,138,138,138	0
53	MG	CA	2057	1/1	0.60	0.11	99,99,99,99	0
53	MG	AA	2014	1/1	0.61	0.18	112,112,112,112	0
53	MG	AE	201	1/1	0.62	0.09	144,144,144,144	0
53	MG	DB	3066	1/1	0.66	0.09	146,146,146,146	0
53	MG	CA	2023	1/1	0.67	0.27	137,137,137,137	0
53	MG	CA	2038	1/1	0.67	0.11	128,128,128,128	0
53	MG	CA	2036	1/1	0.68	0.15	101,101,101,101	0
53	MG	CA	2011	1/1	0.69	0.08	132,132,132,132	0
53	MG	AA	2057	1/1	0.72	0.14	141,141,141,141	0
53	MG	AA	2045	1/1	0.76	0.23	92,92,92,92	0
53	MG	CA	2021	1/1	0.78	0.24	125,125,125,125	0
53	MG	BB	3042	1/1	0.79	0.11	168,168,168,168	0
53	MG	CA	2015	1/1	0.80	0.07	149,149,149,149	0
53	MG	CA	2027	1/1	0.80	0.08	50,50,50,50	1
53	MG	BB	3090	1/1	0.80	0.09	112,112,112,112	0
53	MG	DB	3058	1/1	0.82	0.19	151,151,151,151	0
54	HYG	CA	2062	36/36	0.82	0.12	45,45,45,45	0
53	MG	AA	2008	1/1	0.83	0.08	125,125,125,125	0
54	HYG	AA	2059	36/36	0.84	0.10	52,52,52,52	0
53	MG	AA	2044	1/1	0.84	0.09	112,112,112,112	0
53	MG	DB	3047	1/1	0.85	0.04	14,14,14,14	0
53	MG	AA	2035	1/1	0.87	0.17	137,137,137,137	0
53	MG	AA	2025	1/1	0.89	0.07	58,58,58,58	0
53	MG	BB	3072	1/1	0.89	0.15	17,17,17,17	0
53	MG	CA	2059	1/1	0.89	0.06	94,94,94,94	0
53	MG	AA	2043	1/1	0.89	0.07	96,96,96,96	0
53	MG	CE	201	1/1	0.90	0.07	127,127,127,127	0
53	MG	AA	2004	1/1	0.90	0.11	56,56,56,56	0
53	MG	AA	2018	1/1	0.90	0.05	131,131,131,131	0
53	MG	CA	2054	1/1	0.90	0.07	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	AA	2022	1/1	0.90	0.13	82,82,82,82	0
53	MG	AA	2013	1/1	0.90	0.05	122,122,122,122	0
53	MG	AA	2056	1/1	0.91	0.05	124,124,124,124	0
53	MG	BB	3097	1/1	0.91	0.10	114,114,114,114	0
53	MG	AN	201	1/1	0.91	0.08	69,69,69,69	0
53	MG	CA	2052	1/1	0.91	0.06	73,73,73,73	0
53	MG	DB	3013	1/1	0.91	0.13	51,51,51,51	0
53	MG	BB	3033	1/1	0.92	0.09	125,125,125,125	0
53	MG	AA	2054	1/1	0.92	0.08	110,110,110,110	0
53	MG	DB	3060	1/1	0.92	0.12	112,112,112,112	0
53	MG	DB	3029	1/1	0.93	0.06	88,88,88,88	0
53	MG	BB	3100	1/1	0.93	0.06	129,129,129,129	0
53	MG	AA	2050	1/1	0.93	0.07	105,105,105,105	0
53	MG	DB	3059	1/1	0.93	0.05	180,180,180,180	0
53	MG	AA	2031	1/1	0.94	0.06	58,58,58,58	0
53	MG	AA	2002	1/1	0.94	0.04	99,99,99,99	0
53	MG	BB	3047	1/1	0.94	0.09	75,75,75,75	0
53	MG	DB	3061	1/1	0.94	0.07	69,69,69,69	0
53	MG	CA	2026	1/1	0.94	0.09	26,26,26,26	1
53	MG	AA	2012	1/1	0.94	0.08	84,84,84,84	0
53	MG	DB	3057	1/1	0.94	0.05	71,71,71,71	0
53	MG	BB	3080	1/1	0.95	0.12	39,39,39,39	0
53	MG	AA	2055	1/1	0.95	0.12	102,102,102,102	0
53	MG	CA	2014	1/1	0.95	0.09	47,47,47,47	0
53	MG	DB	3018	1/1	0.95	0.02	22,22,22,22	0
53	MG	BB	3043	1/1	0.95	0.05	104,104,104,104	0
53	MG	CA	2028	1/1	0.95	0.07	75,75,75,75	0
53	MG	CA	2058	1/1	0.95	0.04	106,106,106,106	0
53	MG	BB	3106	1/1	0.96	0.08	62,62,62,62	0
53	MG	AA	2005	1/1	0.96	0.04	69,69,69,69	0
53	MG	AA	2047	1/1	0.96	0.03	100,100,100,100	0
53	MG	CA	2035	1/1	0.96	0.04	89,89,89,89	0
53	MG	AA	2019	1/1	0.96	0.04	107,107,107,107	0
53	MG	BB	3010	1/1	0.96	0.06	44,44,44,44	0
53	MG	DB	3083	1/1	0.96	0.06	85,85,85,85	0
53	MG	DB	3092	1/1	0.96	0.05	66,66,66,66	0
53	MG	DB	3111	1/1	0.96	0.06	38,38,38,38	0
53	MG	CA	2022	1/1	0.96	0.05	63,63,63,63	0
53	MG	BB	3054	1/1	0.96	0.04	77,77,77,77	0
55	ZN	D4	101	1/1	0.96	0.09	46,46,46,46	0
53	MG	AA	2049	1/1	0.97	0.05	75,75,75,75	0
53	MG	CA	2019	1/1	0.97	0.06	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	CA	2020	1/1	0.97	0.12	73,73,73,73	0
53	MG	BB	3051	1/1	0.97	0.06	35,35,35,35	0
53	MG	AA	2030	1/1	0.97	0.09	99,99,99,99	0
53	MG	DB	3045	1/1	0.97	0.03	57,57,57,57	0
53	MG	AA	2052	1/1	0.97	0.04	78,78,78,78	0
53	MG	DB	3050	1/1	0.97	0.05	90,90,90,90	0
53	MG	DB	3052	1/1	0.97	0.06	100,100,100,100	0
53	MG	BB	3008	1/1	0.97	0.07	89,89,89,89	0
53	MG	AA	2053	1/1	0.97	0.07	79,79,79,79	0
53	MG	BB	3091	1/1	0.97	0.14	16,16,16,16	0
53	MG	CA	2029	1/1	0.97	0.04	23,23,23,23	1
53	MG	BB	3093	1/1	0.97	0.17	71,71,71,71	0
53	MG	BB	3020	1/1	0.97	0.09	26,26,26,26	0
53	MG	BB	3032	1/1	0.97	0.04	56,56,56,56	0
53	MG	CA	2042	1/1	0.97	0.04	58,58,58,58	0
53	MG	DB	3095	1/1	0.97	0.08	89,89,89,89	0
53	MG	DB	3103	1/1	0.97	0.05	27,27,27,27	0
53	MG	AA	2007	1/1	0.97	0.06	31,31,31,31	0
53	MG	CA	2008	1/1	0.97	0.07	93,93,93,93	0
53	MG	AA	2033	1/1	0.97	0.05	99,99,99,99	0
55	ZN	B4	101	1/1	0.97	0.05	80,80,80,80	0
53	MG	AA	2048	1/1	0.97	0.04	99,99,99,99	0
53	MG	CA	2048	1/1	0.98	0.11	58,58,58,58	0
53	MG	CA	2049	1/1	0.98	0.04	74,74,74,74	0
53	MG	BB	3014	1/1	0.98	0.04	50,50,50,50	0
53	MG	BB	3044	1/1	0.98	0.04	53,53,53,53	0
53	MG	BB	3108	1/1	0.98	0.06	47,47,47,47	0
53	MG	BB	3109	1/1	0.98	0.06	54,54,54,54	0
53	MG	CA	2005	1/1	0.98	0.04	24,24,24,24	0
53	MG	CA	2060	1/1	0.98	0.03	80,80,80,80	0
53	MG	CA	2006	1/1	0.98	0.04	95,95,95,95	0
53	MG	DB	3003	1/1	0.98	0.14	63,63,63,63	0
53	MG	CA	2007	1/1	0.98	0.03	46,46,46,46	0
53	MG	AA	2026	1/1	0.98	0.05	65,65,65,65	0
53	MG	CA	2009	1/1	0.98	0.03	67,67,67,67	0
53	MG	DB	3032	1/1	0.98	0.04	63,63,63,63	0
53	MG	DB	3034	1/1	0.98	0.09	52,52,52,52	0
53	MG	DB	3036	1/1	0.98	0.04	30,30,30,30	0
53	MG	BB	3048	1/1	0.98	0.04	44,44,44,44	0
53	MG	BB	3026	1/1	0.98	0.05	39,39,39,39	0
53	MG	BB	3028	1/1	0.98	0.12	86,86,86,86	0
53	MG	BB	3068	1/1	0.98	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BB	3071	1/1	0.98	0.10	26,26,26,26	0
53	MG	BB	3031	1/1	0.98	0.09	41,41,41,41	0
53	MG	BB	3077	1/1	0.98	0.05	36,36,36,36	0
53	MG	BB	3078	1/1	0.98	0.07	70,70,70,70	0
53	MG	AA	2051	1/1	0.98	0.04	41,41,41,41	0
53	MG	BB	3081	1/1	0.98	0.07	46,46,46,46	0
53	MG	DB	3070	1/1	0.98	0.03	45,45,45,45	0
53	MG	BB	3082	1/1	0.98	0.10	46,46,46,46	0
53	MG	DB	3088	1/1	0.98	0.04	25,25,25,25	0
53	MG	DB	3090	1/1	0.98	0.05	37,37,37,37	0
53	MG	BB	3085	1/1	0.98	0.05	103,103,103,103	0
53	MG	CA	2033	1/1	0.98	0.07	56,56,56,56	0
53	MG	DB	3097	1/1	0.98	0.05	38,38,38,38	0
53	MG	AA	2017	1/1	0.98	0.08	87,87,87,87	0
53	MG	DB	3108	1/1	0.98	0.04	37,37,37,37	0
53	MG	DB	3110	1/1	0.98	0.09	21,21,21,21	0
53	MG	BB	3034	1/1	0.98	0.08	35,35,35,35	0
53	MG	CA	2037	1/1	0.98	0.04	94,94,94,94	0
53	MG	BB	3037	1/1	0.98	0.04	23,23,23,23	0
53	MG	AA	2040	1/1	0.98	0.05	83,83,83,83	0
53	MG	CA	2047	1/1	0.98	0.03	121,121,121,121	0
53	MG	AA	2010	1/1	0.99	0.04	60,60,60,60	0
53	MG	AA	2036	1/1	0.99	0.03	31,31,31,31	0
53	MG	CA	2016	1/1	0.99	0.04	53,53,53,53	0
53	MG	AA	2015	1/1	0.99	0.05	24,24,24,24	0
53	MG	AA	2038	1/1	0.99	0.08	71,71,71,71	0
53	MG	BB	3045	1/1	0.99	0.02	31,31,31,31	0
53	MG	BB	3046	1/1	0.99	0.04	22,22,22,22	0
53	MG	AA	2039	1/1	0.99	0.07	64,64,64,64	0
53	MG	CA	2024	1/1	0.99	0.04	29,29,29,29	0
53	MG	CA	2025	1/1	0.99	0.03	50,50,50,50	0
53	MG	AA	2058	1/1	0.99	0.07	86,86,86,86	0
53	MG	AA	2024	1/1	0.99	0.08	5,5,5,5	1
53	MG	BB	3052	1/1	0.99	0.05	38,38,38,38	0
53	MG	AA	2041	1/1	0.99	0.03	83,83,83,83	0
53	MG	CA	2031	1/1	0.99	0.04	28,28,28,28	0
53	MG	CA	2032	1/1	0.99	0.05	33,33,33,33	0
53	MG	BB	3055	1/1	0.99	0.04	17,17,17,17	0
53	MG	CA	2034	1/1	0.99	0.03	6,6,6,6	0
53	MG	BB	3059	1/1	0.99	0.11	26,26,26,26	0
53	MG	BB	3061	1/1	0.99	0.04	48,48,48,48	0
53	MG	BB	3063	1/1	0.99	0.03	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BB	3064	1/1	0.99	0.04	35,35,35,35	0
53	MG	CA	2040	1/1	0.99	0.04	48,48,48,48	0
53	MG	CA	2041	1/1	0.99	0.04	46,46,46,46	0
53	MG	BB	3065	1/1	0.99	0.02	29,29,29,29	0
53	MG	CA	2043	1/1	0.99	0.07	19,19,19,19	0
53	MG	CA	2044	1/1	0.99	0.04	59,59,59,59	0
53	MG	CA	2046	1/1	0.99	0.02	57,57,57,57	0
53	MG	BB	3067	1/1	0.99	0.03	44,44,44,44	0
53	MG	BB	3001	1/1	0.99	0.03	51,51,51,51	0
53	MG	BB	3070	1/1	0.99	0.03	37,37,37,37	0
53	MG	CA	2051	1/1	0.99	0.03	39,39,39,39	0
53	MG	BB	3003	1/1	0.99	0.06	32,32,32,32	0
53	MG	CA	2053	1/1	0.99	0.05	30,30,30,30	0
53	MG	BB	3004	1/1	0.99	0.06	32,32,32,32	0
53	MG	BB	3074	1/1	0.99	0.02	28,28,28,28	0
53	MG	BB	3007	1/1	0.99	0.07	82,82,82,82	0
53	MG	AA	2042	1/1	0.99	0.02	69,69,69,69	0
53	MG	BB	3079	1/1	0.99	0.09	19,19,19,19	0
53	MG	BB	3009	1/1	0.99	0.04	46,46,46,46	0
53	MG	AA	2016	1/1	0.99	0.04	89,89,89,89	0
53	MG	DB	3007	1/1	0.99	0.04	18,18,18,18	0
53	MG	DB	3008	1/1	0.99	0.04	6,6,6,6	0
53	MG	DB	3011	1/1	0.99	0.05	17,17,17,17	0
53	MG	BB	3012	1/1	0.99	0.06	32,32,32,32	0
53	MG	DB	3015	1/1	0.99	0.03	33,33,33,33	0
53	MG	DB	3017	1/1	0.99	0.04	13,13,13,13	0
53	MG	BB	3083	1/1	0.99	0.09	12,12,12,12	0
53	MG	DB	3022	1/1	0.99	0.03	25,25,25,25	0
53	MG	DB	3024	1/1	0.99	0.04	63,63,63,63	0
53	MG	DB	3026	1/1	0.99	0.04	34,34,34,34	0
53	MG	BB	3013	1/1	0.99	0.03	43,43,43,43	0
53	MG	DB	3031	1/1	0.99	0.03	8,8,8,8	0
53	MG	BB	3086	1/1	0.99	0.11	42,42,42,42	0
53	MG	BB	3087	1/1	0.99	0.03	57,57,57,57	0
53	MG	DB	3035	1/1	0.99	0.04	55,55,55,55	0
53	MG	BB	3088	1/1	0.99	0.02	28,28,28,28	0
53	MG	DB	3037	1/1	0.99	0.09	28,28,28,28	0
53	MG	DB	3039	1/1	0.99	0.10	22,22,22,22	0
53	MG	DB	3041	1/1	0.99	0.04	29,29,29,29	0
53	MG	DB	3044	1/1	0.99	0.04	24,24,24,24	0
53	MG	BB	3089	1/1	0.99	0.04	56,56,56,56	0
53	MG	DB	3046	1/1	0.99	0.04	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	AA	2011	1/1	0.99	0.03	85,85,85,85	0
53	MG	DB	3048	1/1	0.99	0.09	28,28,28,28	0
53	MG	BB	3017	1/1	0.99	0.03	34,34,34,34	0
53	MG	DB	3051	1/1	0.99	0.07	23,23,23,23	0
53	MG	AA	2028	1/1	0.99	0.05	100,100,100,100	0
53	MG	BB	3094	1/1	0.99	0.04	28,28,28,28	0
53	MG	BB	3095	1/1	0.99	0.03	33,33,33,33	0
53	MG	BB	3021	1/1	0.99	0.11	30,30,30,30	0
53	MG	BB	3099	1/1	0.99	0.07	40,40,40,40	0
53	MG	BB	3022	1/1	0.99	0.09	34,34,34,34	0
53	MG	DB	3062	1/1	0.99	0.04	77,77,77,77	0
53	MG	DB	3063	1/1	0.99	0.06	43,43,43,43	0
53	MG	DB	3064	1/1	0.99	0.05	20,20,20,20	0
53	MG	BB	3102	1/1	0.99	0.03	20,20,20,20	0
53	MG	BB	3103	1/1	0.99	0.04	5,5,5,5	0
53	MG	DB	3071	1/1	0.99	0.06	16,16,16,16	0
53	MG	DB	3072	1/1	0.99	0.03	18,18,18,18	0
53	MG	DB	3073	1/1	0.99	0.03	14,14,14,14	0
53	MG	DB	3075	1/1	0.99	0.03	57,57,57,57	0
53	MG	DB	3077	1/1	0.99	0.04	54,54,54,54	0
53	MG	DB	3079	1/1	0.99	0.04	28,28,28,28	0
53	MG	DB	3082	1/1	0.99	0.03	30,30,30,30	0
53	MG	BB	3104	1/1	0.99	0.04	36,36,36,36	0
53	MG	DB	3087	1/1	0.99	0.04	53,53,53,53	0
53	MG	BB	3105	1/1	0.99	0.03	20,20,20,20	0
53	MG	BB	3025	1/1	0.99	0.03	30,30,30,30	0
53	MG	AA	2029	1/1	0.99	0.02	39,39,39,39	0
53	MG	AA	2001	1/1	0.99	0.04	35,35,35,35	0
53	MG	BB	3029	1/1	0.99	0.03	14,14,14,14	0
53	MG	DB	3099	1/1	0.99	0.04	7,7,7,7	0
53	MG	DB	3100	1/1	0.99	0.05	13,13,13,13	0
53	MG	DB	3102	1/1	0.99	0.02	12,12,12,12	0
53	MG	AA	2006	1/1	0.99	0.02	60,60,60,60	0
53	MG	DB	3106	1/1	0.99	0.04	23,23,23,23	0
53	MG	AA	2032	1/1	0.99	0.03	62,62,62,62	0
53	MG	AA	2021	1/1	0.99	0.21	5,5,5,5	1
53	MG	AA	2034	1/1	0.99	0.03	68,68,68,68	0
53	MG	CA	2010	1/1	0.99	0.03	33,33,33,33	0
53	MG	BB	3036	1/1	0.99	0.06	42,42,42,42	0
53	MG	CA	2012	1/1	0.99	0.02	93,93,93,93	0
53	MG	CA	2013	1/1	0.99	0.03	73,73,73,73	0
53	MG	DB	3010	1/1	1.00	0.02	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BB	3075	1/1	1.00	0.06	40,40,40,40	0
53	MG	DB	3012	1/1	1.00	0.03	9,9,9,9	0
53	MG	BB	3076	1/1	1.00	0.04	38,38,38,38	0
53	MG	DB	3014	1/1	1.00	0.08	5,5,5,5	0
53	MG	AA	2003	1/1	1.00	0.04	39,39,39,39	0
53	MG	DB	3016	1/1	1.00	0.04	15,15,15,15	0
53	MG	AA	2009	1/1	1.00	0.02	7,7,7,7	0
53	MG	AA	2046	1/1	1.00	0.04	5,5,5,5	0
53	MG	DB	3019	1/1	1.00	0.01	5,5,5,5	0
53	MG	DB	3020	1/1	1.00	0.06	5,5,5,5	0
53	MG	DB	3021	1/1	1.00	0.07	11,11,11,11	0
53	MG	BB	3023	1/1	1.00	0.02	5,5,5,5	0
53	MG	DB	3023	1/1	1.00	0.03	32,32,32,32	0
53	MG	CA	2017	1/1	1.00	0.03	5,5,5,5	0
53	MG	DB	3025	1/1	1.00	0.03	5,5,5,5	0
53	MG	CA	2018	1/1	1.00	0.06	6,6,6,6	0
53	MG	DB	3027	1/1	1.00	0.03	6,6,6,6	0
53	MG	DB	3028	1/1	1.00	0.10	24,24,24,24	0
53	MG	BB	3024	1/1	1.00	0.02	15,15,15,15	0
53	MG	DB	3030	1/1	1.00	0.05	6,6,6,6	0
53	MG	BB	3002	1/1	1.00	0.02	5,5,5,5	0
53	MG	BB	3011	1/1	1.00	0.03	5,5,5,5	0
53	MG	DB	3033	1/1	1.00	0.01	9,9,9,9	0
53	MG	BB	3084	1/1	1.00	0.02	24,24,24,24	0
53	MG	BB	3049	1/1	1.00	0.02	10,10,10,10	0
53	MG	BB	3050	1/1	1.00	0.04	28,28,28,28	0
53	MG	BB	3027	1/1	1.00	0.05	33,33,33,33	0
53	MG	DB	3038	1/1	1.00	0.04	5,5,5,5	0
53	MG	AA	2020	1/1	1.00	0.11	5,5,5,5	0
53	MG	DB	3040	1/1	1.00	0.07	5,5,5,5	0
53	MG	BB	3053	1/1	1.00	0.04	28,28,28,28	0
53	MG	DB	3042	1/1	1.00	0.02	6,6,6,6	0
53	MG	DB	3043	1/1	1.00	0.02	5,5,5,5	0
53	MG	AA	2027	1/1	1.00	0.02	36,36,36,36	0
53	MG	BB	3030	1/1	1.00	0.02	35,35,35,35	0
53	MG	CA	2030	1/1	1.00	0.15	7,7,7,7	0
53	MG	BB	3092	1/1	1.00	0.02	54,54,54,54	0
53	MG	BB	3056	1/1	1.00	0.03	26,26,26,26	0
53	MG	DB	3049	1/1	1.00	0.01	36,36,36,36	0
53	MG	BB	3057	1/1	1.00	0.11	28,28,28,28	0
53	MG	BB	3058	1/1	1.00	0.03	22,22,22,22	0
53	MG	BB	3096	1/1	1.00	0.03	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3053	1/1	1.00	0.03	35,35,35,35	0
53	MG	DB	3054	1/1	1.00	0.11	19,19,19,19	0
53	MG	DB	3055	1/1	1.00	0.04	26,26,26,26	0
53	MG	DB	3056	1/1	1.00	0.01	5,5,5,5	0
53	MG	BB	3005	1/1	1.00	0.06	5,5,5,5	0
53	MG	BB	3098	1/1	1.00	0.03	35,35,35,35	0
53	MG	BB	3060	1/1	1.00	0.03	19,19,19,19	0
53	MG	CA	2039	1/1	1.00	0.04	16,16,16,16	0
53	MG	BB	3015	1/1	1.00	0.02	13,13,13,13	0
53	MG	BB	3101	1/1	1.00	0.01	24,24,24,24	0
53	MG	BB	3062	1/1	1.00	0.04	14,14,14,14	0
53	MG	BB	3016	1/1	1.00	0.06	38,38,38,38	0
53	MG	DB	3065	1/1	1.00	0.04	37,37,37,37	0
53	MG	BB	3006	1/1	1.00	0.04	5,5,5,5	0
53	MG	DB	3067	1/1	1.00	0.06	5,5,5,5	0
53	MG	DB	3068	1/1	1.00	0.03	5,5,5,5	0
53	MG	DB	3069	1/1	1.00	0.04	11,11,11,11	0
53	MG	CA	2045	1/1	1.00	0.04	48,48,48,48	0
53	MG	BB	3035	1/1	1.00	0.03	15,15,15,15	0
53	MG	BB	3066	1/1	1.00	0.02	23,23,23,23	0
53	MG	BB	3107	1/1	1.00	0.01	6,6,6,6	0
53	MG	DB	3074	1/1	1.00	0.03	12,12,12,12	0
53	MG	BB	3018	1/1	1.00	0.02	32,32,32,32	0
53	MG	DB	3076	1/1	1.00	0.03	5,5,5,5	0
53	MG	CA	2050	1/1	1.00	0.01	8,8,8,8	0
53	MG	DB	3078	1/1	1.00	0.03	27,27,27,27	0
53	MG	BB	3019	1/1	1.00	0.03	22,22,22,22	0
53	MG	DB	3080	1/1	1.00	0.02	10,10,10,10	0
53	MG	DB	3081	1/1	1.00	0.01	18,18,18,18	0
53	MG	BB	3110	1/1	1.00	0.05	23,23,23,23	0
53	MG	CA	2001	1/1	1.00	0.06	5,5,5,5	0
53	MG	DB	3084	1/1	1.00	0.08	5,5,5,5	0
53	MG	DB	3085	1/1	1.00	0.02	5,5,5,5	0
53	MG	DB	3086	1/1	1.00	0.02	11,11,11,11	0
53	MG	CA	2002	1/1	1.00	0.01	5,5,5,5	0
53	MG	CA	2055	1/1	1.00	0.01	11,11,11,11	0
53	MG	DB	3089	1/1	1.00	0.04	7,7,7,7	0
53	MG	CA	2056	1/1	1.00	0.03	5,5,5,5	0
53	MG	DB	3091	1/1	1.00	0.07	13,13,13,13	0
53	MG	CA	2003	1/1	1.00	0.05	35,35,35,35	0
53	MG	DB	3093	1/1	1.00	0.07	11,11,11,11	0
53	MG	DB	3094	1/1	1.00	0.03	29,29,29,29	0

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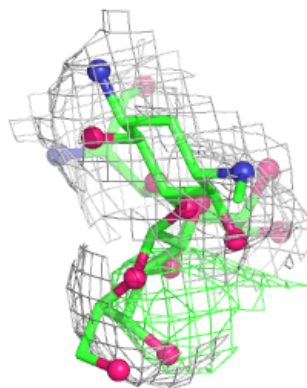
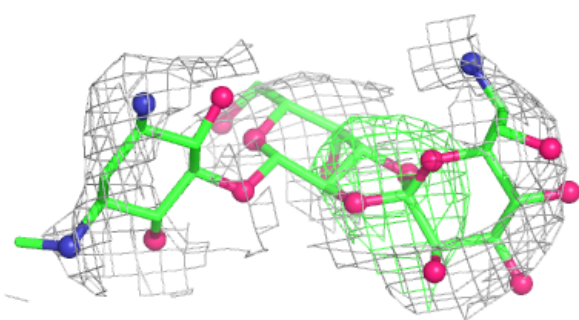
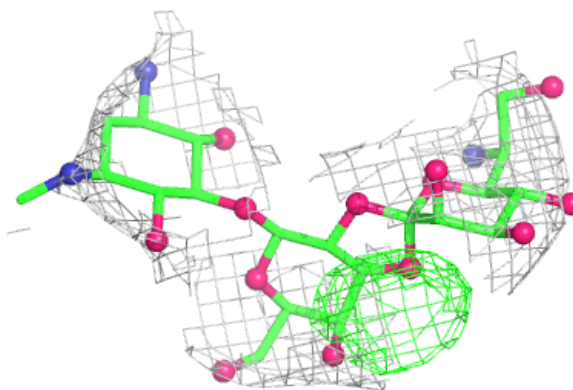
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	CA	2004	1/1	1.00	0.10	8,8,8,8	0
53	MG	DB	3096	1/1	1.00	0.04	6,6,6,6	0
53	MG	BB	3069	1/1	1.00	0.02	17,17,17,17	0
53	MG	DB	3098	1/1	1.00	0.07	44,44,44,44	0
53	MG	BB	3038	1/1	1.00	0.03	71,71,71,71	0
53	MG	CA	2061	1/1	1.00	0.02	23,23,23,23	0
53	MG	DB	3101	1/1	1.00	0.02	5,5,5,5	0
53	MG	BB	3039	1/1	1.00	0.05	7,7,7,7	0
53	MG	DB	3001	1/1	1.00	0.01	5,5,5,5	0
53	MG	DB	3104	1/1	1.00	0.02	33,33,33,33	0
53	MG	DB	3105	1/1	1.00	0.03	23,23,23,23	0
53	MG	DB	3002	1/1	1.00	0.05	12,12,12,12	0
53	MG	DB	3107	1/1	1.00	0.01	10,10,10,10	0
53	MG	BB	3040	1/1	1.00	0.07	26,26,26,26	0
53	MG	DB	3109	1/1	1.00	0.01	9,9,9,9	0
53	MG	DB	3004	1/1	1.00	0.01	6,6,6,6	0
53	MG	DB	3005	1/1	1.00	0.01	10,10,10,10	0
53	MG	DB	3006	1/1	1.00	0.02	5,5,5,5	0
53	MG	BB	3073	1/1	1.00	0.03	39,39,39,39	0
53	MG	BB	3041	1/1	1.00	0.01	7,7,7,7	0
53	MG	DB	3009	1/1	1.00	0.03	29,29,29,29	0

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

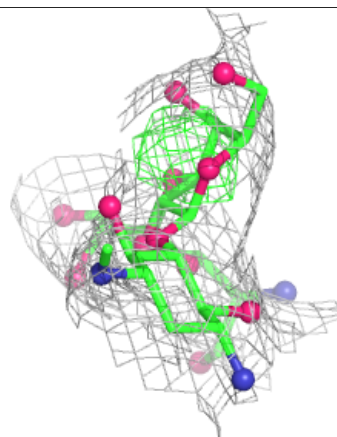
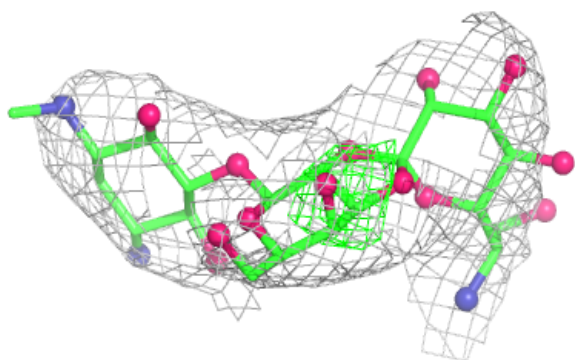
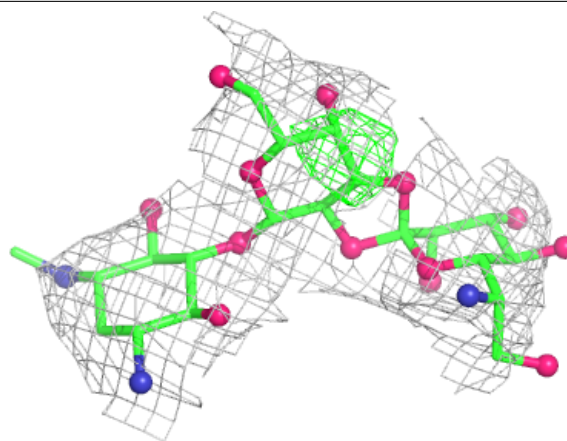
Electron density around HYG CA 2062:

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



Electron density around HYG AA 2059:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.