



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 17, 2023 – 10:13 AM EST

PDB ID : 4U27
Title : Crystal structure of the E. coli ribosome bound to flopristin and linopristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-07-16
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

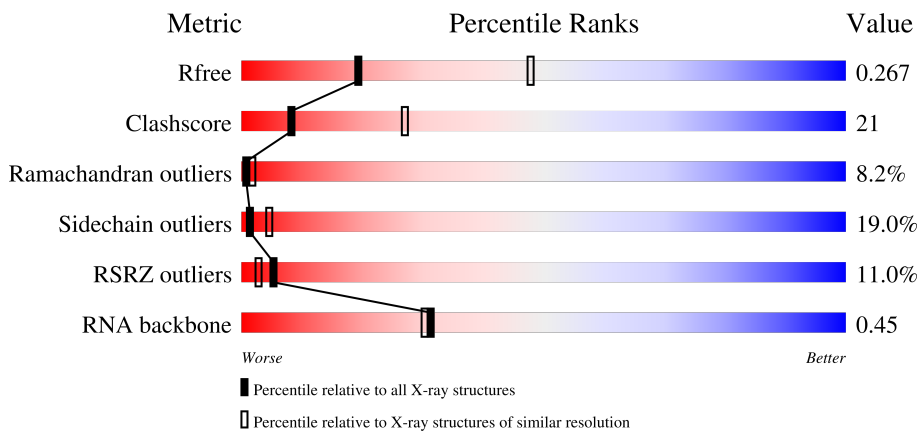
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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	1539	 2% 34% 49% 16%
1	CA	1539	 4% 33% 52% 15%
2	AB	218	 9% 25% 45% 23% 6%
2	CB	218	 25% 25% 55% 17% 8%

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Mol	Chain	Length	Quality of chain
3	AC	206	46% 39% 13% 2%
3	CC	206	11% 51% 37% 1%
4	AD	205	4% 35% 42% 20%
4	CD	205	2% 40% 43% 15%
5	AE	150	41% 39% 18% 2%
5	CE	150	2% 39% 38% 20%
6	AF	100	38% 37% 20% 5%
6	CF	100	3% 32% 45% 19%
7	AG	151	8% 39% 45% 16%
7	CG	151	58% 40% 45% 13%
8	AH	129	40% 45% 15%
8	CH	129	4% 51% 37% 9%
9	AI	127	12% 37% 35% 26%
9	CI	127	28% 37% 43% 18%
10	AJ	98	6% 33% 41% 23%
10	CJ	98	48% 42% 37% 19%
11	AK	117	9% 44% 38% 16%
11	CK	117	3% 36% 48% 15%
12	AL	123	4% 47% 43% 7%
12	CL	123	5% 37% 42% 16%
13	AM	114	40% 42% 16% 4%
13	CM	114	58% 40% 44% 15%
14	AN	100	10% 37% 38% 19%
14	CN	100	34% 37% 43% 15%
15	AO	88	2% 58% 33% 9%

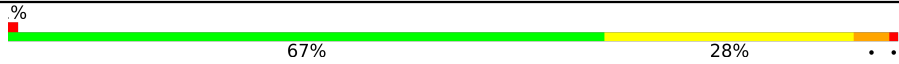

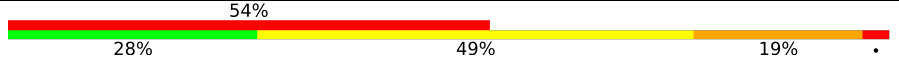
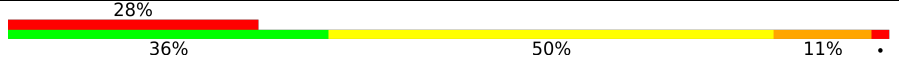


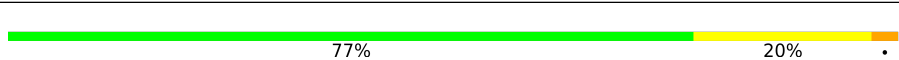
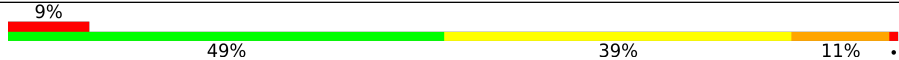
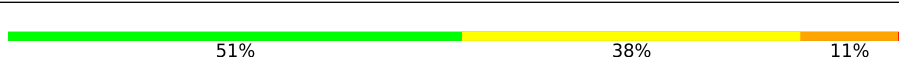
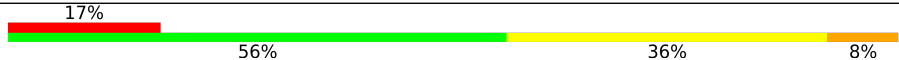
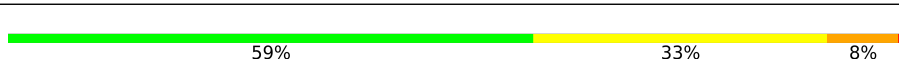
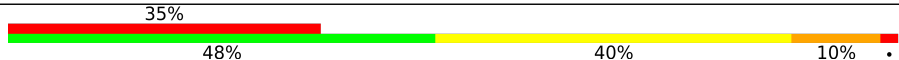


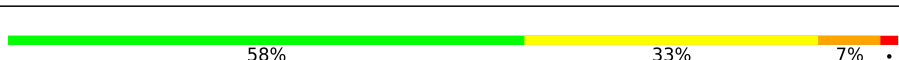
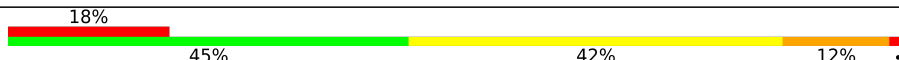
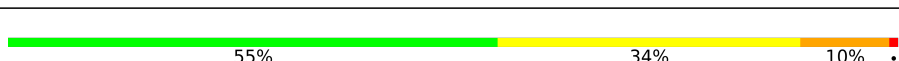
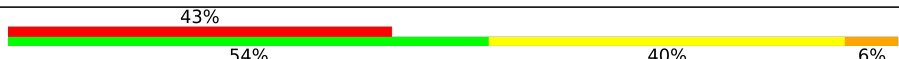
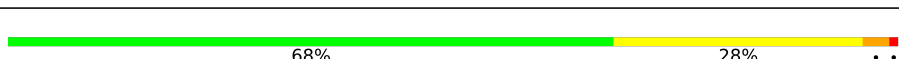
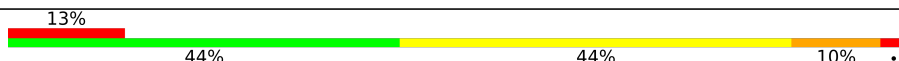
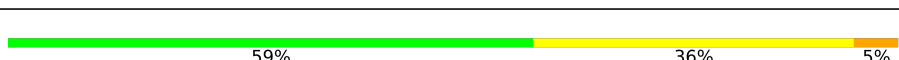
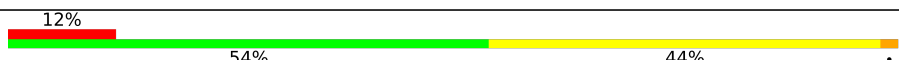
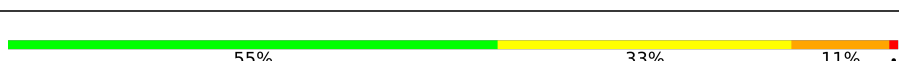

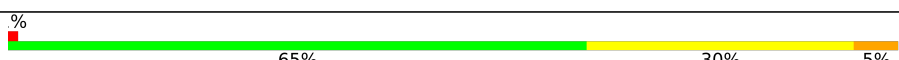
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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
27	DF	177	

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Mol	Chain	Length	Quality of chain
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
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	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	76	
44	DW	76	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	

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Mol	Chain	Length	Quality of chain
53	B5	228	<p>81%</p> <p>48% 24% 12% 16%</p>
54	B6	7	<p>14% 71% 14%</p>
54	D6	7	<p>14% 71% 14%</p>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MHW	B6	1	-	X	-	-
54	MHW	D6	1	-	-	X	-
54	004	D6	7	-	X	-	-
55	MG	AA	1658	-	-	-	X
55	MG	AA	1660	-	-	-	X
55	MG	AA	1662	-	-	-	X
55	MG	AA	1672	-	-	-	X
55	MG	CA	1656	-	-	-	X
55	MG	DA	3008	-	-	-	X
55	MG	DA	3016	-	-	-	X
55	MG	DA	3027	-	-	-	X
55	MG	DA	3063	-	-	-	X
55	MG	DA	3093	-	-	-	X
55	MG	DA	3113	-	-	-	X
55	MG	DA	3132	-	-	-	X
55	MG	DA	3134	-	-	-	X
55	MG	DA	3138	-	-	-	X
55	MG	DA	3165	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 288396 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1538	Total 32995	C 14716	N 6050	O 10691	P 1538	0	0	0
1	CA	1539	Total 33015	C 14725	N 6052	O 10699	P 1539	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AB	218	Total 1705	C 1081	N 305	O 312	S 7	0	0	0
2	CB	218	Total 1705	C 1081	N 305	O 312	S 7	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	206	Total 1625	C 1028	N 305	O 289	S 3	0	0	0
3	CC	206	Total 1625	C 1028	N 305	O 289	S 3	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	CG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	CM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			
15	CO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	AP	82	Total 649	C 406	N 128	O 114	S 1	0	0	0
16	CP	82	Total 649	C 406	N 128	O 114	S 1	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	AQ	80	Total 649	C 411	N 121	O 114	S 3	0	0	0
17	CQ	80	Total 649	C 411	N 121	O 114	S 3	0	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	AR	55	Total 456	C 288	N 86	O 82	0	0	0
18	CR	55	Total 456	C 288	N 86	O 82	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AS	79	Total 638	C 408	N 120	O 108	S 2	0	0	0
19	CS	79	Total 638	C 408	N 120	O 108	S 2	0	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- 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
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
22	DA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
23	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	BF	177	1411	899	249	257	6	0	0	0
27	DF	177	1411	899	249	257	6	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	BH	149	1110	699	197	213	1	0	0	0
29	DH	149	1110	699	197	213	1	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- 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
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	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
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	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	0	0	0
			780	492	146	142			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	DU	102	780	492	146	142	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	BW	76	580	359	117	103	1	0	0	0
44	DW	75	569	353	113	102	1	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BX	77	625	388	129	106	2	0	0	0
45	DX	77	625	388	129	106	2	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	BY	63	509	313	99	95	2	0	0	0
46	DY	63	509	313	99	95	2	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	BZ	58	449	281	87	79	2	0	0	0
47	DZ	58	449	281	87	79	2	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	B5	191	Total	C	N	O	0	0	1
			1142	691	221	230			

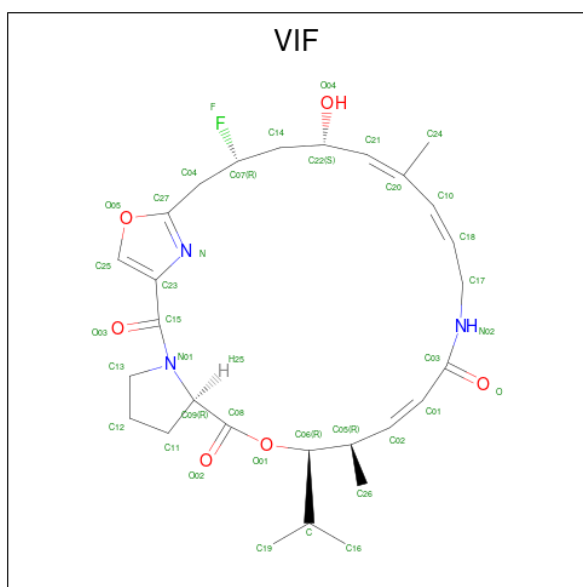
- Molecule 54 is a protein called Linopristin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	B6	7	Total	C	N	O	0	0	0
			69	50	9	10			
54	D6	7	Total	C	N	O	0	0	0
			69	50	9	10			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	72	Total	Mg	0	0
			72	72		
55	BA	193	Total	Mg	0	0
			193	193		
55	BB	4	Total	Mg	0	0
			4	4		
55	BD	1	Total	Mg	0	0
			1	1		
55	BQ	1	Total	Mg	0	0
			1	1		
55	CA	56	Total	Mg	0	0
			56	56		
55	DA	167	Total	Mg	0	0
			167	167		
55	DB	3	Total	Mg	0	0
			3	3		
55	D2	1	Total	Mg	0	0
			1	1		

- Molecule 56 is Flopristin (three-letter code: VIF) (formula: C₂₈H₃₈FN₃O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
56	BA	1	Total	C	F	N	O	0	0
			38	28	1	3	6		
56	DA	1	Total	C	F	N	O	0	0
			38	28	1	3	6		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	193	Total	O	0	0
			193	193		
58	AL	2	Total	O	0	0
			2	2		
58	AN	5	Total	O	0	0
			5	5		
58	AT	2	Total	O	0	0
			2	2		
58	AU	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	BA	623	Total O 623 623	0	0
58	BB	14	Total O 14 14	0	0
58	BC	6	Total O 6 6	0	0
58	BD	3	Total O 3 3	0	0
58	BE	4	Total O 4 4	0	0
58	BF	1	Total O 1 1	0	0
58	BG	1	Total O 1 1	0	0
58	BL	4	Total O 4 4	0	0
58	BN	3	Total O 3 3	0	0
58	BS	1	Total O 1 1	0	0
58	BT	1	Total O 1 1	0	0
58	B2	1	Total O 1 1	0	0
58	B3	2	Total O 2 2	0	0
58	B4	2	Total O 2 2	0	0
58	CA	192	Total O 192 192	0	0
58	CL	1	Total O 1 1	0	0
58	CN	3	Total O 3 3	0	0
58	CT	1	Total O 1 1	0	0
58	CU	1	Total O 1 1	0	0
58	DA	608	Total O 608 608	0	0
58	DB	13	Total O 13 13	0	0

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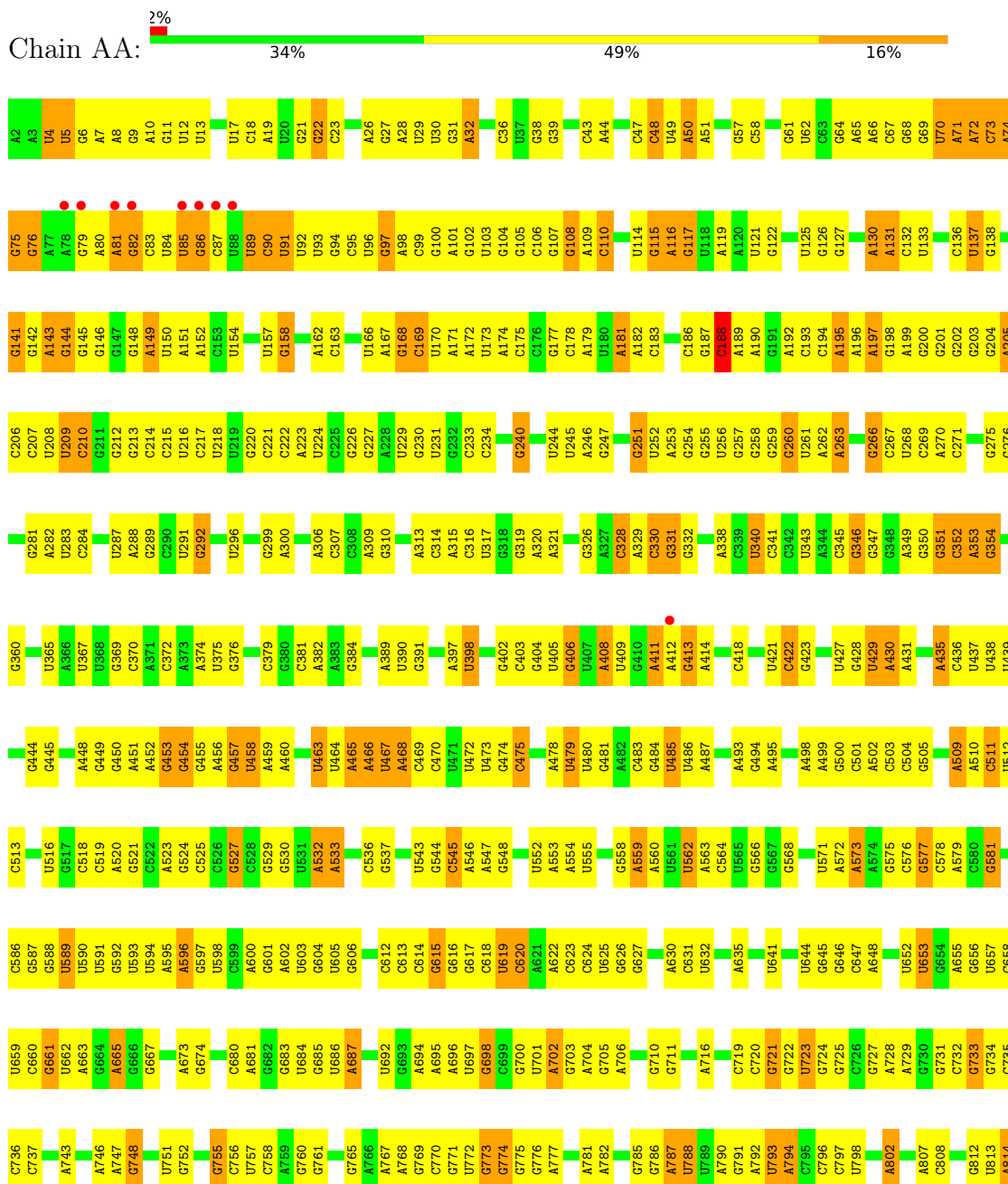
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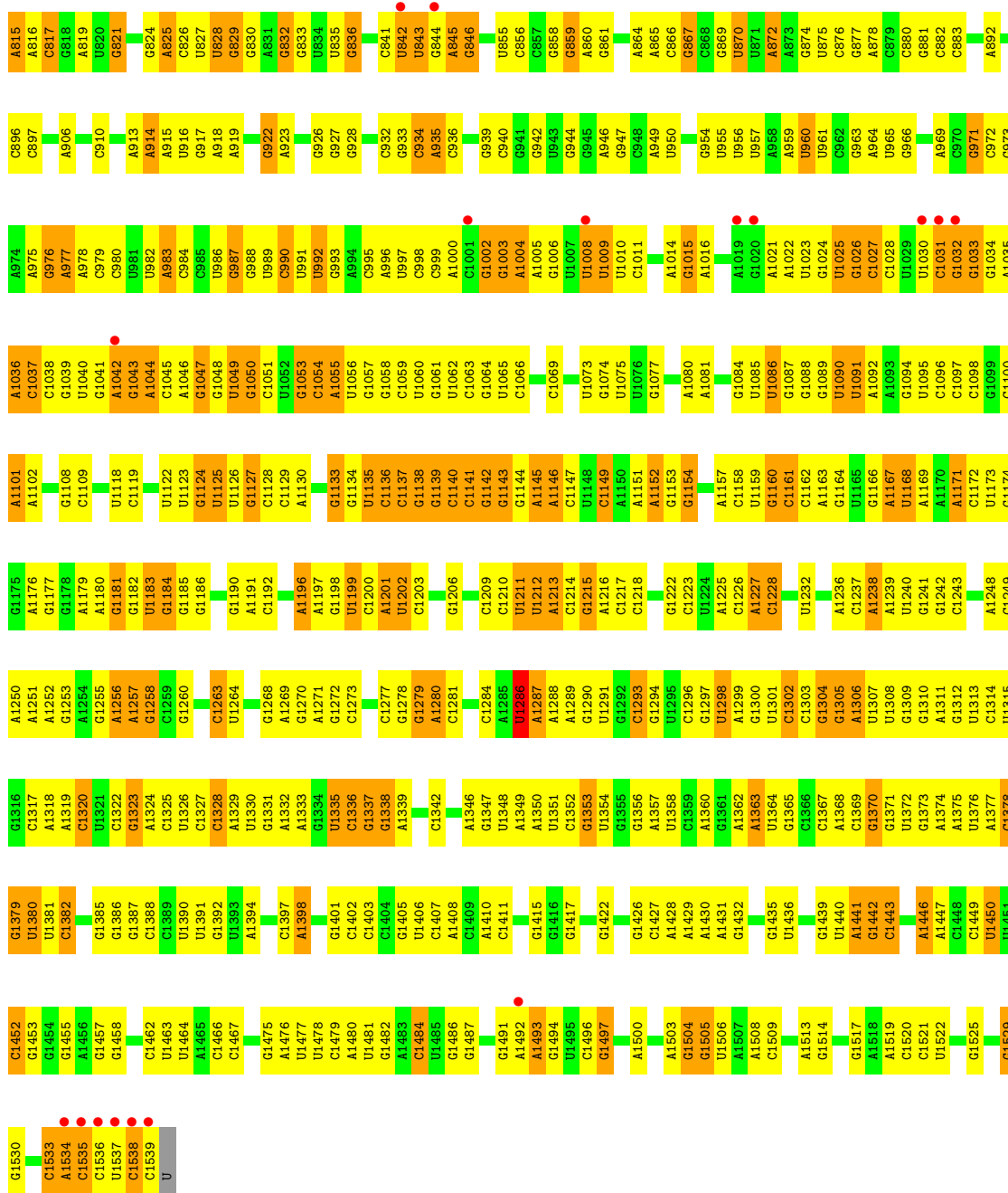
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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58	DD	4	Total 4	O 4	0	0
58	DE	5	Total 5	O 5	0	0
58	DJ	1	Total 1	O 1	0	0
58	DL	4	Total 4	O 4	0	0
58	DN	2	Total 2	O 2	0	0
58	DT	1	Total 1	O 1	0	0
58	DU	1	Total 1	O 1	0	0
58	DV	1	Total 1	O 1	0	0
58	D0	1	Total 1	O 1	0	0
58	D2	1	Total 1	O 1	0	0
58	D3	2	Total 2	O 2	0	0
58	D4	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

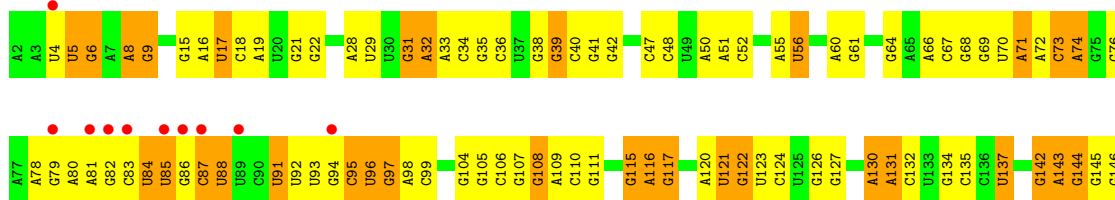
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S rRNA

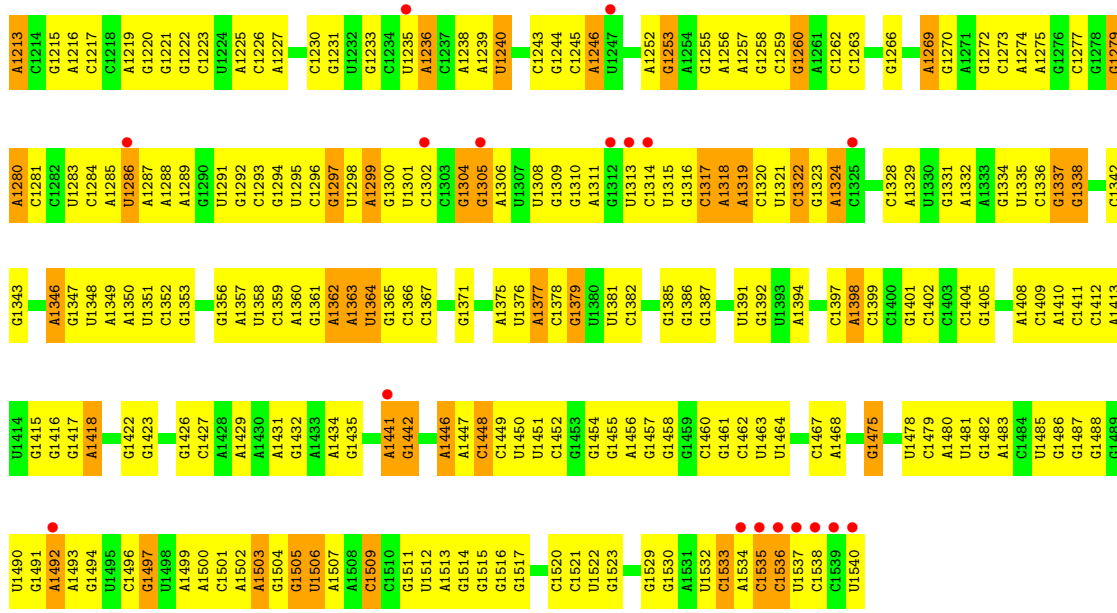




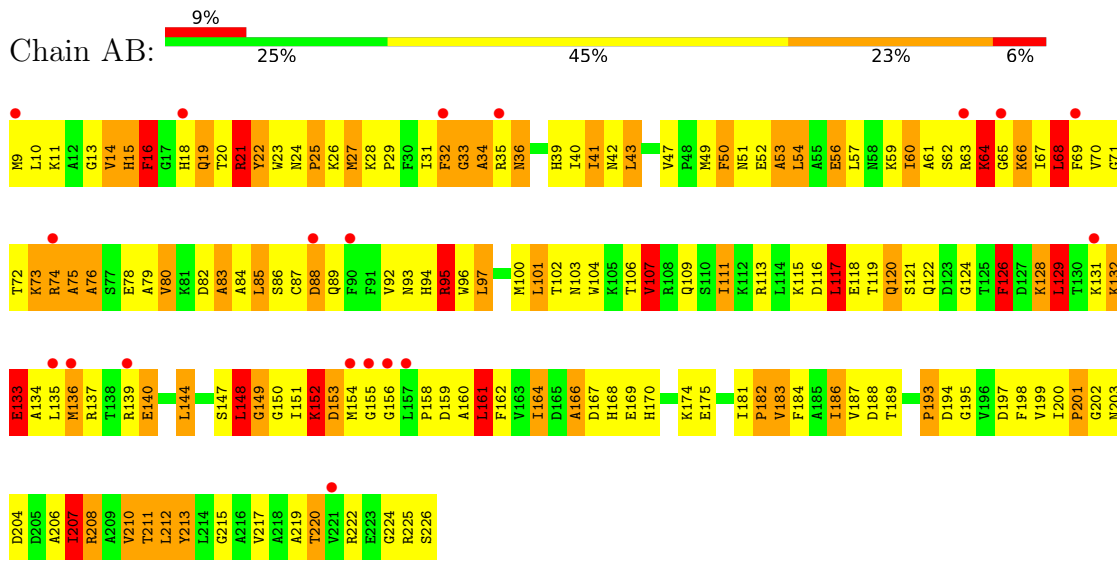
• Molecule 1: 16S rRNA



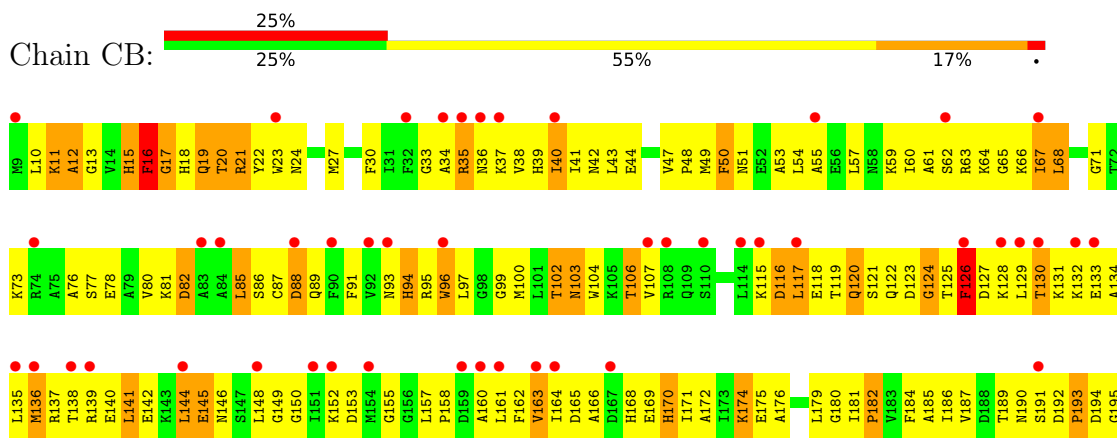
C1149	G1015	U798	G730	U657	G567	A502	A431	G360	G289	G212	G147
A1150	A1016	U801	G731	U662	G568	C503	A432	G361	C290	G213	G148
A1151	U1017	A802	G732	A663	U571	C504	C436	U367	C291	C214	A149
A1152	G1018	G803	G733	A664	A572	G505	U437	U368	G292	C215	U150
G1153	A1019	U804	G734	A665	A573	U508	U438	G369	G293	C216	A151
G1154	G1020	C805	G735	A666	A574	A509	U439	C370	U294	U218	A152
A1155	A1021	C806	G736	G666	G575	A510	C440	A371	C295	U219	C153
A1156	A1022	C807	G737	G667	G576	A511	A441	C372	U296	G220	U154
U1091	U1023	G808	U740	A671	G577	U512	A442	A373	C297	G221	A155
U1092	G1024	C809	U741	A672	G578	C513	C443	A374	G298	C222	C156
U1093	U1025	G809	G742	A673	A579	C514	C444	A375	A298	U157	U157
A1094	G1026	A579	G743	A674	C580	C515	C445	U376	G299	G158	G158
U1095	C1027	C811	A743	A675	C581	C516	C446	G376	A300	U224	G159
C1096	C1028	G812	C744	A676	C582	U516	G446	G377	G301	G225	A160
U1029	U1029	U813	U746	U677	C583	G517	G447	G378	G302	G226	A161
C1098	U1030	A814	G746	U678	A596	C518	A448	C379	A306	G227	A162
C1099	G1031	A815	A747	C680	G597	C519	A449	G380	A307	G228	G163
A1100	C1032	C816	G748	C681	U598	A520	C450	A381	C307	A228	G164
A1101	G1033	A817	A749	A682	U599	G521	A451	A383	C308	G237	G165
A1102	C1034	C818	A753	G683	A596	C522	A452	C384	A309	G240	U166
A1035	A1035	A819	A753	G684	G597	C523	G453	C385	C312	G241	A167
A1170	C1036	U820	C754	U684	G597	C524	C454	C386	G242	G242	G168
G1104	C1037	G821	G755	U685	U598	C525	C455	U387	A313	G243	G169
A1105	C1038	U822	C756	U686	U599	G527	A456	A388	C314	A243	C169
A1172	C1039	U823	U757	A687	G604	C528	C457	A389	U170	U244	U170
G1106	U1040	G826	C758	G688	U605	G529	U458	U390	A315	U245	A171
G1107	U1041	U827	C759	G689	U606	G530	A459	G391	C316	U246	A172
G1108	C1042	U828	G760	G690	A607	G531	A460	C392	A320	A247	U173
U1112	A1043	G829	A761	G691	A608	A532	U463	A393	A321	G248	A174
U1115	U1044	U830	G765	U692	A609	A533	U464	A394	A322	U249	C175
U1116	C1045	G833	A766	A695	U695	H534	A465	A397	H393	G251	C176
A1117	A1046	U834	A766	A696	U696	A535	A466	U398	A324	G252	G177
U1118	G1047	U834	G769	A696	U697	G537	U467	G399	A325	U252	C178
U1123	U1048	G834	C770	A696	U699	G538	C469	C400	G326	A253	A178
U1124	U1049	C940	A771	A702	A621	A468	C469	C401	A327	G254	U180
U1125	A913	C941	U772	G703	G622	A488	G474	C403	C328	G255	A181
U1126	A918	U842	G773	A704	C623	A489	C475	C404	A329	U256	C182
U1127	A919	U843	G774	G705	C624	A490	C476	G404	C330	G257	A183
U1128	U920	G844	G775	U706	U625	C544	C477	U405	G331	G258	G184
C1084	U921	A845	G776	U707	U626	C545	C478	U406	G332	G259	U185
A1055	U922	G846	G777	C708	U628	C546	A478	U407	G337	A262	A189
U1062	A923	G847	A778	U709	U632	A547	U479	U408	A338	G263	C194
U1062	C924	G847	C779	G710	U633	C549	U480	U409	A339	C264	A195
U1065	C925	G851	A780	G711	G633	C549	C481	G410	C344	G265	A196
C1066	G926	G852	A781	A712	U636	C550	A482	A411	C345	C266	C196
A1067	G927	G858	A782	A713	G637	U551	A483	A412	C346	C267	A197
G1068	C927	G859	C783	G714	C637	U552	C484	A413	C347	U268	G198
C1069	U930	G860	A784	A715	U638	A553	U485	A414	C348	U269	A199
G1070	C931	A861	G785	A716	A642	U554	U486	C418	G348	C269	G206
C1071	C931	G861	G786	U717	C643	U555	U487	C419	G349	A270	C207
G1072	C934	C862	A787	A718	U644	C556	A488	C421	G350	G273	U208
U1073	U938	U863	A788	A719	G645	U557	A489	C422	G351	U274	U209
G1074	A938	A864	A790	C720	U646	A558	C494	C423	C352	A275	C210
C1141	G939	A865	G791	G721	U652	A559	A495	C424	A353	G278	G206
G1077	C940	G866	A792	G722	U653	A559	A496	C425	G354	U279	C207
U1078	U939	G867	U793	U723	U654	A560	A497	C426	C355	C280	U208
G1079	C941	C868	A794	G724	C651	U562	C497	U426	A356	G281	U208
A1080	G945	G869	A795	G725	U655	A563	C498	U427	A357	C282	U209
C1103	A946	U946	C795	A728	U656	C564	A499	U428	U358	A282	C211
A1014	A946	A872	C797	A729	U657	U565	C501	A430	G359	U283	G211

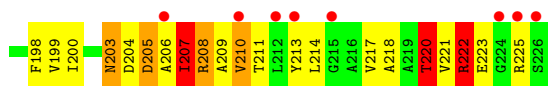


● Molecule 2: 30S ribosomal protein S2

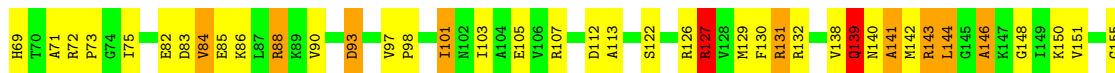
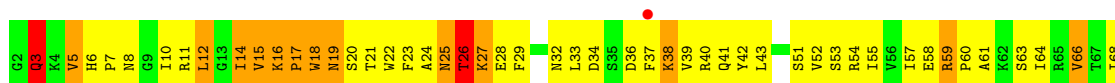


● Molecule 2: 30S ribosomal protein S2

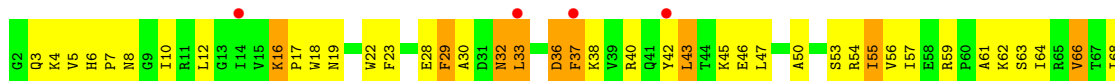




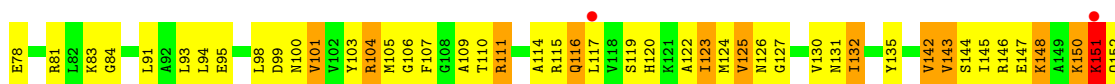
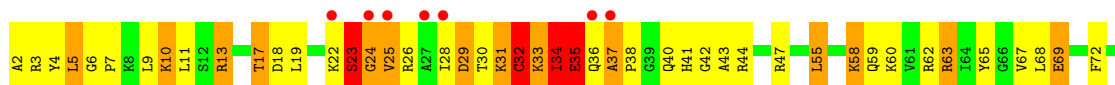
- Molecule 3: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S3

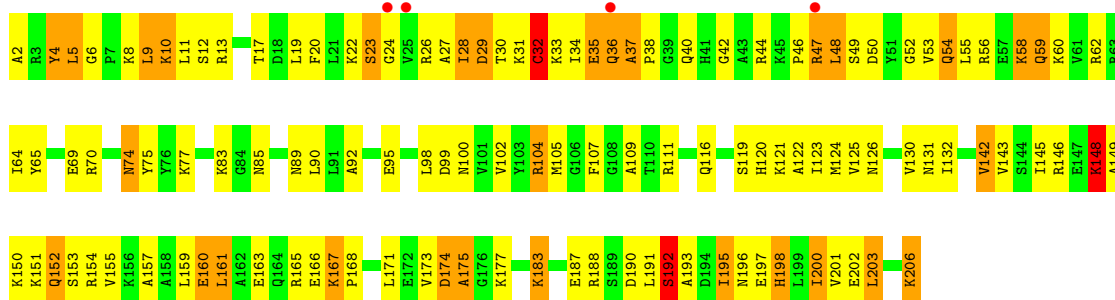


- Molecule 4: 30S ribosomal protein S4

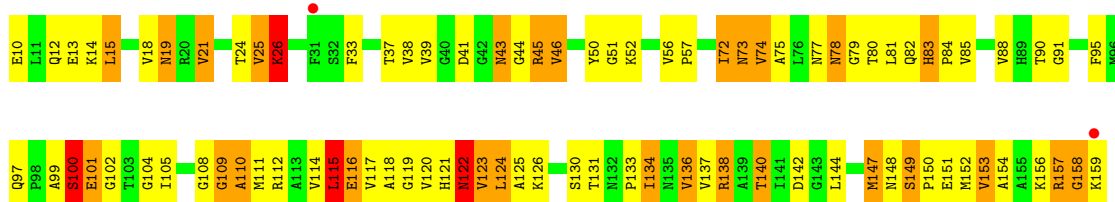


- Molecule 4: 30S ribosomal protein S4

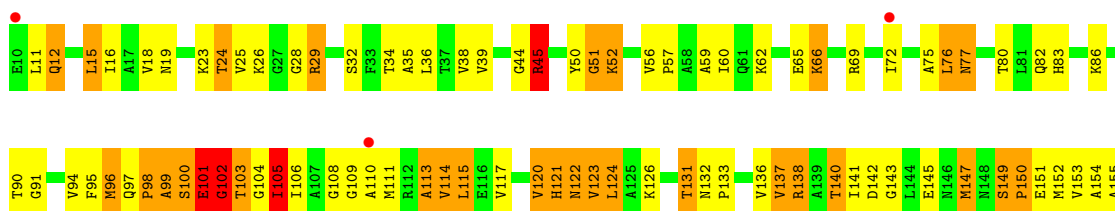




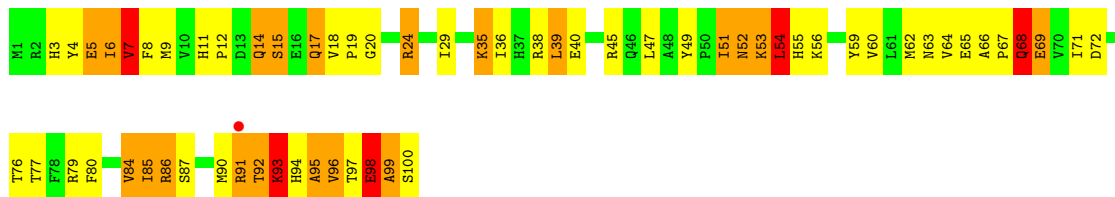
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5

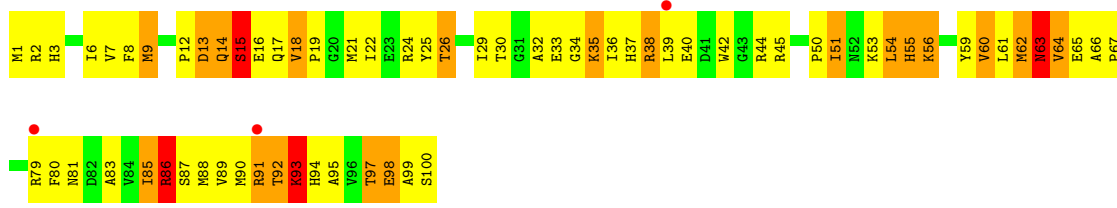


- Molecule 6: 30S ribosomal protein S6

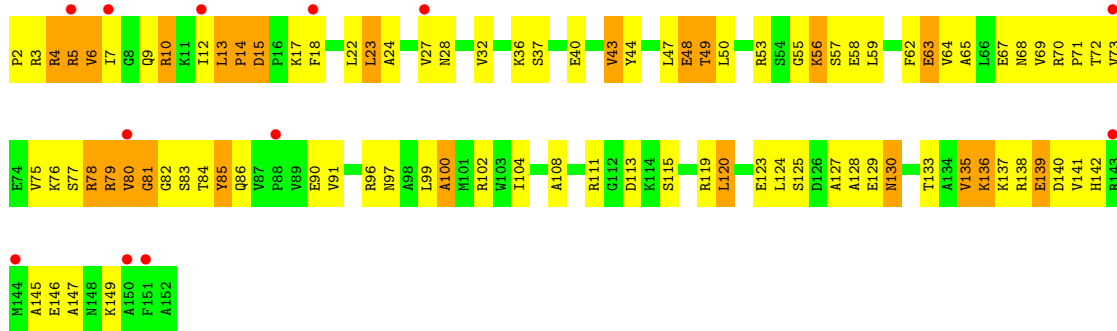


- Molecule 6: 30S ribosomal protein S6

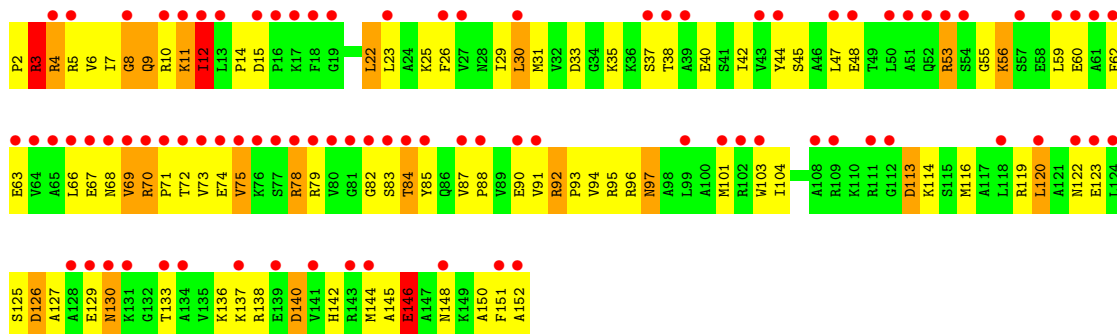




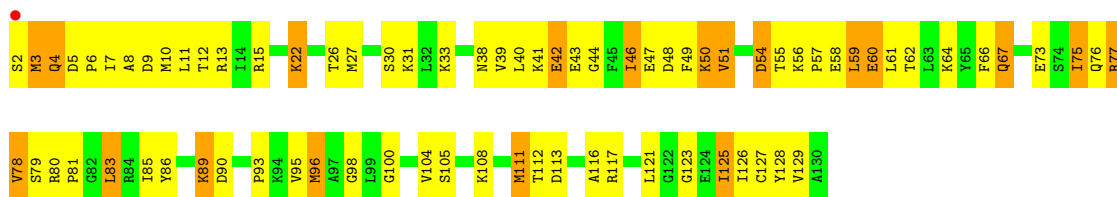
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7

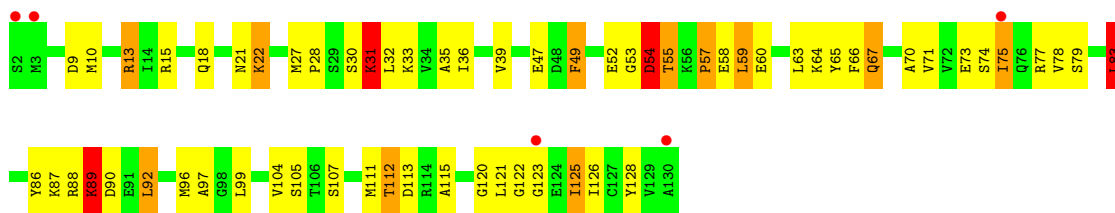


• Molecule 8: 30S ribosomal protein S8

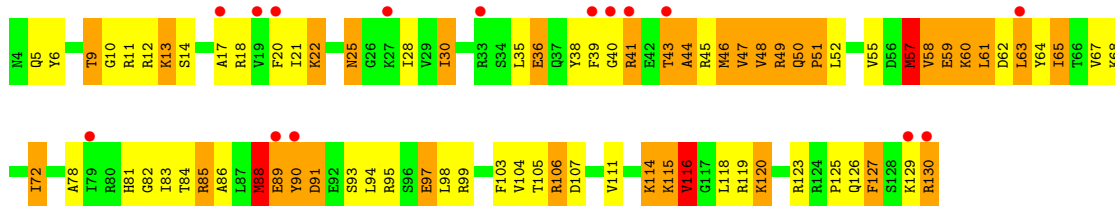


• Molecule 8: 30S ribosomal protein S8

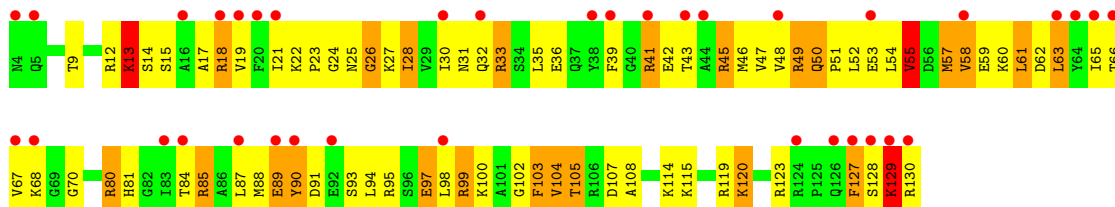
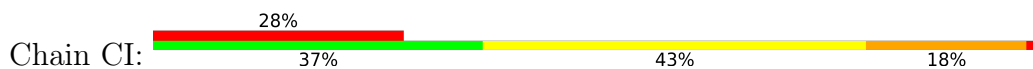




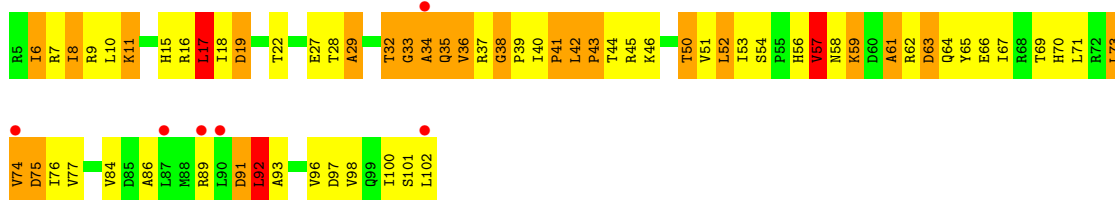
• Molecule 9: 30S ribosomal protein S9



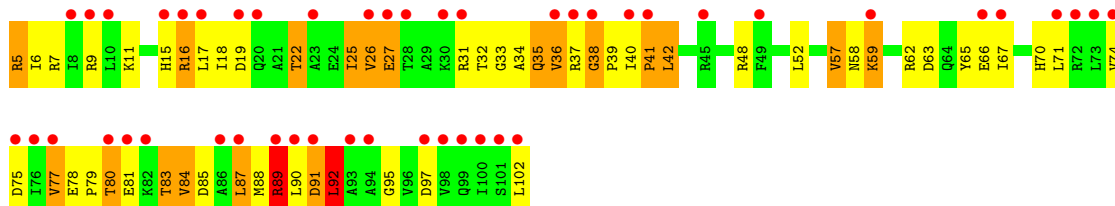
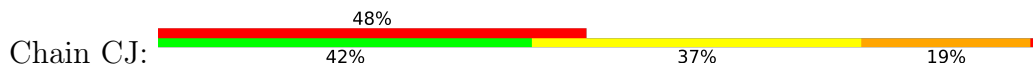
• Molecule 9: 30S ribosomal protein S9



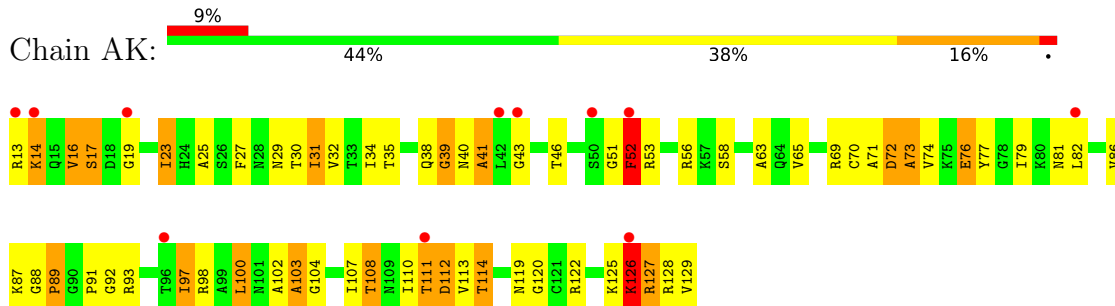
• Molecule 10: 30S ribosomal protein S10



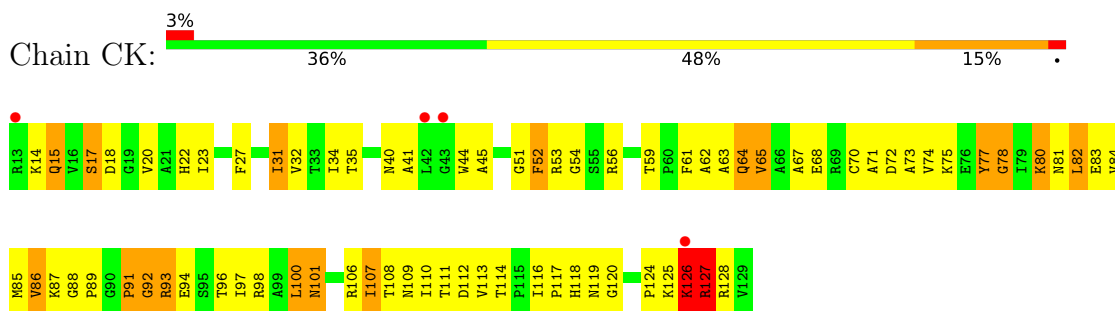
• Molecule 10: 30S ribosomal protein S10



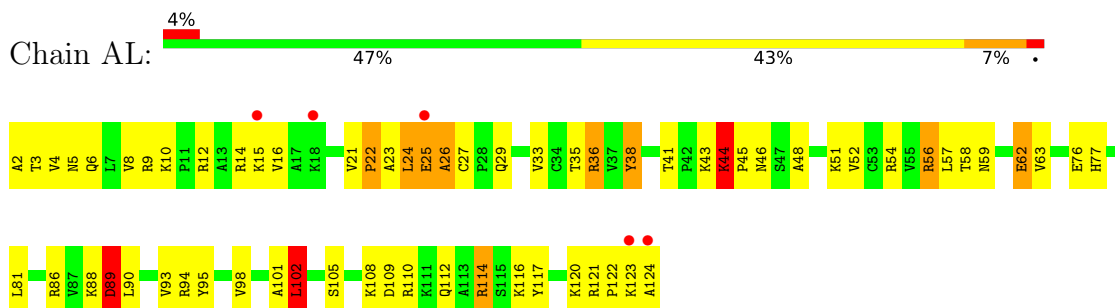
- Molecule 11: 30S ribosomal protein S11



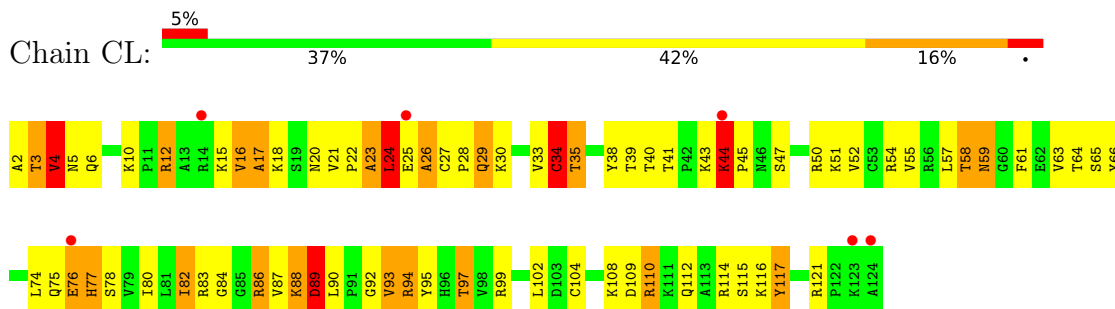
- Molecule 11: 30S ribosomal protein S11



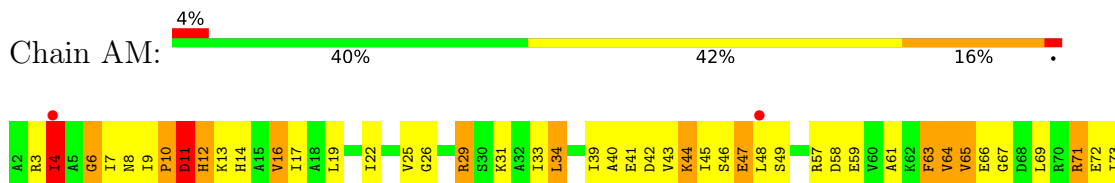
- Molecule 12: 30S ribosomal protein S12

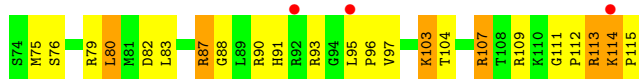


- Molecule 12: 30S ribosomal protein S12

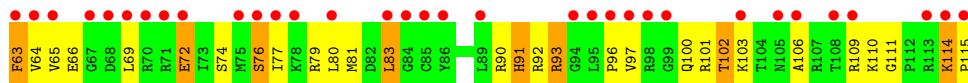
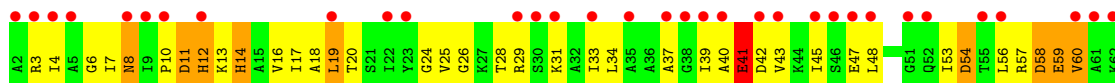
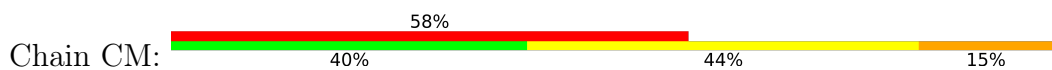


- Molecule 13: 30S ribosomal protein S13

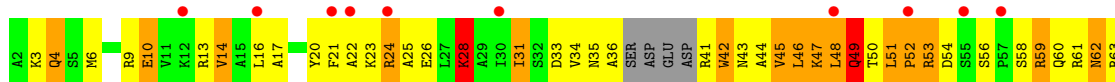




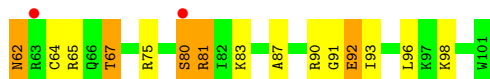
- Molecule 13: 30S ribosomal protein S13



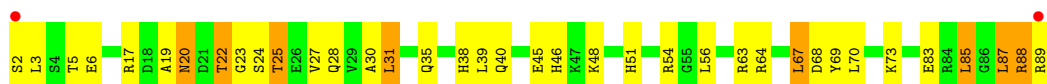
- Molecule 14: 30S ribosomal protein S14



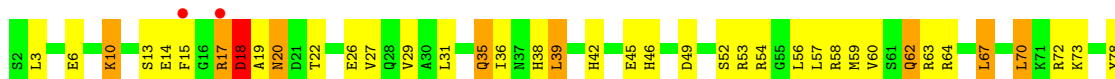
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

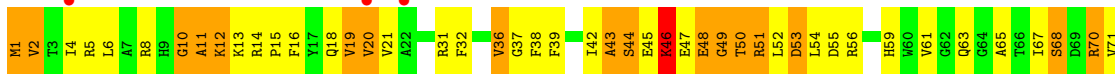


- Molecule 15: 30S ribosomal protein S15

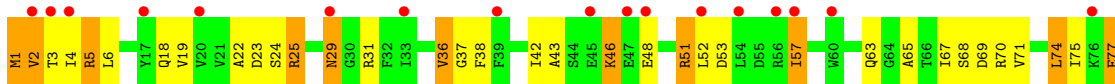




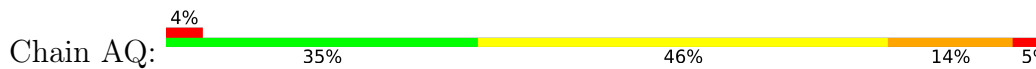
- Molecule 16: 30S ribosomal protein S16



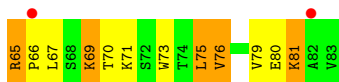
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

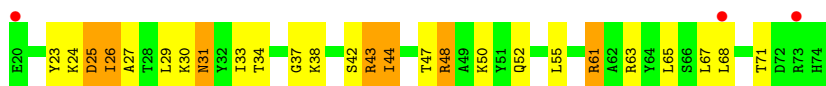


- Molecule 17: 30S ribosomal protein S17

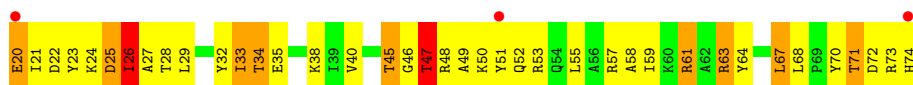


- Molecule 18: 30S ribosomal protein S18

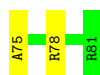




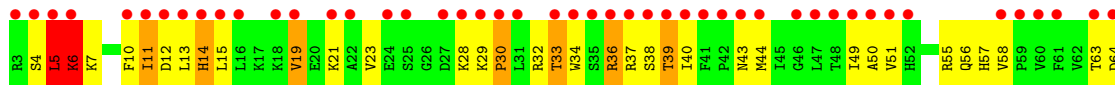
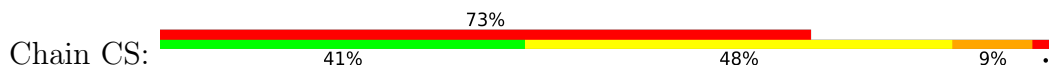
• Molecule 18: 30S ribosomal protein S18



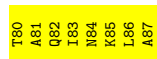
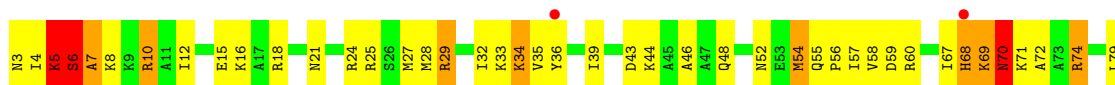
• Molecule 19: 30S ribosomal protein S19



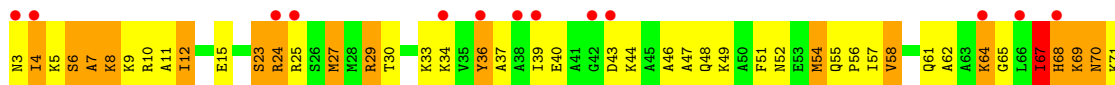
• Molecule 19: 30S ribosomal protein S19

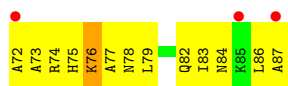


• Molecule 20: 30S ribosomal protein S20

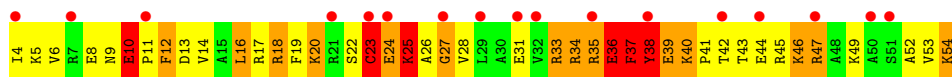
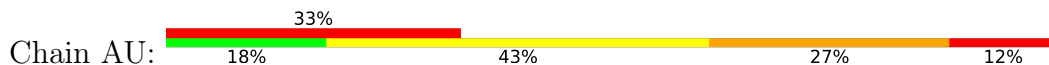


• Molecule 20: 30S ribosomal protein S20

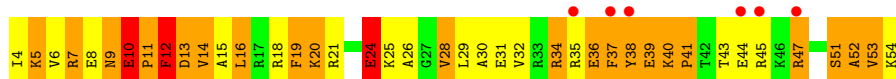
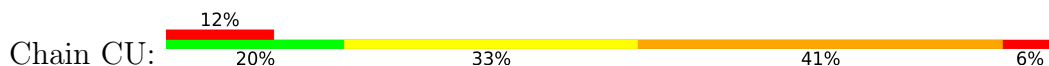




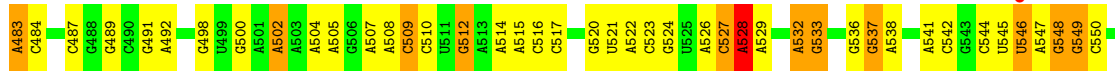
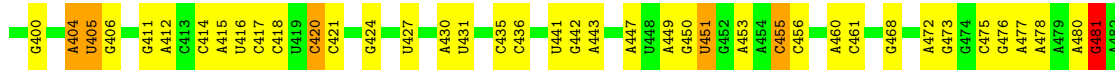
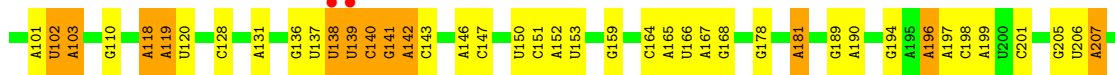
● Molecule 21: 30S ribosomal protein S21

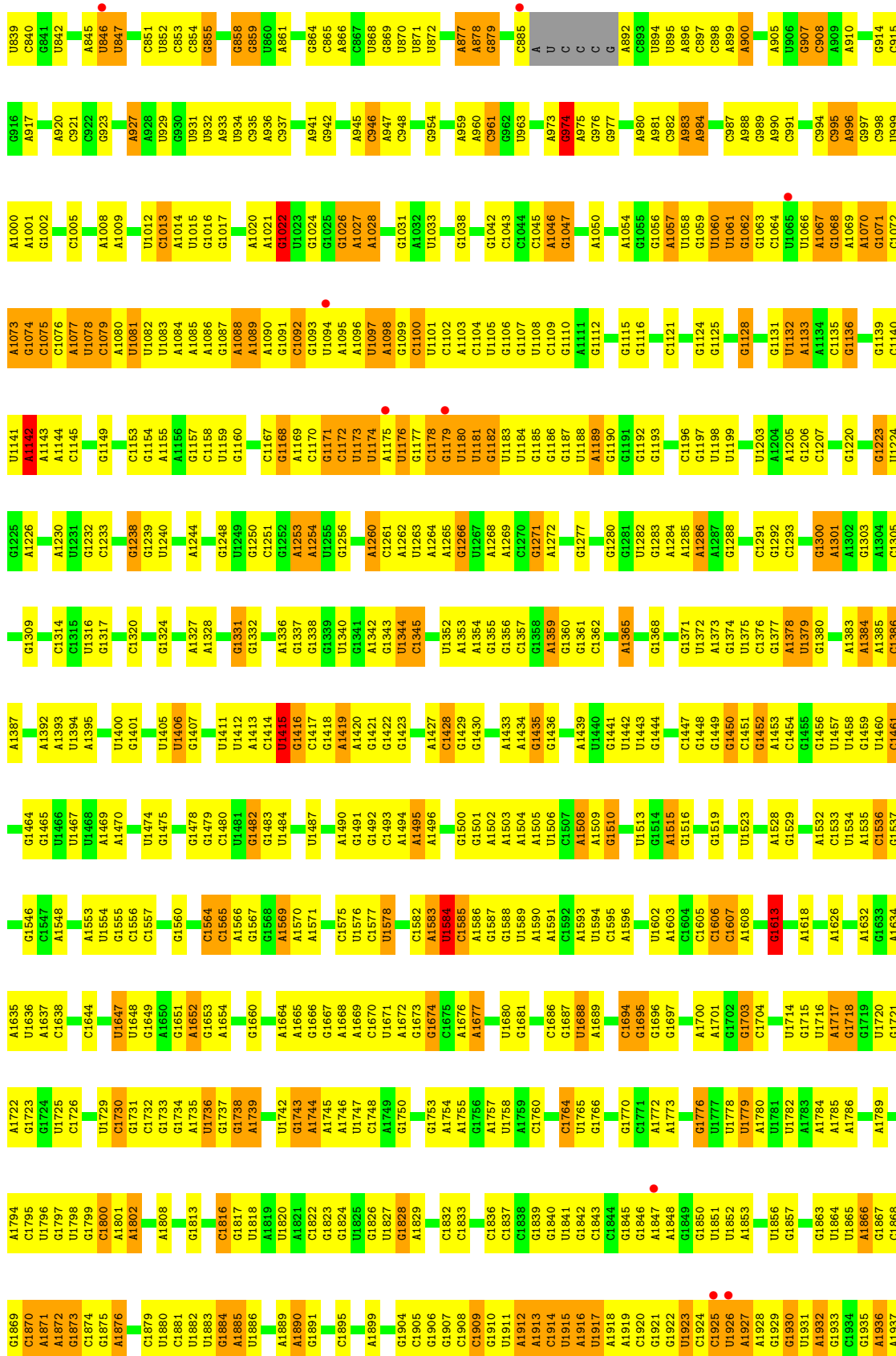


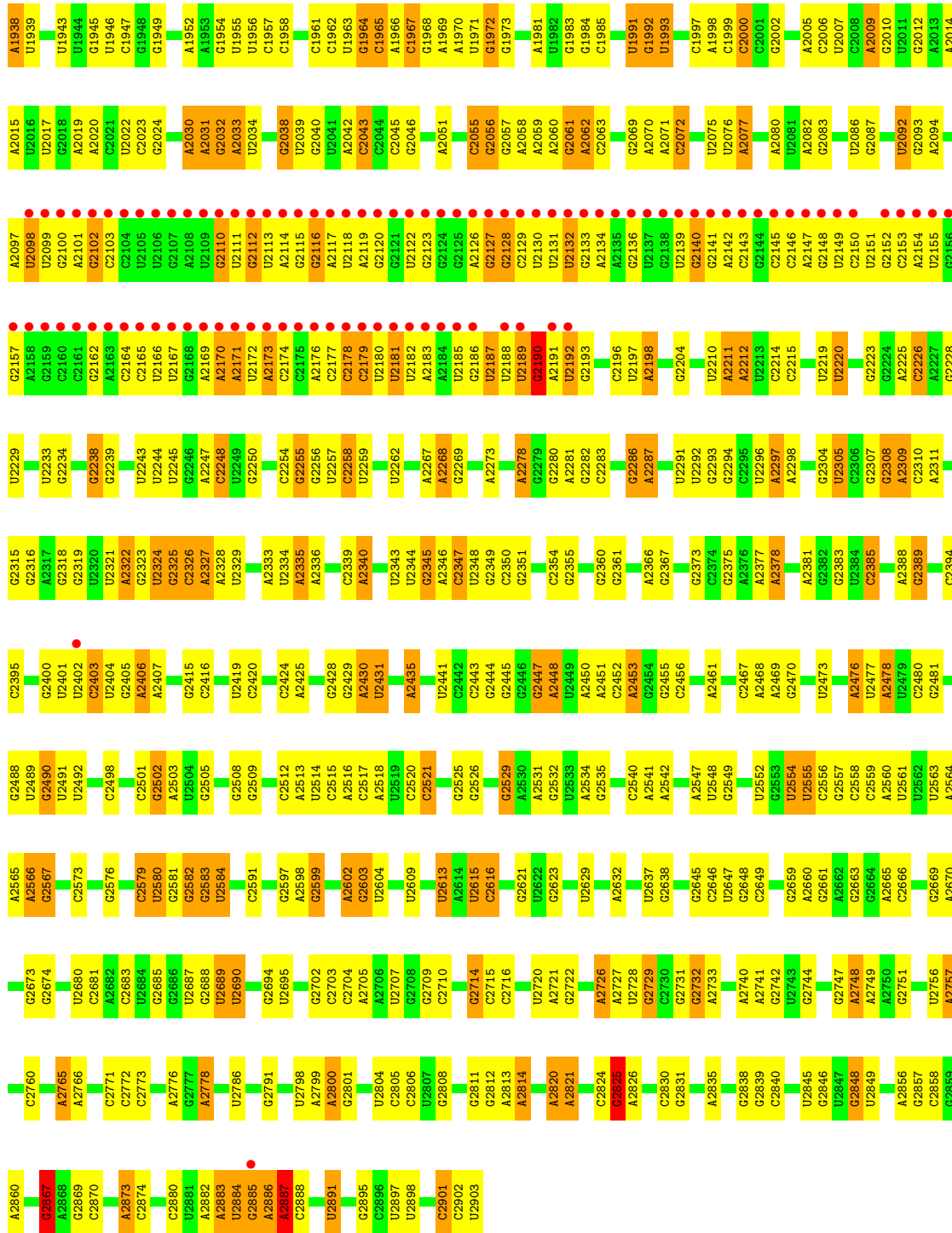
● Molecule 21: 30S ribosomal protein S21



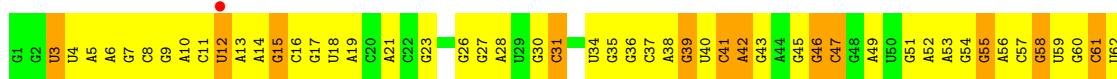
● Molecule 22: 23S rRNA

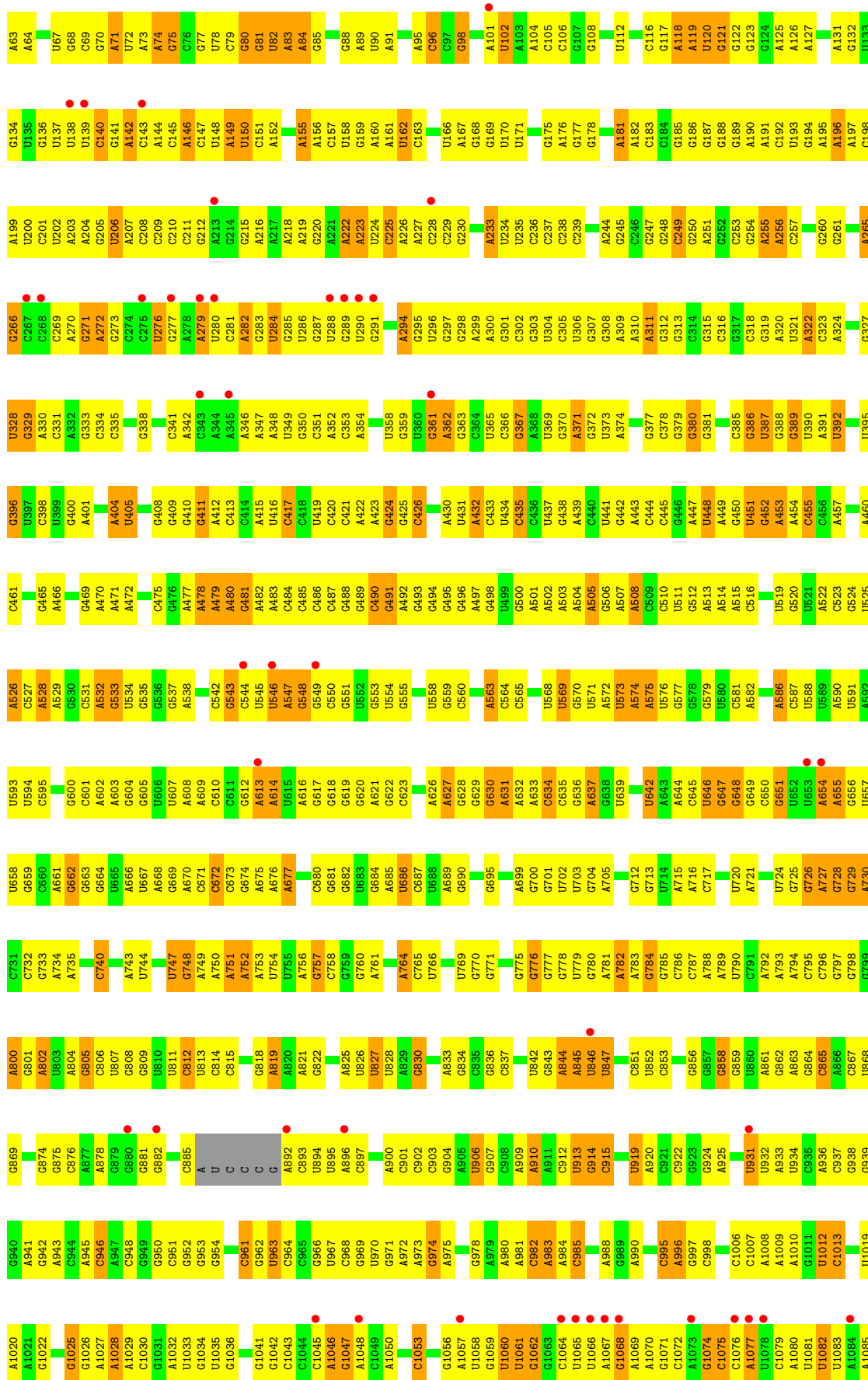


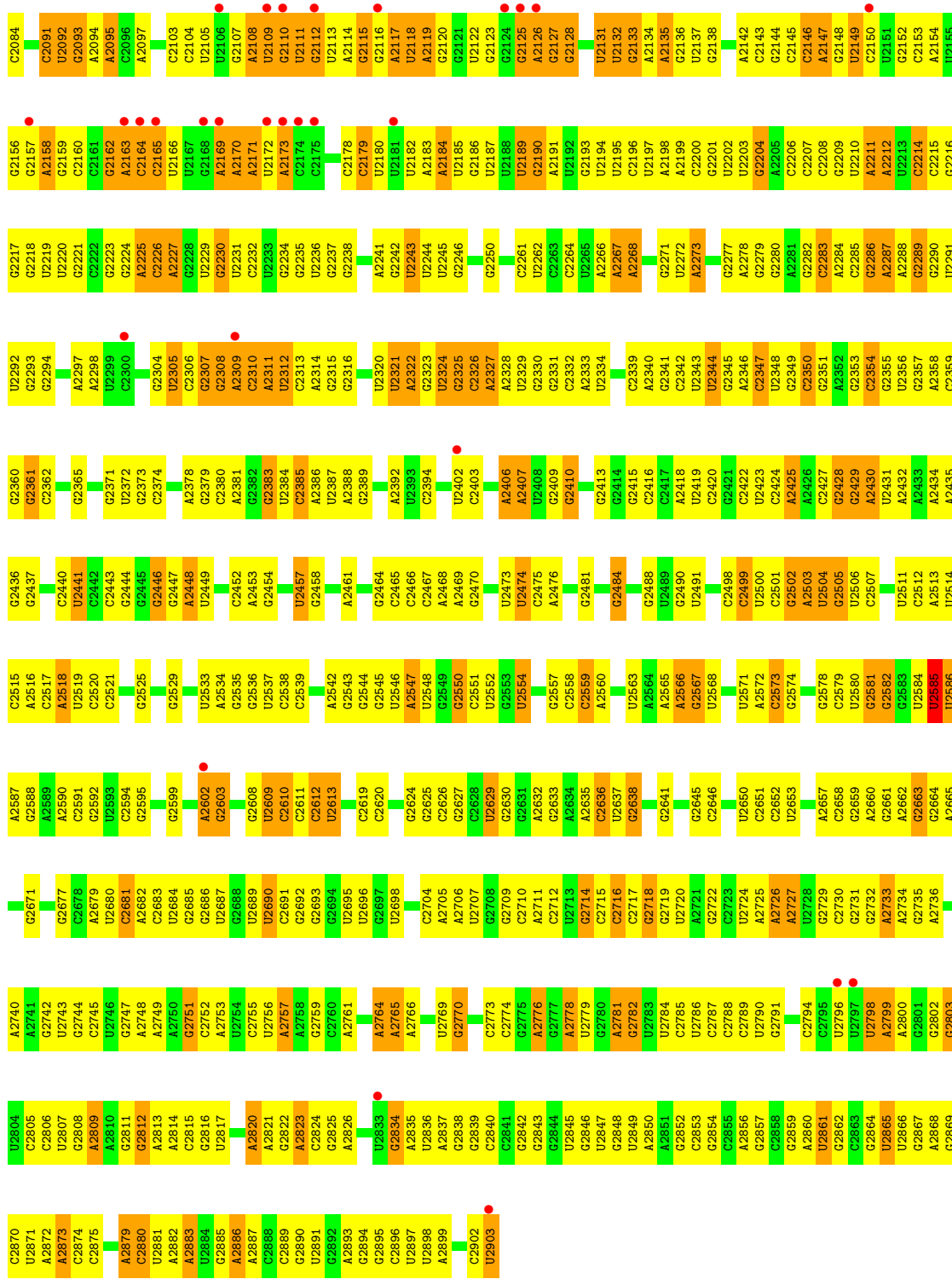




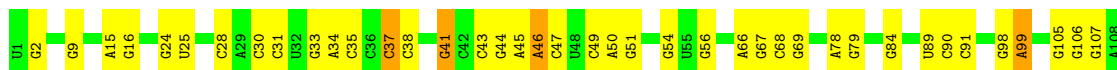
● Molecule 22: 23S rRNA





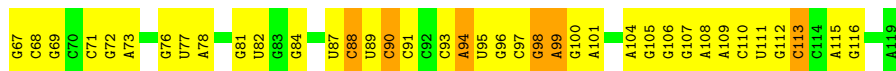
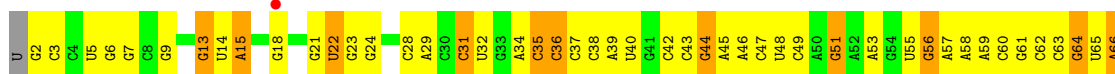


• Molecule 23: 5S rRNA

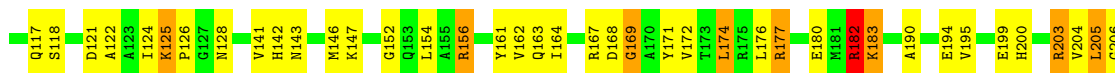
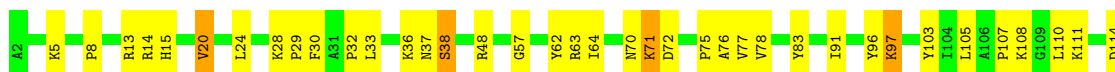




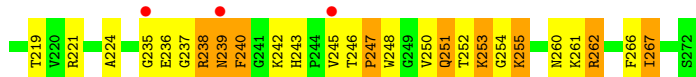
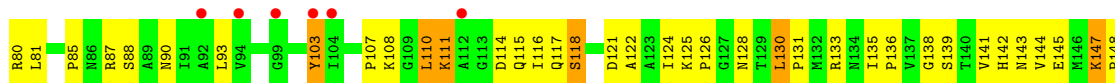
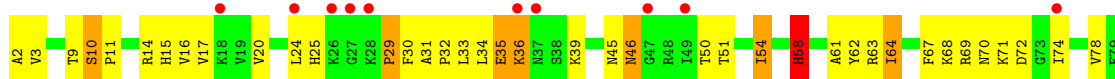
- Molecule 23: 5S rRNA



- Molecule 24: 50S ribosomal protein L2

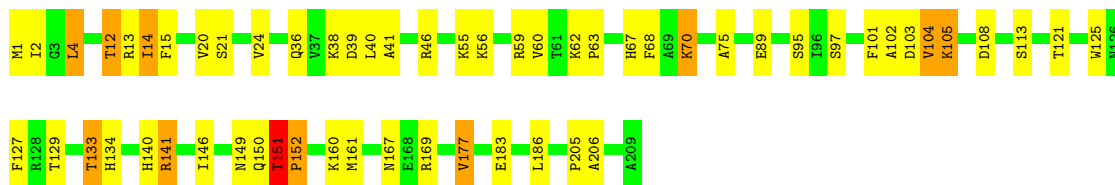


- Molecule 24: 50S ribosomal protein L2

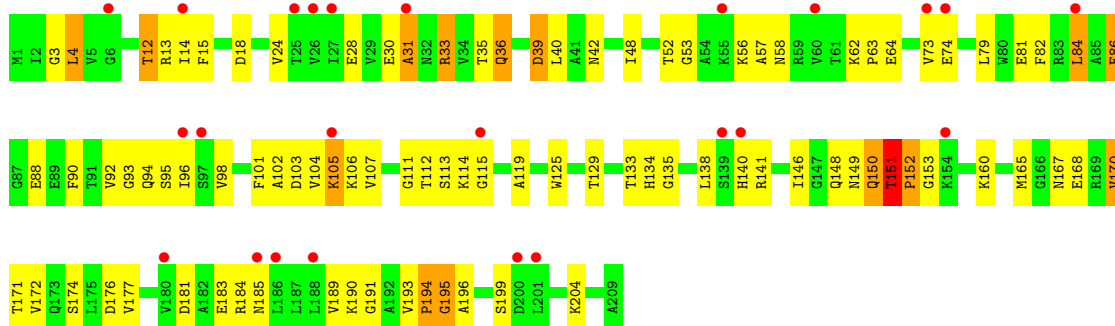


- Molecule 25: 50S ribosomal protein L3

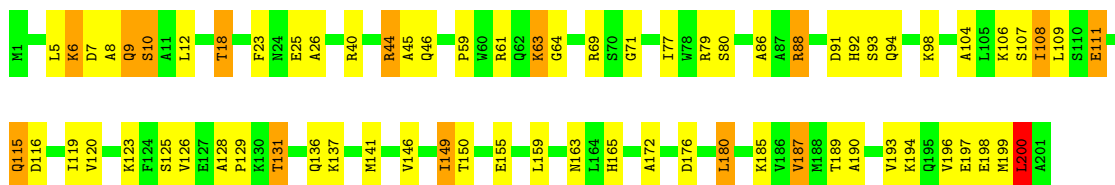




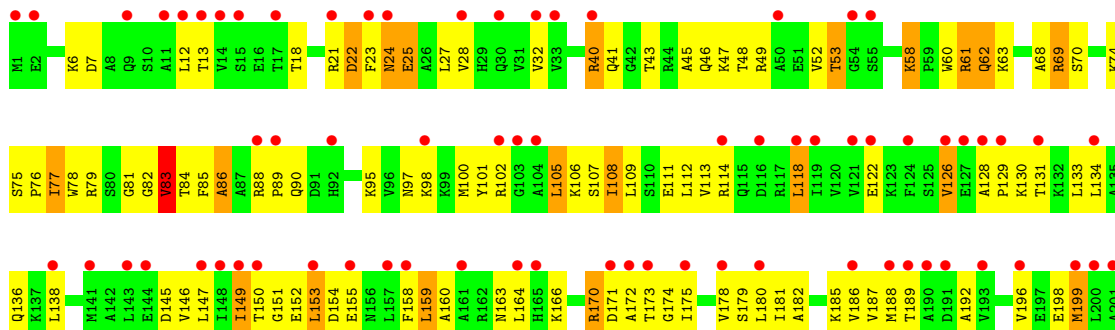
- Molecule 25: 50S ribosomal protein L3



- Molecule 26: 50S ribosomal protein L4

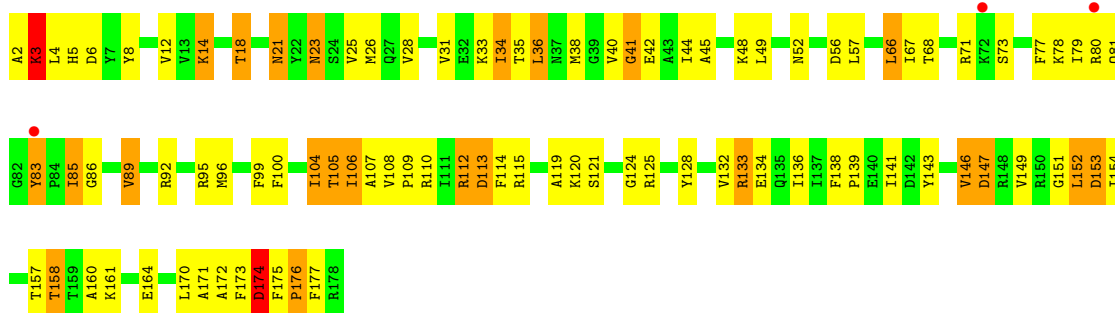


- Molecule 26: 50S ribosomal protein L4

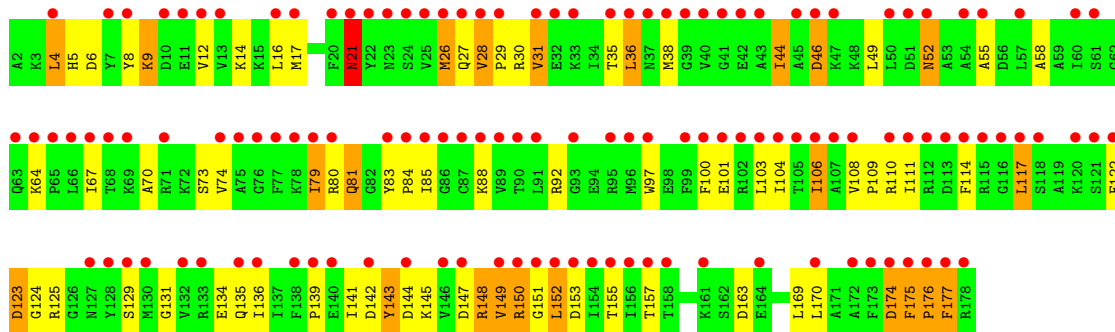
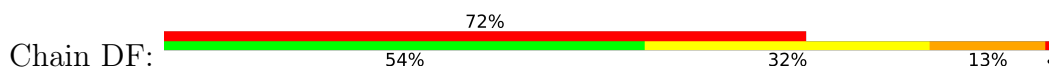


- Molecule 27: 50S ribosomal protein L5

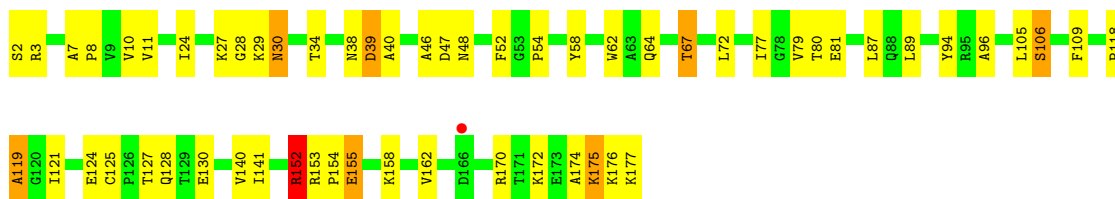




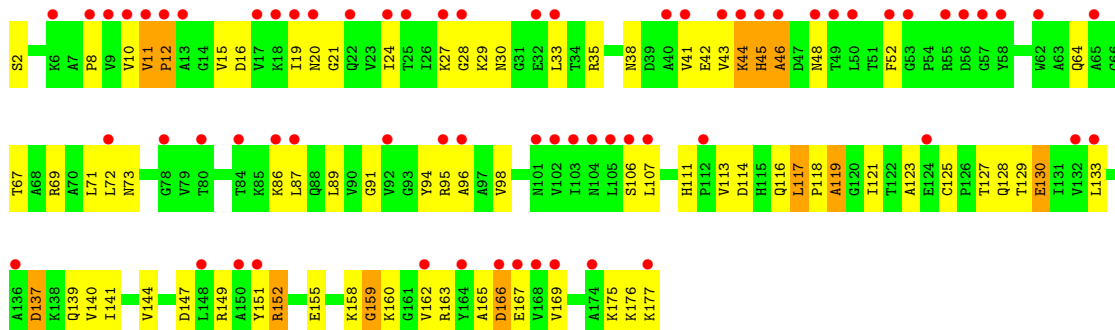
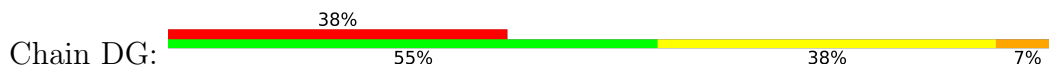
- Molecule 27: 50S ribosomal protein L5



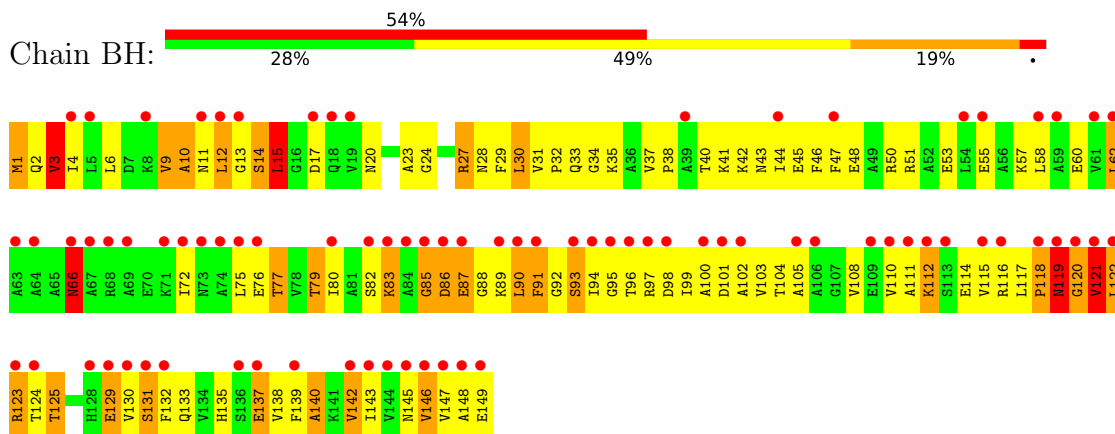
- Molecule 28: 50S ribosomal protein L6



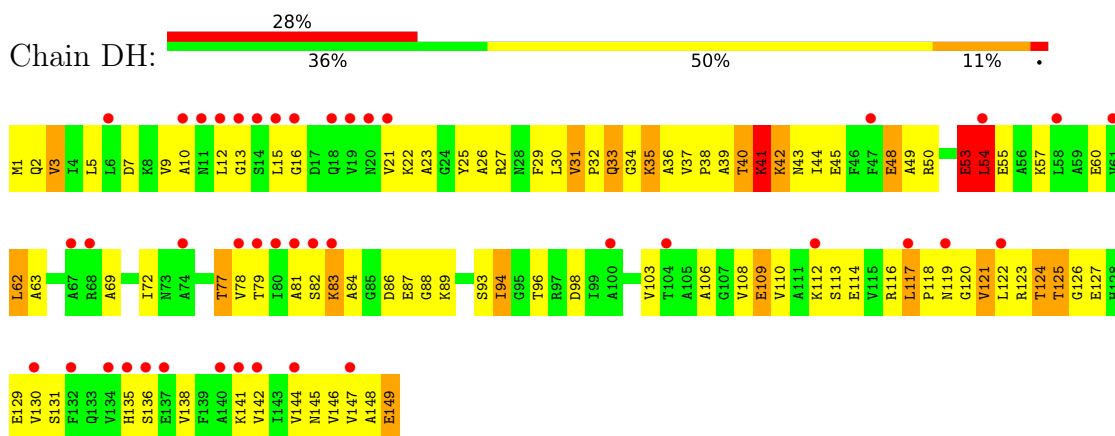
- Molecule 28: 50S ribosomal protein L6



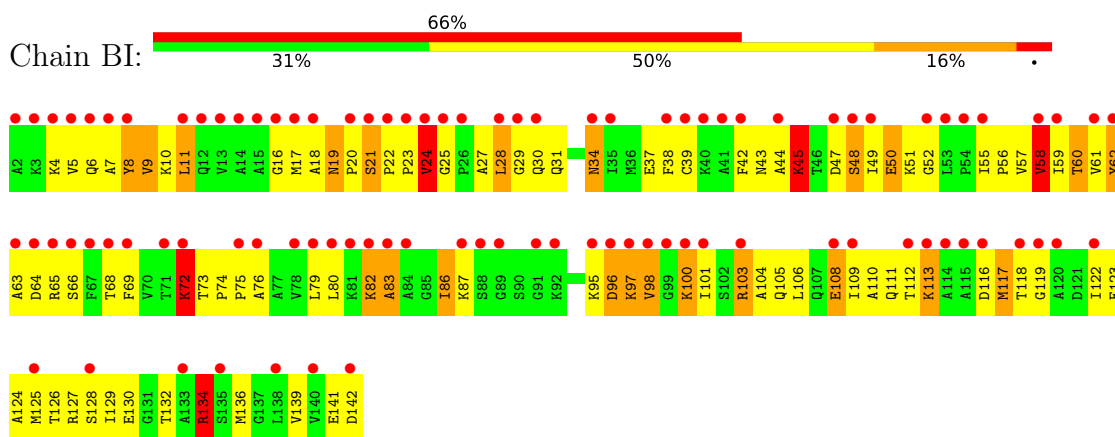
- Molecule 29: 50S ribosomal protein L9



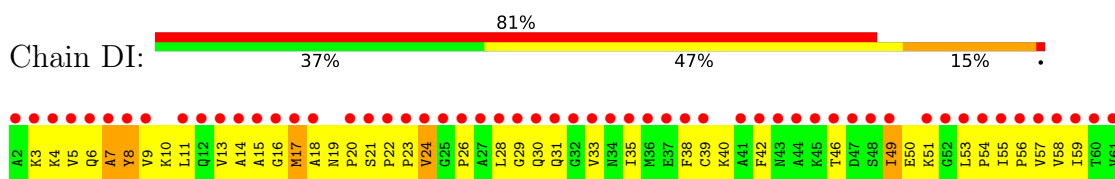
• Molecule 29: 50S ribosomal protein L9

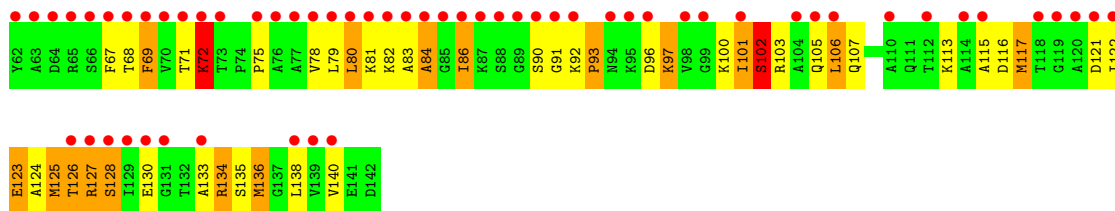


• Molecule 30: 50S ribosomal protein L11

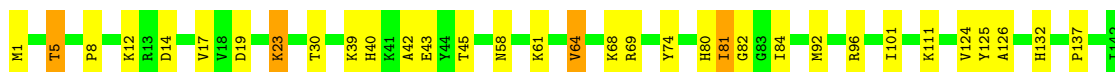
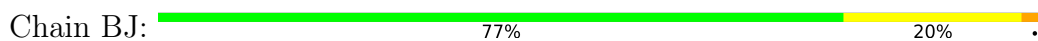


• Molecule 30: 50S ribosomal protein L11

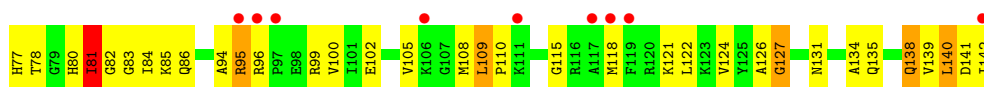




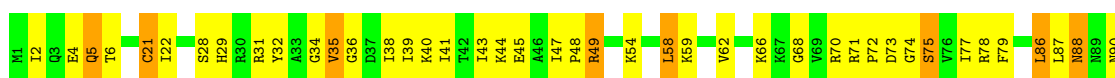
- Molecule 31: 50S ribosomal protein L13



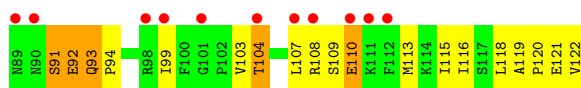
- Molecule 31: 50S ribosomal protein L13



- Molecule 32: 50S ribosomal protein L14



- Molecule 32: 50S ribosomal protein L14

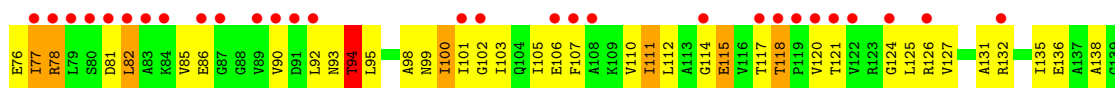


- Molecule 33: 50S ribosomal protein L15

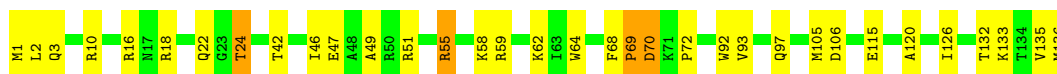
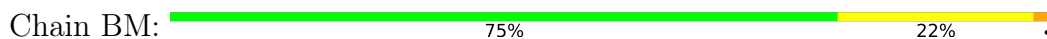




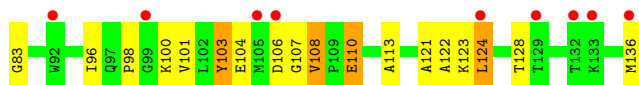
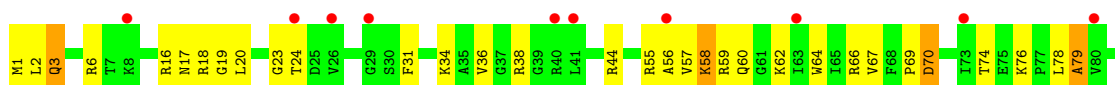
- Molecule 33: 50S ribosomal protein L15



- Molecule 34: 50S ribosomal protein L16



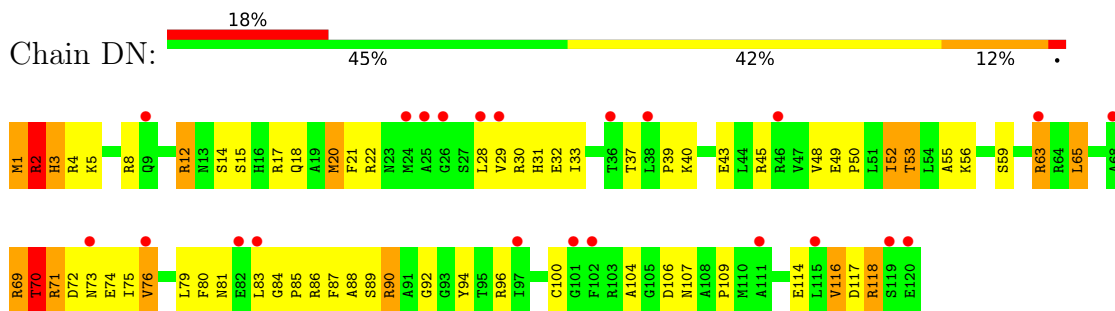
- Molecule 34: 50S ribosomal protein L16



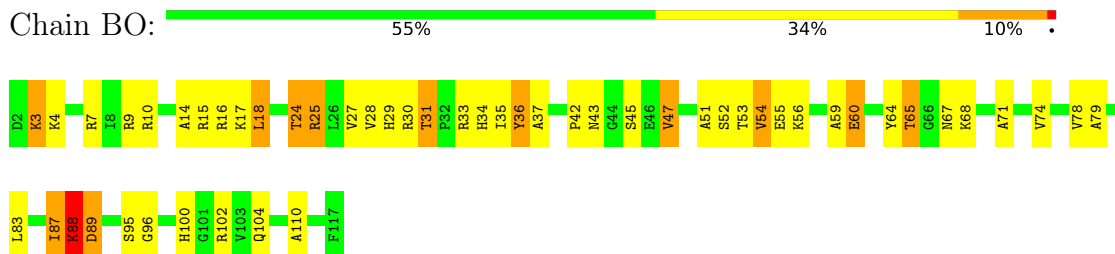
- Molecule 35: 50S ribosomal protein L17



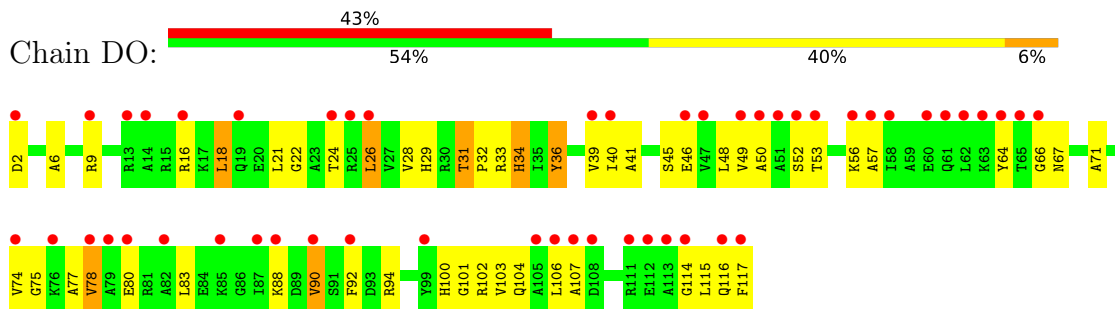
- Molecule 35: 50S ribosomal protein L17



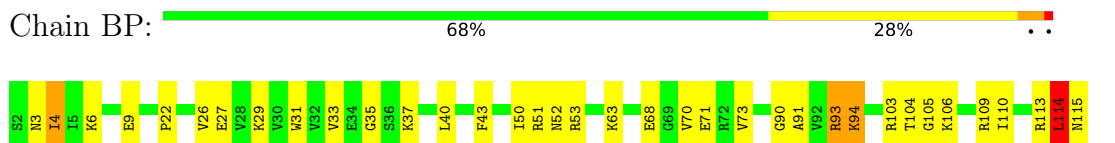
- Molecule 36: 50S ribosomal protein L18



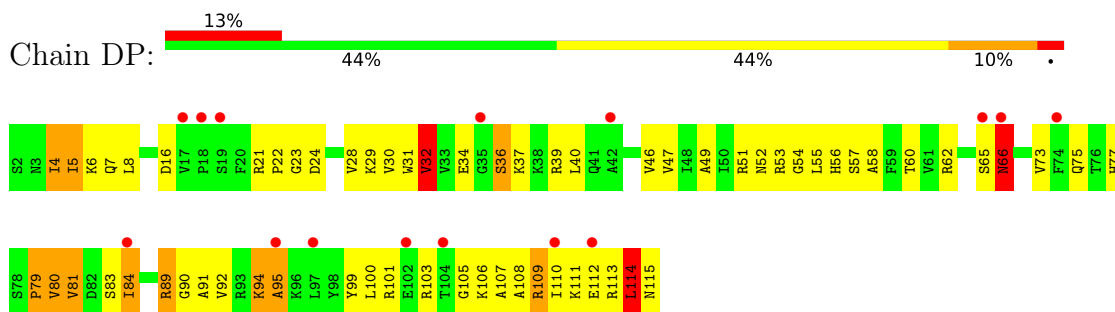
- Molecule 36: 50S ribosomal protein L18



- Molecule 37: 50S ribosomal protein L19

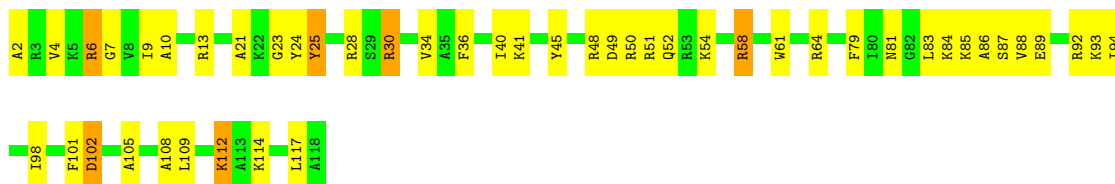


- Molecule 37: 50S ribosomal protein L19



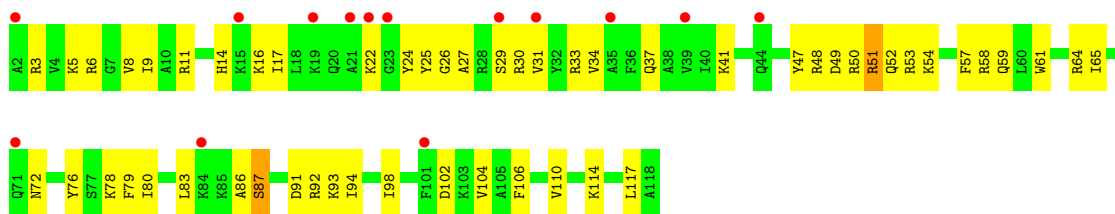
- Molecule 38: 50S ribosomal protein L20

Chain BQ:  59% 36% 5%



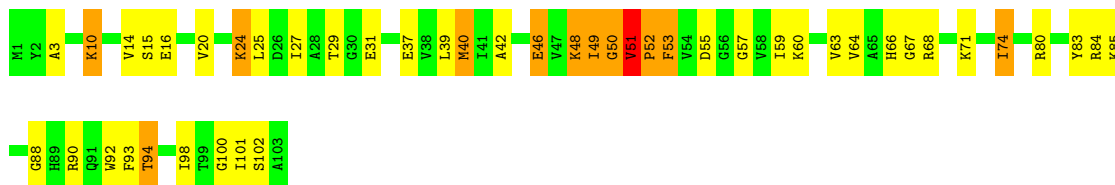
• Molecule 38: 50S ribosomal protein L20

Chain DQ:  12% 54% 44%



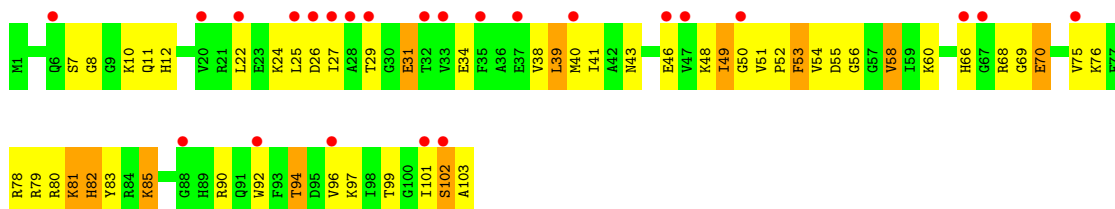
• Molecule 39: 50S ribosomal protein L21

Chain BR:  55% 33% 11%



• Molecule 39: 50S ribosomal protein L21

Chain DR:  23% 50% 40% 11%



• Molecule 40: 50S ribosomal protein L22

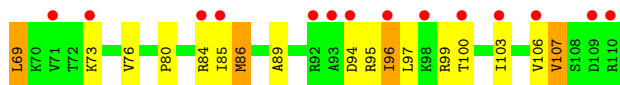
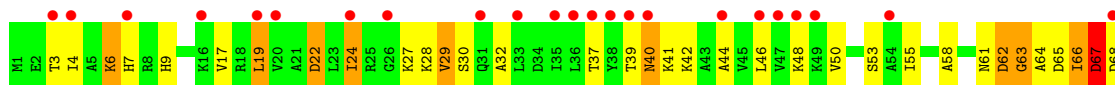
Chain BS:  65% 30% 5%



H110

- Molecule 40: 50S ribosomal protein L22

Chain DS: 



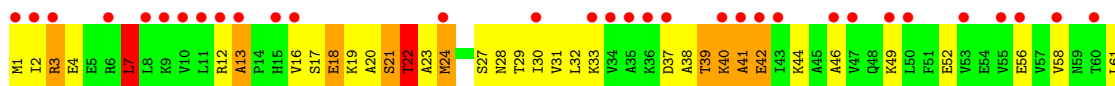
- Molecule 41: 50S ribosomal protein L23

Chain BT: 



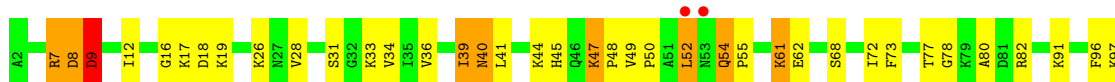
- Molecule 41: 50S ribosomal protein L23

Chain DT: 



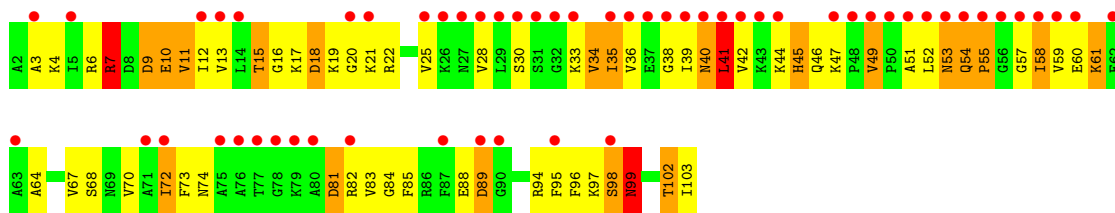
- Molecule 42: 50S ribosomal protein L24

Chain BU: 



- Molecule 42: 50S ribosomal protein L24

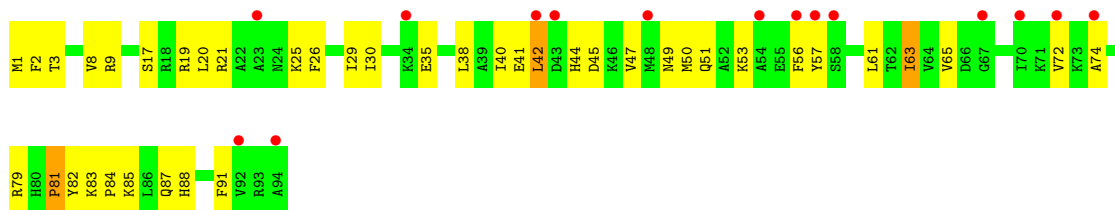
Chain DU: 



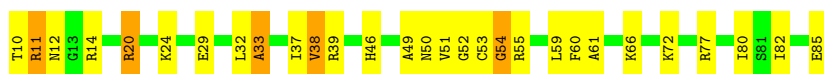
- Molecule 43: 50S ribosomal protein L25



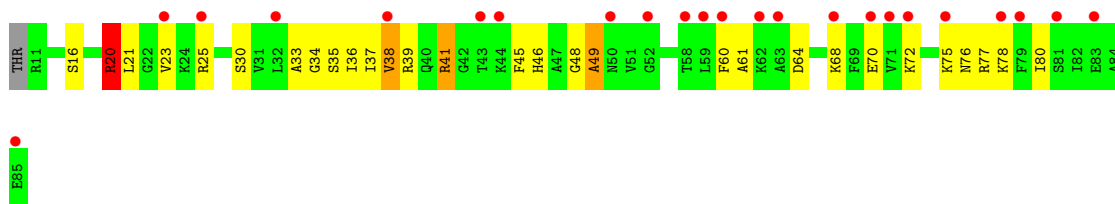
- Molecule 43: 50S ribosomal protein L25



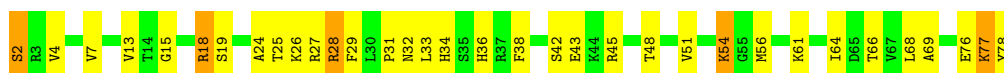
- Molecule 44: 50S ribosomal protein L27



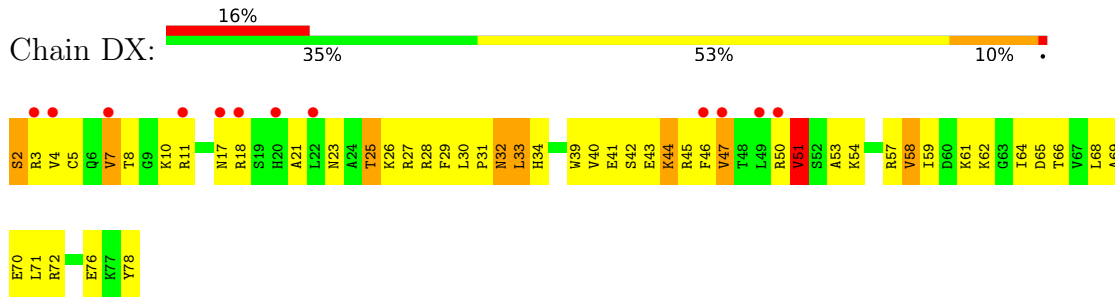
- Molecule 44: 50S ribosomal protein L27



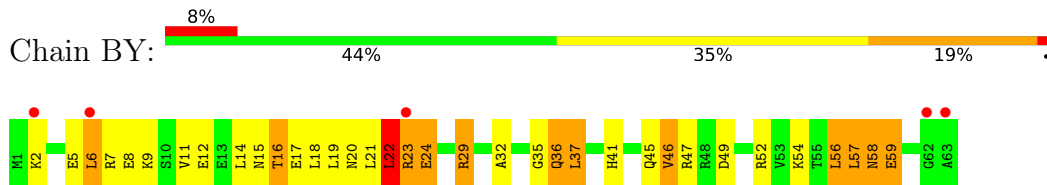
- Molecule 45: 50S ribosomal protein L28



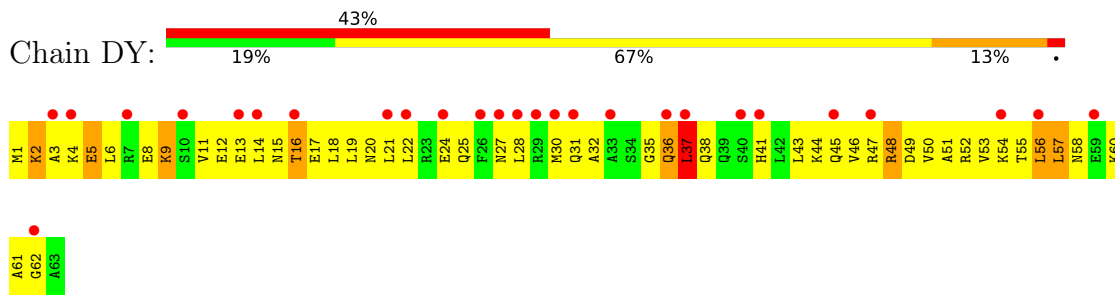
- Molecule 45: 50S ribosomal protein L28



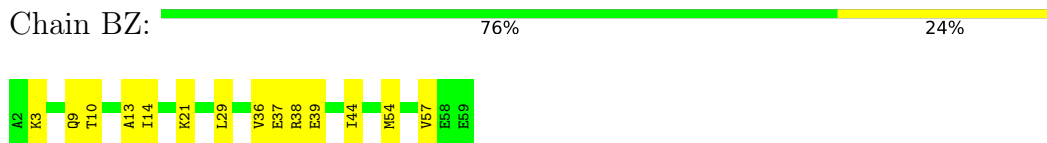
- Molecule 46: 50S ribosomal protein L29



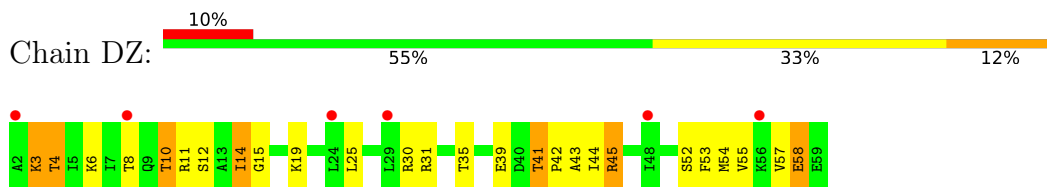
- Molecule 46: 50S ribosomal protein L29



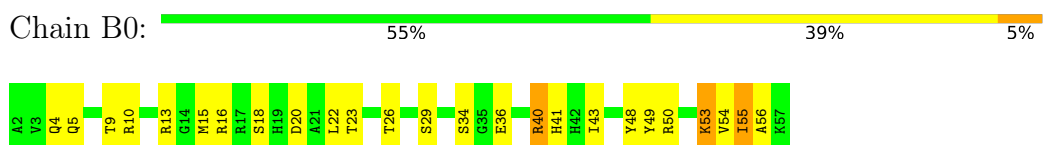
- Molecule 47: 50S ribosomal protein L30



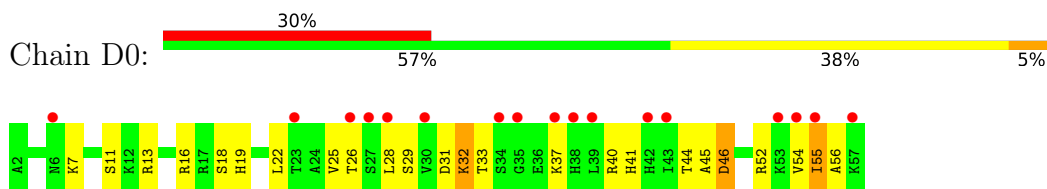
- Molecule 47: 50S ribosomal protein L30



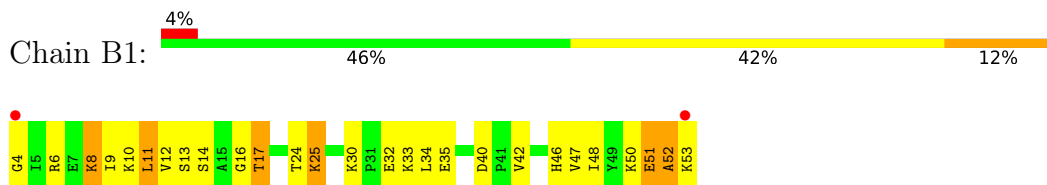
- Molecule 48: 50S ribosomal protein L32



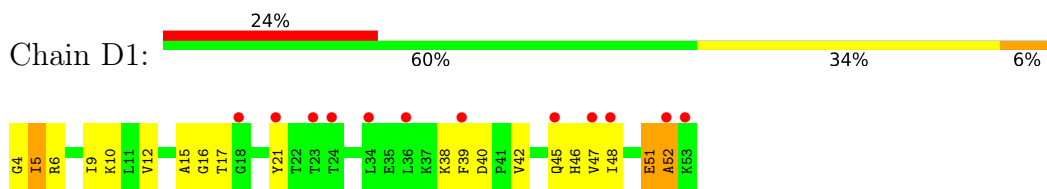
- Molecule 48: 50S ribosomal protein L32



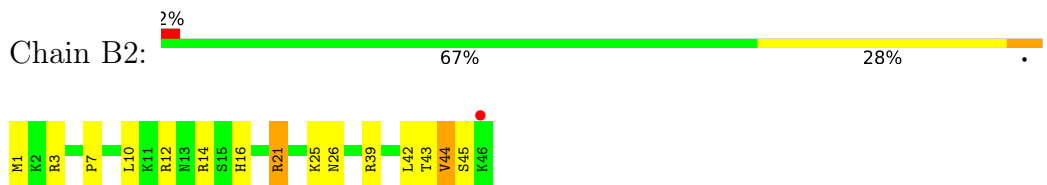
- Molecule 49: 50S ribosomal protein L33



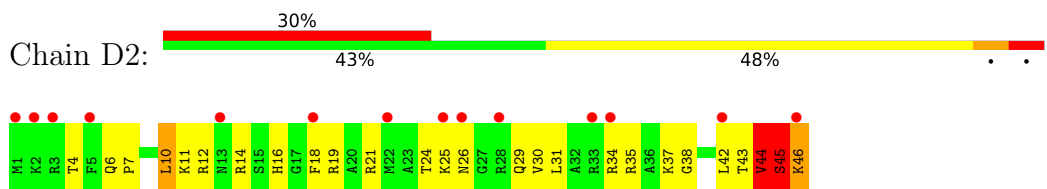
- Molecule 49: 50S ribosomal protein L33



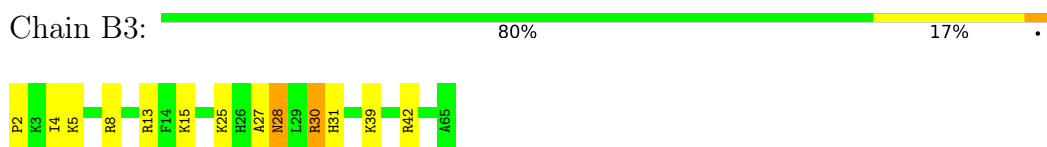
- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34

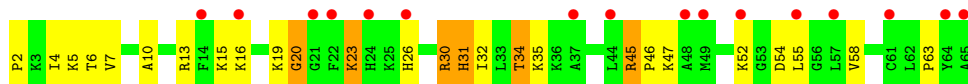


- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35

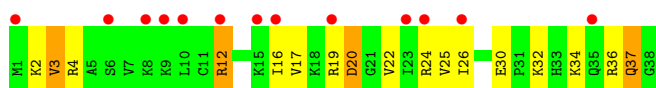




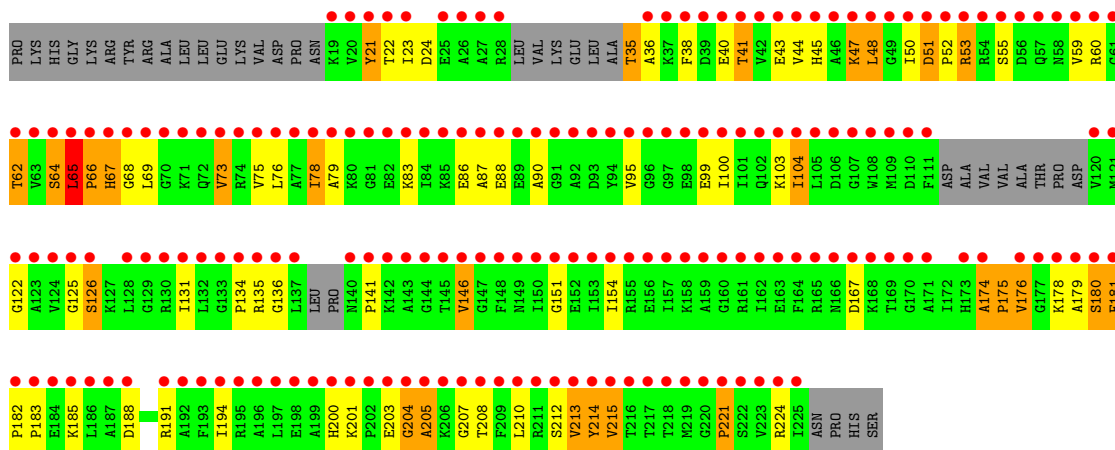
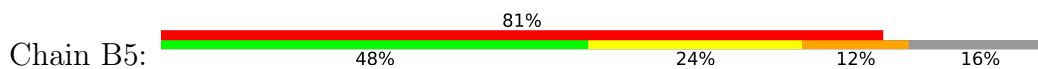
• Molecule 52: 50S ribosomal protein L36



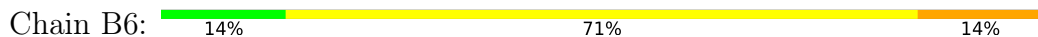
• Molecule 52: 50S ribosomal protein L36



• Molecule 53: 50S ribosomal protein L1



• Molecule 54: Linopristin



• Molecule 54: Linopristin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.97Å 434.65Å 623.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.36 – 2.80 69.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.2 (69.36-2.80) 89.2 (69.36-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.215 , 0.260 0.222 , 0.267	Depositor DCC
R_{free} test set	5006 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtrriage
Anisotropy	0.182	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288396	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: DBB, ZN, VIF, 004, 04X, MG, MHW, MHU

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	0.35	0/36944	0.82	6/57632 (0.0%)
1	CA	0.29	0/36966	0.79	2/57666 (0.0%)
2	AB	0.29	0/1736	0.58	0/2338
2	CB	0.26	0/1736	0.52	0/2338
3	AC	0.28	0/1652	0.54	0/2225
3	CC	0.26	0/1652	0.50	0/2225
4	AD	0.29	0/1665	0.55	0/2227
4	CD	0.32	0/1665	0.57	0/2227
5	AE	0.32	0/1119	0.61	0/1504
5	CE	0.31	0/1119	0.64	0/1504
6	AF	0.31	0/836	0.61	1/1128 (0.1%)
6	CF	0.27	0/836	0.60	1/1128 (0.1%)
7	AG	0.26	0/1196	0.50	0/1602
7	CG	0.26	0/1196	0.50	0/1602
8	AH	0.31	0/989	0.54	0/1326
8	CH	0.26	0/989	0.50	0/1326
9	AI	0.27	0/1034	0.58	0/1375
9	CI	0.27	0/1034	0.54	0/1375
10	AJ	0.29	0/797	0.56	0/1077
10	CJ	0.27	0/797	0.55	0/1077
11	AK	0.28	0/893	0.57	0/1205
11	CK	0.28	0/893	0.58	0/1205
12	AL	0.32	0/969	0.62	0/1300
12	CL	0.30	0/969	0.61	0/1300
13	AM	0.27	0/893	0.56	0/1193
13	CM	0.26	0/893	0.55	0/1193
14	AN	0.29	0/785	0.56	0/1043
14	CN	0.25	0/785	0.48	0/1043
15	AO	0.27	0/718	0.53	0/959
15	CO	0.26	0/718	0.48	0/959
16	AP	0.30	0/659	0.58	0/884
16	CP	0.27	0/659	0.52	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.30	0/658	0.58	0/881
17	CQ	0.29	0/658	0.54	0/881
18	AR	0.27	0/463	0.53	0/621
18	CR	0.28	0/463	0.54	0/621
19	AS	0.29	0/653	0.58	0/877
19	CS	0.28	0/653	0.52	0/877
20	AT	0.30	0/671	0.56	0/888
20	CT	0.26	0/671	0.51	0/888
21	AU	0.35	0/431	0.64	0/570
21	CU	0.35	0/431	0.60	0/570
22	BA	0.60	5/69659 (0.0%)	1.01	98/108672 (0.1%)
22	DA	0.28	0/69659	0.80	8/108672 (0.0%)
23	BB	0.53	0/2850	0.95	0/4444
23	DB	0.24	0/2828	0.79	0/4410
24	BC	0.39	0/2122	0.63	1/2852 (0.0%)
24	DC	0.28	0/2122	0.54	0/2852
25	BD	0.42	0/1586	0.65	1/2134 (0.0%)
25	DD	0.28	0/1586	0.53	0/2134
26	BE	0.38	0/1571	0.60	0/2113
26	DE	0.27	0/1571	0.52	0/2113
27	BF	0.31	0/1435	0.53	0/1926
27	DF	0.26	0/1435	0.48	0/1926
28	BG	0.31	0/1343	0.57	0/1816
28	DG	0.25	0/1343	0.47	0/1816
29	BH	0.36	0/1121	0.66	1/1515 (0.1%)
29	DH	0.35	0/1121	0.56	0/1515
30	BI	0.28	0/1046	0.56	0/1410
30	DI	0.29	0/1046	0.54	0/1410
31	BJ	0.44	0/1152	0.62	0/1551
31	DJ	0.27	0/1152	0.51	0/1551
32	BK	0.44	0/948	0.66	0/1268
32	DK	0.28	0/948	0.51	0/1268
33	BL	0.40	0/1054	0.68	0/1403
33	DL	0.27	0/1054	0.57	0/1403
34	BM	0.43	0/1093	0.64	0/1460
34	DM	0.26	0/1093	0.47	0/1460
35	BN	0.46	0/974	0.68	1/1301 (0.1%)
35	DN	0.27	0/974	0.51	0/1301
36	BO	0.34	0/902	0.59	0/1209
36	DO	0.26	0/902	0.48	0/1209
37	BP	0.39	0/929	0.57	0/1242
37	DP	0.28	0/929	0.53	0/1242
38	BQ	0.48	0/960	0.68	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.27	0/960	0.48	0/1278
39	BR	0.47	0/829	0.73	1/1107 (0.1%)
39	DR	0.27	0/829	0.55	0/1107
40	BS	0.51	0/864	0.69	0/1156
40	DS	0.27	0/864	0.52	0/1156
41	BT	0.35	0/745	0.58	0/994
41	DT	0.27	0/745	0.53	0/994
42	BU	0.36	0/788	0.60	0/1051
42	DU	0.30	0/788	0.55	0/1051
43	BV	0.36	0/766	0.59	0/1025
43	DV	0.25	0/766	0.45	0/1025
44	BW	0.43	0/587	0.63	0/776
44	DW	0.26	0/576	0.48	0/762
45	BX	0.35	0/635	0.59	0/848
45	DX	0.28	0/635	0.52	0/848
46	BY	0.32	0/510	0.60	0/677
46	DY	0.26	0/510	0.54	0/677
47	BZ	0.46	0/453	0.60	0/605
47	DZ	0.26	0/453	0.52	0/605
48	B0	0.43	0/450	0.63	0/599
48	D0	0.29	0/450	0.55	0/599
49	B1	0.35	0/417	0.56	0/554
49	D1	0.27	0/417	0.48	0/554
50	B2	0.45	0/380	0.71	0/498
50	D2	0.29	0/380	0.52	0/498
51	B3	0.39	0/513	0.61	0/676
51	D3	0.26	0/513	0.48	0/676
52	B4	0.46	0/303	0.72	0/397
52	D4	0.25	0/303	0.50	0/397
53	B5	0.26	0/1145	0.50	0/1556
54	B6	4.15	4/13 (30.8%)	3.77	4/15 (26.7%)
54	D6	3.89	4/13 (30.8%)	3.55	1/15 (6.7%)
All	All	0.40	13/310652 (0.0%)	0.81	126/464396 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	CE	0	1
6	CF	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	AK	0	1
12	AL	0	1
12	CL	0	1
21	AU	0	1
21	CU	0	1
24	BC	0	1
25	BD	0	1
25	DD	0	1
All	All	0	10

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-10.72	1.31	1.37
22	BA	984	A	N9-C4	-9.17	1.32	1.37
22	BA	1936	A	N9-C4	-7.33	1.33	1.37
22	BA	974	G	N9-C8	6.97	1.42	1.37
54	B6	2	THR	CB-OG1	-6.86	1.29	1.43

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	984	A	C2-N3-C4	-10.54	105.33	110.60
22	BA	1142	A	C2-N3-C4	-9.69	105.75	110.60
22	BA	1142	A	N3-C4-C5	9.46	133.42	126.80
22	BA	984	A	N3-C4-C5	9.37	133.36	126.80
22	BA	974	G	C4-C5-N7	9.29	114.51	110.80

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
12	AL	38	TYR	Peptide
21	AU	39	GLU	Peptide
24	BC	232	HIS	Peptide
25	BD	151	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	1047	0
1	CA	33015	0	16617	1004	0
2	AB	1705	0	1732	177	0
2	CB	1705	0	1732	125	0
3	AC	1625	0	1696	75	0
3	CC	1625	0	1696	64	0
4	AD	1643	0	1707	134	0
4	CD	1643	0	1707	121	0
5	AE	1106	0	1148	75	0
5	CE	1106	0	1148	101	0
6	AF	818	0	808	60	0
6	CF	818	0	808	56	0
7	AG	1182	0	1238	58	0
7	CG	1182	0	1238	54	0
8	AH	979	0	1031	74	0
8	CH	979	0	1031	42	0
9	AI	1022	0	1070	82	0
9	CI	1022	0	1070	70	0
10	AJ	787	0	828	69	0
10	CJ	787	0	828	59	0
11	AK	877	0	887	66	0
11	CK	877	0	887	65	0
12	AL	955	0	1016	61	0
12	CL	955	0	1016	72	0
13	AM	884	0	941	61	0
13	CM	884	0	941	49	0
14	AN	774	0	824	59	0
14	CN	774	0	824	45	0
15	AO	710	0	728	27	0
15	CO	710	0	728	31	0
16	AP	649	0	666	60	0
16	CP	649	0	666	29	0
17	AQ	649	0	691	65	0
17	CQ	649	0	691	59	0
18	AR	456	0	478	17	0
18	CR	456	0	478	40	0
19	AS	638	0	665	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	638	0	665	37	0
20	AT	665	0	714	50	0
20	CT	665	0	714	46	0
21	AU	426	0	449	49	0
21	CU	426	0	449	59	0
22	BA	62195	0	31280	1407	0
22	DA	62195	0	31280	2116	0
23	BB	2549	0	1291	30	0
23	DB	2529	0	1281	80	0
24	BC	2083	0	2154	82	0
24	DC	2083	0	2154	116	0
25	BD	1565	0	1616	52	0
25	DD	1565	0	1616	80	0
26	BE	1552	0	1619	46	0
26	DE	1552	0	1619	79	0
27	BF	1411	0	1444	89	0
27	DF	1411	0	1444	55	0
28	BG	1323	0	1371	43	0
28	DG	1323	0	1371	54	0
29	BH	1110	0	1147	151	0
29	DH	1110	0	1148	87	0
30	BI	1032	0	1085	81	0
30	DI	1032	0	1085	78	0
31	BJ	1129	0	1162	22	0
31	DJ	1129	0	1162	52	0
32	BK	939	0	1012	48	0
32	DK	939	0	1012	42	0
33	BL	1045	0	1117	55	0
33	DL	1045	0	1117	66	0
34	BM	1074	0	1157	25	0
34	DM	1074	0	1157	35	0
35	BN	961	0	1000	46	0
35	DN	961	0	1000	58	0
36	BO	892	0	923	37	0
36	DO	892	0	923	39	0
37	BP	917	0	962	28	0
37	DP	917	0	962	47	0
38	BQ	947	0	1019	39	0
38	DQ	947	0	1019	47	0
39	BR	816	0	839	56	0
39	DR	816	0	839	46	0
40	BS	857	0	922	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DS	857	0	922	40	0
41	BT	739	0	807	37	0
41	DT	739	0	807	47	0
42	BU	780	0	831	27	0
42	DU	780	0	831	64	0
43	BV	753	0	780	20	0
43	DV	753	0	780	27	0
44	BW	580	0	594	18	0
44	DW	569	0	581	25	0
45	BX	625	0	652	22	0
45	DX	625	0	652	45	0
46	BY	509	0	543	35	0
46	DY	509	0	543	45	0
47	BZ	449	0	488	9	0
47	DZ	449	0	488	13	0
48	B0	444	0	458	23	0
48	D0	444	0	458	18	0
49	B1	410	0	440	22	0
49	D1	410	0	440	11	0
50	B2	377	0	418	17	0
50	D2	377	0	418	24	0
51	B3	504	0	572	12	0
51	D3	504	0	572	27	0
52	B4	302	0	340	23	0
52	D4	302	0	340	15	0
53	B5	1142	0	865	52	0
54	B6	69	0	60	1	0
54	D6	69	0	61	20	0
55	AA	72	0	0	0	0
55	BA	193	0	0	0	0
55	BB	4	0	0	0	0
55	BD	1	0	0	0	0
55	BQ	1	0	0	0	0
55	CA	56	0	0	0	0
55	D2	1	0	0	0	0
55	DA	167	0	0	0	0
55	DB	3	0	0	0	0
56	BA	38	0	38	2	0
56	DA	38	0	37	11	0
57	B4	1	0	0	0	0
57	D4	1	0	0	0	0
58	AA	193	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	AL	2	0	0	0	0
58	AN	5	0	0	0	0
58	AT	2	0	0	0	0
58	AU	1	0	0	0	0
58	B2	1	0	0	0	0
58	B3	2	0	0	0	0
58	B4	2	0	0	0	0
58	BA	623	0	0	64	0
58	BB	14	0	0	0	0
58	BC	6	0	0	1	0
58	BD	3	0	0	2	0
58	BE	4	0	0	0	0
58	BF	1	0	0	1	0
58	BG	1	0	0	1	0
58	BL	4	0	0	2	0
58	BN	3	0	0	0	0
58	BS	1	0	0	0	0
58	BT	1	0	0	0	0
58	CA	192	0	0	21	0
58	CL	1	0	0	0	0
58	CN	3	0	0	0	0
58	CT	1	0	0	0	0
58	CU	1	0	0	1	0
58	D0	1	0	0	0	0
58	D2	1	0	0	0	0
58	D3	2	0	0	0	0
58	D4	1	0	0	0	0
58	DA	608	0	0	99	0
58	DB	13	0	0	1	0
58	DC	11	0	0	0	0
58	DD	4	0	0	2	0
58	DE	5	0	0	2	0
58	DJ	1	0	0	0	0
58	DL	4	0	0	2	0
58	DN	2	0	0	0	0
58	DT	1	0	0	0	0
58	DU	1	0	0	0	0
58	DV	1	0	0	0	0
All	All	288396	0	192983	10007	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 21.

The worst 5 of 10007 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)
29:BH:123:ARG:HH22	1:CA:367:U:P	1.57	1.26
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14
22:BA:2498:C:OP2	58:BA:3690:HOH:O	1.65	1.12
1:AA:533:A:OP1	58:AA:1848:HOH:O	1.68	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	127 (59%)	39 (18%)	50 (23%)	0	0
2	CB	216/218 (99%)	137 (63%)	46 (21%)	33 (15%)	0	0
3	AC	204/206 (99%)	149 (73%)	34 (17%)	21 (10%)	0	1
3	CC	204/206 (99%)	149 (73%)	44 (22%)	11 (5%)	2	5
4	AD	203/205 (99%)	135 (66%)	38 (19%)	30 (15%)	0	0
4	CD	203/205 (99%)	150 (74%)	32 (16%)	21 (10%)	0	1
5	AE	148/150 (99%)	105 (71%)	23 (16%)	20 (14%)	0	0
5	CE	148/150 (99%)	92 (62%)	36 (24%)	20 (14%)	0	0
6	AF	98/100 (98%)	60 (61%)	25 (26%)	13 (13%)	0	0
6	CF	98/100 (98%)	66 (67%)	17 (17%)	15 (15%)	0	0
7	AG	149/151 (99%)	111 (74%)	25 (17%)	13 (9%)	1	1
7	CG	149/151 (99%)	119 (80%)	18 (12%)	12 (8%)	1	2
8	AH	127/129 (98%)	88 (69%)	32 (25%)	7 (6%)	2	5
8	CH	127/129 (98%)	102 (80%)	16 (13%)	9 (7%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AI	125/127 (98%)	89 (71%)	20 (16%)	16 (13%)	0	1
9	CI	125/127 (98%)	86 (69%)	28 (22%)	11 (9%)	1	1
10	AJ	96/98 (98%)	63 (66%)	15 (16%)	18 (19%)	0	0
10	CJ	96/98 (98%)	70 (73%)	15 (16%)	11 (12%)	0	1
11	AK	115/117 (98%)	84 (73%)	20 (17%)	11 (10%)	0	1
11	CK	115/117 (98%)	81 (70%)	25 (22%)	9 (8%)	1	2
12	AL	121/123 (98%)	92 (76%)	20 (16%)	9 (7%)	1	2
12	CL	121/123 (98%)	88 (73%)	18 (15%)	15 (12%)	0	1
13	AM	112/114 (98%)	87 (78%)	12 (11%)	13 (12%)	0	1
13	CM	112/114 (98%)	81 (72%)	23 (20%)	8 (7%)	1	2
14	AN	92/100 (92%)	58 (63%)	19 (21%)	15 (16%)	0	0
14	CN	92/100 (92%)	60 (65%)	15 (16%)	17 (18%)	0	0
15	AO	86/88 (98%)	68 (79%)	15 (17%)	3 (4%)	3	12
15	CO	86/88 (98%)	72 (84%)	10 (12%)	4 (5%)	2	7
16	AP	80/82 (98%)	54 (68%)	13 (16%)	13 (16%)	0	0
16	CP	80/82 (98%)	61 (76%)	14 (18%)	5 (6%)	1	3
17	AQ	78/80 (98%)	52 (67%)	21 (27%)	5 (6%)	1	3
17	CQ	78/80 (98%)	56 (72%)	13 (17%)	9 (12%)	0	1
18	AR	53/55 (96%)	39 (74%)	12 (23%)	2 (4%)	3	10
18	CR	53/55 (96%)	34 (64%)	12 (23%)	7 (13%)	0	0
19	AS	77/79 (98%)	50 (65%)	18 (23%)	9 (12%)	0	1
19	CS	77/79 (98%)	60 (78%)	12 (16%)	5 (6%)	1	3
20	AT	83/85 (98%)	66 (80%)	11 (13%)	6 (7%)	1	2
20	CT	83/85 (98%)	62 (75%)	16 (19%)	5 (6%)	1	4
21	AU	49/51 (96%)	28 (57%)	8 (16%)	13 (26%)	0	0
21	CU	49/51 (96%)	24 (49%)	12 (24%)	13 (26%)	0	0
24	BC	269/271 (99%)	217 (81%)	42 (16%)	10 (4%)	3	11
24	DC	269/271 (99%)	205 (76%)	47 (18%)	17 (6%)	1	3
25	BD	207/209 (99%)	180 (87%)	22 (11%)	5 (2%)	6	20
25	DD	207/209 (99%)	162 (78%)	33 (16%)	12 (6%)	1	4
26	BE	199/201 (99%)	172 (86%)	22 (11%)	5 (2%)	5	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	DE	199/201 (99%)	158 (79%)	30 (15%)	11 (6%)	2	5
27	BF	175/177 (99%)	144 (82%)	22 (13%)	9 (5%)	2	6
27	DF	175/177 (99%)	133 (76%)	29 (17%)	13 (7%)	1	2
28	BG	174/176 (99%)	150 (86%)	19 (11%)	5 (3%)	4	15
28	DG	174/176 (99%)	136 (78%)	30 (17%)	8 (5%)	2	7
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	0
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	0	1
30	BI	139/141 (99%)	82 (59%)	37 (27%)	20 (14%)	0	0
30	DI	139/141 (99%)	77 (55%)	47 (34%)	15 (11%)	0	1
31	BJ	140/142 (99%)	125 (89%)	14 (10%)	1 (1%)	22	53
31	DJ	140/142 (99%)	119 (85%)	13 (9%)	8 (6%)	1	5
32	BK	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	1	3
32	DK	120/122 (98%)	94 (78%)	19 (16%)	7 (6%)	1	4
33	BL	141/143 (99%)	110 (78%)	25 (18%)	6 (4%)	2	8
33	DL	141/143 (99%)	96 (68%)	33 (23%)	12 (8%)	1	1
34	BM	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	10	33
34	DM	134/136 (98%)	108 (81%)	18 (13%)	8 (6%)	1	4
35	BN	118/120 (98%)	106 (90%)	9 (8%)	3 (2%)	5	19
35	DN	118/120 (98%)	97 (82%)	13 (11%)	8 (7%)	1	3
36	BO	114/116 (98%)	93 (82%)	18 (16%)	3 (3%)	5	18
36	DO	114/116 (98%)	87 (76%)	20 (18%)	7 (6%)	1	4
37	BP	112/114 (98%)	100 (89%)	7 (6%)	5 (4%)	2	8
37	DP	112/114 (98%)	84 (75%)	15 (13%)	13 (12%)	0	1
38	BQ	115/117 (98%)	111 (96%)	1 (1%)	3 (3%)	5	18
38	DQ	115/117 (98%)	97 (84%)	16 (14%)	2 (2%)	9	29
39	BR	101/103 (98%)	86 (85%)	6 (6%)	9 (9%)	1	1
39	DR	101/103 (98%)	74 (73%)	20 (20%)	7 (7%)	1	3
40	BS	108/110 (98%)	95 (88%)	10 (9%)	3 (3%)	5	17
40	DS	108/110 (98%)	84 (78%)	16 (15%)	8 (7%)	1	2
41	BT	91/93 (98%)	72 (79%)	13 (14%)	6 (7%)	1	3
41	DT	91/93 (98%)	54 (59%)	23 (25%)	14 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BU	100/102 (98%)	79 (79%)	12 (12%)	9 (9%)	1	1
42	DU	100/102 (98%)	68 (68%)	19 (19%)	13 (13%)	0	1
43	BV	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
43	DV	92/94 (98%)	77 (84%)	13 (14%)	2 (2%)	6	22
44	BW	74/76 (97%)	69 (93%)	2 (3%)	3 (4%)	3	9
44	DW	73/76 (96%)	64 (88%)	7 (10%)	2 (3%)	5	17
45	BX	75/77 (97%)	70 (93%)	4 (5%)	1 (1%)	12	36
45	DX	75/77 (97%)	52 (69%)	16 (21%)	7 (9%)	0	1
46	BY	61/63 (97%)	42 (69%)	13 (21%)	6 (10%)	0	1
46	DY	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	3
47	BZ	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
47	DZ	56/58 (97%)	48 (86%)	5 (9%)	3 (5%)	2	5
48	B0	54/56 (96%)	43 (80%)	9 (17%)	2 (4%)	3	11
48	D0	54/56 (96%)	36 (67%)	15 (28%)	3 (6%)	2	5
49	B1	48/50 (96%)	37 (77%)	9 (19%)	2 (4%)	3	9
49	D1	48/50 (96%)	37 (77%)	8 (17%)	3 (6%)	1	3
50	B2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	6	21
50	D2	44/46 (96%)	35 (80%)	7 (16%)	2 (4%)	2	8
51	B3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	31
51	D3	62/64 (97%)	46 (74%)	14 (23%)	2 (3%)	4	13
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	17
53	B5	183/228 (80%)	100 (55%)	50 (27%)	33 (18%)	0	0
54	B6	2/7 (29%)	2 (100%)	0	0	100	100
54	D6	2/7 (29%)	0	1 (50%)	1 (50%)	0	0
All	All	11422/11686 (98%)	8617 (75%)	1868 (16%)	937 (8%)	1	2

5 of 937 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE
2	AB	21	ARG
2	AB	22	TYR

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Mol	Chain	Res	Type
2	AB	25	PRO
2	AB	34	ALA

5.3.2 Protein sidechains [i](#)

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	AB	180/180 (100%)	134 (74%)	46 (26%)	0	1
2	CB	180/180 (100%)	131 (73%)	49 (27%)	0	1
3	AC	170/170 (100%)	128 (75%)	42 (25%)	0	2
3	CC	170/170 (100%)	136 (80%)	34 (20%)	1	4
4	AD	172/172 (100%)	135 (78%)	37 (22%)	1	3
4	CD	172/172 (100%)	140 (81%)	32 (19%)	1	5
5	AE	113/113 (100%)	82 (73%)	31 (27%)	0	1
5	CE	113/113 (100%)	86 (76%)	27 (24%)	0	2
6	AF	87/87 (100%)	64 (74%)	23 (26%)	0	1
6	CF	87/87 (100%)	63 (72%)	24 (28%)	0	1
7	AG	124/124 (100%)	91 (73%)	33 (27%)	0	1
7	CG	124/124 (100%)	86 (69%)	38 (31%)	0	1
8	AH	104/104 (100%)	84 (81%)	20 (19%)	1	4
8	CH	104/104 (100%)	82 (79%)	22 (21%)	1	3
9	AI	105/105 (100%)	71 (68%)	34 (32%)	0	0
9	CI	105/105 (100%)	73 (70%)	32 (30%)	0	1
10	AJ	86/86 (100%)	65 (76%)	21 (24%)	0	2
10	CJ	86/86 (100%)	68 (79%)	18 (21%)	1	3
11	AK	90/90 (100%)	70 (78%)	20 (22%)	1	2
11	CK	90/90 (100%)	65 (72%)	25 (28%)	0	1
12	AL	103/103 (100%)	86 (84%)	17 (16%)	2	7
12	CL	103/103 (100%)	81 (79%)	22 (21%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AM	92/92 (100%)	70 (76%)	22 (24%)	0	2
13	CM	92/92 (100%)	66 (72%)	26 (28%)	0	1
14	AN	79/83 (95%)	64 (81%)	15 (19%)	1	4
14	CN	79/83 (95%)	67 (85%)	12 (15%)	3	8
15	AO	75/76 (99%)	61 (81%)	14 (19%)	1	5
15	CO	75/76 (99%)	59 (79%)	16 (21%)	1	3
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	2
16	CP	65/65 (100%)	49 (75%)	16 (25%)	0	2
17	AQ	74/74 (100%)	53 (72%)	21 (28%)	0	1
17	CQ	74/74 (100%)	49 (66%)	25 (34%)	0	0
18	AR	48/48 (100%)	36 (75%)	12 (25%)	0	2
18	CR	48/48 (100%)	38 (79%)	10 (21%)	1	3
19	AS	70/70 (100%)	56 (80%)	14 (20%)	1	4
19	CS	70/70 (100%)	57 (81%)	13 (19%)	1	5
20	AT	65/65 (100%)	49 (75%)	16 (25%)	0	2
20	CT	65/65 (100%)	48 (74%)	17 (26%)	0	1
21	AU	44/44 (100%)	25 (57%)	19 (43%)	0	0
21	CU	44/44 (100%)	27 (61%)	17 (39%)	0	0
24	BC	216/216 (100%)	189 (88%)	27 (12%)	4	14
24	DC	216/216 (100%)	180 (83%)	36 (17%)	2	6
25	BD	164/164 (100%)	152 (93%)	12 (7%)	14	38
25	DD	164/164 (100%)	147 (90%)	17 (10%)	7	21
26	BE	165/165 (100%)	139 (84%)	26 (16%)	2	8
26	DE	165/165 (100%)	135 (82%)	30 (18%)	1	5
27	BF	148/148 (100%)	114 (77%)	34 (23%)	1	2
27	DF	148/148 (100%)	123 (83%)	25 (17%)	2	6
28	BG	137/137 (100%)	125 (91%)	12 (9%)	10	29
28	DG	137/137 (100%)	117 (85%)	20 (15%)	3	9
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	2
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	2
30	BI	109/109 (100%)	76 (70%)	33 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	DI	109/109 (100%)	78 (72%)	31 (28%)	0	1
31	BJ	116/116 (100%)	103 (89%)	13 (11%)	6	18
31	DJ	116/116 (100%)	96 (83%)	20 (17%)	2	6
32	BK	103/103 (100%)	90 (87%)	13 (13%)	4	14
32	DK	103/103 (100%)	96 (93%)	7 (7%)	16	42
33	BL	102/102 (100%)	88 (86%)	14 (14%)	3	11
33	DL	102/102 (100%)	85 (83%)	17 (17%)	2	6
34	BM	109/109 (100%)	101 (93%)	8 (7%)	14	38
34	DM	109/109 (100%)	100 (92%)	9 (8%)	11	32
35	BN	100/100 (100%)	89 (89%)	11 (11%)	6	19
35	DN	100/100 (100%)	78 (78%)	22 (22%)	1	2
36	BO	86/86 (100%)	68 (79%)	18 (21%)	1	3
36	DO	86/86 (100%)	73 (85%)	13 (15%)	3	9
37	BP	99/99 (100%)	90 (91%)	9 (9%)	9	27
37	DP	99/99 (100%)	84 (85%)	15 (15%)	3	8
38	BQ	89/89 (100%)	81 (91%)	8 (9%)	9	28
38	DQ	89/89 (100%)	76 (85%)	13 (15%)	3	9
39	BR	84/84 (100%)	73 (87%)	11 (13%)	4	12
39	DR	84/84 (100%)	66 (79%)	18 (21%)	1	3
40	BS	93/93 (100%)	80 (86%)	13 (14%)	3	11
40	DS	93/93 (100%)	81 (87%)	12 (13%)	4	13
41	BT	80/80 (100%)	65 (81%)	15 (19%)	1	5
41	DT	80/80 (100%)	65 (81%)	15 (19%)	1	5
42	BU	83/83 (100%)	70 (84%)	13 (16%)	2	8
42	DU	83/83 (100%)	65 (78%)	18 (22%)	1	3
43	BV	78/78 (100%)	69 (88%)	9 (12%)	5	17
43	DV	78/78 (100%)	64 (82%)	14 (18%)	2	5
44	BW	57/58 (98%)	52 (91%)	5 (9%)	10	29
44	DW	56/58 (97%)	51 (91%)	5 (9%)	9	28
45	BX	67/67 (100%)	55 (82%)	12 (18%)	2	5
45	DX	67/67 (100%)	54 (81%)	13 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BY	55/55 (100%)	47 (86%)	8 (14%)	3	9
46	DY	55/55 (100%)	40 (73%)	15 (27%)	0	1
47	BZ	48/48 (100%)	45 (94%)	3 (6%)	18	46
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	3
48	B0	47/47 (100%)	43 (92%)	4 (8%)	10	31
48	D0	47/47 (100%)	43 (92%)	4 (8%)	10	31
49	B1	45/45 (100%)	40 (89%)	5 (11%)	6	19
49	D1	45/45 (100%)	40 (89%)	5 (11%)	6	19
50	B2	38/38 (100%)	34 (90%)	4 (10%)	7	20
50	D2	38/38 (100%)	30 (79%)	8 (21%)	1	3
51	B3	51/51 (100%)	48 (94%)	3 (6%)	19	49
51	D3	51/51 (100%)	44 (86%)	7 (14%)	3	11
52	B4	34/34 (100%)	27 (79%)	7 (21%)	1	3
52	D4	34/34 (100%)	29 (85%)	5 (15%)	3	9
53	B5	61/180 (34%)	46 (75%)	15 (25%)	0	2
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7602 (81%)	1788 (19%)	1	4

5 of 1788 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CC	80	LYS
50	D2	44	VAL
11	CK	77	TYR
47	DZ	39	GLU
36	DO	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
18	CR	74	HIS
41	DT	15	HIS
20	CT	68	HIS
29	DH	128	HIS

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Mol	Chain	Res	Type
46	DY	15	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	344 (22%)	12 (0%)
1	CA	1538/1539 (99%)	340 (22%)	9 (0%)
22	BA	2895/2903 (99%)	542 (18%)	21 (0%)
22	DA	2895/2903 (99%)	673 (23%)	28 (0%)
23	BB	118/119 (99%)	19 (16%)	0
23	DB	117/119 (98%)	24 (20%)	0
All	All	9100/9122 (99%)	1942 (21%)	70 (0%)

5 of 1942 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	13	U

5 of 70 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	DA	1738	G
22	DA	2109	U
22	DA	2286	G
22	BA	1606	C
22	BA	1378	A

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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	004	D6	7	54	9,10,11	3.27	7 (77%)	9,12,14	2.11	3 (33%)
54	004	B6	7	54	9,10,11	3.96	7 (77%)	9,12,14	0.93	0
54	MHU	D6	5	54	14,15,16	2.75	7 (50%)	18,19,21	2.45	2 (11%)
54	MHW	B6	1	54	9,9,10	3.33	4 (44%)	10,11,13	2.29	6 (60%)
54	MHW	D6	1	54	9,9,10	3.31	4 (44%)	10,11,13	2.22	5 (50%)
54	DBB	D6	3	54	4,5,6	0.63	0	1,5,7	0.36	0
54	MHU	B6	5	54	14,15,16	2.81	8 (57%)	18,19,21	2.81	5 (27%)
54	04X	D6	6	54	14,16,17	1.17	1 (7%)	11,20,22	4.89	7 (63%)
54	DBB	B6	3	54	4,5,6	0.36	0	1,5,7	1.39	0
54	04X	B6	6	54	14,16,17	1.46	1 (7%)	11,20,22	4.75	6 (54%)

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	004	D6	7	54	-	4/4/6/8	0/1/1/1
54	004	B6	7	54	-	2/4/6/8	0/1/1/1
54	MHU	D6	5	54	-	2/9/12/14	0/1/1/1
54	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	D6	3	54	-	1/3/4/6	-
54	MHU	B6	5	54	-	0/9/12/14	0/1/1/1
54	04X	D6	6	54	-	3/4/24/26	0/2/2/2
54	DBB	B6	3	54	-	0/3/4/6	-
54	04X	B6	6	54	-	2/4/24/26	0/2/2/2

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	7	004	CB-CA	-8.53	1.43	1.52
54	B6	1	MHW	CA-N	-6.09	1.27	1.35
54	D6	1	MHW	CA-N	-5.92	1.27	1.35
54	B6	5	MHU	CE1-CD1	5.79	1.49	1.38
54	D6	7	004	CB-CA	-5.67	1.46	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	04X	C0-N1-C1	13.77	132.45	111.09
54	B6	6	04X	C0-N1-C1	13.33	131.77	111.09
54	B6	5	MHU	CB-CA-N	7.72	122.61	110.65
54	D6	5	MHU	CB-CA-N	7.49	122.26	110.65
54	B6	5	MHU	O-C-CA	-7.08	106.23	124.78

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	D6	3	DBB	O-C-CA-CB
54	B6	6	04X	CD-C0-N1-C1
54	D6	6	04X	CD-C0-N1-C1
54	D6	5	MHU	CA-CB-CG-CD2
54	D6	6	04X	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	D6	7	004	2	0
54	D6	5	MHU	5	0
54	B6	1	MHW	1	0
54	D6	1	MHW	6	0
54	D6	3	DBB	2	0
54	D6	6	04X	4	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 502 ligands modelled in this entry, 500 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
56	VIF	BA	3001	-	35,40,40	2.34	15 (42%)	43,55,55	2.14	14 (32%)
56	VIF	DA	3001	-	35,40,40	2.34	14 (40%)	43,55,55	2.06	12 (27%)

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
56	VIF	BA	3001	-	-	3/42/58/58	0/2/3/3
56	VIF	DA	3001	-	-	5/42/58/58	0/2/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BA	3001	VIF	O01-C06	-4.73	1.37	1.44
56	DA	3001	VIF	O01-C06	-4.48	1.38	1.44
56	BA	3001	VIF	O01-C08	-4.41	1.24	1.34
56	BA	3001	VIF	C11-C09	-4.40	1.43	1.53
56	DA	3001	VIF	O04-C22	-4.39	1.35	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BA	3001	VIF	C02-C01-C03	-6.39	106.72	122.69
56	DA	3001	VIF	C18-C10-C20	-6.01	116.82	125.89
56	DA	3001	VIF	C02-C01-C03	-5.99	107.71	122.69
56	BA	3001	VIF	O01-C08-C09	4.36	120.38	110.78
56	BA	3001	VIF	C18-C10-C20	-4.27	119.44	125.89

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

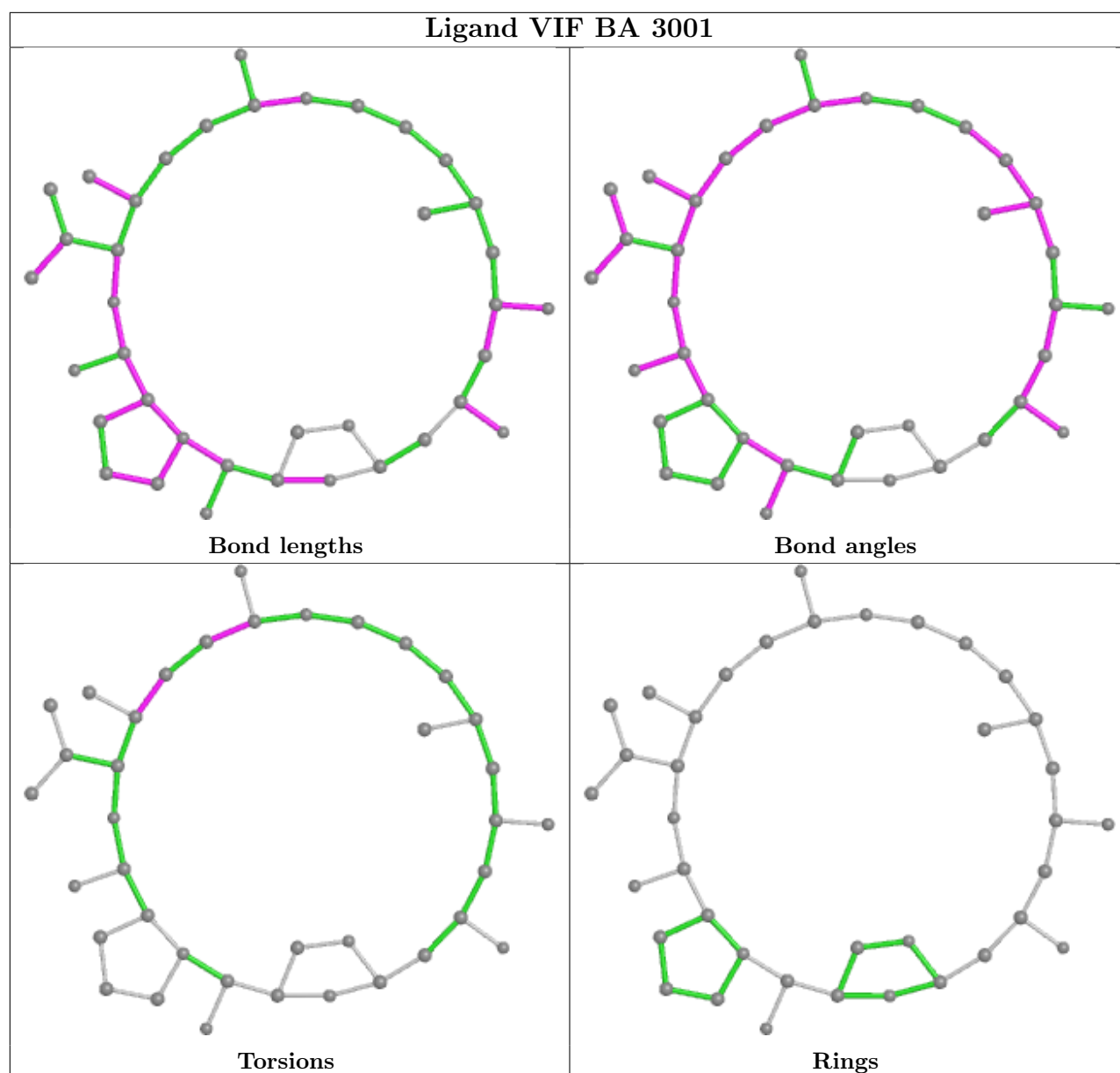
Mol	Chain	Res	Type	Atoms
56	DA	3001	VIF	F-C07-C14-C22
56	BA	3001	VIF	C02-C01-C03-O
56	BA	3001	VIF	C02-C01-C03-N02
56	DA	3001	VIF	C05-C06-O01-C08
56	DA	3001	VIF	C-C06-O01-C08

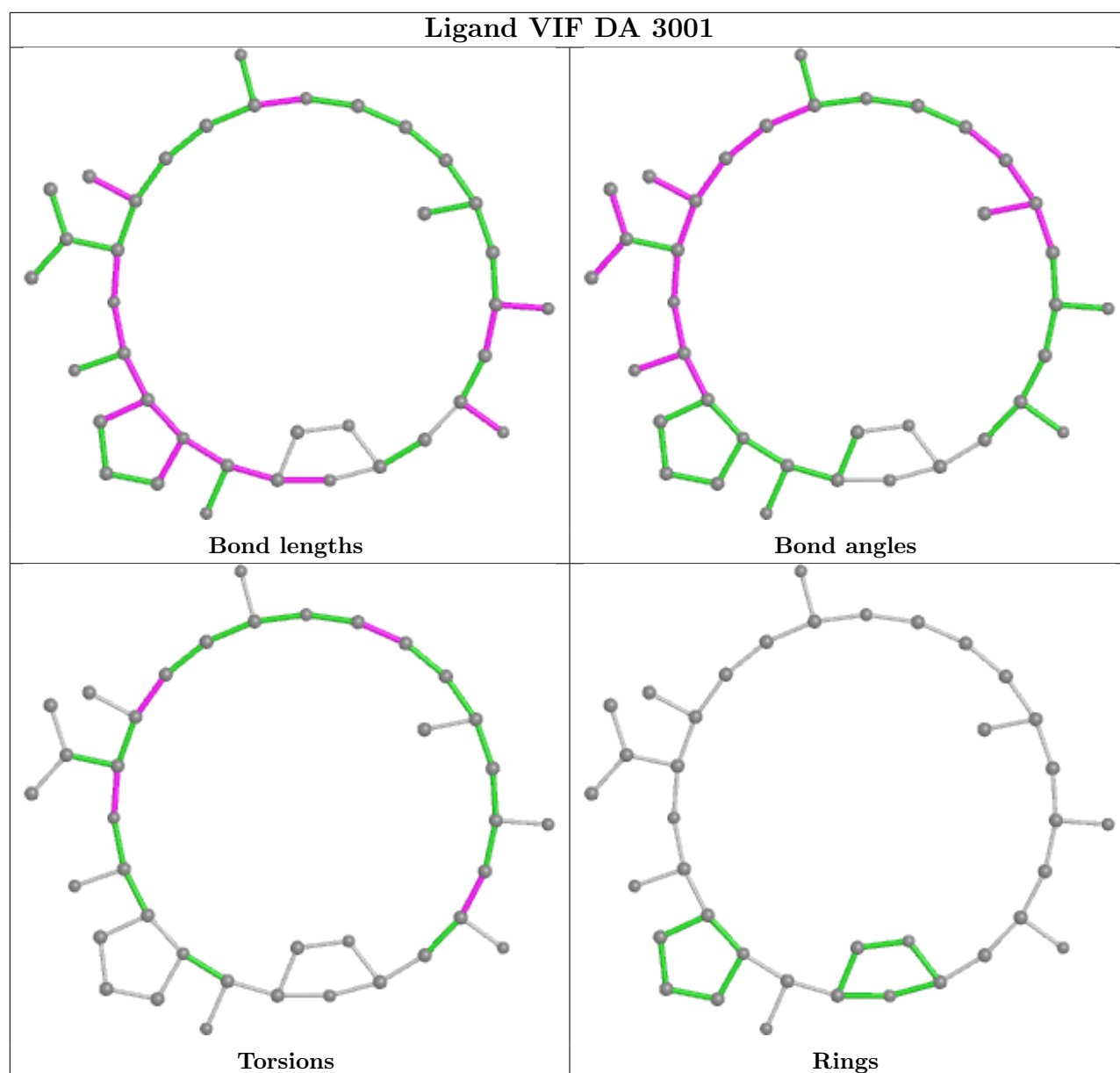
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BA	3001	VIF	2	0
56	DA	3001	VIF	11	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	1538/1539 (99%)	-0.21	26 (1%) 70 63	13, 50, 135, 180	0
1	CA	1539/1539 (100%)	0.02	56 (3%) 42 32	27, 70, 145, 177	0
2	AB	218/218 (100%)	0.65	19 (8%) 10 5	38, 73, 99, 121	0
2	CB	218/218 (100%)	1.06	55 (25%) 0 0	61, 87, 107, 125	0
3	AC	206/206 (100%)	-0.07	3 (1%) 73 68	33, 57, 78, 93	0
3	CC	206/206 (100%)	0.69	22 (10%) 6 3	48, 78, 95, 105	0
4	AD	205/205 (100%)	0.17	9 (4%) 34 24	32, 55, 79, 105	0
4	CD	205/205 (100%)	-0.16	4 (1%) 65 56	18, 38, 64, 88	0
5	AE	150/150 (100%)	-0.01	2 (1%) 77 72	30, 48, 79, 102	0
5	CE	150/150 (100%)	0.11	3 (2%) 65 56	32, 56, 82, 104	0
6	AF	100/100 (100%)	-0.15	1 (1%) 82 77	34, 58, 73, 86	0
6	CF	100/100 (100%)	-0.03	3 (3%) 50 40	44, 74, 93, 105	0
7	AG	151/151 (100%)	0.34	12 (7%) 12 7	54, 77, 96, 102	0
7	CG	151/151 (100%)	2.44	87 (57%) 0 0	81, 100, 109, 114	0
8	AH	129/129 (100%)	-0.12	1 (0%) 86 81	27, 48, 66, 76	0
8	CH	129/129 (100%)	0.17	5 (3%) 39 29	49, 65, 80, 90	0
9	AI	127/127 (100%)	0.88	15 (11%) 4 2	43, 73, 96, 109	0
9	CI	127/127 (100%)	1.38	36 (28%) 0 0	71, 93, 110, 122	0
10	AJ	98/98 (100%)	0.39	6 (6%) 21 13	40, 64, 92, 122	0
10	CJ	98/98 (100%)	2.18	47 (47%) 0 0	72, 93, 111, 125	0
11	AK	117/117 (100%)	0.55	11 (9%) 8 4	27, 65, 91, 115	0
11	CK	117/117 (100%)	0.14	4 (3%) 45 35	39, 66, 79, 93	0
12	AL	123/123 (100%)	0.05	5 (4%) 37 27	18, 35, 64, 96	0
12	CL	123/123 (100%)	0.23	6 (4%) 29 20	38, 52, 78, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.17	5 (4%) 34 24	45, 68, 92, 102	0
13	CM	114/114 (100%)	2.60	66 (57%) 0 0	96, 108, 116, 119	0
14	AN	96/100 (96%)	0.71	10 (10%) 6 3	37, 58, 94, 103	0
14	CN	96/100 (96%)	1.91	34 (35%) 0 0	69, 94, 111, 120	0
15	AO	88/88 (100%)	0.02	2 (2%) 60 51	28, 51, 65, 90	0
15	CO	88/88 (100%)	0.07	2 (2%) 60 51	40, 62, 80, 98	0
16	AP	82/82 (100%)	0.27	5 (6%) 21 13	31, 47, 85, 101	0
16	CP	82/82 (100%)	1.00	19 (23%) 0 0	44, 61, 87, 105	0
17	AQ	80/80 (100%)	0.25	3 (3%) 40 30	27, 49, 77, 122	0
17	CQ	80/80 (100%)	0.97	13 (16%) 1 1	44, 75, 97, 102	0
18	AR	55/55 (100%)	-0.14	3 (5%) 25 16	39, 52, 78, 108	0
18	CR	55/55 (100%)	0.09	3 (5%) 25 16	42, 55, 79, 111	0
19	AS	79/79 (100%)	0.71	11 (13%) 2 1	52, 68, 89, 102	0
19	CS	79/79 (100%)	3.58	58 (73%) 0 0	89, 108, 118, 124	0
20	AT	85/85 (100%)	0.32	2 (2%) 59 49	34, 48, 70, 103	0
20	CT	85/85 (100%)	1.13	16 (18%) 1 1	55, 73, 91, 97	0
21	AU	51/51 (100%)	1.34	17 (33%) 0 0	48, 74, 95, 106	0
21	CU	51/51 (100%)	0.67	6 (11%) 4 2	45, 71, 96, 105	0
22	BA	2897/2903 (99%)	0.04	107 (3%) 41 31	0, 13, 130, 195	0
22	DA	2897/2903 (99%)	0.19	103 (3%) 42 32	40, 82, 145, 181	0
23	BB	119/119 (100%)	-0.39	0 100 100	2, 23, 49, 85	0
23	DB	118/119 (99%)	0.03	1 (0%) 86 81	66, 112, 133, 143	0
24	BC	271/271 (100%)	-0.26	0 100 100	3, 19, 36, 51	0
24	DC	271/271 (100%)	0.48	20 (7%) 14 8	43, 61, 77, 89	0
25	BD	209/209 (100%)	-0.34	0 100 100	0, 10, 34, 68	0
25	DD	209/209 (100%)	0.76	24 (11%) 4 2	49, 68, 83, 96	0
26	BE	201/201 (100%)	-0.36	0 100 100	1, 23, 54, 90	0
26	DE	201/201 (100%)	1.41	71 (35%) 0 0	42, 84, 100, 108	0
27	BF	177/177 (100%)	0.02	3 (1%) 70 63	20, 41, 78, 90	0
27	DF	177/177 (100%)	2.94	127 (71%) 0 0	90, 107, 119, 125	0
28	BG	176/176 (100%)	-0.15	1 (0%) 89 86	17, 37, 62, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	1.81	67 (38%) 0 0	72, 93, 105, 114	0
29	BH	149/149 (100%)	3.13	81 (54%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.34	42 (28%) 0 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.38	93 (65%) 0 0	90, 111, 122, 133	0
30	DI	141/141 (100%)	4.67	114 (80%) 0 0	101, 117, 127, 130	0
31	BJ	142/142 (100%)	-0.42	0 100 100	1, 6, 22, 36	0
31	DJ	142/142 (100%)	0.54	13 (9%) 9 5	50, 66, 79, 96	0
32	BK	122/122 (100%)	-0.49	0 100 100	4, 12, 32, 67	0
32	DK	122/122 (100%)	0.92	21 (17%) 1 1	46, 63, 82, 97	0
33	BL	143/143 (100%)	-0.31	0 100 100	1, 18, 43, 74	0
33	DL	143/143 (100%)	1.61	50 (34%) 0 0	46, 79, 94, 113	0
34	BM	136/136 (100%)	-0.45	0 100 100	1, 9, 29, 84	0
34	DM	136/136 (100%)	0.79	19 (13%) 2 1	45, 69, 82, 101	0
35	BN	120/120 (100%)	-0.35	0 100 100	2, 7, 16, 52	0
35	DN	120/120 (100%)	1.00	22 (18%) 1 1	56, 75, 88, 114	0
36	BO	116/116 (100%)	-0.29	0 100 100	13, 24, 42, 50	0
36	DO	116/116 (100%)	1.83	50 (43%) 0 0	80, 94, 105, 114	0
37	BP	114/114 (100%)	-0.37	0 100 100	6, 18, 42, 64	0
37	DP	114/114 (100%)	0.74	15 (13%) 3 2	57, 69, 86, 91	0
38	BQ	117/117 (100%)	-0.35	0 100 100	1, 4, 13, 31	0
38	DQ	117/117 (100%)	0.63	14 (11%) 4 2	52, 67, 78, 82	0
39	BR	103/103 (100%)	-0.43	0 100 100	0, 11, 33, 66	0
39	DR	103/103 (100%)	1.36	24 (23%) 0 0	51, 77, 88, 99	0
40	BS	110/110 (100%)	-0.36	1 (0%) 84 80	1, 4, 21, 80	0
40	DS	110/110 (100%)	1.60	37 (33%) 0 0	57, 74, 89, 100	0
41	BT	93/93 (100%)	0.03	2 (2%) 62 52	8, 26, 75, 103	0
41	DT	93/93 (100%)	2.46	49 (52%) 0 0	66, 85, 103, 117	0
42	BU	102/102 (100%)	-0.30	2 (1%) 65 56	12, 28, 63, 92	0
42	DU	102/102 (100%)	2.93	56 (54%) 0 0	75, 90, 109, 118	0
43	BV	94/94 (100%)	-0.44	0 100 100	5, 19, 41, 53	0
43	DV	94/94 (100%)	0.88	15 (15%) 1 1	69, 84, 95, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.33	0 100 100	4, 12, 27, 54	0
44	DW	75/76 (98%)	1.53	23 (30%) 0 0	60, 80, 90, 105	0
45	BX	77/77 (100%)	-0.31	0 100 100	6, 24, 51, 73	0
45	DX	77/77 (100%)	0.70	12 (15%) 2 1	51, 71, 84, 87	0
46	BY	63/63 (100%)	0.14	5 (7%) 12 7	20, 40, 73, 93	0
46	DY	63/63 (100%)	1.92	27 (42%) 0 0	78, 94, 100, 105	0
47	BZ	58/58 (100%)	-0.30	0 100 100	2, 6, 23, 42	0
47	DZ	58/58 (100%)	0.58	6 (10%) 6 3	58, 71, 81, 94	0
48	B0	56/56 (100%)	-0.36	0 100 100	0, 9, 36, 68	0
48	D0	56/56 (100%)	1.45	17 (30%) 0 0	56, 78, 92, 102	0
49	B1	50/50 (100%)	-0.16	2 (4%) 38 28	17, 29, 49, 77	0
49	D1	50/50 (100%)	1.46	12 (24%) 0 0	69, 84, 93, 103	0
50	B2	46/46 (100%)	-0.24	1 (2%) 62 52	3, 9, 16, 88	0
50	D2	46/46 (100%)	1.45	14 (30%) 0 0	56, 68, 79, 102	0
51	B3	64/64 (100%)	-0.25	0 100 100	4, 9, 16, 31	0
51	D3	64/64 (100%)	1.07	16 (25%) 0 0	57, 71, 80, 81	0
52	B4	38/38 (100%)	-0.24	0 100 100	8, 16, 35, 52	0
52	D4	38/38 (100%)	1.49	13 (34%) 0 0	58, 75, 87, 101	0
53	B5	191/228 (83%)	5.76	184 (96%) 0 0	99, 115, 127, 135	0
54	B6	2/7 (28%)	-0.26	0 100 100	1, 1, 1, 1	0
54	D6	2/7 (28%)	0.48	0 100 100	47, 47, 47, 57	0
All	All	20738/20808 (99%)	0.45	2289 (11%) 5 3	0, 62, 120, 195	0

The worst 5 of 2289 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BI	53	LEU	20.9
29	BH	97	ARG	16.2
22	BA	2184	A	14.8
30	DI	3	LYS	14.3
30	DI	2	ALA	14.2

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

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(\AA^2)	Q<0.9
54	MHU	D6	5	15/16	0.87	0.27	45,56,65,65	0
54	MHW	D6	1	9/10	0.92	0.19	36,47,54,54	0
54	DBB	D6	3	6/7	0.94	0.28	45,52,56,63	0
54	04X	D6	6	15/16	0.94	0.15	46,56,70,73	0
54	004	D6	7	10/11	0.95	0.18	40,51,56,56	0
54	DBB	B6	3	6/7	0.97	0.19	0,1,1,4	0
54	04X	B6	6	15/16	0.97	0.14	1,3,15,15	0
54	MHW	B6	1	9/10	0.97	0.16	0,1,2,9	0
54	004	B6	7	10/11	0.97	0.22	0,0,1,2	0
54	MHU	B6	5	15/16	0.97	0.21	0,1,3,6	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
55	MG	DA	3049	1/1	0.28	0.29	109,109,109,109	0
55	MG	DA	3045	1/1	0.37	0.26	95,95,95,95	0
55	MG	DA	3137	1/1	0.37	0.11	88,88,88,88	0
55	MG	DA	3005	1/1	0.39	0.28	94,94,94,94	0
55	MG	DA	3072	1/1	0.43	0.16	80,80,80,80	0
55	MG	DA	3120	1/1	0.45	0.31	97,97,97,97	0
55	MG	DA	3101	1/1	0.45	0.27	78,78,78,78	0
55	MG	CA	1630	1/1	0.47	0.21	105,105,105,105	0
55	MG	DA	3042	1/1	0.47	0.33	68,68,68,68	0
55	MG	DA	3093	1/1	0.49	0.43	101,101,101,101	0
55	MG	CA	1649	1/1	0.50	0.18	71,71,71,71	0
55	MG	DA	3114	1/1	0.55	0.28	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3094	1/1	0.55	0.14	93,93,93,93	0
55	MG	DA	3132	1/1	0.55	0.42	89,89,89,89	0
55	MG	BA	3099	1/1	0.55	0.37	64,64,64,64	0
55	MG	DA	3017	1/1	0.56	0.13	84,84,84,84	0
55	MG	CA	1621	1/1	0.56	0.07	71,71,71,71	0
55	MG	DA	3027	1/1	0.58	0.98	96,96,96,96	0
55	MG	DA	3061	1/1	0.58	0.17	80,80,80,80	0
55	MG	CA	1629	1/1	0.61	0.08	80,80,80,80	0
55	MG	DA	3063	1/1	0.61	0.74	93,93,93,93	0
55	MG	DA	3058	1/1	0.62	0.17	73,73,73,73	0
55	MG	DA	3165	1/1	0.62	0.51	68,68,68,68	0
55	MG	DA	3149	1/1	0.63	0.26	54,54,54,54	0
55	MG	CA	1615	1/1	0.66	0.09	55,55,55,55	0
55	MG	BA	3048	1/1	0.66	0.11	53,53,53,53	0
55	MG	DA	3007	1/1	0.66	0.21	101,101,101,101	0
55	MG	CA	1646	1/1	0.67	0.34	65,65,65,65	0
55	MG	DA	3014	1/1	0.67	0.16	80,80,80,80	0
55	MG	BA	3003	1/1	0.68	0.11	23,23,23,23	0
55	MG	DA	3016	1/1	0.69	0.42	78,78,78,78	0
55	MG	DA	3080	1/1	0.70	0.10	101,101,101,101	0
55	MG	AA	1660	1/1	0.70	1.03	70,70,70,70	0
55	MG	D2	101	1/1	0.70	0.12	77,77,77,77	0
55	MG	DA	3148	1/1	0.71	0.14	58,58,58,58	0
55	MG	AA	1653	1/1	0.71	0.28	51,51,51,51	0
55	MG	DA	3150	1/1	0.71	0.20	61,61,61,61	0
55	MG	DA	3134	1/1	0.71	0.64	100,100,100,100	0
55	MG	DA	3020	1/1	0.71	0.19	83,83,83,83	0
55	MG	DA	3136	1/1	0.72	0.27	84,84,84,84	0
55	MG	DA	3006	1/1	0.72	0.11	98,98,98,98	0
55	MG	CA	1632	1/1	0.72	0.12	74,74,74,74	0
55	MG	CA	1628	1/1	0.72	0.24	98,98,98,98	0
55	MG	DA	3043	1/1	0.72	0.11	82,82,82,82	0
55	MG	AA	1658	1/1	0.72	0.44	72,72,72,72	0
55	MG	CA	1604	1/1	0.72	0.06	89,89,89,89	0
55	MG	CA	1605	1/1	0.73	0.17	88,88,88,88	0
55	MG	DA	3008	1/1	0.73	0.41	100,100,100,100	0
55	MG	DA	3003	1/1	0.73	0.29	92,92,92,92	0
55	MG	DA	3028	1/1	0.74	0.23	83,83,83,83	0
55	MG	DA	3022	1/1	0.74	0.13	62,62,62,62	0
55	MG	CA	1638	1/1	0.74	0.18	84,84,84,84	0
55	MG	DA	3057	1/1	0.75	0.27	88,88,88,88	0
55	MG	AA	1672	1/1	0.75	0.48	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	DA	3073	1/1	0.75	0.09	72,72,72,72	0
55	MG	DA	3154	1/1	0.75	0.34	70,70,70,70	0
55	MG	DA	3112	1/1	0.75	0.08	70,70,70,70	0
55	MG	DA	3019	1/1	0.75	0.17	85,85,85,85	0
55	MG	DA	3100	1/1	0.76	0.33	81,81,81,81	0
55	MG	DA	3128	1/1	0.76	0.13	71,71,71,71	0
55	MG	DA	3113	1/1	0.76	0.62	77,77,77,77	0
55	MG	AA	1667	1/1	0.76	0.36	54,54,54,54	0
55	MG	DA	3059	1/1	0.77	0.24	70,70,70,70	0
55	MG	DA	3074	1/1	0.77	0.11	68,68,68,68	0
55	MG	DA	3107	1/1	0.77	0.14	48,48,48,48	0
55	MG	CA	1609	1/1	0.77	0.12	77,77,77,77	0
55	MG	BA	3016	1/1	0.77	0.36	59,59,59,59	0
55	MG	CA	1617	1/1	0.77	0.09	40,40,40,40	0
55	MG	DA	3030	1/1	0.78	0.19	72,72,72,72	0
55	MG	DA	3138	1/1	0.78	0.43	52,52,52,52	0
55	MG	DA	3146	1/1	0.78	0.08	84,84,84,84	0
55	MG	BA	3037	1/1	0.78	0.15	35,35,35,35	0
55	MG	CA	1650	1/1	0.78	0.26	44,44,44,44	0
55	MG	CA	1635	1/1	0.78	0.25	120,120,120,120	0
55	MG	DA	3153	1/1	0.78	0.34	62,62,62,62	0
55	MG	DA	3047	1/1	0.78	0.10	80,80,80,80	0
55	MG	AA	1616	1/1	0.78	0.12	50,50,50,50	0
55	MG	DB	203	1/1	0.78	0.07	83,83,83,83	0
55	MG	BA	3002	1/1	0.78	0.07	15,15,15,15	0
55	MG	BA	3089	1/1	0.79	0.09	22,22,22,22	0
55	MG	CA	1636	1/1	0.79	0.19	113,113,113,113	0
55	MG	AA	1662	1/1	0.79	0.54	47,47,47,47	0
55	MG	CA	1656	1/1	0.79	0.75	53,53,53,53	0
55	MG	DA	3110	1/1	0.80	0.23	48,48,48,48	0
55	MG	DA	3055	1/1	0.80	0.10	41,41,41,41	0
55	MG	AA	1668	1/1	0.80	0.20	58,58,58,58	0
55	MG	BA	3084	1/1	0.80	0.25	49,49,49,49	0
55	MG	DA	3033	1/1	0.81	0.16	71,71,71,71	0
55	MG	DA	3108	1/1	0.81	0.12	72,72,72,72	0
55	MG	CA	1647	1/1	0.81	0.22	45,45,45,45	0
55	MG	BA	3174	1/1	0.81	0.22	27,27,27,27	0
55	MG	BA	3189	1/1	0.81	0.27	44,44,44,44	0
55	MG	BA	3077	1/1	0.81	0.25	61,61,61,61	0
55	MG	BA	3081	1/1	0.81	0.12	16,16,16,16	0
55	MG	AA	1614	1/1	0.81	0.12	55,55,55,55	0
55	MG	AA	1647	1/1	0.81	0.25	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1649	1/1	0.81	0.18	46,46,46,46	0
55	MG	BA	3100	1/1	0.81	0.09	14,14,14,14	0
55	MG	CA	1625	1/1	0.82	0.13	43,43,43,43	0
55	MG	BA	3049	1/1	0.82	0.07	13,13,13,13	0
55	MG	BA	3102	1/1	0.82	0.19	10,10,10,10	0
55	MG	BA	3133	1/1	0.82	0.07	37,37,37,37	0
55	MG	DA	3125	1/1	0.82	0.45	92,92,92,92	0
55	MG	BA	3006	1/1	0.82	0.08	51,51,51,51	0
55	MG	DA	3104	1/1	0.82	0.15	67,67,67,67	0
55	MG	AA	1638	1/1	0.82	0.06	77,77,77,77	0
55	MG	CA	1602	1/1	0.82	0.15	69,69,69,69	0
55	MG	DA	3076	1/1	0.82	0.15	70,70,70,70	0
55	MG	CA	1626	1/1	0.83	0.06	43,43,43,43	0
55	MG	AA	1644	1/1	0.83	0.52	58,58,58,58	0
55	MG	AA	1670	1/1	0.83	0.34	56,56,56,56	0
55	MG	BA	3058	1/1	0.83	0.24	45,45,45,45	0
55	MG	DA	3041	1/1	0.84	0.11	92,92,92,92	0
55	MG	AA	1652	1/1	0.84	0.36	56,56,56,56	0
55	MG	DA	3092	1/1	0.84	0.10	77,77,77,77	0
55	MG	DA	3025	1/1	0.84	0.39	56,56,56,56	0
55	MG	BA	3151	1/1	0.84	0.24	49,49,49,49	0
55	MG	DA	3096	1/1	0.84	0.18	75,75,75,75	0
55	MG	DA	3097	1/1	0.84	0.15	51,51,51,51	0
55	MG	AA	1630	1/1	0.84	0.13	63,63,63,63	0
55	MG	AA	1645	1/1	0.84	0.37	53,53,53,53	0
55	MG	BA	3112	1/1	0.84	0.17	8,8,8,8	0
55	MG	DA	3056	1/1	0.84	0.07	66,66,66,66	0
55	MG	DA	3071	1/1	0.85	0.08	96,96,96,96	0
55	MG	CA	1633	1/1	0.85	0.34	78,78,78,78	0
55	MG	BA	3173	1/1	0.85	0.20	32,32,32,32	0
55	MG	CA	1622	1/1	0.85	0.10	51,51,51,51	0
55	MG	DA	3116	1/1	0.85	0.34	96,96,96,96	0
55	MG	BA	3136	1/1	0.85	0.11	34,34,34,34	0
55	MG	DA	3021	1/1	0.85	0.08	64,64,64,64	0
55	MG	DA	3085	1/1	0.85	0.08	78,78,78,78	0
55	MG	DA	3086	1/1	0.85	0.08	72,72,72,72	0
55	MG	DA	3157	1/1	0.85	0.49	63,63,63,63	0
55	MG	DA	3133	1/1	0.85	0.11	53,53,53,53	0
55	MG	DB	202	1/1	0.85	0.08	65,65,65,65	0
55	MG	BA	3154	1/1	0.85	0.17	34,34,34,34	0
55	MG	DA	3135	1/1	0.85	0.11	53,53,53,53	0
55	MG	DA	3011	1/1	0.86	0.08	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1624	1/1	0.86	0.11	47,47,47,47	0
55	MG	CA	1655	1/1	0.86	0.13	51,51,51,51	0
55	MG	DA	3036	1/1	0.86	0.08	70,70,70,70	0
55	MG	BA	3168	1/1	0.86	0.23	35,35,35,35	0
55	MG	AA	1651	1/1	0.86	0.25	40,40,40,40	0
55	MG	DA	3070	1/1	0.86	0.19	86,86,86,86	0
55	MG	DA	3004	1/1	0.86	0.10	65,65,65,65	0
55	MG	AA	1605	1/1	0.86	0.15	33,33,33,33	0
55	MG	BA	3020	1/1	0.86	0.18	8,8,8,8	0
55	MG	DB	201	1/1	0.86	0.06	97,97,97,97	0
55	MG	BA	3026	1/1	0.86	0.14	36,36,36,36	0
55	MG	AA	1627	1/1	0.86	0.13	58,58,58,58	0
55	MG	DA	3079	1/1	0.86	0.12	92,92,92,92	0
55	MG	BA	3137	1/1	0.87	0.69	66,66,66,66	0
55	MG	DA	3121	1/1	0.87	0.27	78,78,78,78	0
55	MG	DA	3002	1/1	0.87	0.08	65,65,65,65	0
55	MG	DA	3126	1/1	0.87	0.17	59,59,59,59	0
55	MG	BA	3171	1/1	0.87	0.21	24,24,24,24	0
55	MG	DA	3064	1/1	0.87	0.19	48,48,48,48	0
55	MG	DA	3068	1/1	0.87	0.10	47,47,47,47	0
55	MG	DA	3160	1/1	0.87	0.11	74,74,74,74	0
55	MG	BA	3148	1/1	0.87	0.45	24,24,24,24	0
55	MG	BA	3075	1/1	0.87	0.07	29,29,29,29	0
55	MG	BA	3083	1/1	0.87	0.13	20,20,20,20	0
55	MG	CA	1651	1/1	0.87	0.29	50,50,50,50	0
55	MG	BA	3190	1/1	0.87	0.21	39,39,39,39	0
55	MG	AA	1664	1/1	0.88	0.33	42,42,42,42	0
55	MG	AA	1613	1/1	0.88	0.11	30,30,30,30	0
55	MG	DA	3026	1/1	0.88	0.24	67,67,67,67	0
55	MG	DA	3050	1/1	0.88	0.15	83,83,83,83	0
55	MG	BA	3055	1/1	0.88	0.12	6,6,6,6	0
55	MG	DA	3012	1/1	0.88	0.20	74,74,74,74	0
55	MG	AA	1624	1/1	0.88	0.09	35,35,35,35	0
55	MG	DA	3032	1/1	0.88	0.10	63,63,63,63	0
55	MG	DA	3151	1/1	0.88	0.27	49,49,49,49	0
55	MG	BA	3145	1/1	0.88	0.39	41,41,41,41	0
55	MG	DA	3091	1/1	0.88	0.07	76,76,76,76	0
55	MG	DA	3034	1/1	0.88	0.11	62,62,62,62	0
55	MG	BA	3062	1/1	0.88	0.83	57,57,57,57	0
55	MG	DA	3161	1/1	0.88	0.19	49,49,49,49	0
55	MG	BA	3065	1/1	0.88	0.17	0,0,0,0	0
55	MG	DA	3095	1/1	0.88	0.12	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3070	1/1	0.88	0.07	50,50,50,50	0
55	MG	DA	3069	1/1	0.88	0.08	60,60,60,60	0
55	MG	AA	1601	1/1	0.88	0.07	41,41,41,41	0
55	MG	AA	1639	1/1	0.89	0.06	60,60,60,60	0
55	MG	BA	3103	1/1	0.89	0.11	13,13,13,13	0
55	MG	BA	3159	1/1	0.89	0.14	21,21,21,21	0
55	MG	DA	3109	1/1	0.89	0.17	50,50,50,50	0
55	MG	CA	1631	1/1	0.89	0.14	92,92,92,92	0
55	MG	CA	1614	1/1	0.89	0.09	49,49,49,49	0
55	MG	DA	3089	1/1	0.89	0.07	78,78,78,78	0
55	MG	DA	3090	1/1	0.89	0.18	80,80,80,80	0
55	MG	DA	3040	1/1	0.89	0.14	60,60,60,60	0
55	MG	AA	1634	1/1	0.89	0.12	42,42,42,42	0
55	MG	BA	3121	1/1	0.89	0.07	7,7,7,7	0
55	MG	BA	3074	1/1	0.89	0.13	14,14,14,14	0
55	MG	BA	3086	1/1	0.89	0.11	5,5,5,5	0
55	MG	AA	1612	1/1	0.89	0.14	37,37,37,37	0
55	MG	DA	3167	1/1	0.89	0.40	43,43,43,43	0
55	MG	AA	1666	1/1	0.89	0.57	41,41,41,41	0
55	MG	DA	3098	1/1	0.89	0.14	73,73,73,73	0
55	MG	BA	3079	1/1	0.89	0.08	37,37,37,37	0
55	MG	DA	3029	1/1	0.89	0.12	65,65,65,65	0
55	MG	DA	3018	1/1	0.90	0.15	51,51,51,51	0
55	MG	DA	3145	1/1	0.90	0.38	67,67,67,67	0
55	MG	BA	3119	1/1	0.90	0.09	14,14,14,14	0
55	MG	BA	3053	1/1	0.90	0.12	6,6,6,6	0
55	MG	BA	3177	1/1	0.90	0.19	29,29,29,29	0
55	MG	BA	3186	1/1	0.90	0.14	32,32,32,32	0
55	MG	AA	1607	1/1	0.90	0.14	41,41,41,41	0
55	MG	DA	3046	1/1	0.90	0.10	77,77,77,77	0
55	MG	CA	1637	1/1	0.90	0.11	64,64,64,64	0
55	MG	DA	3156	1/1	0.90	0.11	42,42,42,42	0
55	MG	BA	3157	1/1	0.90	0.26	27,27,27,27	0
55	MG	DA	3158	1/1	0.90	0.20	49,49,49,49	0
55	MG	DA	3127	1/1	0.90	0.15	86,86,86,86	0
55	MG	CA	1601	1/1	0.90	0.10	45,45,45,45	0
55	MG	DA	3075	1/1	0.90	0.08	63,63,63,63	0
55	MG	AA	1636	1/1	0.90	0.09	42,42,42,42	0
55	MG	CA	1627	1/1	0.90	0.11	76,76,76,76	0
55	MG	AA	1650	1/1	0.90	0.16	37,37,37,37	0
55	MG	BA	3170	1/1	0.90	0.15	33,33,33,33	0
55	MG	AA	1632	1/1	0.90	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3141	1/1	0.91	0.37	41,41,41,41	0
55	MG	BA	3182	1/1	0.91	0.21	20,20,20,20	0
55	MG	BA	3150	1/1	0.91	0.14	45,45,45,45	0
55	MG	AA	1665	1/1	0.91	0.07	48,48,48,48	0
55	MG	AA	1669	1/1	0.91	0.32	51,51,51,51	0
55	MG	CA	1641	1/1	0.91	0.45	67,67,67,67	0
55	MG	BA	3115	1/1	0.91	0.14	17,17,17,17	0
55	MG	DA	3124	1/1	0.91	0.16	51,51,51,51	0
55	MG	DA	3048	1/1	0.91	0.09	53,53,53,53	0
55	MG	DA	3010	1/1	0.91	0.09	68,68,68,68	0
55	MG	BA	3047	1/1	0.91	0.15	9,9,9,9	0
55	MG	AA	1602	1/1	0.91	0.10	46,46,46,46	0
55	MG	DA	3159	1/1	0.91	0.37	61,61,61,61	0
55	MG	BA	3088	1/1	0.91	0.15	37,37,37,37	0
55	MG	BA	3015	1/1	0.91	0.12	6,6,6,6	0
55	MG	AA	1671	1/1	0.91	0.47	47,47,47,47	0
55	MG	DA	3084	1/1	0.91	0.20	72,72,72,72	0
55	MG	BA	3054	1/1	0.91	0.15	2,2,2,2	0
55	MG	AA	1661	1/1	0.91	0.11	53,53,53,53	0
55	MG	DA	3087	1/1	0.91	0.10	69,69,69,69	0
55	MG	DA	3139	1/1	0.91	0.43	49,49,49,49	0
55	MG	BA	3080	1/1	0.92	0.14	17,17,17,17	0
55	MG	AA	1663	1/1	0.92	0.13	41,41,41,41	0
55	MG	BA	3180	1/1	0.92	0.23	40,40,40,40	0
55	MG	AA	1609	1/1	0.92	0.09	35,35,35,35	0
55	MG	BA	3032	1/1	0.92	0.08	5,5,5,5	0
55	MG	BA	3060	1/1	0.92	0.12	9,9,9,9	0
55	MG	BA	3004	1/1	0.92	0.12	25,25,25,25	0
55	MG	BA	3149	1/1	0.92	0.15	27,27,27,27	0
55	MG	BA	3044	1/1	0.92	0.04	19,19,19,19	0
55	MG	BA	3092	1/1	0.92	0.04	55,55,55,55	0
55	MG	DA	3111	1/1	0.92	0.15	43,43,43,43	0
55	MG	BA	3005	1/1	0.92	0.08	42,42,42,42	0
55	MG	CA	1608	1/1	0.92	0.13	63,63,63,63	0
55	MG	BA	3156	1/1	0.92	0.23	23,23,23,23	0
55	MG	BA	3073	1/1	0.92	0.18	2,2,2,2	0
55	MG	DA	3117	1/1	0.92	0.57	73,73,73,73	0
55	MG	AA	1631	1/1	0.92	0.10	48,48,48,48	0
55	MG	BA	3160	1/1	0.92	0.22	29,29,29,29	0
55	MG	DA	3054	1/1	0.92	0.12	41,41,41,41	0
55	MG	CA	1619	1/1	0.92	0.09	40,40,40,40	0
55	MG	DA	3164	1/1	0.92	0.21	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	DA	3024	1/1	0.92	0.07	61,61,61,61	0
55	MG	DA	3166	1/1	0.92	0.20	57,57,57,57	0
55	MG	AA	1623	1/1	0.92	0.07	46,46,46,46	0
55	MG	DA	3168	1/1	0.92	0.10	47,47,47,47	0
55	MG	BA	3050	1/1	0.92	0.19	6,6,6,6	0
55	MG	BA	3078	1/1	0.92	0.08	31,31,31,31	0
55	MG	AA	1655	1/1	0.92	0.25	45,45,45,45	0
55	MG	DA	3062	1/1	0.92	1.19	104,104,104,104	0
55	MG	BA	3193	1/1	0.93	0.15	42,42,42,42	0
55	MG	DA	3143	1/1	0.93	0.20	39,39,39,39	0
55	MG	CA	1652	1/1	0.93	0.07	62,62,62,62	0
55	MG	CA	1654	1/1	0.93	0.24	58,58,58,58	0
55	MG	BA	3166	1/1	0.93	0.17	36,36,36,36	0
55	MG	BA	3061	1/1	0.93	0.25	28,28,28,28	0
55	MG	DA	3081	1/1	0.93	0.12	84,84,84,84	0
55	MG	DA	3052	1/1	0.93	0.09	49,49,49,49	0
55	MG	BA	3147	1/1	0.93	0.19	39,39,39,39	0
55	MG	AA	1604	1/1	0.93	0.05	58,58,58,58	0
55	MG	BA	3172	1/1	0.93	0.17	32,32,32,32	0
55	MG	BA	3063	1/1	0.93	0.17	6,6,6,6	0
55	MG	CA	1610	1/1	0.93	0.10	64,64,64,64	0
55	MG	AA	1610	1/1	0.93	0.19	63,63,63,63	0
55	MG	BA	3091	1/1	0.93	0.10	23,23,23,23	0
55	MG	DA	3009	1/1	0.93	0.20	81,81,81,81	0
55	MG	DA	3162	1/1	0.93	0.12	35,35,35,35	0
55	MG	DA	3163	1/1	0.93	0.42	71,71,71,71	0
55	MG	AA	1656	1/1	0.93	0.22	36,36,36,36	0
55	MG	BA	3094	1/1	0.93	0.06	30,30,30,30	0
55	MG	DA	3067	1/1	0.93	0.08	42,42,42,42	0
55	MG	DA	3038	1/1	0.93	0.08	75,75,75,75	0
55	MG	CA	1620	1/1	0.93	0.04	65,65,65,65	0
55	MG	AA	1626	1/1	0.93	0.15	19,19,19,19	0
55	MG	BA	3038	1/1	0.93	0.25	0,0,0,0	0
55	MG	BA	3141	1/1	0.93	0.18	26,26,26,26	0
55	MG	BA	3191	1/1	0.93	0.16	20,20,20,20	0
55	MG	BA	3120	1/1	0.94	0.18	32,32,32,32	0
55	MG	BA	3095	1/1	0.94	0.06	20,20,20,20	0
55	MG	BA	3185	1/1	0.94	0.25	25,25,25,25	0
55	MG	BA	3152	1/1	0.94	0.15	18,18,18,18	0
55	MG	BA	3187	1/1	0.94	0.13	25,25,25,25	0
55	MG	BA	3122	1/1	0.94	0.08	39,39,39,39	0
55	MG	BA	3125	1/1	0.94	0.14	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3031	1/1	0.94	0.07	57,57,57,57	0
55	MG	BA	3129	1/1	0.94	0.14	5,5,5,5	0
55	MG	DA	3142	1/1	0.94	0.27	40,40,40,40	0
55	MG	DA	3065	1/1	0.94	0.21	43,43,43,43	0
55	MG	DA	3066	1/1	0.94	0.15	39,39,39,39	0
55	MG	BA	3076	1/1	0.94	0.17	4,4,4,4	0
55	MG	DA	3102	1/1	0.94	0.08	58,58,58,58	0
55	MG	BA	3134	1/1	0.94	0.34	47,47,47,47	0
55	MG	DA	3105	1/1	0.94	0.08	67,67,67,67	0
55	MG	DA	3106	1/1	0.94	0.19	72,72,72,72	0
55	MG	DA	3152	1/1	0.94	0.16	47,47,47,47	0
55	MG	AA	1640	1/1	0.94	0.05	45,45,45,45	0
55	MG	DA	3037	1/1	0.94	0.09	54,54,54,54	0
55	MG	AA	1635	1/1	0.94	0.19	65,65,65,65	0
55	MG	BA	3138	1/1	0.94	0.38	4,4,4,4	0
55	MG	CA	1606	1/1	0.94	0.15	70,70,70,70	0
55	MG	CA	1607	1/1	0.94	0.09	47,47,47,47	0
55	MG	BA	3018	1/1	0.94	0.17	0,0,0,0	0
55	MG	BA	3111	1/1	0.94	0.08	24,24,24,24	0
55	MG	CA	1639	1/1	0.94	0.09	49,49,49,49	0
55	MG	BA	3008	1/1	0.94	0.04	22,22,22,22	0
55	MG	CA	1643	1/1	0.94	0.25	56,56,56,56	0
55	MG	DA	3083	1/1	0.94	0.12	49,49,49,49	0
55	MG	BA	3041	1/1	0.94	0.38	2,2,2,2	0
55	MG	BA	3043	1/1	0.94	0.14	11,11,11,11	0
55	MG	BA	3178	1/1	0.94	0.14	13,13,13,13	0
55	MG	BA	3179	1/1	0.94	0.20	34,34,34,34	0
55	MG	DA	3088	1/1	0.94	0.07	52,52,52,52	0
55	MG	DA	3130	1/1	0.94	0.18	39,39,39,39	0
55	MG	DA	3131	1/1	0.94	0.07	67,67,67,67	0
56	VIF	DA	3001	38/38	0.94	0.23	34,47,57,61	0
55	MG	DA	3099	1/1	0.95	0.16	50,50,50,50	0
55	MG	CA	1634	1/1	0.95	0.11	52,52,52,52	0
55	MG	BA	3135	1/1	0.95	0.15	2,2,2,2	0
55	MG	DA	3039	1/1	0.95	0.12	63,63,63,63	0
55	MG	DA	3103	1/1	0.95	0.31	83,83,83,83	0
55	MG	BA	3097	1/1	0.95	0.16	5,5,5,5	0
55	MG	AA	1659	1/1	0.95	0.32	61,61,61,61	0
55	MG	AA	1606	1/1	0.95	0.10	41,41,41,41	0
55	MG	AA	1620	1/1	0.95	0.07	59,59,59,59	0
55	MG	DA	3015	1/1	0.95	0.05	44,44,44,44	0
55	MG	AA	1621	1/1	0.95	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3078	1/1	0.95	0.24	83,83,83,83	0
55	MG	BA	3104	1/1	0.95	0.06	18,18,18,18	0
55	MG	CA	1644	1/1	0.95	0.49	55,55,55,55	0
55	MG	CA	1645	1/1	0.95	0.19	40,40,40,40	0
55	MG	DA	3082	1/1	0.95	0.08	66,66,66,66	0
55	MG	BA	3066	1/1	0.95	0.14	1,1,1,1	0
55	MG	DA	3051	1/1	0.95	0.13	54,54,54,54	0
55	MG	DA	3118	1/1	0.95	0.10	66,66,66,66	0
55	MG	BA	3068	1/1	0.95	0.20	0,0,0,0	0
55	MG	BA	3085	1/1	0.95	0.08	16,16,16,16	0
55	MG	BA	3024	1/1	0.95	0.14	4,4,4,4	0
55	MG	BA	3072	1/1	0.95	0.08	23,23,23,23	0
55	MG	BA	3014	1/1	0.95	0.19	0,0,0,0	0
55	MG	BA	3155	1/1	0.95	0.16	26,26,26,26	0
55	MG	BA	3090	1/1	0.95	0.14	1,1,1,1	0
55	MG	BA	3057	1/1	0.95	0.06	3,3,3,3	0
55	MG	BA	3126	1/1	0.95	0.15	4,4,4,4	0
55	MG	BB	203	1/1	0.95	0.06	15,15,15,15	0
55	MG	BA	3045	1/1	0.95	0.10	21,21,21,21	0
55	MG	BA	3059	1/1	0.95	0.05	13,13,13,13	0
55	MG	BA	3030	1/1	0.95	0.05	12,12,12,12	0
55	MG	BA	3169	1/1	0.95	0.09	34,34,34,34	0
55	MG	BA	3131	1/1	0.96	0.19	0,0,0,0	0
55	MG	BA	3132	1/1	0.96	0.28	50,50,50,50	0
55	MG	AA	1625	1/1	0.96	0.11	33,33,33,33	0
55	MG	BA	3158	1/1	0.96	0.20	15,15,15,15	0
55	MG	BA	3033	1/1	0.96	0.15	4,4,4,4	0
55	MG	DA	3013	1/1	0.96	0.16	34,34,34,34	0
55	MG	BA	3192	1/1	0.96	0.22	34,34,34,34	0
55	MG	BA	3105	1/1	0.96	0.19	0,0,0,0	0
55	MG	BB	202	1/1	0.96	0.10	2,2,2,2	0
55	MG	BA	3163	1/1	0.96	0.12	31,31,31,31	0
55	MG	BB	204	1/1	0.96	0.39	21,21,21,21	0
55	MG	BD	301	1/1	0.96	0.17	27,27,27,27	0
55	MG	BA	3165	1/1	0.96	0.17	5,5,5,5	0
55	MG	BA	3034	1/1	0.96	0.21	0,0,0,0	0
55	MG	DA	3147	1/1	0.96	0.10	60,60,60,60	0
55	MG	BA	3167	1/1	0.96	0.12	21,21,21,21	0
55	MG	DA	3023	1/1	0.96	0.13	42,42,42,42	0
55	MG	CA	1640	1/1	0.96	0.08	31,31,31,31	0
55	MG	AA	1619	1/1	0.96	0.15	37,37,37,37	0
55	MG	CA	1642	1/1	0.96	0.24	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3052	1/1	0.96	0.15	3,3,3,3	0
55	MG	BA	3116	1/1	0.96	0.22	50,50,50,50	0
55	MG	DA	3155	1/1	0.96	0.15	45,45,45,45	0
55	MG	BA	3118	1/1	0.96	0.13	1,1,1,1	0
55	MG	BA	3146	1/1	0.96	0.26	15,15,15,15	0
55	MG	BA	3093	1/1	0.96	0.04	38,38,38,38	0
55	MG	CA	1611	1/1	0.96	0.21	82,82,82,82	0
55	MG	CA	1612	1/1	0.96	0.07	44,44,44,44	0
55	MG	CA	1613	1/1	0.96	0.11	24,24,24,24	0
55	MG	DA	3115	1/1	0.96	0.11	51,51,51,51	0
55	MG	BA	3022	1/1	0.96	0.15	0,0,0,0	0
55	MG	BA	3176	1/1	0.96	0.11	13,13,13,13	0
55	MG	CA	1616	1/1	0.96	0.11	33,33,33,33	0
55	MG	BA	3039	1/1	0.96	0.14	0,0,0,0	0
55	MG	AA	1633	1/1	0.96	0.10	41,41,41,41	0
55	MG	AA	1654	1/1	0.96	0.23	30,30,30,30	0
55	MG	BA	3027	1/1	0.96	0.09	4,4,4,4	0
55	MG	BA	3181	1/1	0.96	0.18	19,19,19,19	0
55	MG	DA	3044	1/1	0.96	0.13	47,47,47,47	0
55	MG	BA	3153	1/1	0.96	0.28	11,11,11,11	0
55	MG	AA	1637	1/1	0.96	0.11	16,16,16,16	0
55	MG	DA	3060	1/1	0.97	0.10	43,43,43,43	0
55	MG	BA	3114	1/1	0.97	0.22	0,0,0,0	0
55	MG	BA	3087	1/1	0.97	0.20	1,1,1,1	0
55	MG	AA	1643	1/1	0.97	0.12	25,25,25,25	0
55	MG	BA	3117	1/1	0.97	0.10	3,3,3,3	0
55	MG	CA	1618	1/1	0.97	0.12	45,45,45,45	0
55	MG	DA	3140	1/1	0.97	0.29	28,28,28,28	0
55	MG	BA	3069	1/1	0.97	0.18	0,0,0,0	0
55	MG	CA	1653	1/1	0.97	0.10	42,42,42,42	0
55	MG	AA	1603	1/1	0.97	0.13	48,48,48,48	0
55	MG	DA	3144	1/1	0.97	0.21	30,30,30,30	0
55	MG	BA	3019	1/1	0.97	0.15	12,12,12,12	0
55	MG	BA	3035	1/1	0.97	0.19	47,47,47,47	0
55	MG	CA	1623	1/1	0.97	0.10	35,35,35,35	0
55	MG	BA	3188	1/1	0.97	0.17	16,16,16,16	0
55	MG	BA	3036	1/1	0.97	0.14	0,0,0,0	0
55	MG	BA	3123	1/1	0.97	0.20	0,0,0,0	0
55	MG	BA	3124	1/1	0.97	0.15	5,5,5,5	0
55	MG	AA	1617	1/1	0.97	0.05	51,51,51,51	0
55	MG	DA	3077	1/1	0.97	0.13	65,65,65,65	0
55	MG	BA	3056	1/1	0.97	0.14	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	BA	3128	1/1	0.97	0.13	0,0,0,0	0
55	MG	BA	3162	1/1	0.97	0.13	37,37,37,37	0
55	MG	BA	3021	1/1	0.97	0.07	2,2,2,2	0
55	MG	AA	1615	1/1	0.97	0.07	50,50,50,50	0
55	MG	BA	3040	1/1	0.97	0.17	3,3,3,3	0
55	MG	DA	3119	1/1	0.97	0.07	46,46,46,46	0
55	MG	BA	3101	1/1	0.97	0.09	2,2,2,2	0
55	MG	BA	3010	1/1	0.97	0.13	0,0,0,0	0
55	MG	DA	3122	1/1	0.97	0.08	44,44,44,44	0
55	MG	DA	3123	1/1	0.97	0.17	37,37,37,37	0
55	MG	BA	3013	1/1	0.97	0.17	0,0,0,0	0
55	MG	AA	1648	1/1	0.97	0.11	57,57,57,57	0
55	MG	BA	3028	1/1	0.97	0.06	15,15,15,15	0
55	MG	BA	3106	1/1	0.97	0.26	0,0,0,0	0
55	MG	BA	3140	1/1	0.97	0.36	3,3,3,3	0
55	MG	BA	3110	1/1	0.97	0.22	0,0,0,0	0
55	MG	BA	3175	1/1	0.97	0.13	33,33,33,33	0
55	MG	BA	3029	1/1	0.97	0.15	2,2,2,2	0
56	VIF	BA	3001	38/38	0.97	0.20	0,2,7,10	0
55	MG	AA	1641	1/1	0.97	0.14	15,15,15,15	0
55	MG	BA	3007	1/1	0.98	0.09	17,17,17,17	0
55	MG	BA	3017	1/1	0.98	0.06	1,1,1,1	0
55	MG	BA	3042	1/1	0.98	0.14	11,11,11,11	0
55	MG	BA	3142	1/1	0.98	0.39	5,5,5,5	0
55	MG	BQ	201	1/1	0.98	0.26	1,1,1,1	0
55	MG	AA	1618	1/1	0.98	0.09	41,41,41,41	0
55	MG	BA	3031	1/1	0.98	0.15	2,2,2,2	0
55	MG	CA	1603	1/1	0.98	0.12	36,36,36,36	0
55	MG	BA	3009	1/1	0.98	0.14	5,5,5,5	0
55	MG	AA	1628	1/1	0.98	0.05	35,35,35,35	0
55	MG	BA	3098	1/1	0.98	0.14	2,2,2,2	0
55	MG	BA	3011	1/1	0.98	0.18	1,1,1,1	0
55	MG	BA	3012	1/1	0.98	0.09	25,25,25,25	0
55	MG	BA	3064	1/1	0.98	0.20	0,0,0,0	0
55	MG	BA	3082	1/1	0.98	0.17	0,0,0,0	0
55	MG	BA	3023	1/1	0.98	0.17	0,0,0,0	0
55	MG	DA	3053	1/1	0.98	0.07	45,45,45,45	0
55	MG	BA	3127	1/1	0.98	0.20	6,6,6,6	0
55	MG	BA	3051	1/1	0.98	0.08	5,5,5,5	0
55	MG	BA	3183	1/1	0.98	0.21	24,24,24,24	0
55	MG	BA	3184	1/1	0.98	0.17	10,10,10,10	0
55	MG	BA	3067	1/1	0.98	0.17	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1648	1/1	0.98	0.21	30,30,30,30	0
55	MG	AA	1642	1/1	0.98	0.15	15,15,15,15	0
55	MG	DA	3129	1/1	0.98	0.14	75,75,75,75	0
55	MG	BA	3108	1/1	0.98	0.14	9,9,9,9	0
55	MG	BA	3109	1/1	0.98	0.20	1,1,1,1	0
55	MG	BA	3161	1/1	0.98	0.13	13,13,13,13	0
55	MG	AA	1622	1/1	0.98	0.20	17,17,17,17	0
55	MG	AA	1657	1/1	0.98	0.21	46,46,46,46	0
55	MG	BA	3071	1/1	0.98	0.09	5,5,5,5	0
55	MG	BA	3113	1/1	0.98	0.08	13,13,13,13	0
55	MG	BA	3194	1/1	0.98	0.08	32,32,32,32	0
55	MG	DA	3035	1/1	0.98	0.09	41,41,41,41	0
55	MG	BB	201	1/1	0.98	0.08	29,29,29,29	0
55	MG	BA	3025	1/1	0.99	0.15	0,0,0,0	0
55	MG	BA	3046	1/1	0.99	0.12	2,2,2,2	0
55	MG	AA	1629	1/1	0.99	0.05	54,54,54,54	0
55	MG	BA	3096	1/1	0.99	0.05	10,10,10,10	0
55	MG	AA	1611	1/1	0.99	0.10	19,19,19,19	0
55	MG	AA	1646	1/1	0.99	0.16	55,55,55,55	0
55	MG	BA	3139	1/1	0.99	0.40	0,0,0,0	0
55	MG	BA	3164	1/1	0.99	0.31	19,19,19,19	0
55	MG	BA	3130	1/1	0.99	0.15	0,0,0,0	0
55	MG	AA	1608	1/1	0.99	0.19	16,16,16,16	0
55	MG	BA	3107	1/1	0.99	0.24	0,0,0,0	0
55	MG	BA	3143	1/1	0.99	0.30	14,14,14,14	0
55	MG	BA	3144	1/1	0.99	0.28	8,8,8,8	0
57	ZN	D4	101	1/1	0.99	0.10	86,86,86,86	0
57	ZN	B4	101	1/1	1.00	0.14	24,24,24,24	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.