



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 17, 2023 – 04:42 PM EST

PDB ID : 4U1V
Title : Crystal structure of the E. coli ribosome bound to linopristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-07-16
Resolution : 3.00 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

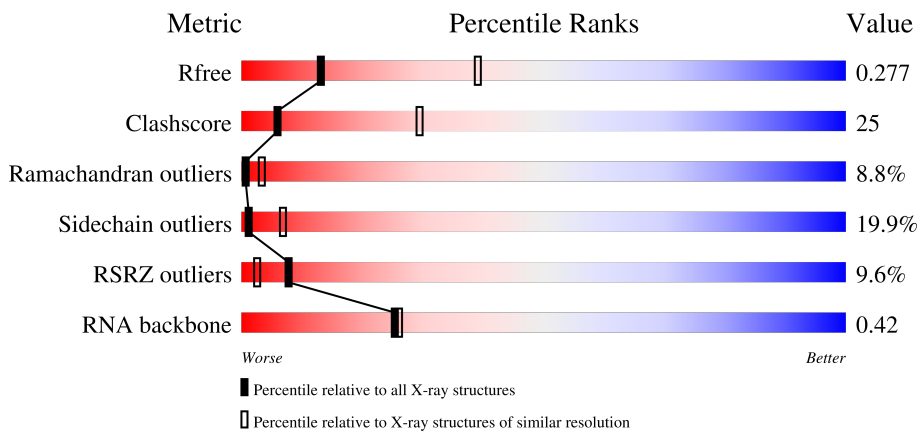
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	
1	CA	1539	
2	AB	218	
2	CB	218	

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	
7	CG	151	
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
13	CM	114	
14	AN	100	
14	CN	100	
15	AO	88	



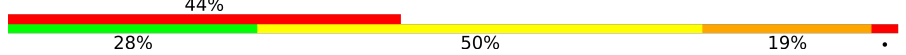







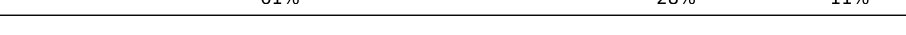






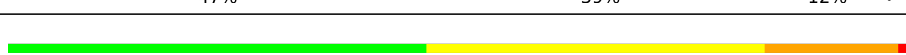



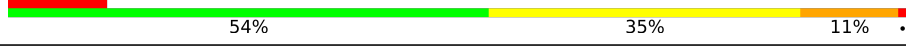



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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD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


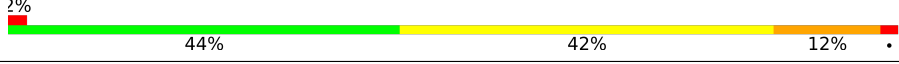
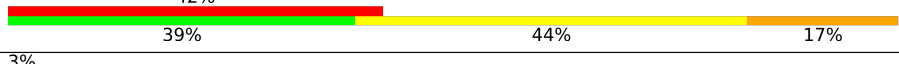
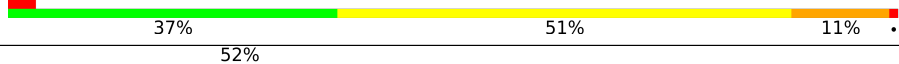
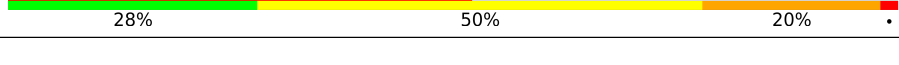

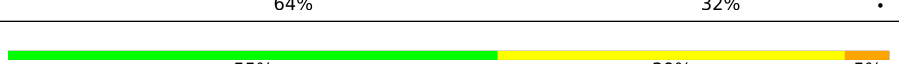
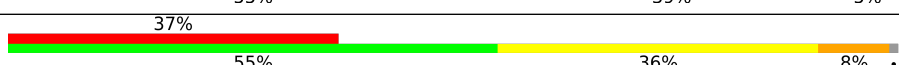
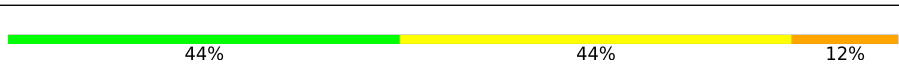

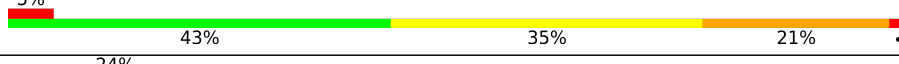
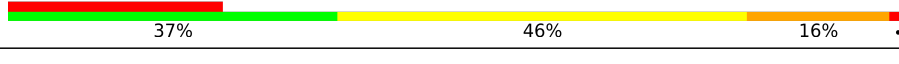


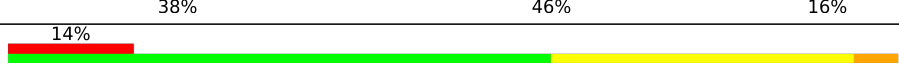
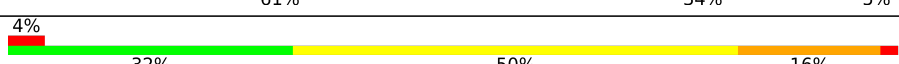


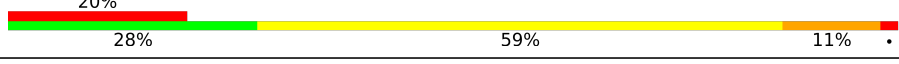






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Mol	Chain	Length	Quality of chain
28	BG	176	 55% 38% 7%
28	DG	176	 22% 54% 36% 9%
29	BH	149	 44% 28% 50% 19%
29	DH	149	 24% 35% 52% 11%
30	BI	141	 47% 34% 40% 25%
30	DI	141	 69% 42% 40% 17%
31	BJ	142	 56% 38% 6%
31	DJ	142	 8% 52% 42% 6%
32	BK	122	 35% 50% 15%
32	DK	122	 11% 61% 28% 11%
33	BL	143	 58% 30% 11%
33	DL	143	 25% 43% 41% 16%
34	BM	136	 49% 41% 8%
34	DM	136	 13% 54% 36% 10%
35	BN	120	 51% 38% 8%
35	DN	120	 14% 47% 39% 12%
36	BO	116	 47% 38% 15%
36	DO	116	 39% 53% 40% 8%
37	BP	114	 53% 39% 7%
37	DP	114	 11% 54% 35% 11%
38	BQ	117	 48% 44% 9%
38	DQ	117	 8% 52% 44%
39	BR	103	 37% 49% 14%
39	DR	103	 17% 51% 40% 9%
40	BS	110	 39% 48% 13%

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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>74% 49% 26% 9% 16%</p>
54	B6	7	<p>43% 57%</p>
54	D6	7	<p>29% 57% 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	X	-
55	MG	AA	1627	-	-	-	X
55	MG	AA	1644	-	-	-	X
55	MG	AA	1665	-	-	-	X
55	MG	AA	1667	-	-	-	X
55	MG	AA	1670	-	-	-	X
55	MG	BA	3015	-	-	-	X
55	MG	BA	3098	-	-	-	X
55	MG	BA	3115	-	-	-	X
55	MG	BA	3190	-	-	-	X
55	MG	CA	1655	-	-	-	X
55	MG	DA	3002	-	-	-	X
55	MG	DA	3015	-	-	-	X
55	MG	DA	3016	-	-	-	X
55	MG	DA	3028	-	-	-	X
55	MG	DA	3041	-	-	-	X
55	MG	DA	3061	-	-	-	X
55	MG	DA	3062	-	-	-	X
55	MG	DA	3071	-	-	-	X
55	MG	DA	3072	-	-	-	X
55	MG	DA	3092	-	-	-	X
55	MG	DA	3120	-	-	-	X
55	MG	DA	3132	-	-	-	X
55	MG	DA	3134	-	-	-	X
55	MG	DA	3151	-	-	-	X
55	MG	DA	3158	-	-	-	X
55	MG	DA	3164	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288320 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	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

- 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	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- 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	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- 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	C	N	O	S	0	0	0
			1643	1026	315	298	4			
4	CD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- 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
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	CP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

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

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

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

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

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

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

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

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

- 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	S	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
			Total	C	N	O			
53	B5	191	1142	691	221	230	0	0	1

- Molecule 54 is a protein called Linopristin.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	71	Total 71	Mg 71	0	0
55	AM	1	Total 1	Mg 1	0	0
55	BA	195	Total 195	Mg 195	0	0
55	BB	4	Total 4	Mg 4	0	0
55	CA	55	Total 55	Mg 55	0	0
55	CM	1	Total 1	Mg 1	0	0
55	DA	167	Total 167	Mg 167	0	0
55	DB	3	Total 3	Mg 3	0	0
55	DQ	1	Total 1	Mg 1	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	194	Total O 194 194	0	0
57	AL	1	Total O 1 1	0	0
57	AN	5	Total O 5 5	0	0
57	AT	2	Total O 2 2	0	0
57	AU	1	Total O 1 1	0	0
57	BA	615	Total O 615 615	0	0
57	BB	14	Total O 14 14	0	0
57	BC	10	Total O 10 10	0	0
57	BD	4	Total O 4 4	0	0
57	BE	4	Total O 4 4	0	0
57	BF	1	Total O 1 1	0	0
57	BG	1	Total O 1 1	0	0
57	BJ	1	Total O 1 1	0	0
57	BL	6	Total O 6 6	0	0
57	BN	2	Total O 2 2	0	0
57	BS	1	Total O 1 1	0	0
57	BU	1	Total O 1 1	0	0
57	B2	1	Total O 1 1	0	0
57	B3	3	Total O 3 3	0	0
57	B4	2	Total O 2 2	0	0
57	CA	189	Total O 189 189	0	0
57	CL	1	Total O 1 1	0	0

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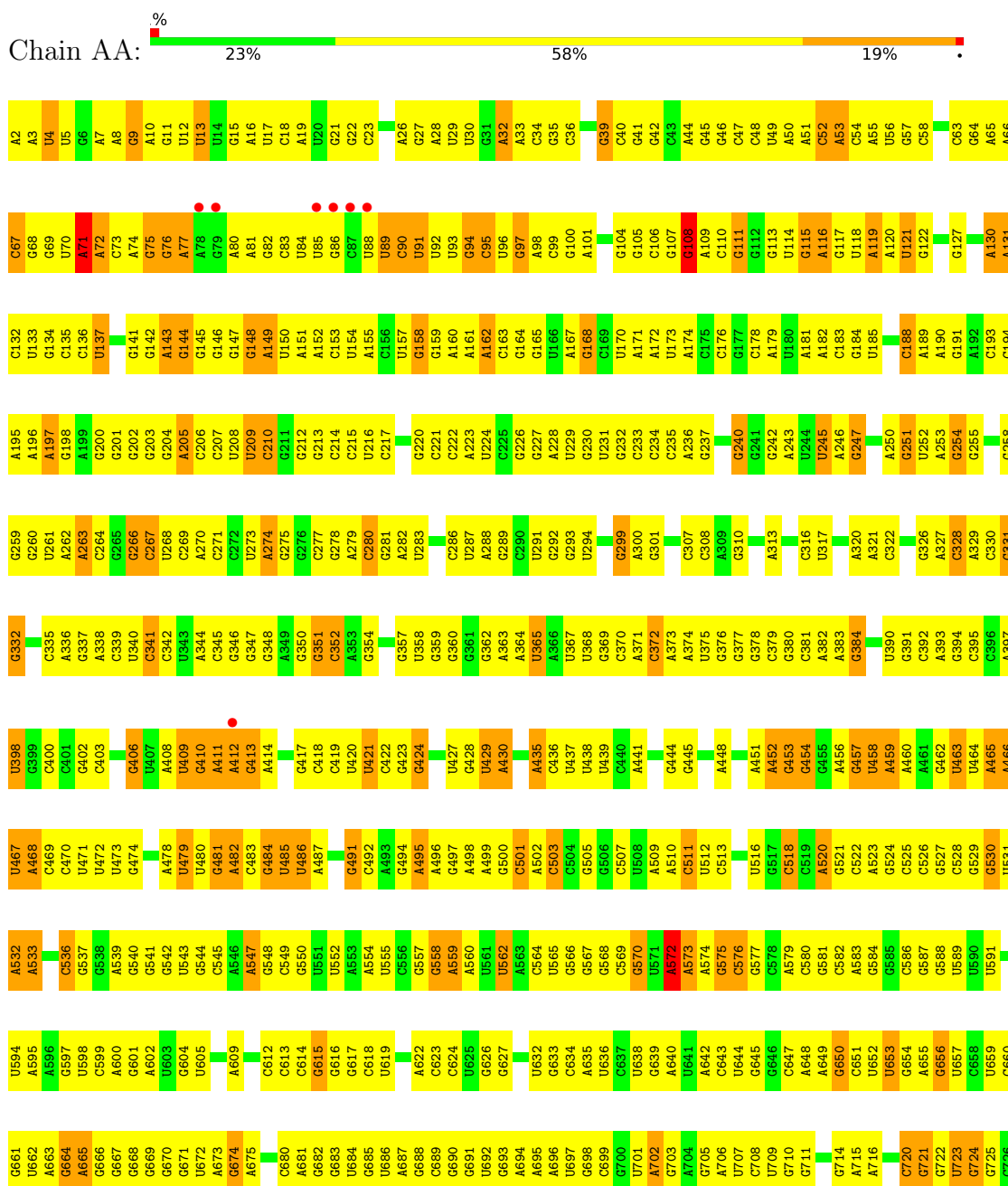
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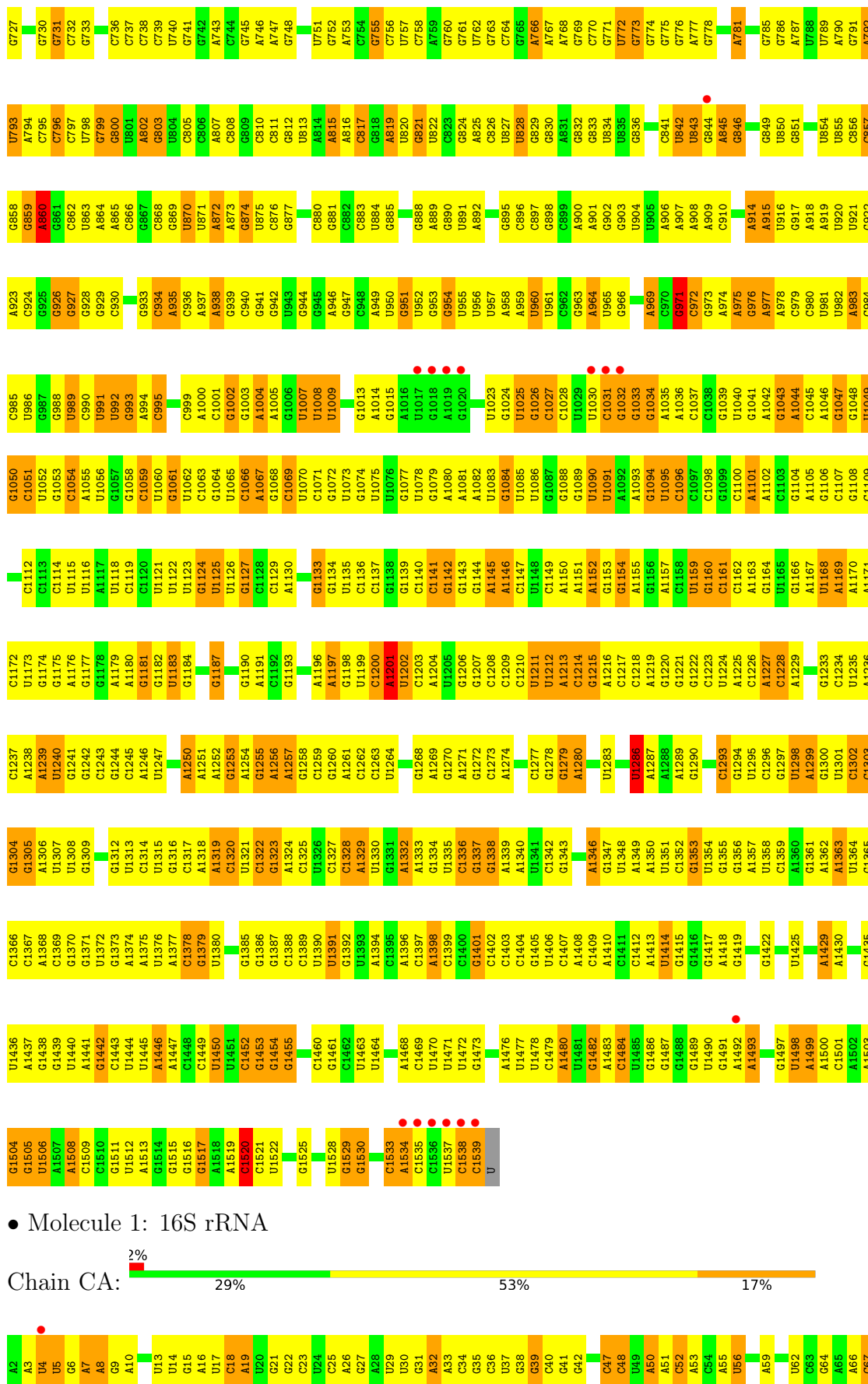
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57	CT	3	Total O 3 3	0	0
57	CU	2	Total O 2 2	0	0
57	DA	607	Total O 607 607	0	0
57	DB	13	Total O 13 13	0	0
57	DC	9	Total O 9 9	0	0
57	DD	4	Total O 4 4	0	0
57	DE	6	Total O 6 6	0	0
57	DL	5	Total O 5 5	0	0
57	DN	2	Total O 2 2	0	0
57	DT	2	Total O 2 2	0	0
57	DU	1	Total O 1 1	0	0
57	DV	1	Total O 1 1	0	0
57	D0	1	Total O 1 1	0	0
57	D2	2	Total O 2 2	0	0
57	D3	2	Total O 2 2	0	0
57	D4	1	Total O 1 1	0	0

3 Residue-property plots

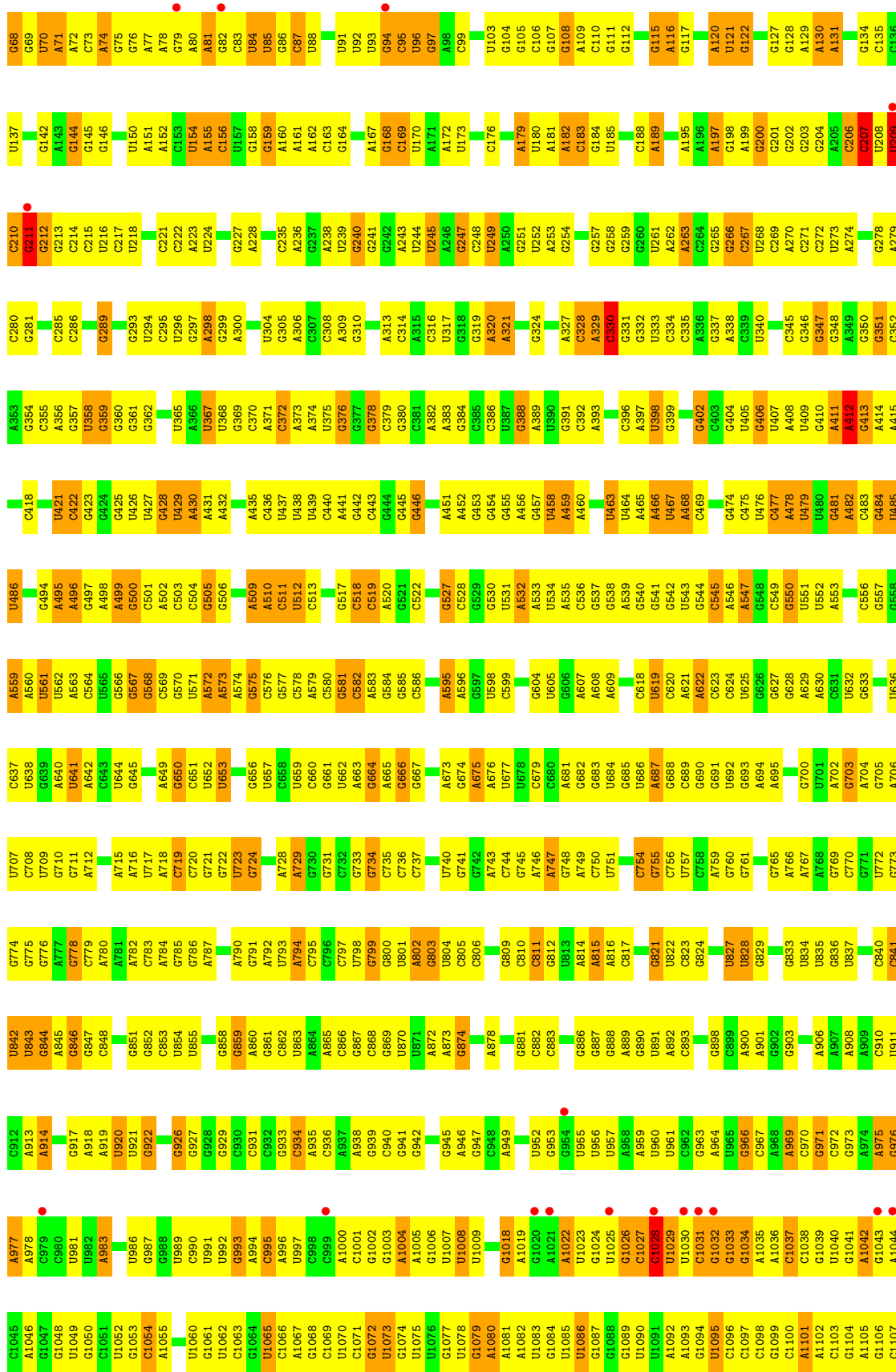
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

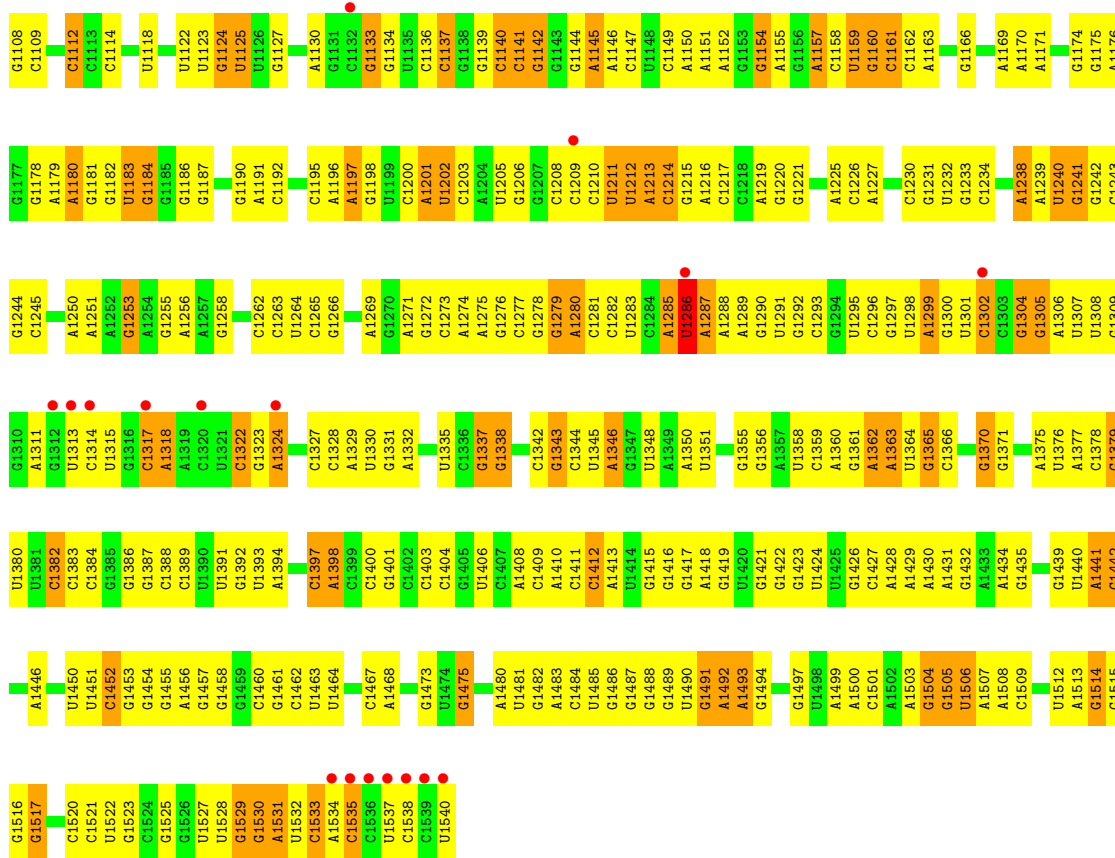
- Molecule 1: 16S rRNA



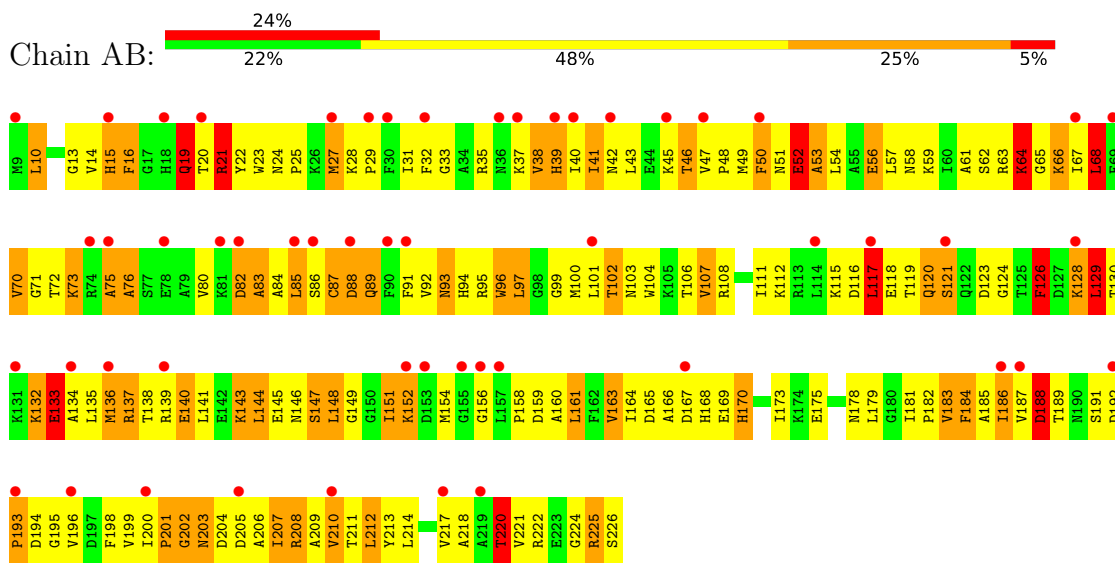


● Molecule 1: 16S rRNA

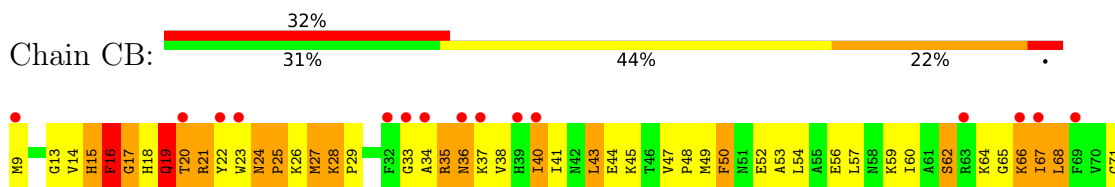


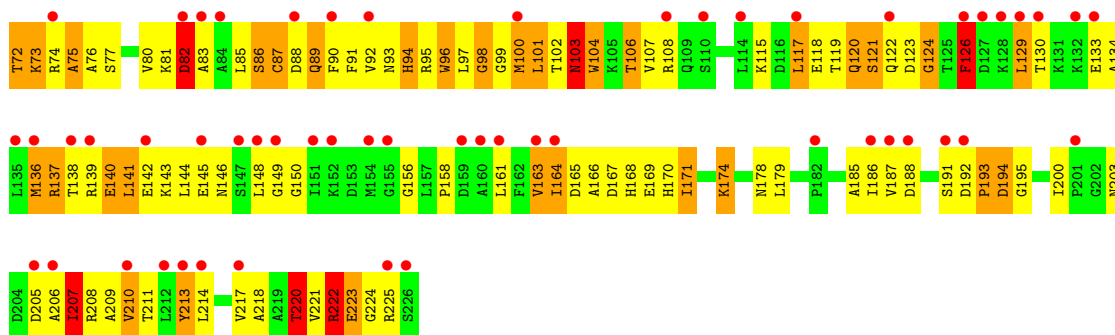


• Molecule 2: 30S ribosomal protein S2

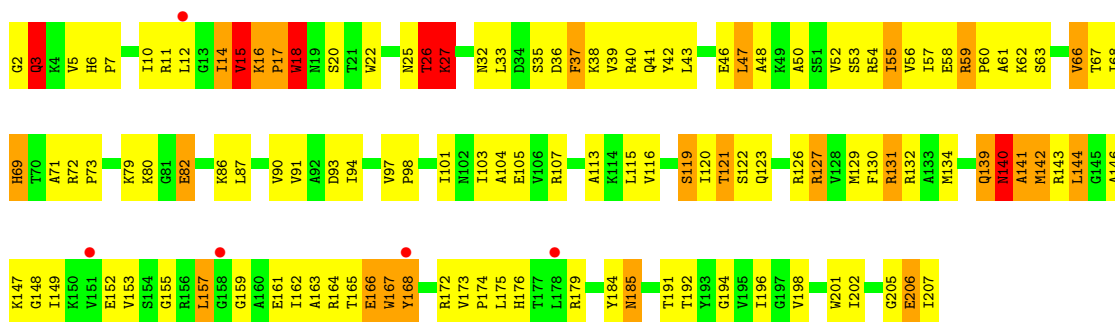
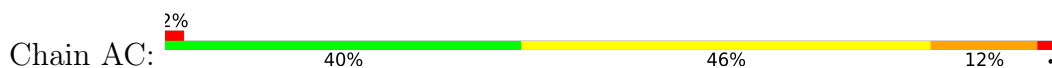


• Molecule 2: 30S ribosomal protein S2

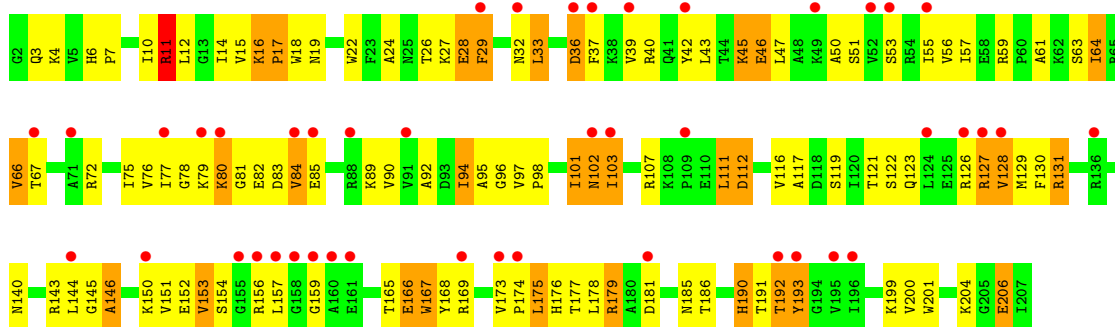
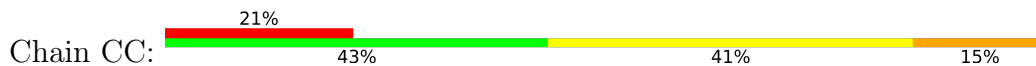




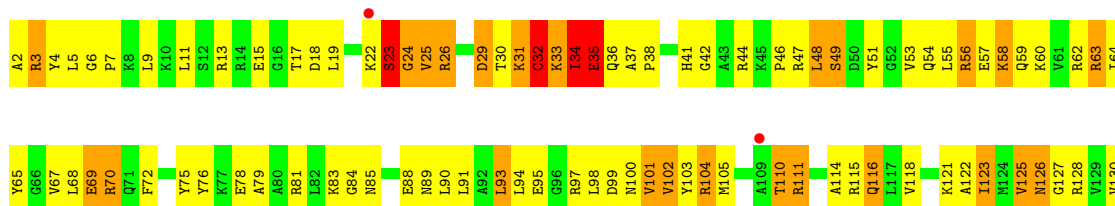
- Molecule 3: 30S ribosomal protein S3

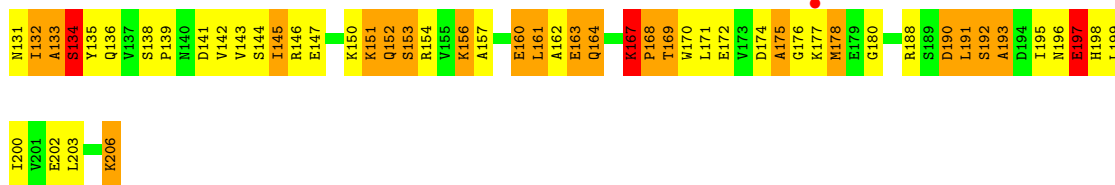


- Molecule 3: 30S ribosomal protein S3

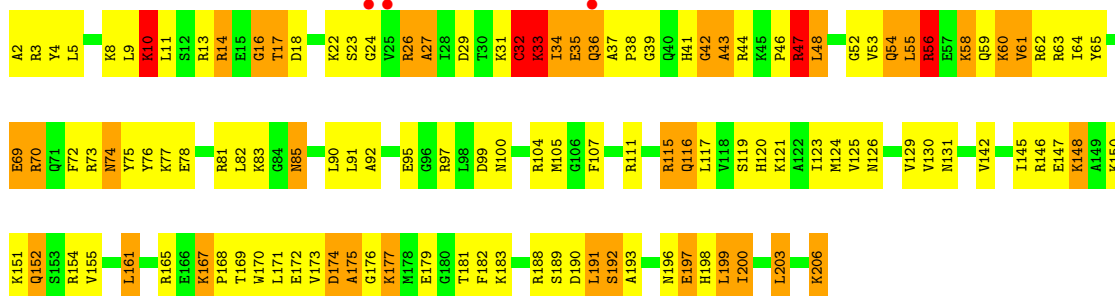
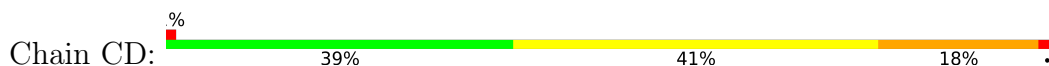


- Molecule 4: 30S ribosomal protein S4

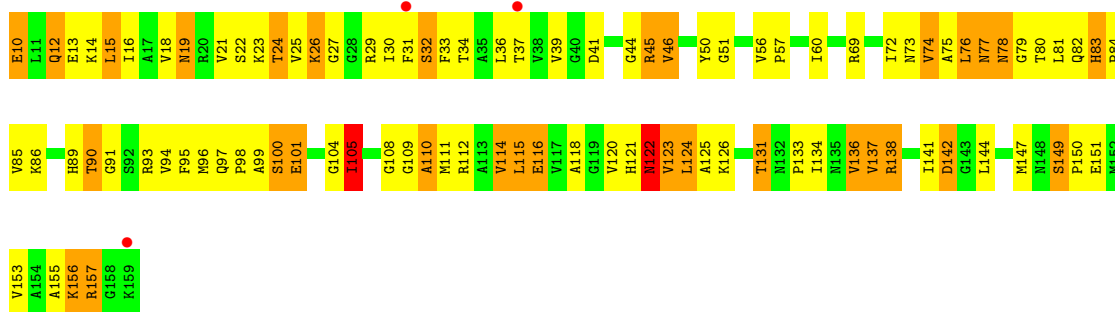




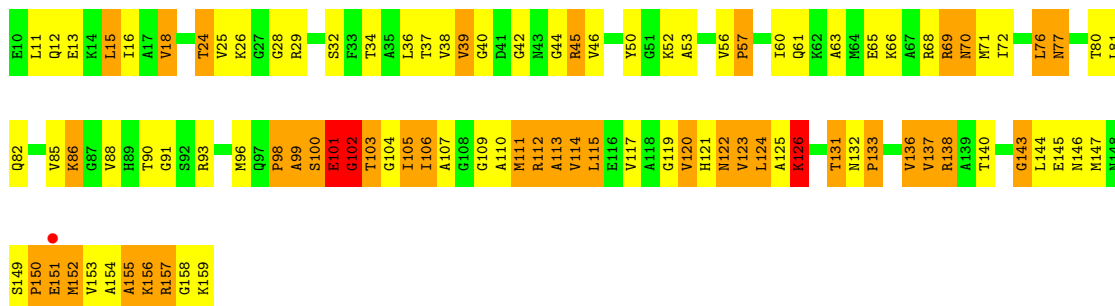
• Molecule 4: 30S ribosomal protein S4



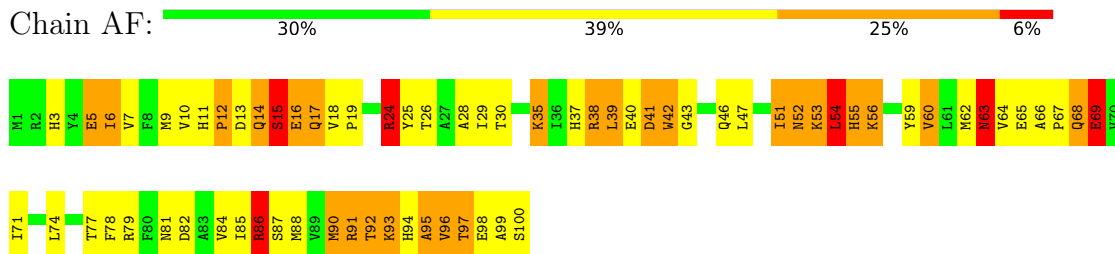
• Molecule 5: 30S ribosomal protein S5



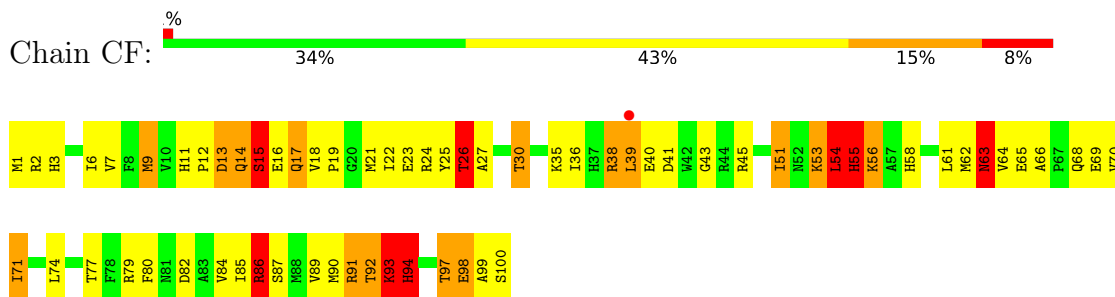
• Molecule 5: 30S ribosomal protein S5



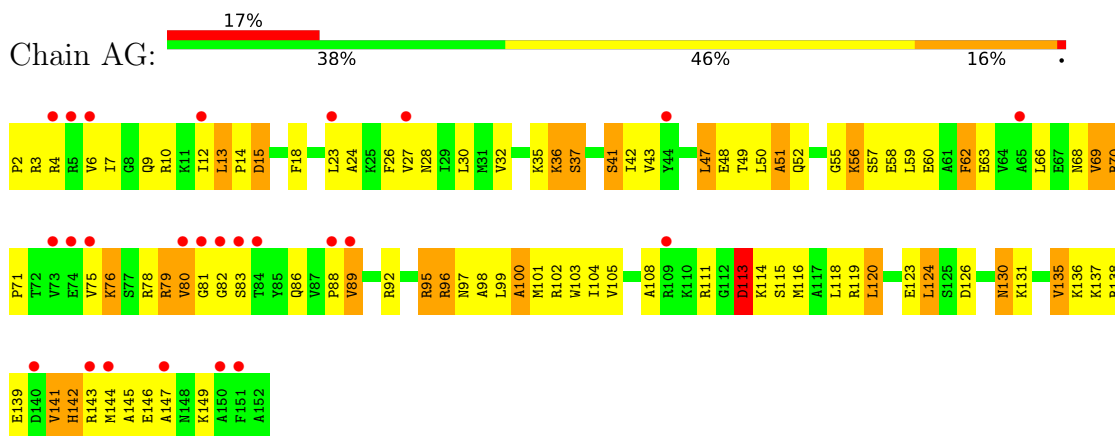
• Molecule 6: 30S ribosomal protein S6



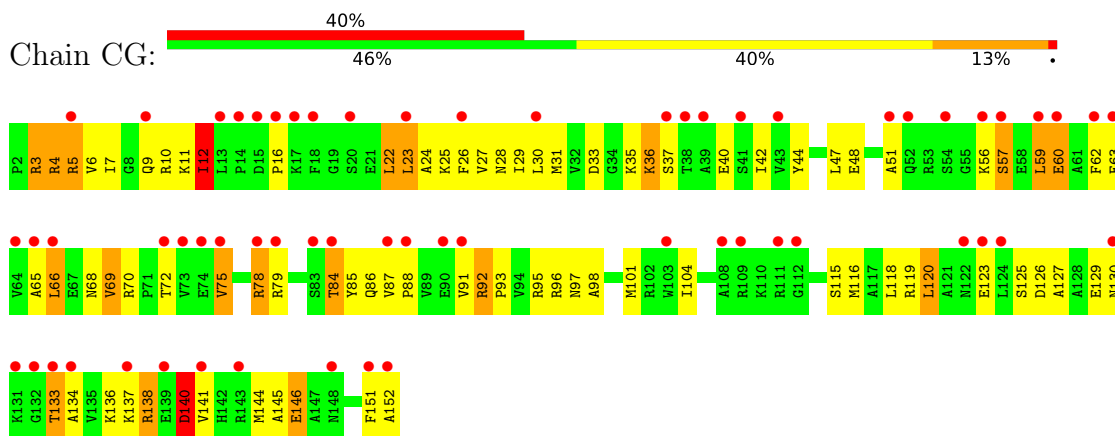
- Molecule 6: 30S ribosomal protein S6



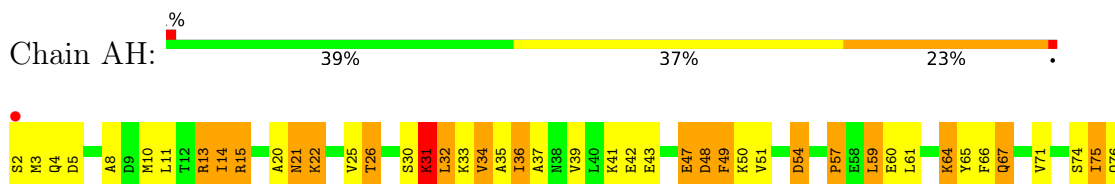
- Molecule 7: 30S ribosomal protein S7



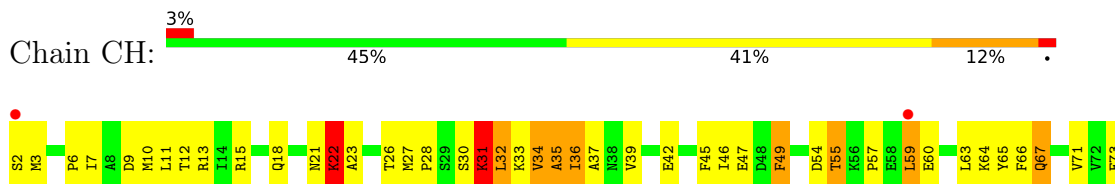
- Molecule 7: 30S ribosomal protein S7



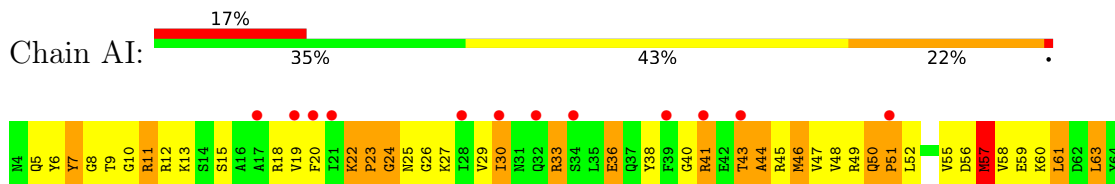
- Molecule 8: 30S ribosomal protein S8



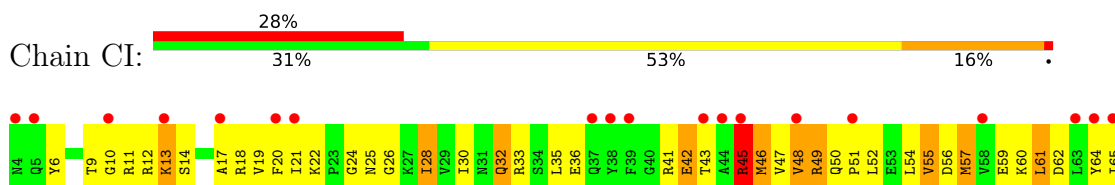
- Molecule 8: 30S ribosomal protein S8



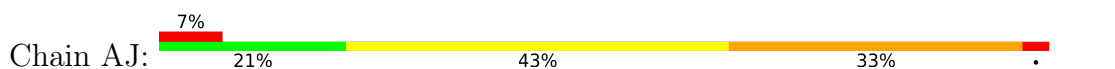
- Molecule 9: 30S ribosomal protein S9

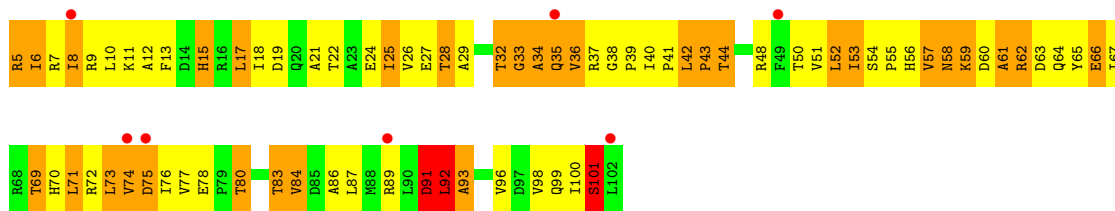


- Molecule 9: 30S ribosomal protein S9

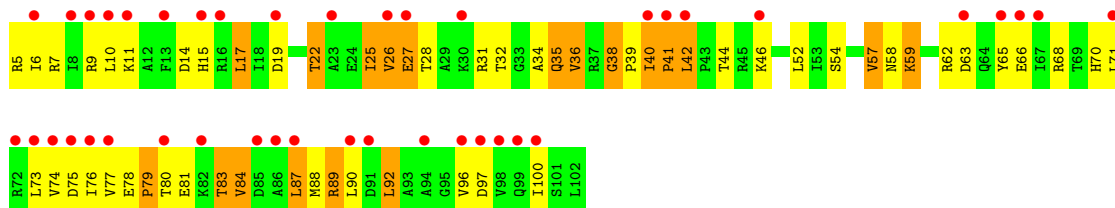
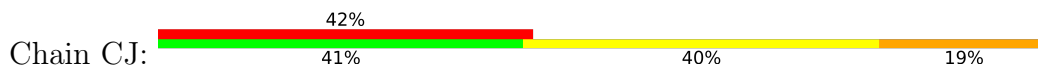


- Molecule 10: 30S ribosomal protein S10

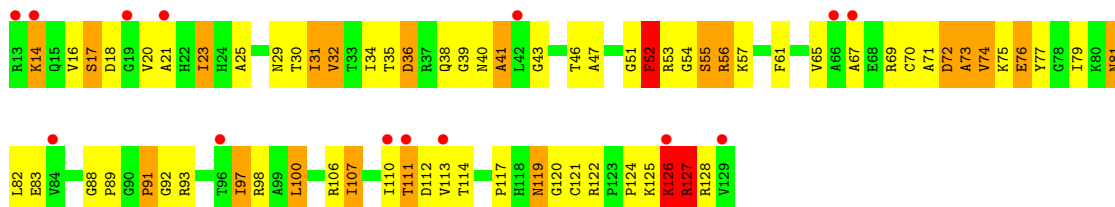
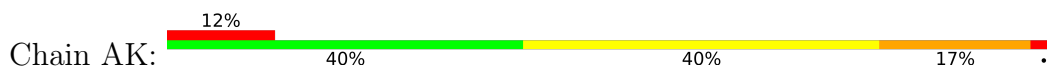




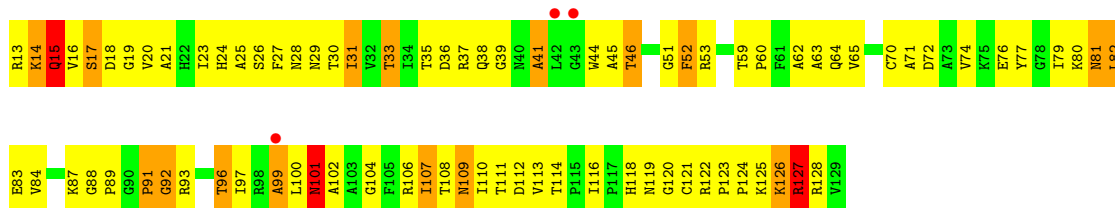
• Molecule 10: 30S ribosomal protein S10



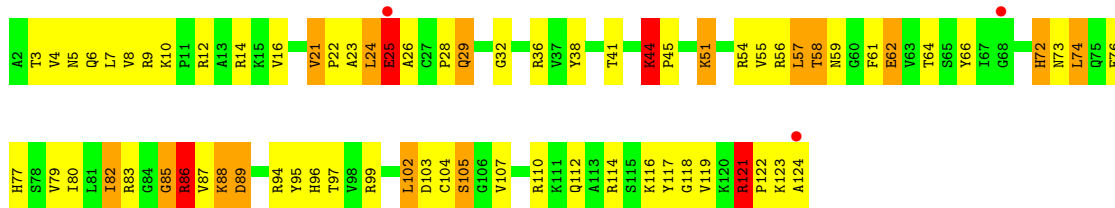
• Molecule 11: 30S ribosomal protein S11



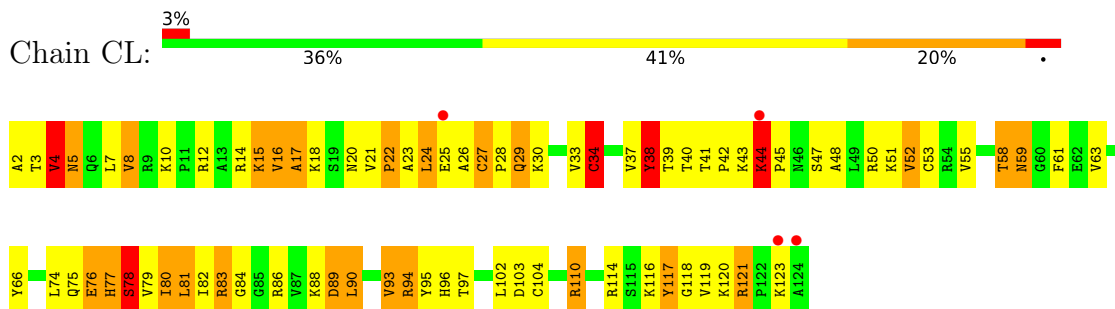
• Molecule 11: 30S ribosomal protein S11



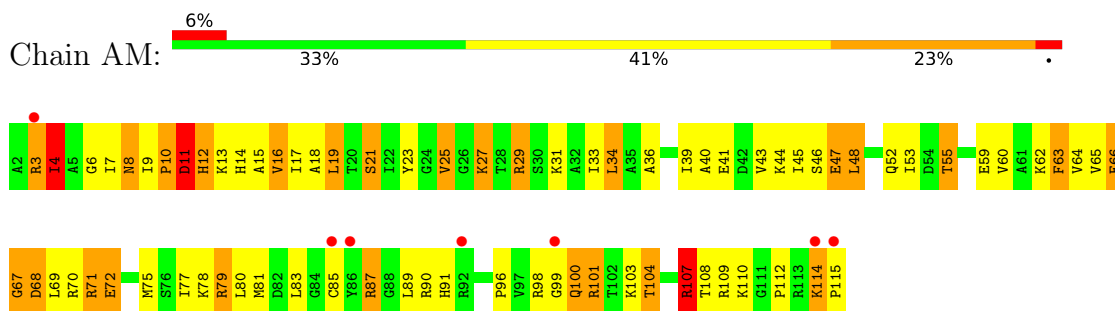
• Molecule 12: 30S ribosomal protein S12



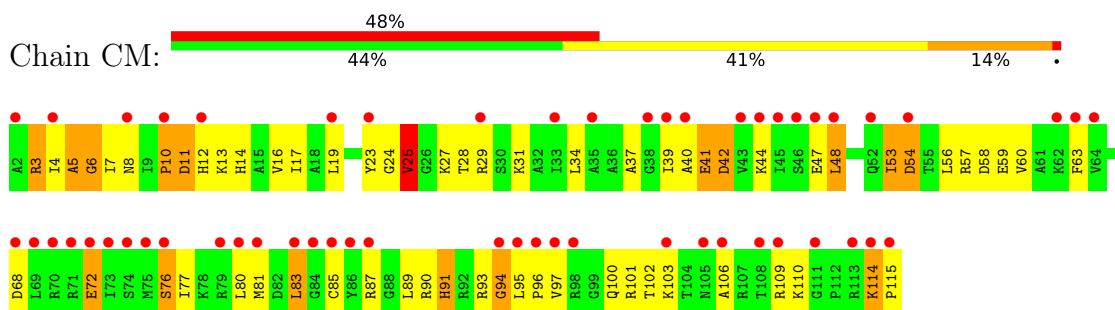
- Molecule 12: 30S ribosomal protein S12



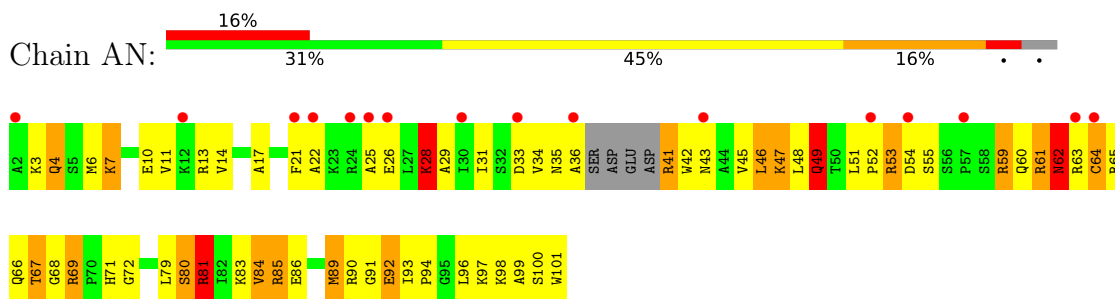
- Molecule 13: 30S ribosomal protein S13



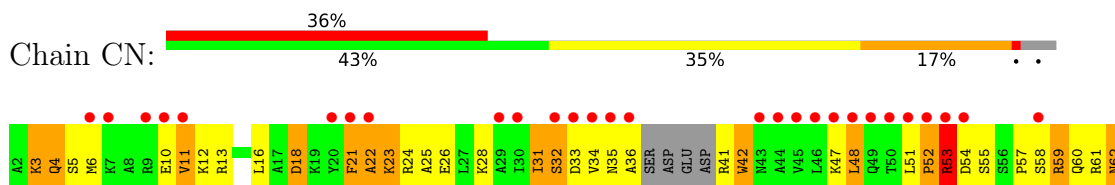
- Molecule 13: 30S ribosomal protein S13

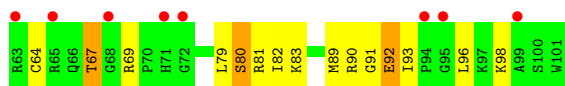


- Molecule 14: 30S ribosomal protein S14

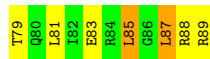
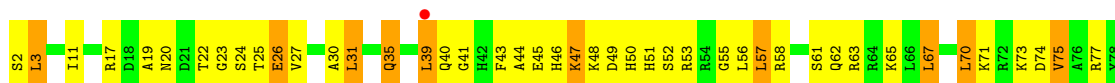
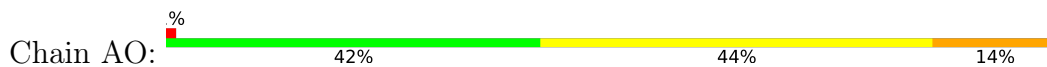


- Molecule 14: 30S ribosomal protein S14

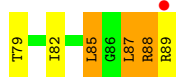
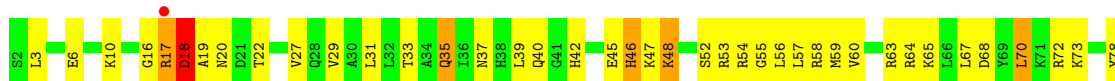




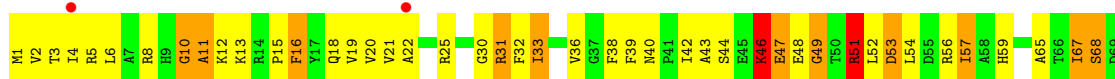
- Molecule 15: 30S ribosomal protein S15



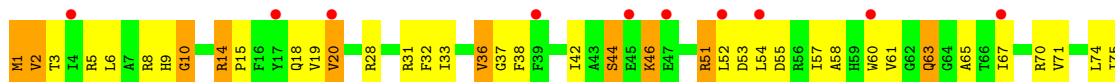
- Molecule 15: 30S ribosomal protein S15



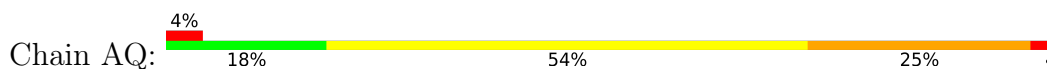
- Molecule 16: 30S ribosomal protein S16

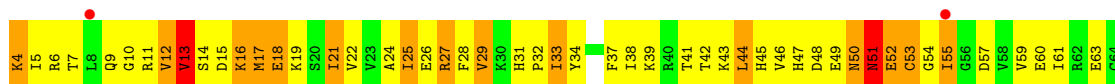


- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

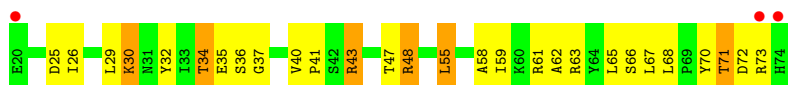




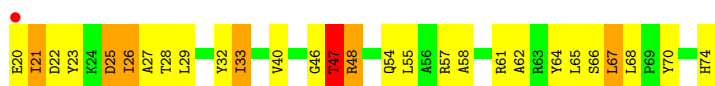
• Molecule 17: 30S ribosomal protein S17



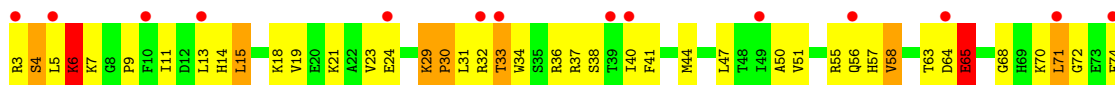
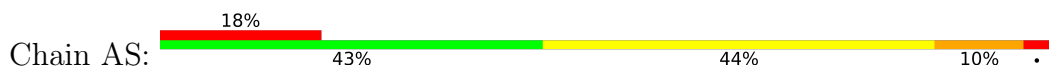
• Molecule 18: 30S ribosomal protein S18



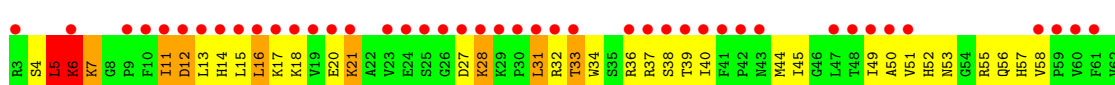
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19

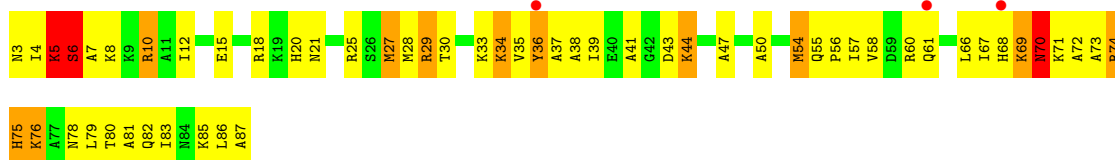
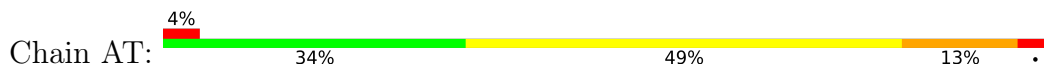


• Molecule 19: 30S ribosomal protein S19

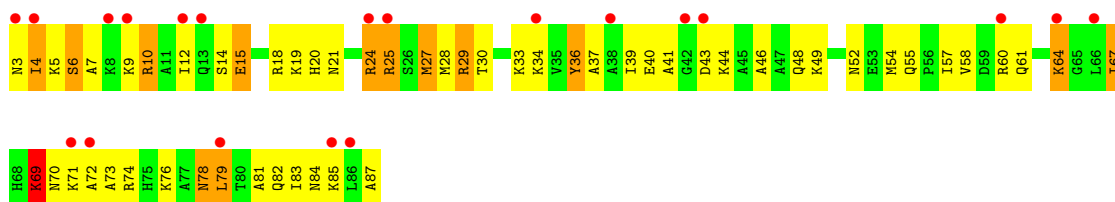




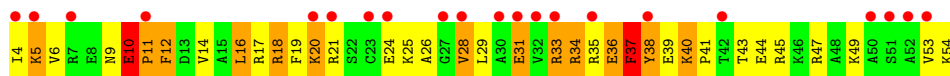
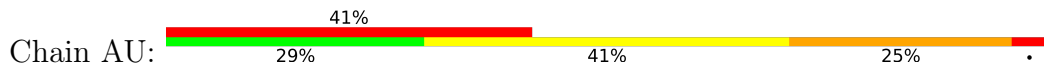
• Molecule 20: 30S ribosomal protein S20



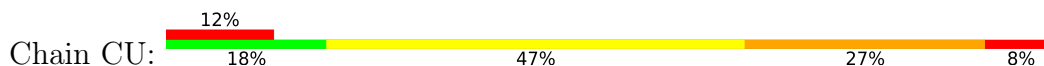
• Molecule 20: 30S ribosomal protein S20



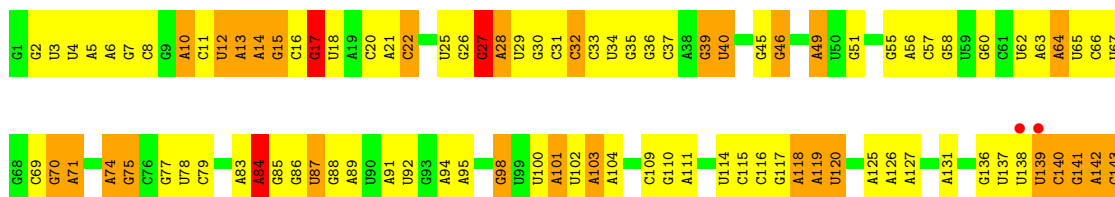
• Molecule 21: 30S ribosomal protein S21



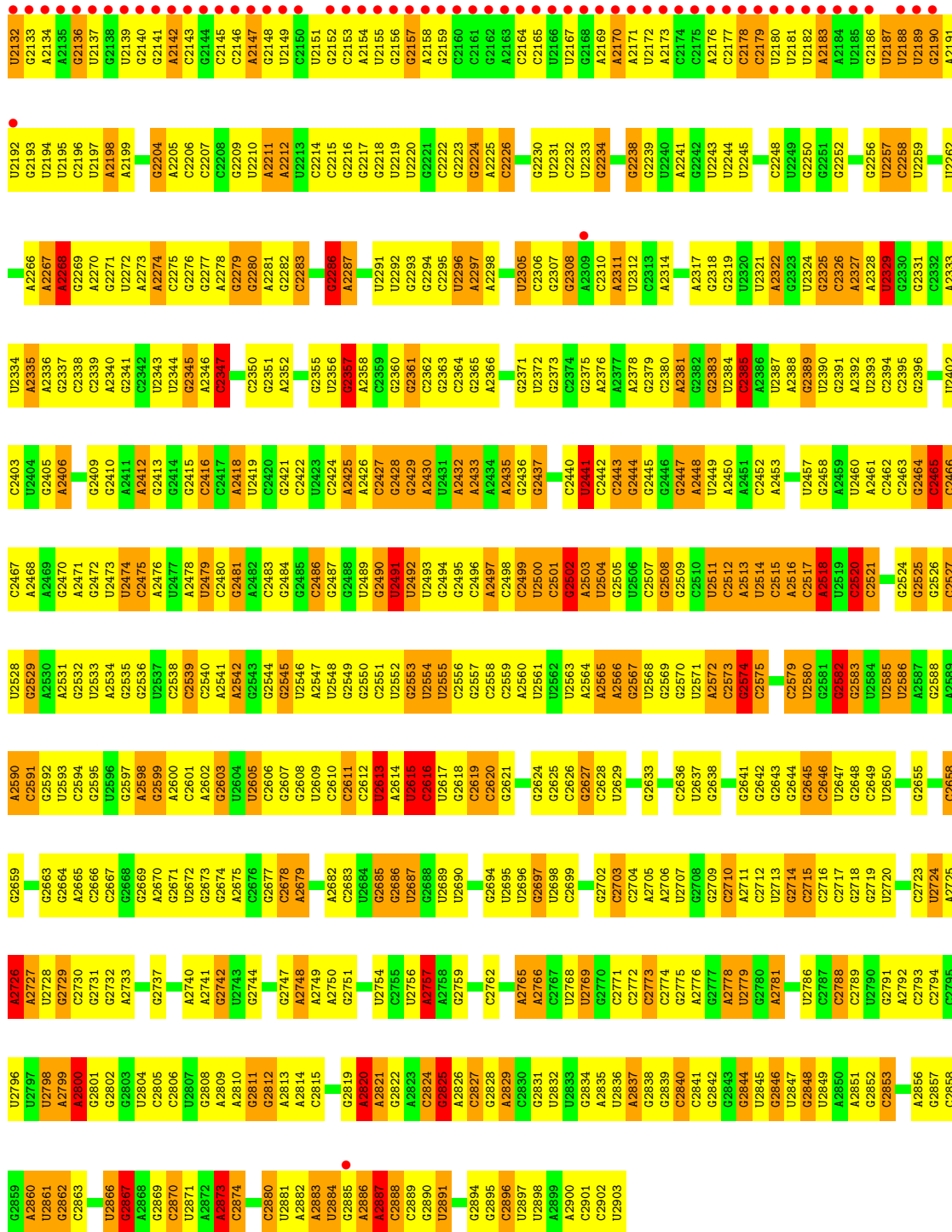
• Molecule 21: 30S ribosomal protein S21



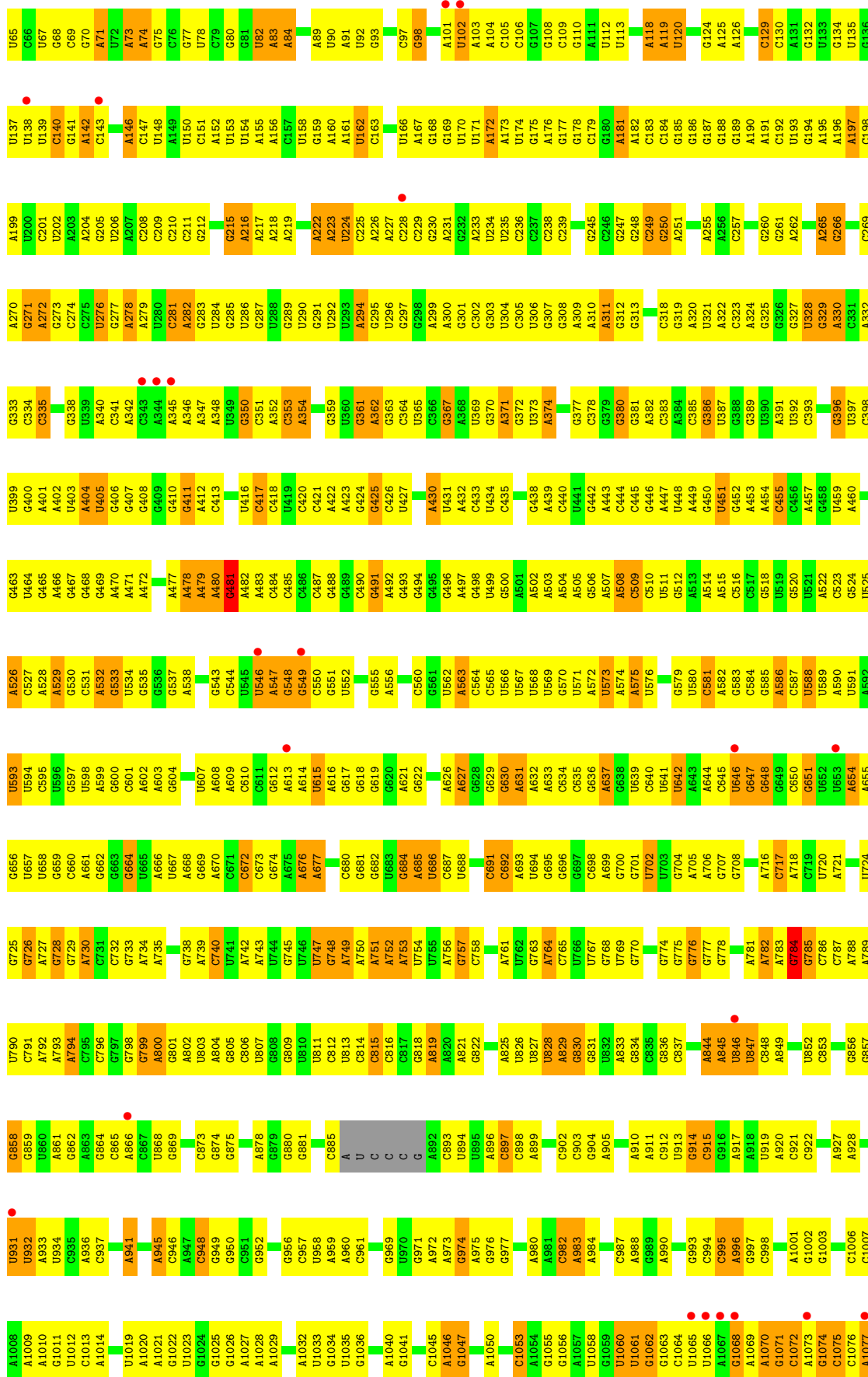
• Molecule 22: 23S rRNA

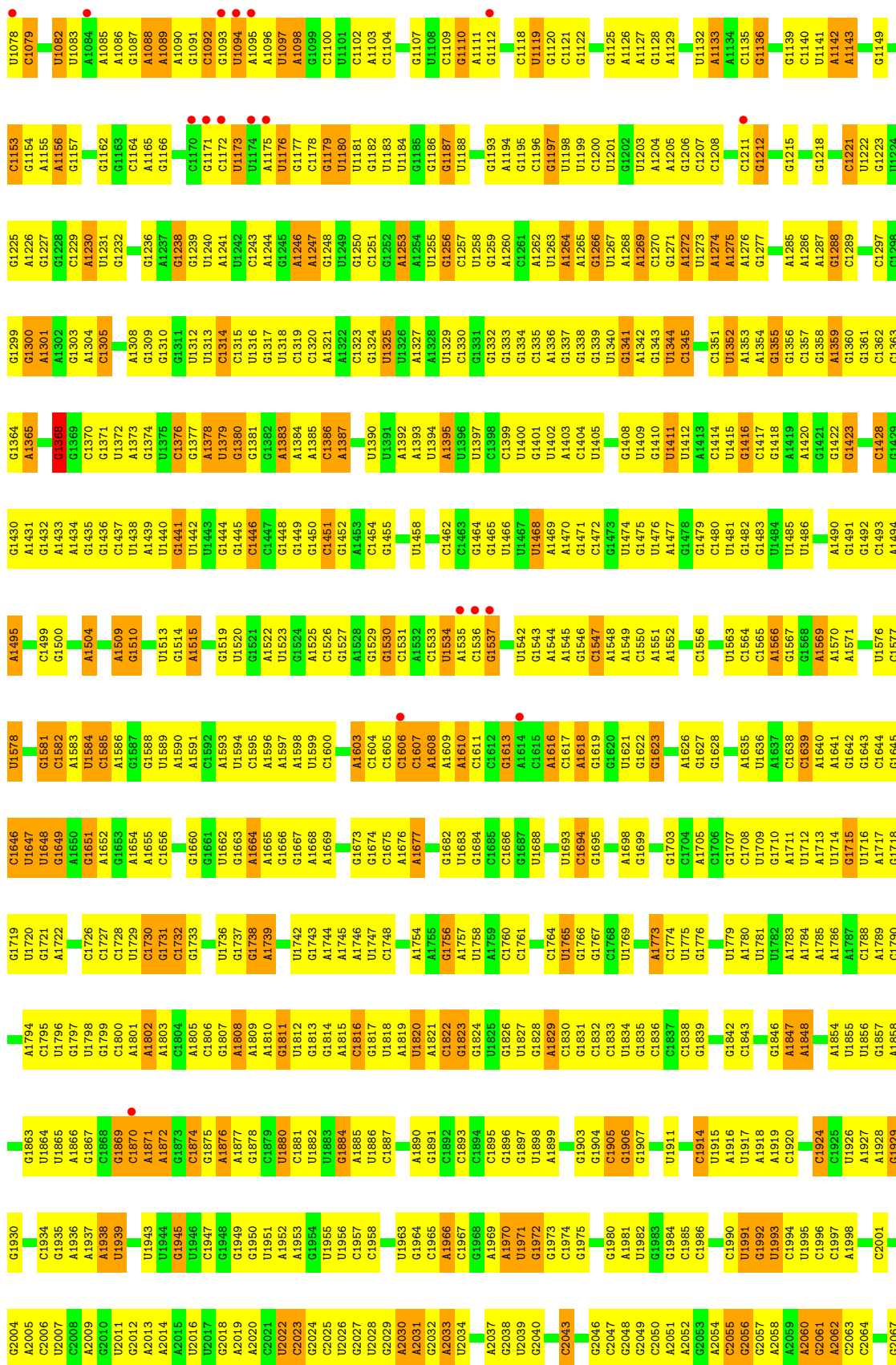


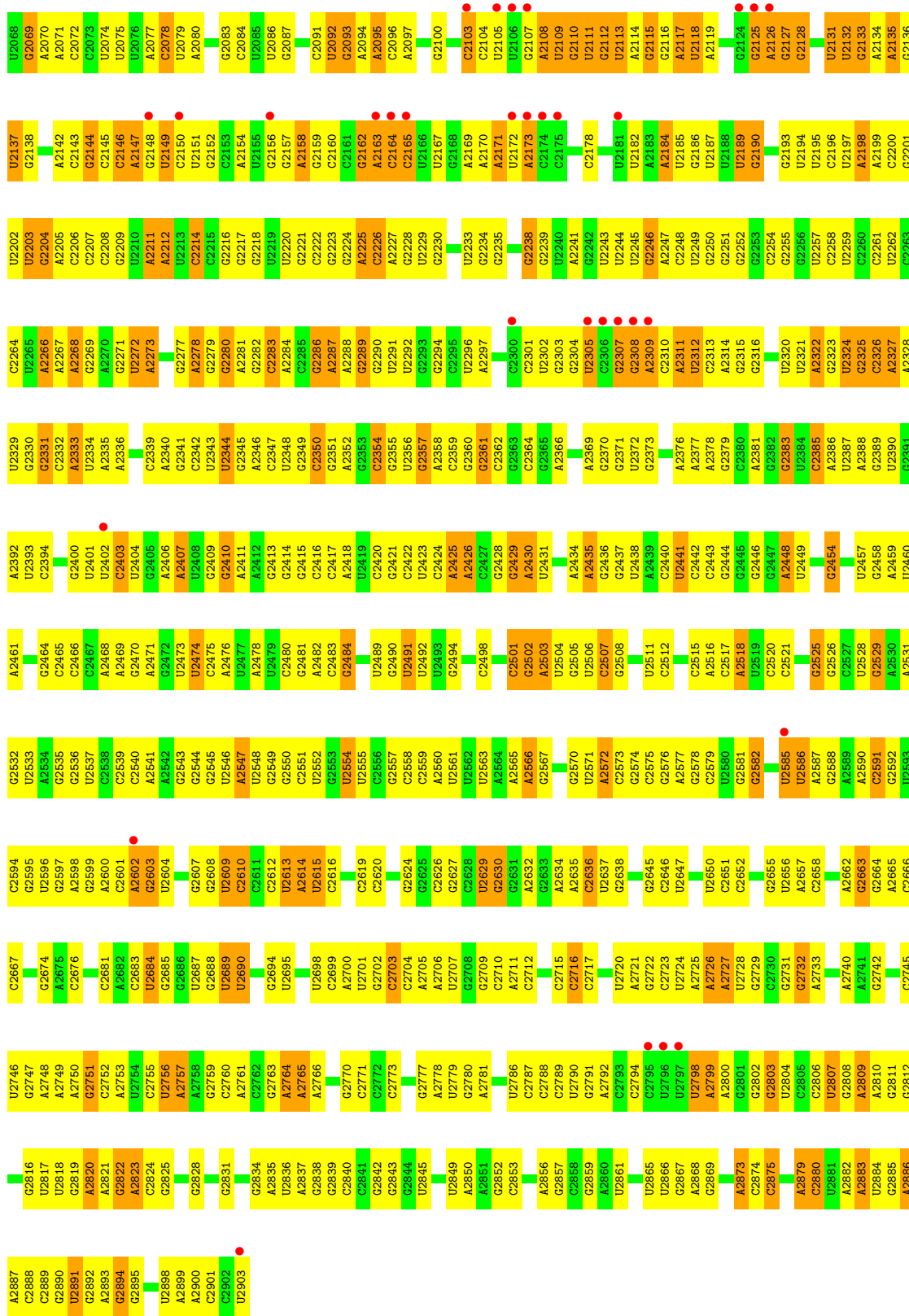
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U1798	G1799	G1800	A1801	A1802	A1805	A1806	G1807	A1808	A1809	A1810	G1811	U1812	G1813	G1816	G1817	U1818	A1819	U1820	G1821	G1822	G1823	U1824	U1825	G1826	U1827	A1828	A1829	C1830	G1833	U1834	C1838	G1839	G1840	U1841	G1842	C1843	G1846	A1847	A1848	G1849	U1850	U1851	U1852	A1853	A1854	U1855	U1856	G1857	A1858	U1859	G1863	U1864	U1865																																						
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U1586	G1587	G1588	U1589	A1590	A1591	G1592	A1593	A1594	A1595	U1599	G1600	G1601	A1602	A1603	A1604	G1606	C1607	A1608	A1609	A1610	G1613	A1614	C1617	G1618	G1619	G1620	A1621	A1622	U1623	G1624	G1625	A1626	G1627	G1628	G1631	A1632	G1633	A1634	A1635	A1636	A1637	C1638	G1639	A1640	G1643	A1644	A1645	A1646	A1647	A1648	A1649	A1650	A1651	A1652	A1653	A1654	A1655	A1656	A1657	A1658	A1659	A1660	A1661	A1662	A1663	A1664	A1665																								
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• Molecule 22: 23S rRNA

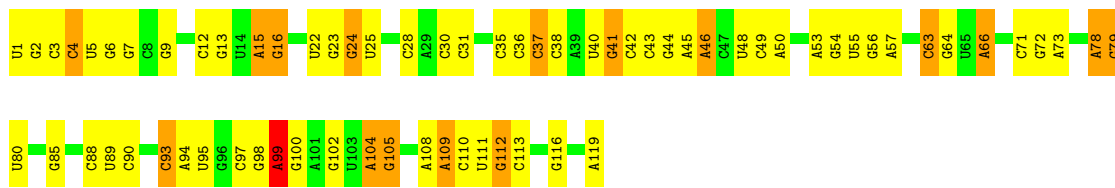




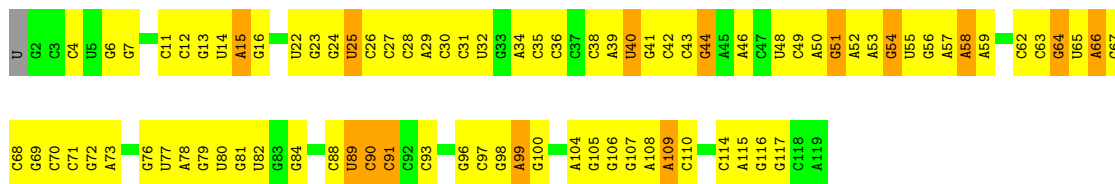


• Molecule 23: 5S rRNA

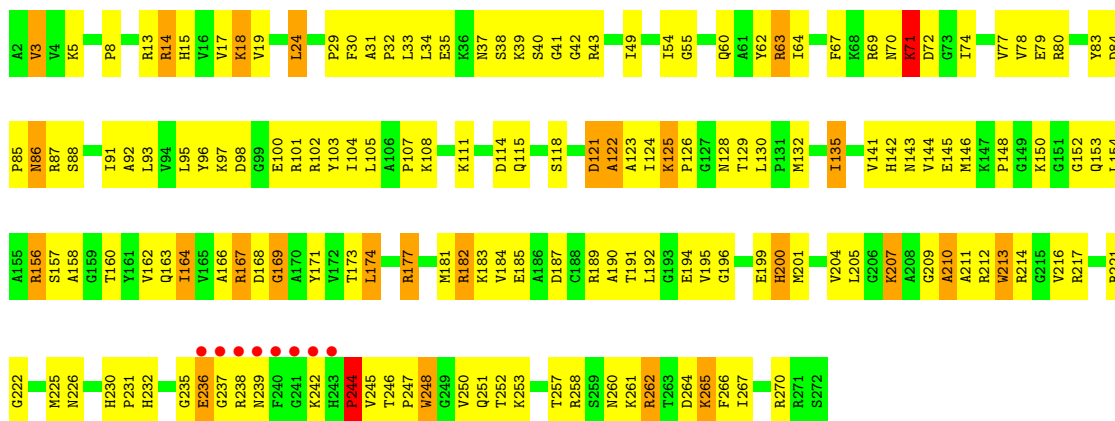




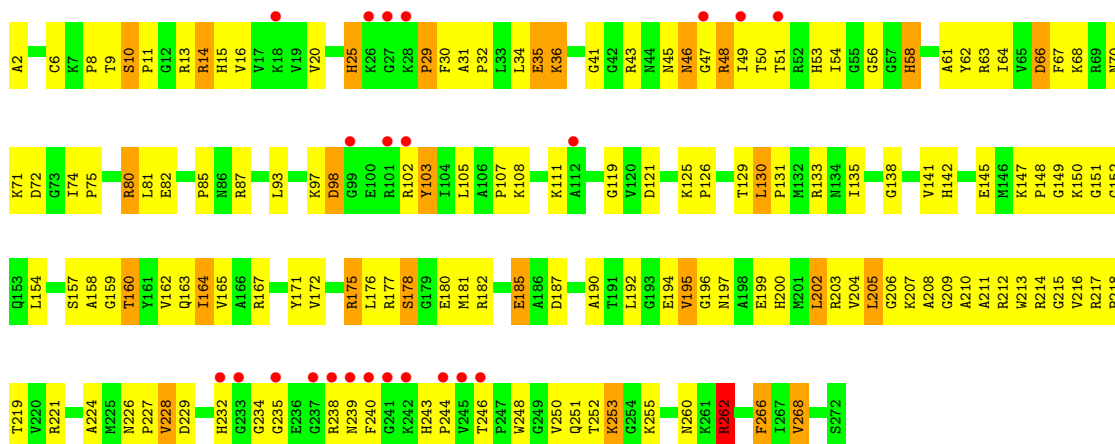
• Molecule 23: 5S rRNA



• Molecule 24: 50S ribosomal protein L2

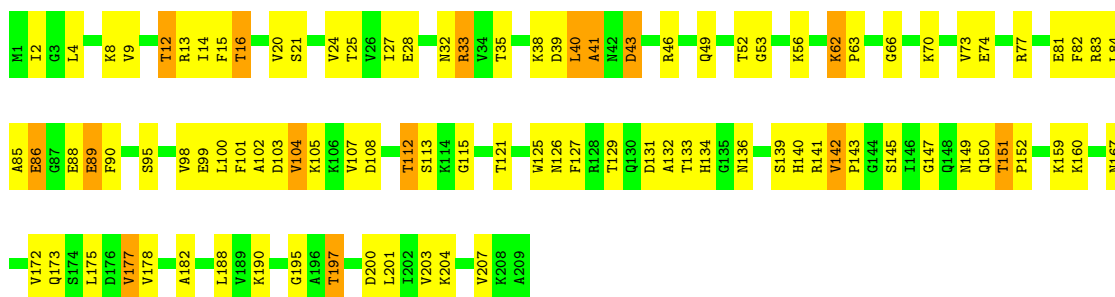


• Molecule 24: 50S ribosomal protein L2



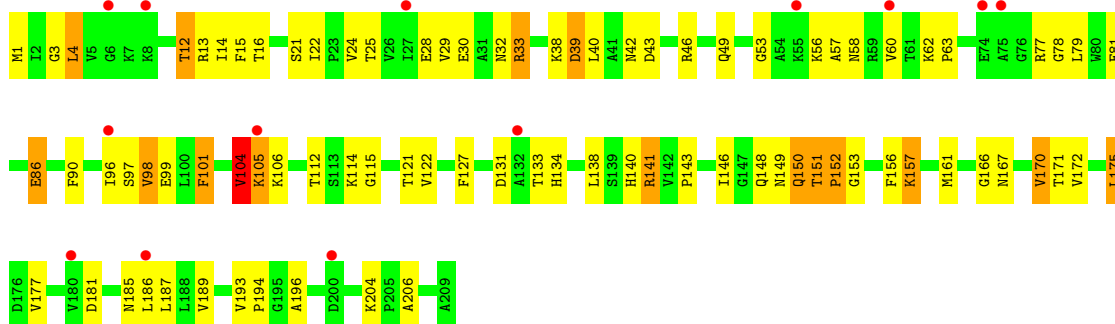
- Molecule 25: 50S ribosomal protein L3

Chain BD: 



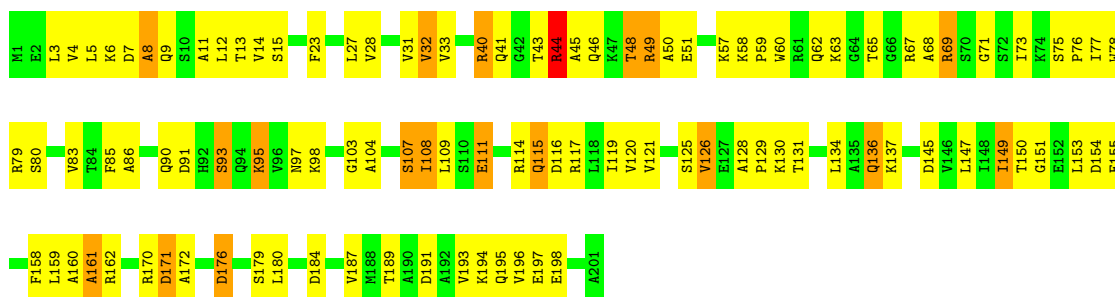
- Molecule 25: 50S ribosomal protein L3

Chain DD: 



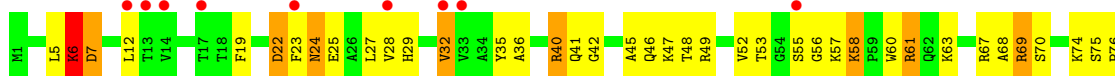
- Molecule 26: 50S ribosomal protein L4

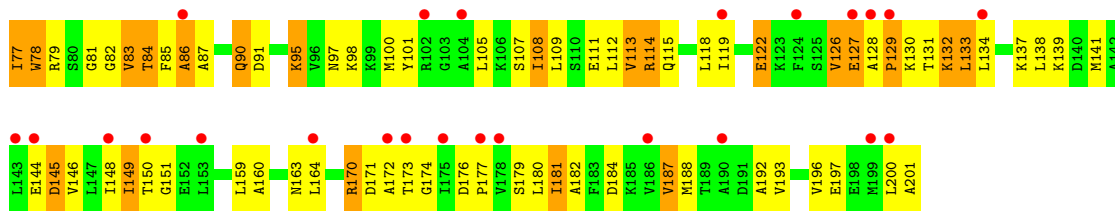
Chain BE: 



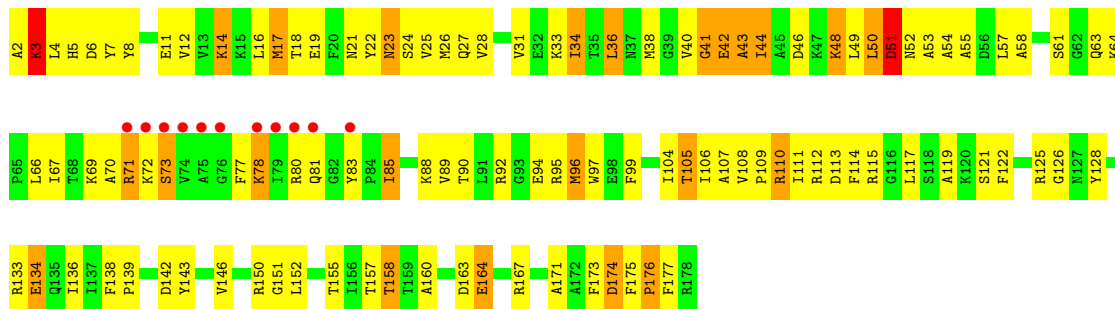
- Molecule 26: 50S ribosomal protein L4

Chain DE: 

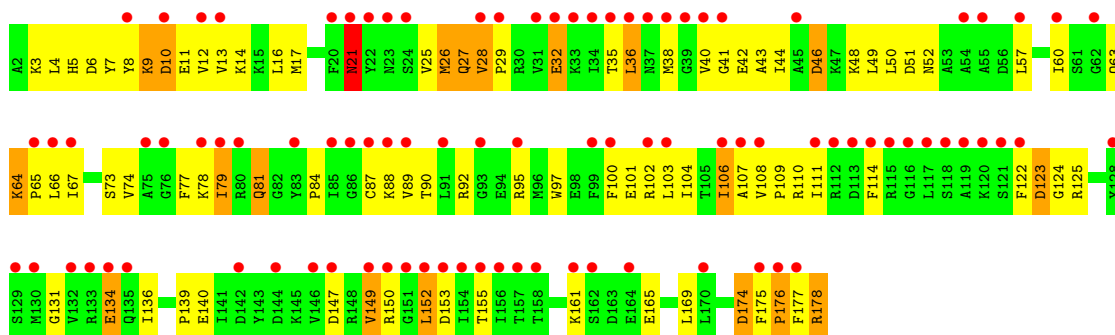




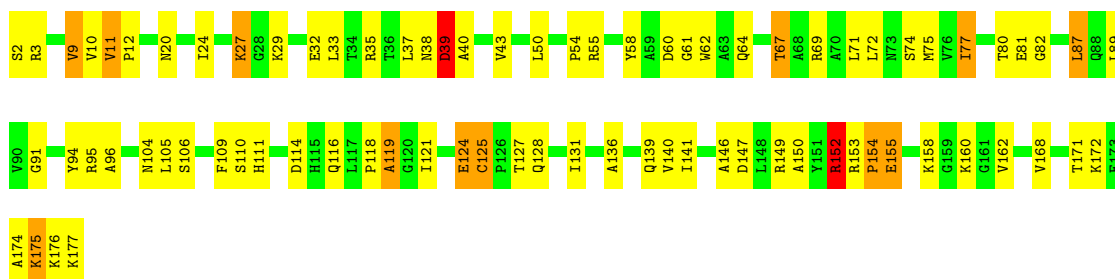
• Molecule 27: 50S ribosomal protein L5



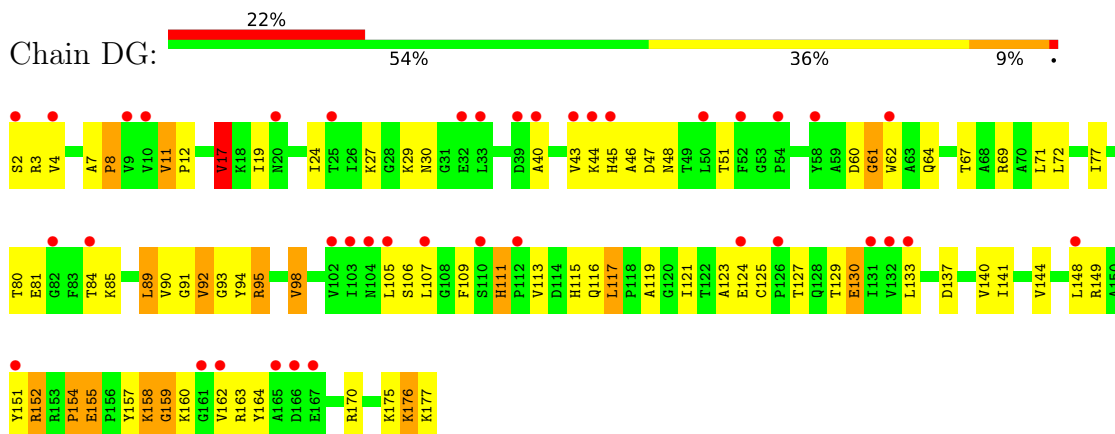
• Molecule 27: 50S ribosomal protein L5



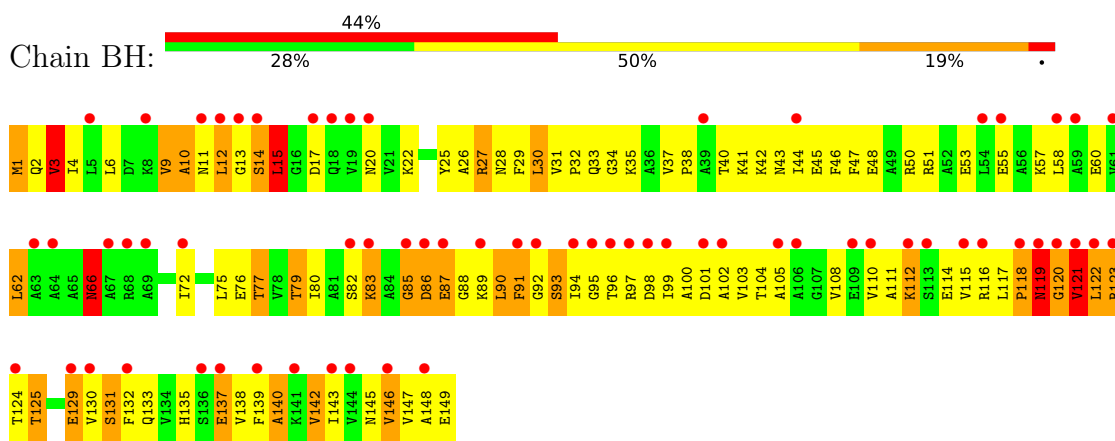
• Molecule 28: 50S ribosomal protein L6



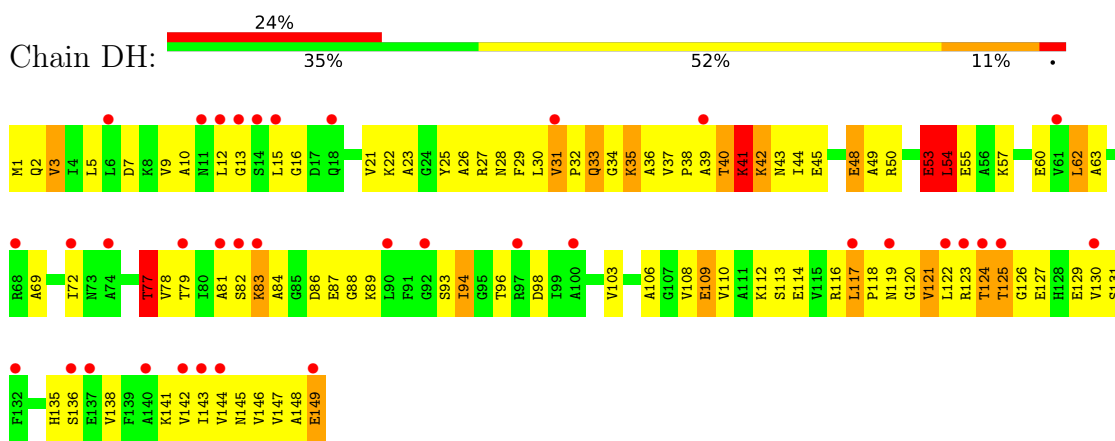
• Molecule 28: 50S ribosomal protein L6



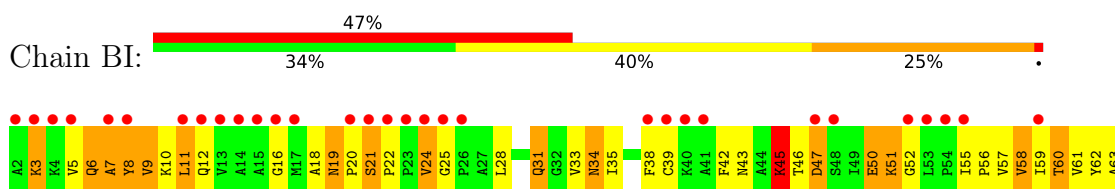
• Molecule 29: 50S ribosomal protein L9

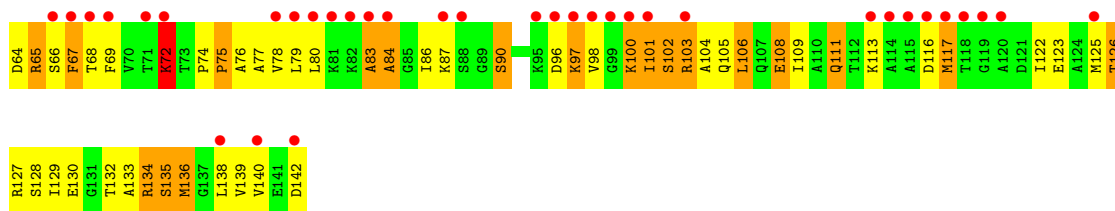


• Molecule 29: 50S ribosomal protein L9

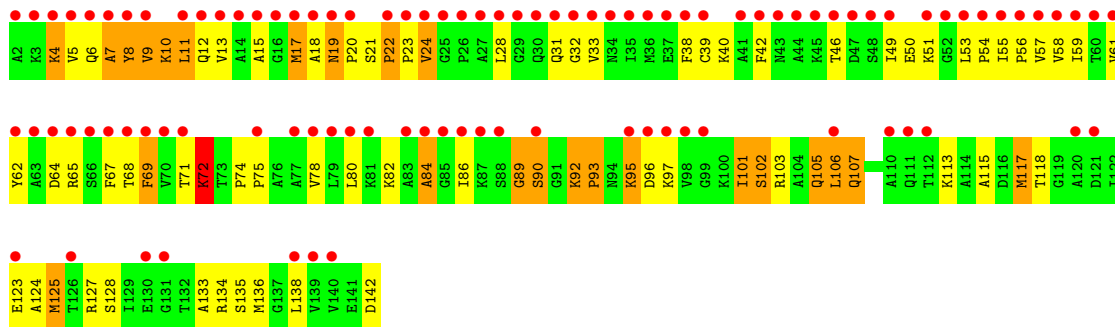
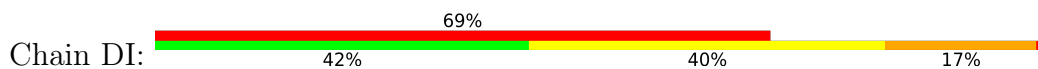


• Molecule 30: 50S ribosomal protein L11

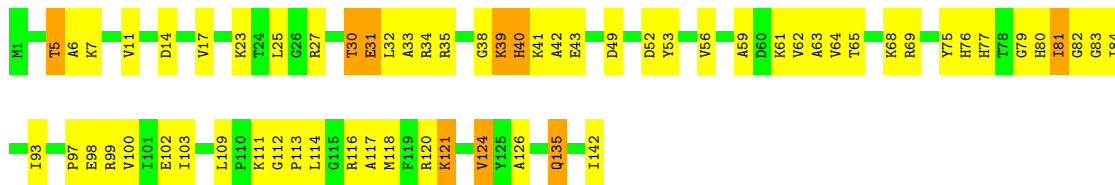




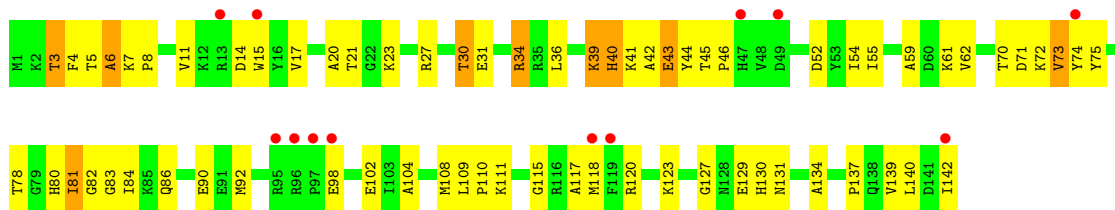
● Molecule 30: 50S ribosomal protein L11



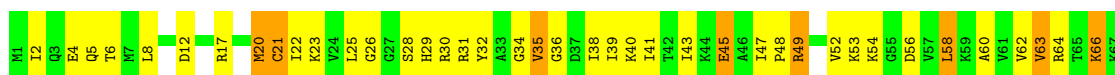
● Molecule 31: 50S ribosomal protein L13



● Molecule 31: 50S ribosomal protein L13

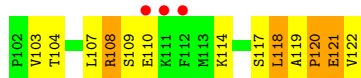


● Molecule 32: 50S ribosomal protein L14

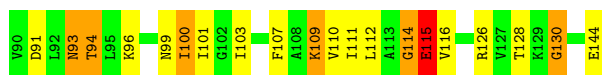




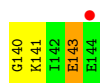
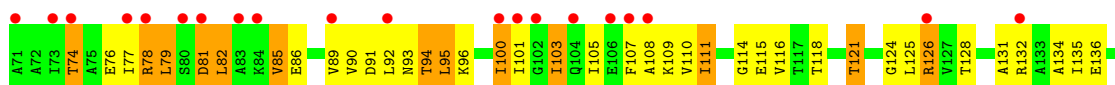
- Molecule 32: 50S ribosomal protein L14



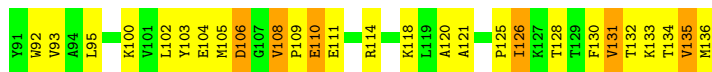
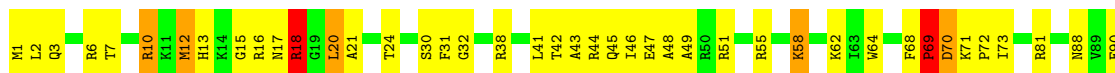
- Molecule 33: 50S ribosomal protein L15



- Molecule 33: 50S ribosomal protein L15

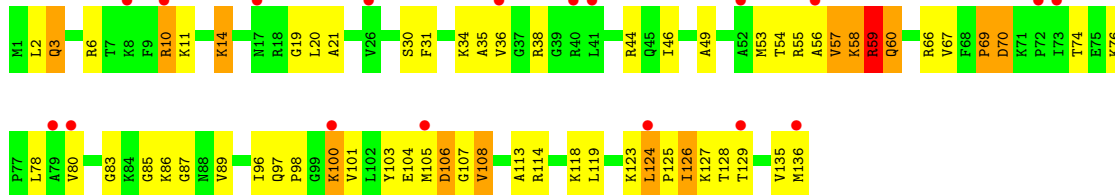


- Molecule 34: 50S ribosomal protein L16



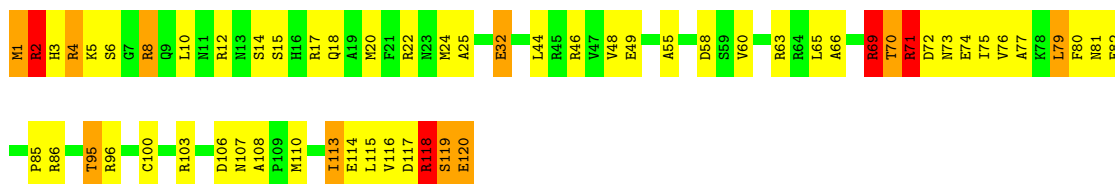
- Molecule 34: 50S ribosomal protein L16

Chain DM: 



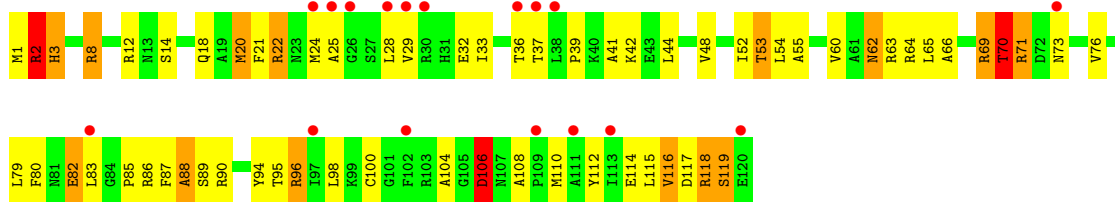
- Molecule 35: 50S ribosomal protein L17

Chain BN: 



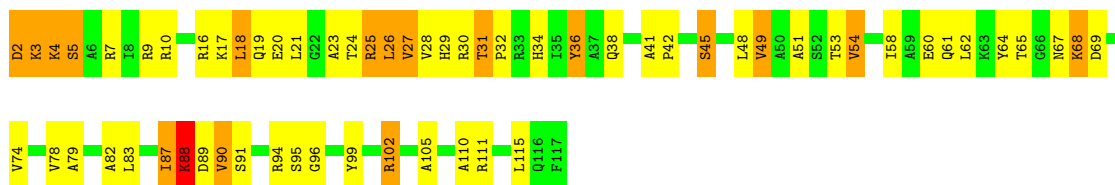
- Molecule 35: 50S ribosomal protein L17

Chain DN: 




- Molecule 36: 50S ribosomal protein L18

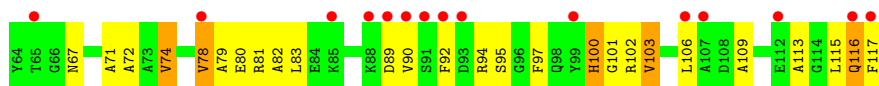
Chain BO: 



- Molecule 36: 50S ribosomal protein L18

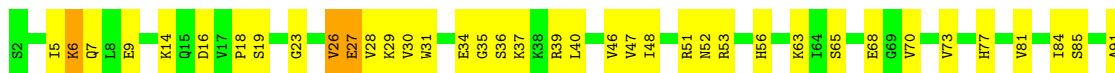
Chain DO: 





- Molecule 37: 50S ribosomal protein L19

Chain BP: 53% 39% 7%



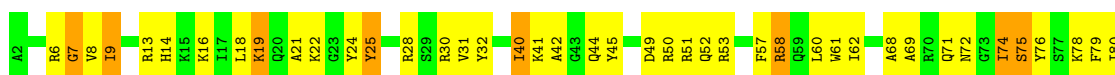
- Molecule 37: 50S ribosomal protein L19

Chain DP: 11% 54% 35% 11%



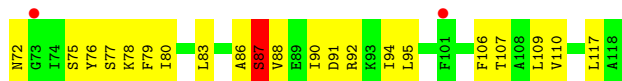
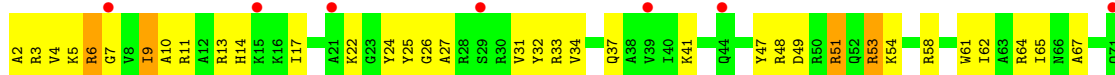
- Molecule 38: 50S ribosomal protein L20

Chain BQ: 48% 44% 9%



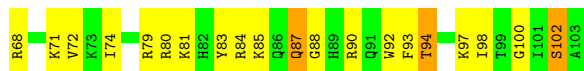
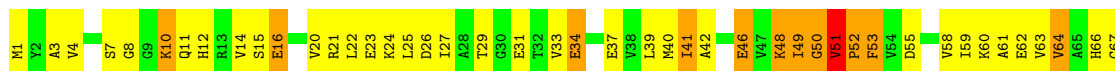
- Molecule 38: 50S ribosomal protein L20

Chain DQ: 8% 52% 44% 2%

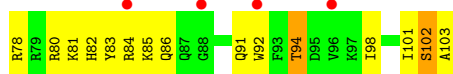
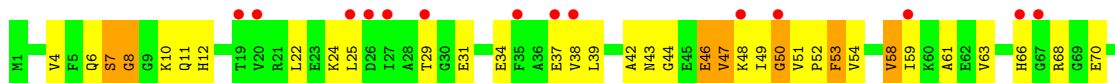


- Molecule 39: 50S ribosomal protein L21

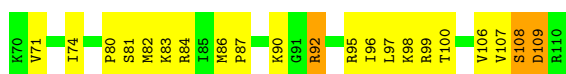
Chain BR: 37% 49% 14%



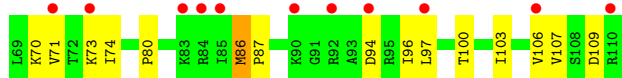
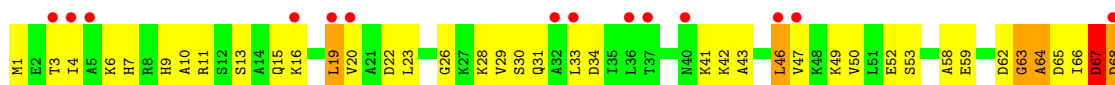
- Molecule 39: 50S ribosomal protein L21



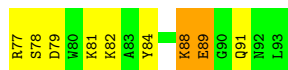
- Molecule 40: 50S ribosomal protein L22



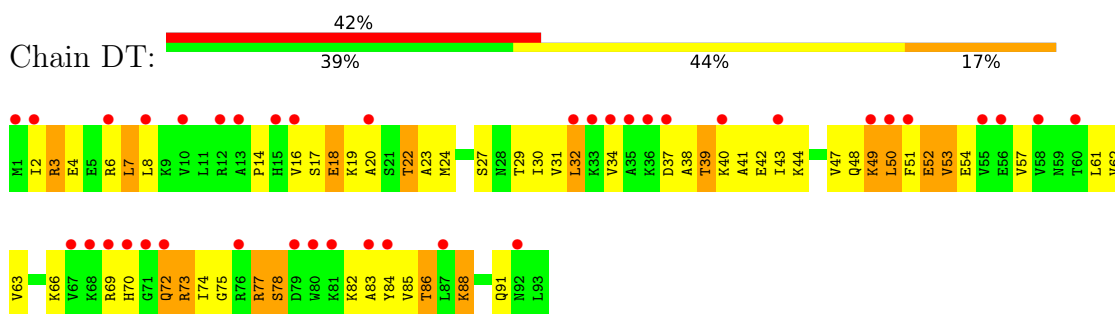
- Molecule 40: 50S ribosomal protein L22



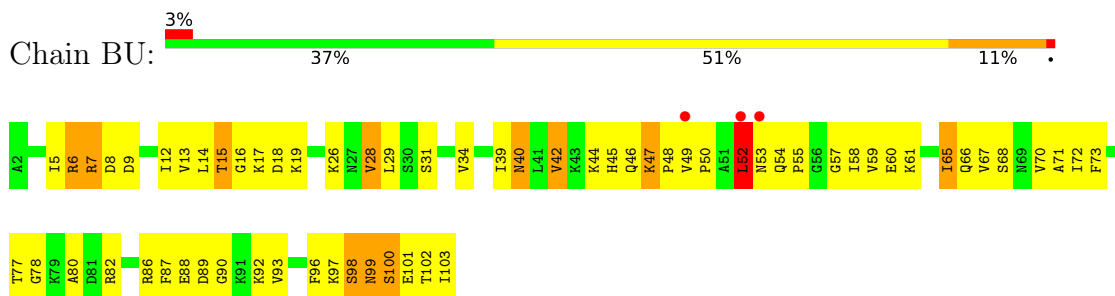
- Molecule 41: 50S ribosomal protein L23



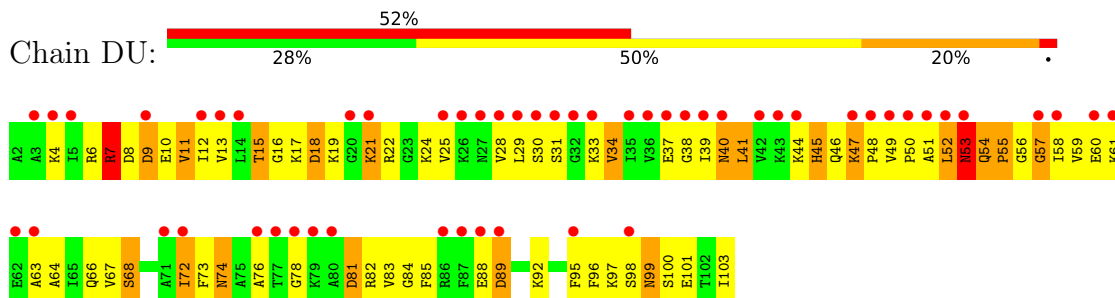
- Molecule 41: 50S ribosomal protein L23



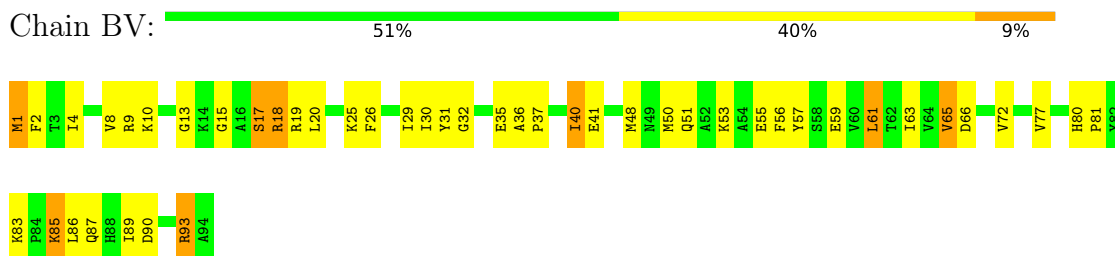
- Molecule 42: 50S ribosomal protein L24



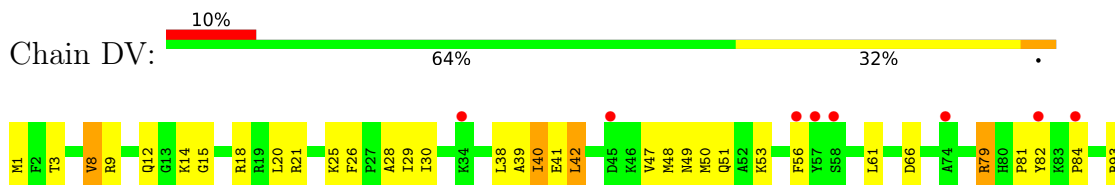
- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25



- Molecule 43: 50S ribosomal protein L25



A94

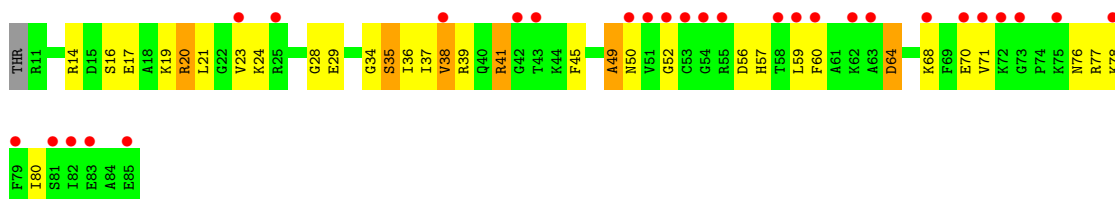
- Molecule 44: 50S ribosomal protein L27

Chain BW: 55% 39% 5%



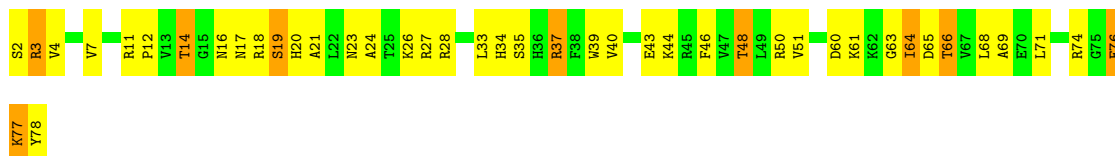
- Molecule 44: 50S ribosomal protein L27

Chain DW: 37% 55% 36% 8%



- Molecule 45: 50S ribosomal protein L28

Chain BX: 44% 44% 12%



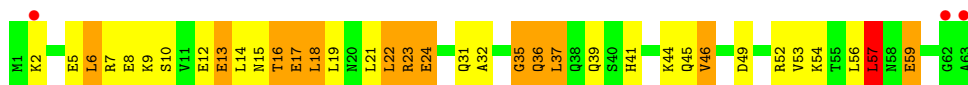
- Molecule 45: 50S ribosomal protein L28

Chain DX: 18% 34% 55% 12%

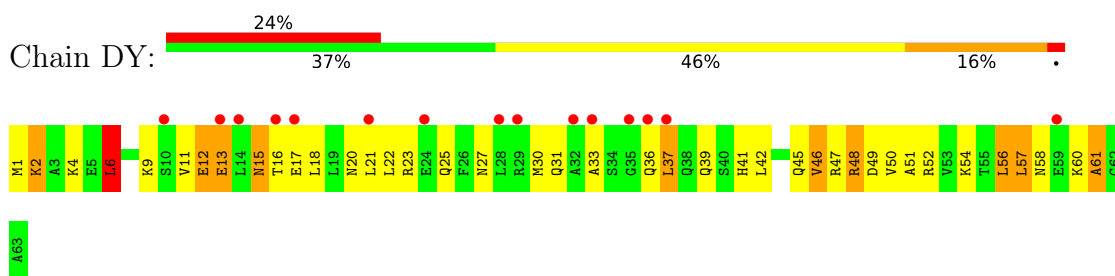


- Molecule 46: 50S ribosomal protein L29

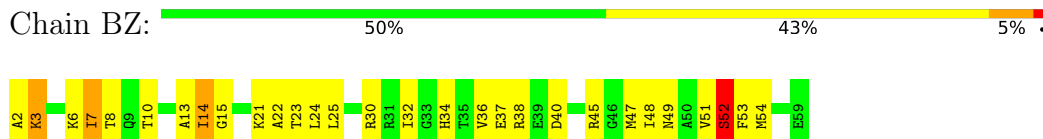
Chain BY: 5% 43% 35% 21%



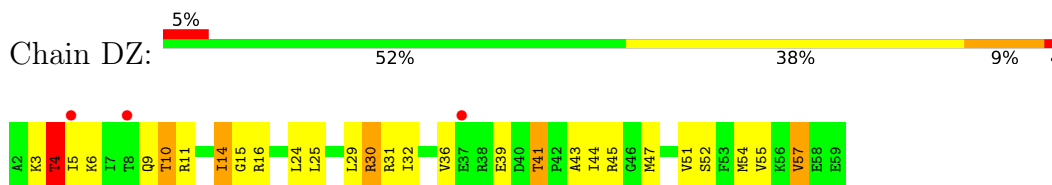
- Molecule 46: 50S ribosomal protein L29



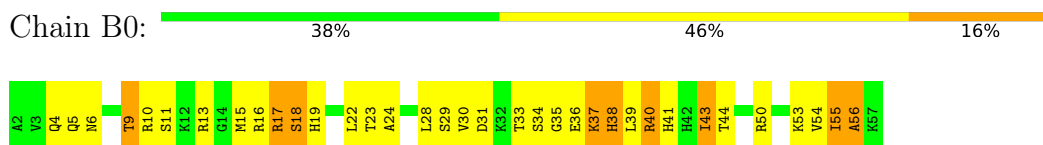
- Molecule 47: 50S ribosomal protein L30



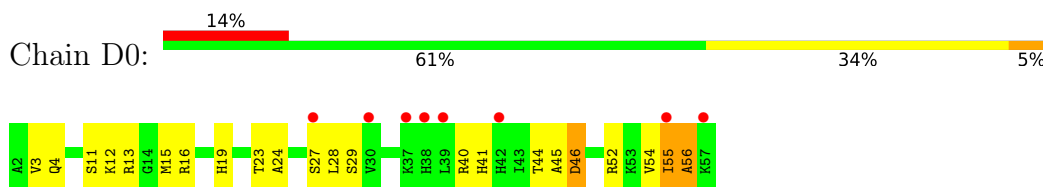
- Molecule 47: 50S ribosomal protein L30



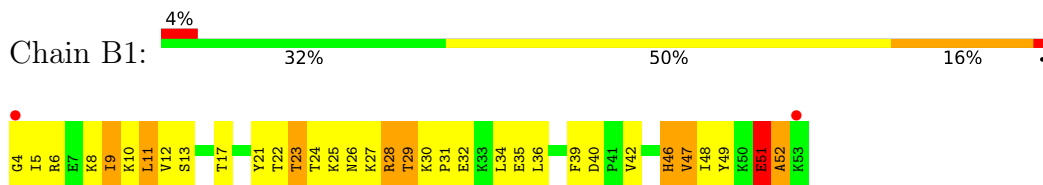
- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32

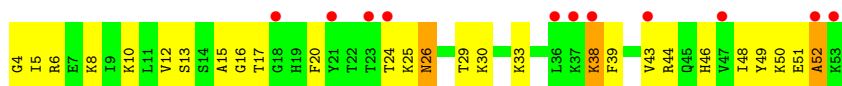


- Molecule 49: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L33





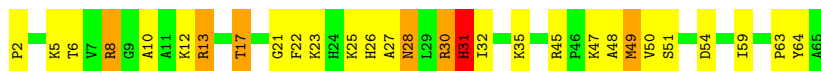
- Molecule 50: 50S ribosomal protein L34



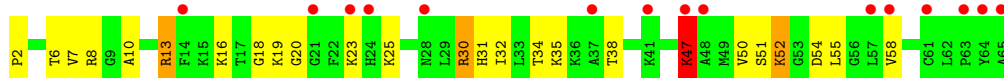
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



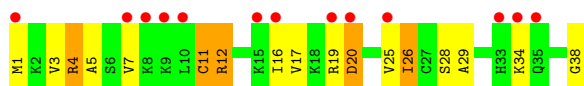
- Molecule 51: 50S ribosomal protein L35



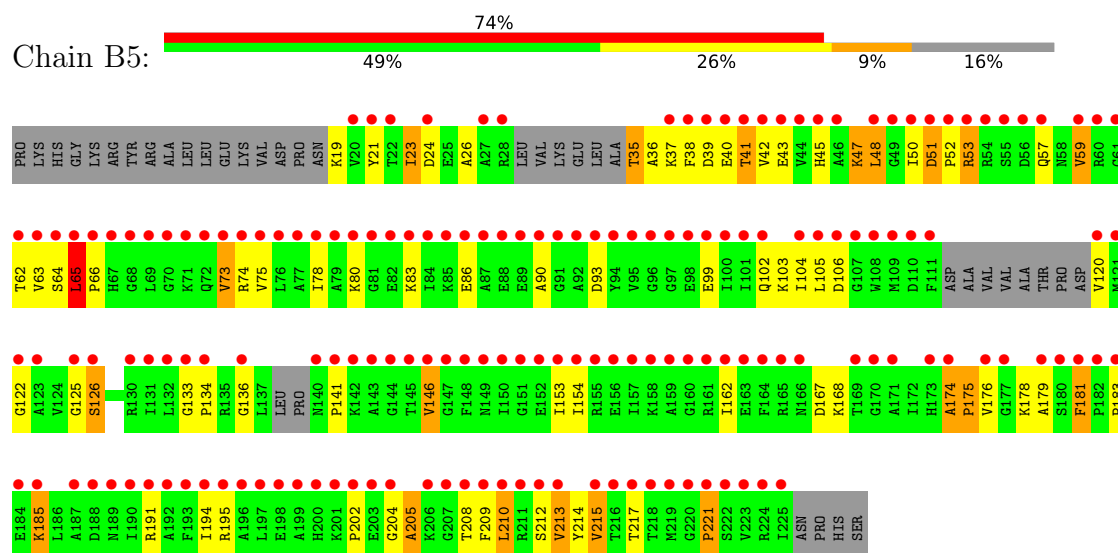
- Molecule 52: 50S ribosomal protein L36



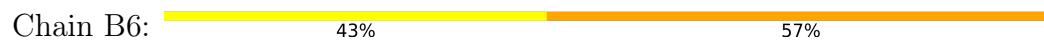
- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L1



- Molecule 54: Linopristin



MHW1	T2	T3	P4	F5	O4X6	O047
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- Molecule 54: Linopristin



MHW1	T2	T3	P4	F5	O4X6	O047
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.49Å 433.90Å 621.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.15 – 3.00 69.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (69.15-3.00) 90.2 (69.15-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.225 , 0.274 0.228 , 0.277	Depositor DCC
R_{free} test set	4092 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288320	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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, 004, MG, 04X, MHU, MHW

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	0.52	0/36944	1.02	48/57632 (0.1%)
1	CA	0.45	0/36966	0.96	27/57666 (0.0%)
2	AB	0.44	0/1736	0.65	0/2338
2	CB	0.38	0/1736	0.59	0/2338
3	AC	0.39	0/1652	0.61	0/2225
3	CC	0.37	0/1652	0.58	1/2225 (0.0%)
4	AD	0.39	0/1665	0.64	0/2227
4	CD	0.43	0/1665	0.65	0/2227
5	AE	0.41	0/1119	0.75	0/1504
5	CE	0.41	0/1119	0.73	0/1504
6	AF	0.41	0/836	0.77	2/1128 (0.2%)
6	CF	0.35	0/836	0.64	1/1128 (0.1%)
7	AG	0.37	0/1196	0.60	0/1602
7	CG	0.38	0/1196	0.54	0/1602
8	AH	0.40	0/989	0.63	0/1326
8	CH	0.34	0/989	0.57	0/1326
9	AI	0.39	0/1034	0.65	0/1375
9	CI	0.36	0/1034	0.59	0/1375
10	AJ	0.37	0/797	0.62	0/1077
10	CJ	0.36	0/797	0.61	0/1077
11	AK	0.38	0/893	0.63	0/1205
11	CK	0.37	0/893	0.61	0/1205
12	AL	0.41	0/969	0.71	0/1300
12	CL	0.41	0/969	0.73	0/1300
13	AM	0.38	0/893	0.70	1/1193 (0.1%)
13	CM	0.39	0/893	0.62	0/1193
14	AN	0.38	0/785	0.61	0/1043
14	CN	0.34	0/785	0.52	0/1043
15	AO	0.34	0/718	0.59	0/959
15	CO	0.32	0/718	0.57	0/959
16	AP	0.40	0/659	0.70	1/884 (0.1%)
16	CP	0.36	0/659	0.60	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/658	0.66	0/881
17	CQ	0.39	0/658	0.61	0/881
18	AR	0.37	0/463	0.61	0/621
18	CR	0.37	0/463	0.58	0/621
19	AS	0.43	0/653	0.66	0/877
19	CS	0.38	0/653	0.58	0/877
20	AT	0.43	0/671	0.63	0/888
20	CT	0.35	0/671	0.56	0/888
21	AU	0.50	0/431	0.71	0/570
21	CU	0.44	0/431	0.66	0/570
22	BA	0.90	44/69659 (0.1%)	1.39	725/108672 (0.7%)
22	DA	0.45	0/69659	0.95	28/108672 (0.0%)
23	BB	0.78	2/2850 (0.1%)	1.29	20/4444 (0.5%)
23	DB	0.39	0/2828	0.89	0/4410
24	BC	0.56	1/2122 (0.0%)	0.75	1/2852 (0.0%)
24	DC	0.37	0/2122	0.61	0/2852
25	BD	0.62	0/1586	0.80	1/2134 (0.0%)
25	DD	0.34	0/1586	0.55	0/2134
26	BE	0.54	0/1571	0.70	0/2113
26	DE	0.38	0/1571	0.60	0/2113
27	BF	0.41	0/1435	0.62	0/1926
27	DF	0.37	0/1435	0.53	0/1926
28	BG	0.45	0/1343	0.67	0/1816
28	DG	0.34	0/1343	0.52	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	0.44	0/1046	0.62	0/1410
30	DI	0.43	0/1046	0.59	0/1410
31	BJ	0.61	0/1152	0.75	1/1551 (0.1%)
31	DJ	0.35	0/1152	0.57	0/1551
32	BK	0.64	0/948	0.81	0/1268
32	DK	0.37	0/948	0.57	0/1268
33	BL	0.52	0/1054	0.75	0/1403
33	DL	0.38	0/1054	0.62	0/1403
34	BM	0.62	0/1093	0.80	1/1460 (0.1%)
34	DM	0.33	0/1093	0.56	0/1460
35	BN	0.61	0/974	0.88	3/1301 (0.2%)
35	DN	0.36	0/974	0.56	0/1301
36	BO	0.48	0/902	0.71	0/1209
36	DO	0.34	0/902	0.53	0/1209
37	BP	0.54	0/929	0.75	1/1242 (0.1%)
37	DP	0.37	0/929	0.58	0/1242
38	BQ	0.73	0/960	0.82	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.36	0/960	0.54	0/1278
39	BR	0.66	0/829	0.91	2/1107 (0.2%)
39	DR	0.36	0/829	0.59	0/1107
40	BS	0.72	0/864	0.81	0/1156
40	DS	0.36	0/864	0.63	0/1156
41	BT	0.49	0/745	0.68	0/994
41	DT	0.38	0/745	0.60	0/994
42	BU	0.48	0/788	0.72	0/1051
42	DU	0.43	0/788	0.61	0/1051
43	BV	0.52	0/766	0.70	0/1025
43	DV	0.32	0/766	0.48	0/1025
44	BW	0.64	0/587	0.79	0/776
44	DW	0.33	0/576	0.54	0/762
45	BX	0.45	0/635	0.73	0/848
45	DX	0.36	0/635	0.60	0/848
46	BY	0.46	0/510	0.71	0/677
46	DY	0.39	0/510	0.61	0/677
47	BZ	0.61	0/453	0.82	1/605 (0.2%)
47	DZ	0.32	0/453	0.58	0/605
48	B0	0.64	0/450	0.91	2/599 (0.3%)
48	D0	0.35	0/450	0.58	0/599
49	B1	0.46	0/417	0.67	0/554
49	D1	0.35	0/417	0.51	0/554
50	B2	0.55	0/380	0.83	0/498
50	D2	0.38	0/380	0.61	0/498
51	B3	0.58	0/513	0.75	0/676
51	D3	0.33	0/513	0.57	0/676
52	B4	0.60	0/303	0.71	0/397
52	D4	0.32	0/303	0.54	0/397
53	B5	0.39	0/1145	0.56	0/1556
54	B6	3.67	4/13 (30.8%)	4.12	3/15 (20.0%)
54	D6	3.86	3/13 (23.1%)	3.82	4/15 (26.7%)
All	All	0.59	54/310652 (0.0%)	1.02	876/464396 (0.2%)

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	CL	0	2
21	AU	0	1
25	BD	0	1
25	DD	0	1
33	BL	0	1
48	B0	0	1
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-12.83	1.30	1.37
22	BA	528	A	N9-C4	-10.27	1.31	1.37
22	BA	528	A	N3-C4	-8.70	1.29	1.34
22	BA	974	G	N9-C4	-8.12	1.31	1.38
22	BA	979	A	N9-C4	-7.80	1.33	1.37

The worst 5 of 876 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	974	G	C4-C5-N7	15.39	116.95	110.80
22	BA	974	G	C5-N7-C8	-15.02	96.79	104.30
22	BA	752	A	N1-C6-N6	14.90	127.54	118.60
22	BA	974	G	N1-C6-O6	14.51	128.61	119.90
22	BA	1779	U	N3-C4-O4	-13.09	110.24	119.40

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
48	B0	24	ALA	Peptide
25	BD	151	THR	Peptide
33	BL	28	GLY	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	1338	4
1	CA	33015	0	16617	1198	0
2	AB	1705	0	1732	164	0
2	CB	1705	0	1732	121	0
3	AC	1625	0	1696	89	0
3	CC	1625	0	1696	80	0
4	AD	1643	0	1707	133	0
4	CD	1643	0	1707	144	0
5	AE	1106	0	1148	83	0
5	CE	1106	0	1148	104	0
6	AF	818	0	808	62	0
6	CF	818	0	808	56	0
7	AG	1182	0	1238	65	0
7	CG	1182	0	1238	59	0
8	AH	979	0	1031	67	0
8	CH	979	0	1031	47	0
9	AI	1022	0	1070	77	0
9	CI	1022	0	1070	69	0
10	AJ	787	0	828	87	0
10	CJ	787	0	828	48	0
11	AK	877	0	887	79	0
11	CK	877	0	887	72	0
12	AL	955	0	1016	65	0
12	CL	955	0	1016	61	0
13	AM	884	0	941	80	0
13	CM	884	0	941	46	0
14	AN	774	0	824	66	0
14	CN	774	0	824	44	0
15	AO	710	0	728	35	0
15	CO	710	0	728	42	0
16	AP	649	0	666	53	0
16	CP	649	0	666	30	0
17	AQ	649	0	691	69	0
17	CQ	649	0	691	50	0
18	AR	456	0	478	22	0
18	CR	456	0	478	23	0
19	AS	638	0	665	48	0
19	CS	638	0	665	38	0
20	AT	665	0	714	54	0
20	CT	665	0	714	38	0
21	AU	426	0	449	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CU	426	0	449	37	0
22	BA	62195	0	31280	2134	0
22	DA	62195	0	31280	2174	0
23	BB	2549	0	1291	56	0
23	DB	2529	0	1281	72	0
24	BC	2083	0	2154	157	0
24	DC	2083	0	2154	123	0
25	BD	1565	0	1616	92	0
25	DD	1565	0	1616	81	0
26	BE	1552	0	1619	75	0
26	DE	1552	0	1619	103	0
27	BF	1411	0	1444	105	0
27	DF	1411	0	1444	63	0
28	BG	1323	0	1371	61	0
28	DG	1323	0	1371	56	0
29	BH	1110	0	1147	154	0
29	DH	1110	0	1148	90	4
30	BI	1032	0	1085	82	0
30	DI	1032	0	1085	72	0
31	BJ	1129	0	1162	64	0
31	DJ	1129	0	1162	55	0
32	BK	939	0	1012	75	0
32	DK	939	0	1012	38	0
33	BL	1045	0	1117	51	0
33	DL	1045	0	1117	81	0
34	BM	1074	0	1157	47	0
34	DM	1074	0	1157	43	0
35	BN	961	0	1000	51	0
35	DN	961	0	1000	55	0
36	BO	892	0	923	57	0
36	DO	892	0	923	50	0
37	BP	917	0	962	48	0
37	DP	917	0	962	47	0
38	BQ	947	0	1019	61	0
38	DQ	947	0	1019	55	0
39	BR	816	0	839	84	0
39	DR	816	0	839	47	0
40	BS	857	0	922	64	0
40	DS	857	0	922	39	0
41	BT	739	0	807	46	0
41	DT	739	0	807	44	0
42	BU	780	0	831	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DU	780	0	831	65	0
43	BV	753	0	780	31	0
43	DV	753	0	780	25	0
44	BW	580	0	594	23	0
44	DW	569	0	581	26	0
45	BX	625	0	652	35	0
45	DX	625	0	652	55	0
46	BY	509	0	543	29	0
46	DY	509	0	543	38	0
47	BZ	449	0	488	19	0
47	DZ	449	0	488	14	0
48	B0	444	0	458	33	0
48	D0	444	0	458	18	0
49	B1	410	0	440	32	0
49	D1	410	0	440	19	0
50	B2	377	0	418	19	0
50	D2	377	0	418	34	0
51	B3	504	0	572	22	0
51	D3	504	0	572	29	0
52	B4	302	0	340	12	0
52	D4	302	0	342	17	0
53	B5	1142	0	865	49	0
54	B6	69	0	60	5	0
54	D6	69	0	60	14	0
55	AA	71	0	0	0	0
55	AM	1	0	0	0	0
55	BA	195	0	0	0	0
55	BB	4	0	0	0	0
55	CA	55	0	0	0	0
55	CM	1	0	0	0	0
55	DA	167	0	0	0	0
55	DB	3	0	0	0	0
55	DQ	1	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	194	0	0	23	0
57	AL	1	0	0	0	0
57	AN	5	0	0	1	0
57	AT	2	0	0	1	0
57	AU	1	0	0	1	0
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B4	2	0	0	0	0
57	BA	615	0	0	101	0
57	BB	14	0	0	0	0
57	BC	10	0	0	0	0
57	BD	4	0	0	2	0
57	BE	4	0	0	0	0
57	BF	1	0	0	1	0
57	BG	1	0	0	0	0
57	BJ	1	0	0	0	0
57	BL	6	0	0	0	0
57	BN	2	0	0	0	0
57	BS	1	0	0	0	0
57	BU	1	0	0	0	0
57	CA	189	0	0	20	0
57	CL	1	0	0	0	0
57	CN	3	0	0	2	0
57	CT	3	0	0	0	0
57	CU	2	0	0	0	0
57	D0	1	0	0	0	0
57	D2	2	0	0	0	0
57	D3	2	0	0	0	0
57	D4	1	0	0	0	0
57	DA	607	0	0	82	0
57	DB	13	0	0	3	0
57	DC	9	0	0	1	0
57	DD	4	0	0	2	0
57	DE	6	0	0	1	0
57	DL	5	0	0	1	0
57	DN	2	0	0	0	0
57	DT	2	0	0	0	0
57	DU	1	0	0	1	0
57	DV	1	0	0	0	0
All	All	288320	0	192909	11780	4

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 25.

The worst 5 of 11780 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)
22:BA:1006:C:OP2	57:BA:3781:HOH:O	1.56	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
22:BA:2714:G:OP2	57:BA:3548:HOH:O	1.61	1.18
22:BA:1603:A:OP1	57:BA:3411:HOH:O	1.61	1.15
54:D6:4:PRO:HB2	54:D6:5:MHU:HM1	1.15	1.14

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:368:U:OP2	29:DH:123:ARG:NE[4_455]	1.78	0.42
1:AA:368:U:OP1	29:DH:93:SER:OG[4_455]	1.93	0.27
1:AA:368:U:OP2	29:DH:123:ARG:NH2[4_455]	2.03	0.17
1:AA:368:U:OP2	29:DH:123:ARG:CZ[4_455]	2.07	0.13

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%)	135 (62%)	36 (17%)	45 (21%)	0	0
2	CB	216/218 (99%)	143 (66%)	36 (17%)	37 (17%)	0	0
3	AC	204/206 (99%)	142 (70%)	42 (21%)	20 (10%)	0	2
3	CC	204/206 (99%)	145 (71%)	41 (20%)	18 (9%)	1	3
4	AD	203/205 (99%)	133 (66%)	36 (18%)	34 (17%)	0	0
4	CD	203/205 (99%)	129 (64%)	48 (24%)	26 (13%)	0	1
5	AE	148/150 (99%)	98 (66%)	33 (22%)	17 (12%)	0	2
5	CE	148/150 (99%)	96 (65%)	29 (20%)	23 (16%)	0	1
6	AF	98/100 (98%)	61 (62%)	19 (19%)	18 (18%)	0	0
6	CF	98/100 (98%)	64 (65%)	18 (18%)	16 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	110 (74%)	27 (18%)	12 (8%)	1	4
7	CG	149/151 (99%)	120 (80%)	21 (14%)	8 (5%)	2	11
8	AH	127/129 (98%)	80 (63%)	29 (23%)	18 (14%)	0	1
8	CH	127/129 (98%)	100 (79%)	19 (15%)	8 (6%)	1	7
9	AI	125/127 (98%)	90 (72%)	24 (19%)	11 (9%)	1	3
9	CI	125/127 (98%)	89 (71%)	27 (22%)	9 (7%)	1	5
10	AJ	96/98 (98%)	68 (71%)	7 (7%)	21 (22%)	0	0
10	CJ	96/98 (98%)	69 (72%)	18 (19%)	9 (9%)	0	3
11	AK	115/117 (98%)	83 (72%)	17 (15%)	15 (13%)	0	1
11	CK	115/117 (98%)	77 (67%)	28 (24%)	10 (9%)	1	3
12	AL	121/123 (98%)	92 (76%)	19 (16%)	10 (8%)	1	4
12	CL	121/123 (98%)	89 (74%)	17 (14%)	15 (12%)	0	1
13	AM	112/114 (98%)	79 (70%)	22 (20%)	11 (10%)	0	2
13	CM	112/114 (98%)	86 (77%)	15 (13%)	11 (10%)	0	2
14	AN	92/100 (92%)	57 (62%)	20 (22%)	15 (16%)	0	1
14	CN	92/100 (92%)	59 (64%)	20 (22%)	13 (14%)	0	1
15	AO	86/88 (98%)	60 (70%)	21 (24%)	5 (6%)	1	10
15	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	3	20
16	AP	80/82 (98%)	52 (65%)	16 (20%)	12 (15%)	0	1
16	CP	80/82 (98%)	54 (68%)	20 (25%)	6 (8%)	1	5
17	AQ	78/80 (98%)	52 (67%)	16 (20%)	10 (13%)	0	1
17	CQ	78/80 (98%)	55 (70%)	13 (17%)	10 (13%)	0	1
18	AR	53/55 (96%)	40 (76%)	12 (23%)	1 (2%)	8	36
18	CR	53/55 (96%)	45 (85%)	4 (8%)	4 (8%)	1	5
19	AS	77/79 (98%)	52 (68%)	19 (25%)	6 (8%)	1	4
19	CS	77/79 (98%)	59 (77%)	14 (18%)	4 (5%)	2	12
20	AT	83/85 (98%)	51 (61%)	23 (28%)	9 (11%)	0	2
20	CT	83/85 (98%)	66 (80%)	11 (13%)	6 (7%)	1	5
21	AU	49/51 (96%)	23 (47%)	18 (37%)	8 (16%)	0	1
21	CU	49/51 (96%)	25 (51%)	10 (20%)	14 (29%)	0	0
24	BC	269/271 (99%)	208 (77%)	49 (18%)	12 (4%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	DC	269/271 (99%)	206 (77%)	42 (16%)	21 (8%)	1	4
25	BD	207/209 (99%)	176 (85%)	22 (11%)	9 (4%)	2	15
25	DD	207/209 (99%)	175 (84%)	24 (12%)	8 (4%)	3	17
26	BE	199/201 (99%)	164 (82%)	26 (13%)	9 (4%)	2	14
26	DE	199/201 (99%)	160 (80%)	27 (14%)	12 (6%)	1	9
27	BF	175/177 (99%)	136 (78%)	24 (14%)	15 (9%)	1	3
27	DF	175/177 (99%)	141 (81%)	23 (13%)	11 (6%)	1	7
28	BG	174/176 (99%)	146 (84%)	20 (12%)	8 (5%)	2	14
28	DG	174/176 (99%)	132 (76%)	33 (19%)	9 (5%)	2	12
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	1
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	0	2
30	BI	139/141 (99%)	79 (57%)	34 (24%)	26 (19%)	0	0
30	DI	139/141 (99%)	79 (57%)	42 (30%)	18 (13%)	0	1
31	BJ	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	7	33
31	DJ	140/142 (99%)	116 (83%)	18 (13%)	6 (4%)	2	15
32	BK	120/122 (98%)	94 (78%)	15 (12%)	11 (9%)	1	3
32	DK	120/122 (98%)	96 (80%)	14 (12%)	10 (8%)	1	4
33	BL	141/143 (99%)	108 (77%)	23 (16%)	10 (7%)	1	5
33	DL	141/143 (99%)	104 (74%)	28 (20%)	9 (6%)	1	7
34	BM	134/136 (98%)	114 (85%)	16 (12%)	4 (3%)	4	24
34	DM	134/136 (98%)	115 (86%)	13 (10%)	6 (4%)	2	14
35	BN	118/120 (98%)	97 (82%)	18 (15%)	3 (2%)	5	28
35	DN	118/120 (98%)	94 (80%)	16 (14%)	8 (7%)	1	6
36	BO	114/116 (98%)	87 (76%)	22 (19%)	5 (4%)	2	15
36	DO	114/116 (98%)	97 (85%)	15 (13%)	2 (2%)	8	37
37	BP	112/114 (98%)	97 (87%)	10 (9%)	5 (4%)	2	14
37	DP	112/114 (98%)	86 (77%)	19 (17%)	7 (6%)	1	7
38	BQ	115/117 (98%)	96 (84%)	15 (13%)	4 (4%)	3	20
38	DQ	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	17	55
39	BR	101/103 (98%)	89 (88%)	5 (5%)	7 (7%)	1	6
39	DR	101/103 (98%)	77 (76%)	17 (17%)	7 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	91 (84%)	11 (10%)	6 (6%)	2	10
40	DS	108/110 (98%)	87 (81%)	14 (13%)	7 (6%)	1	7
41	BT	91/93 (98%)	69 (76%)	13 (14%)	9 (10%)	0	2
41	DT	91/93 (98%)	62 (68%)	19 (21%)	10 (11%)	0	2
42	BU	100/102 (98%)	75 (75%)	17 (17%)	8 (8%)	1	4
42	DU	100/102 (98%)	72 (72%)	15 (15%)	13 (13%)	0	1
43	BV	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
43	DV	92/94 (98%)	76 (83%)	12 (13%)	4 (4%)	2	15
44	BW	74/76 (97%)	65 (88%)	9 (12%)	0	100	100
44	DW	73/76 (96%)	58 (80%)	10 (14%)	5 (7%)	1	6
45	BX	75/77 (97%)	64 (85%)	7 (9%)	4 (5%)	2	11
45	DX	75/77 (97%)	56 (75%)	15 (20%)	4 (5%)	2	11
46	BY	61/63 (97%)	38 (62%)	13 (21%)	10 (16%)	0	1
46	DY	61/63 (97%)	44 (72%)	11 (18%)	6 (10%)	0	2
47	BZ	56/58 (97%)	49 (88%)	4 (7%)	3 (5%)	2	11
47	DZ	56/58 (97%)	48 (86%)	5 (9%)	3 (5%)	2	11
48	B0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	0	3
48	D0	54/56 (96%)	42 (78%)	8 (15%)	4 (7%)	1	5
49	B1	48/50 (96%)	39 (81%)	4 (8%)	5 (10%)	0	2
49	D1	48/50 (96%)	39 (81%)	6 (12%)	3 (6%)	1	7
50	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	2	14
50	D2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	1	6
51	B3	62/64 (97%)	51 (82%)	9 (14%)	2 (3%)	4	22
51	D3	62/64 (97%)	50 (81%)	9 (14%)	3 (5%)	2	13
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	5	25
53	B5	183/228 (80%)	100 (55%)	53 (29%)	30 (16%)	0	1
54	B6	2/7 (29%)	2 (100%)	0	0	100	100
54	D6	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
All	All	11422/11686 (98%)	8514 (74%)	1907 (17%)	1001 (9%)	1	3

5 of 1001 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	22	TYR
2	AB	64	LYS
2	AB	68	LEU
2	AB	73	LYS
2	AB	75	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%)	125 (69%)	55 (31%)	0	1
2	CB	180/180 (100%)	126 (70%)	54 (30%)	0	1
3	AC	170/170 (100%)	137 (81%)	33 (19%)	1	7
3	CC	170/170 (100%)	130 (76%)	40 (24%)	1	3
4	AD	172/172 (100%)	128 (74%)	44 (26%)	0	3
4	CD	172/172 (100%)	140 (81%)	32 (19%)	1	8
5	AE	113/113 (100%)	85 (75%)	28 (25%)	0	3
5	CE	113/113 (100%)	83 (74%)	30 (26%)	0	2
6	AF	87/87 (100%)	63 (72%)	24 (28%)	0	2
6	CF	87/87 (100%)	58 (67%)	29 (33%)	0	1
7	AG	124/124 (100%)	88 (71%)	36 (29%)	0	2
7	CG	124/124 (100%)	92 (74%)	32 (26%)	0	2
8	AH	104/104 (100%)	80 (77%)	24 (23%)	1	4
8	CH	104/104 (100%)	79 (76%)	25 (24%)	0	3
9	AI	105/105 (100%)	73 (70%)	32 (30%)	0	1
9	CI	105/105 (100%)	73 (70%)	32 (30%)	0	1
10	AJ	86/86 (100%)	61 (71%)	25 (29%)	0	2
10	CJ	86/86 (100%)	70 (81%)	16 (19%)	1	8
11	AK	90/90 (100%)	70 (78%)	20 (22%)	1	4
11	CK	90/90 (100%)	67 (74%)	23 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	78 (76%)	25 (24%)	0	3
12	CL	103/103 (100%)	78 (76%)	25 (24%)	0	3
13	AM	92/92 (100%)	65 (71%)	27 (29%)	0	2
13	CM	92/92 (100%)	69 (75%)	23 (25%)	0	3
14	AN	79/83 (95%)	63 (80%)	16 (20%)	1	6
14	CN	79/83 (95%)	69 (87%)	10 (13%)	4	19
15	AO	75/76 (99%)	61 (81%)	14 (19%)	1	8
15	CO	75/76 (99%)	64 (85%)	11 (15%)	3	15
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	4
16	CP	65/65 (100%)	52 (80%)	13 (20%)	1	7
17	AQ	74/74 (100%)	50 (68%)	24 (32%)	0	1
17	CQ	74/74 (100%)	54 (73%)	20 (27%)	0	2
18	AR	48/48 (100%)	40 (83%)	8 (17%)	2	11
18	CR	48/48 (100%)	43 (90%)	5 (10%)	7	27
19	AS	70/70 (100%)	59 (84%)	11 (16%)	2	13
19	CS	70/70 (100%)	53 (76%)	17 (24%)	0	3
20	AT	65/65 (100%)	49 (75%)	16 (25%)	0	3
20	CT	65/65 (100%)	49 (75%)	16 (25%)	0	3
21	AU	44/44 (100%)	29 (66%)	15 (34%)	0	1
21	CU	44/44 (100%)	29 (66%)	15 (34%)	0	1
24	BC	216/216 (100%)	182 (84%)	34 (16%)	2	13
24	DC	216/216 (100%)	189 (88%)	27 (12%)	4	20
25	BD	164/164 (100%)	145 (88%)	19 (12%)	5	23
25	DD	164/164 (100%)	145 (88%)	19 (12%)	5	23
26	BE	165/165 (100%)	137 (83%)	28 (17%)	2	10
26	DE	165/165 (100%)	131 (79%)	34 (21%)	1	6
27	BF	148/148 (100%)	121 (82%)	27 (18%)	1	9
27	DF	148/148 (100%)	116 (78%)	32 (22%)	1	5
28	BG	137/137 (100%)	118 (86%)	19 (14%)	3	16
28	DG	137/137 (100%)	119 (87%)	18 (13%)	4	18
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	4
30	BI	109/109 (100%)	80 (73%)	29 (27%)	0	2
30	DI	109/109 (100%)	85 (78%)	24 (22%)	1	4
31	BJ	116/116 (100%)	106 (91%)	10 (9%)	10	37
31	DJ	116/116 (100%)	103 (89%)	13 (11%)	6	24
32	BK	103/103 (100%)	90 (87%)	13 (13%)	4	20
32	DK	103/103 (100%)	93 (90%)	10 (10%)	8	31
33	BL	102/102 (100%)	86 (84%)	16 (16%)	2	13
33	DL	102/102 (100%)	80 (78%)	22 (22%)	1	5
34	BM	109/109 (100%)	92 (84%)	17 (16%)	2	13
34	DM	109/109 (100%)	93 (85%)	16 (15%)	3	15
35	BN	100/100 (100%)	83 (83%)	17 (17%)	2	10
35	DN	100/100 (100%)	77 (77%)	23 (23%)	1	4
36	BO	86/86 (100%)	63 (73%)	23 (27%)	0	2
36	DO	86/86 (100%)	71 (83%)	15 (17%)	2	10
37	BP	99/99 (100%)	84 (85%)	15 (15%)	3	14
37	DP	99/99 (100%)	83 (84%)	16 (16%)	2	12
38	BQ	89/89 (100%)	75 (84%)	14 (16%)	2	13
38	DQ	89/89 (100%)	76 (85%)	13 (15%)	3	15
39	BR	84/84 (100%)	69 (82%)	15 (18%)	2	9
39	DR	84/84 (100%)	73 (87%)	11 (13%)	4	18
40	BS	93/93 (100%)	75 (81%)	18 (19%)	1	7
40	DS	93/93 (100%)	80 (86%)	13 (14%)	3	16
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	14
41	DT	80/80 (100%)	64 (80%)	16 (20%)	1	7
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	6
42	DU	83/83 (100%)	60 (72%)	23 (28%)	0	2
43	BV	78/78 (100%)	62 (80%)	16 (20%)	1	6
43	DV	78/78 (100%)	67 (86%)	11 (14%)	3	16
44	BW	57/58 (98%)	50 (88%)	7 (12%)	4	21
44	DW	56/58 (97%)	51 (91%)	5 (9%)	9	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	56 (84%)	11 (16%)	2	11
45	DX	67/67 (100%)	57 (85%)	10 (15%)	3	14
46	BY	55/55 (100%)	47 (86%)	8 (14%)	3	15
46	DY	55/55 (100%)	45 (82%)	10 (18%)	1	9
47	BZ	48/48 (100%)	42 (88%)	6 (12%)	4	20
47	DZ	48/48 (100%)	35 (73%)	13 (27%)	0	2
48	B0	47/47 (100%)	40 (85%)	7 (15%)	3	14
48	D0	47/47 (100%)	43 (92%)	4 (8%)	10	38
49	B1	45/45 (100%)	37 (82%)	8 (18%)	2	9
49	D1	45/45 (100%)	39 (87%)	6 (13%)	4	17
50	B2	38/38 (100%)	33 (87%)	5 (13%)	4	18
50	D2	38/38 (100%)	32 (84%)	6 (16%)	2	12
51	B3	51/51 (100%)	40 (78%)	11 (22%)	1	5
51	D3	51/51 (100%)	47 (92%)	4 (8%)	12	42
52	B4	34/34 (100%)	29 (85%)	5 (15%)	3	15
52	D4	34/34 (100%)	29 (85%)	5 (15%)	3	15
53	B5	61/180 (34%)	47 (77%)	14 (23%)	1	4
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%)	7518 (80%)	1872 (20%)	1	7

5 of 1872 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	B2	24	THR
41	DT	86	THR
7	CG	5	ARG
40	DS	68	ASP
30	DI	96	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
18	CR	52	GLN

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Mol	Chain	Res	Type
37	DP	41	GLN
20	CT	68	HIS
28	DG	115	HIS
51	D3	31	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	361 (23%)	17 (1%)
1	CA	1538/1539 (99%)	335 (21%)	16 (1%)
22	BA	2895/2903 (99%)	672 (23%)	36 (1%)
22	DA	2895/2903 (99%)	609 (21%)	33 (1%)
23	BB	118/119 (99%)	27 (22%)	1 (0%)
23	DB	117/119 (98%)	25 (21%)	0
All	All	9100/9122 (99%)	2029 (22%)	103 (1%)

5 of 2029 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	13	U
1	AA	32	A

5 of 103 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	209	U
22	DA	83	A
22	DA	2501	C
1	CA	429	U
1	CA	873	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	MHU	B6	5	54	14,15,16	2.87	7 (50%)	18,19,21	2.71	5 (27%)
54	MHW	D6	1	54	9,9,10	3.18	4 (44%)	10,11,13	2.22	7 (70%)
54	DBB	D6	3	54	4,5,6	0.76	0	1,5,7	0.74	0
54	004	D6	7	54	9,10,11	3.28	7 (77%)	9,12,14	2.38	2 (22%)
54	MHU	D6	5	54	14,15,16	2.80	6 (42%)	18,19,21	2.69	4 (22%)
54	04X	B6	6	54	14,16,17	1.22	1 (7%)	11,20,22	4.65	6 (54%)
54	MHW	B6	1	54	9,9,10	2.88	4 (44%)	10,11,13	3.44	8 (80%)
54	DBB	B6	3	54	4,5,6	0.86	0	1,5,7	0.96	0
54	004	B6	7	54	9,10,11	3.36	6 (66%)	9,12,14	1.59	2 (22%)
54	04X	D6	6	54	14,16,17	1.14	2 (14%)	11,20,22	5.43	7 (63%)

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

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	7	004	CB-CA	-6.34	1.45	1.52
54	D6	5	MHU	CE1-CD1	6.06	1.49	1.38
54	D6	7	004	CB-CA	-5.93	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	1	MHW	CG2-CB	-5.61	1.29	1.39
54	B6	1	MHW	CG2-CB	-5.54	1.29	1.39

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	04X	C0-N1-C1	15.71	135.46	111.09
54	B6	6	04X	C0-N1-C1	13.07	131.37	111.09
54	D6	5	MHU	CB-CA-N	7.71	122.60	110.65
54	B6	1	MHW	O-C-CA	-7.51	117.11	124.22
54	B6	5	MHU	CB-CA-N	7.43	122.16	110.65

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	B6	1	MHW	O-C-CA-N
54	B6	3	DBB	C-CA-CB-CG
54	D6	3	DBB	O-C-CA-CB
54	D6	3	DBB	C-CA-CB-CG
54	D6	5	MHU	O-C-CA-CB

There are no ring outliers.

8 monomers are involved in 18 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 500 ligands modelled in this entry, 500 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	B6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	2:THR	C	3:DBB	N	1.61

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%)	-0.39	22 (1%) 75 49	14, 54, 137, 179	0
1	CA	1539/1539 (100%)	-0.19	35 (2%) 60 31	27, 72, 145, 177	0
2	AB	218/218 (100%)	1.16	53 (24%) 0 0	43, 76, 100, 125	0
2	CB	218/218 (100%)	1.54	69 (31%) 0 0	63, 86, 106, 126	0
3	AC	206/206 (100%)	0.10	5 (2%) 59 30	39, 61, 83, 96	0
3	CC	206/206 (100%)	1.24	44 (21%) 0 0	57, 79, 97, 109	0
4	AD	205/205 (100%)	0.04	3 (1%) 73 46	35, 58, 79, 106	0
4	CD	205/205 (100%)	-0.20	3 (1%) 73 46	21, 40, 71, 90	0
5	AE	150/150 (100%)	0.01	3 (2%) 65 36	27, 51, 82, 106	0
5	CE	150/150 (100%)	0.02	1 (0%) 87 69	34, 59, 87, 104	0
6	AF	100/100 (100%)	-0.31	0 100 100	38, 59, 76, 84	0
6	CF	100/100 (100%)	-0.14	1 (1%) 82 59	46, 74, 96, 104	0
7	AG	151/151 (100%)	0.82	25 (16%) 1 0	54, 78, 98, 108	0
7	CG	151/151 (100%)	1.77	61 (40%) 0 0	77, 97, 107, 113	0
8	AH	129/129 (100%)	-0.07	1 (0%) 86 65	30, 50, 73, 81	0
8	CH	129/129 (100%)	0.08	4 (3%) 49 21	45, 65, 81, 90	0
9	AI	127/127 (100%)	1.01	22 (17%) 1 0	51, 73, 97, 113	0
9	CI	127/127 (100%)	1.42	36 (28%) 0 0	71, 91, 109, 126	0
10	AJ	98/98 (100%)	0.44	7 (7%) 16 5	46, 68, 92, 122	0
10	CJ	98/98 (100%)	1.87	41 (41%) 0 0	71, 93, 110, 124	0
11	AK	117/117 (100%)	0.58	14 (11%) 4 1	32, 64, 91, 110	0
11	CK	117/117 (100%)	0.11	3 (2%) 56 27	44, 68, 82, 91	0
12	AL	123/123 (100%)	0.11	3 (2%) 59 30	23, 39, 68, 94	0
12	CL	123/123 (100%)	0.07	4 (3%) 46 20	39, 52, 79, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.42	7 (6%) 21 7	49, 71, 92, 105	0
13	CM	114/114 (100%)	1.96	55 (48%) 0 0	90, 103, 116, 120	0
14	AN	96/100 (96%)	0.83	16 (16%) 1 0	43, 63, 94, 106	0
14	CN	96/100 (96%)	1.89	36 (37%) 0 0	69, 91, 110, 118	0
15	AO	88/88 (100%)	-0.01	1 (1%) 80 56	31, 51, 68, 98	0
15	CO	88/88 (100%)	-0.02	2 (2%) 60 31	43, 63, 81, 105	0
16	AP	82/82 (100%)	0.48	4 (4%) 29 11	35, 49, 84, 100	0
16	CP	82/82 (100%)	0.66	12 (14%) 2 1	45, 62, 88, 106	0
17	AQ	80/80 (100%)	-0.03	3 (3%) 40 16	27, 54, 81, 124	0
17	CQ	80/80 (100%)	0.49	5 (6%) 20 6	44, 72, 96, 105	0
18	AR	55/55 (100%)	-0.14	3 (5%) 25 9	39, 53, 81, 112	0
18	CR	55/55 (100%)	0.01	1 (1%) 68 40	46, 56, 82, 111	0
19	AS	79/79 (100%)	1.00	14 (17%) 1 0	55, 72, 92, 101	0
19	CS	79/79 (100%)	3.08	55 (69%) 0 0	87, 103, 114, 123	0
20	AT	85/85 (100%)	0.10	3 (3%) 44 18	35, 51, 74, 111	0
20	CT	85/85 (100%)	1.25	20 (23%) 0 0	53, 72, 93, 96	0
21	AU	51/51 (100%)	1.69	21 (41%) 0 0	56, 76, 95, 108	0
21	CU	51/51 (100%)	0.40	6 (11%) 4 1	48, 72, 94, 108	0
22	BA	2897/2903 (99%)	-0.13	105 (3%) 42 17	0, 14, 130, 195	0
22	DA	2897/2903 (99%)	-0.07	71 (2%) 57 29	42, 83, 144, 183	0
23	BB	119/119 (100%)	-0.52	0 100 100	1, 24, 54, 90	0
23	DB	118/119 (99%)	-0.35	0 100 100	66, 111, 133, 141	0
24	BC	271/271 (100%)	-0.24	8 (2%) 50 22	3, 21, 43, 55	0
24	DC	271/271 (100%)	0.42	23 (8%) 10 3	42, 62, 76, 91	0
25	BD	209/209 (100%)	-0.45	0 100 100	0, 9, 38, 71	0
25	DD	209/209 (100%)	0.38	13 (6%) 20 7	46, 66, 81, 99	0
26	BE	201/201 (100%)	-0.43	0 100 100	0, 24, 56, 91	0
26	DE	201/201 (100%)	0.93	33 (16%) 1 0	45, 81, 98, 106	0
27	BF	177/177 (100%)	0.26	11 (6%) 20 7	15, 46, 88, 97	0
27	DF	177/177 (100%)	2.38	92 (51%) 0 0	85, 102, 117, 125	0
28	BG	176/176 (100%)	-0.16	0 100 100	15, 38, 64, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	1.19	39 (22%) 0 0	71, 90, 104, 117	0
29	BH	149/149 (100%)	2.29	65 (43%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.15	36 (24%) 0 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	2.43	66 (46%) 0 0	84, 108, 121, 136	0
30	DI	141/141 (100%)	3.62	97 (68%) 0 0	96, 114, 123, 127	0
31	BJ	142/142 (100%)	-0.46	0 100 100	1, 5, 23, 43	0
31	DJ	142/142 (100%)	0.41	12 (8%) 10 3	48, 64, 79, 96	0
32	BK	122/122 (100%)	-0.54	0 100 100	2, 11, 37, 67	0
32	DK	122/122 (100%)	0.64	14 (11%) 4 1	48, 61, 81, 96	0
33	BL	143/143 (100%)	-0.35	0 100 100	0, 21, 48, 76	0
33	DL	143/143 (100%)	1.25	36 (25%) 0 0	42, 77, 91, 113	0
34	BM	136/136 (100%)	-0.49	0 100 100	1, 9, 30, 87	0
34	DM	136/136 (100%)	0.80	18 (13%) 3 1	42, 67, 82, 108	0
35	BN	120/120 (100%)	-0.47	0 100 100	1, 6, 17, 62	0
35	DN	120/120 (100%)	0.58	17 (14%) 2 1	54, 74, 88, 110	0
36	BO	116/116 (100%)	-0.26	0 100 100	14, 27, 46, 52	0
36	DO	116/116 (100%)	1.68	45 (38%) 0 0	74, 91, 102, 114	0
37	BP	114/114 (100%)	-0.31	0 100 100	5, 19, 48, 70	0
37	DP	114/114 (100%)	0.58	13 (11%) 5 1	56, 68, 84, 93	0
38	BQ	117/117 (100%)	-0.45	0 100 100	0, 3, 11, 42	0
38	DQ	117/117 (100%)	0.40	9 (7%) 13 4	52, 66, 77, 84	0
39	BR	103/103 (100%)	-0.48	0 100 100	0, 9, 31, 63	0
39	DR	103/103 (100%)	0.87	18 (17%) 1 0	50, 75, 87, 97	0
40	BS	110/110 (100%)	-0.38	0 100 100	1, 3, 23, 84	0
40	DS	110/110 (100%)	1.07	25 (22%) 0 0	56, 73, 89, 96	0
41	BT	93/93 (100%)	-0.02	2 (2%) 62 33	10, 27, 80, 101	0
41	DT	93/93 (100%)	1.82	39 (41%) 0 0	63, 83, 103, 110	0
42	BU	102/102 (100%)	-0.10	3 (2%) 51 23	10, 30, 61, 92	0
42	DU	102/102 (100%)	2.61	53 (51%) 0 0	70, 88, 106, 112	0
43	BV	94/94 (100%)	-0.36	0 100 100	4, 22, 43, 54	0
43	DV	94/94 (100%)	0.46	9 (9%) 8 2	65, 82, 94, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.42	0 100 100	3, 10, 27, 48	0
44	DW	75/76 (98%)	1.49	28 (37%) 0 0	54, 79, 88, 108	0
45	BX	77/77 (100%)	-0.36	0 100 100	6, 24, 52, 77	0
45	DX	77/77 (100%)	0.61	14 (18%) 1 0	49, 69, 86, 89	0
46	BY	63/63 (100%)	0.05	3 (4%) 30 11	22, 44, 74, 96	0
46	DY	63/63 (100%)	1.28	15 (23%) 0 0	71, 90, 99, 103	0
47	BZ	58/58 (100%)	-0.38	0 100 100	2, 7, 29, 41	0
47	DZ	58/58 (100%)	0.26	3 (5%) 27 10	52, 70, 84, 89	0
48	B0	56/56 (100%)	-0.53	0 100 100	0, 8, 35, 70	0
48	D0	56/56 (100%)	0.86	8 (14%) 2 1	53, 74, 91, 104	0
49	B1	50/50 (100%)	-0.28	2 (4%) 38 15	13, 31, 54, 87	0
49	D1	50/50 (100%)	1.17	11 (22%) 0 0	68, 84, 93, 105	0
50	B2	46/46 (100%)	-0.31	1 (2%) 62 33	3, 9, 17, 90	0
50	D2	46/46 (100%)	1.18	9 (19%) 1 0	53, 66, 79, 100	0
51	B3	64/64 (100%)	-0.32	0 100 100	4, 9, 18, 31	0
51	D3	64/64 (100%)	0.94	15 (23%) 0 0	58, 71, 79, 85	0
52	B4	38/38 (100%)	-0.08	0 100 100	11, 20, 35, 52	0
52	D4	38/38 (100%)	1.59	13 (34%) 0 0	63, 74, 85, 99	0
53	B5	191/228 (83%)	4.42	168 (87%) 0 0	85, 111, 123, 134	0
54	B6	2/7 (28%)	0.27	0 100 100	5, 5, 5, 9	0
54	D6	2/7 (28%)	0.74	0 100 100	53, 53, 53, 62	0
All	All	20738/20808 (99%)	0.28	1986 (9%) 8 2	0, 64, 119, 195	0

The worst 5 of 1986 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	DI	6	GLN	16.5
30	BI	53	LEU	16.3
22	BA	2100	G	15.9
30	DI	2	ALA	15.0
22	BA	2104	C	14.5

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(Å ²)	Q<0.9
54	MHU	D6	5	15/16	0.82	0.38	45,58,69,72	0
54	DBB	D6	3	6/7	0.88	0.50	45,50,65,70	0
54	04X	D6	6	15/16	0.90	0.27	47,59,67,73	0
54	MHU	B6	5	15/16	0.93	0.24	3,7,15,15	0
54	MHW	D6	1	9/10	0.94	0.18	55,59,63,66	0
54	DBB	B6	3	6/7	0.94	0.28	8,14,20,33	0
54	004	D6	7	10/11	0.95	0.23	47,52,61,64	0
54	MHW	B6	1	9/10	0.97	0.20	8,13,21,30	0
54	004	B6	7	10/11	0.97	0.28	2,4,6,6	0
54	04X	B6	6	15/16	0.97	0.19	6,11,15,20	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(Å ²)	Q<0.9
55	MG	AA	1627	1/1	0.17	0.55	76,76,76,76	0
55	MG	DA	3071	1/1	0.18	0.59	93,93,93,93	0
55	MG	DA	3072	1/1	0.23	0.50	89,89,89,89	0
55	MG	AA	1644	1/1	0.24	0.69	49,49,49,49	0
55	MG	DA	3061	1/1	0.25	1.80	97,97,97,97	0
55	MG	DA	3093	1/1	0.26	0.35	99,99,99,99	0
55	MG	CA	1631	1/1	0.35	0.26	98,98,98,98	0
55	MG	DA	3011	1/1	0.41	0.30	74,74,74,74	0
55	MG	DA	3057	1/1	0.41	0.29	82,82,82,82	0
55	MG	DA	3116	1/1	0.43	0.34	92,92,92,92	0
55	MG	DA	3005	1/1	0.44	0.12	90,90,90,90	0
55	MG	DA	3041	1/1	0.46	0.42	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	CA	1629	1/1	0.49	0.10	84,84,84,84	0
55	MG	CA	1621	1/1	0.51	0.09	67,67,67,67	0
55	MG	CA	1637	1/1	0.52	0.37	80,80,80,80	0
55	MG	DA	3132	1/1	0.53	0.79	85,85,85,85	0
55	MG	DA	3027	1/1	0.55	0.12	82,82,82,82	0
55	MG	DA	3104	1/1	0.56	0.18	76,76,76,76	0
55	MG	BA	3055	1/1	0.58	0.25	50,50,50,50	0
55	MG	DA	3120	1/1	0.58	0.56	95,95,95,95	0
55	MG	DA	3085	1/1	0.58	0.19	78,78,78,78	0
55	MG	DA	3134	1/1	0.58	0.58	87,87,87,87	0
55	MG	CA	1628	1/1	0.59	0.28	100,100,100,100	0
55	MG	DA	3070	1/1	0.60	0.11	93,93,93,93	0
55	MG	DA	3016	1/1	0.60	0.42	84,84,84,84	0
55	MG	CA	1627	1/1	0.61	0.29	88,88,88,88	0
55	MG	DA	3077	1/1	0.62	0.26	76,76,76,76	0
55	MG	AA	1665	1/1	0.63	0.74	53,53,53,53	0
55	MG	AA	1635	1/1	0.63	0.27	76,76,76,76	0
55	MG	BA	3119	1/1	0.64	0.36	49,49,49,49	0
55	MG	BA	3135	1/1	0.65	0.27	48,48,48,48	0
55	MG	CA	1609	1/1	0.67	0.09	78,78,78,78	0
55	MG	DA	3032	1/1	0.67	0.20	78,78,78,78	0
55	MG	DA	3062	1/1	0.68	0.77	70,70,70,70	0
55	MG	DA	3079	1/1	0.68	0.08	94,94,94,94	0
55	MG	DA	3056	1/1	0.68	0.28	80,80,80,80	0
55	MG	DA	3028	1/1	0.69	0.56	86,86,86,86	0
55	MG	DA	3111	1/1	0.69	0.12	81,81,81,81	0
55	MG	DA	3008	1/1	0.70	0.16	80,80,80,80	0
55	MG	CA	1636	1/1	0.70	0.29	97,97,97,97	0
55	MG	BA	3016	1/1	0.70	0.22	31,31,31,31	0
55	MG	DA	3021	1/1	0.70	0.34	62,62,62,62	0
55	MG	AA	1651	1/1	0.70	0.34	55,55,55,55	0
55	MG	DA	3137	1/1	0.70	0.27	84,84,84,84	0
55	MG	DA	3153	1/1	0.70	0.12	68,68,68,68	0
55	MG	DA	3078	1/1	0.71	0.20	95,95,95,95	0
55	MG	AA	1667	1/1	0.72	0.68	54,54,54,54	0
55	MG	DA	3082	1/1	0.72	0.11	65,65,65,65	0
55	MG	BA	3011	1/1	0.72	0.16	30,30,30,30	0
55	MG	BA	3115	1/1	0.73	0.51	76,76,76,76	0
55	MG	BA	3048	1/1	0.73	0.08	26,26,26,26	0
55	MG	BA	3090	1/1	0.73	0.20	33,33,33,33	0
55	MG	BA	3098	1/1	0.73	0.59	73,73,73,73	0
55	MG	DA	3024	1/1	0.73	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	AA	1670	1/1	0.74	0.40	45,45,45,45	0
55	MG	BA	3047	1/1	0.74	0.11	40,40,40,40	0
55	MG	DA	3121	1/1	0.74	0.16	60,60,60,60	0
55	MG	DA	3122	1/1	0.74	0.08	64,64,64,64	0
55	MG	DA	3155	1/1	0.74	0.28	37,37,37,37	0
55	MG	DA	3165	1/1	0.74	0.38	43,43,43,43	0
55	MG	CA	1635	1/1	0.75	0.10	94,94,94,94	0
55	MG	AA	1634	1/1	0.75	0.09	49,49,49,49	0
55	MG	DA	3150	1/1	0.75	0.21	50,50,50,50	0
55	MG	DA	3151	1/1	0.75	0.47	40,40,40,40	0
55	MG	DA	3094	1/1	0.75	0.20	83,83,83,83	0
55	MG	BA	3154	1/1	0.75	0.23	21,21,21,21	0
55	MG	CA	1605	1/1	0.75	0.25	78,78,78,78	0
55	MG	CA	1655	1/1	0.76	1.02	67,67,67,67	0
55	MG	DA	3010	1/1	0.76	0.10	64,64,64,64	0
55	MG	AA	1601	1/1	0.76	0.11	61,61,61,61	0
55	MG	DA	3145	1/1	0.76	0.09	68,68,68,68	0
55	MG	DA	3164	1/1	0.76	0.76	56,56,56,56	0
55	MG	DA	3149	1/1	0.76	0.19	49,49,49,49	0
55	MG	DB	201	1/1	0.76	0.05	96,96,96,96	0
55	MG	AA	1646	1/1	0.77	0.21	50,50,50,50	0
55	MG	AA	1648	1/1	0.77	0.26	39,39,39,39	0
55	MG	DA	3019	1/1	0.77	0.15	84,84,84,84	0
55	MG	DA	3091	1/1	0.77	0.13	79,79,79,79	0
55	MG	DA	3029	1/1	0.77	0.37	66,66,66,66	0
55	MG	DA	3002	1/1	0.77	0.52	81,81,81,81	0
55	MG	DA	3106	1/1	0.78	0.31	70,70,70,70	0
55	MG	BA	3031	1/1	0.78	0.11	7,7,7,7	0
55	MG	DA	3038	1/1	0.78	0.14	63,63,63,63	0
55	MG	DA	3084	1/1	0.78	0.15	75,75,75,75	0
55	MG	BA	3190	1/1	0.78	0.53	42,42,42,42	0
55	MG	DA	3042	1/1	0.78	0.14	69,69,69,69	0
55	MG	DA	3158	1/1	0.78	0.46	58,58,58,58	0
55	MG	DA	3160	1/1	0.78	0.20	47,47,47,47	0
55	MG	DA	3048	1/1	0.78	0.22	93,93,93,93	0
55	MG	CA	1602	1/1	0.78	0.12	69,69,69,69	0
55	MG	CA	1626	1/1	0.78	0.26	66,66,66,66	0
55	MG	DA	3092	1/1	0.79	0.44	94,94,94,94	0
55	MG	BA	3015	1/1	0.79	0.41	61,61,61,61	0
55	MG	AA	1623	1/1	0.79	0.17	49,49,49,49	0
55	MG	DA	3161	1/1	0.79	0.33	48,48,48,48	0
55	MG	DA	3014	1/1	0.79	0.36	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	DA	3015	1/1	0.79	0.57	77,77,77,77	0
55	MG	BA	3025	1/1	0.79	0.18	40,40,40,40	0
55	MG	DA	3126	1/1	0.80	0.17	61,61,61,61	0
55	MG	DA	3040	1/1	0.80	0.21	66,66,66,66	0
55	MG	DA	3136	1/1	0.81	0.42	81,81,81,81	0
55	MG	CA	1652	1/1	0.81	0.11	62,62,62,62	0
55	MG	DA	3044	1/1	0.81	0.21	83,83,83,83	0
55	MG	BA	3004	1/1	0.81	0.14	52,52,52,52	0
55	MG	BA	3070	1/1	0.81	0.11	37,37,37,37	0
55	MG	DA	3133	1/1	0.81	0.19	55,55,55,55	0
55	MG	BA	3019	1/1	0.81	0.26	1,1,1,1	0
55	MG	BA	3029	1/1	0.82	0.12	35,35,35,35	0
55	MG	DA	3090	1/1	0.82	0.08	59,59,59,59	0
55	MG	DA	3154	1/1	0.82	0.24	40,40,40,40	0
55	MG	DA	3033	1/1	0.82	0.09	54,54,54,54	0
55	MG	DA	3098	1/1	0.82	0.08	50,50,50,50	0
55	MG	DB	203	1/1	0.82	0.09	90,90,90,90	0
55	MG	DA	3013	1/1	0.83	0.11	64,64,64,64	0
55	MG	BA	3157	1/1	0.83	0.34	34,34,34,34	0
55	MG	AA	1652	1/1	0.83	0.13	40,40,40,40	0
55	MG	AA	1657	1/1	0.83	0.34	37,37,37,37	0
55	MG	AA	1662	1/1	0.83	0.27	49,49,49,49	0
55	MG	CA	1638	1/1	0.83	0.16	74,74,74,74	0
55	MG	DA	3058	1/1	0.83	0.16	70,70,70,70	0
55	MG	DA	3166	1/1	0.83	0.19	44,44,44,44	0
55	MG	AA	1630	1/1	0.83	0.15	67,67,67,67	0
55	MG	DA	3099	1/1	0.83	0.41	82,82,82,82	0
55	MG	DA	3009	1/1	0.84	0.09	69,69,69,69	0
55	MG	DA	3055	1/1	0.84	0.07	57,57,57,57	0
55	MG	DA	3115	1/1	0.84	0.09	79,79,79,79	0
55	MG	BA	3161	1/1	0.84	0.17	15,15,15,15	0
55	MG	BA	3168	1/1	0.84	0.24	21,21,21,21	0
55	MG	DA	3006	1/1	0.84	0.22	98,98,98,98	0
55	MG	CA	1611	1/1	0.84	0.17	69,69,69,69	0
55	MG	DA	3060	1/1	0.85	0.22	72,72,72,72	0
55	MG	BA	3113	1/1	0.85	0.12	2,2,2,2	0
55	MG	CA	1615	1/1	0.85	0.23	56,56,56,56	0
55	MG	AA	1659	1/1	0.85	0.48	32,32,32,32	0
55	MG	BA	3045	1/1	0.85	0.12	4,4,4,4	0
55	MG	DA	3046	1/1	0.85	0.11	62,62,62,62	0
55	MG	DA	3127	1/1	0.85	0.13	88,88,88,88	0
55	MG	AA	1671	1/1	0.85	0.34	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	CA	1604	1/1	0.85	0.07	78,78,78,78	0
55	MG	DA	3100	1/1	0.85	0.31	73,73,73,73	0
55	MG	CM	201	1/1	0.85	0.38	50,50,50,50	0
55	MG	AA	1617	1/1	0.85	0.11	62,62,62,62	0
55	MG	DA	3144	1/1	0.85	0.30	58,58,58,58	0
55	MG	BA	3109	1/1	0.85	0.21	1,1,1,1	0
55	MG	CA	1620	1/1	0.86	0.13	81,81,81,81	0
55	MG	BA	3076	1/1	0.86	0.28	56,56,56,56	0
55	MG	DA	3102	1/1	0.86	0.31	72,72,72,72	0
55	MG	DA	3018	1/1	0.86	0.11	68,68,68,68	0
55	MG	BA	3129	1/1	0.86	0.13	0,0,0,0	0
55	MG	DA	3004	1/1	0.86	0.48	87,87,87,87	0
55	MG	DA	3112	1/1	0.86	0.13	64,64,64,64	0
55	MG	DA	3054	1/1	0.87	0.08	62,62,62,62	0
55	MG	DA	3135	1/1	0.87	0.08	46,46,46,46	0
55	MG	AA	1624	1/1	0.87	0.10	50,50,50,50	0
55	MG	DA	3063	1/1	0.87	0.12	53,53,53,53	0
55	MG	DA	3069	1/1	0.87	0.20	77,77,77,77	0
55	MG	BA	3150	1/1	0.87	0.20	37,37,37,37	0
55	MG	BA	3093	1/1	0.87	0.10	26,26,26,26	0
55	MG	BA	3028	1/1	0.87	0.10	3,3,3,3	0
55	MG	DA	3073	1/1	0.87	0.10	35,35,35,35	0
55	MG	BA	3080	1/1	0.87	0.09	24,24,24,24	0
55	MG	BA	3003	1/1	0.88	0.10	29,29,29,29	0
55	MG	AA	1607	1/1	0.88	0.12	48,48,48,48	0
55	MG	BA	3061	1/1	0.88	0.64	66,66,66,66	0
55	MG	CA	1606	1/1	0.88	0.25	76,76,76,76	0
55	MG	BA	3160	1/1	0.88	0.20	5,5,5,5	0
55	MG	BA	3124	1/1	0.88	0.09	9,9,9,9	0
55	MG	BA	3166	1/1	0.88	0.20	37,37,37,37	0
55	MG	CA	1646	1/1	0.88	0.23	36,36,36,36	0
55	MG	DA	3103	1/1	0.88	0.28	67,67,67,67	0
55	MG	CA	1650	1/1	0.88	0.63	50,50,50,50	0
55	MG	BA	3167	1/1	0.88	0.17	22,22,22,22	0
55	MG	DA	3152	1/1	0.88	0.32	55,55,55,55	0
55	MG	CA	1654	1/1	0.88	0.20	26,26,26,26	0
55	MG	AA	1639	1/1	0.88	0.10	67,67,67,67	0
55	MG	DA	3081	1/1	0.88	0.12	62,62,62,62	0
55	MG	CA	1622	1/1	0.88	0.12	57,57,57,57	0
55	MG	DA	3118	1/1	0.88	0.11	73,73,73,73	0
55	MG	BA	3180	1/1	0.88	0.62	25,25,25,25	0
55	MG	DA	3025	1/1	0.88	0.12	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3088	1/1	0.88	0.08	69,69,69,69	0
55	MG	DA	3125	1/1	0.88	0.17	86,86,86,86	0
55	MG	DA	3089	1/1	0.88	0.62	91,91,91,91	0
55	MG	BA	3002	1/1	0.88	0.09	18,18,18,18	0
55	MG	DQ	201	1/1	0.88	0.30	40,40,40,40	0
55	MG	BA	3118	1/1	0.89	0.14	34,34,34,34	0
55	MG	AA	1636	1/1	0.89	0.18	42,42,42,42	0
55	MG	DA	3113	1/1	0.89	0.46	75,75,75,75	0
55	MG	DA	3157	1/1	0.89	0.14	29,29,29,29	0
55	MG	CA	1608	1/1	0.89	0.12	65,65,65,65	0
55	MG	CA	1648	1/1	0.89	0.14	51,51,51,51	0
55	MG	BA	3056	1/1	0.89	0.19	22,22,22,22	0
55	MG	BA	3020	1/1	0.89	0.13	5,5,5,5	0
55	MG	DA	3045	1/1	0.89	0.21	61,61,61,61	0
55	MG	BB	202	1/1	0.89	0.10	4,4,4,4	0
55	MG	CA	1633	1/1	0.89	0.80	82,82,82,82	0
55	MG	BA	3133	1/1	0.89	0.34	57,57,57,57	0
55	MG	AA	1614	1/1	0.89	0.19	66,66,66,66	0
55	MG	BA	3026	1/1	0.90	0.10	6,6,6,6	0
55	MG	AA	1658	1/1	0.90	0.16	35,35,35,35	0
55	MG	BA	3077	1/1	0.90	0.07	38,38,38,38	0
55	MG	AA	1643	1/1	0.90	0.15	23,23,23,23	0
55	MG	DA	3138	1/1	0.90	0.36	37,37,37,37	0
55	MG	DA	3139	1/1	0.90	0.56	47,47,47,47	0
55	MG	BA	3088	1/1	0.90	0.08	29,29,29,29	0
55	MG	DA	3043	1/1	0.90	0.07	67,67,67,67	0
55	MG	BA	3052	1/1	0.90	0.09	21,21,21,21	0
55	MG	BA	3091	1/1	0.90	0.05	48,48,48,48	0
55	MG	CA	1624	1/1	0.90	0.07	52,52,52,52	0
55	MG	DA	3047	1/1	0.90	0.14	71,71,71,71	0
55	MG	BA	3007	1/1	0.90	0.09	32,32,32,32	0
55	MG	DA	3049	1/1	0.90	0.10	69,69,69,69	0
55	MG	DA	3083	1/1	0.90	0.24	65,65,65,65	0
55	MG	DA	3053	1/1	0.90	0.13	39,39,39,39	0
55	MG	BB	203	1/1	0.90	0.09	7,7,7,7	0
55	MG	DA	3087	1/1	0.90	0.05	58,58,58,58	0
55	MG	BA	3145	1/1	0.90	0.16	26,26,26,26	0
55	MG	BA	3036	1/1	0.90	0.15	23,23,23,23	0
55	MG	CA	1630	1/1	0.90	0.65	102,102,102,102	0
55	MG	BA	3099	1/1	0.90	0.16	21,21,21,21	0
55	MG	DA	3130	1/1	0.90	0.19	43,43,43,43	0
55	MG	DB	202	1/1	0.90	0.13	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	CA	1632	1/1	0.90	0.07	75,75,75,75	0
55	MG	BA	3044	1/1	0.90	0.21	8,8,8,8	0
55	MG	DA	3142	1/1	0.91	0.40	39,39,39,39	0
55	MG	BA	3050	1/1	0.91	0.07	7,7,7,7	0
55	MG	AA	1631	1/1	0.91	0.16	52,52,52,52	0
55	MG	DA	3147	1/1	0.91	0.15	35,35,35,35	0
55	MG	DA	3065	1/1	0.91	0.07	41,41,41,41	0
55	MG	BA	3054	1/1	0.91	0.08	7,7,7,7	0
55	MG	CA	1645	1/1	0.91	0.12	32,32,32,32	0
55	MG	BA	3112	1/1	0.91	0.09	20,20,20,20	0
55	MG	BA	3073	1/1	0.91	0.15	9,9,9,9	0
55	MG	BA	3173	1/1	0.91	0.29	30,30,30,30	0
55	MG	BA	3075	1/1	0.91	0.14	6,6,6,6	0
55	MG	DA	3035	1/1	0.91	0.13	71,71,71,71	0
55	MG	DA	3128	1/1	0.91	0.07	74,74,74,74	0
55	MG	CA	1653	1/1	0.91	0.38	48,48,48,48	0
55	MG	DA	3101	1/1	0.91	0.08	63,63,63,63	0
55	MG	DA	3163	1/1	0.91	0.21	47,47,47,47	0
55	MG	DA	3080	1/1	0.91	0.10	91,91,91,91	0
55	MG	BA	3152	1/1	0.91	0.27	8,8,8,8	0
55	MG	CA	1618	1/1	0.91	0.21	35,35,35,35	0
55	MG	DA	3059	1/1	0.91	0.09	42,42,42,42	0
55	MG	DA	3107	1/1	0.91	0.19	56,56,56,56	0
55	MG	BA	3092	1/1	0.91	0.19	42,42,42,42	0
55	MG	BA	3040	1/1	0.91	0.39	2,2,2,2	0
55	MG	BA	3178	1/1	0.92	0.35	12,12,12,12	0
55	MG	AA	1668	1/1	0.92	0.38	33,33,33,33	0
55	MG	BA	3059	1/1	0.92	0.12	5,5,5,5	0
55	MG	DA	3108	1/1	0.92	0.14	55,55,55,55	0
55	MG	AA	1669	1/1	0.92	0.27	34,34,34,34	0
55	MG	DA	3146	1/1	0.92	0.11	41,41,41,41	0
55	MG	BA	3136	1/1	0.92	0.57	43,43,43,43	0
55	MG	DA	3148	1/1	0.92	0.22	51,51,51,51	0
55	MG	CA	1601	1/1	0.92	0.17	52,52,52,52	0
55	MG	DA	3031	1/1	0.92	0.14	59,59,59,59	0
55	MG	BA	3144	1/1	0.92	0.24	24,24,24,24	0
55	MG	BA	3095	1/1	0.92	0.08	14,14,14,14	0
55	MG	DA	3007	1/1	0.92	0.37	80,80,80,80	0
55	MG	BA	3066	1/1	0.92	0.14	2,2,2,2	0
55	MG	AA	1610	1/1	0.92	0.15	51,51,51,51	0
55	MG	DA	3064	1/1	0.92	0.19	48,48,48,48	0
55	MG	AA	1604	1/1	0.92	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3111	1/1	0.92	0.08	27,27,27,27	0
55	MG	DA	3095	1/1	0.92	0.24	69,69,69,69	0
55	MG	DA	3129	1/1	0.92	0.13	70,70,70,70	0
55	MG	DA	3096	1/1	0.92	0.09	54,54,54,54	0
55	MG	AA	1661	1/1	0.92	0.35	23,23,23,23	0
55	MG	AA	1616	1/1	0.92	0.09	62,62,62,62	0
55	MG	AA	1663	1/1	0.92	0.23	49,49,49,49	0
55	MG	AA	1602	1/1	0.92	0.38	53,53,53,53	0
55	MG	AA	1609	1/1	0.92	0.08	33,33,33,33	0
55	MG	BA	3034	1/1	0.92	0.13	5,5,5,5	0
55	MG	AA	1655	1/1	0.93	0.14	20,20,20,20	0
55	MG	BA	3179	1/1	0.93	0.34	30,30,30,30	0
55	MG	BA	3057	1/1	0.93	0.21	20,20,20,20	0
55	MG	BA	3181	1/1	0.93	0.12	26,26,26,26	0
55	MG	BA	3038	1/1	0.93	0.14	1,1,1,1	0
55	MG	BA	3023	1/1	0.93	0.17	0,0,0,0	0
55	MG	AA	1605	1/1	0.93	0.20	29,29,29,29	0
55	MG	AA	1606	1/1	0.93	0.06	58,58,58,58	0
55	MG	BA	3071	1/1	0.93	0.14	17,17,17,17	0
55	MG	BA	3102	1/1	0.93	0.18	17,17,17,17	0
55	MG	BA	3151	1/1	0.93	0.14	23,23,23,23	0
55	MG	BA	3027	1/1	0.93	0.35	36,36,36,36	0
55	MG	CA	1639	1/1	0.93	0.13	43,43,43,43	0
55	MG	CA	1640	1/1	0.93	0.15	36,36,36,36	0
55	MG	BA	3074	1/1	0.93	0.21	32,32,32,32	0
55	MG	BA	3014	1/1	0.93	0.19	26,26,26,26	0
55	MG	DA	3159	1/1	0.93	0.26	57,57,57,57	0
55	MG	BA	3001	1/1	0.93	0.05	21,21,21,21	0
55	MG	AA	1619	1/1	0.93	0.15	65,65,65,65	0
55	MG	BA	3032	1/1	0.93	0.12	2,2,2,2	0
55	MG	CA	1619	1/1	0.93	0.12	27,27,27,27	0
55	MG	AA	1629	1/1	0.93	0.17	54,54,54,54	0
55	MG	BA	3120	1/1	0.93	0.12	11,11,11,11	0
55	MG	BA	3171	1/1	0.93	0.17	20,20,20,20	0
55	MG	DA	3036	1/1	0.93	0.12	57,57,57,57	0
55	MG	CA	1623	1/1	0.93	0.17	66,66,66,66	0
55	MG	BA	3123	1/1	0.93	0.13	11,11,11,11	0
55	MG	BA	3138	1/1	0.94	0.30	0,0,0,0	0
55	MG	DA	3030	1/1	0.94	0.27	61,61,61,61	0
55	MG	BA	3140	1/1	0.94	0.15	7,7,7,7	0
55	MG	AM	201	1/1	0.94	0.61	50,50,50,50	0
55	MG	CA	1641	1/1	0.94	0.40	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	AA	1650	1/1	0.94	0.25	20,20,20,20	0
55	MG	AA	1638	1/1	0.94	0.11	63,63,63,63	0
55	MG	BA	3108	1/1	0.94	0.16	5,5,5,5	0
55	MG	BA	3053	1/1	0.94	0.18	0,0,0,0	0
55	MG	AA	1613	1/1	0.94	0.07	23,23,23,23	0
55	MG	BA	3155	1/1	0.94	0.18	2,2,2,2	0
55	MG	CA	1610	1/1	0.94	0.07	58,58,58,58	0
55	MG	AA	1640	1/1	0.94	0.10	57,57,57,57	0
55	MG	DA	3141	1/1	0.94	0.42	45,45,45,45	0
55	MG	CA	1614	1/1	0.94	0.05	52,52,52,52	0
55	MG	DA	3001	1/1	0.94	0.08	37,37,37,37	0
55	MG	BA	3159	1/1	0.94	0.14	24,24,24,24	0
55	MG	CA	1616	1/1	0.94	0.10	38,38,38,38	0
55	MG	BA	3079	1/1	0.94	0.09	21,21,21,21	0
55	MG	AA	1608	1/1	0.94	0.15	20,20,20,20	0
55	MG	BA	3087	1/1	0.94	0.09	27,27,27,27	0
55	MG	BA	3041	1/1	0.94	0.10	11,11,11,11	0
55	MG	BA	3089	1/1	0.94	0.14	1,1,1,1	0
55	MG	BA	3122	1/1	0.94	0.17	0,0,0,0	0
55	MG	AA	1625	1/1	0.94	0.09	51,51,51,51	0
55	MG	BA	3174	1/1	0.94	0.14	5,5,5,5	0
55	MG	BA	3175	1/1	0.94	0.10	9,9,9,9	0
55	MG	BA	3177	1/1	0.94	0.10	9,9,9,9	0
55	MG	AA	1615	1/1	0.94	0.13	63,63,63,63	0
55	MG	BA	3065	1/1	0.94	0.12	1,1,1,1	0
55	MG	BA	3046	1/1	0.94	0.17	3,3,3,3	0
55	MG	AA	1620	1/1	0.94	0.06	55,55,55,55	0
55	MG	DA	3068	1/1	0.94	0.07	60,60,60,60	0
55	MG	DA	3022	1/1	0.94	0.13	43,43,43,43	0
55	MG	BA	3183	1/1	0.94	0.26	22,22,22,22	0
55	MG	DA	3119	1/1	0.94	0.07	58,58,58,58	0
55	MG	DA	3167	1/1	0.94	0.13	30,30,30,30	0
55	MG	BA	3097	1/1	0.94	0.12	0,0,0,0	0
55	MG	DA	3026	1/1	0.94	0.70	75,75,75,75	0
55	MG	BA	3193	1/1	0.94	0.17	12,12,12,12	0
55	MG	BB	201	1/1	0.94	0.08	28,28,28,28	0
55	MG	DA	3051	1/1	0.95	0.05	33,33,33,33	0
55	MG	DA	3052	1/1	0.95	0.06	47,47,47,47	0
55	MG	CA	1642	1/1	0.95	0.20	25,25,25,25	0
55	MG	BA	3182	1/1	0.95	0.22	14,14,14,14	0
55	MG	AA	1660	1/1	0.95	0.09	41,41,41,41	0
55	MG	CA	1647	1/1	0.95	0.31	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	BA	3184	1/1	0.95	0.13	8,8,8,8	0
55	MG	BA	3039	1/1	0.95	0.22	1,1,1,1	0
55	MG	DA	3097	1/1	0.95	0.15	67,67,67,67	0
55	MG	CA	1651	1/1	0.95	0.25	72,72,72,72	0
55	MG	BA	3084	1/1	0.95	0.10	7,7,7,7	0
55	MG	DA	3143	1/1	0.95	0.18	35,35,35,35	0
55	MG	BA	3194	1/1	0.95	0.19	22,22,22,22	0
55	MG	BA	3195	1/1	0.95	0.14	36,36,36,36	0
55	MG	BA	3137	1/1	0.95	0.29	2,2,2,2	0
55	MG	BA	3096	1/1	0.95	0.18	2,2,2,2	0
55	MG	AA	1666	1/1	0.95	0.25	32,32,32,32	0
55	MG	DA	3066	1/1	0.95	0.12	45,45,45,45	0
55	MG	BA	3169	1/1	0.95	0.10	4,4,4,4	0
55	MG	DA	3034	1/1	0.95	0.20	58,58,58,58	0
55	MG	BA	3064	1/1	0.95	0.15	0,0,0,0	0
55	MG	CA	1603	1/1	0.95	0.15	45,45,45,45	0
55	MG	DA	3037	1/1	0.95	0.08	76,76,76,76	0
55	MG	DA	3114	1/1	0.95	0.09	52,52,52,52	0
55	MG	BA	3024	1/1	0.95	0.07	3,3,3,3	0
55	MG	DA	3039	1/1	0.95	0.10	53,53,53,53	0
55	MG	BA	3101	1/1	0.95	0.09	11,11,11,11	0
55	MG	AA	1618	1/1	0.95	0.09	34,34,34,34	0
55	MG	BA	3176	1/1	0.95	0.27	24,24,24,24	0
55	MG	BA	3104	1/1	0.95	0.26	0,0,0,0	0
55	MG	BA	3105	1/1	0.95	0.22	0,0,0,0	0
55	MG	DA	3123	1/1	0.95	0.15	44,44,44,44	0
55	MG	DA	3124	1/1	0.95	0.16	41,41,41,41	0
55	MG	DA	3012	1/1	0.95	0.14	39,39,39,39	0
55	MG	BA	3125	1/1	0.95	0.17	2,2,2,2	0
55	MG	CA	1612	1/1	0.95	0.05	43,43,43,43	0
55	MG	BA	3156	1/1	0.95	0.15	9,9,9,9	0
55	MG	BA	3068	1/1	0.95	0.17	1,1,1,1	0
55	MG	BA	3117	1/1	0.96	0.16	1,1,1,1	0
55	MG	AA	1633	1/1	0.96	0.08	35,35,35,35	0
55	MG	DA	3003	1/1	0.96	0.13	66,66,66,66	0
55	MG	BA	3082	1/1	0.96	0.07	6,6,6,6	0
55	MG	BA	3083	1/1	0.96	0.22	34,34,34,34	0
55	MG	BA	3185	1/1	0.96	0.14	5,5,5,5	0
55	MG	BA	3186	1/1	0.96	0.23	12,12,12,12	0
55	MG	BA	3188	1/1	0.96	0.10	35,35,35,35	0
55	MG	BA	3121	1/1	0.96	0.06	14,14,14,14	0
55	MG	BA	3191	1/1	0.96	0.18	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3192	1/1	0.96	0.23	11,11,11,11	0
55	MG	BA	3069	1/1	0.96	0.15	64,64,64,64	0
55	MG	BA	3100	1/1	0.96	0.10	9,9,9,9	0
55	MG	BA	3085	1/1	0.96	0.17	11,11,11,11	0
55	MG	AA	1626	1/1	0.96	0.21	26,26,26,26	0
55	MG	CA	1634	1/1	0.96	0.06	58,58,58,58	0
55	MG	BA	3163	1/1	0.96	0.14	27,27,27,27	0
55	MG	BA	3165	1/1	0.96	0.12	3,3,3,3	0
55	MG	BA	3126	1/1	0.96	0.15	3,3,3,3	0
55	MG	BA	3103	1/1	0.96	0.07	7,7,7,7	0
55	MG	DA	3023	1/1	0.96	0.10	60,60,60,60	0
55	MG	BA	3012	1/1	0.96	0.16	0,0,0,0	0
55	MG	DA	3105	1/1	0.96	0.12	52,52,52,52	0
55	MG	BA	3049	1/1	0.96	0.14	3,3,3,3	0
55	MG	BA	3170	1/1	0.96	0.26	22,22,22,22	0
55	MG	BA	3022	1/1	0.96	0.15	0,0,0,0	0
55	MG	DA	3110	1/1	0.96	0.24	45,45,45,45	0
55	MG	CA	1644	1/1	0.96	0.38	36,36,36,36	0
55	MG	DA	3156	1/1	0.96	0.13	58,58,58,58	0
55	MG	CA	1607	1/1	0.96	0.14	55,55,55,55	0
55	MG	BA	3172	1/1	0.96	0.12	16,16,16,16	0
55	MG	BA	3013	1/1	0.96	0.17	0,0,0,0	0
55	MG	BA	3110	1/1	0.96	0.11	26,26,26,26	0
55	MG	AA	1637	1/1	0.96	0.14	16,16,16,16	0
55	MG	DA	3117	1/1	0.96	0.12	55,55,55,55	0
55	MG	BA	3143	1/1	0.96	0.32	3,3,3,3	0
55	MG	DA	3075	1/1	0.96	0.26	61,61,61,61	0
55	MG	DA	3076	1/1	0.96	0.13	59,59,59,59	0
55	MG	CA	1613	1/1	0.96	0.14	17,17,17,17	0
55	MG	BA	3005	1/1	0.96	0.17	43,43,43,43	0
55	MG	BA	3094	1/1	0.96	0.12	20,20,20,20	0
55	MG	BA	3146	1/1	0.96	0.21	22,22,22,22	0
55	MG	BA	3067	1/1	0.96	0.20	0,0,0,0	0
55	MG	BA	3127	1/1	0.97	0.10	2,2,2,2	0
55	MG	BA	3162	1/1	0.97	0.14	23,23,23,23	0
55	MG	BA	3062	1/1	0.97	0.11	4,4,4,4	0
55	MG	BB	204	1/1	0.97	0.36	0,0,0,0	0
55	MG	BA	3130	1/1	0.97	0.17	2,2,2,2	0
55	MG	DA	3020	1/1	0.97	0.19	44,44,44,44	0
55	MG	BA	3131	1/1	0.97	0.32	37,37,37,37	0
55	MG	BA	3132	1/1	0.97	0.20	32,32,32,32	0
55	MG	DA	3140	1/1	0.97	0.23	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	BA	3043	1/1	0.97	0.06	23,23,23,23	0
55	MG	BA	3134	1/1	0.97	0.09	3,3,3,3	0
55	MG	BA	3009	1/1	0.97	0.08	2,2,2,2	0
55	MG	CA	1643	1/1	0.97	0.37	41,41,41,41	0
55	MG	AA	1649	1/1	0.97	0.12	28,28,28,28	0
55	MG	AA	1603	1/1	0.97	0.21	57,57,57,57	0
55	MG	AA	1641	1/1	0.97	0.12	7,7,7,7	0
55	MG	AA	1611	1/1	0.97	0.07	21,21,21,21	0
55	MG	DA	3109	1/1	0.97	0.19	30,30,30,30	0
55	MG	BA	3142	1/1	0.97	0.21	0,0,0,0	0
55	MG	BA	3030	1/1	0.97	0.16	3,3,3,3	0
55	MG	AA	1653	1/1	0.97	0.18	34,34,34,34	0
55	MG	BA	3116	1/1	0.97	0.19	30,30,30,30	0
55	MG	BA	3072	1/1	0.97	0.19	2,2,2,2	0
55	MG	BA	3147	1/1	0.97	0.14	11,11,11,11	0
55	MG	CA	1617	1/1	0.97	0.09	41,41,41,41	0
55	MG	BA	3148	1/1	0.97	0.14	13,13,13,13	0
55	MG	BA	3149	1/1	0.97	0.23	0,0,0,0	0
55	MG	AA	1664	1/1	0.97	0.13	51,51,51,51	0
55	MG	BA	3018	1/1	0.97	0.08	10,10,10,10	0
55	MG	AA	1654	1/1	0.97	0.14	41,41,41,41	0
55	MG	DA	3162	1/1	0.97	0.11	48,48,48,48	0
55	MG	BA	3153	1/1	0.97	0.16	2,2,2,2	0
55	MG	AA	1632	1/1	0.97	0.13	40,40,40,40	0
55	MG	BA	3189	1/1	0.97	0.20	0,0,0,0	0
55	MG	AA	1628	1/1	0.97	0.04	39,39,39,39	0
55	MG	BA	3006	1/1	0.97	0.07	13,13,13,13	0
55	MG	BA	3058	1/1	0.97	0.07	15,15,15,15	0
55	MG	BA	3158	1/1	0.97	0.12	15,15,15,15	0
55	MG	AA	1622	1/1	0.97	0.22	21,21,21,21	0
55	MG	BA	3042	1/1	0.97	0.14	1,1,1,1	0
56	ZN	D4	101	1/1	0.97	0.07	74,74,74,74	0
55	MG	CA	1625	1/1	0.98	0.17	18,18,18,18	0
55	MG	BA	3106	1/1	0.98	0.24	0,0,0,0	0
55	MG	BA	3081	1/1	0.98	0.10	0,0,0,0	0
55	MG	BA	3021	1/1	0.98	0.15	2,2,2,2	0
55	MG	BA	3139	1/1	0.98	0.27	0,0,0,0	0
55	MG	CA	1649	1/1	0.98	0.22	24,24,24,24	0
55	MG	BA	3060	1/1	0.98	0.13	29,29,29,29	0
55	MG	BA	3051	1/1	0.98	0.14	4,4,4,4	0
55	MG	DA	3131	1/1	0.98	0.13	50,50,50,50	0
55	MG	BA	3035	1/1	0.98	0.07	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3017	1/1	0.98	0.18	39,39,39,39	0
55	MG	BA	3008	1/1	0.98	0.13	0,0,0,0	0
55	MG	DA	3086	1/1	0.98	0.12	61,61,61,61	0
55	MG	BA	3128	1/1	0.98	0.19	3,3,3,3	0
55	MG	BA	3114	1/1	0.98	0.09	28,28,28,28	0
55	MG	BA	3037	1/1	0.98	0.19	0,0,0,0	0
55	MG	BA	3164	1/1	0.98	0.30	6,6,6,6	0
55	MG	BA	3017	1/1	0.98	0.16	0,0,0,0	0
55	MG	AA	1612	1/1	0.98	0.13	38,38,38,38	0
55	MG	BA	3078	1/1	0.98	0.04	38,38,38,38	0
55	MG	BA	3010	1/1	0.98	0.09	1,1,1,1	0
55	MG	AA	1621	1/1	0.98	0.09	37,37,37,37	0
55	MG	BA	3187	1/1	0.98	0.21	3,3,3,3	0
55	MG	DA	3050	1/1	0.98	0.12	52,52,52,52	0
55	MG	DA	3074	1/1	0.98	0.08	47,47,47,47	0
55	MG	AA	1642	1/1	0.99	0.07	25,25,25,25	0
55	MG	BA	3107	1/1	0.99	0.14	3,3,3,3	0
55	MG	BA	3086	1/1	0.99	0.20	0,0,0,0	0
55	MG	BA	3141	1/1	0.99	0.40	0,0,0,0	0
55	MG	DA	3067	1/1	0.99	0.18	43,43,43,43	0
55	MG	AA	1656	1/1	0.99	0.07	32,32,32,32	0
55	MG	BA	3063	1/1	0.99	0.13	2,2,2,2	0
55	MG	BA	3033	1/1	0.99	0.20	0,0,0,0	0
55	MG	AA	1647	1/1	0.99	0.17	44,44,44,44	0
55	MG	AA	1645	1/1	0.99	0.09	42,42,42,42	0
56	ZN	B4	101	1/1	1.00	0.08	76,76,76,76	0

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

There are no such residues in this entry.