wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 11:50 PM EDT

PDB ID	:	6BY1
Title	:	E. coli pH03H9 complex
Authors	:	Amiri, H.; Noller, H.F.
Deposited on	:	2017-12-19
Resolution	:	3.94 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 (i) 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 (i)) were used in the production of this report:

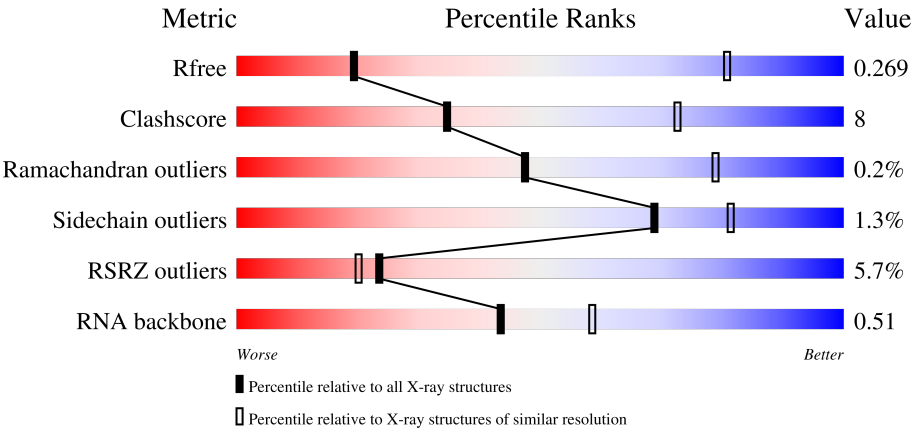
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 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	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)
RNA backbone	3102	1041 (4.84-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	1541	45% 44% 10%
1	BA	1541	44% 45% 9%
2	CA	2904	52% 39% 8%
2	DA	2904	48% 42% 9%

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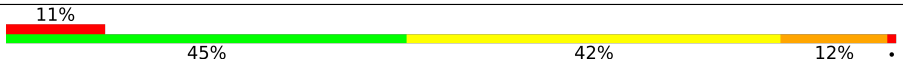
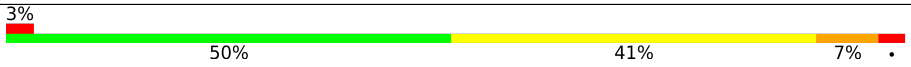
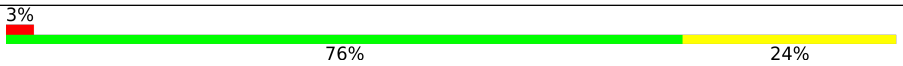
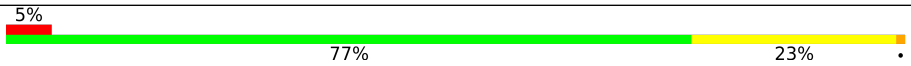
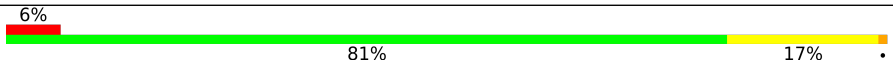
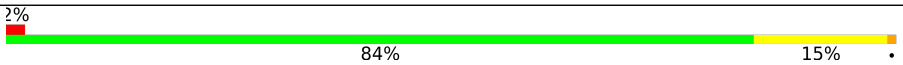
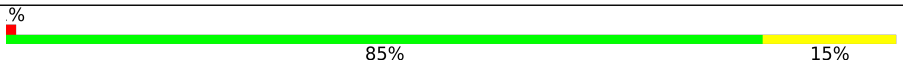
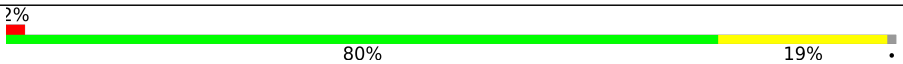
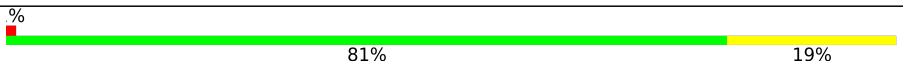
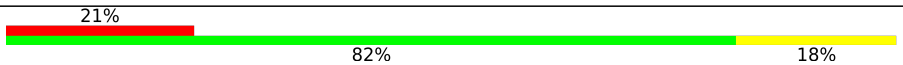
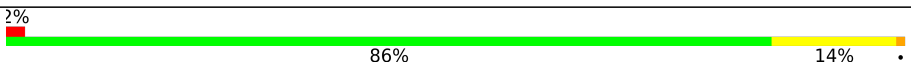
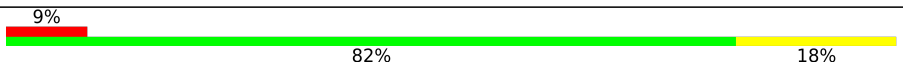
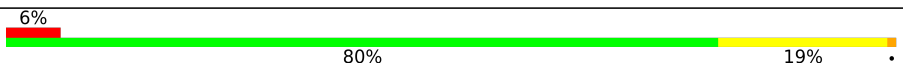
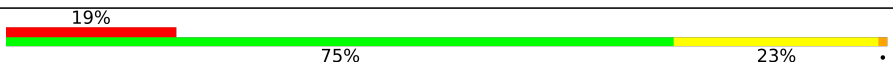
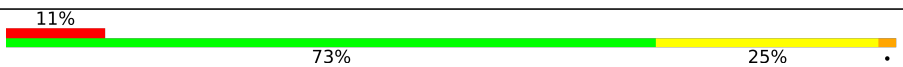
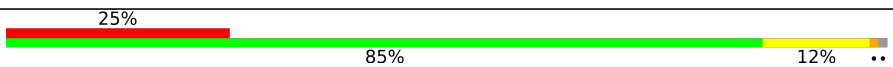
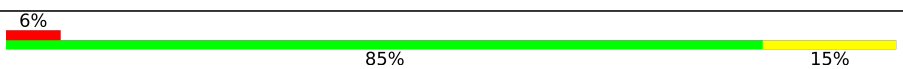
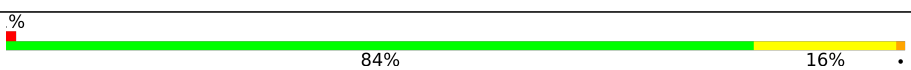
Mol	Chain	Length	Quality of chain
3	CB	118	
3	DB	118	
4	AV	76	
4	AW	76	
4	AY	76	
4	BV	76	
4	BW	76	
5	CC	271	
5	DC	271	
6	CD	209	
6	DD	209	
7	CE	181	
7	DE	181	
8	CF	177	
8	DF	177	
9	CG	176	
9	DG	176	
10	CH	149	
10	DH	149	
11	C5	109	
12	CI	72	
12	DI	72	
13	CJ	142	
13	DJ	142	
14	CK	122	

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Mol	Chain	Length	Quality of chain
14	DK	122	6% 77% 23%
15	CL	143	6% 75% 24%
15	DL	143	5% 80% 20%
16	CM	136	90% 8%
16	DM	136	18% 79% 21%
17	CN	121	73% 26%
17	DN	121	2% 81% 17%
18	CO	116	3% 76% 23%
18	DO	116	25% 79% 20%
19	CP	114	5% 82% 18%
19	DP	114	4% 73% 26%
20	CQ	117	87% 13%
20	DQ	117	82% 18%
21	CR	103	86% 13%
21	DR	103	2% 80% 20%
22	CS	110	5% 85% 15%
22	DS	110	7% 85% 15%
23	CT	93	9% 80% 16%
23	DT	93	3% 90% 9%
24	CU	102	2% 85% 15%
24	DU	102	13% 79% 20%
25	CV	94	6% 78% 22%
25	DV	94	3% 82% 18%
26	CW	75	5% 77% 21%
26	DW	75	17% 79% 21%

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Mol	Chain	Length	Quality of chain
27	CX	77	4% 86% 13%
27	DX	77	5% 81% 19%
28	CY	63	87% 10%
28	DY	63	5% 76% 24%
29	CZ	58	3% 76% 22%
29	DZ	58	9% 81% 19%
30	C0	39	15% 69% 31%
30	D0	39	26% 59% 36% 5%
31	C1	56	82% 18%
31	D1	56	79% 21%
32	C2	50	62% 78% 22%
32	D2	50	78% 80% 20%
33	C3	46	80% 20%
33	D3	46	76% 22%
34	C4	62	19% 79% 19%
34	D4	62	39% 77% 23%
35	C6	38	68% 32%
35	D6	38	34% 55% 45%
36	AX	46	33% 26% 33% 7% 35%
36	BX	46	37% 33% 30% 35%
37	AB	225	12% 83% 17%
37	BB	225	7% 80% 19%
38	AC	206	% 83% 15%
38	BC	206	10% 74% 25%
39	AD	205	12% 73% 26%

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Mol	Chain	Length	Quality of chain
39	BD	205	2% 72% 27%
40	AE	150	11% 76% 24%
40	BE	150	7% 77% 21%
41	AF	100	% 72% 28%
41	BF	100	15% 72% 26%
42	AG	179	8% 61% 15% 25%
42	BG	179	13% 62% 12% 26%
43	AH	129	6% 86% 13%
43	BH	129	3% 81% 19%
44	AI	130	14% 75% 19% 5%
44	BI	130	9% 58% 38%
45	AJ	98	16% 62% 37%
45	BJ	98	12% 71% 27%
46	AK	117	74% 25%
46	BK	117	14% 73% 26%
47	AL	123	16% 73% 26%
47	BL	123	7% 64% 34%
48	AM	114	10% 75% 24%
48	BM	114	7% 71% 28%
49	AN	101	12% 78% 17% 5%
49	BN	101	7% 72% 23% 5%
50	AO	89	80% 17%
50	BO	89	9% 85% 11%
51	AP	82	43% 85% 12%
51	BP	82	30% 78% 21%

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Mol	Chain	Length	Quality of chain
52	AQ	80	10% 71% 25%
52	BQ	80	20% 78% 21%
53	AR	55	7% 67% 31%
53	BR	55	15% 87% 13%
54	AS	79	10% 81% 19%
54	BS	79	20% 80% 20%
55	AT	85	4% 79% 20%
55	BT	85	6% 86% 14%

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
56	MG	AA	1640	-	-	-	X
56	MG	AA	1644	-	-	-	X
56	MG	BA	1608	-	-	-	X
56	MG	BA	1620	-	-	-	X
56	MG	BA	1628	-	-	-	X
56	MG	CA	3068	-	-	-	X
56	MG	DA	3094	-	-	-	X

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 296390 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1540	Total	C	N	O	P	0	1	0
			33037	14735	6057	10705	1540			
1	BA	1541	Total	C	N	O	P	0	0	0
			33057	14744	6059	10713	1541			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CA	2867	Total	C	N	O	P	0	0	0
			61550	27457	11328	19898	2867			
2	DA	2869	Total	C	N	O	P	0	0	0
			61593	27477	11339	19908	2869			

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
3	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 4 is a RNA chain called Valine-specific transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AV	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			
4	AY	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			
4	AW	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			
4	BV	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	BW	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	CE	181	Total	C	N	O	S	0	0	0
			1404	881	261	258	4			
7	DE	180	Total	C	N	O	S	0	0	0
			1393	875	257	257	4			

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	C5	109	Total	C	N	O	S	0	0	0
			825	521	149	151	4			

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	CI	71	Total	C	N	O	S	0	0	0
			511	313	93	102	3			
12	DI	72	Total	C	N	O	S	0	0	0
			518	317	94	104	3			

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	CL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	CM	135	Total	C	N	O	S	0	0	0
			1065	681	204	175	5			
16	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	CN	121	Total	C	N	O	S	0	0	0
			969	599	198	167	5			
17	DN	121	Total	C	N	O	S	0	0	0
			969	599	198	167	5			

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	CQ	117	Total	C	N	O	0	0	0
			947	604	192	151			
20	DQ	117	Total	C	N	O	0	0	0
			947	604	192	151			

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	CT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
23	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 24 is a protein called 50S ribosomal protein L24.

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

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CW	75	Total	C	N	O	S	0	0	0
			574	356	116	101	1			
26	DW	75	Total	C	N	O	S	0	0	0
			574	356	116	101	1			

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CY	61	Total	C	N	O	S	0	0	0
			499	308	97	92	2			
28	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	C0	39	Total	C	N	O	S	0	0	0
			293	179	52	57	5			
30	D0	39	Total	C	N	O	S	0	0	0
			293	179	52	57	5			

- Molecule 31 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	C1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	C2	50	Total	C	N	O	0	0	0
			410	263	75	72			
32	D2	50	Total	C	N	O	0	0	0
			410	263	75	72			

- Molecule 33 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	C3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
33	D3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 34 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	C4	61	Total	C	N	O	S	0	0	0
			479	306	102	69	2			
34	D4	62	Total	C	N	O	S	0	0	0
			486	311	103	70	2			

- Molecule 35 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	C6	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
35	D6	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 36 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AX	30	Total	C	N	O	P	0	0	0
			653	293	130	200	30			
36	BX	30	Total	C	N	O	P	0	0	0
			653	293	130	200	30			

- Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AB	225	Total	C	N	O	S	0	0	0
			1757	1111	315	323	8			
37	BB	225	Total	C	N	O	S	0	0	0
			1757	1111	315	323	8			

- Molecule 38 is a protein called 30S ribosomal protein S3.

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

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

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

- Molecule 41 is a protein called 30S ribosomal protein S6.

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

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AG	135	Total	C	N	O	S	0	0	0
			1058	659	203	192	4			
42	BG	132	Total	C	N	O	S	0	0	0
			1035	644	200	187	4			

- Molecule 43 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AH	128	Total	C	N	O	S	0	0	0
			973	613	172	182	6			
43	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 44 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AI	124	Total	C	N	O	S	0	0	0
			995	619	199	174	3			
44	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 45 is a protein called 30S ribosomal protein S10.

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

- Molecule 46 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	AK	116	Total	C	N	O	S	0	0	0
			869	535	173	158	3			
46	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 47 is a protein called 30S ribosomal protein S12.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 48 is a protein called 30S ribosomal protein S13.

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

- Molecule 49 is a protein called 30S ribosomal protein S14.

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

- Molecule 50 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
50	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

- Molecule 53 is a protein called 30S ribosomal protein S18.

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

- Molecule 54 is a protein called 30S ribosomal protein S19.

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

- Molecule 55 is a protein called 30S ribosomal protein S20.

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	50	Total 50	Mg 50	0	0
56	CA	167	Total 167	Mg 167	0	0
56	CB	3	Total 3	Mg 3	0	0
56	CC	1	Total 1	Mg 1	0	0
56	CN	2	Total 2	Mg 2	0	0
56	CQ	1	Total 1	Mg 1	0	0
56	C4	1	Total 1	Mg 1	0	0
56	BA	49	Total 49	Mg 49	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DA	166	Total Mg 166 166	0	0
56	DB	3	Total Mg 3 3	0	0
56	DN	1	Total Mg 1 1	0	0
56	DQ	1	Total Mg 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	C0	1	Total Zn 1 1	0	0
57	C6	1	Total Zn 1 1	0	0
57	D0	1	Total Zn 1 1	0	0
57	D6	1	Total Zn 1 1	0	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AA	481	Total O 481 481	0	0
58	CA	1106	Total O 1106 1106	0	0
58	CB	49	Total O 49 49	0	0
58	AV	28	Total O 28 28	0	0
58	AY	5	Total O 5 5	0	0
58	CC	13	Total O 13 13	0	0
58	CD	10	Total O 10 10	0	0
58	CE	16	Total O 16 16	0	0
58	CF	14	Total O 14 14	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	CG	18	Total O 18 18	0	0
58	CH	8	Total O 8 8	0	0
58	C5	7	Total O 7 7	0	0
58	CI	4	Total O 4 4	0	0
58	CJ	9	Total O 9 9	0	0
58	CK	7	Total O 7 7	0	0
58	CL	8	Total O 8 8	0	0
58	CM	4	Total O 4 4	0	0
58	CN	6	Total O 6 6	0	0
58	CO	8	Total O 8 8	0	0
58	CP	8	Total O 8 8	0	0
58	CQ	2	Total O 2 2	0	0
58	CR	7	Total O 7 7	0	0
58	CS	3	Total O 3 3	0	0
58	CT	7	Total O 7 7	0	0
58	CU	13	Total O 13 13	0	0
58	CV	10	Total O 10 10	0	0
58	CW	4	Total O 4 4	0	0
58	CX	3	Total O 3 3	0	0
58	CY	3	Total O 3 3	0	0
58	CZ	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	C1	5	Total O 5 5	0	0
58	C2	1	Total O 1 1	0	0
58	C3	2	Total O 2 2	0	0
58	C4	2	Total O 2 2	0	0
58	C6	3	Total O 3 3	0	0
58	AX	4	Total O 4 4	0	0
58	AW	32	Total O 32 32	0	0
58	AB	7	Total O 7 7	0	0
58	AC	15	Total O 15 15	0	0
58	AD	10	Total O 10 10	0	0
58	AE	12	Total O 12 12	0	0
58	AF	6	Total O 6 6	0	0
58	AG	5	Total O 5 5	0	0
58	AH	7	Total O 7 7	0	0
58	AI	6	Total O 6 6	0	0
58	AJ	4	Total O 4 4	0	0
58	AK	10	Total O 10 10	0	0
58	AL	9	Total O 9 9	0	0
58	AM	6	Total O 6 6	0	0
58	AN	3	Total O 3 3	0	0
58	AO	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AP	4	Total O 4 4	0	0
58	AQ	8	Total O 8 8	0	0
58	AR	1	Total O 1 1	0	0
58	AS	4	Total O 4 4	0	0
58	AT	4	Total O 4 4	0	0
58	BA	461	Total O 461 461	0	0
58	DA	1005	Total O 1005 1005	0	0
58	DB	32	Total O 32 32	0	0
58	BV	13	Total O 13 13	0	0
58	DC	28	Total O 28 28	0	0
58	DD	15	Total O 15 15	0	0
58	DE	12	Total O 12 12	0	0
58	DF	4	Total O 4 4	0	0
58	DG	6	Total O 6 6	0	0
58	DH	4	Total O 4 4	0	0
58	DJ	3	Total O 3 3	0	0
58	DK	5	Total O 5 5	0	0
58	DL	10	Total O 10 10	0	0
58	DM	6	Total O 6 6	0	0
58	DN	6	Total O 6 6	0	0
58	DO	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	DP	6	Total O 6 6	0	0
58	DQ	5	Total O 5 5	0	0
58	DR	13	Total O 13 13	0	0
58	DS	9	Total O 9 9	0	0
58	DT	10	Total O 10 10	0	0
58	DU	14	Total O 14 14	0	0
58	DV	7	Total O 7 7	0	0
58	DW	3	Total O 3 3	0	0
58	DX	3	Total O 3 3	0	0
58	DY	7	Total O 7 7	0	0
58	DZ	2	Total O 2 2	0	0
58	D0	2	Total O 2 2	0	0
58	D1	11	Total O 11 11	0	0
58	D2	2	Total O 2 2	0	0
58	D3	2	Total O 2 2	0	0
58	D6	1	Total O 1 1	0	0
58	BX	5	Total O 5 5	0	0
58	BW	23	Total O 23 23	0	0
58	BB	2	Total O 2 2	0	0
58	BC	8	Total O 8 8	0	0
58	BD	24	Total O 24 24	0	0

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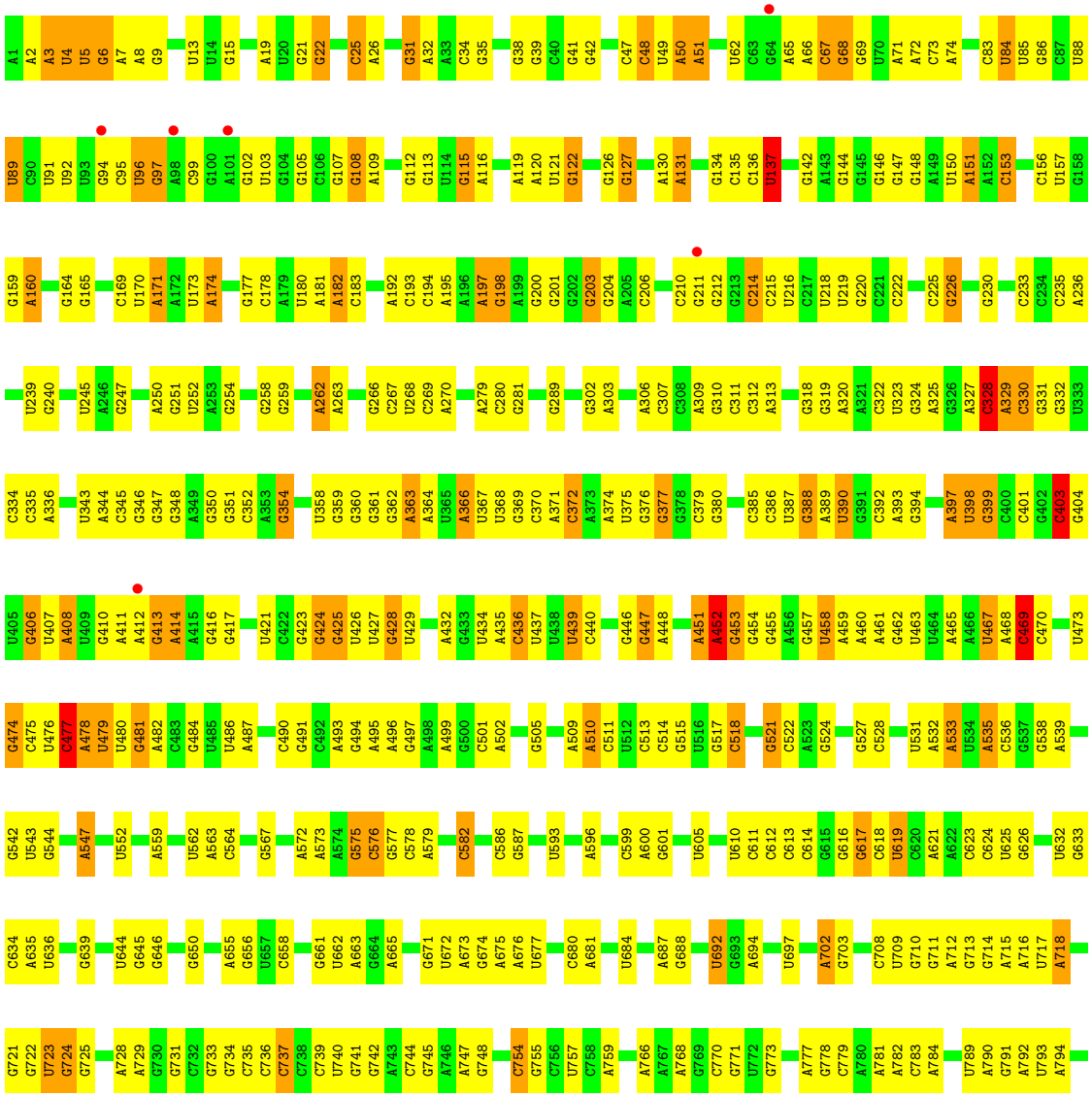
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	BE	18	Total O 18 18	0	0
58	BF	6	Total O 6 6	0	0
58	BG	4	Total O 4 4	0	0
58	BH	12	Total O 12 12	0	0
58	BI	9	Total O 9 9	0	0
58	BJ	8	Total O 8 8	0	0
58	BK	5	Total O 5 5	0	0
58	BL	8	Total O 8 8	0	0
58	BM	6	Total O 6 6	0	0
58	BN	5	Total O 5 5	0	0
58	BO	2	Total O 2 2	0	0
58	BP	5	Total O 5 5	0	0
58	BQ	10	Total O 10 10	0	0
58	BR	1	Total O 1 1	0	0
58	BS	3	Total O 3 3	0	0
58	BT	2	Total O 2 2	0	0

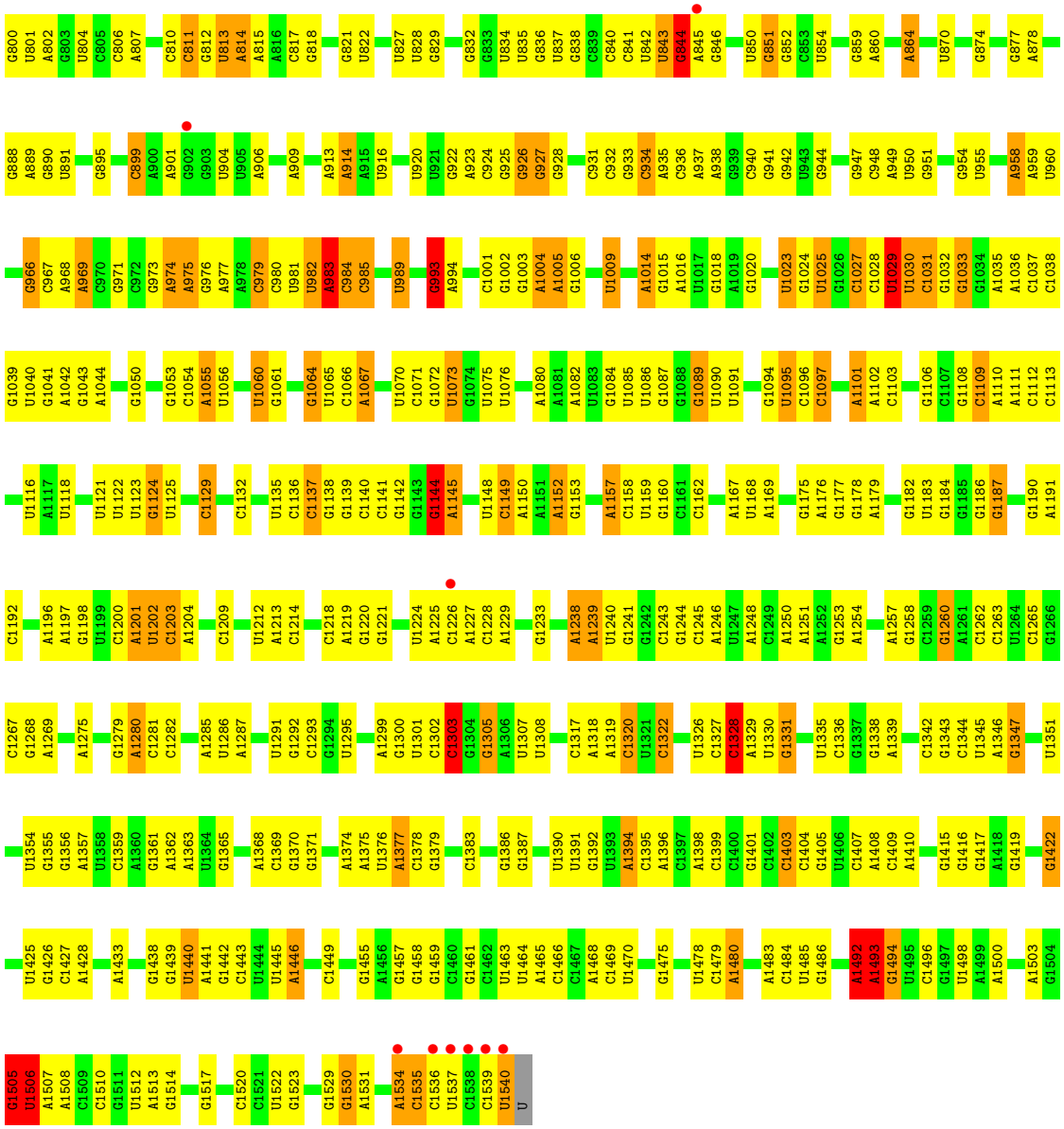
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

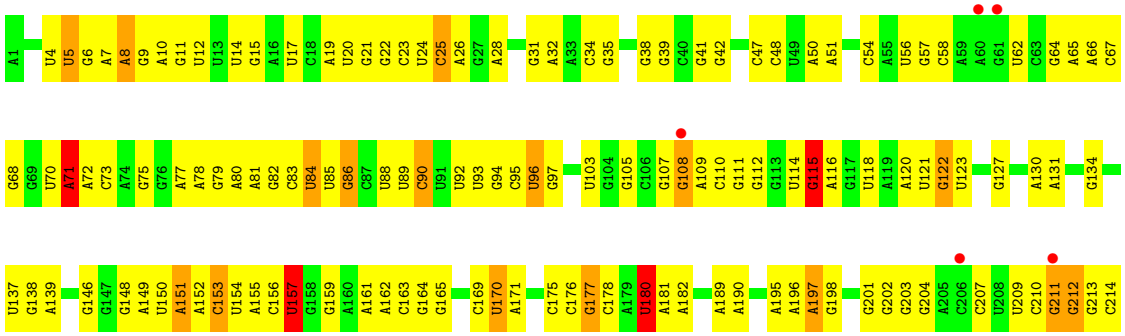
Chain AA:

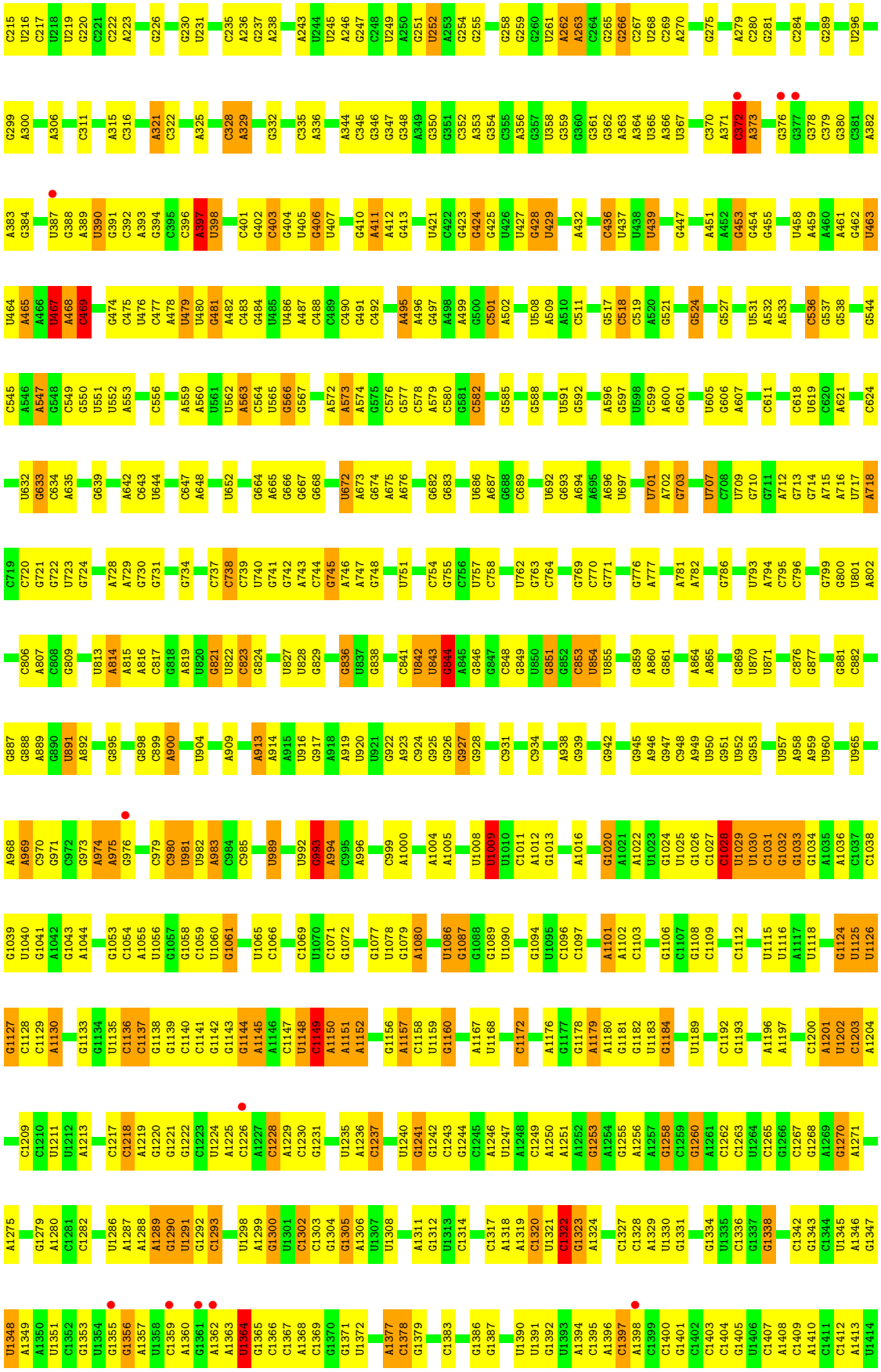


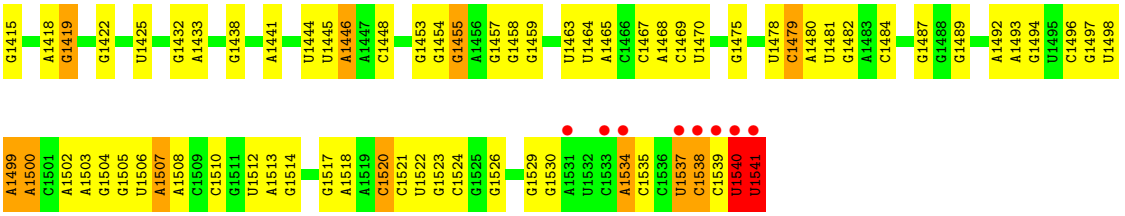


• Molecule 1: 16S ribosomal RNA

Chain BA:

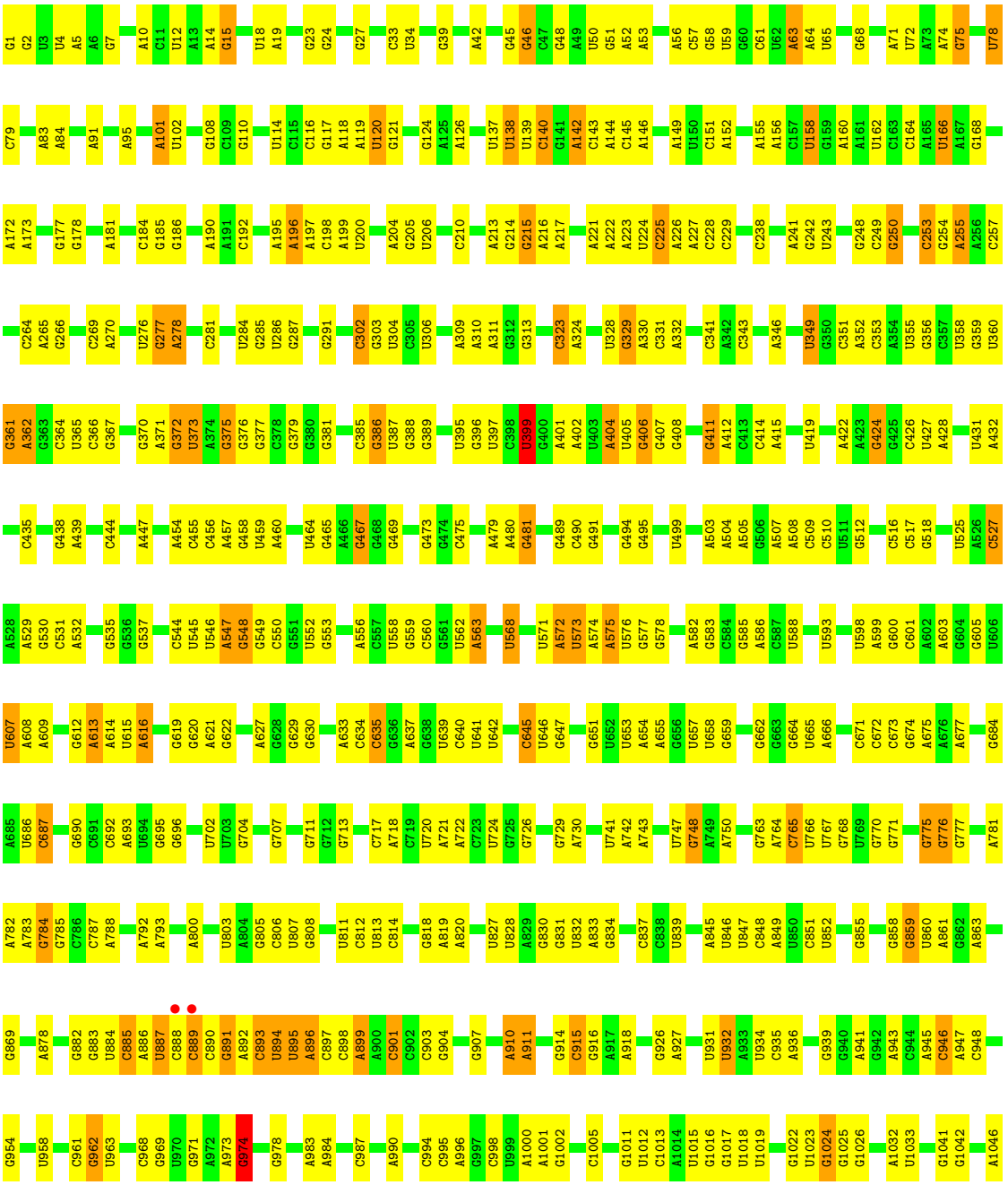


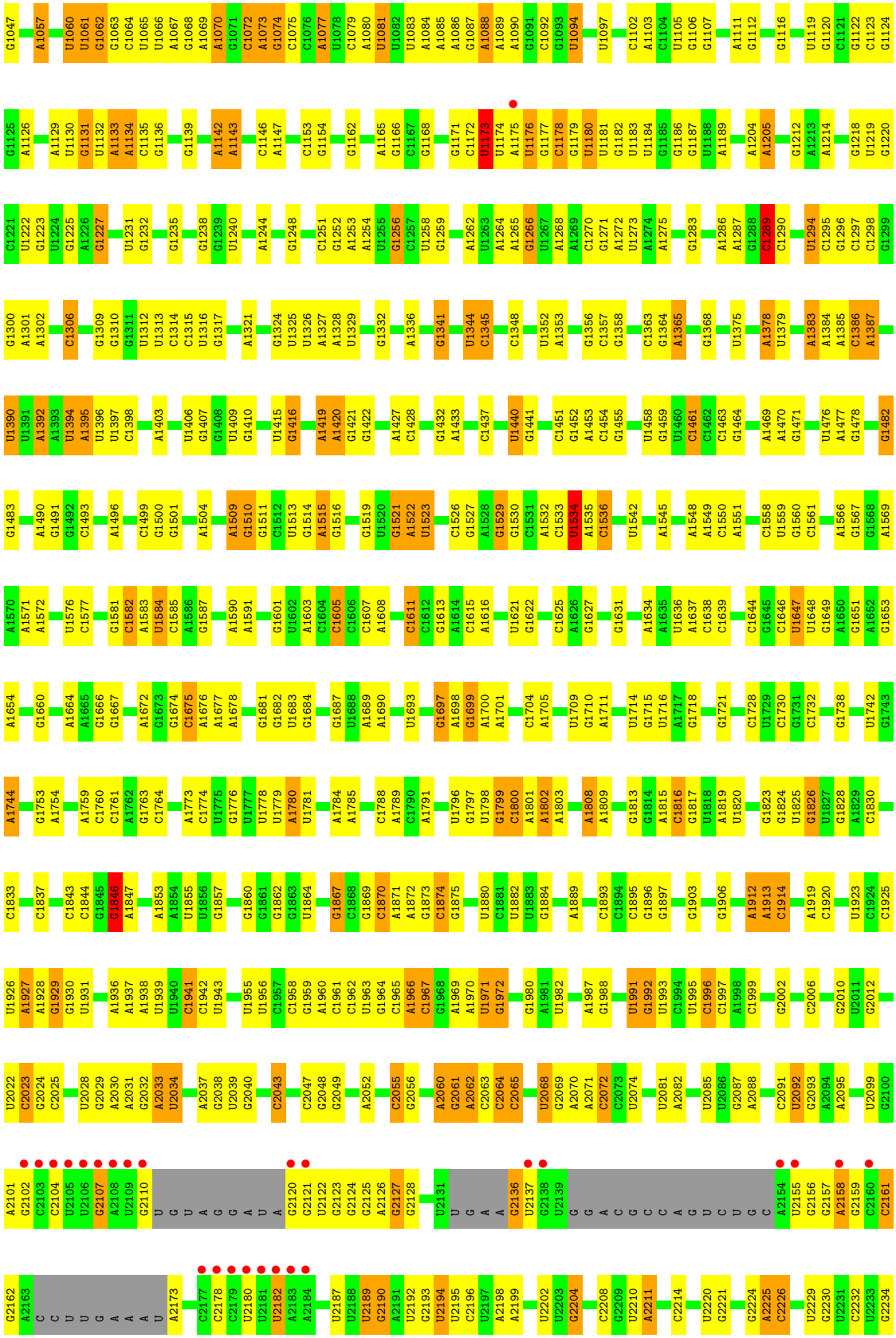




• Molecule 2: 23S ribosomal RNA

Chain CA:




G1047 A1057 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 U1097 C1102 A1103 C1104 U1105 G1106 G1107 A1111 G1112 G1116 U1119 G1120 C1121 G1122 C1123 G1124
G1125 A1126 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136 G1139 A1142 A1143 C1146 A1147 C1153 G1154 G1162 A1165 G1166 C1167 G1168 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1185 G1186 G1187 U1188 A1189 A1204 A1205 G1212 A1213 A1214 G1218 U1219 G1220
C1221 U1222 G1223 U1224 G1225 A1226 G1227 U1231 G1232 G1235 G1238 G1239 U1240 A1244 G1248 C1251 G1252 A1253 A1254 U1255 G1256 C1257 U1258 G1259 A1262 U1263 A1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 G1283 A1286 A1287 G1288 C1289 C1290 U1294 C1295 G1296 C1297 C1298 G1299
G1300 A1301 A1302 C1306 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 G1317 A1321 G1324 U1325 U1326 A1327 A1328 U1329 G1332 A1336 G1341 U1344 C1345 C1348 U1352 A1353 G1356 C1357 G1358 C1363 G1364 A1365 G1368 U1375 A1378 U1379 A1383 A1384 A1385 C1386 A1387
U1390 U1391 A1392 A1393 U1394 A1395 U1396 U1397 C1398 A1403 U1406 G1407 G1408 U1409 G1410 U1415 G1416 A1419 A1420 G1421 G1422 A1427 C1428 G1432 A1433 C1437 U1440 G1441 C1451 G1452 A1453 C1454 G1455 U1458 G1459 U1460 C1461 C1462 C1463 G1464 A1469 A1470 G1471 U1476 A1477 G1478 G1482
G1483 A1490 G1491 G1492 C1493 A1496 C1499 G1500 G1501 A1504 A1509 G1510 G1511 C1512 U1513 G1514 A1515 G1516 G1519 U1520 G1521 A1522 U1523 C1526 G1527 A1528 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 U1542 A1545 A1548 A1549 C1550 A1551 C1558 U1559 G1560 C1561 A1566 G1567 G1568 A1569
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A1654 G1660 A1664 A1665 G1666 G1667 A1672 G1673 G1674 C1675 A1676 A1677 A1678 G1681 G1682 U1683 G1684 G1687 U1688 A1689 A1690 U1693 G1697 A1698 G1699 A1700 A1701 C1704 A1705 U1709 G1710 A1711 U1714 G1715 U1716 A1717 G1718 G1721 C1728 U1729 C1730 G1731 C1732 G1738 U1742 G1743
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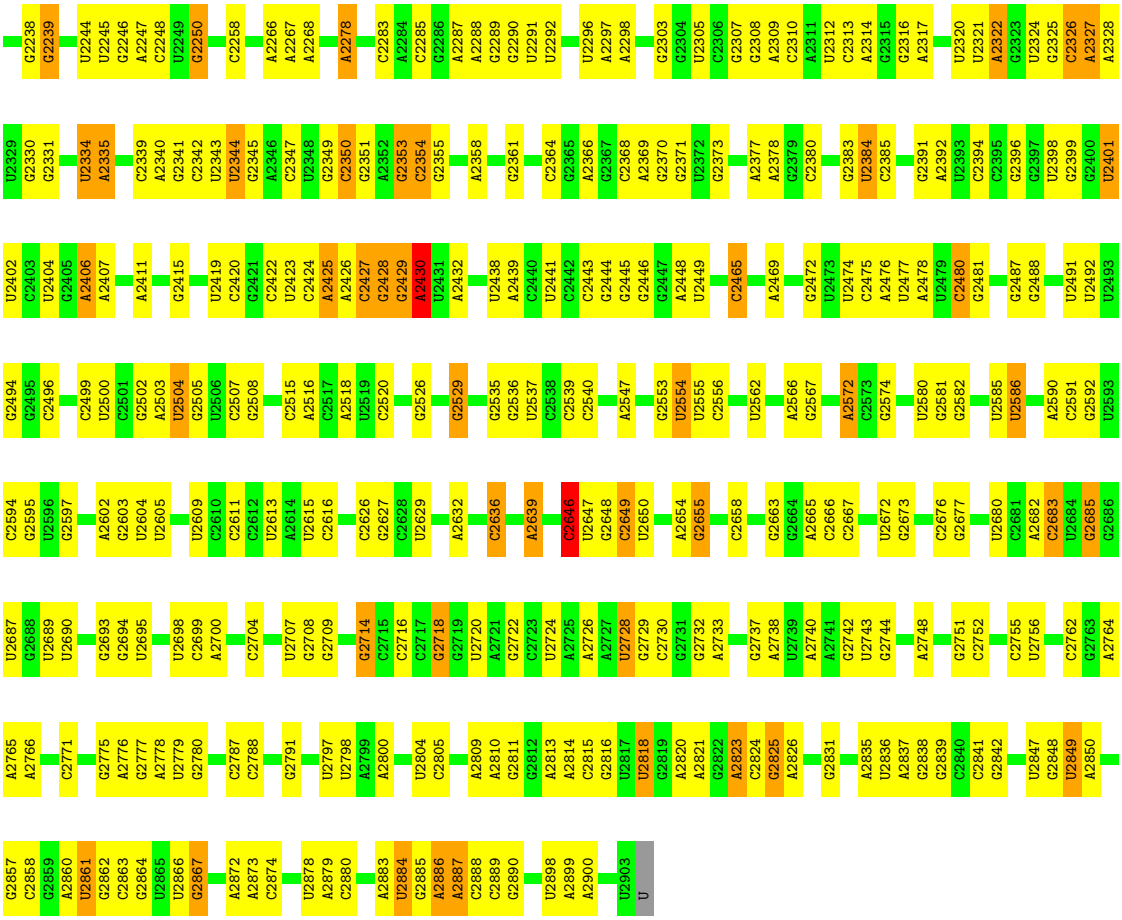
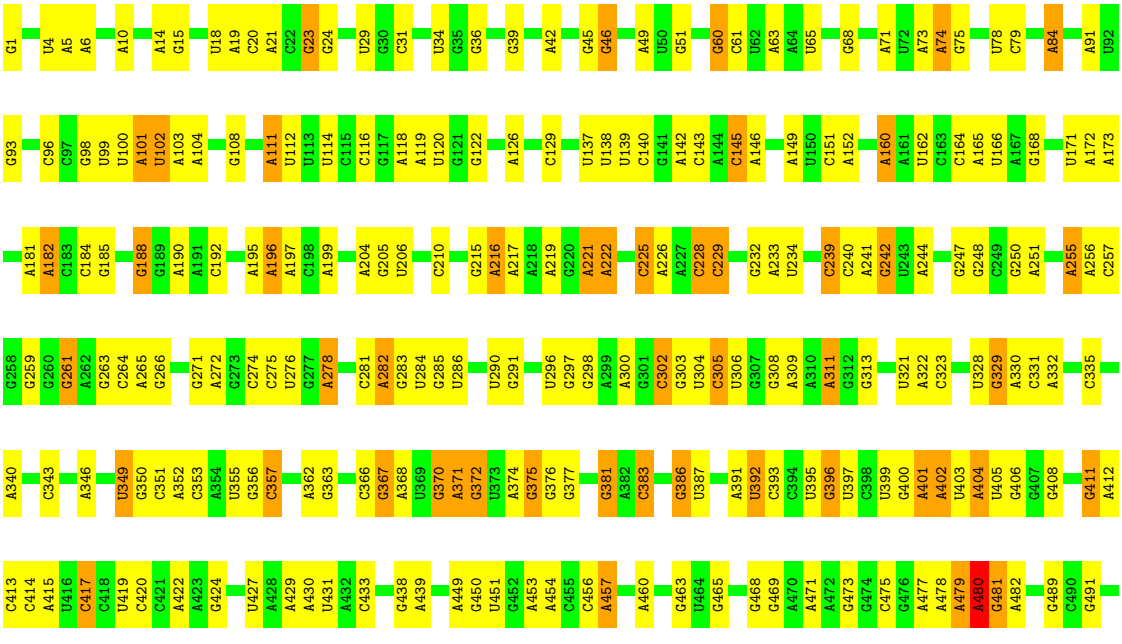
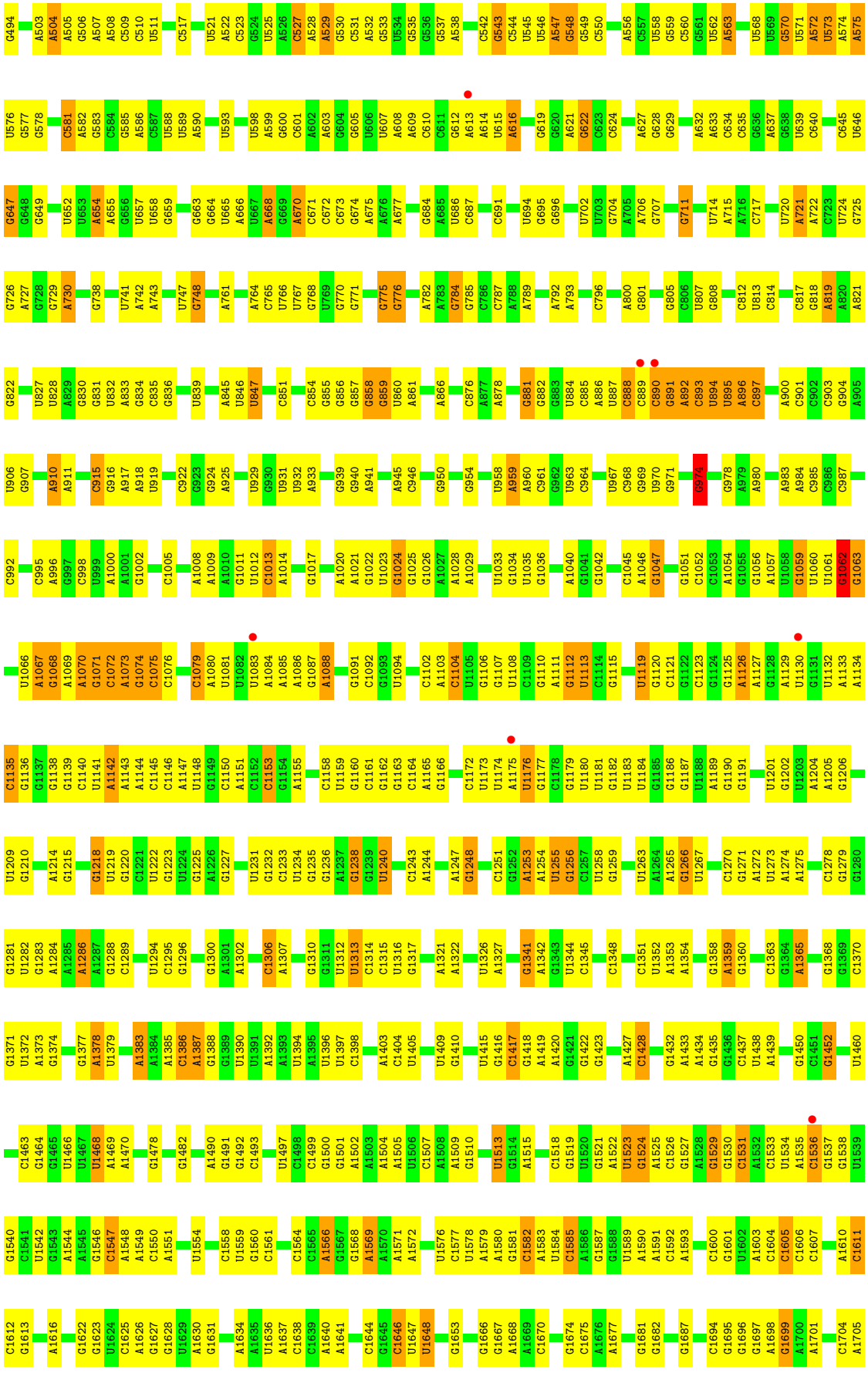
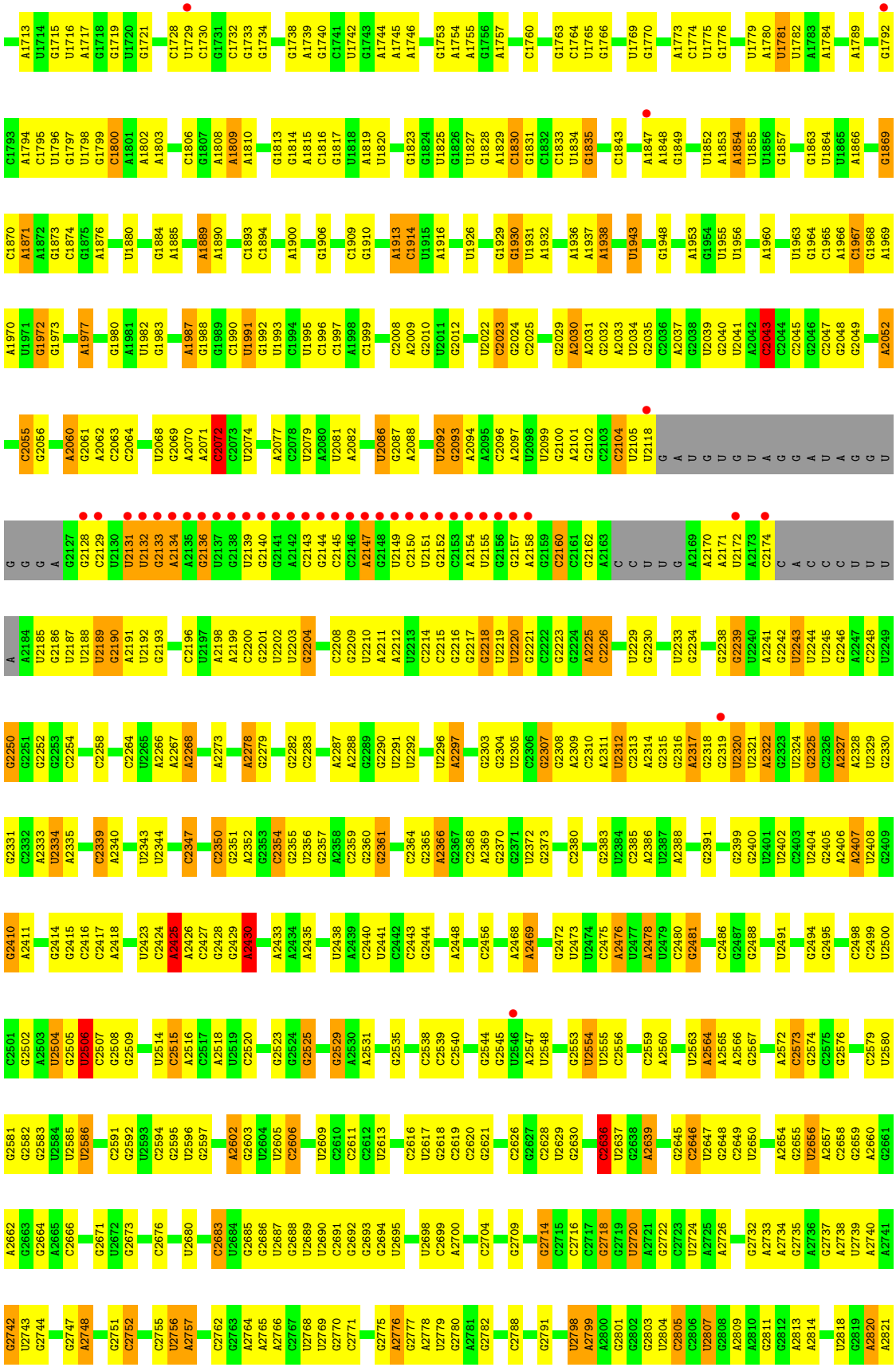


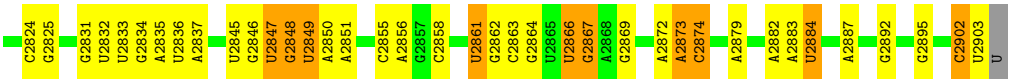
• Molecule 2: 23S ribosomal RNA

Chain DA:



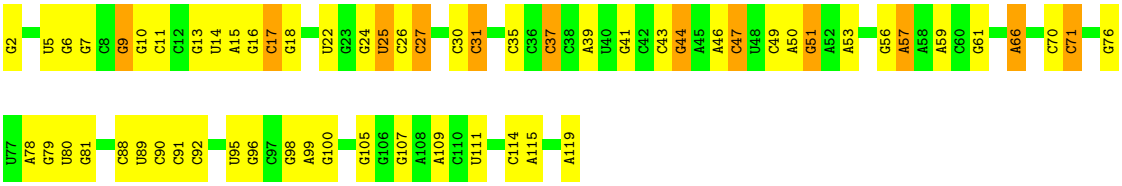






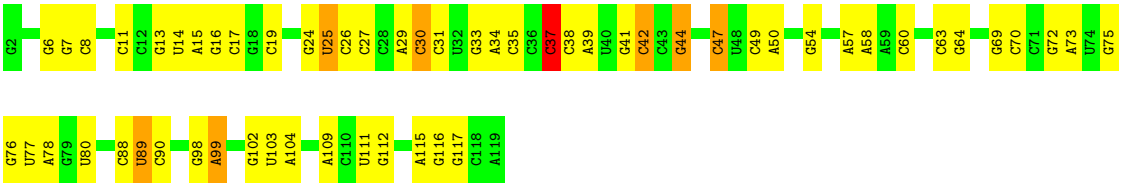
• Molecule 3: 5S ribosomal RNA

Chain CB:



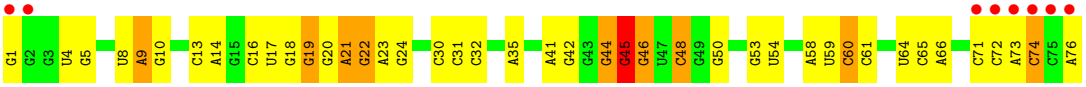
• Molecule 3: 5S ribosomal RNA

Chain DB:



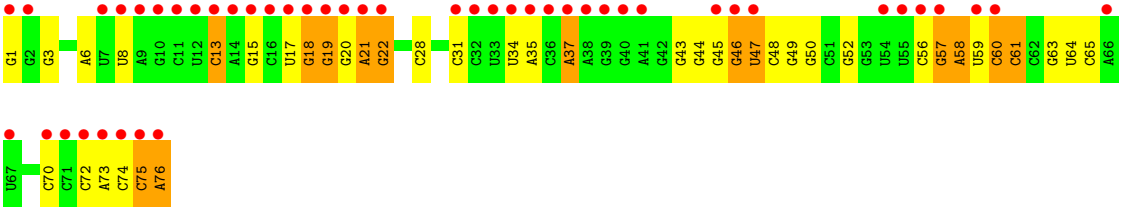
• Molecule 4: Valine-specific transfer RNA

Chain AV:



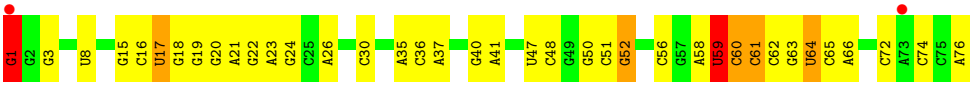
• Molecule 4: Valine-specific transfer RNA

Chain AY:



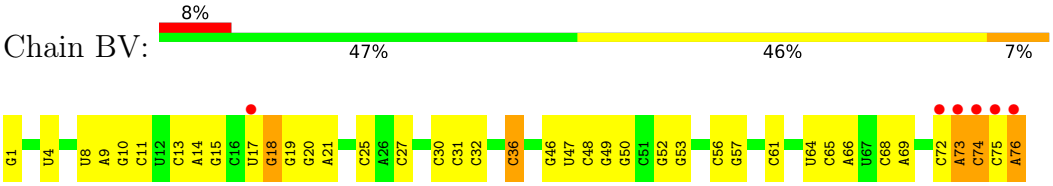
• Molecule 4: Valine-specific transfer RNA

Chain AW:



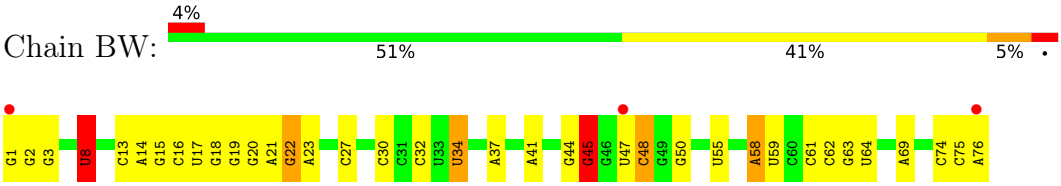
• Molecule 4: Valine-specific transfer RNA

Chain BV:



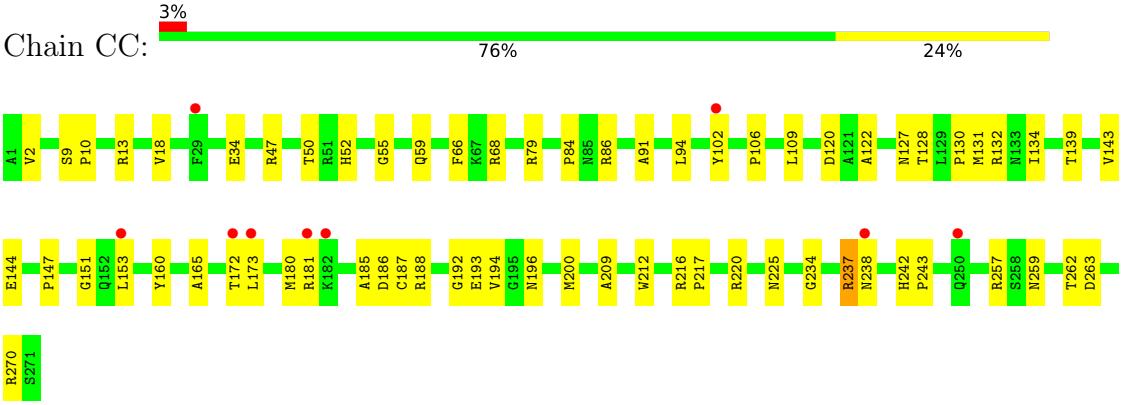
• Molecule 4: Valine-specific transfer RNA

Chain BW:



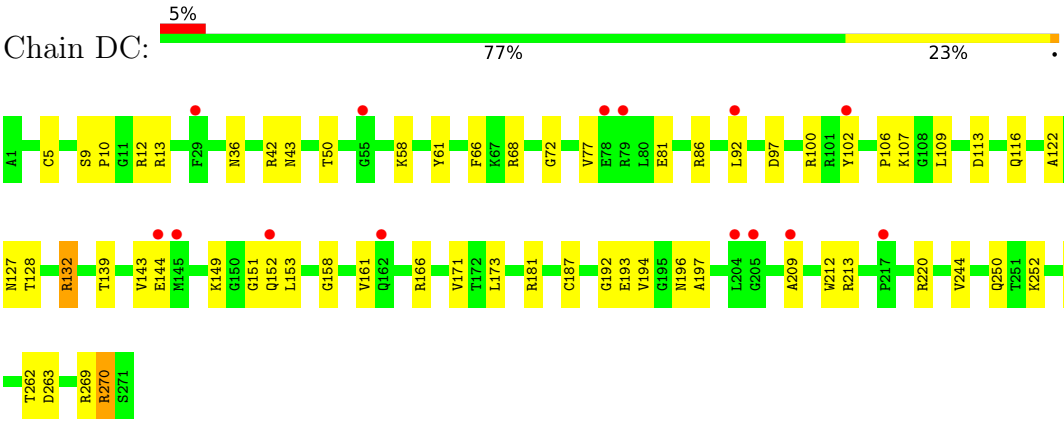
• Molecule 5: 50S ribosomal protein L2

Chain CC:



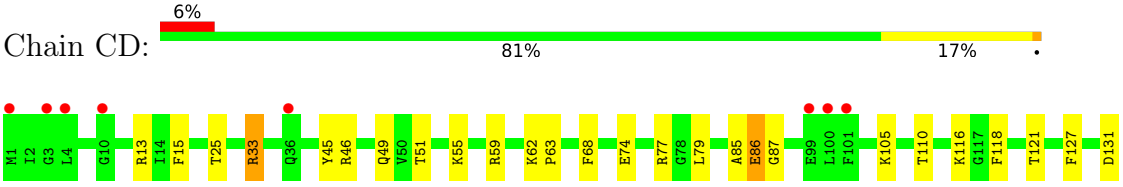
• Molecule 5: 50S ribosomal protein L2

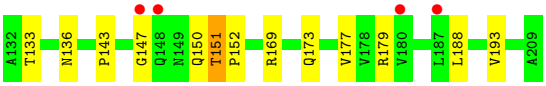
Chain DC:



• Molecule 6: 50S ribosomal protein L3

Chain CD:





• Molecule 6: 50S ribosomal protein L3

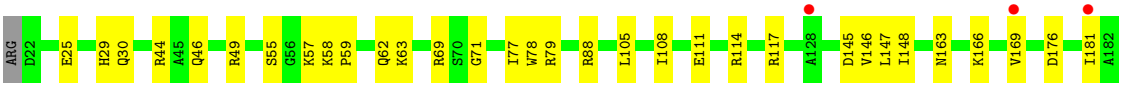
Chain DD:

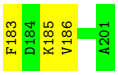
• Molecule 7: 50S ribosomal protein L4

Chain CE:

• Molecule 7: 50S ribosomal protein L4

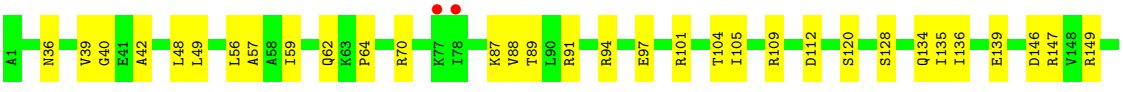
Chain DE:





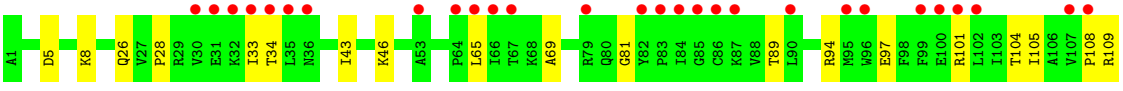
• Molecule 8: 50S ribosomal protein L5

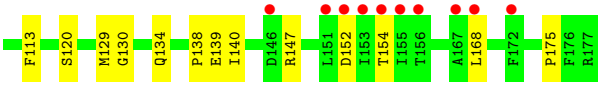
Chain CF:



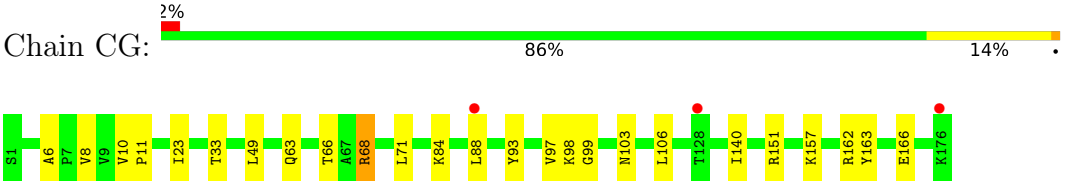
• Molecule 8: 50S ribosomal protein L5

Chain DF:

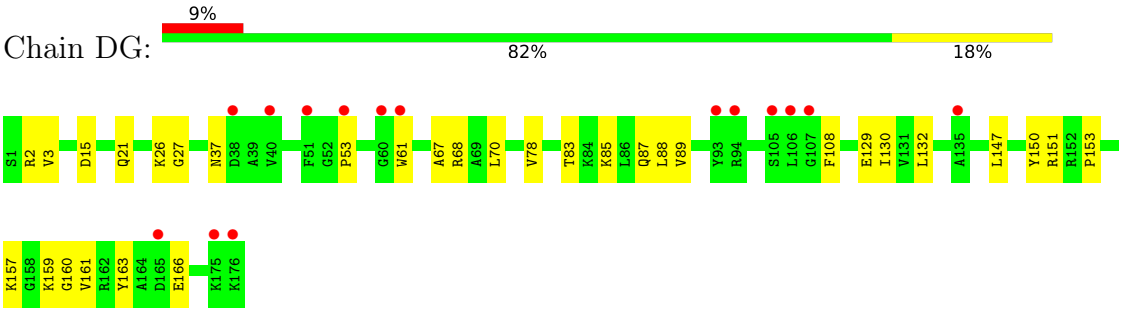




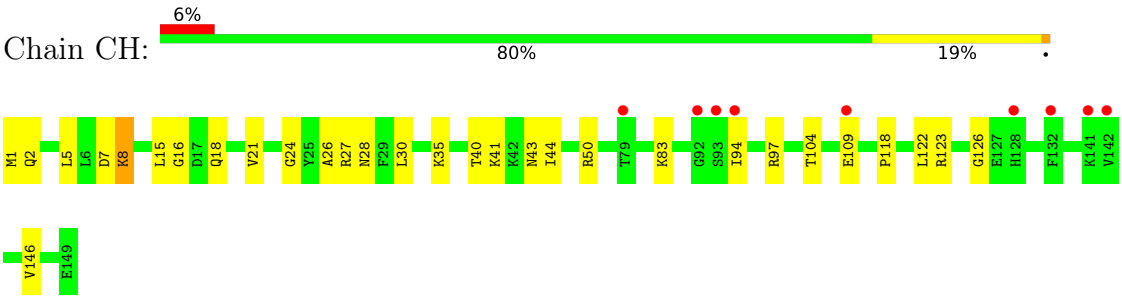
• Molecule 9: 50S ribosomal protein L6



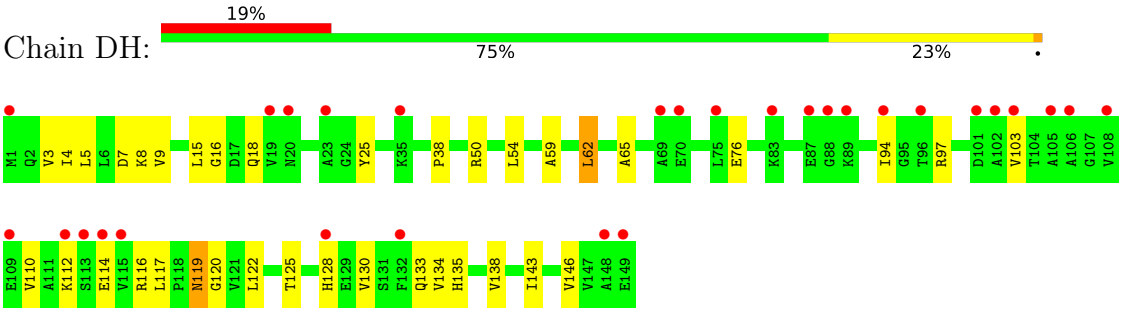
• Molecule 9: 50S ribosomal protein L6



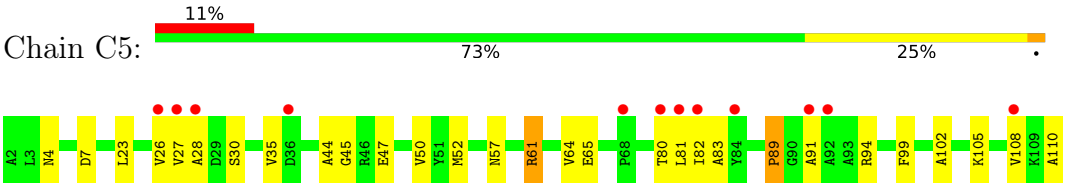
• Molecule 10: 50S ribosomal protein L9



• Molecule 10: 50S ribosomal protein L9

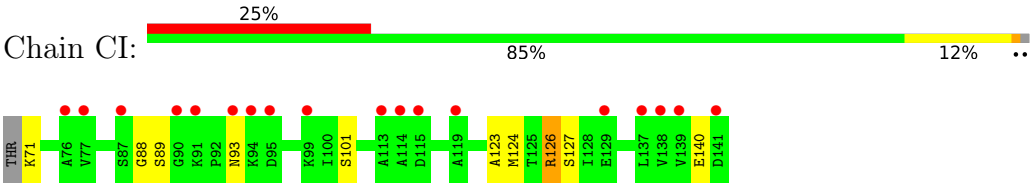


• Molecule 11: 50S ribosomal protein L10



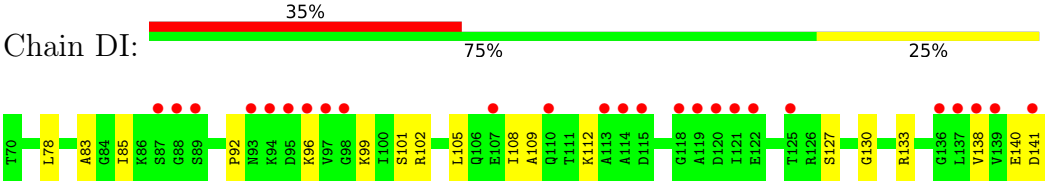
• Molecule 12: 50S ribosomal protein L11

Chain CI:



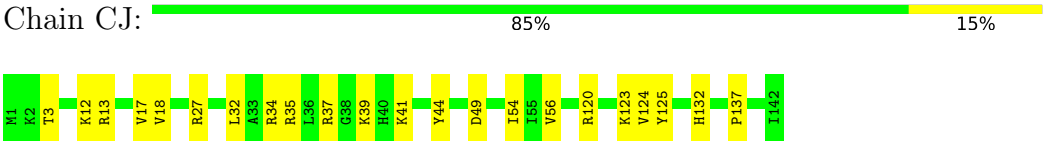
• Molecule 12: 50S ribosomal protein L11

Chain DI:



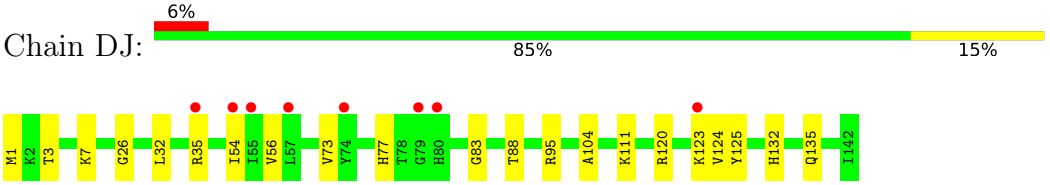
• Molecule 13: 50S ribosomal protein L13

Chain CJ:



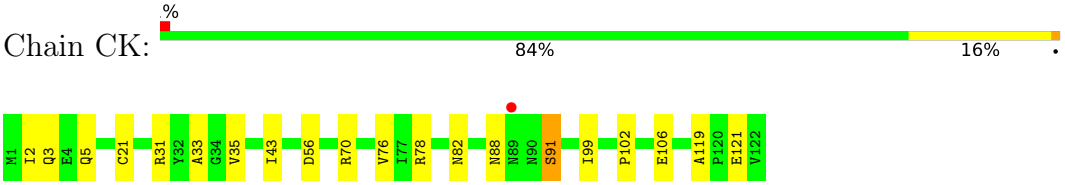
• Molecule 13: 50S ribosomal protein L13

Chain DJ:



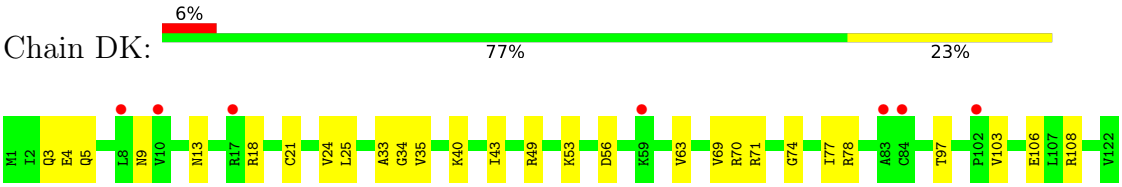
• Molecule 14: 50S ribosomal protein L14

Chain CK:



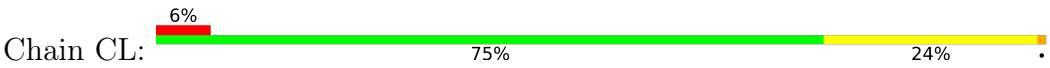
• Molecule 14: 50S ribosomal protein L14

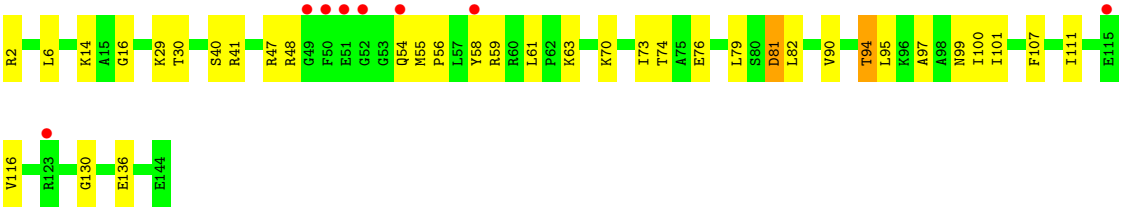
Chain DK:



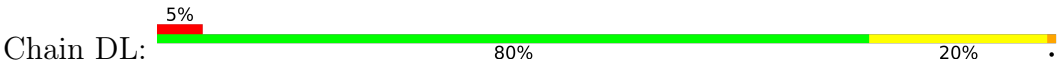
• Molecule 15: 50S ribosomal protein L15

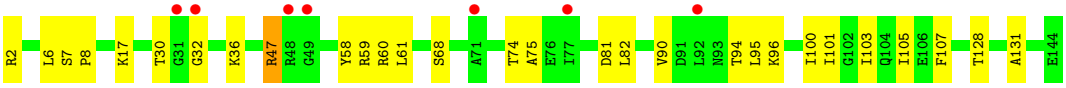
Chain CL:



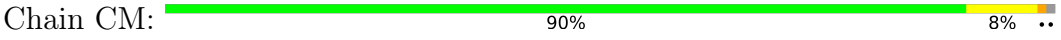


• Molecule 15: 50S ribosomal protein L15

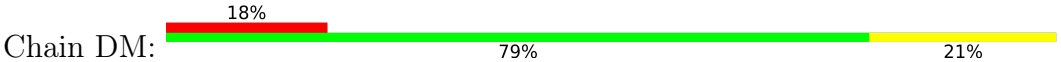


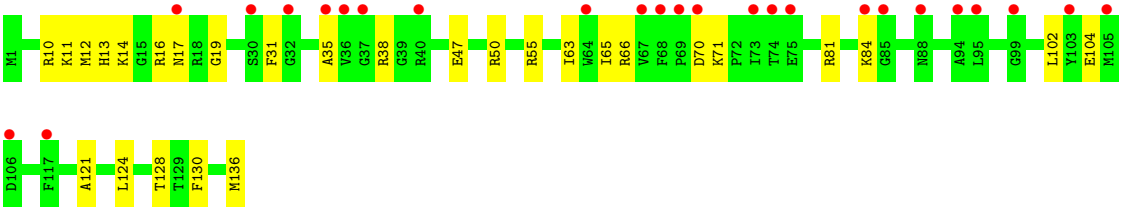


• Molecule 16: 50S ribosomal protein L16



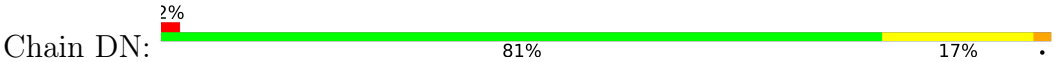
• Molecule 16: 50S ribosomal protein L16

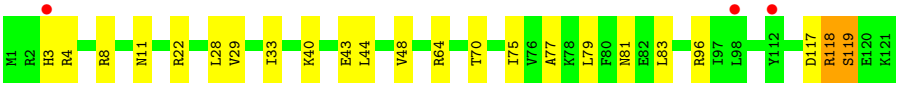




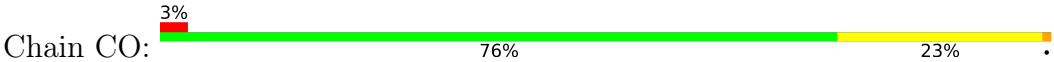
• Molecule 17: 50S ribosomal protein L17

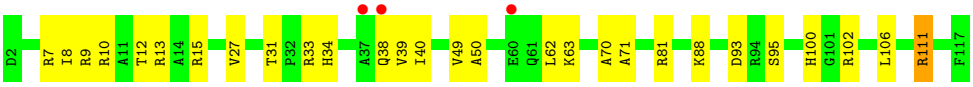
• Molecule 17: 50S ribosomal protein L17



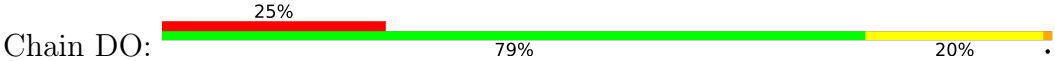


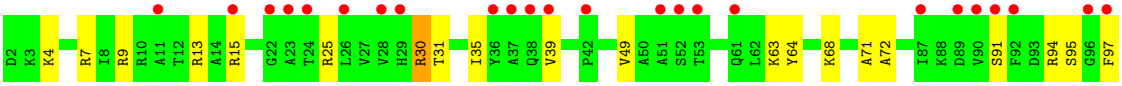
• Molecule 18: 50S ribosomal protein L18



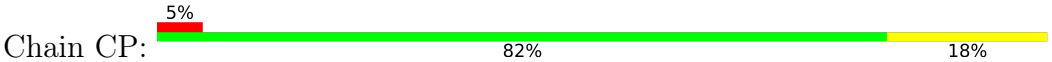


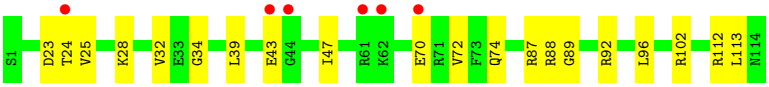
• Molecule 18: 50S ribosomal protein L18



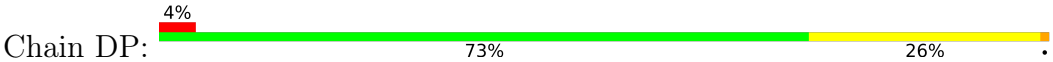


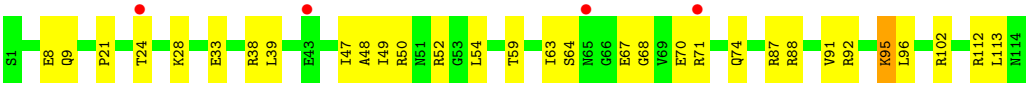
• Molecule 19: 50S ribosomal protein L19



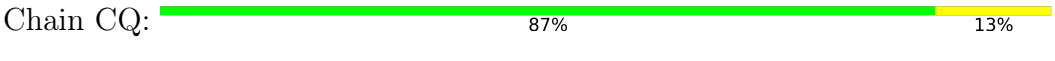


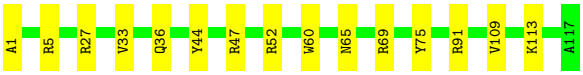
• Molecule 19: 50S ribosomal protein L19



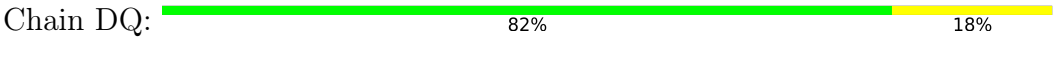


• Molecule 20: 50S ribosomal protein L20

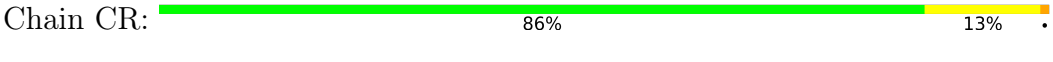


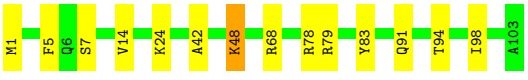


• Molecule 20: 50S ribosomal protein L20



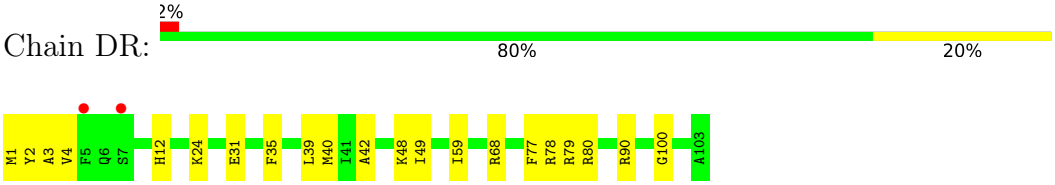
• Molecule 21: 50S ribosomal protein L21





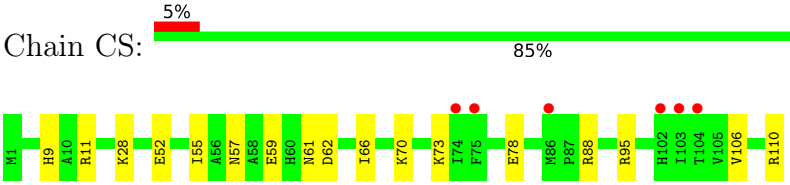
• Molecule 21: 50S ribosomal protein L21

Chain DR:



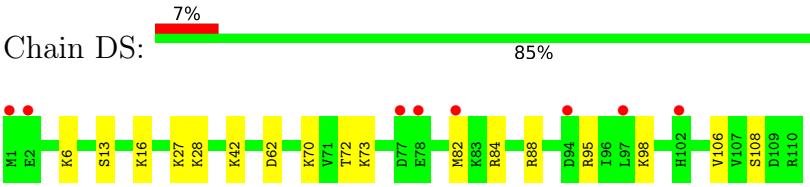
• Molecule 22: 50S ribosomal protein L22

Chain CS:



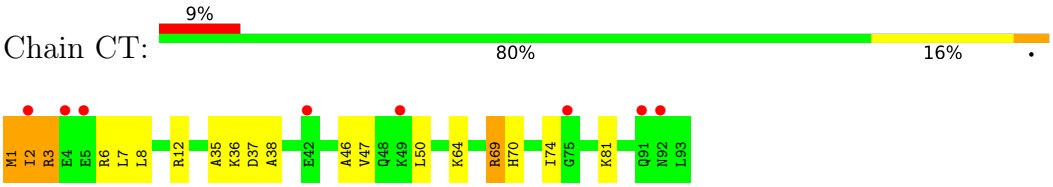
• Molecule 22: 50S ribosomal protein L22

Chain DS:



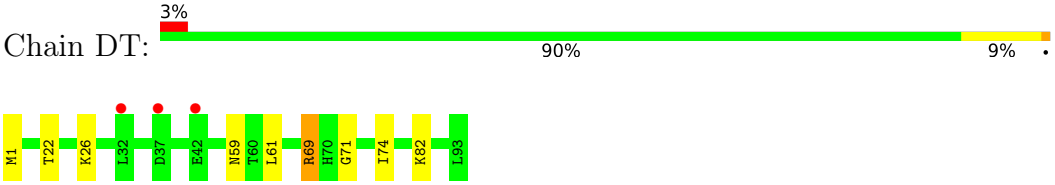
• Molecule 23: 50S ribosomal protein L23

Chain CT:



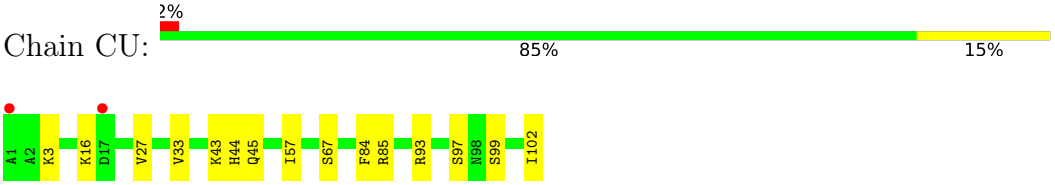
• Molecule 23: 50S ribosomal protein L23

Chain DT:



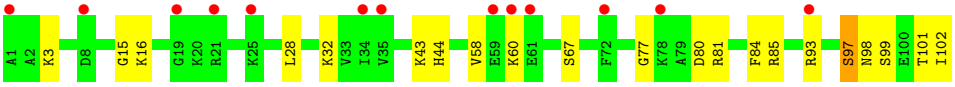
• Molecule 24: 50S ribosomal protein L24

Chain CU:

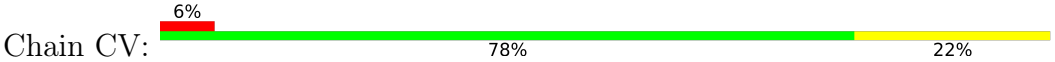


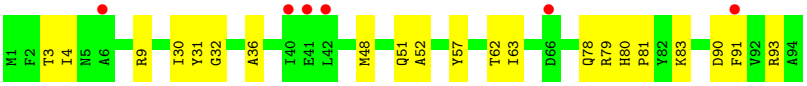
• Molecule 24: 50S ribosomal protein L24

Chain DU:

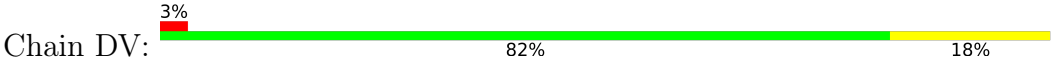


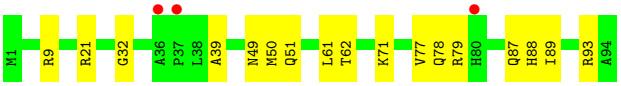
• Molecule 25: 50S ribosomal protein L25



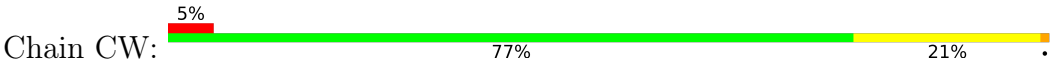


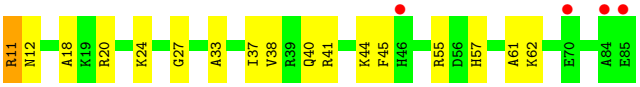
• Molecule 25: 50S ribosomal protein L25



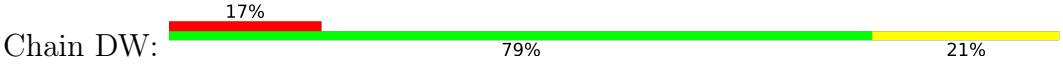


• Molecule 26: 50S ribosomal protein L27

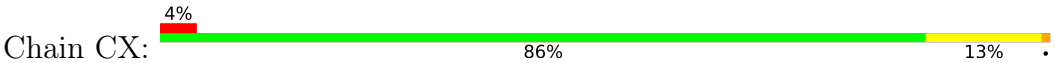


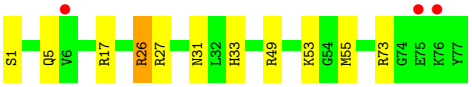


• Molecule 26: 50S ribosomal protein L27

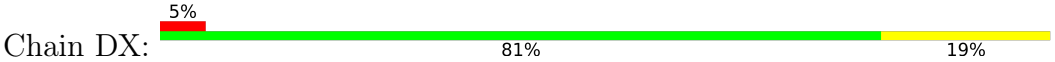


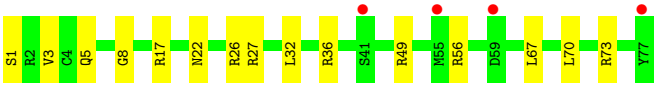
• Molecule 27: 50S ribosomal protein L28





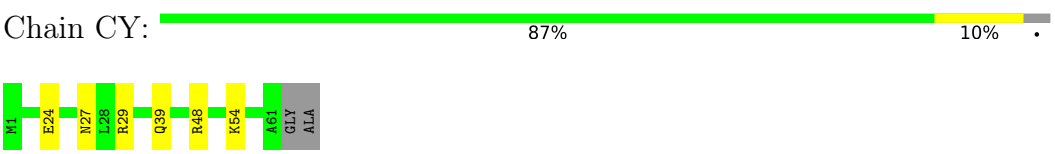
• Molecule 27: 50S ribosomal protein L28





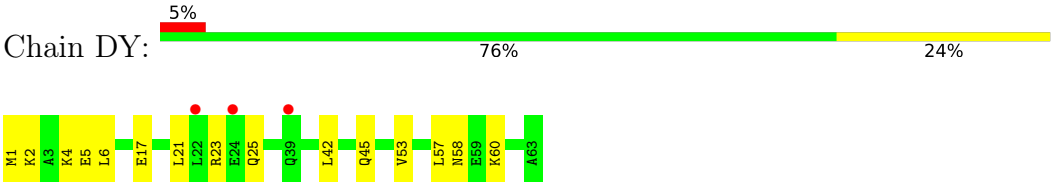
• Molecule 28: 50S ribosomal protein L29

Chain CY:



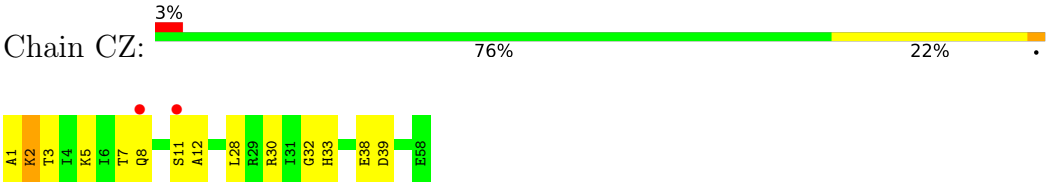
• Molecule 28: 50S ribosomal protein L29

Chain DY:



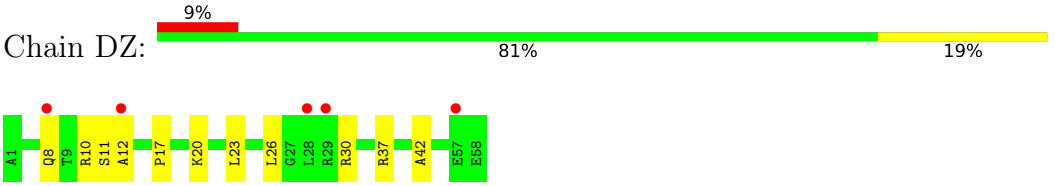
• Molecule 29: 50S ribosomal protein L30

Chain CZ:



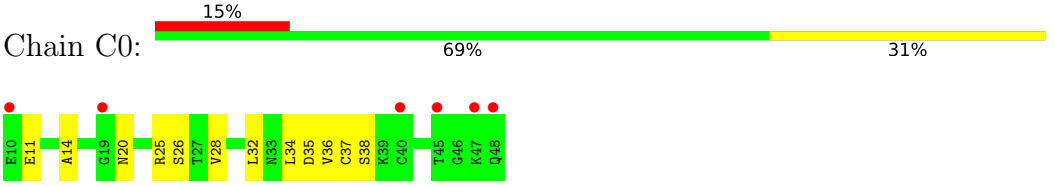
• Molecule 29: 50S ribosomal protein L30

Chain DZ:



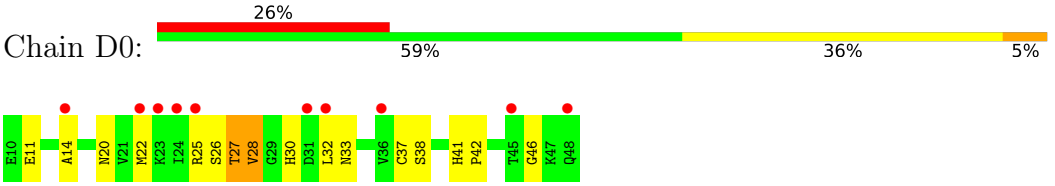
• Molecule 30: 50S ribosomal protein L31

Chain C0:



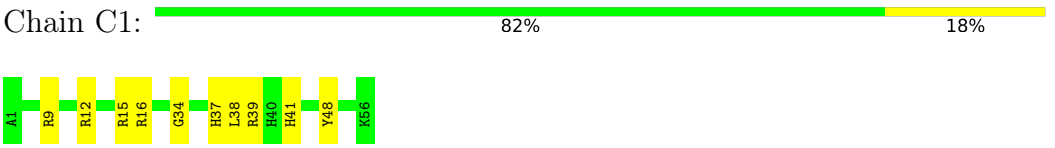
• Molecule 30: 50S ribosomal protein L31

Chain D0:



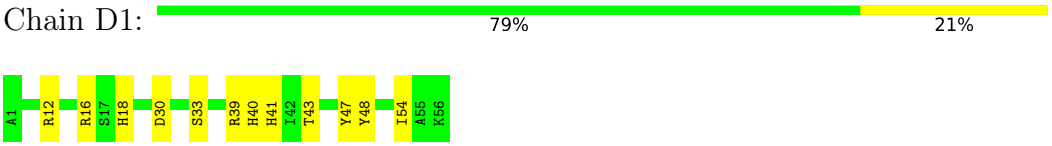
• Molecule 31: 50S ribosomal protein L32

Chain C1:



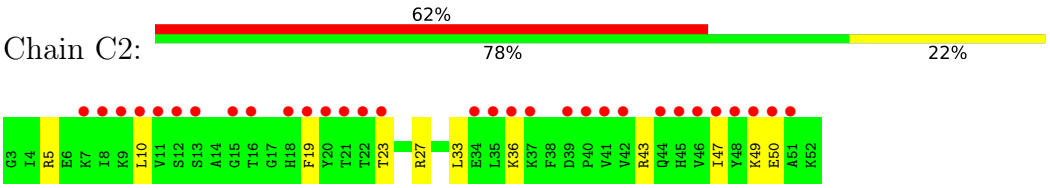
• Molecule 31: 50S ribosomal protein L32

Chain D1:



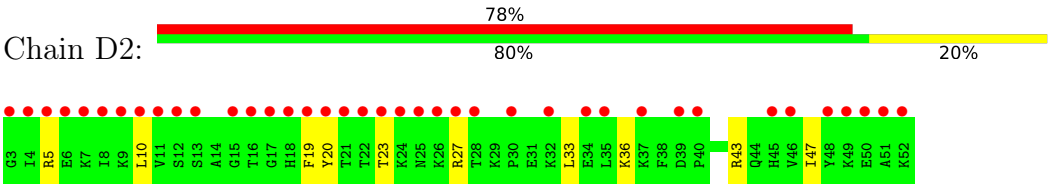
• Molecule 32: 50S ribosomal protein L33

Chain C2:



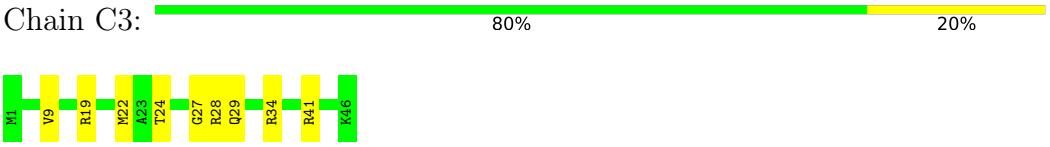
• Molecule 32: 50S ribosomal protein L33

Chain D2:



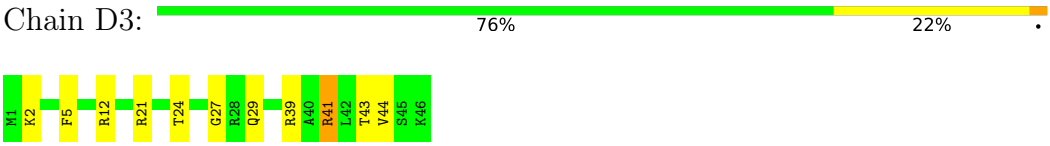
• Molecule 33: 50S ribosomal protein L34

Chain C3:



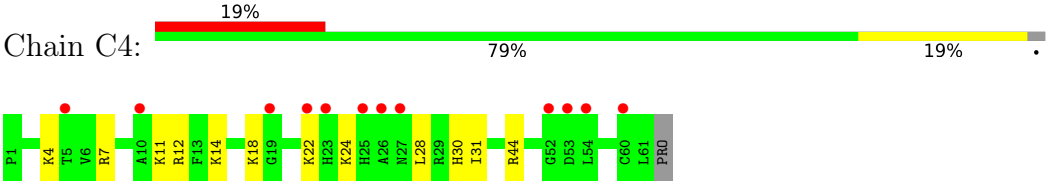
• Molecule 33: 50S ribosomal protein L34

Chain D3:



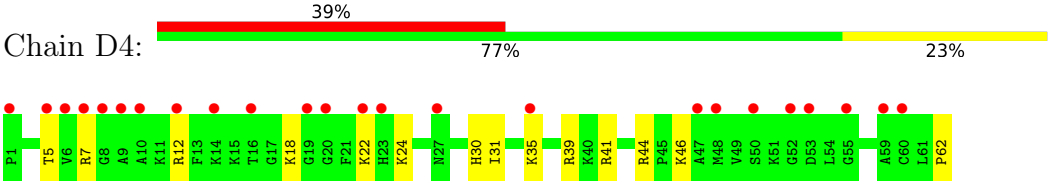
• Molecule 34: 50S ribosomal protein L35

Chain C4:



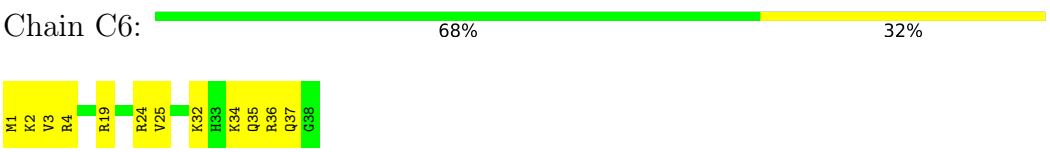
• Molecule 34: 50S ribosomal protein L35

Chain D4:



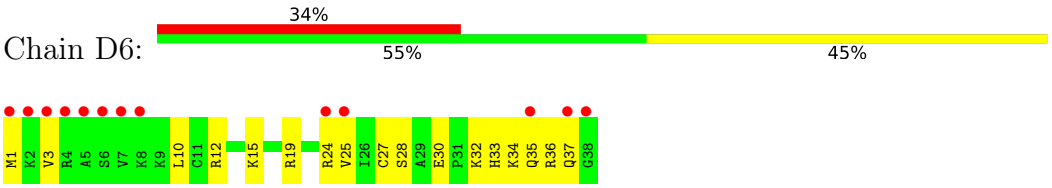
• Molecule 35: 50S ribosomal protein L36

Chain C6:



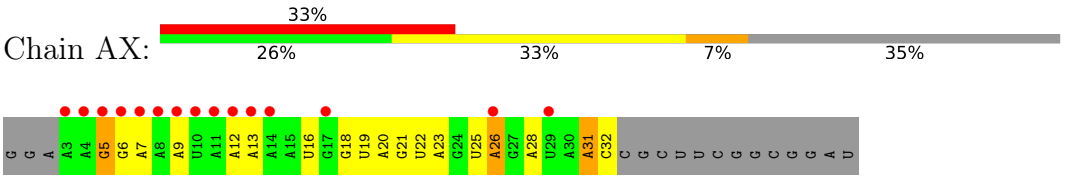
• Molecule 35: 50S ribosomal protein L36

Chain D6:



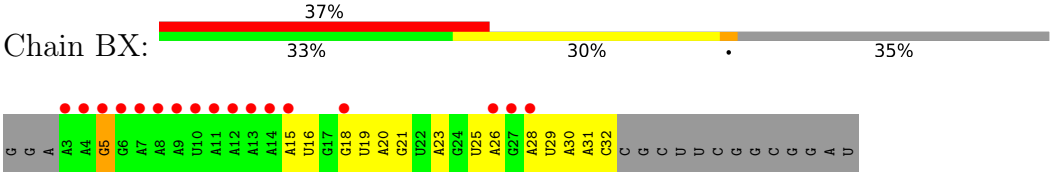
• Molecule 36: Messenger RNA

Chain AX:



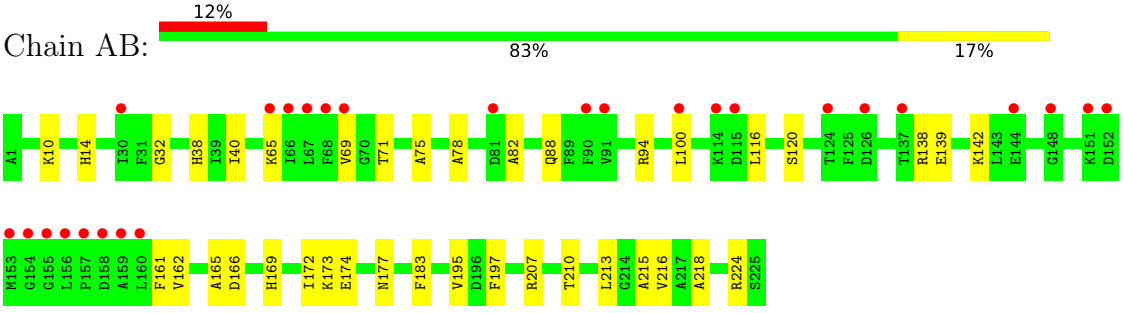
• Molecule 36: Messenger RNA

Chain BX:



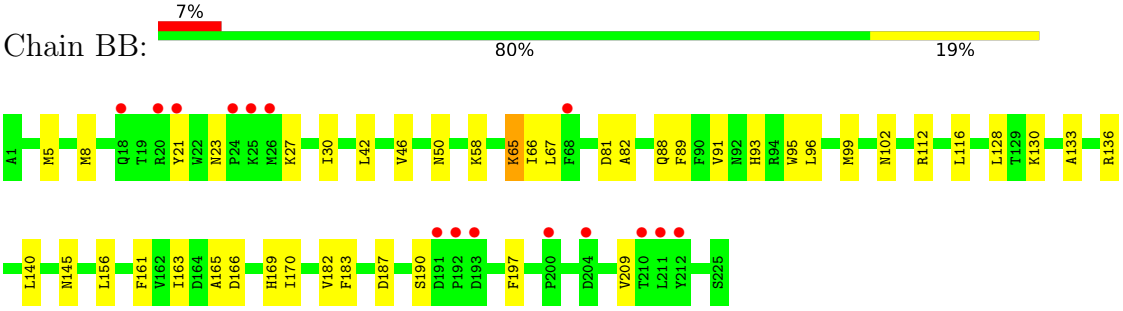
• Molecule 37: 30S ribosomal protein S2

Chain AB:



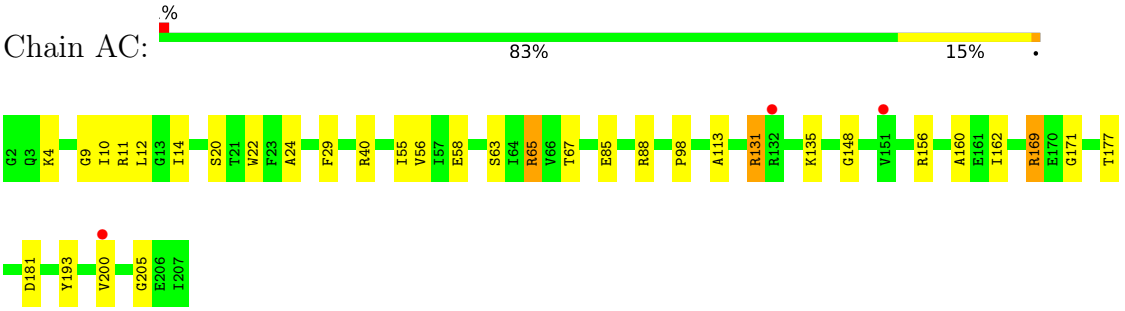
• Molecule 37: 30S ribosomal protein S2

Chain BB:



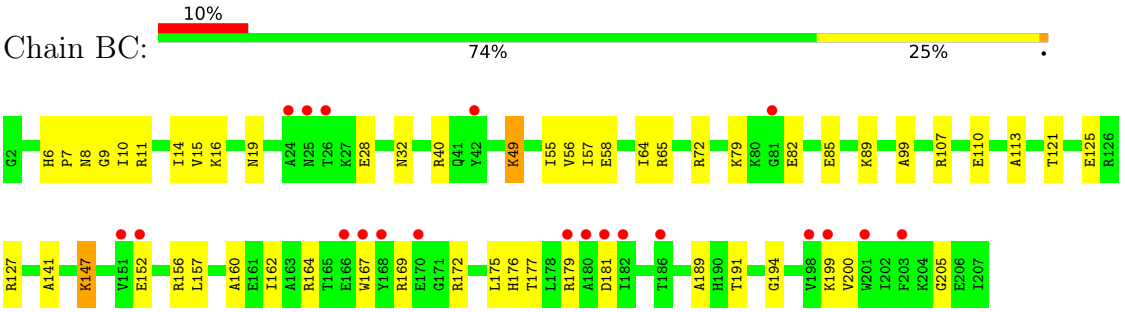
• Molecule 38: 30S ribosomal protein S3

Chain AC:



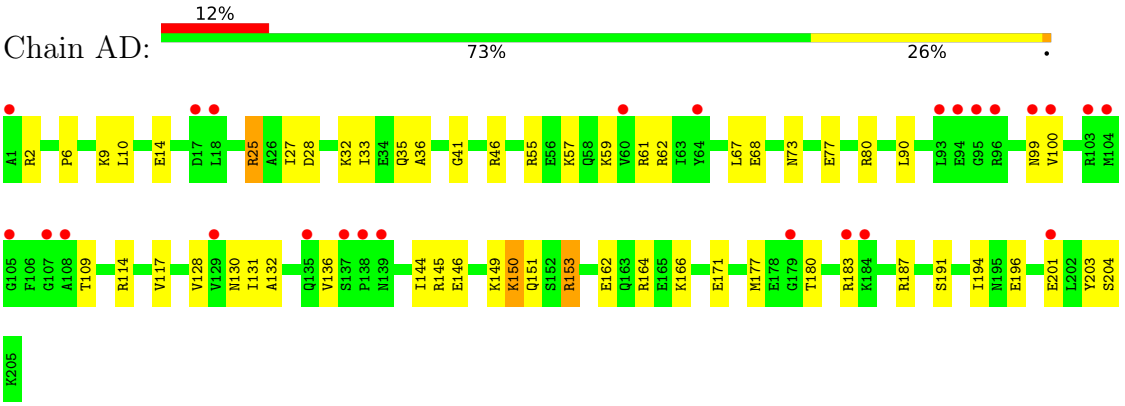
• Molecule 38: 30S ribosomal protein S3

Chain BC:



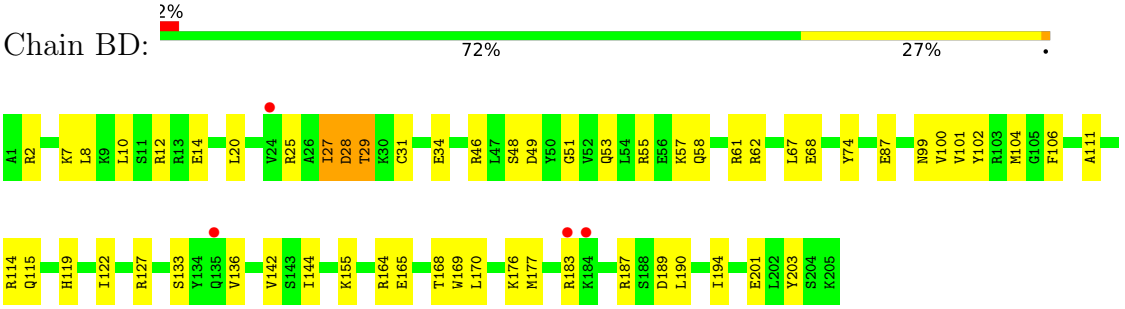
• Molecule 39: 30S ribosomal protein S4

Chain AD:



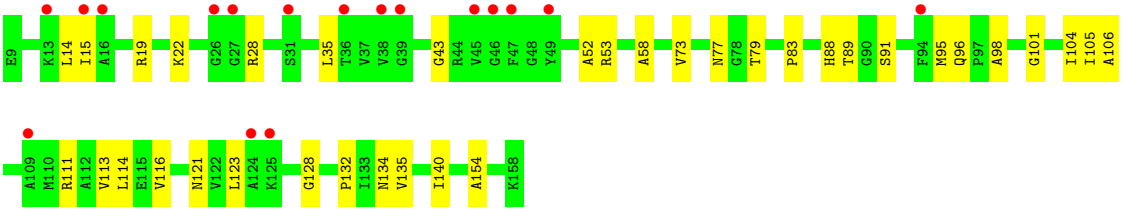
• Molecule 39: 30S ribosomal protein S4

Chain BD:



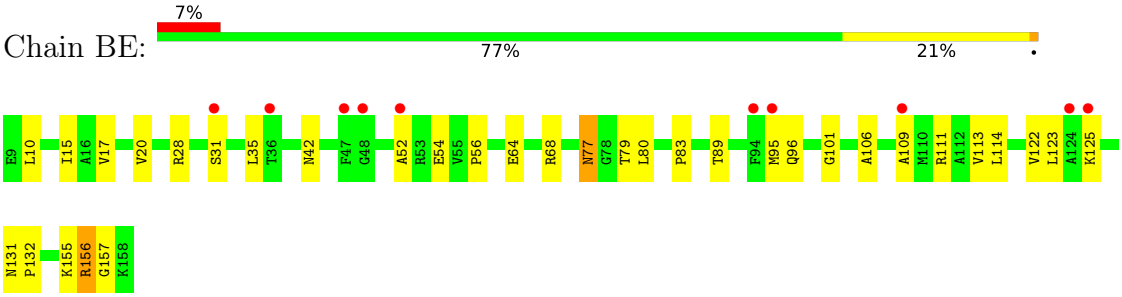
• Molecule 40: 30S ribosomal protein S5

Chain AE:



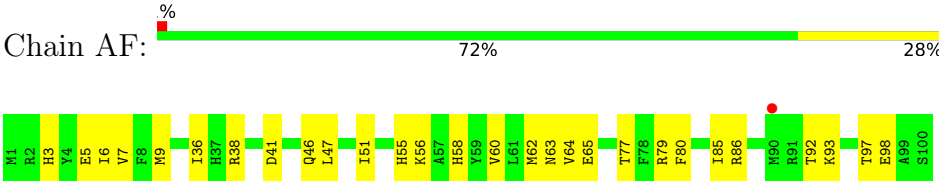
• Molecule 40: 30S ribosomal protein S5

Chain BE:



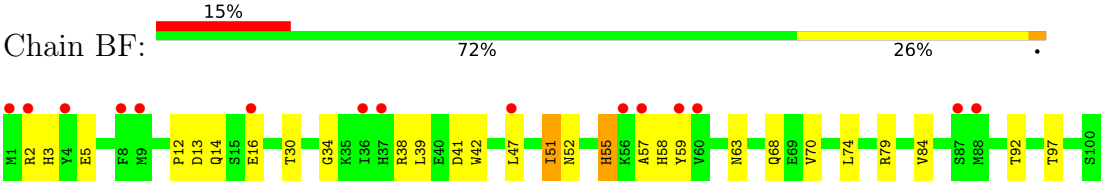
• Molecule 41: 30S ribosomal protein S6

Chain AF:



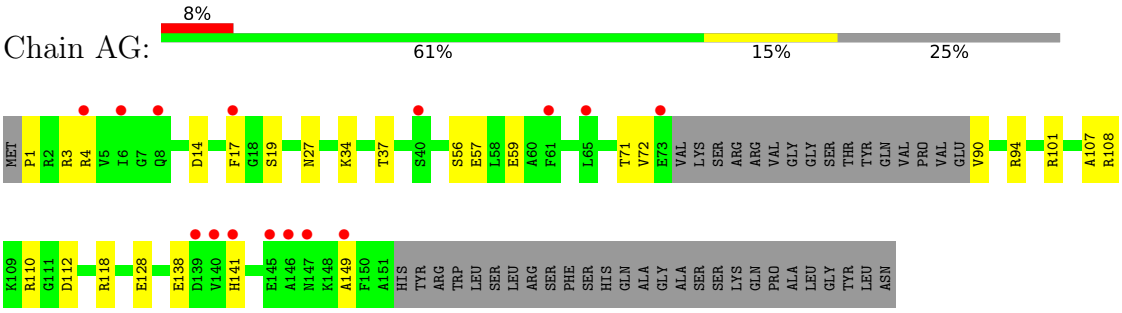
• Molecule 41: 30S ribosomal protein S6

Chain BF:



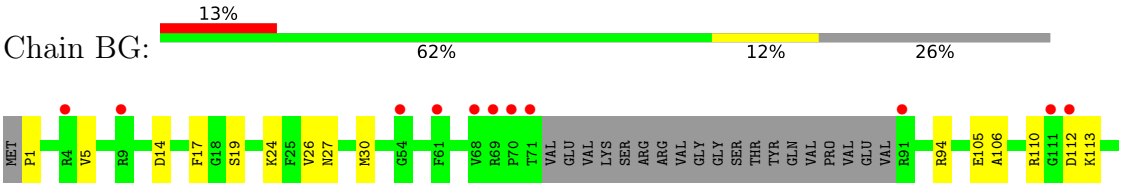
• Molecule 42: 30S ribosomal protein S7

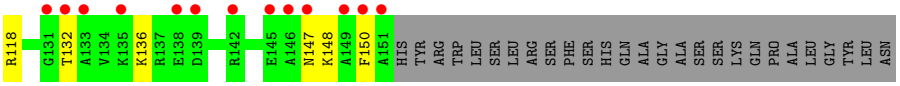
Chain AG:



• Molecule 42: 30S ribosomal protein S7

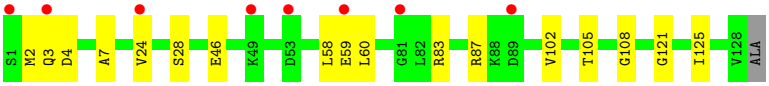
Chain BG:





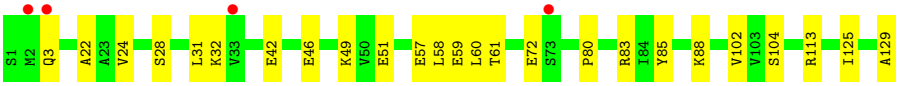
• Molecule 43: 30S ribosomal protein S8

Chain AH:



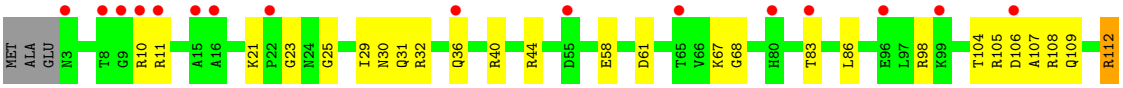
• Molecule 43: 30S ribosomal protein S8

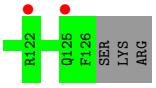
Chain BH:



• Molecule 44: 30S ribosomal protein S9

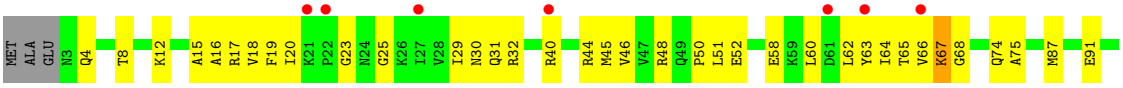
Chain AI:





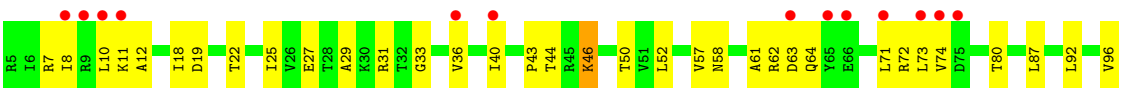
• Molecule 44: 30S ribosomal protein S9

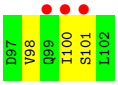
Chain BI:



• Molecule 45: 30S ribosomal protein S10

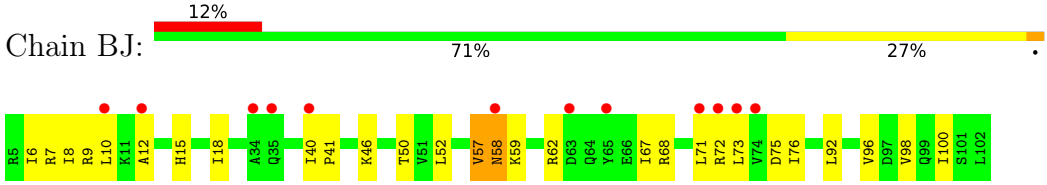
Chain AJ:





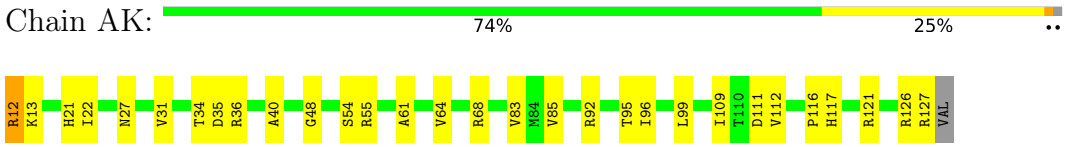
• Molecule 45: 30S ribosomal protein S10

Chain BJ:



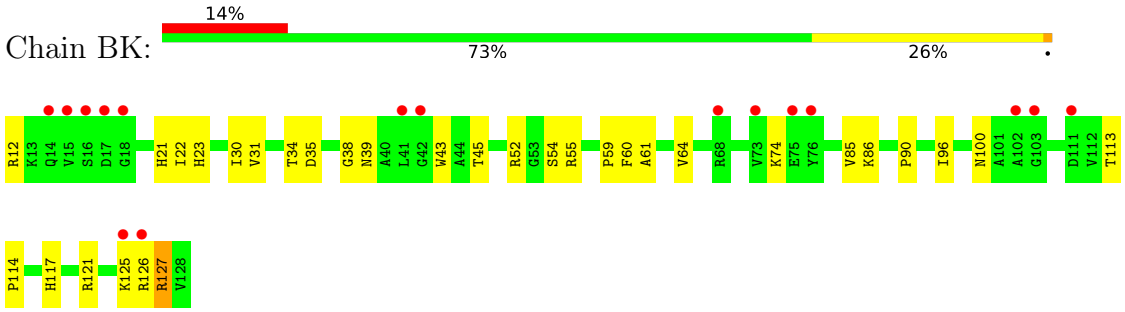
• Molecule 46: 30S ribosomal protein S11

Chain AK:



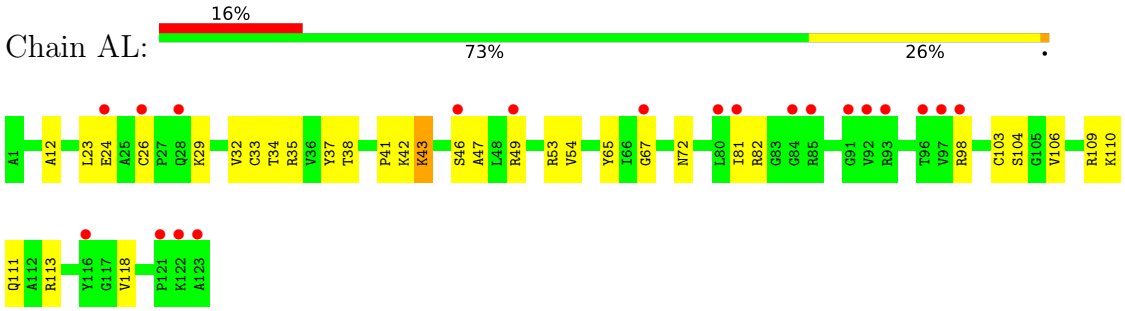
• Molecule 46: 30S ribosomal protein S11

Chain BK:



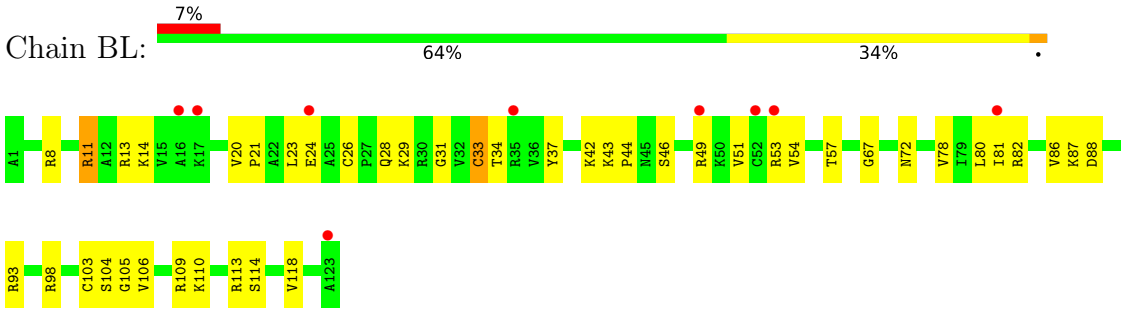
• Molecule 47: 30S ribosomal protein S12

Chain AL:



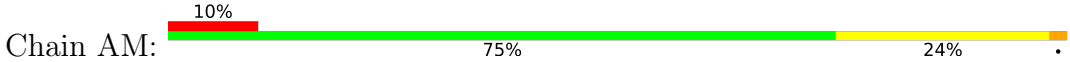
• Molecule 47: 30S ribosomal protein S12

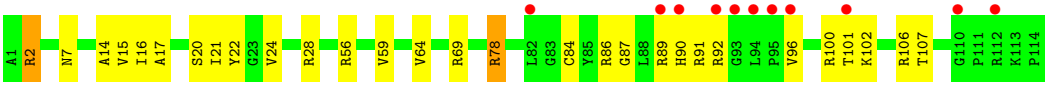
Chain BL:



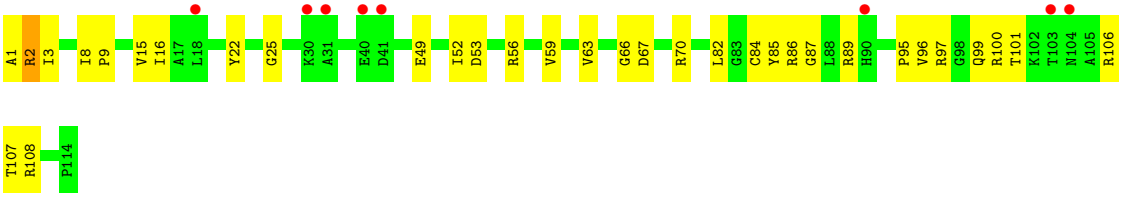
• Molecule 48: 30S ribosomal protein S13

Chain AM:

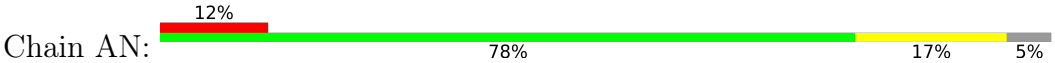


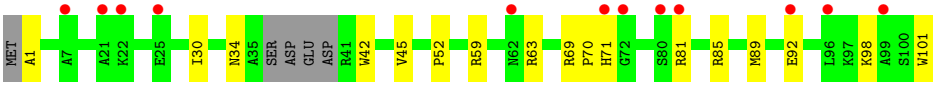


• Molecule 48: 30S ribosomal protein S13

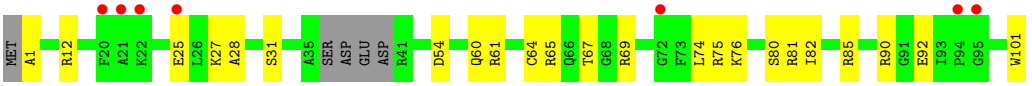


• Molecule 49: 30S ribosomal protein S14

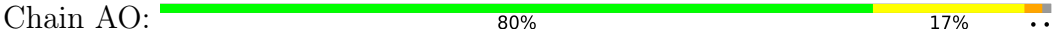


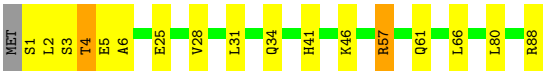


• Molecule 49: 30S ribosomal protein S14

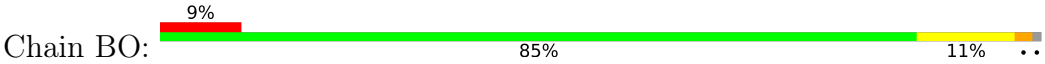


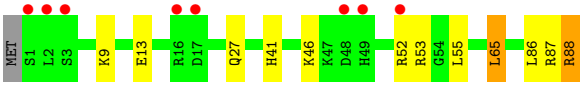
• Molecule 50: 30S ribosomal protein S15



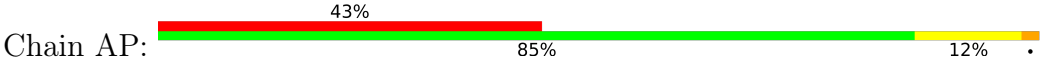


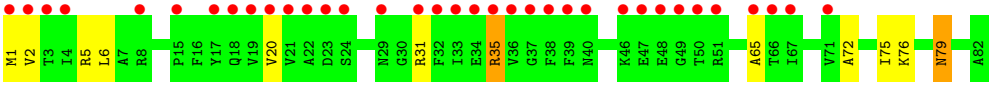
• Molecule 50: 30S ribosomal protein S15





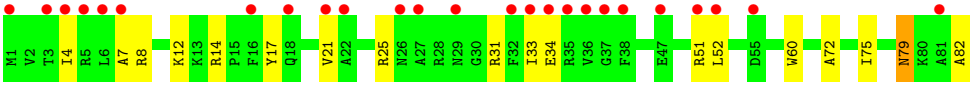
• Molecule 51: 30S ribosomal protein S16





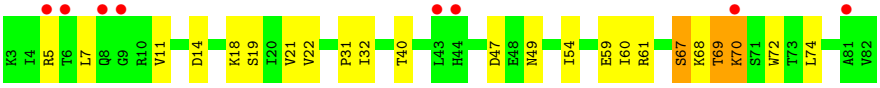
• Molecule 51: 30S ribosomal protein S16

Chain BP:



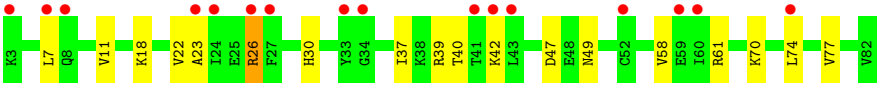
• Molecule 52: 30S ribosomal protein S17

Chain AQ:



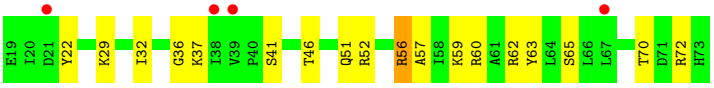
• Molecule 52: 30S ribosomal protein S17

Chain BQ:



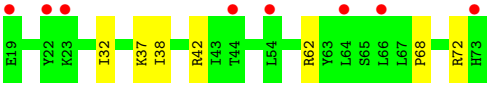
• Molecule 53: 30S ribosomal protein S18

Chain AR:



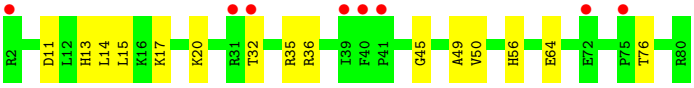
• Molecule 53: 30S ribosomal protein S18

Chain BR:



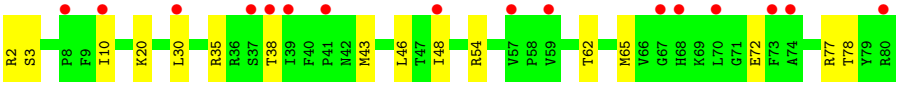
• Molecule 54: 30S ribosomal protein S19

Chain AS:

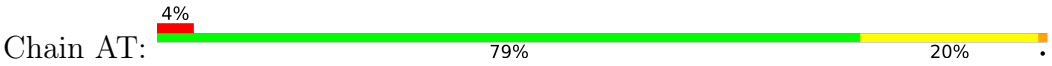


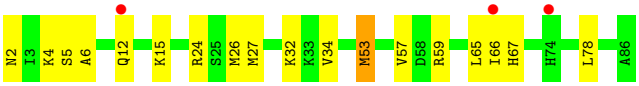
• Molecule 54: 30S ribosomal protein S19

Chain BS:

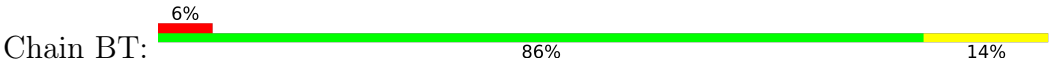


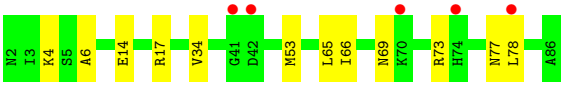
• Molecule 55: 30S ribosomal protein S20





• Molecule 55: 30S ribosomal protein S20





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	211.66Å 433.91Å 623.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.99 – 3.94 59.99 – 3.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.99-3.94) 99.9 (59.99-3.94)	Depositor EDS
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.249 , 0.269 0.249 , 0.269	Depositor DCC
R_{free} test set	10092 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	137.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 71.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	296390	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.44	0/36967	1.12	179/57663 (0.3%)
1	BA	0.47	0/37009	1.18	224/57723 (0.4%)
2	CA	0.49	2/68933 (0.0%)	1.10	263/107532 (0.2%)
2	DA	0.45	1/68974 (0.0%)	1.11	303/107576 (0.3%)
3	CB	0.47	0/2828	1.14	19/4410 (0.4%)
3	DB	0.39	0/2828	1.14	21/4410 (0.5%)
4	AV	0.47	1/1813 (0.1%)	1.16	18/2823 (0.6%)
4	AW	0.51	1/1813 (0.1%)	1.22	21/2823 (0.7%)
4	AY	0.42	1/1813 (0.1%)	1.06	5/2823 (0.2%)
4	BV	0.47	1/1813 (0.1%)	1.10	10/2823 (0.4%)
4	BW	0.48	1/1813 (0.1%)	1.18	13/2823 (0.5%)
5	CC	0.32	0/2122	0.60	0/2852
5	DC	0.31	0/2122	0.61	0/2852
6	CD	0.36	0/1586	0.60	0/2134
6	DD	0.33	0/1586	0.59	0/2134
7	CE	0.31	0/1422	0.57	0/1911
7	DE	0.30	0/1411	0.53	0/1897
8	CF	0.35	0/1435	0.64	0/1926
8	DF	0.36	0/1435	0.63	0/1926
9	CG	0.33	0/1343	0.55	0/1816
9	DG	0.30	0/1343	0.55	0/1816
10	CH	0.30	0/1121	0.62	0/1515
10	DH	0.32	0/1121	0.65	1/1515 (0.1%)
11	C5	0.31	0/835	0.63	0/1123
12	CI	0.29	0/513	0.54	0/684
12	DI	0.30	0/520	0.62	0/694
13	CJ	0.33	0/1152	0.55	0/1551
13	DJ	0.32	0/1152	0.53	0/1551
14	CK	0.33	0/948	0.61	0/1268
14	DK	0.33	0/948	0.63	0/1268
15	CL	0.32	0/1054	0.68	1/1403 (0.1%)
15	DL	0.30	0/1054	0.65	1/1403 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	CM	0.34	0/1084	0.66	1/1450 (0.1%)
16	DM	0.33	0/1093	0.65	1/1460 (0.1%)
17	CN	0.31	0/982	0.61	0/1312
17	DN	0.31	0/982	0.62	0/1312
18	CO	0.30	0/902	0.57	0/1209
18	DO	0.31	0/902	0.65	0/1209
19	CP	0.32	0/929	0.57	1/1242 (0.1%)
19	DP	0.31	0/929	0.59	1/1242 (0.1%)
20	CQ	0.34	0/960	0.50	0/1278
20	DQ	0.30	0/960	0.47	0/1278
21	CR	0.33	0/829	0.62	0/1107
21	DR	0.30	0/829	0.60	0/1107
22	CS	0.32	0/864	0.56	0/1156
22	DS	0.29	0/864	0.54	0/1156
23	CT	0.32	0/745	0.59	0/994
23	DT	0.29	0/745	0.57	0/994
24	CU	0.35	0/788	0.65	1/1051 (0.1%)
24	DU	0.33	0/788	0.63	1/1051 (0.1%)
25	CV	0.33	0/766	0.58	0/1025
25	DV	0.29	0/766	0.56	0/1025
26	CW	0.32	0/581	0.53	0/769
26	DW	0.31	0/581	0.55	0/769
27	CX	0.34	0/635	0.57	0/848
27	DX	0.29	0/635	0.53	0/848
28	CY	0.30	0/500	0.64	0/665
28	DY	0.29	0/510	0.61	0/677
29	CZ	0.30	0/453	0.56	0/605
29	DZ	0.30	0/453	0.58	0/605
30	C0	0.54	0/297	1.05	2/398 (0.5%)
30	D0	0.65	1/297 (0.3%)	0.89	1/398 (0.3%)
31	C1	0.32	0/450	0.61	0/599
31	D1	0.28	0/450	0.59	0/599
32	C2	0.30	0/417	0.61	0/554
32	D2	0.28	0/417	0.60	0/554
33	C3	0.30	0/380	0.53	0/498
33	D3	0.30	0/380	0.54	0/498
34	C4	0.30	0/486	0.57	0/639
34	D4	0.29	0/494	0.59	0/651
35	C6	0.36	0/303	0.65	0/397
35	D6	0.33	0/303	0.61	0/397
36	AX	0.43	0/735	1.26	7/1145 (0.6%)
36	BX	0.55	1/735 (0.1%)	1.34	9/1145 (0.8%)
37	AB	0.31	0/1788	0.60	0/2408

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	BB	0.31	0/1788	0.64	1/2408 (0.0%)
38	AC	0.31	0/1652	0.60	1/2225 (0.0%)
38	BC	0.30	0/1652	0.56	0/2225
39	AD	0.31	0/1665	0.65	1/2227 (0.0%)
39	BD	0.34	0/1665	0.65	0/2227
40	AE	0.33	0/1119	0.68	0/1504
40	BE	0.34	0/1119	0.69	0/1504
41	AF	0.32	0/836	0.64	0/1128
41	BF	0.32	0/836	0.69	1/1128 (0.1%)
42	AG	0.29	0/1069	0.54	0/1430
42	BG	0.28	0/1046	0.56	0/1398
43	AH	0.30	0/983	0.55	0/1319
43	BH	0.30	0/989	0.54	0/1326
44	AI	0.29	0/1007	0.60	0/1342
44	BI	0.29	0/1034	0.62	0/1375
45	AJ	0.29	0/797	0.70	1/1077 (0.1%)
45	BJ	0.29	0/797	0.67	1/1077 (0.1%)
46	AK	0.31	0/885	0.58	0/1195
46	BK	0.29	0/893	0.60	0/1205
47	AL	0.30	0/969	0.67	1/1300 (0.1%)
47	BL	0.32	0/969	0.65	1/1300 (0.1%)
48	AM	0.36	0/893	0.73	2/1193 (0.2%)
48	BM	0.44	1/893 (0.1%)	0.68	1/1193 (0.1%)
49	AN	0.29	0/785	0.60	0/1043
49	BN	0.28	0/785	0.60	0/1043
50	AO	0.30	0/722	0.63	0/964
50	BO	0.27	0/722	0.62	1/964 (0.1%)
51	AP	0.29	0/659	0.64	0/884
51	BP	0.30	0/659	0.62	0/884
52	AQ	0.35	0/658	0.75	1/881 (0.1%)
52	BQ	0.32	0/658	0.69	0/881
53	AR	0.28	0/463	0.56	0/621
53	BR	0.27	0/463	0.55	0/621
54	AS	0.30	0/653	0.59	0/877
54	BS	0.28	0/653	0.58	0/877
55	AT	0.29	0/671	0.57	0/888
55	BT	0.30	0/671	0.55	0/888
All	All	0.43	11/317592 (0.0%)	1.02	1117/475614 (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	CC	0	2
6	CD	0	1
6	DD	0	1
8	CF	0	1
10	DH	0	2
11	C5	0	1
14	CK	0	1
14	DK	0	1
15	CL	0	1
19	DP	0	1
23	CT	0	1
23	DT	0	1
25	DV	0	1
33	D3	0	1
34	C4	0	1
34	D4	0	1
37	AB	0	1
38	AC	0	1
39	AD	0	2
39	BD	0	2
40	BE	0	2
41	AF	0	1
41	BF	0	1
42	AG	0	1
45	BJ	0	1
48	AM	0	1
49	AN	0	1
52	AQ	0	1
52	BQ	0	1
All	All	0	34

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BW	1	G	OP3-P	-10.75	1.48	1.61
4	BV	1	G	OP3-P	-10.71	1.48	1.61
4	AV	1	G	OP3-P	-10.67	1.48	1.61
4	AY	1	G	OP3-P	-10.64	1.48	1.61
4	AW	1	G	OP3-P	-10.49	1.48	1.61

The worst 5 of 1117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BA	71	A	OP2-P-O3'	-33.97	30.46	105.20
2	DA	2219	U	O5'-P-OP1	-27.34	77.89	110.70
2	DA	2219	U	OP1-P-OP2	-24.36	83.07	119.60
2	DA	2219	U	O5'-P-OP2	19.93	134.61	110.70
2	CA	1521	G	OP2-P-O3'	-15.81	70.41	105.20

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	C5	89	PRO	Peptide
5	CC	120	ASP	Peptide
5	CC	237	ARG	Peptide
6	CD	151	THR	Peptide
8	CF	174	PHE	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	33037	0	16628	487	3
1	BA	33057	0	16640	516	0
2	CA	61550	0	30959	698	0
2	DA	61593	0	30990	812	3
3	CB	2529	0	1281	36	0
3	DB	2529	0	1281	34	0
4	AV	1623	0	823	18	0
4	AW	1623	0	823	28	0
4	AY	1623	0	823	12	0
4	BV	1623	0	823	19	0
4	BW	1623	0	823	20	0
5	CC	2083	0	2157	48	0
5	DC	2083	0	2157	46	0
6	CD	1565	0	1616	30	2
6	DD	1565	0	1616	25	0
7	CE	1404	0	1466	22	0
7	DE	1393	0	1453	24	0
8	CF	1411	0	1447	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	DF	1411	0	1447	23	0
9	CG	1323	0	1374	15	0
9	DG	1323	0	1374	17	0
10	CH	1110	0	1148	17	0
10	DH	1110	0	1148	24	3
11	C5	825	0	856	17	0
12	CI	511	0	544	7	0
12	DI	518	0	551	12	0
13	CJ	1129	0	1162	15	0
13	DJ	1129	0	1162	15	0
14	CK	939	0	1012	14	0
14	DK	939	0	1012	16	0
15	CL	1045	0	1117	24	1
15	DL	1045	0	1117	23	0
16	CM	1065	0	1148	7	0
16	DM	1074	0	1157	20	0
17	CN	969	0	1012	32	0
17	DN	969	0	1013	20	0
18	CO	892	0	923	21	2
18	DO	892	0	923	15	0
19	CP	917	0	965	14	0
19	DP	917	0	965	22	0
20	CQ	947	0	1022	13	0
20	DQ	947	0	1022	20	0
21	CR	816	0	839	10	0
21	DR	816	0	839	17	2
22	CS	857	0	922	12	0
22	DS	857	0	922	12	0
23	CT	739	0	807	14	0
23	DT	739	0	807	5	0
24	CU	780	0	834	10	0
24	DU	780	0	834	16	0
25	CV	753	0	780	16	0
25	DV	753	0	780	12	0
26	CW	574	0	592	16	0
26	DW	574	0	592	14	0
27	CX	625	0	655	10	0
27	DX	625	0	655	11	0
28	CY	499	0	535	6	0
28	DY	509	0	543	9	0
29	CZ	449	0	491	16	1
29	DZ	449	0	491	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	C0	293	0	283	9	0
30	D0	293	0	284	18	0
31	C1	444	0	461	9	1
31	D1	444	0	461	9	0
32	C2	410	0	440	7	0
32	D2	410	0	440	7	0
33	C3	377	0	418	6	0
33	D3	377	0	418	8	0
34	C4	479	0	553	10	0
34	D4	486	0	560	10	0
35	C6	302	0	340	8	0
35	D6	302	0	340	11	0
36	AX	653	0	325	29	0
36	BX	653	0	325	24	0
37	AB	1757	0	1787	23	0
37	BB	1757	0	1787	25	0
38	AC	1625	0	1696	28	0
38	BC	1625	0	1696	40	0
39	AD	1643	0	1710	46	3
39	BD	1643	0	1710	41	0
40	AE	1106	0	1148	24	0
40	BE	1106	0	1148	21	0
41	AF	818	0	808	18	0
41	BF	818	0	808	13	3
42	AG	1058	0	1111	19	0
42	BG	1035	0	1087	16	0
43	AH	973	0	1029	11	0
43	BH	979	0	1034	20	0
44	AI	995	0	1039	42	0
44	BI	1022	0	1070	51	0
45	AJ	787	0	828	27	0
45	BJ	787	0	828	19	0
46	AK	869	0	878	23	0
46	BK	877	0	887	23	0
47	AL	955	0	1019	21	0
47	BL	955	0	1019	33	0
48	AM	884	0	944	23	0
48	BM	884	0	944	34	0
49	AN	774	0	827	12	0
49	BN	774	0	827	19	0
50	AO	714	0	737	23	0
50	BO	714	0	737	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	AP	649	0	666	9	0
51	BP	649	0	666	12	0
52	AQ	649	0	691	13	0
52	BQ	649	0	691	11	0
53	AR	456	0	478	15	0
53	BR	456	0	478	5	0
54	AS	638	0	665	16	0
54	BS	638	0	665	16	0
55	AT	665	0	714	14	0
55	BT	665	0	714	7	0
56	AA	50	0	0	0	0
56	BA	49	0	0	0	0
56	C4	1	0	0	0	0
56	CA	167	0	0	0	0
56	CB	3	0	0	0	0
56	CC	1	0	0	0	0
56	CN	2	0	0	0	0
56	CQ	1	0	0	0	0
56	DA	166	0	0	0	0
56	DB	3	0	0	0	0
56	DN	1	0	0	0	0
56	DQ	1	0	0	0	0
57	C0	1	0	0	0	0
57	C6	1	0	0	0	0
57	D0	1	0	0	0	0
57	D6	1	0	0	0	0
58	AA	481	0	0	8	0
58	AB	7	0	0	0	0
58	AC	15	0	0	0	0
58	AD	10	0	0	1	0
58	AE	12	0	0	1	0
58	AF	6	0	0	0	0
58	AG	5	0	0	0	0
58	AH	7	0	0	1	0
58	AI	6	0	0	0	0
58	AJ	4	0	0	0	0
58	AK	10	0	0	2	0
58	AL	9	0	0	0	0
58	AM	6	0	0	0	0
58	AN	3	0	0	0	0
58	AO	7	0	0	1	0
58	AP	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	AQ	8	0	0	1	0
58	AR	1	0	0	0	0
58	AS	4	0	0	1	0
58	AT	4	0	0	1	0
58	AV	28	0	0	0	0
58	AW	32	0	0	0	0
58	AX	4	0	0	0	0
58	AY	5	0	0	0	0
58	BA	461	0	0	14	0
58	BB	2	0	0	0	0
58	BC	8	0	0	1	0
58	BD	24	0	0	2	0
58	BE	18	0	0	0	0
58	BF	6	0	0	0	0
58	BG	4	0	0	0	0
58	BH	12	0	0	2	0
58	BI	9	0	0	0	0
58	BJ	8	0	0	1	0
58	BK	5	0	0	0	0
58	BL	8	0	0	0	0
58	BM	6	0	0	1	0
58	BN	5	0	0	0	0
58	BO	2	0	0	1	0
58	BP	5	0	0	1	0
58	BQ	10	0	0	0	0
58	BR	1	0	0	1	0
58	BS	3	0	0	0	0
58	BT	2	0	0	0	0
58	BV	13	0	0	0	0
58	BW	23	0	0	0	0
58	BX	5	0	0	0	0
58	C1	5	0	0	0	0
58	C2	1	0	0	0	0
58	C3	2	0	0	0	0
58	C4	2	0	0	0	0
58	C5	7	0	0	0	0
58	C6	3	0	0	0	0
58	CA	1106	0	0	22	0
58	CB	49	0	0	1	0
58	CC	13	0	0	0	0
58	CD	10	0	0	0	0
58	CE	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	CF	14	0	0	2	0
58	CG	18	0	0	0	0
58	CH	8	0	0	1	0
58	CI	4	0	0	0	0
58	CJ	9	0	0	0	0
58	CK	7	0	0	0	0
58	CL	8	0	0	1	0
58	CM	4	0	0	0	0
58	CN	6	0	0	2	0
58	CO	8	0	0	2	0
58	CP	8	0	0	0	0
58	CQ	2	0	0	0	0
58	CR	7	0	0	0	0
58	CS	3	0	0	0	0
58	CT	7	0	0	1	0
58	CU	13	0	0	0	0
58	CV	10	0	0	5	0
58	CW	4	0	0	0	0
58	CX	3	0	0	0	0
58	CY	3	0	0	0	0
58	CZ	1	0	0	0	0
58	D0	2	0	0	2	0
58	D1	11	0	0	0	0
58	D2	2	0	0	0	0
58	D3	2	0	0	0	0
58	D6	1	0	0	0	0
58	DA	1005	0	0	22	0
58	DB	32	0	0	1	0
58	DC	28	0	0	1	0
58	DD	15	0	0	0	0
58	DE	12	0	0	0	0
58	DF	4	0	0	0	0
58	DG	6	0	0	0	0
58	DH	4	0	0	0	0
58	DJ	3	0	0	0	0
58	DK	5	0	0	0	0
58	DL	10	0	0	0	0
58	DM	6	0	0	1	0
58	DN	6	0	0	0	0
58	DO	4	0	0	0	0
58	DP	6	0	0	0	0
58	DQ	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	DR	13	0	0	0	0
58	DS	9	0	0	0	0
58	DT	10	0	0	0	0
58	DU	14	0	0	1	0
58	DV	7	0	0	0	0
58	DW	3	0	0	0	0
58	DX	3	0	0	1	0
58	DY	7	0	0	0	0
58	DZ	2	0	0	0	0
All	All	296390	0	195117	3829	12

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 8.

The worst 5 of 3829 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)
1:BA:1029:U:O2'	1:BA:1033:G:N2	1.59	1.29
30:D0:46:GLY:HA2	58:D0:201:HOH:O	1.29	1.28
2:CA:2278:A:OP2	26:CW:12:ASN:ND2	1.73	1.19
50:AO:2:LEU:HD13	50:AO:34:GLN:NE2	1.58	1.18
17:CN:94:TYR:C	17:CN:116:VAL:HG23	1.72	1.08

The worst 5 of 12 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)
18:CO:111:ARG:NH1	21:DR:31:GLU:OE1[3_445]	1.60	0.60
29:CZ:5:LYS:NZ	31:C1:34:GLY:O[4_445]	1.69	0.51
39:AD:164:ARG:CD	41:BF:14:GLN:OE1[4_455]	1.79	0.41
1:AA:368:U:N3	10:DH:97:ARG:NH1[4_455]	1.88	0.32
39:AD:25:ARG:O	41:BF:13:ASP:OD2[4_455]	1.93	0.27

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	
5	CC	269/271 (99%)	240 (89%)	29 (11%)	0	100	100
5	DC	269/271 (99%)	249 (93%)	20 (7%)	0	100	100
6	CD	207/209 (99%)	192 (93%)	13 (6%)	2 (1%)	15	52
6	DD	207/209 (99%)	195 (94%)	11 (5%)	1 (0%)	29	66
7	CE	179/181 (99%)	172 (96%)	7 (4%)	0	100	100
7	DE	178/181 (98%)	169 (95%)	9 (5%)	0	100	100
8	CF	175/177 (99%)	150 (86%)	25 (14%)	0	100	100
8	DF	175/177 (99%)	152 (87%)	23 (13%)	0	100	100
9	CG	174/176 (99%)	163 (94%)	11 (6%)	0	100	100
9	DG	174/176 (99%)	162 (93%)	12 (7%)	0	100	100
10	CH	147/149 (99%)	120 (82%)	26 (18%)	1 (1%)	22	60
10	DH	147/149 (99%)	118 (80%)	29 (20%)	0	100	100
11	C5	107/109 (98%)	91 (85%)	16 (15%)	0	100	100
12	CI	69/72 (96%)	65 (94%)	4 (6%)	0	100	100
12	DI	70/72 (97%)	59 (84%)	11 (16%)	0	100	100
13	CJ	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
13	DJ	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
14	CK	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
14	DK	120/122 (98%)	104 (87%)	16 (13%)	0	100	100
15	CL	141/143 (99%)	122 (86%)	19 (14%)	0	100	100
15	DL	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
16	CM	133/136 (98%)	127 (96%)	4 (3%)	2 (2%)	10	45
16	DM	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
17	CN	119/121 (98%)	108 (91%)	11 (9%)	0	100	100
17	DN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	9	42
18	CO	114/116 (98%)	105 (92%)	9 (8%)	0	100	100
18	DO	114/116 (98%)	100 (88%)	13 (11%)	1 (1%)	17	54
19	CP	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
19	DP	112/114 (98%)	104 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	CQ	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
20	DQ	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
21	CR	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
21	DR	101/103 (98%)	90 (89%)	11 (11%)	0	100	100
22	CS	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
22	DS	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
23	CT	91/93 (98%)	84 (92%)	6 (7%)	1 (1%)	14	50
23	DT	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
24	CU	100/102 (98%)	86 (86%)	14 (14%)	0	100	100
24	DU	100/102 (98%)	85 (85%)	14 (14%)	1 (1%)	15	52
25	CV	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
25	DV	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
26	CW	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
26	DW	73/75 (97%)	64 (88%)	9 (12%)	0	100	100
27	CX	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
27	DX	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
28	CY	59/63 (94%)	52 (88%)	7 (12%)	0	100	100
28	DY	61/63 (97%)	54 (88%)	6 (10%)	1 (2%)	9	44
29	CZ	56/58 (97%)	53 (95%)	2 (4%)	1 (2%)	8	41
29	DZ	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
30	C0	37/39 (95%)	33 (89%)	4 (11%)	0	100	100
30	D0	37/39 (95%)	33 (89%)	4 (11%)	0	100	100
31	C1	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
31	D1	54/56 (96%)	48 (89%)	6 (11%)	0	100	100
32	C2	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
32	D2	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
33	C3	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
33	D3	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
34	C4	59/62 (95%)	52 (88%)	6 (10%)	1 (2%)	9	42
34	D4	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	9	42
35	C6	36/38 (95%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	D6	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
37	AB	223/225 (99%)	198 (89%)	25 (11%)	0	100	100
37	BB	223/225 (99%)	186 (83%)	37 (17%)	0	100	100
38	AC	204/206 (99%)	174 (85%)	30 (15%)	0	100	100
38	BC	204/206 (99%)	186 (91%)	18 (9%)	0	100	100
39	AD	203/205 (99%)	179 (88%)	24 (12%)	0	100	100
39	BD	203/205 (99%)	174 (86%)	27 (13%)	2 (1%)	15	52
40	AE	148/150 (99%)	117 (79%)	31 (21%)	0	100	100
40	BE	148/150 (99%)	122 (82%)	26 (18%)	0	100	100
41	AF	98/100 (98%)	80 (82%)	17 (17%)	1 (1%)	15	52
41	BF	98/100 (98%)	79 (81%)	18 (18%)	1 (1%)	15	52
42	AG	131/179 (73%)	117 (89%)	14 (11%)	0	100	100
42	BG	128/179 (72%)	117 (91%)	11 (9%)	0	100	100
43	AH	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
43	BH	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
44	AI	122/130 (94%)	107 (88%)	15 (12%)	0	100	100
44	BI	125/130 (96%)	104 (83%)	21 (17%)	0	100	100
45	AJ	96/98 (98%)	85 (88%)	11 (12%)	0	100	100
45	BJ	96/98 (98%)	80 (83%)	15 (16%)	1 (1%)	15	52
46	AK	114/117 (97%)	101 (89%)	13 (11%)	0	100	100
46	BK	115/117 (98%)	99 (86%)	16 (14%)	0	100	100
47	AL	121/123 (98%)	104 (86%)	16 (13%)	1 (1%)	19	57
47	BL	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
48	AM	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
48	BM	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
49	AN	92/101 (91%)	80 (87%)	12 (13%)	0	100	100
49	BN	92/101 (91%)	77 (84%)	15 (16%)	0	100	100
50	AO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13	49
50	BO	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
51	AP	80/82 (98%)	71 (89%)	8 (10%)	1 (1%)	12	47
51	BP	80/82 (98%)	68 (85%)	11 (14%)	1 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
52	AQ	78/80 (98%)	64 (82%)	12 (15%)	2 (3%)	5 34
52	BQ	78/80 (98%)	63 (81%)	15 (19%)	0	100 100
53	AR	53/55 (96%)	49 (92%)	4 (8%)	0	100 100
53	BR	53/55 (96%)	49 (92%)	4 (8%)	0	100 100
54	AS	77/79 (98%)	65 (84%)	12 (16%)	0	100 100
54	BS	77/79 (98%)	68 (88%)	9 (12%)	0	100 100
55	AT	83/85 (98%)	78 (94%)	5 (6%)	0	100 100
55	BT	83/85 (98%)	75 (90%)	8 (10%)	0	100 100
All	All	11101/11427 (97%)	9933 (90%)	1142 (10%)	26 (0%)	47 79

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	CT	3	ARG
41	AF	55	HIS
52	AQ	70	LYS
17	DN	118	ARG
39	BD	28	ASP

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
5	CC	216/216 (100%)	214 (99%)	2 (1%)	78 87
5	DC	216/216 (100%)	213 (99%)	3 (1%)	67 80
6	CD	164/164 (100%)	163 (99%)	1 (1%)	86 91
6	DD	164/164 (100%)	163 (99%)	1 (1%)	86 91
7	CE	148/148 (100%)	147 (99%)	1 (1%)	84 90
7	DE	147/148 (99%)	145 (99%)	2 (1%)	67 80
8	CF	148/148 (100%)	148 (100%)	0	100 100
8	DF	148/148 (100%)	147 (99%)	1 (1%)	84 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	CG	137/137 (100%)	136 (99%)	1 (1%)	84 90
9	DG	137/137 (100%)	136 (99%)	1 (1%)	84 90
10	CH	114/114 (100%)	110 (96%)	4 (4%)	36 61
10	DH	114/114 (100%)	113 (99%)	1 (1%)	78 87
11	C5	83/83 (100%)	81 (98%)	2 (2%)	49 69
12	CI	53/54 (98%)	50 (94%)	3 (6%)	20 49
12	DI	54/54 (100%)	54 (100%)	0	100 100
13	CJ	116/116 (100%)	115 (99%)	1 (1%)	78 87
13	DJ	116/116 (100%)	114 (98%)	2 (2%)	60 78
14	CK	103/103 (100%)	103 (100%)	0	100 100
14	DK	103/103 (100%)	101 (98%)	2 (2%)	57 75
15	CL	102/102 (100%)	99 (97%)	3 (3%)	42 64
15	DL	102/102 (100%)	100 (98%)	2 (2%)	55 73
16	CM	108/109 (99%)	108 (100%)	0	100 100
16	DM	109/109 (100%)	108 (99%)	1 (1%)	78 87
17	CN	101/101 (100%)	100 (99%)	1 (1%)	76 85
17	DN	101/101 (100%)	101 (100%)	0	100 100
18	CO	86/86 (100%)	84 (98%)	2 (2%)	50 70
18	DO	86/86 (100%)	84 (98%)	2 (2%)	50 70
19	CP	99/99 (100%)	99 (100%)	0	100 100
19	DP	99/99 (100%)	98 (99%)	1 (1%)	76 85
20	CQ	89/89 (100%)	89 (100%)	0	100 100
20	DQ	89/89 (100%)	89 (100%)	0	100 100
21	CR	84/84 (100%)	83 (99%)	1 (1%)	71 83
21	DR	84/84 (100%)	84 (100%)	0	100 100
22	CS	93/93 (100%)	92 (99%)	1 (1%)	73 84
22	DS	93/93 (100%)	92 (99%)	1 (1%)	73 84
23	CT	80/80 (100%)	78 (98%)	2 (2%)	47 68
23	DT	80/80 (100%)	79 (99%)	1 (1%)	69 81
24	CU	83/83 (100%)	83 (100%)	0	100 100
24	DU	83/83 (100%)	83 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	CV	78/78 (100%)	78 (100%)	0	100	100
25	DV	78/78 (100%)	77 (99%)	1 (1%)	69	81
26	CW	57/57 (100%)	56 (98%)	1 (2%)	59	77
26	DW	57/57 (100%)	57 (100%)	0	100	100
27	CX	67/67 (100%)	66 (98%)	1 (2%)	65	79
27	DX	67/67 (100%)	66 (98%)	1 (2%)	65	79
28	CY	55/55 (100%)	55 (100%)	0	100	100
28	DY	55/55 (100%)	55 (100%)	0	100	100
29	CZ	48/48 (100%)	47 (98%)	1 (2%)	53	72
29	DZ	48/48 (100%)	48 (100%)	0	100	100
30	C0	35/35 (100%)	35 (100%)	0	100	100
30	D0	35/35 (100%)	34 (97%)	1 (3%)	42	64
31	C1	47/47 (100%)	47 (100%)	0	100	100
31	D1	47/47 (100%)	47 (100%)	0	100	100
32	C2	45/45 (100%)	44 (98%)	1 (2%)	52	71
32	D2	45/45 (100%)	44 (98%)	1 (2%)	52	71
33	C3	38/38 (100%)	37 (97%)	1 (3%)	46	67
33	D3	38/38 (100%)	37 (97%)	1 (3%)	46	67
34	C4	49/50 (98%)	49 (100%)	0	100	100
34	D4	50/50 (100%)	49 (98%)	1 (2%)	55	73
35	C6	34/34 (100%)	34 (100%)	0	100	100
35	D6	34/34 (100%)	34 (100%)	0	100	100
37	AB	186/186 (100%)	185 (100%)	1 (0%)	88	93
37	BB	186/186 (100%)	182 (98%)	4 (2%)	52	71
38	AC	170/170 (100%)	169 (99%)	1 (1%)	86	91
38	BC	170/170 (100%)	165 (97%)	5 (3%)	42	64
39	AD	172/172 (100%)	168 (98%)	4 (2%)	50	70
39	BD	172/172 (100%)	167 (97%)	5 (3%)	42	64
40	AE	113/113 (100%)	111 (98%)	2 (2%)	59	77
40	BE	113/113 (100%)	109 (96%)	4 (4%)	36	61
41	AF	87/87 (100%)	86 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	BF	87/87 (100%)	86 (99%)	1 (1%)	73	84
42	AG	110/147 (75%)	110 (100%)	0	100	100
42	BG	107/147 (73%)	107 (100%)	0	100	100
43	AH	104/104 (100%)	103 (99%)	1 (1%)	76	85
43	BH	104/104 (100%)	104 (100%)	0	100	100
44	AI	102/107 (95%)	100 (98%)	2 (2%)	55	73
44	BI	105/107 (98%)	102 (97%)	3 (3%)	42	64
45	AJ	86/86 (100%)	85 (99%)	1 (1%)	71	83
45	BJ	86/86 (100%)	85 (99%)	1 (1%)	71	83
46	AK	89/90 (99%)	87 (98%)	2 (2%)	52	71
46	BK	90/90 (100%)	85 (94%)	5 (6%)	21	49
47	AL	103/103 (100%)	102 (99%)	1 (1%)	76	85
47	BL	103/103 (100%)	102 (99%)	1 (1%)	76	85
48	AM	92/92 (100%)	91 (99%)	1 (1%)	73	84
48	BM	92/92 (100%)	92 (100%)	0	100	100
49	AN	79/84 (94%)	79 (100%)	0	100	100
49	BN	79/84 (94%)	79 (100%)	0	100	100
50	AO	76/77 (99%)	74 (97%)	2 (3%)	46	67
50	BO	76/77 (99%)	73 (96%)	3 (4%)	32	58
51	AP	65/65 (100%)	64 (98%)	1 (2%)	65	79
51	BP	65/65 (100%)	65 (100%)	0	100	100
52	AQ	74/74 (100%)	73 (99%)	1 (1%)	67	80
52	BQ	74/74 (100%)	72 (97%)	2 (3%)	44	66
53	AR	48/48 (100%)	47 (98%)	1 (2%)	53	72
53	BR	48/48 (100%)	48 (100%)	0	100	100
54	AS	70/70 (100%)	70 (100%)	0	100	100
54	BS	70/70 (100%)	69 (99%)	1 (1%)	67	80
55	AT	65/65 (100%)	64 (98%)	1 (2%)	65	79
55	BT	65/65 (100%)	64 (98%)	1 (2%)	65	79
All	All	9222/9323 (99%)	9106 (99%)	116 (1%)	69	81

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	DE	49	ARG
50	BO	53	ARG
19	DP	95	LYS
50	BO	46	LYS
44	BI	67	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
21	DR	66	HIS
38	BC	6	HIS
23	DT	59	ASN
28	DY	25	GLN
39	BD	130	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1536/1541 (99%)	390 (25%)	7 (0%)
1	BA	1536/1541 (99%)	356 (23%)	11 (0%)
2	CA	2862/2904 (98%)	585 (20%)	18 (0%)
2	DA	2856/2904 (98%)	636 (22%)	16 (0%)
3	CB	117/118 (99%)	23 (19%)	0
3	DB	117/118 (99%)	18 (15%)	0
36	AX	29/46 (63%)	2 (6%)	2 (6%)
36	BX	29/46 (63%)	1 (3%)	0
4	AV	75/76 (98%)	21 (28%)	0
4	AW	76/76 (100%)	17 (22%)	2 (2%)
4	AY	75/76 (98%)	32 (42%)	0
4	BV	75/76 (98%)	17 (22%)	0
4	BW	75/76 (98%)	15 (20%)	0
All	All	9458/9598 (98%)	2113 (22%)	56 (0%)

5 of 2113 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	3	A
1	AA	4	U
1	AA	5	U
1	AA	6	G

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	AW	17	U
2	DA	2756	U
1	BA	848	C
2	DA	2425	A
2	DA	1869	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 449 ligands modelled in this entry, 449 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
2	DA	9
1	BA	4

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Mol	Chain	Number of breaks
1	AA	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DA	2105:U	O3'	2118:U	P	30.28
1	DA	2185:U	O3'	2186:G	P	7.24
1	DA	2103:C	O3'	2104:C	P	6.01
1	DA	1887:C	O3'	1888:G	P	5.11
1	DA	2140:G	O3'	2141:G	P	3.75

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1540/1541 (99%)	-0.27	15 (0%) 82 74	95, 154, 227, 359	2 (0%)
1	BA	1541/1541 (100%)	-0.25	24 (1%) 72 62	110, 157, 208, 259	3 (0%)
2	CA	2867/2904 (98%)	-0.48	28 (0%) 82 74	69, 94, 175, 298	33 (1%)
2	DA	2869/2904 (98%)	-0.33	45 (1%) 72 62	86, 126, 219, 320	26 (0%)
3	CB	118/118 (100%)	-0.68	0 100 100	81, 108, 131, 159	0
3	DB	118/118 (100%)	-0.52	0 100 100	133, 191, 210, 222	0
4	AV	76/76 (100%)	0.18	8 (10%) 6 6	125, 166, 186, 201	0
4	AW	76/76 (100%)	-0.11	2 (2%) 56 46	119, 157, 180, 196	0
4	AY	76/76 (100%)	3.17	47 (61%) 0 0	120, 227, 240, 243	76 (100%)
4	BV	76/76 (100%)	0.10	6 (7%) 12 11	138, 193, 215, 225	0
4	BW	76/76 (100%)	-0.06	3 (3%) 39 31	142, 195, 208, 221	0
5	CC	271/271 (100%)	0.09	9 (3%) 46 37	71, 99, 117, 127	0
5	DC	271/271 (100%)	0.18	14 (5%) 27 24	98, 122, 143, 158	0
6	CD	209/209 (100%)	0.31	12 (5%) 23 20	70, 90, 110, 165	0
6	DD	209/209 (100%)	0.15	4 (1%) 66 58	89, 113, 130, 143	0
7	CE	181/181 (100%)	-0.05	2 (1%) 80 72	68, 95, 111, 133	0
7	DE	180/181 (99%)	0.13	3 (1%) 70 60	92, 128, 142, 151	0
8	CF	177/177 (100%)	-0.01	2 (1%) 80 72	113, 134, 158, 170	0
8	DF	177/177 (100%)	0.90	38 (21%) 0 1	136, 191, 224, 239	0
9	CG	176/176 (100%)	-0.03	3 (1%) 70 60	88, 105, 120, 148	0
9	DG	176/176 (100%)	0.46	15 (8%) 10 9	132, 150, 165, 176	0
10	CH	149/149 (100%)	0.32	9 (6%) 21 17	101, 151, 164, 168	0
10	DH	149/149 (100%)	1.00	29 (19%) 1 1	139, 210, 238, 243	0
11	C5	109/109 (100%)	0.38	12 (11%) 5 5	131, 173, 190, 197	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
12	CI	71/72 (98%)	1.30	18 (25%) 0 0	191, 212, 223, 225	71 (100%)
12	DI	72/72 (100%)	1.62	25 (34%) 0 0	262, 278, 291, 295	0
13	CJ	142/142 (100%)	0.13	0 100 100	68, 86, 104, 121	0
13	DJ	142/142 (100%)	0.23	8 (5%) 24 21	97, 114, 129, 147	0
14	CK	122/122 (100%)	-0.14	1 (0%) 86 79	77, 92, 114, 125	0
14	DK	122/122 (100%)	0.33	7 (5%) 23 20	97, 114, 129, 139	0
15	CL	143/143 (100%)	0.26	8 (5%) 24 21	74, 99, 116, 130	0
15	DL	143/143 (100%)	0.33	7 (4%) 29 25	98, 150, 167, 182	0
16	CM	135/136 (99%)	0.07	0 100 100	78, 94, 113, 127	0
16	DM	136/136 (100%)	0.96	25 (18%) 1 1	117, 138, 151, 164	0
17	CN	121/121 (100%)	-0.07	0 100 100	72, 87, 99, 100	0
17	DN	121/121 (100%)	0.04	3 (2%) 57 47	89, 106, 122, 146	0
18	CO	116/116 (100%)	0.13	3 (2%) 56 46	93, 111, 126, 131	0
18	DO	116/116 (100%)	1.16	29 (25%) 0 0	169, 188, 201, 208	0
19	CP	114/114 (100%)	0.20	6 (5%) 26 23	76, 96, 125, 135	0
19	DP	114/114 (100%)	0.31	4 (3%) 44 35	108, 121, 142, 154	0
20	CQ	117/117 (100%)	-0.27	0 100 100	68, 80, 97, 112	0
20	DQ	117/117 (100%)	-0.38	0 100 100	84, 108, 120, 127	0
21	CR	103/103 (100%)	0.09	0 100 100	70, 94, 109, 119	0
21	DR	103/103 (100%)	-0.03	2 (1%) 66 58	99, 116, 130, 141	0
22	CS	110/110 (100%)	0.44	6 (5%) 25 22	69, 87, 102, 121	0
22	DS	110/110 (100%)	0.51	8 (7%) 15 12	84, 104, 119, 131	0
23	CT	93/93 (100%)	0.47	8 (8%) 10 9	78, 97, 123, 138	0
23	DT	93/93 (100%)	0.32	3 (3%) 47 37	107, 127, 150, 166	0
24	CU	102/102 (100%)	0.14	2 (1%) 65 56	77, 96, 118, 137	0
24	DU	102/102 (100%)	0.71	13 (12%) 3 4	97, 123, 149, 165	0
25	CV	94/94 (100%)	0.16	6 (6%) 19 15	78, 101, 116, 119	0
25	DV	94/94 (100%)	0.14	3 (3%) 47 37	132, 146, 157, 161	0
26	CW	75/75 (100%)	0.33	4 (5%) 26 23	82, 95, 110, 155	0
26	DW	75/75 (100%)	0.83	13 (17%) 1 2	129, 148, 161, 172	0
27	CX	77/77 (100%)	0.25	3 (3%) 39 31	83, 98, 117, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	DX	77/77 (100%)	0.70	4 (5%) 27 24	118, 135, 151, 156	0
28	CY	61/63 (96%)	-0.36	0 100 100	94, 109, 122, 145	0
28	DY	63/63 (100%)	0.11	3 (4%) 30 26	118, 133, 150, 154	0
29	CZ	58/58 (100%)	0.53	2 (3%) 45 36	74, 88, 108, 128	0
29	DZ	58/58 (100%)	0.82	5 (8%) 10 9	121, 137, 146, 152	0
30	C0	39/39 (100%)	0.91	6 (15%) 2 2	150, 167, 178, 182	39 (100%)
30	D0	39/39 (100%)	1.43	10 (25%) 0 0	179, 195, 204, 205	39 (100%)
31	C1	56/56 (100%)	-0.23	0 100 100	67, 91, 115, 127	0
31	D1	56/56 (100%)	-0.19	0 100 100	89, 110, 123, 135	0
32	C2	50/50 (100%)	2.64	31 (62%) 0 0	128, 140, 154, 158	0
32	D2	50/50 (100%)	4.10	39 (78%) 0 0	158, 174, 180, 184	50 (100%)
33	C3	46/46 (100%)	0.04	0 100 100	68, 87, 102, 108	0
33	D3	46/46 (100%)	0.16	0 100 100	101, 110, 120, 140	0
34	C4	61/62 (98%)	1.26	12 (19%) 1 1	79, 108, 121, 123	0
34	D4	62/62 (100%)	1.91	24 (38%) 0 0	135, 160, 171, 175	0
35	C6	38/38 (100%)	0.06	0 100 100	88, 103, 122, 149	0
35	D6	38/38 (100%)	1.27	13 (34%) 0 0	126, 137, 150, 178	0
36	AX	30/46 (65%)	2.49	15 (50%) 0 0	123, 203, 227, 257	1 (3%)
36	BX	30/46 (65%)	2.59	17 (56%) 0 0	140, 188, 233, 239	2 (6%)
37	AB	225/225 (100%)	0.54	27 (12%) 4 5	161, 181, 193, 207	0
37	BB	225/225 (100%)	0.31	15 (6%) 17 14	168, 197, 211, 218	0
38	AC	206/206 (100%)	-0.12	3 (1%) 73 64	147, 163, 176, 198	0
38	BC	206/206 (100%)	0.32	20 (9%) 7 7	140, 159, 171, 180	0
39	AD	205/205 (100%)	0.62	25 (12%) 4 5	138, 166, 180, 185	0
39	BD	205/205 (100%)	0.04	4 (1%) 65 56	126, 144, 156, 172	0
40	AE	150/150 (100%)	0.55	17 (11%) 5 5	121, 145, 160, 165	0
40	BE	150/150 (100%)	0.38	10 (6%) 17 14	126, 149, 161, 171	0
41	AF	100/100 (100%)	-0.28	1 (1%) 82 74	113, 136, 153, 159	0
41	BF	100/100 (100%)	0.63	15 (15%) 2 2	145, 158, 171, 178	0
42	AG	135/179 (75%)	0.66	15 (11%) 5 5	149, 173, 188, 200	0
42	BG	132/179 (73%)	0.79	24 (18%) 1 2	169, 196, 215, 225	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	AH	128/129 (99%)	0.31	8 (6%) 20 16	135, 146, 164, 171	0
43	BH	129/129 (100%)	0.14	4 (3%) 49 38	141, 154, 164, 172	0
44	AI	124/130 (95%)	1.00	18 (14%) 2 3	146, 178, 189, 200	0
44	BI	127/130 (97%)	0.73	12 (9%) 8 8	161, 193, 206, 210	0
45	AJ	98/98 (100%)	0.85	16 (16%) 1 2	149, 182, 197, 200	0
45	BJ	98/98 (100%)	0.65	12 (12%) 4 5	151, 176, 189, 193	0
46	AK	116/117 (99%)	-0.27	0 100 100	96, 131, 147, 161	0
46	BK	117/117 (100%)	0.61	16 (13%) 3 3	142, 170, 187, 192	0
47	AL	123/123 (100%)	0.91	20 (16%) 1 2	116, 134, 148, 176	0
47	BL	123/123 (100%)	0.48	9 (7%) 15 12	111, 128, 142, 153	0
48	AM	114/114 (100%)	0.36	11 (9%) 8 7	135, 168, 206, 227	0
48	BM	114/114 (100%)	0.32	8 (7%) 16 13	164, 190, 212, 243	0
49	AN	96/101 (95%)	0.69	12 (12%) 3 5	147, 168, 180, 189	0
49	BN	96/101 (95%)	0.38	7 (7%) 15 12	153, 166, 177, 185	0
50	AO	88/89 (98%)	-0.03	0 100 100	112, 131, 150, 159	0
50	BO	88/89 (98%)	0.32	8 (9%) 9 8	135, 153, 167, 172	0
51	AP	82/82 (100%)	1.95	35 (42%) 0 0	147, 169, 179, 195	0
51	BP	82/82 (100%)	1.16	25 (30%) 0 0	122, 148, 174, 189	0
52	AQ	80/80 (100%)	0.61	8 (10%) 7 7	126, 151, 163, 170	0
52	BQ	80/80 (100%)	0.94	16 (20%) 1 1	131, 150, 161, 173	0
53	AR	55/55 (100%)	0.66	4 (7%) 15 12	126, 139, 157, 161	0
53	BR	55/55 (100%)	0.94	8 (14%) 2 3	152, 162, 183, 200	0
54	AS	79/79 (100%)	0.64	8 (10%) 7 7	156, 170, 179, 184	0
54	BS	79/79 (100%)	0.91	16 (20%) 1 1	165, 179, 188, 193	0
55	AT	85/85 (100%)	0.15	3 (3%) 44 35	134, 154, 166, 176	0
55	BT	85/85 (100%)	0.74	5 (5%) 22 18	131, 151, 163, 170	0
All	All	20800/21025 (98%)	0.09	1191 (5%) 23 20	67, 135, 203, 359	342 (1%)

The worst 5 of 1191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	DA	2153	C	15.4
2	DA	2145	C	11.7

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Mol	Chain	Res	Type	RSRZ
4	AV	76	A	11.0
30	D0	22	MET	10.7
4	AY	17	U	10.7

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

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

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, 95^{th} 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
56	MG	AA	1640	1/1	0.06	0.66	127,127,127,127	0
56	MG	AA	1642	1/1	0.44	0.34	122,122,122,122	0
56	MG	AA	1610	1/1	0.50	0.30	114,114,114,114	0
56	MG	AA	1644	1/1	0.56	0.57	164,164,164,164	0
56	MG	BA	1628	1/1	0.56	1.70	120,120,120,120	0
56	MG	BA	1618	1/1	0.57	0.19	144,144,144,144	0
56	MG	DA	3097	1/1	0.64	0.33	78,78,78,78	0
57	ZN	D0	101	1/1	0.66	0.10	210,210,210,210	1
57	ZN	C0	101	1/1	0.67	0.10	177,177,177,177	1
56	MG	DA	3090	1/1	0.70	0.26	60,60,60,60	0
56	MG	BA	1641	1/1	0.70	0.29	134,134,134,134	0
56	MG	DA	3160	1/1	0.71	0.37	78,78,78,78	0
56	MG	CA	3070	1/1	0.72	0.29	76,76,76,76	0
56	MG	CA	3090	1/1	0.72	0.39	83,83,83,83	0
56	MG	AA	1605	1/1	0.72	0.21	155,155,155,155	1
56	MG	DA	3094	1/1	0.72	0.48	77,77,77,77	0
56	MG	CA	3068	1/1	0.73	0.45	101,101,101,101	0
56	MG	BA	1620	1/1	0.73	1.03	104,104,104,104	0
56	MG	BA	1632	1/1	0.74	0.06	191,191,191,191	0
56	MG	BA	1645	1/1	0.76	0.32	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	1636	1/1	0.77	0.35	99,99,99,99	0
56	MG	BA	1608	1/1	0.78	0.46	127,127,127,127	0
56	MG	BA	1639	1/1	0.80	0.18	155,155,155,155	1
56	MG	AA	1606	1/1	0.81	0.12	110,110,110,110	0
56	MG	BA	1649	1/1	0.81	0.15	72,72,72,72	0
56	MG	C4	101	1/1	0.82	0.75	73,73,73,73	0
56	MG	BA	1604	1/1	0.82	0.10	147,147,147,147	0
56	MG	CA	3091	1/1	0.83	0.34	98,98,98,98	0
56	MG	DA	3087	1/1	0.83	0.41	104,104,104,104	0
56	MG	AA	1638	1/1	0.84	0.34	55,55,55,55	0
56	MG	BA	1626	1/1	0.85	0.54	114,114,114,114	0
56	MG	BA	1607	1/1	0.85	1.12	87,87,87,87	0
56	MG	AA	1604	1/1	0.85	0.10	182,182,182,182	1
56	MG	AA	1641	1/1	0.85	0.27	171,171,171,171	0
56	MG	AA	1647	1/1	0.85	0.28	105,105,105,105	0
56	MG	CA	3019	1/1	0.86	0.19	78,78,78,78	1
56	MG	AA	1632	1/1	0.86	0.36	151,151,151,151	0
56	MG	AA	1648	1/1	0.86	0.13	149,149,149,149	0
56	MG	BA	1648	1/1	0.86	0.45	109,109,109,109	0
56	MG	DA	3154	1/1	0.87	0.94	68,68,68,68	0
56	MG	BA	1646	1/1	0.87	0.32	81,81,81,81	0
56	MG	DA	3164	1/1	0.87	0.27	60,60,60,60	0
56	MG	DA	3076	1/1	0.87	0.17	76,76,76,76	1
56	MG	DA	3141	1/1	0.87	0.20	151,151,151,151	1
56	MG	DA	3149	1/1	0.88	0.25	68,68,68,68	0
56	MG	CA	3155	1/1	0.88	0.30	81,81,81,81	1
56	MG	BA	1638	1/1	0.88	0.16	154,154,154,154	0
56	MG	DA	3162	1/1	0.88	0.53	77,77,77,77	0
56	MG	DA	3110	1/1	0.88	0.18	108,108,108,108	0
56	MG	DA	3112	1/1	0.88	0.19	101,101,101,101	0
56	MG	DA	3029	1/1	0.88	0.14	72,72,72,72	1
56	MG	AA	1619	1/1	0.89	0.42	124,124,124,124	0
56	MG	BA	1642	1/1	0.89	0.55	107,107,107,107	0
56	MG	DA	3100	1/1	0.89	0.74	76,76,76,76	0
56	MG	DA	3101	1/1	0.89	0.15	125,125,125,125	1
56	MG	CA	3157	1/1	0.89	0.25	52,52,52,52	0
56	MG	CQ	801	1/1	0.89	0.36	56,56,56,56	0
56	MG	AA	1630	1/1	0.89	0.27	158,158,158,158	0
56	MG	BA	1631	1/1	0.89	0.42	155,155,155,155	0
56	MG	AA	1603	1/1	0.89	0.05	148,148,148,148	1
56	MG	DA	3060	1/1	0.89	0.66	73,73,73,73	1
56	MG	DA	3061	1/1	0.89	0.39	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3112	1/1	0.89	0.11	73,73,73,73	1
56	MG	DA	3165	1/1	0.89	1.17	60,60,60,60	0
56	MG	CA	3150	1/1	0.89	0.39	91,91,91,91	0
56	MG	BA	1610	1/1	0.89	0.10	147,147,147,147	0
56	MG	DA	3158	1/1	0.90	0.62	64,64,64,64	0
56	MG	DA	3081	1/1	0.90	0.43	55,55,55,55	0
56	MG	BA	1617	1/1	0.90	0.18	124,124,124,124	0
56	MG	CA	3164	1/1	0.90	0.28	60,60,60,60	0
56	MG	CA	3007	1/1	0.90	0.25	88,88,88,88	0
56	MG	DN	201	1/1	0.90	0.43	84,84,84,84	1
56	MG	DQ	801	1/1	0.90	0.59	60,60,60,60	0
56	MG	BA	1605	1/1	0.90	0.31	104,104,104,104	0
56	MG	BA	1615	1/1	0.90	0.14	115,115,115,115	0
56	MG	BA	1635	1/1	0.91	0.12	141,141,141,141	0
56	MG	DA	3044	1/1	0.91	0.06	125,125,125,125	0
56	MG	DA	3135	1/1	0.91	0.61	92,92,92,92	0
56	MG	AA	1650	1/1	0.91	0.28	86,86,86,86	0
56	MG	BA	1637	1/1	0.91	0.08	150,150,150,150	0
56	MG	CA	3026	1/1	0.91	0.28	70,70,70,70	1
56	MG	CA	3166	1/1	0.91	0.69	60,60,60,60	0
56	MG	DA	3083	1/1	0.91	1.01	73,73,73,73	0
56	MG	CA	3098	1/1	0.91	0.13	98,98,98,98	0
56	MG	CA	3005	1/1	0.91	0.30	90,90,90,90	1
56	MG	CA	3127	1/1	0.91	0.25	42,42,42,42	0
56	MG	CA	3149	1/1	0.91	0.30	95,95,95,95	1
56	MG	AA	1602	1/1	0.91	0.25	177,177,177,177	0
56	MG	CA	3079	1/1	0.91	0.40	64,64,64,64	0
56	MG	DA	3106	1/1	0.91	0.10	90,90,90,90	1
56	MG	DA	3132	1/1	0.92	0.22	105,105,105,105	0
56	MG	DA	3026	1/1	0.92	0.17	102,102,102,102	0
56	MG	CA	3084	1/1	0.92	0.39	85,85,85,85	0
56	MG	DA	3091	1/1	0.92	0.47	132,132,132,132	1
56	MG	DA	3152	1/1	0.92	0.38	103,103,103,103	0
56	MG	DA	3093	1/1	0.92	0.21	76,76,76,76	0
56	MG	BA	1644	1/1	0.92	0.58	78,78,78,78	0
56	MG	DA	3159	1/1	0.92	0.21	95,95,95,95	0
56	MG	DA	3056	1/1	0.92	0.28	84,84,84,84	0
56	MG	DA	3161	1/1	0.92	0.27	92,92,92,92	0
56	MG	CB	202	1/1	0.92	0.19	80,80,80,80	0
56	MG	DA	3163	1/1	0.92	0.38	60,60,60,60	0
56	MG	CA	3087	1/1	0.92	0.27	74,74,74,74	0
56	MG	DA	3103	1/1	0.92	0.09	95,95,95,95	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DB	203	1/1	0.92	0.23	131,131,131,131	0
56	MG	BA	1647	1/1	0.92	0.36	104,104,104,104	0
56	MG	BA	1613	1/1	0.92	0.16	88,88,88,88	0
56	MG	BA	1625	1/1	0.92	0.18	171,171,171,171	0
56	MG	DA	3128	1/1	0.92	0.14	121,121,121,121	1
56	MG	DA	3139	1/1	0.93	0.09	99,99,99,99	0
56	MG	DA	3043	1/1	0.93	0.17	104,104,104,104	0
56	MG	CA	3165	1/1	0.93	0.78	60,60,60,60	0
56	MG	AA	1627	1/1	0.93	0.25	128,128,128,128	0
56	MG	CA	3001	1/1	0.93	0.26	62,62,62,62	1
56	MG	CA	3160	1/1	0.93	0.15	68,68,68,68	0
56	MG	DA	3072	1/1	0.93	0.26	79,79,79,79	0
56	MG	CA	3042	1/1	0.93	0.12	77,77,77,77	1
57	ZN	C6	101	1/1	0.93	0.09	98,98,98,98	0
56	MG	DA	3030	1/1	0.93	0.14	132,132,132,132	1
56	MG	CA	3138	1/1	0.94	0.07	102,102,102,102	0
56	MG	CA	3142	1/1	0.94	0.26	57,57,57,57	0
56	MG	DA	3092	1/1	0.94	0.24	102,102,102,102	0
56	MG	BA	1643	1/1	0.94	0.15	114,114,114,114	1
56	MG	CA	3060	1/1	0.94	0.39	48,48,48,48	0
56	MG	AA	1613	1/1	0.94	0.42	104,104,104,104	0
56	MG	DA	3098	1/1	0.94	0.23	84,84,84,84	0
56	MG	CA	3151	1/1	0.94	0.51	75,75,75,75	0
56	MG	CA	3008	1/1	0.94	0.24	69,69,69,69	0
56	MG	CA	3011	1/1	0.94	0.18	52,52,52,52	0
56	MG	CA	3082	1/1	0.94	0.37	84,84,84,84	0
56	MG	DA	3002	1/1	0.94	0.15	89,89,89,89	0
56	MG	DA	3005	1/1	0.94	0.07	120,120,120,120	0
56	MG	DA	3117	1/1	0.94	0.29	95,95,95,95	0
56	MG	DA	3007	1/1	0.94	0.10	72,72,72,72	0
56	MG	DA	3013	1/1	0.94	0.42	51,51,51,51	0
56	MG	DA	3134	1/1	0.94	0.54	67,67,67,67	0
56	MG	DA	3017	1/1	0.94	0.34	73,73,73,73	0
56	MG	DA	3018	1/1	0.94	0.50	95,95,95,95	0
56	MG	DA	3140	1/1	0.94	0.21	98,98,98,98	1
56	MG	DA	3020	1/1	0.94	0.14	77,77,77,77	0
56	MG	DA	3023	1/1	0.94	0.17	100,100,100,100	1
56	MG	DA	3150	1/1	0.94	0.18	28,28,28,28	1
56	MG	BA	1621	1/1	0.94	0.24	91,91,91,91	0
56	MG	BA	1623	1/1	0.94	0.15	139,139,139,139	0
56	MG	DA	3155	1/1	0.94	0.23	79,79,79,79	0
56	MG	CA	3162	1/1	0.94	0.60	56,56,56,56	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3037	1/1	0.94	0.73	83,83,83,83	0
56	MG	CA	3015	1/1	0.94	0.34	87,87,87,87	0
56	MG	AA	1634	1/1	0.94	0.13	122,122,122,122	1
56	MG	DA	3049	1/1	0.94	0.27	96,96,96,96	0
56	MG	BA	1629	1/1	0.94	0.17	161,161,161,161	0
56	MG	AA	1629	1/1	0.94	0.98	127,127,127,127	0
56	MG	CA	3030	1/1	0.94	0.09	84,84,84,84	1
56	MG	DA	3166	1/1	0.94	0.12	137,137,137,137	0
56	MG	DA	3069	1/1	0.94	0.16	166,166,166,166	0
56	MG	CA	3040	1/1	0.94	0.25	88,88,88,88	1
56	MG	AA	1609	1/1	0.94	0.52	127,127,127,127	1
56	MG	CA	3113	1/1	0.94	0.32	81,81,81,81	0
56	MG	CA	3046	1/1	0.94	0.13	77,77,77,77	1
56	MG	BA	1606	1/1	0.94	0.34	100,100,100,100	0
56	MG	DA	3131	1/1	0.95	0.45	78,78,78,78	0
56	MG	CA	3062	1/1	0.95	0.17	90,90,90,90	1
56	MG	DA	3133	1/1	0.95	0.34	77,77,77,77	0
56	MG	AA	1631	1/1	0.95	0.20	148,148,148,148	1
56	MG	DA	3071	1/1	0.95	0.17	101,101,101,101	1
56	MG	CA	3021	1/1	0.95	0.17	78,78,78,78	0
56	MG	CA	3023	1/1	0.95	0.10	80,80,80,80	1
56	MG	DA	3078	1/1	0.95	0.10	151,151,151,151	0
56	MG	DA	3145	1/1	0.95	0.18	30,30,30,30	1
56	MG	AA	1614	1/1	0.95	0.25	103,103,103,103	0
56	MG	CA	3153	1/1	0.95	0.66	73,73,73,73	1
56	MG	DA	3151	1/1	0.95	0.50	88,88,88,88	0
56	MG	AA	1611	1/1	0.95	0.25	165,165,165,165	1
56	MG	BA	1612	1/1	0.95	0.47	116,116,116,116	0
56	MG	CA	3031	1/1	0.95	0.16	66,66,66,66	1
56	MG	DA	3025	1/1	0.95	0.51	88,88,88,88	0
56	MG	BA	1640	1/1	0.95	0.12	145,145,145,145	0
56	MG	CA	3159	1/1	0.95	0.15	93,93,93,93	0
56	MG	CA	3039	1/1	0.95	0.15	62,62,62,62	0
56	MG	AA	1643	1/1	0.95	0.19	85,85,85,85	0
56	MG	CA	3093	1/1	0.95	0.08	100,100,100,100	0
56	MG	AA	1635	1/1	0.95	0.09	133,133,133,133	1
56	MG	DA	3046	1/1	0.95	0.14	111,111,111,111	1
56	MG	DA	3047	1/1	0.95	0.11	122,122,122,122	0
56	MG	DA	3107	1/1	0.95	0.28	112,112,112,112	0
56	MG	CA	3044	1/1	0.95	0.21	86,86,86,86	1
56	MG	DA	3052	1/1	0.95	0.40	54,54,54,54	0
56	MG	AA	1620	1/1	0.95	0.11	160,160,160,160	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3127	1/1	0.95	0.37	43,43,43,43	0
56	MG	AA	1639	1/1	0.95	0.15	137,137,137,137	1
56	MG	DA	3019	1/1	0.96	0.11	102,102,102,102	1
56	MG	DA	3105	1/1	0.96	0.10	92,92,92,92	0
56	MG	CA	3154	1/1	0.96	0.28	78,78,78,78	1
56	MG	AA	1608	1/1	0.96	0.52	106,106,106,106	0
56	MG	DA	3108	1/1	0.96	0.16	97,97,97,97	0
56	MG	BA	1624	1/1	0.96	0.08	119,119,119,119	0
56	MG	CA	3156	1/1	0.96	0.26	84,84,84,84	0
56	MG	AA	1607	1/1	0.96	0.35	98,98,98,98	0
56	MG	DA	3119	1/1	0.96	0.11	92,92,92,92	0
56	MG	DA	3122	1/1	0.96	0.17	103,103,103,103	0
56	MG	DA	3123	1/1	0.96	0.11	120,120,120,120	1
56	MG	BA	1627	1/1	0.96	0.45	132,132,132,132	0
56	MG	CA	3051	1/1	0.96	0.11	82,82,82,82	1
56	MG	CA	3094	1/1	0.96	0.26	74,74,74,74	0
56	MG	AA	1636	1/1	0.96	0.10	104,104,104,104	1
56	MG	CA	3100	1/1	0.96	0.36	66,66,66,66	0
56	MG	CA	3104	1/1	0.96	0.18	85,85,85,85	1
56	MG	AA	1622	1/1	0.96	0.20	92,92,92,92	0
56	MG	DA	3136	1/1	0.96	0.46	78,78,78,78	0
56	MG	DA	3137	1/1	0.96	0.44	68,68,68,68	0
56	MG	DA	3051	1/1	0.96	0.33	99,99,99,99	1
56	MG	CA	3167	1/1	0.96	0.08	102,102,102,102	0
56	MG	AA	1646	1/1	0.96	0.29	132,132,132,132	0
56	MG	CN	201	1/1	0.96	0.12	86,86,86,86	1
56	MG	CN	202	1/1	0.96	0.28	64,64,64,64	0
56	MG	DA	3063	1/1	0.96	0.16	105,105,105,105	0
56	MG	CA	3119	1/1	0.96	0.15	81,81,81,81	1
56	MG	DA	3070	1/1	0.96	0.14	69,69,69,69	0
56	MG	CA	3120	1/1	0.96	0.09	71,71,71,71	1
56	MG	BA	1601	1/1	0.96	0.21	115,115,115,115	0
56	MG	DA	3075	1/1	0.96	0.19	90,90,90,90	0
56	MG	AA	1616	1/1	0.96	0.34	92,92,92,92	0
56	MG	CA	3128	1/1	0.96	0.16	56,56,56,56	0
56	MG	CA	3129	1/1	0.96	0.18	80,80,80,80	0
56	MG	CA	3134	1/1	0.96	0.27	75,75,75,75	0
56	MG	CA	3072	1/1	0.96	0.14	73,73,73,73	1
56	MG	CA	3140	1/1	0.96	0.14	61,61,61,61	0
56	MG	CA	3037	1/1	0.96	0.31	40,40,40,40	0
56	MG	DA	3004	1/1	0.96	0.09	122,122,122,122	0
56	MG	DB	201	1/1	0.96	0.04	204,204,204,204	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3148	1/1	0.96	0.18	98,98,98,98	0
56	MG	CA	3013	1/1	0.96	0.57	55,55,55,55	0
56	MG	AA	1633	1/1	0.96	0.07	108,108,108,108	1
56	MG	DA	3016	1/1	0.96	0.17	90,90,90,90	0
56	MG	CA	3017	1/1	0.96	0.21	64,64,64,64	0
56	MG	CA	3088	1/1	0.96	0.39	83,83,83,83	1
57	ZN	D6	101	1/1	0.96	0.07	128,128,128,128	0
56	MG	DA	3079	1/1	0.97	0.17	144,144,144,144	0
56	MG	CA	3111	1/1	0.97	0.11	74,74,74,74	0
56	MG	AA	1612	1/1	0.97	0.12	128,128,128,128	0
56	MG	CA	3064	1/1	0.97	0.11	70,70,70,70	0
56	MG	DA	3089	1/1	0.97	0.12	115,115,115,115	0
56	MG	AA	1628	1/1	0.97	0.26	143,143,143,143	0
56	MG	CB	203	1/1	0.97	0.17	77,77,77,77	0
56	MG	CC	301	1/1	0.97	0.11	74,74,74,74	0
56	MG	CA	3069	1/1	0.97	0.13	69,69,69,69	0
56	MG	CA	3036	1/1	0.97	0.10	80,80,80,80	1
56	MG	DA	3096	1/1	0.97	0.09	78,78,78,78	1
56	MG	AA	1615	1/1	0.97	0.32	103,103,103,103	0
56	MG	CA	3074	1/1	0.97	0.06	70,70,70,70	0
56	MG	CA	3130	1/1	0.97	0.13	62,62,62,62	1
56	MG	BA	1602	1/1	0.97	0.10	132,132,132,132	0
56	MG	BA	1603	1/1	0.97	0.14	121,121,121,121	0
56	MG	CA	3132	1/1	0.97	0.13	67,67,67,67	0
56	MG	CA	3075	1/1	0.97	0.26	78,78,78,78	1
56	MG	DA	3009	1/1	0.97	0.13	106,106,106,106	0
56	MG	DA	3011	1/1	0.97	0.12	80,80,80,80	0
56	MG	DA	3109	1/1	0.97	0.09	123,123,123,123	0
56	MG	CA	3135	1/1	0.97	0.41	55,55,55,55	0
56	MG	CA	3136	1/1	0.97	0.17	66,66,66,66	0
56	MG	DA	3116	1/1	0.97	0.17	93,93,93,93	1
56	MG	CA	3137	1/1	0.97	0.27	67,67,67,67	1
56	MG	BA	1609	1/1	0.97	0.18	110,110,110,110	0
56	MG	AA	1621	1/1	0.97	0.14	90,90,90,90	0
56	MG	CA	3018	1/1	0.97	0.08	90,90,90,90	1
56	MG	DA	3125	1/1	0.97	0.11	92,92,92,92	1
56	MG	DA	3021	1/1	0.97	0.12	92,92,92,92	1
56	MG	DA	3022	1/1	0.97	0.14	86,86,86,86	0
56	MG	CA	3141	1/1	0.97	0.24	67,67,67,67	1
56	MG	BA	1614	1/1	0.97	0.10	128,128,128,128	1
56	MG	AA	1601	1/1	0.97	0.18	102,102,102,102	0
56	MG	CA	3143	1/1	0.97	0.29	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3144	1/1	0.97	0.25	57,57,57,57	0
56	MG	DA	3035	1/1	0.97	0.18	96,96,96,96	0
56	MG	DA	3036	1/1	0.97	0.31	102,102,102,102	0
56	MG	BA	1619	1/1	0.97	0.04	133,133,133,133	0
56	MG	DA	3039	1/1	0.97	0.11	74,74,74,74	0
56	MG	DA	3042	1/1	0.97	0.14	97,97,97,97	0
56	MG	CA	3145	1/1	0.97	0.21	69,69,69,69	0
56	MG	DA	3146	1/1	0.97	0.16	96,96,96,96	0
56	MG	DA	3147	1/1	0.97	0.14	100,100,100,100	1
56	MG	CA	3147	1/1	0.97	0.18	93,93,93,93	0
56	MG	BA	1622	1/1	0.97	0.30	105,105,105,105	0
56	MG	CA	3006	1/1	0.97	0.09	90,90,90,90	1
56	MG	CA	3045	1/1	0.97	0.06	83,83,83,83	1
56	MG	DA	3050	1/1	0.97	0.24	79,79,79,79	0
56	MG	AA	1645	1/1	0.97	0.15	148,148,148,148	0
56	MG	DA	3156	1/1	0.97	0.12	109,109,109,109	0
56	MG	CA	3047	1/1	0.97	0.12	94,94,94,94	0
56	MG	CA	3050	1/1	0.97	0.27	56,56,56,56	0
56	MG	CA	3025	1/1	0.97	0.11	66,66,66,66	1
56	MG	CA	3055	1/1	0.97	0.12	71,71,71,71	0
56	MG	BA	1630	1/1	0.97	0.13	160,160,160,160	0
56	MG	DA	3065	1/1	0.97	0.12	85,85,85,85	0
56	MG	DA	3066	1/1	0.97	0.37	81,81,81,81	0
56	MG	DA	3067	1/1	0.97	0.33	129,129,129,129	0
56	MG	DA	3068	1/1	0.97	0.46	84,84,84,84	0
56	MG	CA	3058	1/1	0.97	0.15	74,74,74,74	1
56	MG	DB	202	1/1	0.97	0.27	95,95,95,95	0
56	MG	AA	1625	1/1	0.97	0.11	100,100,100,100	1
56	MG	BA	1634	1/1	0.97	0.14	129,129,129,129	0
56	MG	CA	3105	1/1	0.97	0.18	85,85,85,85	1
56	MG	CA	3106	1/1	0.97	0.14	82,82,82,82	0
56	MG	CA	3107	1/1	0.97	0.16	83,83,83,83	1
56	MG	DA	3077	1/1	0.97	0.12	90,90,90,90	0
56	MG	CA	3110	1/1	0.97	0.14	86,86,86,86	1
56	MG	CA	3004	1/1	0.98	0.18	78,78,78,78	0
56	MG	CA	3041	1/1	0.98	0.08	67,67,67,67	1
56	MG	CA	3022	1/1	0.98	0.09	75,75,75,75	1
56	MG	DA	3024	1/1	0.98	0.27	98,98,98,98	0
56	MG	CA	3158	1/1	0.98	0.11	73,73,73,73	0
56	MG	CA	3114	1/1	0.98	0.15	73,73,73,73	1
56	MG	DA	3102	1/1	0.98	0.07	98,98,98,98	1
56	MG	DA	3028	1/1	0.98	0.25	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3043	1/1	0.98	0.30	59,59,59,59	0
56	MG	AA	1649	1/1	0.98	0.21	140,140,140,140	0
56	MG	DA	3031	1/1	0.98	0.15	116,116,116,116	0
56	MG	DA	3032	1/1	0.98	0.25	93,93,93,93	0
56	MG	DA	3034	1/1	0.98	0.11	99,99,99,99	0
56	MG	CA	3163	1/1	0.98	0.18	81,81,81,81	1
56	MG	DA	3111	1/1	0.98	0.05	108,108,108,108	1
56	MG	CA	3121	1/1	0.98	0.18	86,86,86,86	1
56	MG	DA	3113	1/1	0.98	0.28	85,85,85,85	0
56	MG	DA	3114	1/1	0.98	0.21	98,98,98,98	1
56	MG	DA	3115	1/1	0.98	0.11	139,139,139,139	0
56	MG	CA	3123	1/1	0.98	0.24	83,83,83,83	1
56	MG	DA	3038	1/1	0.98	0.17	75,75,75,75	1
56	MG	DA	3118	1/1	0.98	0.30	103,103,103,103	0
56	MG	CA	3124	1/1	0.98	0.18	75,75,75,75	1
56	MG	DA	3040	1/1	0.98	0.26	90,90,90,90	1
56	MG	BA	1633	1/1	0.98	0.23	102,102,102,102	0
56	MG	CA	3024	1/1	0.98	0.33	59,59,59,59	0
56	MG	DA	3126	1/1	0.98	0.08	93,93,93,93	0
56	MG	CA	3076	1/1	0.98	0.06	68,68,68,68	0
56	MG	CA	3077	1/1	0.98	0.13	101,101,101,101	0
56	MG	DA	3129	1/1	0.98	0.11	92,92,92,92	1
56	MG	DA	3130	1/1	0.98	0.55	100,100,100,100	0
56	MG	CA	3014	1/1	0.98	0.24	72,72,72,72	1
56	MG	CA	3131	1/1	0.98	0.32	53,53,53,53	0
56	MG	AA	1637	1/1	0.98	0.09	186,186,186,186	0
56	MG	CA	3133	1/1	0.98	0.48	47,47,47,47	0
56	MG	CA	3083	1/1	0.98	0.29	81,81,81,81	1
56	MG	DA	3054	1/1	0.98	0.12	70,70,70,70	0
56	MG	CA	3049	1/1	0.98	0.25	73,73,73,73	0
56	MG	DA	3057	1/1	0.98	0.21	101,101,101,101	0
56	MG	CA	3085	1/1	0.98	0.18	71,71,71,71	0
56	MG	CA	3028	1/1	0.98	0.20	58,58,58,58	0
56	MG	DA	3143	1/1	0.98	0.09	53,53,53,53	0
56	MG	DA	3144	1/1	0.98	0.23	112,112,112,112	0
56	MG	CA	3016	1/1	0.98	0.80	20,20,20,20	0
56	MG	CA	3053	1/1	0.98	0.16	72,72,72,72	1
56	MG	CA	3054	1/1	0.98	0.38	65,65,65,65	0
56	MG	AA	1624	1/1	0.98	0.20	130,130,130,130	0
56	MG	CA	3056	1/1	0.98	0.11	73,73,73,73	0
56	MG	DA	3001	1/1	0.98	0.15	71,71,71,71	1
56	MG	CA	3096	1/1	0.98	0.19	68,68,68,68	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3153	1/1	0.98	0.12	93,93,93,93	0
56	MG	DA	3003	1/1	0.98	0.04	121,121,121,121	0
56	MG	CA	3035	1/1	0.98	0.36	37,37,37,37	0
56	MG	DA	3073	1/1	0.98	0.22	93,93,93,93	1
56	MG	BA	1611	1/1	0.98	0.49	130,130,130,130	0
56	MG	CA	3146	1/1	0.98	0.34	78,78,78,78	0
56	MG	CA	3059	1/1	0.98	0.10	60,60,60,60	0
56	MG	CA	3101	1/1	0.98	0.09	84,84,84,84	0
56	MG	DA	3012	1/1	0.98	0.07	81,81,81,81	0
56	MG	DA	3080	1/1	0.98	0.18	98,98,98,98	1
56	MG	CA	3002	1/1	0.98	0.17	67,67,67,67	1
56	MG	DA	3082	1/1	0.98	0.34	106,106,106,106	0
56	MG	DA	3014	1/1	0.98	0.08	95,95,95,95	1
56	MG	DA	3084	1/1	0.98	0.37	85,85,85,85	0
56	MG	DA	3085	1/1	0.98	0.14	112,112,112,112	0
56	MG	DA	3086	1/1	0.98	0.11	125,125,125,125	1
56	MG	DA	3015	1/1	0.98	0.46	73,73,73,73	0
56	MG	CA	3061	1/1	0.98	0.17	95,95,95,95	1
56	MG	CA	3010	1/1	0.98	0.21	89,89,89,89	1
56	MG	CA	3152	1/1	0.98	0.28	57,57,57,57	0
56	MG	CA	3020	1/1	0.98	0.16	45,45,45,45	1
56	MG	CA	3065	1/1	0.98	0.10	76,76,76,76	1
56	MG	CA	3139	1/1	0.99	0.14	88,88,88,88	0
56	MG	DA	3048	1/1	0.99	0.12	93,93,93,93	1
56	MG	CA	3099	1/1	0.99	0.09	84,84,84,84	1
56	MG	CA	3071	1/1	0.99	0.10	77,77,77,77	0
56	MG	CA	3052	1/1	0.99	0.17	76,76,76,76	1
56	MG	CA	3102	1/1	0.99	0.23	55,55,55,55	0
56	MG	DA	3053	1/1	0.99	0.06	98,98,98,98	1
56	MG	CA	3073	1/1	0.99	0.22	73,73,73,73	1
56	MG	DA	3055	1/1	0.99	0.15	85,85,85,85	0
56	MG	CA	3038	1/1	0.99	0.18	67,67,67,67	0
56	MG	CA	3012	1/1	0.99	0.16	67,67,67,67	1
56	MG	DA	3058	1/1	0.99	0.23	83,83,83,83	0
56	MG	DA	3121	1/1	0.99	0.11	100,100,100,100	1
56	MG	DA	3059	1/1	0.99	0.18	94,94,94,94	1
56	MG	DA	3006	1/1	0.99	0.09	114,114,114,114	1
56	MG	DA	3124	1/1	0.99	0.13	104,104,104,104	0
56	MG	CA	3027	1/1	0.99	0.07	74,74,74,74	1
56	MG	DA	3062	1/1	0.99	0.19	95,95,95,95	1
56	MG	DA	3008	1/1	0.99	0.08	103,103,103,103	1
56	MG	DA	3064	1/1	0.99	0.10	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3108	1/1	0.99	0.15	71,71,71,71	0
56	MG	DA	3010	1/1	0.99	0.12	97,97,97,97	0
56	MG	CA	3109	1/1	0.99	0.09	90,90,90,90	1
56	MG	BA	1616	1/1	0.99	0.16	136,136,136,136	0
56	MG	AA	1623	1/1	0.99	0.06	104,104,104,104	1
56	MG	CA	3078	1/1	0.99	0.11	102,102,102,102	1
56	MG	CA	3057	1/1	0.99	0.05	78,78,78,78	1
56	MG	CA	3080	1/1	0.99	0.10	62,62,62,62	1
56	MG	CA	3081	1/1	0.99	0.12	73,73,73,73	1
56	MG	DA	3138	1/1	0.99	0.59	58,58,58,58	0
56	MG	DA	3074	1/1	0.99	0.22	92,92,92,92	0
56	MG	CA	3116	1/1	0.99	0.06	83,83,83,83	1
56	MG	CA	3117	1/1	0.99	0.33	49,49,49,49	0
56	MG	DA	3142	1/1	0.99	0.14	100,100,100,100	0
56	MG	CA	3118	1/1	0.99	0.23	82,82,82,82	1
56	MG	CA	3029	1/1	0.99	0.23	57,57,57,57	1
56	MG	AA	1617	1/1	0.99	0.21	107,107,107,107	0
56	MG	CA	3003	1/1	0.99	0.19	82,82,82,82	0
56	MG	CA	3161	1/1	0.99	0.07	97,97,97,97	0
56	MG	DA	3148	1/1	0.99	0.12	88,88,88,88	0
56	MG	CA	3122	1/1	0.99	0.18	77,77,77,77	1
56	MG	CA	3032	1/1	0.99	0.17	79,79,79,79	0
56	MG	DA	3027	1/1	0.99	0.19	92,92,92,92	0
56	MG	CA	3086	1/1	0.99	0.14	93,93,93,93	1
56	MG	CA	3125	1/1	0.99	0.05	82,82,82,82	1
56	MG	CA	3126	1/1	0.99	0.26	67,67,67,67	0
56	MG	DA	3088	1/1	0.99	0.38	88,88,88,88	1
56	MG	CA	3033	1/1	0.99	0.18	65,65,65,65	0
56	MG	DA	3157	1/1	0.99	0.48	83,83,83,83	0
56	MG	CB	201	1/1	0.99	0.16	113,113,113,113	1
56	MG	DA	3033	1/1	0.99	0.12	104,104,104,104	0
56	MG	CA	3034	1/1	0.99	0.13	68,68,68,68	0
56	MG	CA	3089	1/1	0.99	0.14	92,92,92,92	1
56	MG	CA	3048	1/1	0.99	0.14	80,80,80,80	1
56	MG	DA	3095	1/1	0.99	0.08	76,76,76,76	0
56	MG	CA	3066	1/1	0.99	0.15	80,80,80,80	1
56	MG	CA	3092	1/1	0.99	0.10	85,85,85,85	0
56	MG	CA	3067	1/1	0.99	0.12	68,68,68,68	1
56	MG	DA	3099	1/1	0.99	0.19	114,114,114,114	1
56	MG	CA	3009	1/1	0.99	0.12	69,69,69,69	0
56	MG	DA	3041	1/1	0.99	0.14	100,100,100,100	0
56	MG	CA	3095	1/1	0.99	0.08	86,86,86,86	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1618	1/1	0.99	0.11	106,106,106,106	1
56	MG	DA	3104	1/1	0.99	0.21	101,101,101,101	0
56	MG	CA	3097	1/1	0.99	0.21	67,67,67,67	1
56	MG	DA	3045	1/1	0.99	0.18	102,102,102,102	0
56	MG	AA	1626	1/1	0.99	0.25	107,107,107,107	0
56	MG	DA	3120	1/1	1.00	0.12	98,98,98,98	0
56	MG	CA	3103	1/1	1.00	0.20	80,80,80,80	1
56	MG	CA	3063	1/1	1.00	0.09	94,94,94,94	1
56	MG	CA	3115	1/1	1.00	0.13	70,70,70,70	1

6.5 Other polymers (i)

There are no such residues in this entry.