wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 03:15 AM EDT

PDB ID	:	4V7S
Title	:	Crystal structure of the E. coli ribosome bound to telithromycin.
Authors	:	Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on	:	2010-08-05
Resolution	:	3.25 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:

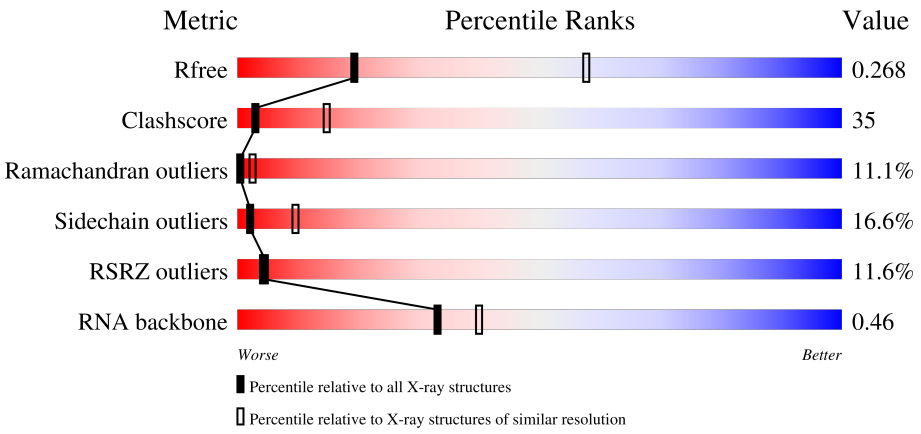
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)
RNA backbone	3102	1072 (3.62-2.90)

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	1533	.% 31% 49% 19% .
2	AB	218	32% 26% 51% 20% .
2	CB	218	39% 35% 50% 14%
3	AC	206	8% 44% 42% 12% .

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Mol	Chain	Length	Quality of chain
3	CC	206	15% 38% 47% 14%
4	AD	205	4% 35% 47% 17%
4	CD	205	39% 41% 17%
5	AE	150	% 31% 47% 19%
5	CE	150	% 37% 45% 17%
6	AF	100	4% 31% 51% 14%
6	CF	100	4% 42% 37% 20%
7	AG	151	11% 41% 46% 11%
8	AH	129	4% 39% 47% 14%
8	CH	129	10% 38% 50% 12%
9	AI	127	20% 36% 48% 14%
9	CI	127	31% 29% 57% 13%
10	AJ	98	14% 24% 58% 16%
10	CJ	98	51% 29% 54% 15%
11	AK	117	17% 44% 42% 12%
11	CK	117	12% 51% 34% 15%
12	AL	123	% 41% 43% 14%
12	CL	123	5% 33% 54% 13%
13	AM	114	10% 39% 51% 10%
14	AN	100	6% 33% 54% 9%
14	CN	100	36% 35% 50% 9% 5%
15	AO	88	% 52% 39% 9%
15	CO	88	2% 45% 47% 7%
16	AP	82	15% 38% 51% 11%
17	AQ	80	9% 26% 50% 20%

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Mol	Chain	Length	Quality of chain
17	CQ	80	14% 34% 46% 19%
18	AR	55	9% 42% 55%
18	CR	55	40% 53% 7%
19	AS	79	34% 34% 54% 8%
19	CS	79	63% 38% 48% 13%
20	AT	85	% 29% 51% 16%
20	CT	85	22% 45% 36% 18%
21	AU	51	57% 24% 51% 22%
21	CU	51	12% 25% 39% 27% 8%
22	BA	2903	% 36% 46% 16%
22	DA	2903	4% 20% 51% 25%
23	BB	118	43% 42% 15%
24	BC	271	3% 35% 44% 19%
24	DC	271	9% 30% 54% 15%
25	BD	209	32% 47% 17%
25	DD	209	19% 30% 52% 17%
26	BE	201	33% 47% 17%
26	DE	201	42% 27% 56% 16%
27	BF	177	11% 37% 49% 13%
28	BG	176	2% 33% 46% 19%
28	DG	176	40% 34% 47% 18%
29	BH	149	46% 36% 43% 16% 5%
29	DH	149	45% 35% 46% 16%
30	BI	141	55% 30% 53% 16%
30	DI	141	75% 40% 50% 9%

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Mol	Chain	Length	Quality of chain
31	BJ	142	32% 51% 14% •
31	DJ	142	23% 35% 48% 15% •
32	BK	122	20% 52% 28%
32	DK	122	22% 26% 47% 27%
33	BL	143	33% 45% 20% •
33	DL	143	26% 34% 45% 17% •
34	BM	136	40% 42% 16% •
34	DM	136	20% 35% 53% 12%
35	BN	120	34% 48% 16% •
35	DN	120	27% 32% 52% 16% •
36	BO	116	33% 52% 16%
36	DO	116	38% 35% 55% 9% •
37	BP	114	% 31% 40% 24% 5%
37	DP	114	16% 20% 61% 18% •
38	BQ	117	% 41% 40% 18% •
38	DQ	117	30% 31% 51% 18%
39	BR	103	% 33% 48% 18% •
39	DR	103	52% 29% 54% 17%
40	BS	110	% 42% 40% 17% •
40	DS	110	50% 43% 44% 13% •
41	BT	93	4% 27% 42% 27% •
41	DT	93	56% 24% 59% 14% •
42	BU	102	3% 37% 40% 20% •
42	DU	102	63% 29% 51% 17% •
43	BV	94	43% 41% 16%

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Mol	Chain	Length	Quality of chain
43	DV	94	33% 39% 49% 12%
44	BW	79	5% 14% 39% 38% 9%
44	DW	79	52% 32% 33% 28% 8%
45	BX	77	31% 58% 8%
45	DX	77	21% 23% 64% 10%
46	BY	63	3% 41% 33% 21% 5%
46	DY	63	27% 33% 56% 11%
47	BZ	58	43% 40% 14%
47	DZ	58	14% 36% 48% 14%
48	B0	56	41% 43% 16%
48	D0	56	27% 30% 48% 21%
49	B1	50	4% 36% 52% 10%
49	D1	50	42% 36% 52% 12%
50	B2	46	30% 54% 15%
50	D2	46	24% 46% 48% 7%
51	B3	64	45% 41% 11%
51	D3	64	47% 30% 52% 16%
52	B4	38	3% 42% 42% 13%
52	D4	38	68% 42% 39% 18%
53	CA	1530	2% 24% 51% 24%
54	CG	150	43% 29% 54% 16%
55	CM	113	50% 30% 58% 11%
56	CP	80	15% 29% 56% 14%
57	DB	117	22% 56% 21%
58	DF	178	55% 26% 49% 22%

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
59	MG	AA	1619	-	-	-	X
59	MG	DA	3002	-	-	-	X
59	MG	DA	3003	-	-	-	X
59	MG	DA	3005	-	-	-	X
59	MG	DA	3007	-	-	-	X
59	MG	DA	3010	-	-	-	X
59	MG	DA	3015	-	-	-	X
59	MG	DA	3016	-	-	-	X
59	MG	DA	3020	-	-	-	X
59	MG	DA	3026	-	-	-	X
59	MG	DA	3028	-	-	-	X
59	MG	DA	3036	-	-	-	X
59	MG	DA	3049	-	-	-	X
59	MG	DA	3060	-	-	-	X
59	MG	DA	3062	-	-	-	X
59	MG	DA	3063	-	-	-	X
59	MG	DA	3064	-	-	-	X
59	MG	DA	3074	-	-	-	X
59	MG	DA	3079	-	-	-	X
59	MG	DA	3106	-	-	-	X
59	MG	DA	3109	-	-	-	X
59	MG	DA	3127	-	-	-	X
59	MG	DA	3129	-	-	-	X
59	MG	DA	3130	-	-	-	X
59	MG	DA	3132	-	-	-	X
59	MG	DJ	201	-	-	-	X
60	TEL	BA	3135	X	-	-	-

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 284525 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1533	32895	14671	6036	10655	1533	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AN	96	774	483	160	128	3	0	0	0
14	CN	95	769	480	159	127	3	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	AU	51	426	265	86	74	1	0	0	0
21	CU	51	426	265	86	74	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	BA	2854	61274	27334	11279	19807	2854	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	DA	2841	60995	27210	11229	19715	2841	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	BB	118	2529	1126	464	821	118	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	BN	120	961	593	196	167	5	0	0	0
35	DN	120	961	593	196	167	5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called 16S rRNA.

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

- Molecule 54 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	CG	150	1175	730	226	215	4	0	0	0

- Molecule 55 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	CM	113	877	541	177	156	3	0	0	0

- Molecule 56 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	CP	80	639	400	126	112	1	0	0	0

- Molecule 57 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
57	DB	117	2507	1116	459	815	117	0	0	0

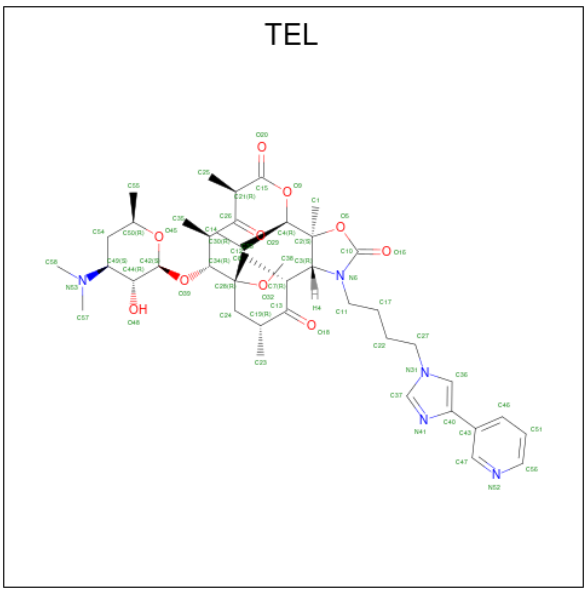
- Molecule 58 is a protein called 50S ribosomal protein L5.

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

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
59	AA	43	43	43	0	0
59	BA	134	134	134	0	0
59	BB	4	4	4	0	0
59	CA	41	41	41	0	0
59	CE	1	1	1	0	0
59	DA	133	133	133	0	0
59	DB	1	1	1	0	0
59	DC	2	2	2	0	0
59	DJ	1	1	1	0	0

- Molecule 60 is TELITHROMYCIN (three-letter code: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
60	BA	1	58	43	5	10	0	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
62	AA	198	198	198	0	0
62	AL	1	1	1	0	0
62	AN	6	6	6	0	0
62	AT	2	2	2	0	0
62	AU	1	1	1	0	0
62	BA	598	598	598	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	BB	20	Total O 20 20	0	0
62	BC	10	Total O 10 10	0	0
62	BD	2	Total O 2 2	0	0
62	BE	1	Total O 1 1	0	0
62	BL	2	Total O 2 2	0	0
62	BN	3	Total O 3 3	0	0
62	BQ	1	Total O 1 1	0	0
62	BR	1	Total O 1 1	0	0
62	BT	1	Total O 1 1	0	0
62	B2	1	Total O 1 1	0	0
62	B3	3	Total O 3 3	0	0
62	B4	1	Total O 1 1	0	0
62	CA	192	Total O 192 192	0	0
62	CE	5	Total O 5 5	0	0
62	CI	1	Total O 1 1	0	0
62	CL	1	Total O 1 1	0	0
62	CN	3	Total O 3 3	0	0
62	CT	3	Total O 3 3	0	0
62	CU	2	Total O 2 2	0	0
62	DA	595	Total O 595 595	0	0
62	DB	4	Total O 4 4	0	0

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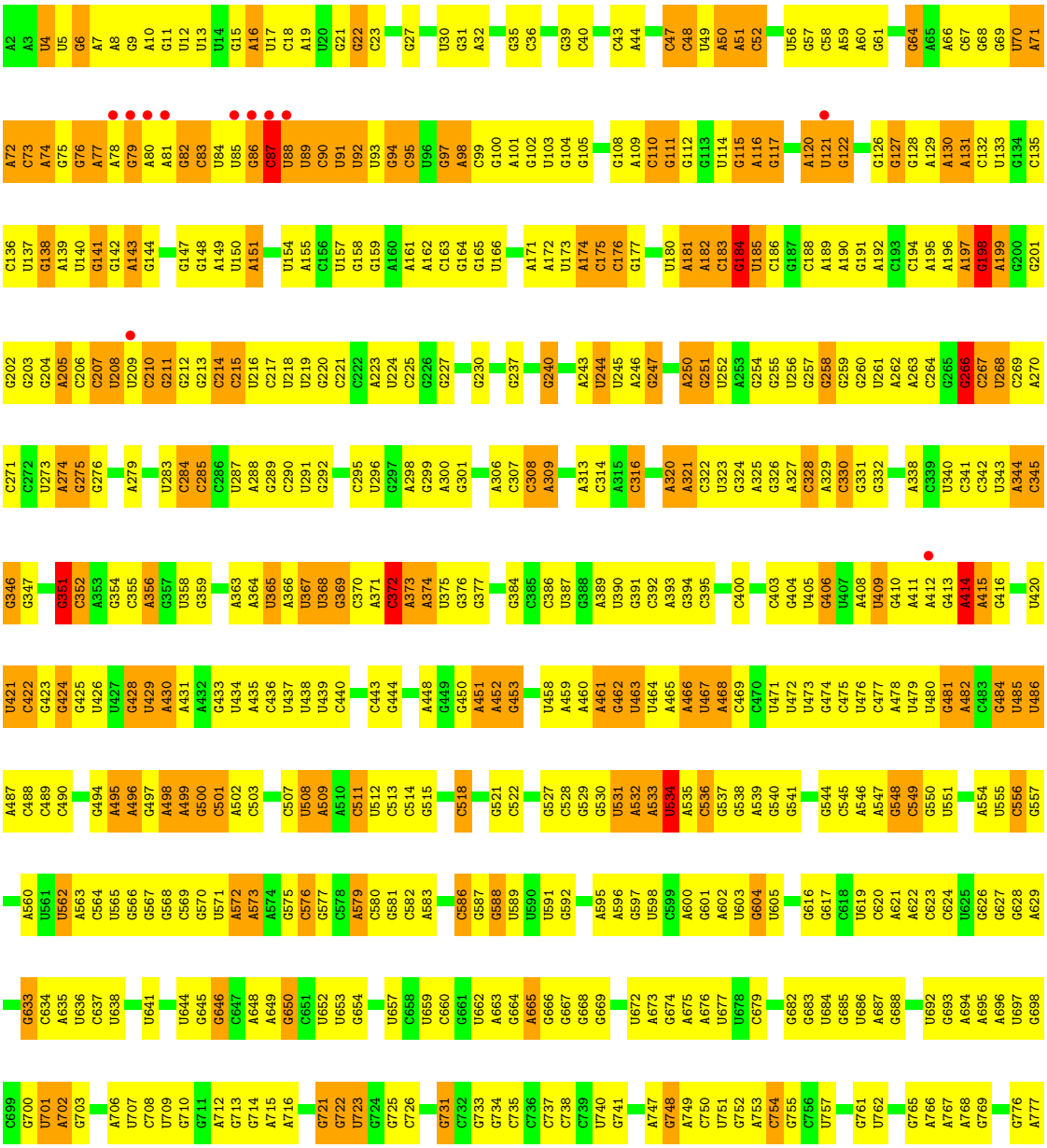
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	DC	13	Total O 13 13	0	0
62	DD	3	Total O 3 3	0	0
62	DE	3	Total O 3 3	0	0
62	DJ	6	Total O 6 6	0	0
62	DL	6	Total O 6 6	0	0
62	DN	2	Total O 2 2	0	0
62	DT	3	Total O 3 3	0	0
62	DU	2	Total O 2 2	0	0
62	DV	1	Total O 1 1	0	0
62	D2	1	Total O 1 1	0	0
62	D3	1	Total O 1 1	0	0
62	D4	3	Total O 3 3	0	0

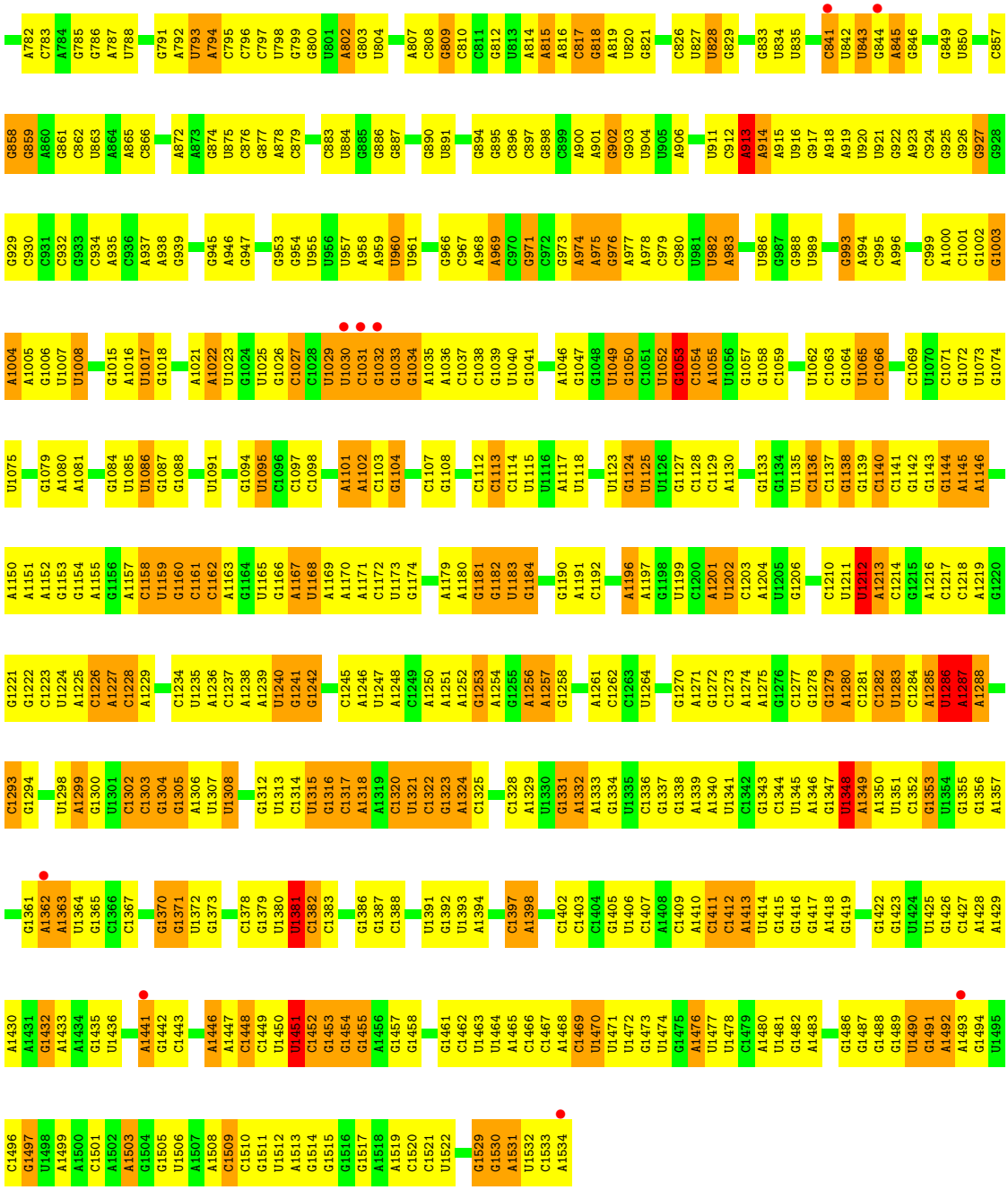
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

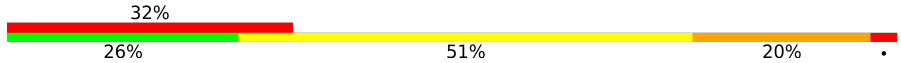
Chain AA:

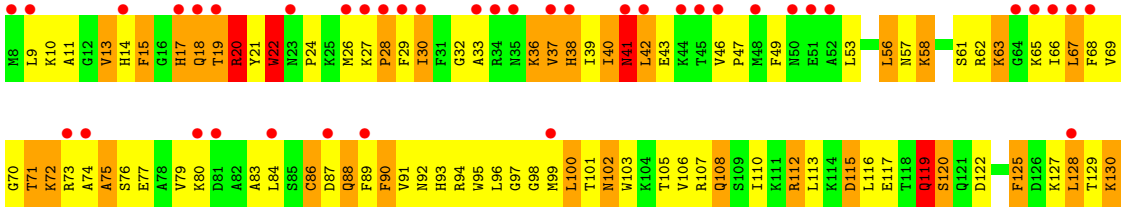


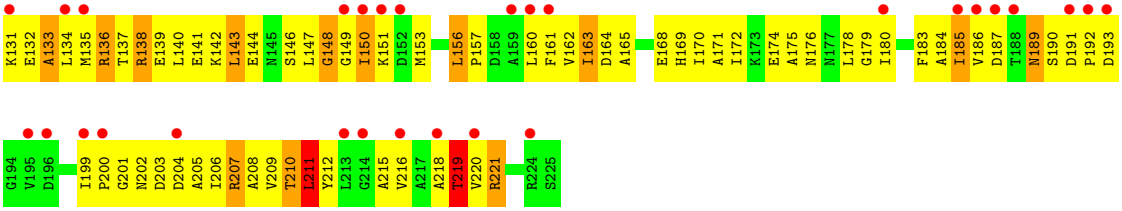


• Molecule 2: 30S ribosomal protein S2

Chain AB:

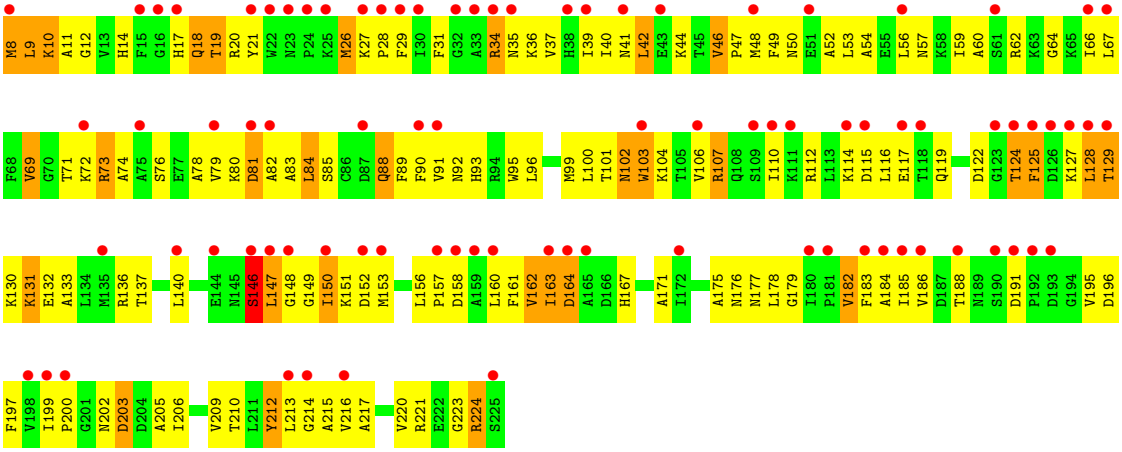






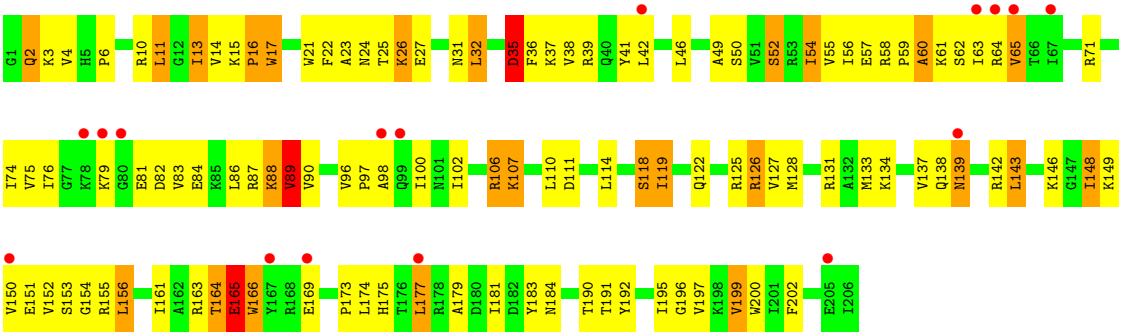
- Molecule 2: 30S ribosomal protein S2

Chain CB:



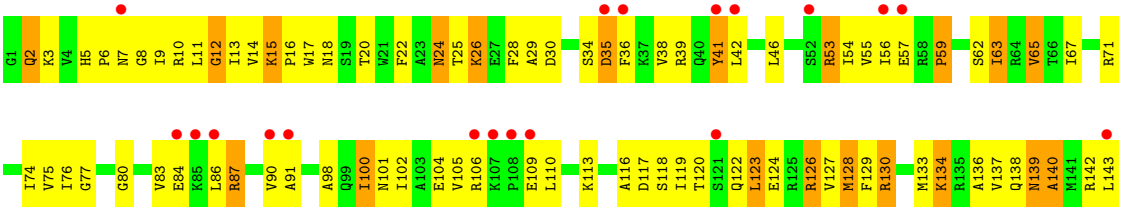
- Molecule 3: 30S ribosomal protein S3

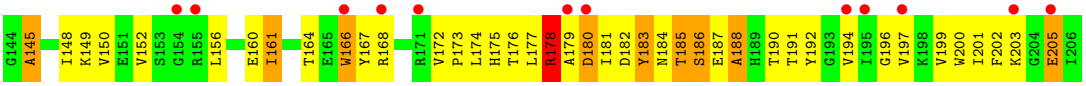
Chain AC:



- Molecule 3: 30S ribosomal protein S3

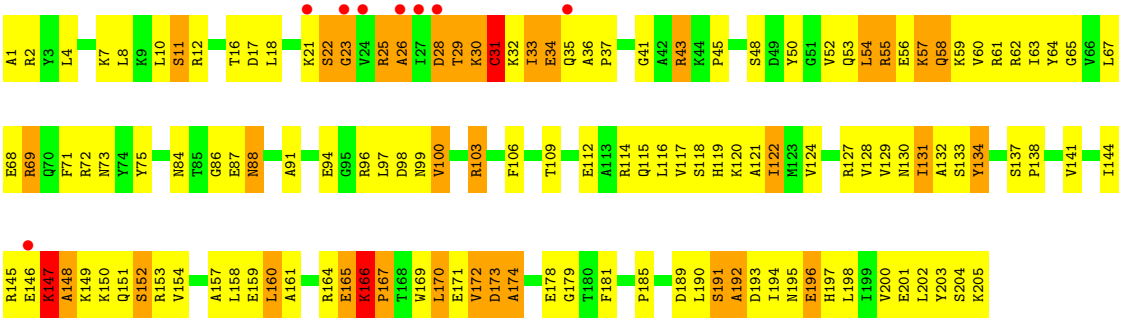
Chain CC:





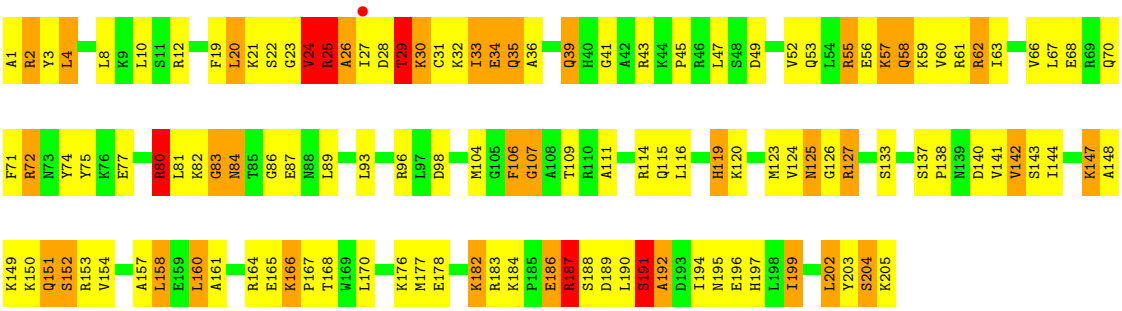
• Molecule 4: 30S ribosomal protein S4

Chain AD:



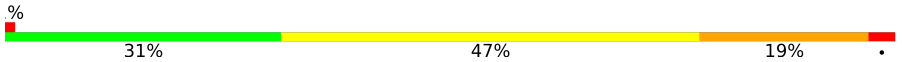
• Molecule 4: 30S ribosomal protein S4

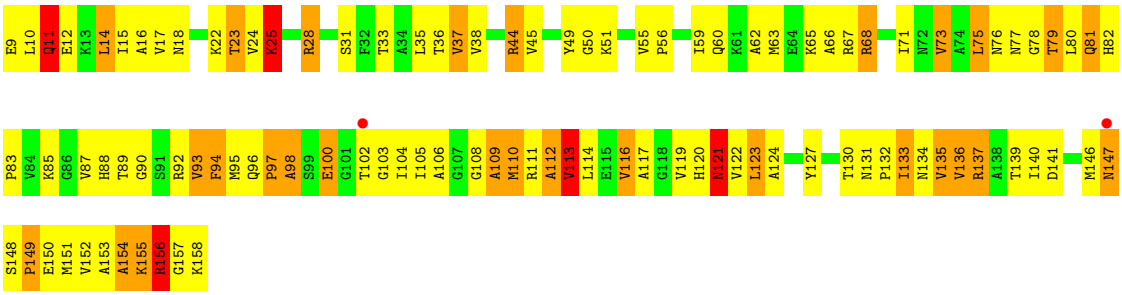
Chain CD:



• Molecule 5: 30S ribosomal protein S5

Chain AE:



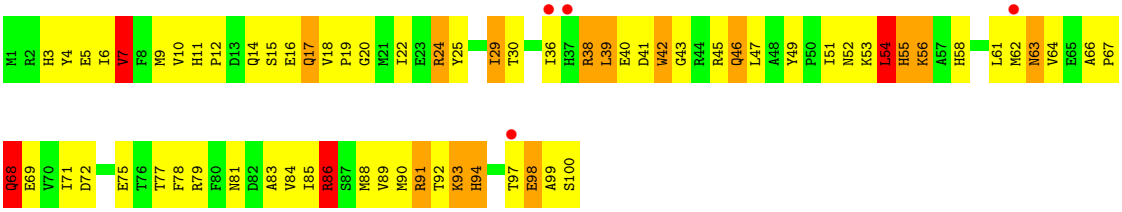


• Molecule 5: 30S ribosomal protein S5

Chain CE:

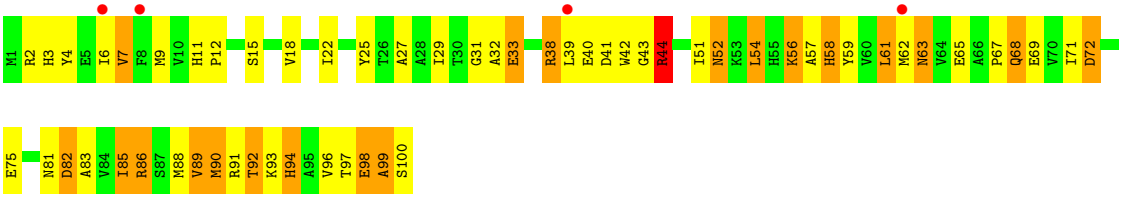
• Molecule 6: 30S ribosomal protein S6

Chain AF:



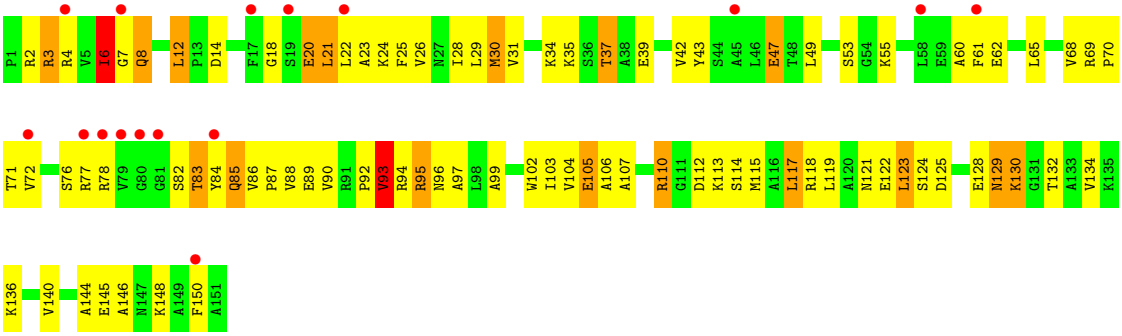
• Molecule 6: 30S ribosomal protein S6

Chain CF:



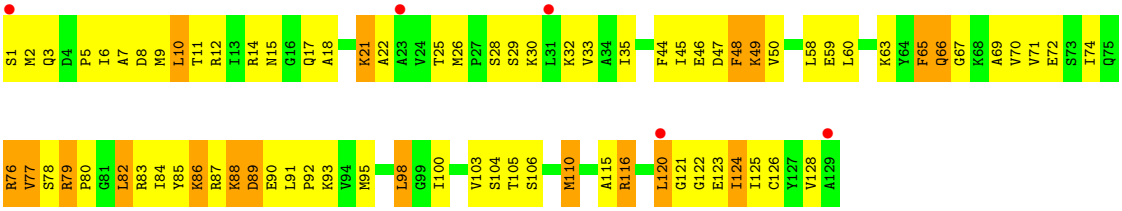
• Molecule 7: 30S ribosomal protein S7

Chain AG:



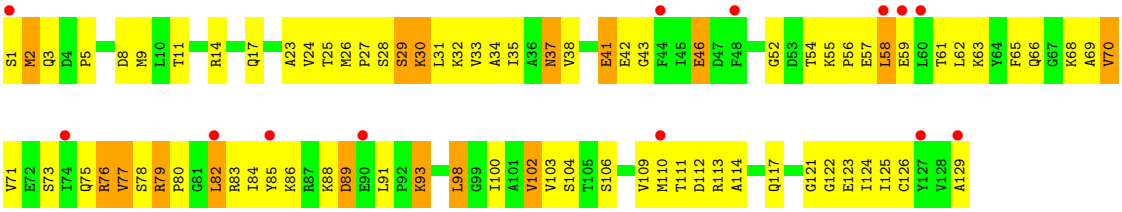
• Molecule 8: 30S ribosomal protein S8

Chain AH:



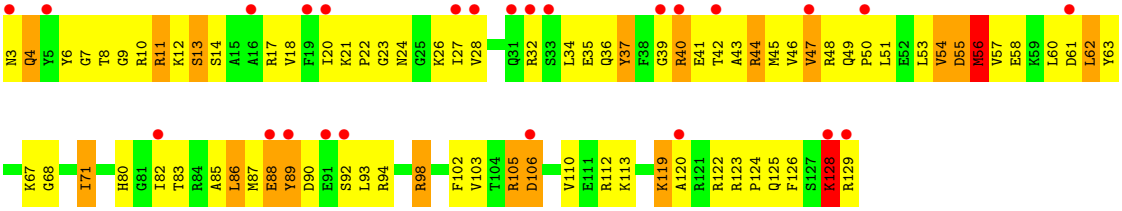
- Molecule 8: 30S ribosomal protein S8

Chain CH:



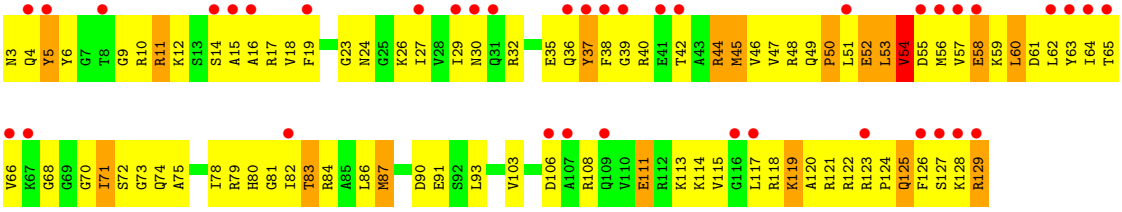
- Molecule 9: 30S ribosomal protein S9

Chain AI:



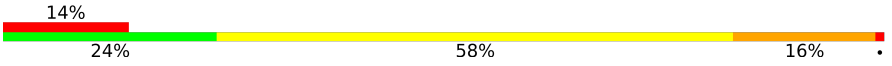
- Molecule 9: 30S ribosomal protein S9

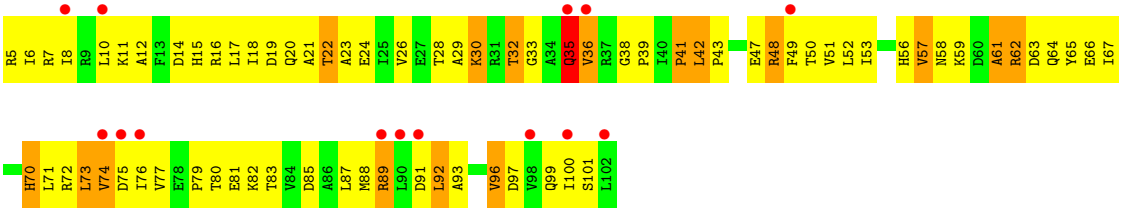
Chain CI:



- Molecule 10: 30S ribosomal protein S10

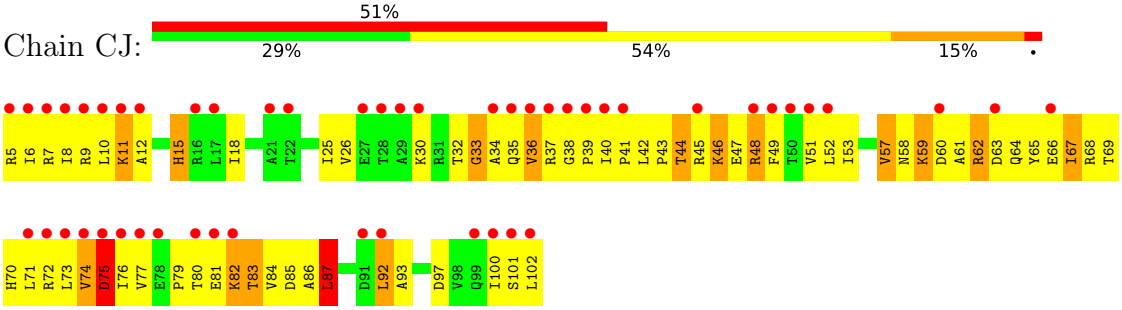
Chain AJ:





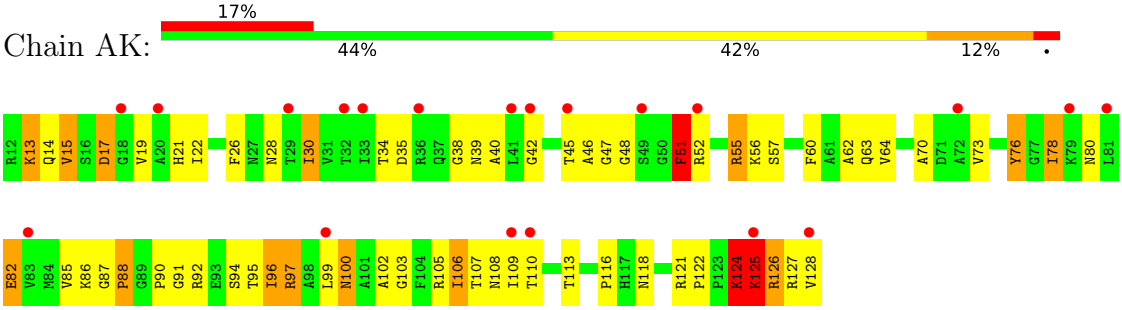
• Molecule 10: 30S ribosomal protein S10

Chain CJ:



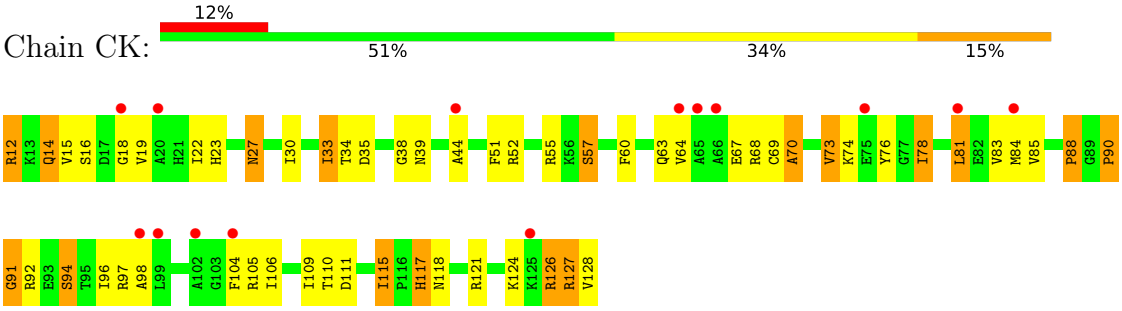
• Molecule 11: 30S ribosomal protein S11

Chain AK:



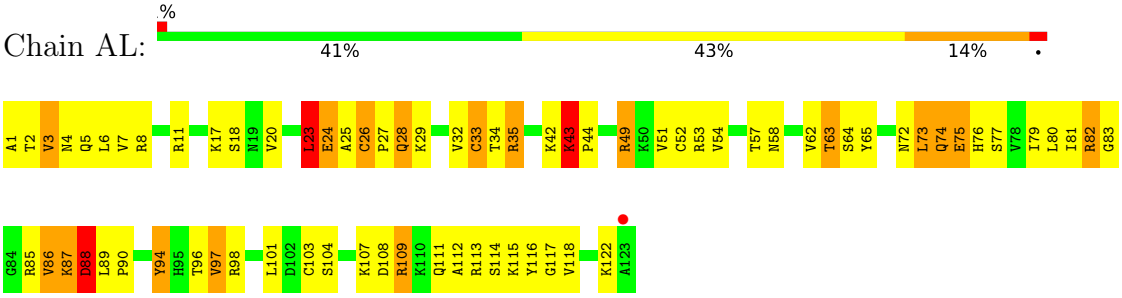
• Molecule 11: 30S ribosomal protein S11

Chain CK:



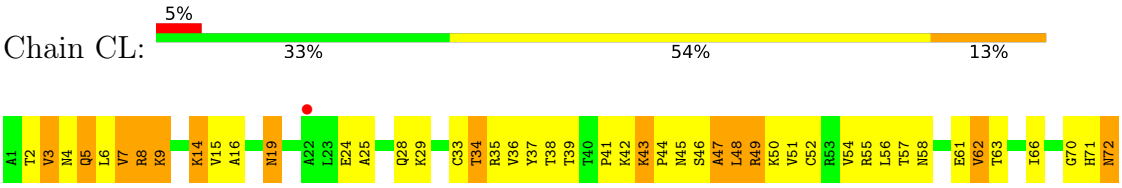
• Molecule 12: 30S ribosomal protein S12

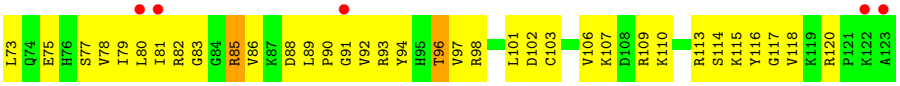
Chain AL:



• Molecule 12: 30S ribosomal protein S12

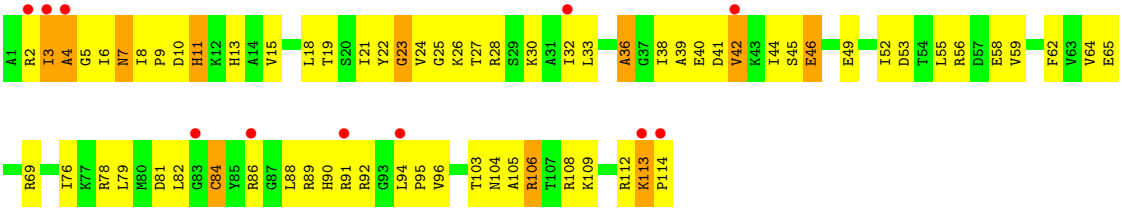
Chain CL:





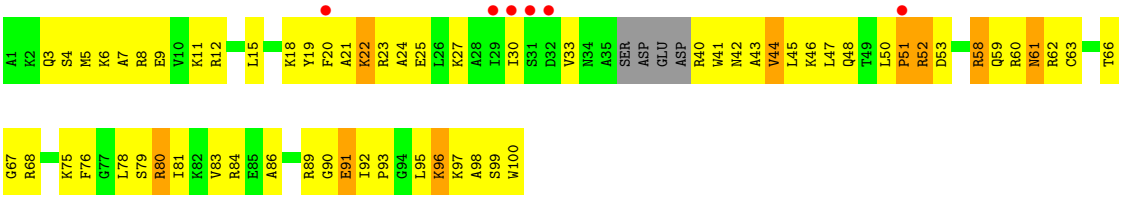
• Molecule 13: 30S ribosomal protein S13

Chain AM:



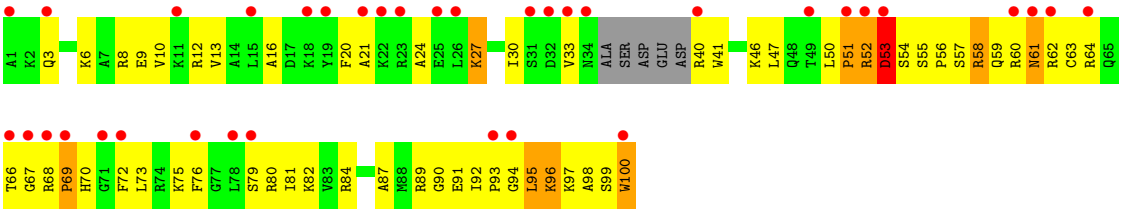
• Molecule 14: 30S ribosomal protein S14

Chain AN:



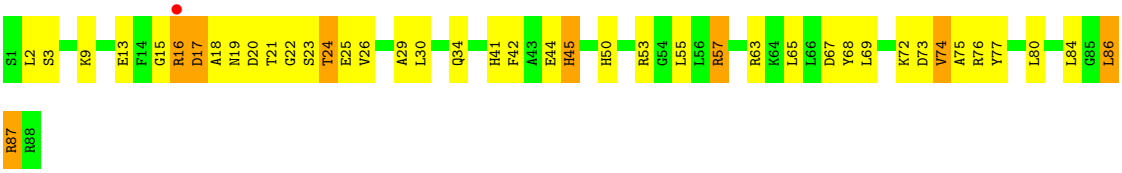
• Molecule 14: 30S ribosomal protein S14

Chain CN:



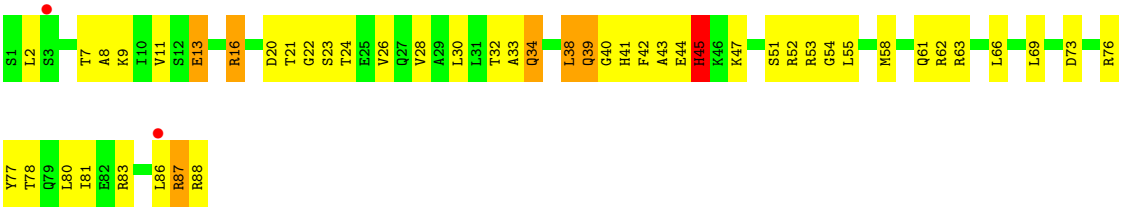
• Molecule 15: 30S ribosomal protein S15

Chain AO:



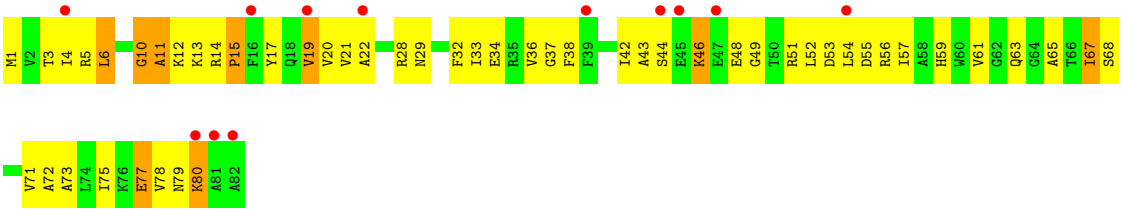
• Molecule 15: 30S ribosomal protein S15

Chain CO:



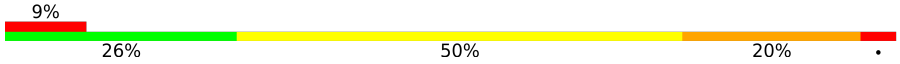
- Molecule 16: 30S ribosomal protein S16

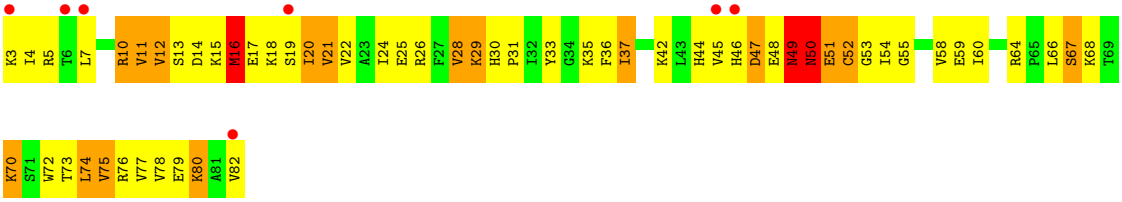
Chain AP:



- Molecule 17: 30S ribosomal protein S17

Chain AQ:





- Molecule 17: 30S ribosomal protein S17

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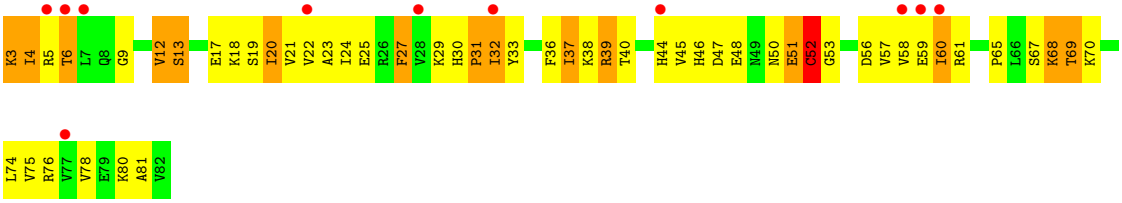
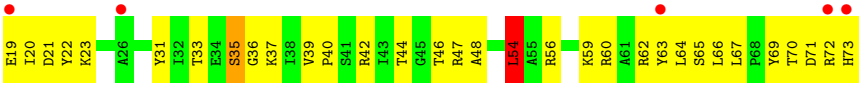


- Molecule 18: 30S ribosomal protein S18

Chain AR:



- Molecule 18: 30S ribosomal protein S18

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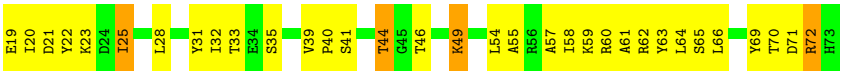

• Molecule 19: 30S ribosomal protein S19

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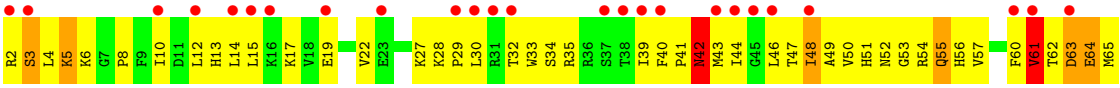

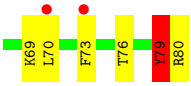

• Molecule 19: 30S ribosomal protein S19

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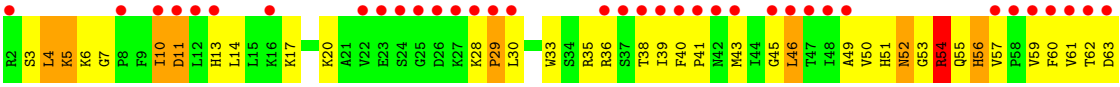

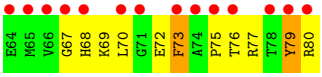

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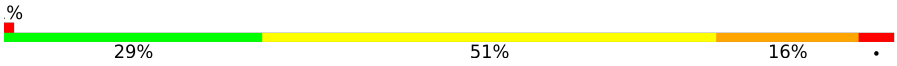
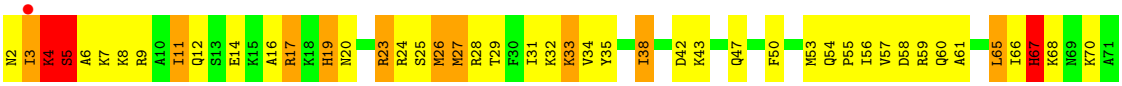
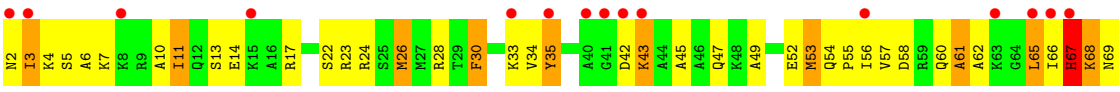
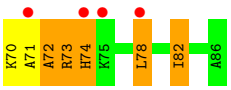




• Molecule 20: 30S ribosomal protein S20

Chain CT:





• Molecule 21: 30S ribosomal protein S21

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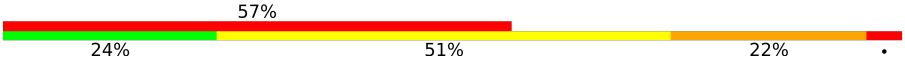

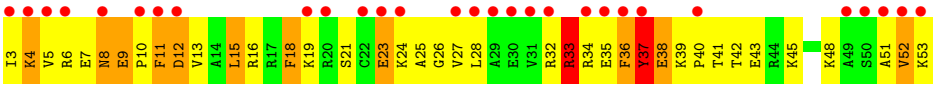

• Molecule 21: 30S ribosomal protein S21

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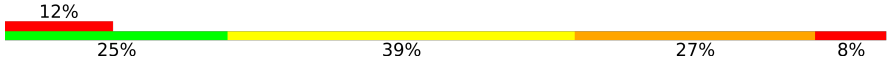
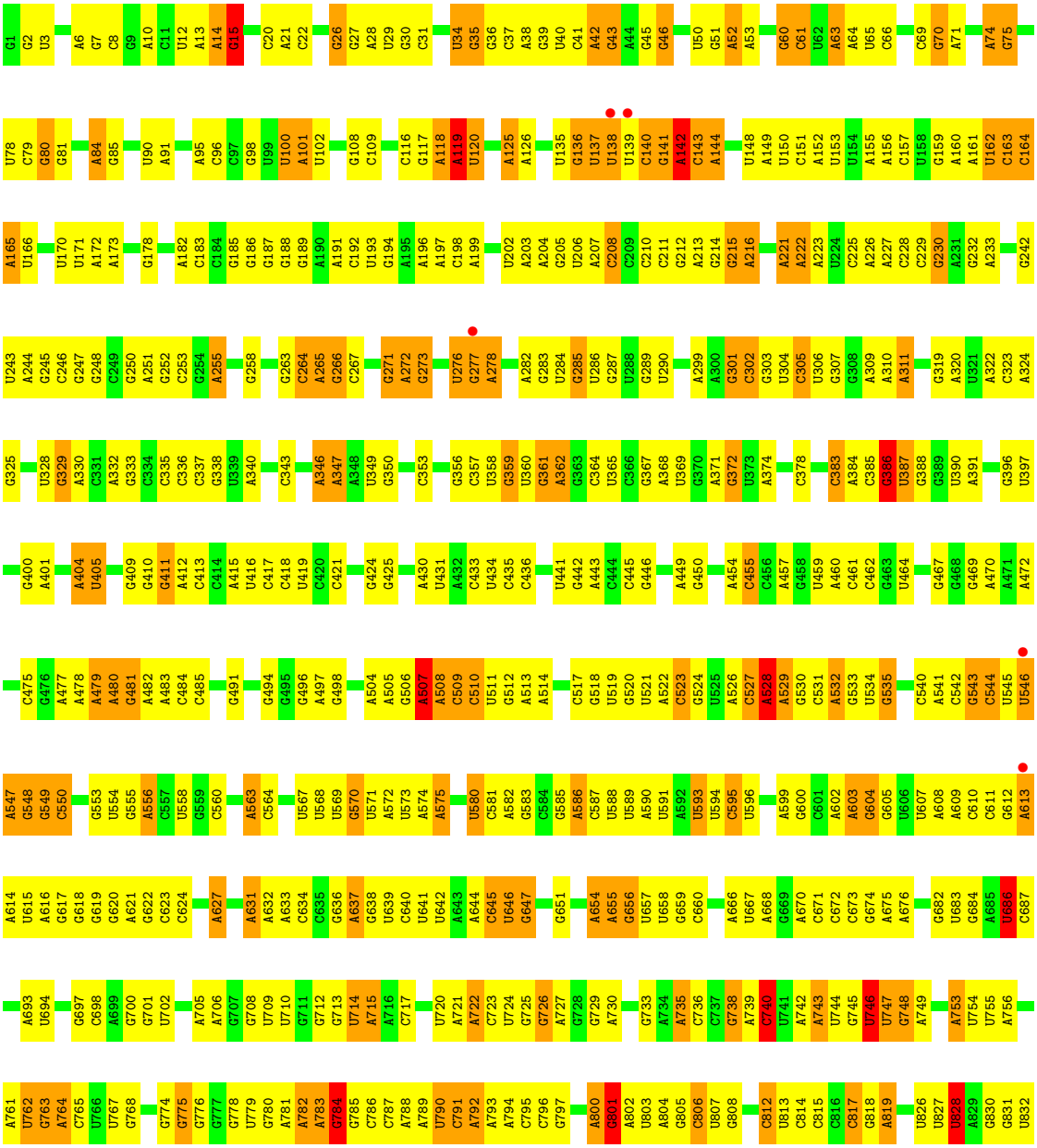
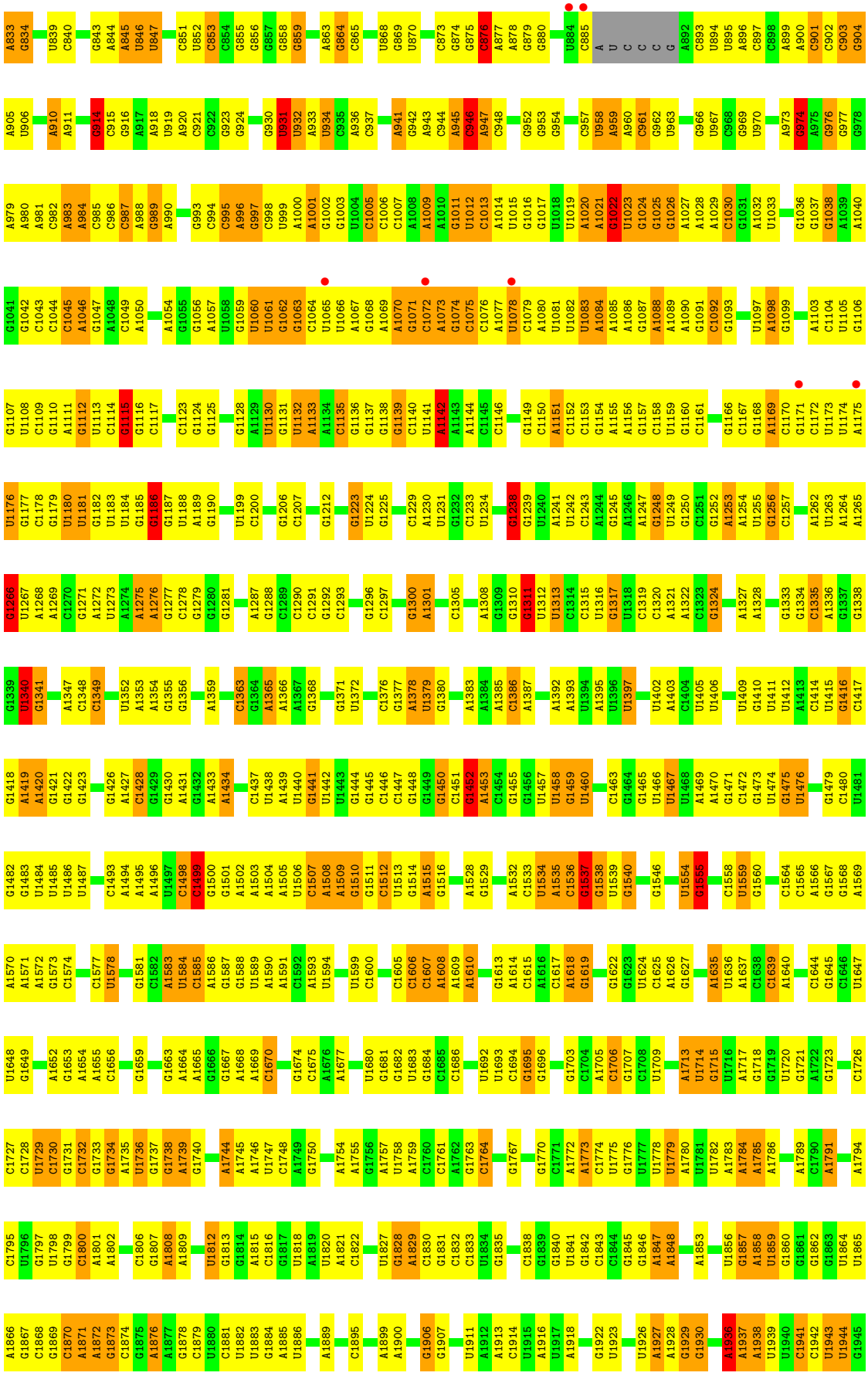


• Molecule 22: 23S rRNA

Chain BA:

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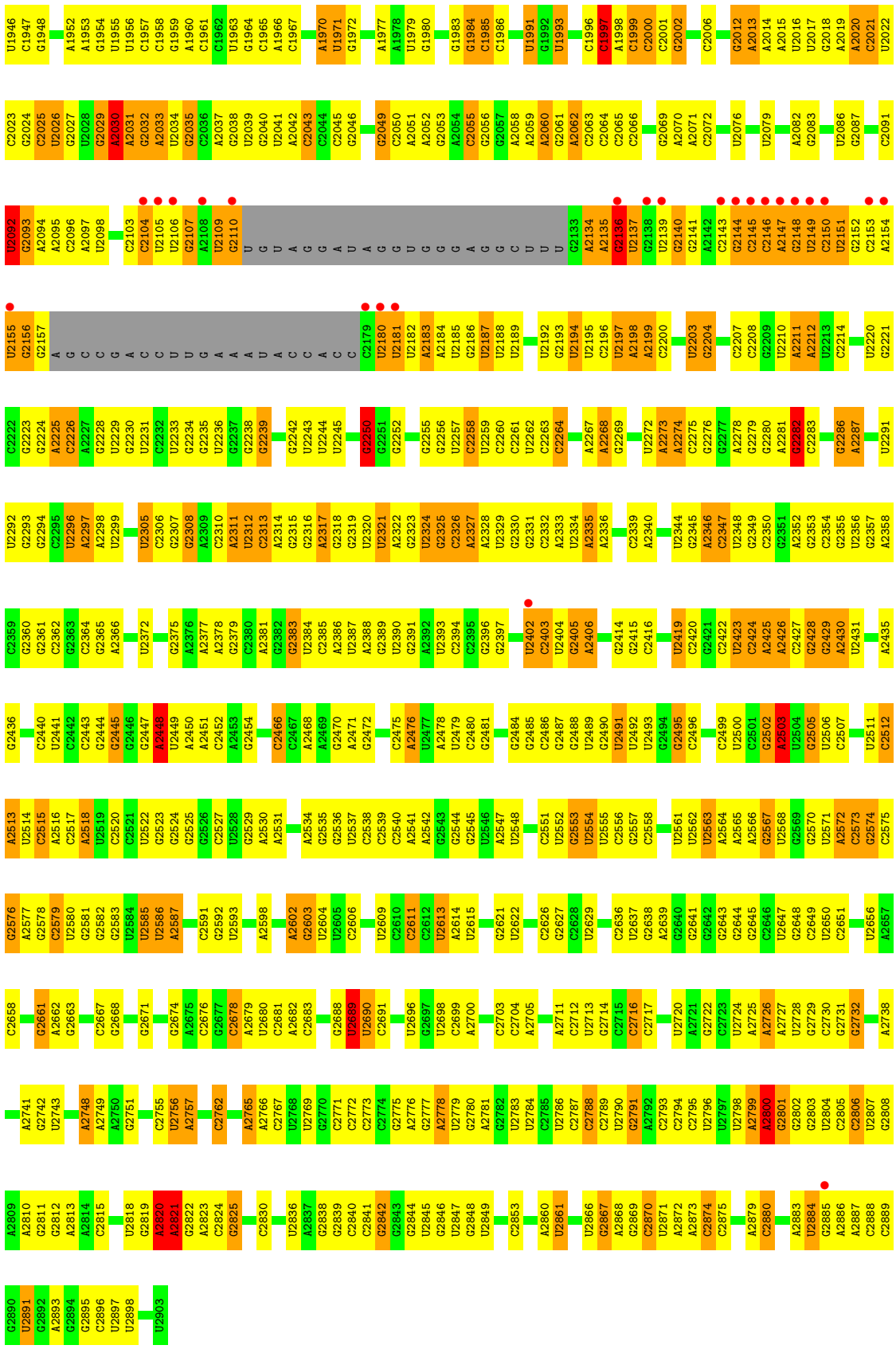
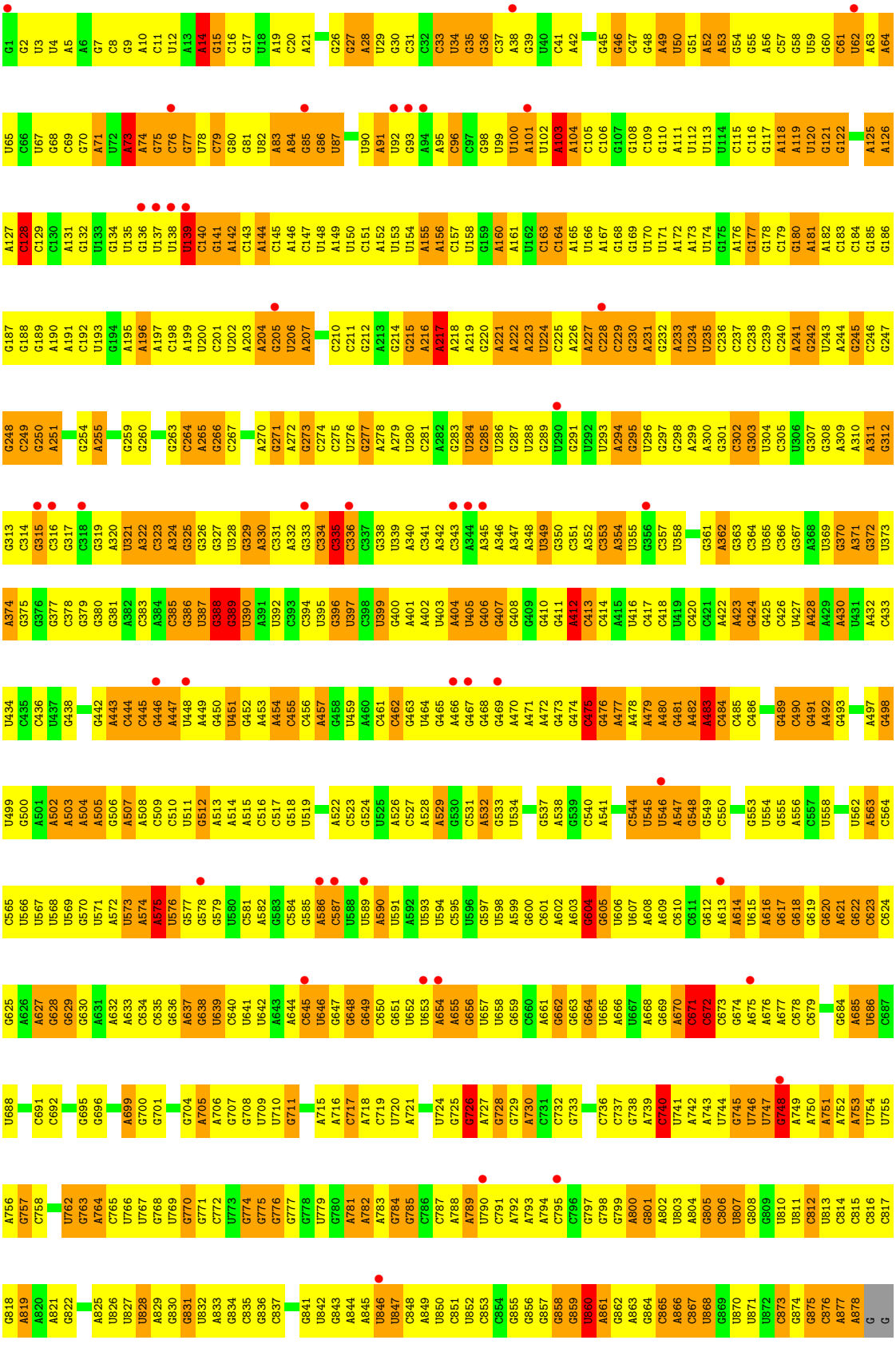
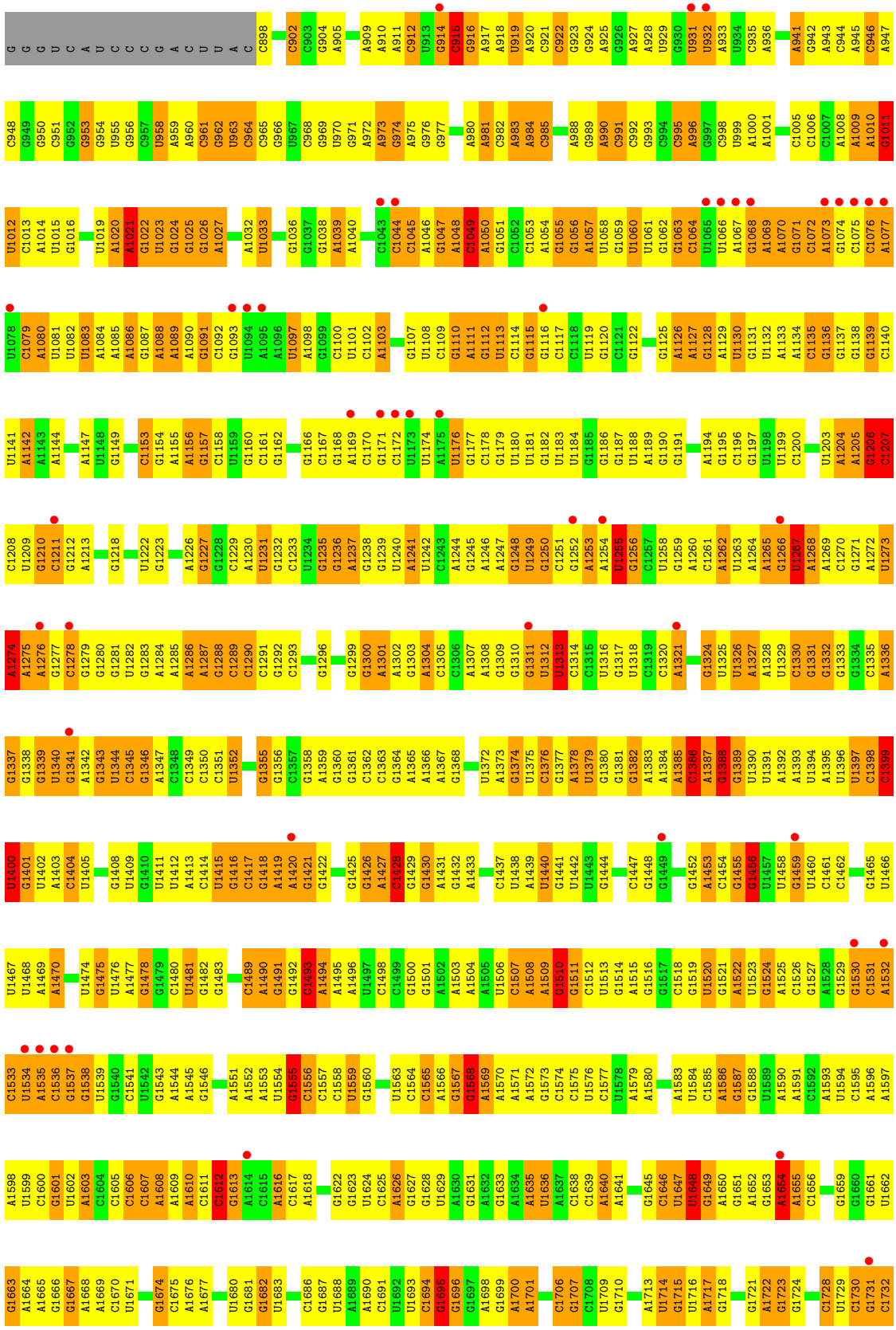


• Molecule 22: 23S rRNA

Chain DA: 4% 20% 51% 25%

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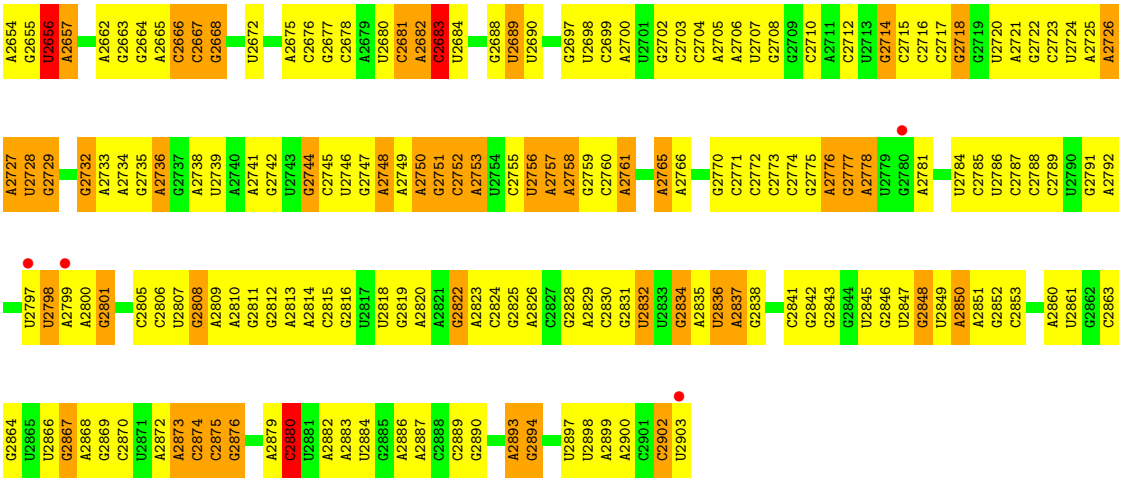
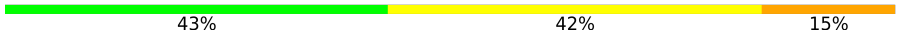
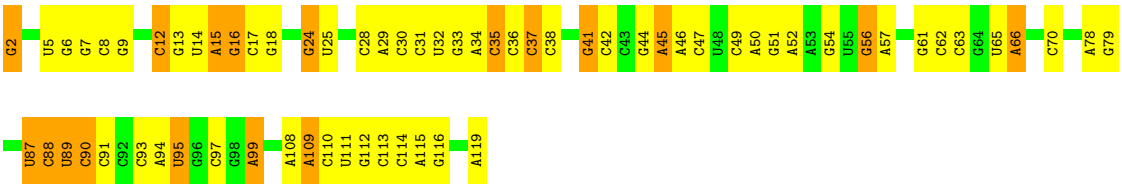


- Molecule 23: 5S rRNA

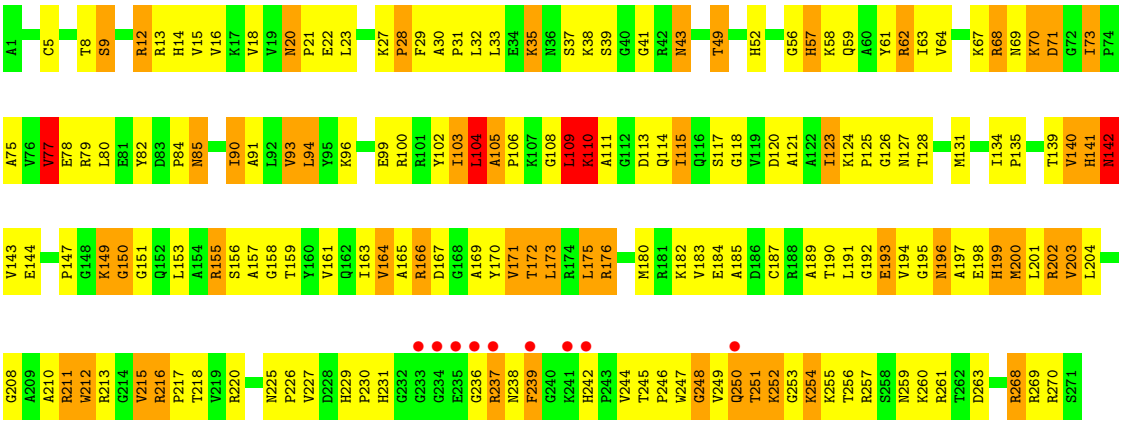
Chain BB:





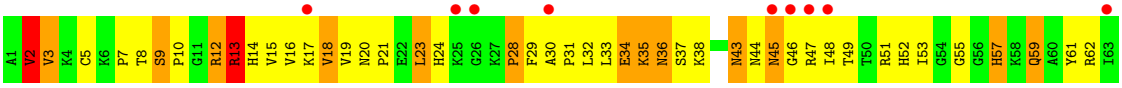
- Molecule 24: 50S ribosomal protein L2

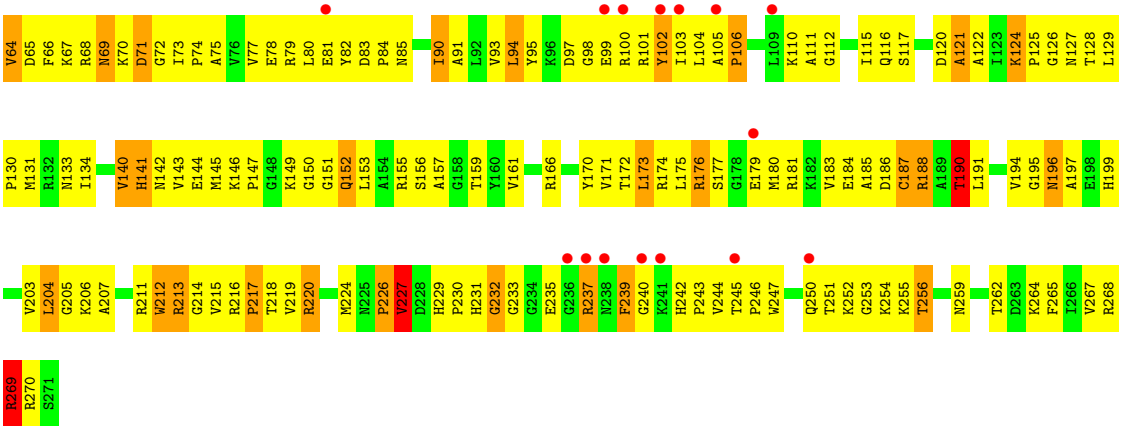
Chain BC:



- Molecule 24: 50S ribosomal protein L2

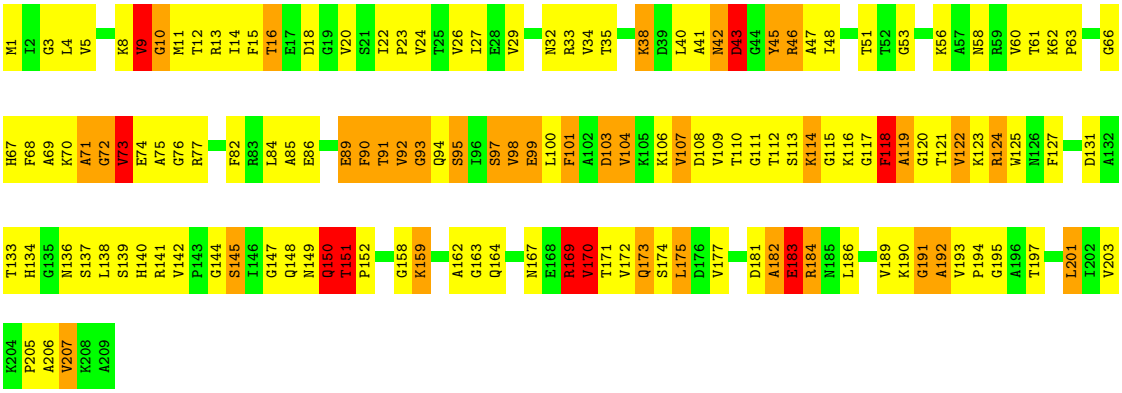
Chain DC:





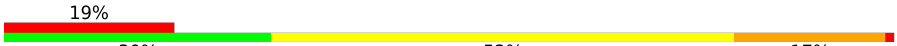
- Molecule 25: 50S ribosomal protein L3

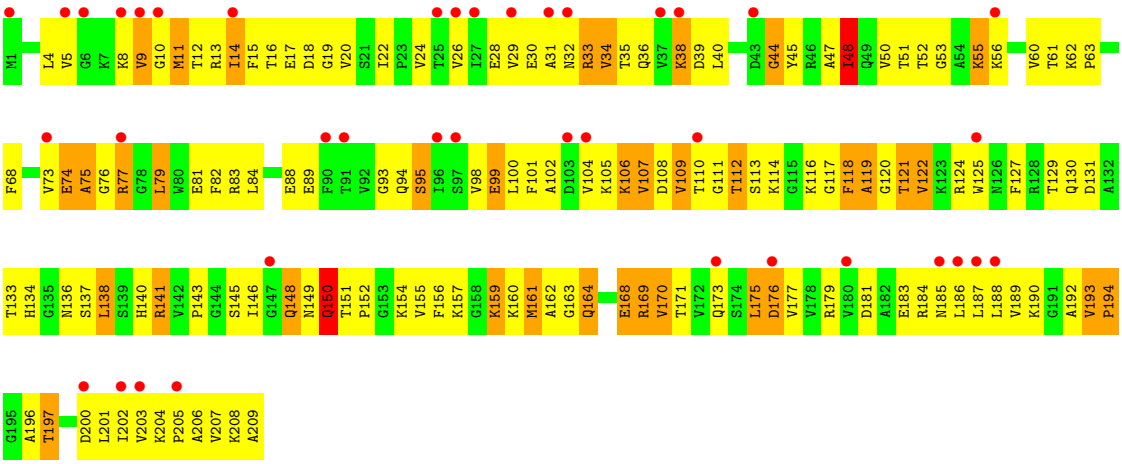
Chain BD:



- Molecule 25: 50S ribosomal protein L3

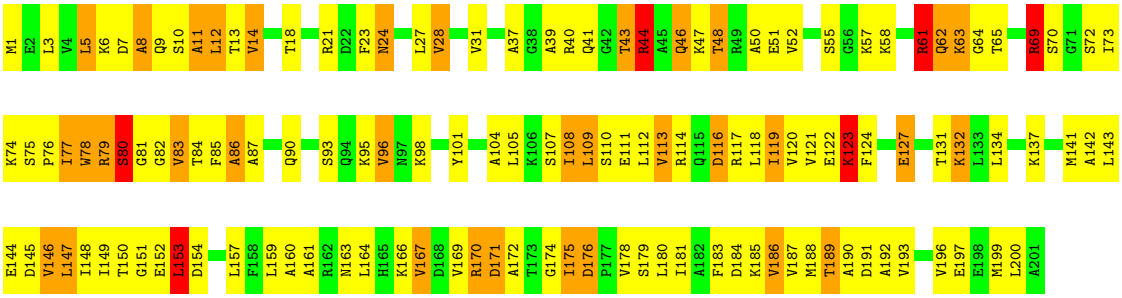
Chain DD:





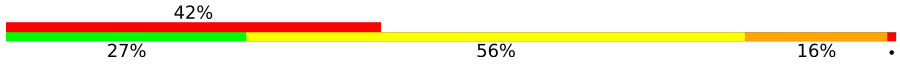
- Molecule 26: 50S ribosomal protein L4

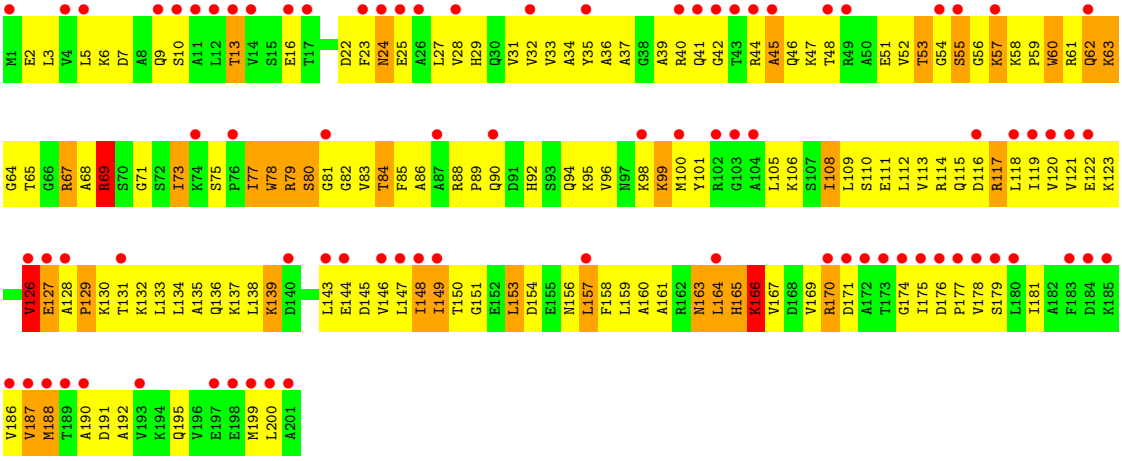
Chain BE:



- Molecule 26: 50S ribosomal protein L4

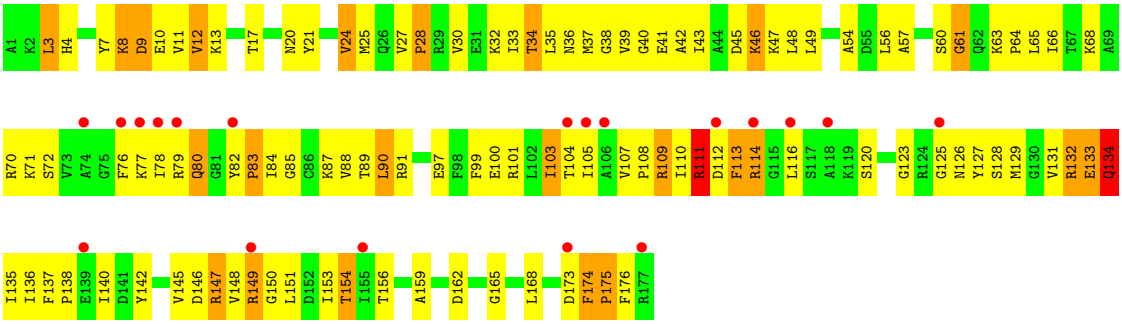
Chain DE:





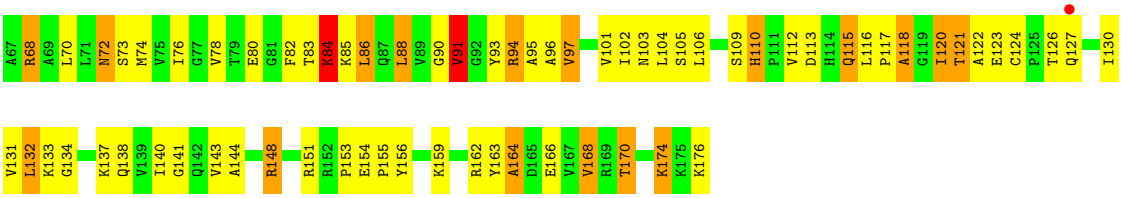
- Molecule 27: 50S ribosomal protein L5

Chain BF:



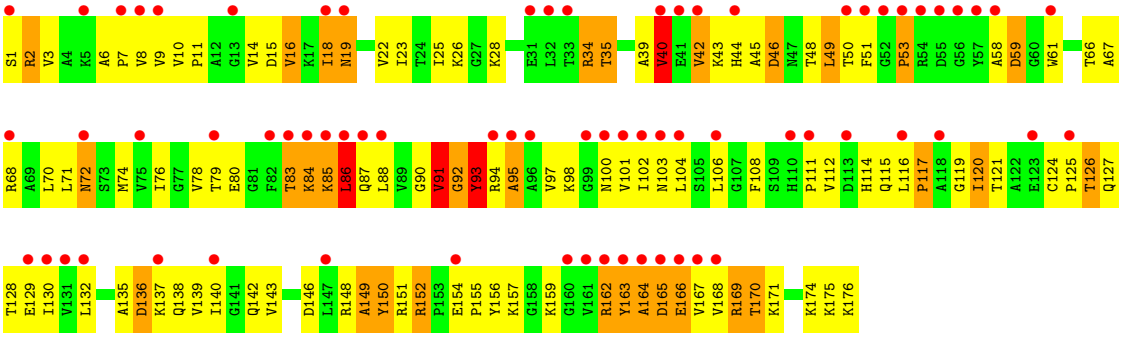
- Molecule 28: 50S ribosomal protein L6

Chain BG:



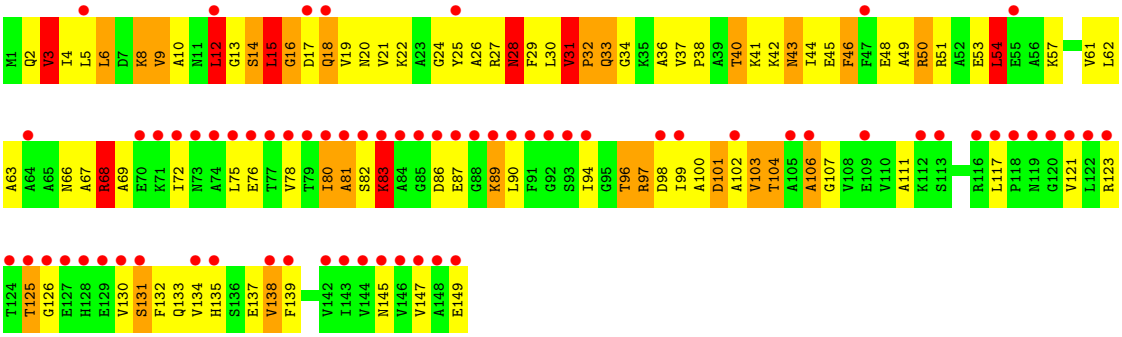
• Molecule 28: 50S ribosomal protein L6

Chain DG:



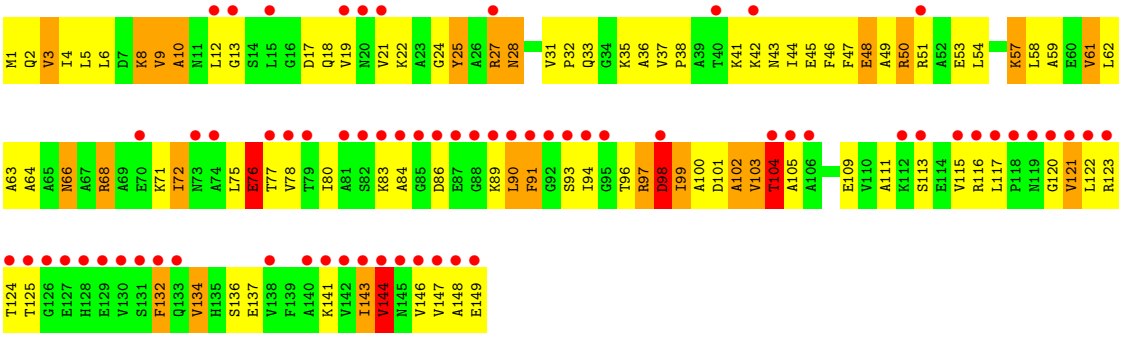
• Molecule 29: 50S ribosomal protein L9

Chain BH:



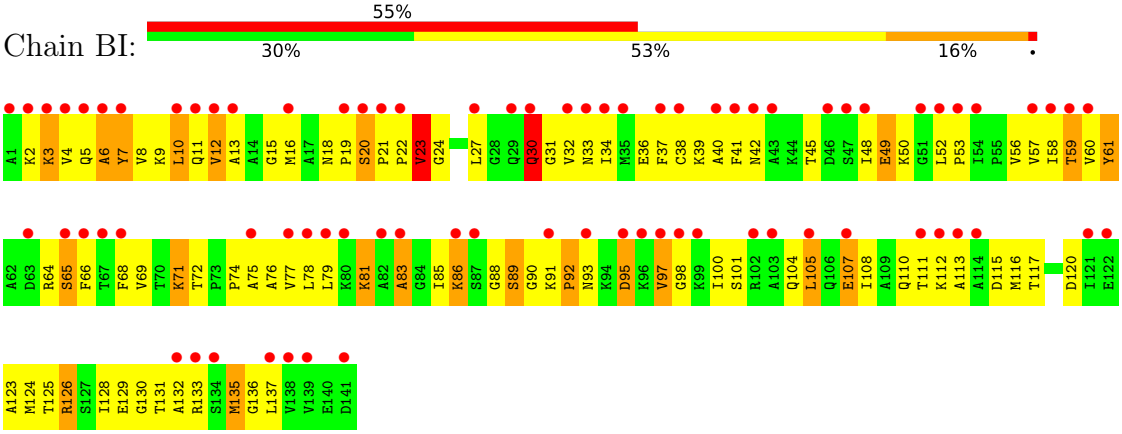
• Molecule 29: 50S ribosomal protein L9

Chain DH:



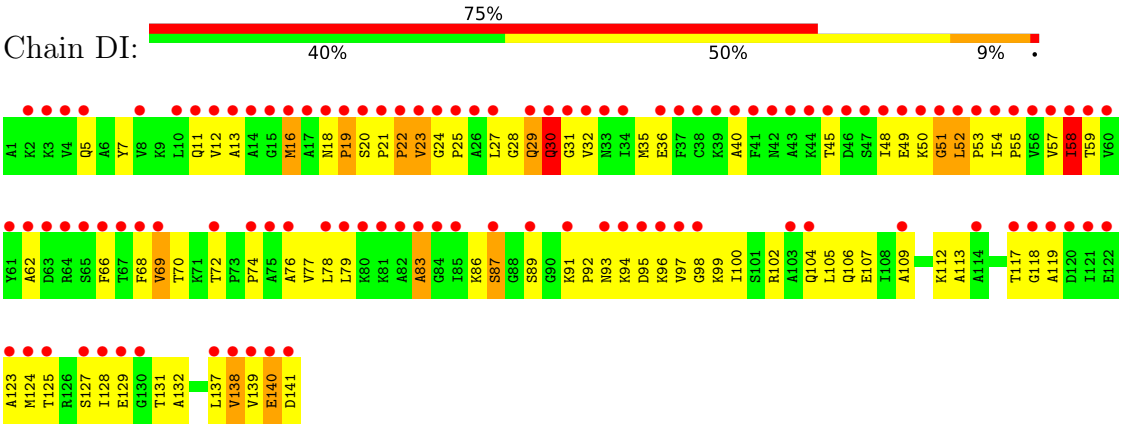
• Molecule 30: 50S ribosomal protein L11

Chain BI:



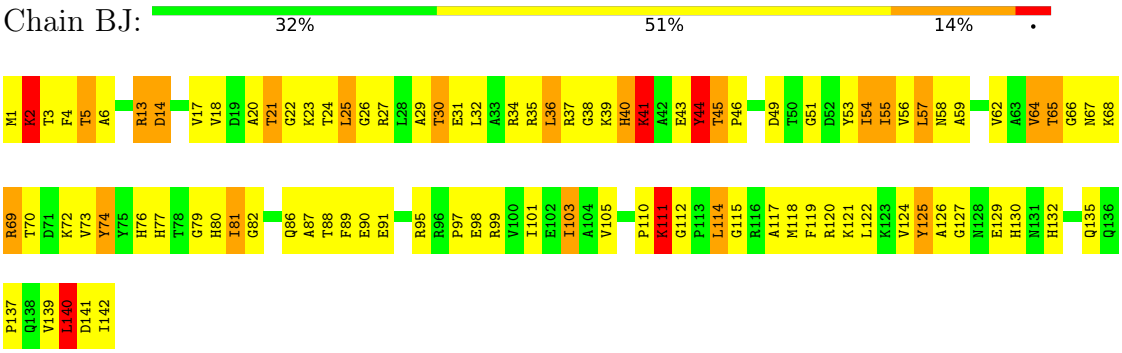
• Molecule 30: 50S ribosomal protein L11

Chain DI:



• Molecule 31: 50S ribosomal protein L13

Chain BJ:



• Molecule 31: 50S ribosomal protein L13

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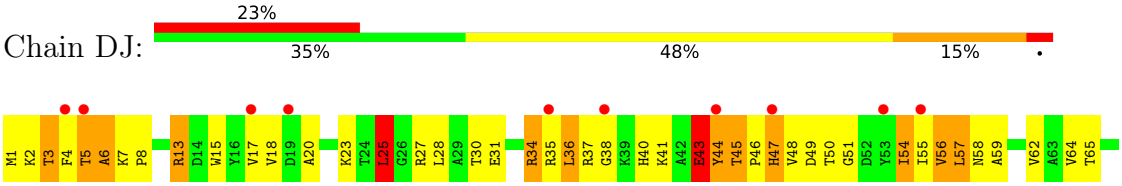
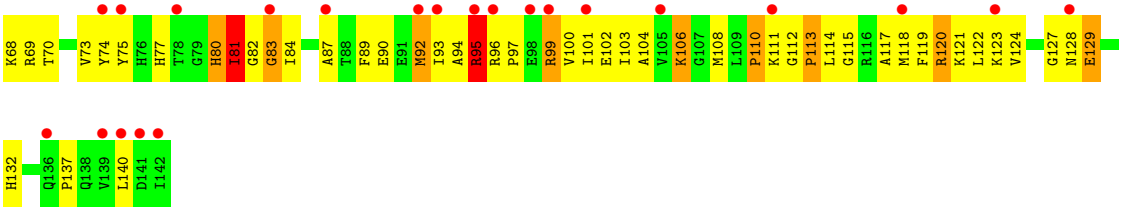
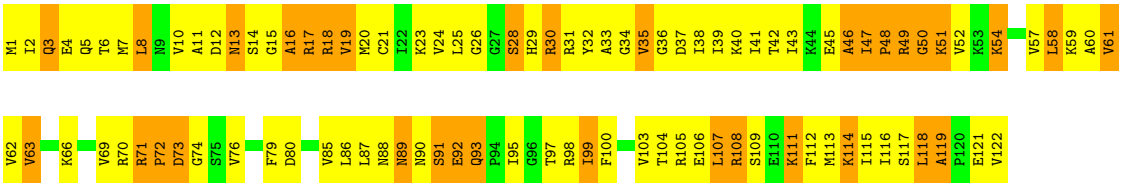




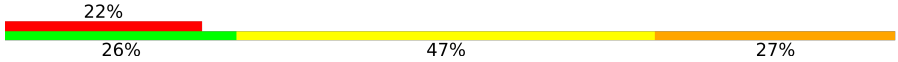
• Molecule 32: 50S ribosomal protein L14

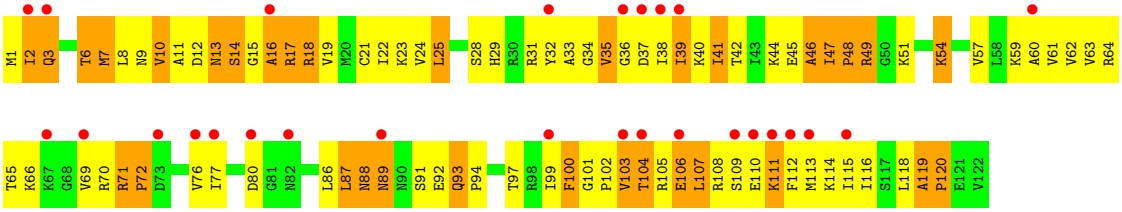
Chain BK:



• Molecule 32: 50S ribosomal protein L14

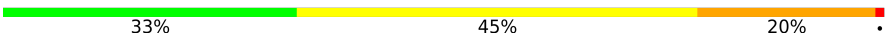
Chain DK:

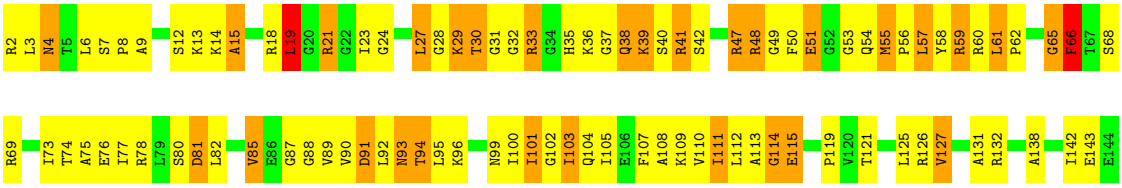




• Molecule 33: 50S ribosomal protein L15

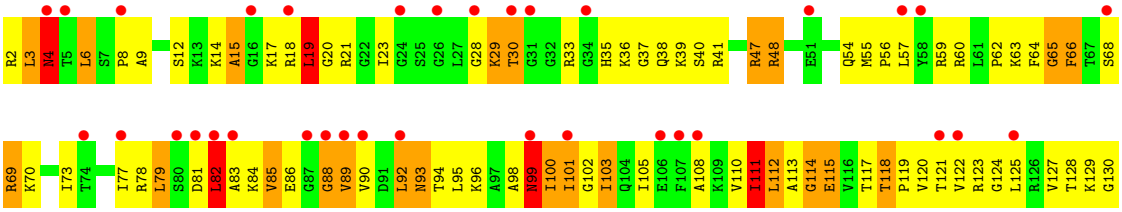
Chain BL:

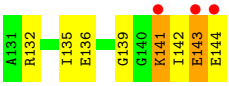




• Molecule 33: 50S ribosomal protein L15

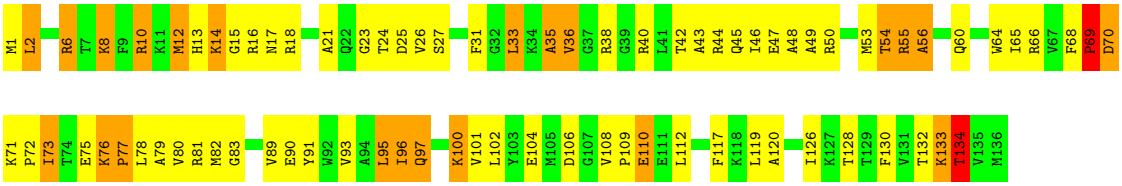
Chain DL:





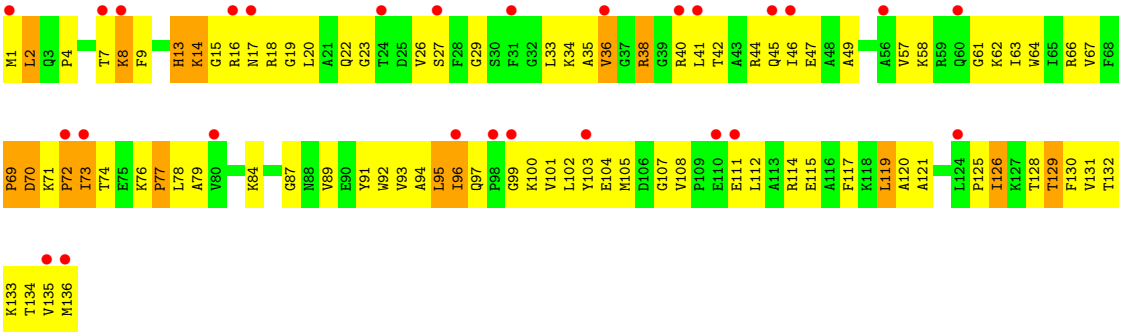
• Molecule 34: 50S ribosomal protein L16

Chain BM:



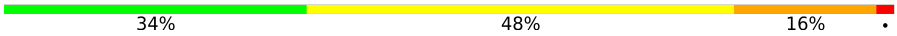
• Molecule 34: 50S ribosomal protein L16

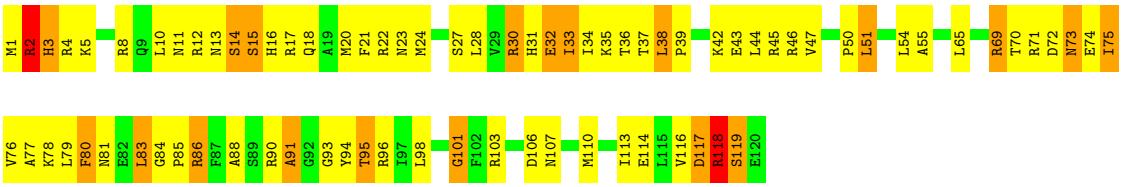
Chain DM:



• Molecule 35: 50S ribosomal protein L17

Chain BN:





• Molecule 35: 50S ribosomal protein L17

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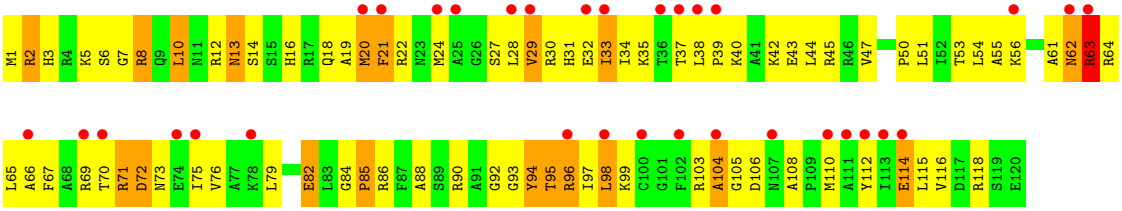
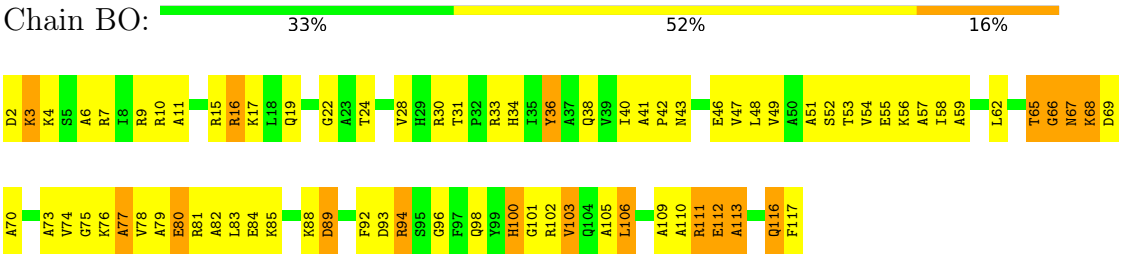


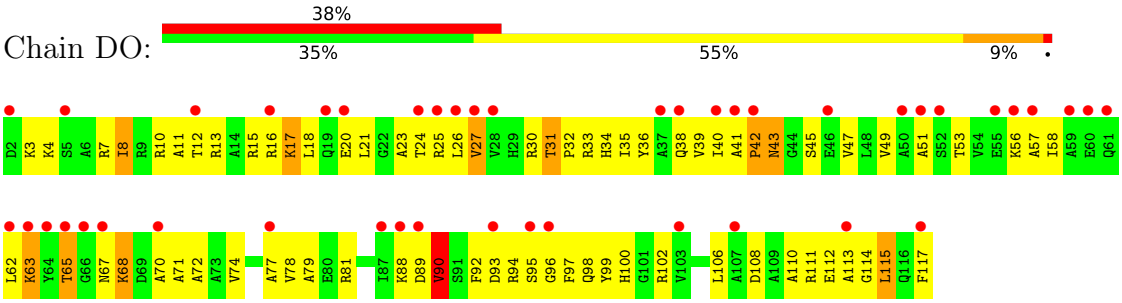
• Molecule 36: 50S ribosomal protein L18

Chain BO:



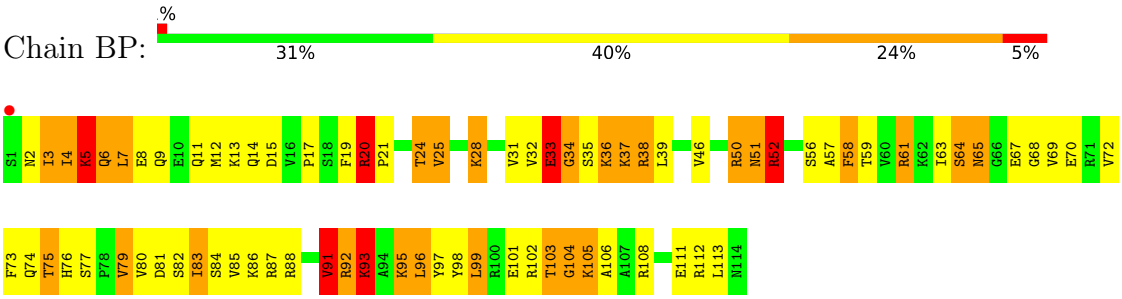
• Molecule 36: 50S ribosomal protein L18

Chain DO:



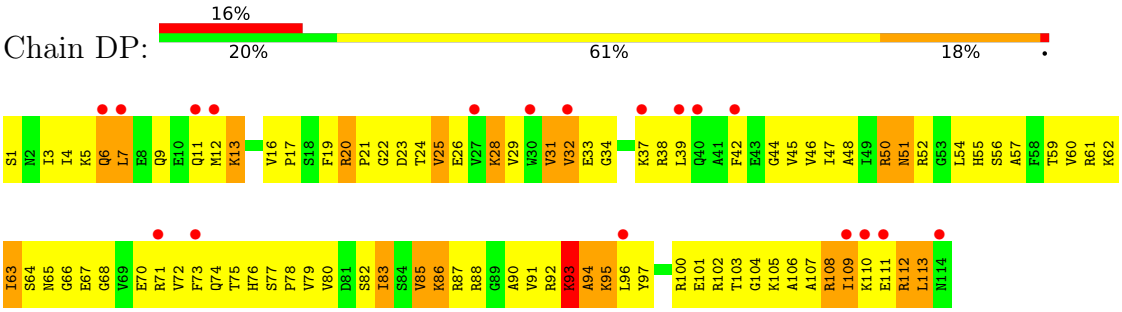
• Molecule 37: 50S ribosomal protein L19

Chain BP:



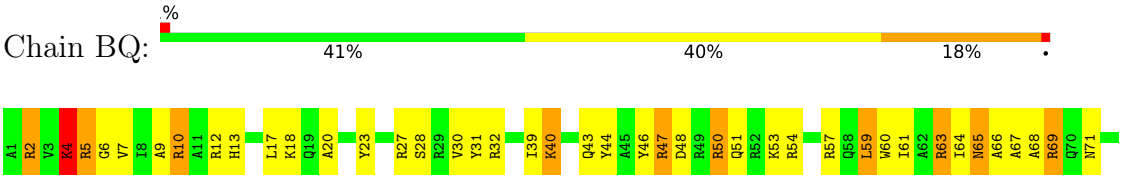
• Molecule 37: 50S ribosomal protein L19

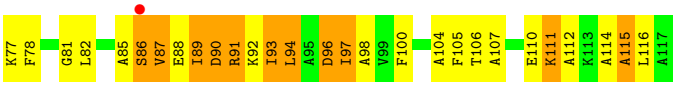
Chain DP:



• Molecule 38: 50S ribosomal protein L20

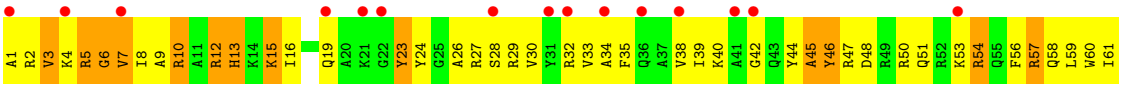
Chain BQ:

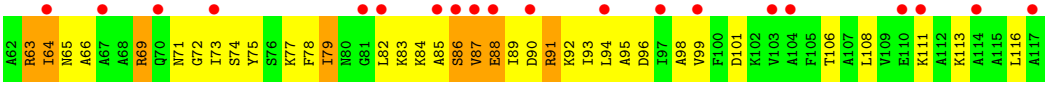




• Molecule 38: 50S ribosomal protein L20

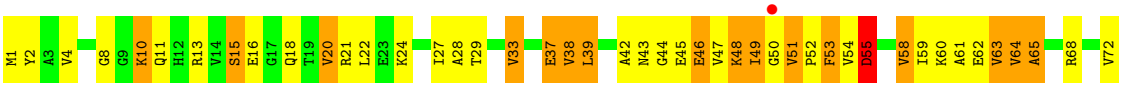
Chain DQ:





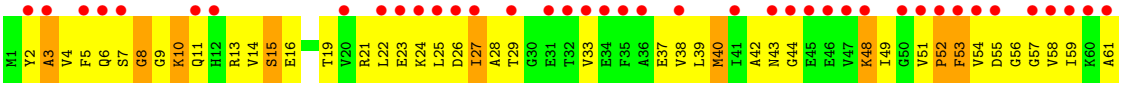
• Molecule 39: 50S ribosomal protein L21

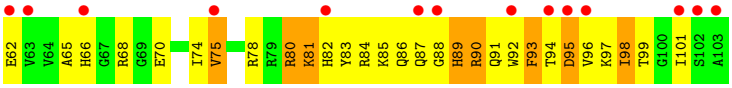
Chain BR:



• Molecule 39: 50S ribosomal protein L21

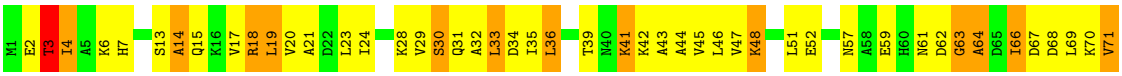
Chain DR:

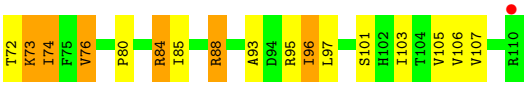




• Molecule 40: 50S ribosomal protein L22

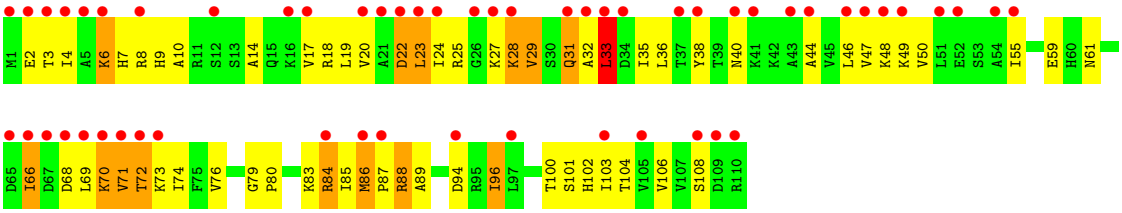
Chain BS:





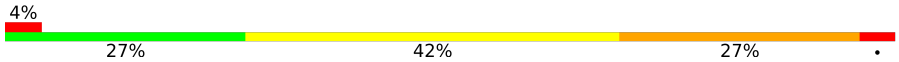
• Molecule 40: 50S ribosomal protein L22

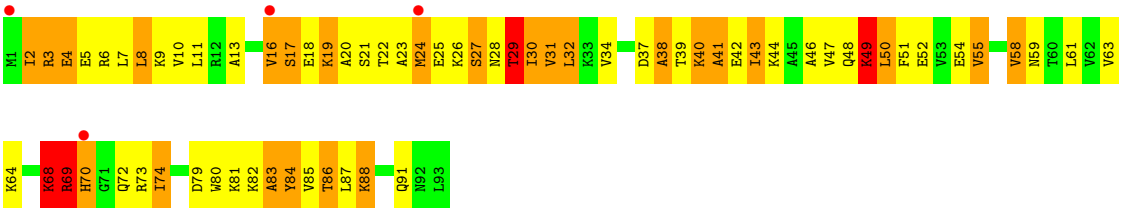
Chain DS:



- Molecule 41: 50S ribosomal protein L23

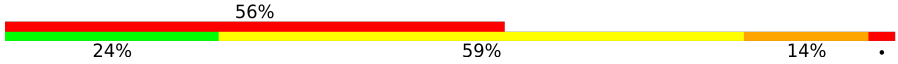
Chain BT:

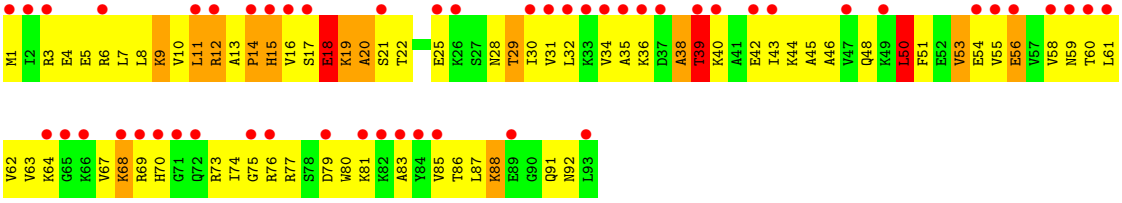




- Molecule 41: 50S ribosomal protein L23

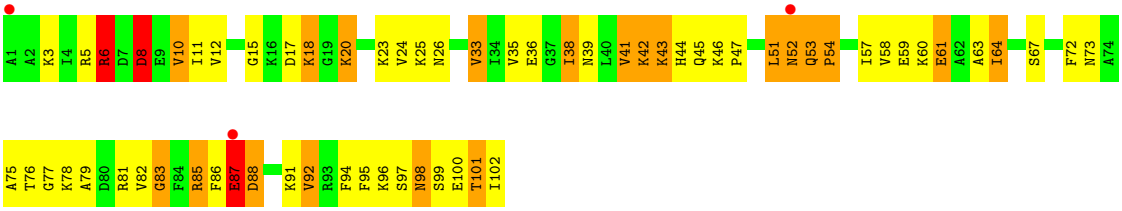
Chain DT:





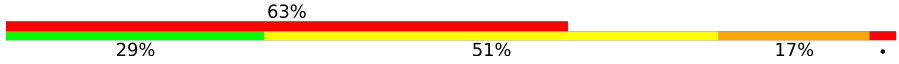
- Molecule 42: 50S ribosomal protein L24

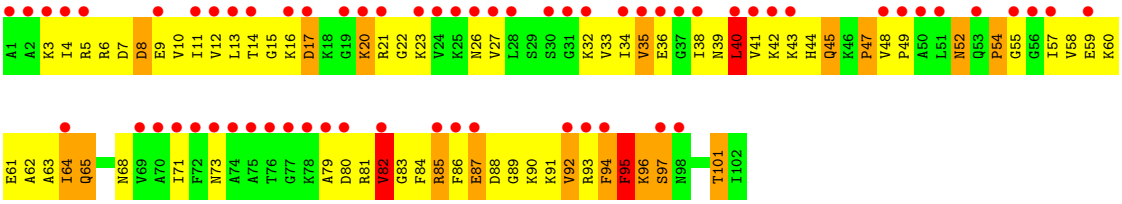
Chain BU:



- Molecule 42: 50S ribosomal protein L24

Chain DU:



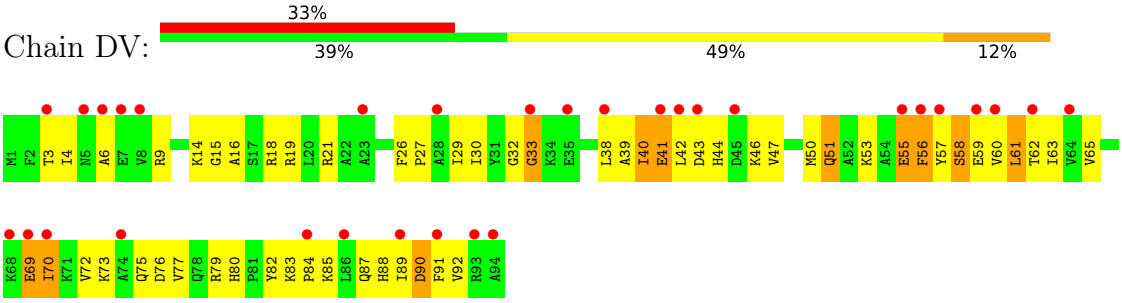


• Molecule 43: 50S ribosomal protein L25

Chain BV:

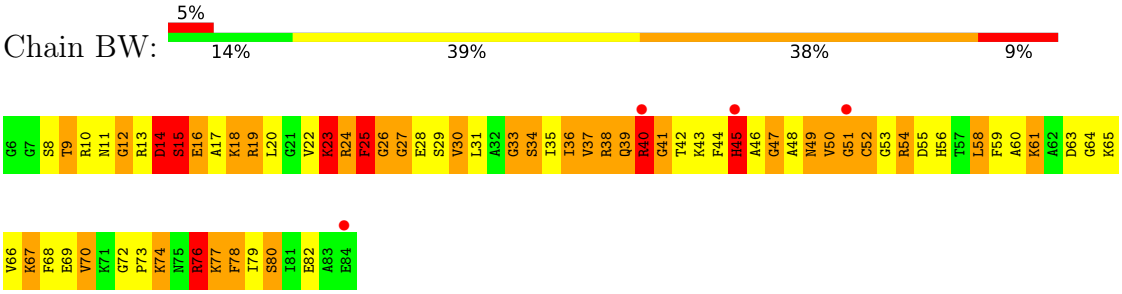
• Molecule 43: 50S ribosomal protein L25

Chain DV:



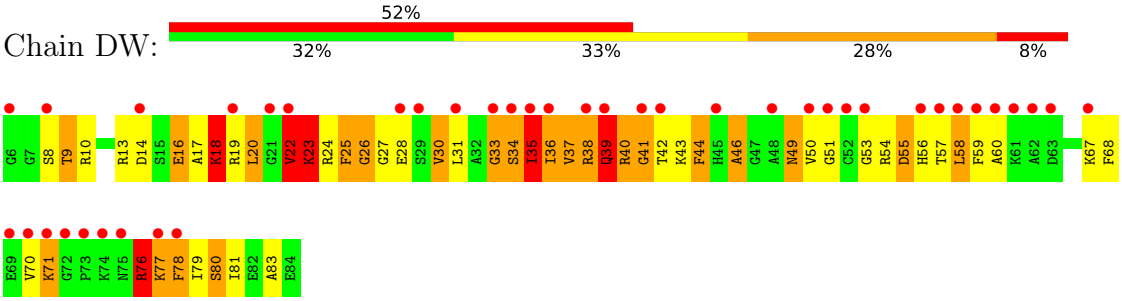
• Molecule 44: 50S ribosomal protein L27

Chain BW:



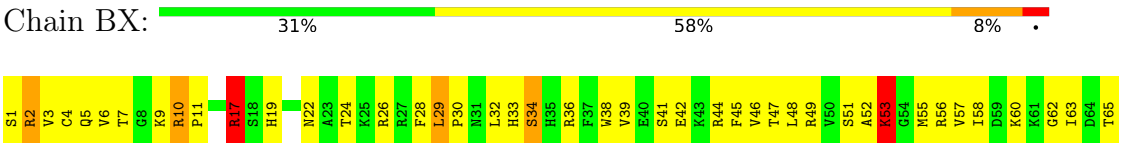
• Molecule 44: 50S ribosomal protein L27

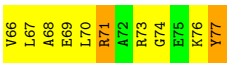
Chain DW:



• Molecule 45: 50S ribosomal protein L28

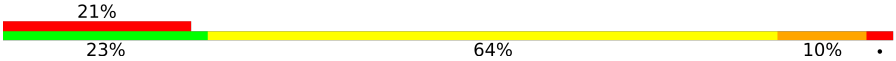
Chain BX:

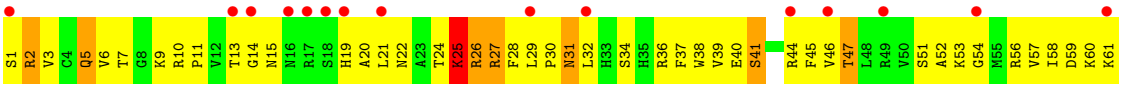




• Molecule 45: 50S ribosomal protein L28

Chain DX:



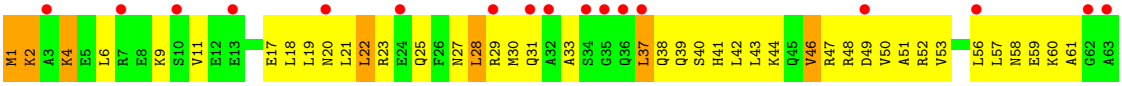


• Molecule 46: 50S ribosomal protein L29

Chain BY:

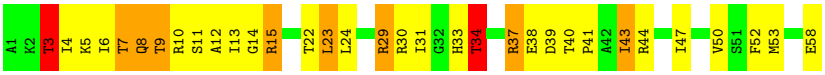
• Molecule 46: 50S ribosomal protein L29

Chain DY:



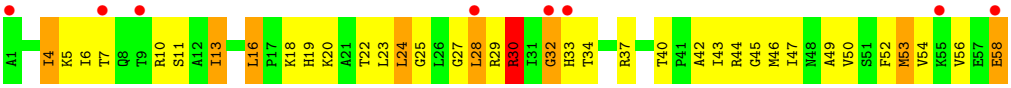
• Molecule 47: 50S ribosomal protein L30

Chain BZ:



• Molecule 47: 50S ribosomal protein L30

Chain DZ:

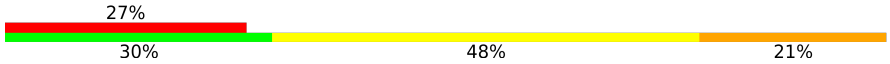


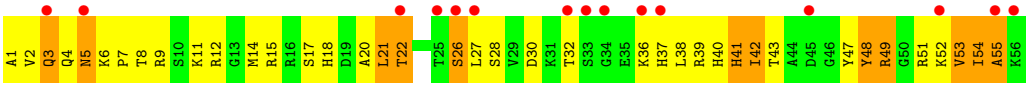
• Molecule 48: 50S ribosomal protein L32

Chain B0:

• Molecule 48: 50S ribosomal protein L32

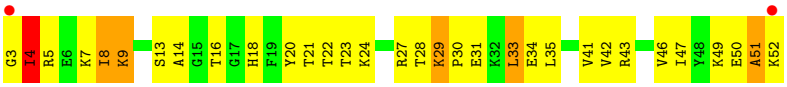
Chain D0:





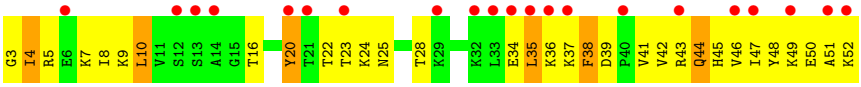
- Molecule 49: 50S ribosomal protein L33

Chain B1:



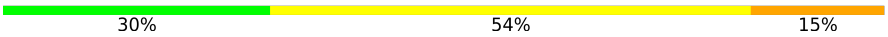
- Molecule 49: 50S ribosomal protein L33

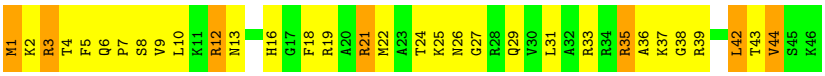
Chain D1:



- Molecule 50: 50S ribosomal protein L34

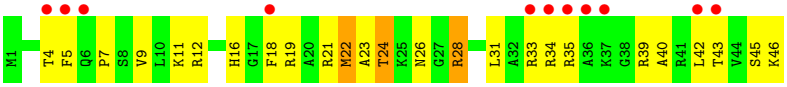
Chain B2:





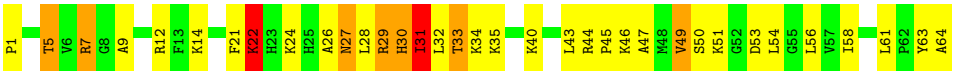
- Molecule 50: 50S ribosomal protein L34

Chain D2:



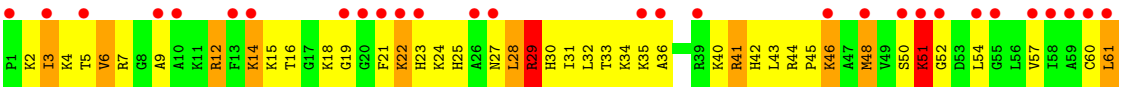
- Molecule 51: 50S ribosomal protein L35

Chain B3:



- Molecule 51: 50S ribosomal protein L35

Chain D3:

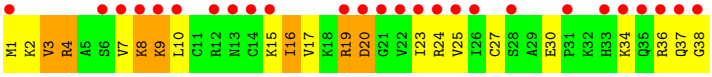


• Molecule 52: 50S ribosomal protein L36

Chain B4:

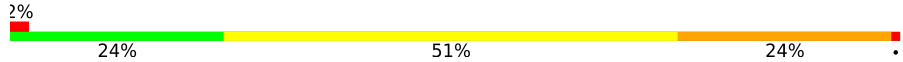
• Molecule 52: 50S ribosomal protein L36

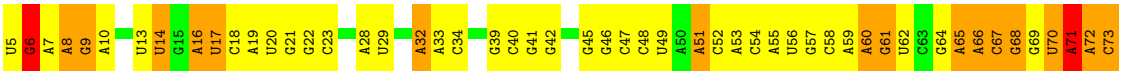
Chain D4:

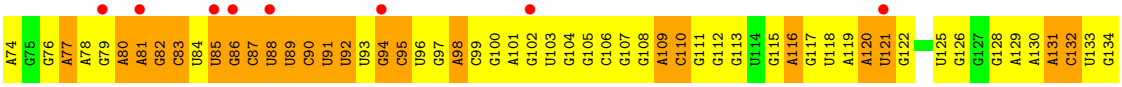


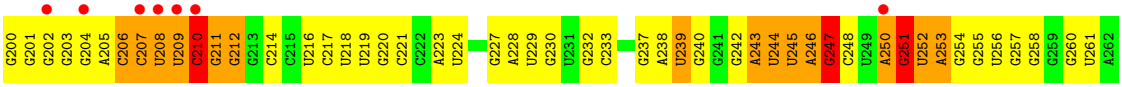
• Molecule 53: 16S rRNA

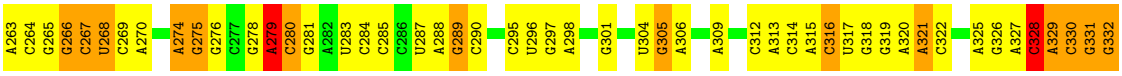
Chain CA:

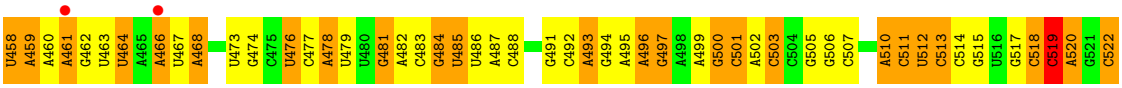


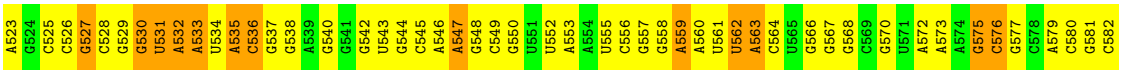


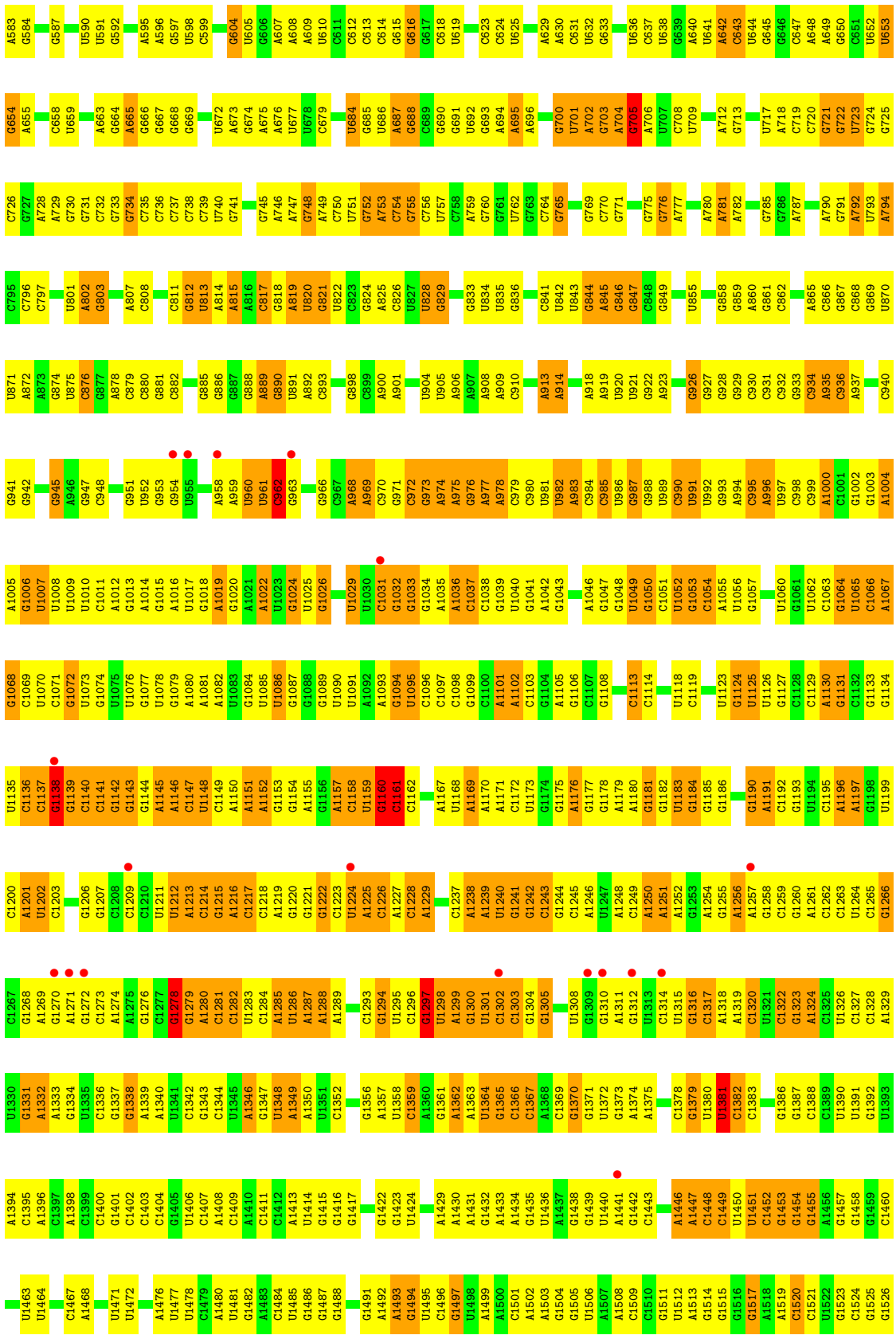








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G654 A655 C658 U659 A663 G664 A665 G666 G667 G668 G669 U672 A673 G674 A675 A676 U677 U678 C679 U684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 G700 U701 A702 G703 A704 G705 A706 U707 C708 U709 A712 G713 U717 A718 C719 C720 G721 G722 U723 G724 G725
C726 G727 A728 A729 G730 G731 C732 G733 G734 C735 C736 C737 C738 C739 U740 G741 G745 A746 A747 G748 A749 C750 U751 G752 A753 C754 G755 C756 U757 C758 A759 G760 G761 U762 G763 C764 G765 G769 C770 G771 G775 G776 A777 A780 A781 A782 G785 G786 A787 A790 G791 G792 U793 A794
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G941 G942 G945 A946 G947 C948 G951 U952 G953 G954 U955 A958 A959 U960 U961 C962 G963 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 U986 G987 G988 U989 C990 U991 U992 G993 A994 C995 A996 U997 C998 C999 A1000 C1001 G1002 G1003 A1004
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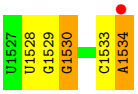
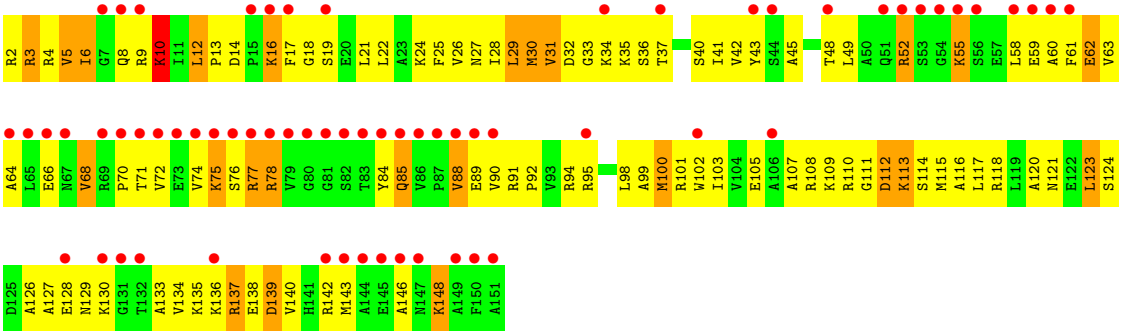
G1068 C1069 U1070 C1071 G1072 U1073 G1074 U1075 U1076 G1077 U1078 G1079 A1080 A1081 A1082 U1083 G1084 U1085 U1086 G1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1113 C1114 U1118 C1119 U1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134
U1135 C1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 A1145 A1146 C1147 U1148 C1149 A1150 A1151 A1152 G1153 G1154 A1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 A1167 U1168 A1169 A1170 A1171 C1172 U1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 U1183 G1184 G1185 G1186 G1190 A1191 C1192 G1193 U1194 C1195 A1196 A1197 G1198 U1199
C1200 A1201 U1202 C1203 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 A1216 C1217 C1218 A1219 G1220 G1221 G1222 C1223 U1224 A1225 G1226 A1227 C1228 A1229 C1237 A1238 A1239 U1240 C1241 G1242 C1243 G1244 C1245 A1246 U1247 A1248 G1249 A1250 A1251 A1252 G1253 A1254 G1255 A1256 A1257 G1258 C1259 G1260 A1261 C1262 C1263 C1264 C1265 G1266
C1267 G1268 A1269 G1270 A1271 G1272 C1273 A1274 A1275 G1276 C1277 G1278 G1279 A1280 C1281 C1282 U1283 C1284 A1285 U1286 A1287 A1288 A1289 C1293 A1294 U1295 C1296 G1297 U1298 A1299 G1300 U1301 C1302 C1303 G1304 G1305 U1308 G1309 G1310 A1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 U1321 C1322 G1323 A1324 C1325 U1326 C1327 C1328 A1329
U1330 G1331 A1332 A1333 G1334 U1335 C1336 G1337 G1338 A1339 A1340 U1341 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1356 A1357 U1358 C1359 A1360 G1361 A1362 A1363 U1364 G1365 C1366 C1367 A1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 C1378 G1379 U1380 U1381 C1382 C1383 G1386 G1387 C1388 C1389 U1390 U1391 G1392 U1393
A1394 C1395 A1396 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 U1406 C1407 A1408 C1409 A1410 C1411 C1412 A1413 U1414 G1415 G1416 G1417 G1422 A1423 U1424 A1429 A1430 A1431 G1432 A1433 A1434 G1435 U1436 A1437 G1438 G1439 U1440 A1441 G1442 C1443 A1446 A1447 C1448 C1449 U1450 U1451 C1452 G1453 G1454 G1455 A1456 G1457 G1458 G1459 C1460
U1463 U1464 C1467 A1468 U1471 U1472 A1476 U1477 U1478 C1479 A1480 U1481 G1482 A1483 C1484 U1485 G1486 G1487 G1488 G1491 A1492 A1493 G1494 U1495 C1496 G1497 U1498 A1499 A1500 C1501 A1502 A1503 G1504 G1505 U1506 A1507 A1508 C1509 C1510 G1511 U1512 A1513 G1514 G1515 G1516 G1517 A1518 A1519 C1520 G1521 U1522 G1523 C1524 G1525 G1526



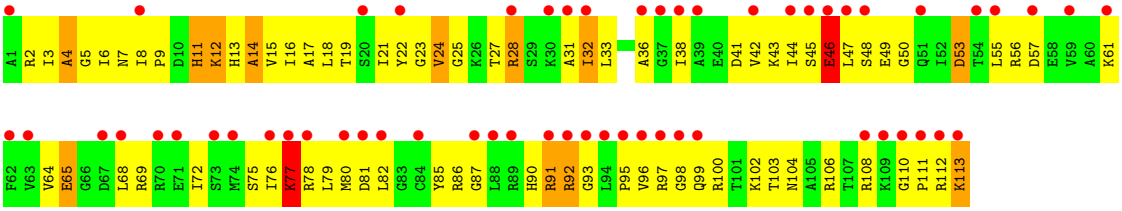
• Molecule 54: 30S ribosomal protein S7

Chain CG:



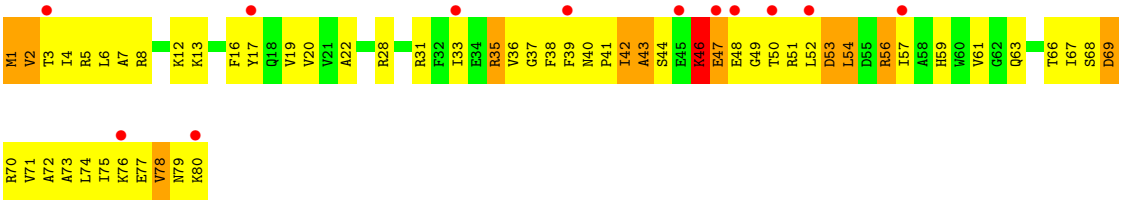
• Molecule 55: 30S ribosomal protein S13

Chain CM:



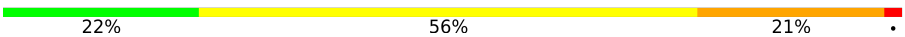
• Molecule 56: 30S ribosomal protein S16

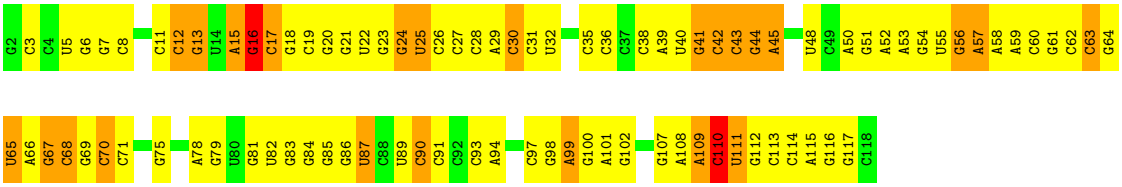
Chain CP:



• Molecule 57: 5S rRNA

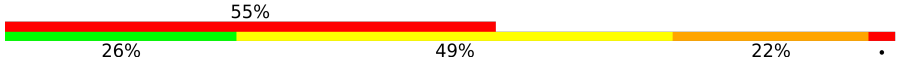
Chain DB:

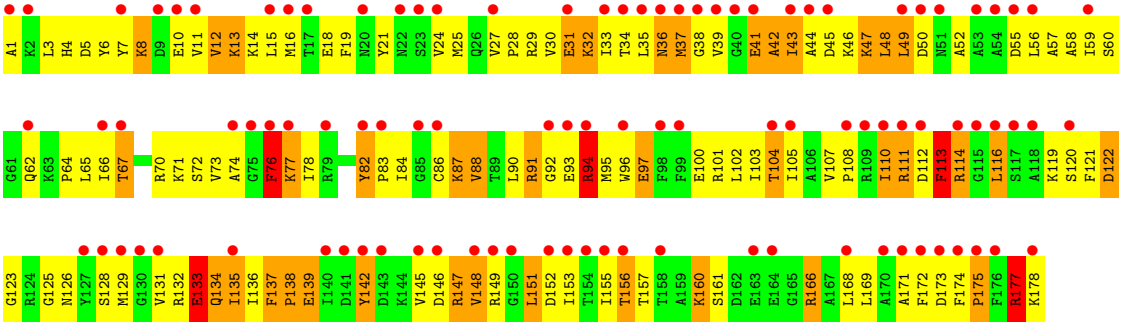




• Molecule 58: 50S ribosomal protein L5

Chain DF:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.76Å 433.27Å 618.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.22 – 3.25 85.13 – 3.25	Depositor EDS
% Data completeness (in resolution range)	85.8 (85.22-3.25) 85.6 (85.13-3.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.6.1_357, PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.193 , 0.245 0.224 , 0.268	Depositor DCC
R_{free} test set	16191 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 73.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	284525	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: TEL, 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	0.45	2/36834 (0.0%)	0.87	33/57462 (0.1%)
2	AB	0.34	1/1736 (0.1%)	0.52	1/2338 (0.0%)
2	CB	0.30	1/1736 (0.1%)	0.58	4/2338 (0.2%)
3	AC	0.28	0/1652	0.50	0/2225
3	CC	0.25	0/1652	0.44	0/2225
4	AD	0.32	0/1665	0.53	0/2227
4	CD	0.39	0/1665	0.61	0/2227
5	AE	0.45	1/1119 (0.1%)	0.66	2/1504 (0.1%)
5	CE	0.36	0/1119	0.58	0/1504
6	AF	0.31	0/836	0.49	0/1128
6	CF	0.30	0/836	0.50	0/1128
7	AG	0.25	0/1196	0.45	0/1602
8	AH	0.33	0/989	0.55	0/1326
8	CH	0.30	0/989	0.52	0/1326
9	AI	0.26	0/1034	0.48	0/1375
9	CI	0.23	0/1034	0.43	0/1375
10	AJ	0.28	0/797	0.48	0/1077
10	CJ	0.24	0/797	0.47	0/1077
11	AK	0.30	0/893	0.53	0/1205
11	CK	0.28	0/893	0.52	0/1205
12	AL	0.38	0/969	0.69	1/1300 (0.1%)
12	CL	0.36	0/969	0.58	0/1300
13	AM	0.25	0/893	0.47	0/1193
14	AN	0.28	0/785	0.50	0/1043
14	CN	0.23	0/780	0.39	0/1036
15	AO	0.29	0/722	0.48	0/964
15	CO	0.39	1/722 (0.1%)	0.48	0/964
16	AP	0.31	0/659	0.51	0/884
17	AQ	0.40	0/658	0.62	0/881
17	CQ	0.34	0/658	0.52	0/881
18	AR	0.31	0/463	0.50	0/621
18	CR	0.31	0/463	0.47	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	AS	0.25	0/653	0.45	0/877
19	CS	0.21	0/653	0.42	0/877
20	AT	0.37	0/671	0.56	0/888
20	CT	0.28	0/671	0.50	0/888
21	AU	0.29	0/431	0.46	0/570
21	CU	0.34	0/431	0.59	0/570
22	BA	0.77	9/68626 (0.0%)	1.12	282/107056 (0.3%)
22	DA	0.39	1/68314 (0.0%)	0.86	83/106569 (0.1%)
23	BB	0.68	0/2828	1.04	4/4410 (0.1%)
24	BC	0.48	0/2122	0.73	1/2852 (0.0%)
24	DC	0.31	0/2122	0.54	0/2852
25	BD	0.55	0/1586	0.78	1/2134 (0.0%)
25	DD	0.31	0/1586	0.58	0/2134
26	BE	0.45	0/1571	0.68	1/2113 (0.0%)
26	DE	0.26	0/1571	0.48	0/2113
27	BF	0.34	0/1435	0.53	0/1926
28	BG	0.39	0/1343	0.62	0/1816
28	DG	0.24	0/1343	0.47	0/1816
29	BH	0.33	0/1122	0.52	0/1515
29	DH	0.38	1/1122 (0.1%)	0.52	0/1515
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.21	0/1046	0.42	0/1410
31	BJ	0.58	0/1152	0.84	1/1551 (0.1%)
31	DJ	0.29	0/1152	0.57	1/1551 (0.1%)
32	BK	0.55	0/948	0.80	0/1268
32	DK	0.35	0/948	0.57	0/1268
33	BL	0.46	0/1054	0.79	1/1403 (0.1%)
33	DL	0.27	0/1054	0.53	0/1403
34	BM	0.54	0/1093	0.73	0/1460
34	DM	0.30	0/1093	0.50	0/1460
35	BN	0.51	0/974	0.75	0/1301
35	DN	0.28	0/974	0.51	0/1301
36	BO	0.43	0/902	0.66	0/1209
36	DO	0.24	0/902	0.43	0/1209
37	BP	0.51	0/929	0.74	0/1242
37	DP	0.32	0/929	0.50	0/1242
38	BQ	0.61	0/960	0.78	0/1278
38	DQ	0.29	0/960	0.47	0/1278
39	BR	0.63	1/829 (0.1%)	0.79	0/1107
39	DR	0.29	0/829	0.51	0/1107
40	BS	0.57	0/864	0.78	0/1156
40	DS	0.28	0/864	0.52	0/1156
41	BT	0.45	0/745	0.70	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	DT	0.24	0/745	0.48	0/994
42	BU	0.43	0/788	0.70	0/1051
42	DU	0.24	0/788	0.46	0/1051
43	BV	0.44	0/766	0.61	0/1025
43	DV	0.25	0/766	0.43	0/1025
44	BW	0.61	0/603	0.89	0/797
44	DW	0.29	0/603	0.51	0/797
45	BX	0.41	0/635	0.70	0/848
45	DX	0.29	0/635	0.56	0/848
46	BY	0.37	0/510	0.64	0/677
46	DY	0.23	0/510	0.44	0/677
47	BZ	0.52	0/453	0.83	0/605
47	DZ	0.28	0/453	0.51	0/605
48	B0	0.48	0/450	0.73	0/599
48	D0	0.29	0/450	0.50	0/599
49	B1	0.38	0/417	0.62	0/554
49	D1	0.27	0/417	0.46	0/554
50	B2	0.53	0/380	0.78	0/498
50	D2	0.27	0/380	0.49	0/498
51	B3	0.49	0/513	0.70	0/676
51	D3	0.29	0/513	0.53	0/676
52	B4	0.53	0/303	0.70	0/397
52	D4	0.45	0/303	0.50	0/397
53	CA	0.41	2/36762 (0.0%)	0.83	32/57350 (0.1%)
54	CG	0.23	0/1188	0.44	0/1591
55	CM	0.20	0/885	0.40	0/1181
56	CP	0.29	0/649	0.53	0/870
57	DB	0.36	1/2803 (0.0%)	0.81	2/4371 (0.0%)
58	DF	0.23	0/1444	0.53	3/1937 (0.2%)
All	All	0.51	21/306773 (0.0%)	0.86	453/458565 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
25	BD	0	1
35	BN	0	1
51	B3	0	1
All	All	0	3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2092	U	O3'-P	-13.97	1.44	1.61
22	DA	2197	U	O3'-P	-13.44	1.45	1.61
53	CA	1396	A	O3'-P	-13.34	1.45	1.61
22	BA	1142	A	N9-C4	-9.96	1.31	1.37
57	DB	107	G	O3'-P	-9.89	1.49	1.61

The worst 5 of 453 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	783	A	C5-N7-C8	-11.37	98.22	103.90
22	BA	974	G	C5-N7-C8	-11.01	98.79	104.30
22	BA	974	G	C4-C5-N7	10.99	115.20	110.80
2	CB	146	SER	O-C-N	-10.79	105.44	122.70
22	BA	2499	C	N1-C2-O2	-10.28	112.73	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	B3	29	ARG	Peptide
25	BD	9	VAL	Peptide
35	BN	101	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32895	0	16553	1232	1
2	AB	1705	0	1732	183	0
2	CB	1705	0	1732	151	0
3	AC	1625	0	1699	109	0
3	CC	1625	0	1699	128	0
4	AD	1643	0	1710	145	0
4	CD	1643	0	1710	157	0
5	AE	1106	0	1148	148	0
5	CE	1106	0	1148	101	0
6	AF	818	0	808	87	0
6	CF	818	0	808	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AG	1182	0	1240	86	0
8	AH	979	0	1034	99	0
8	CH	979	0	1034	92	0
9	AI	1022	0	1070	84	0
9	CI	1022	0	1070	107	0
10	AJ	787	0	828	78	0
10	CJ	787	0	828	91	0
11	AK	877	0	887	91	0
11	CK	877	0	887	71	0
12	AL	955	0	1019	90	0
12	CL	955	0	1019	100	0
13	AM	884	0	944	73	0
14	AN	774	0	827	69	0
14	CN	769	0	822	77	0
15	AO	714	0	737	46	0
15	CO	714	0	737	52	0
16	AP	649	0	666	50	0
17	AQ	649	0	691	71	0
17	CQ	649	0	691	66	0
18	AR	456	0	478	30	0
18	CR	456	0	478	39	0
19	AS	638	0	665	59	0
19	CS	638	0	665	65	0
20	AT	665	0	714	81	0
20	CT	665	0	714	45	0
21	AU	426	0	449	80	0
21	CU	426	0	449	80	0
22	BA	61274	0	30819	1937	6
22	DA	60995	0	30679	3516	8
23	BB	2529	0	1281	73	0
24	BC	2083	0	2157	217	0
24	DC	2083	0	2157	215	0
25	BD	1565	0	1616	196	1
25	DD	1565	0	1616	189	0
26	BE	1552	0	1619	151	0
26	DE	1552	0	1619	180	0
27	BF	1411	0	1447	135	0
28	BG	1323	0	1374	146	0
28	DG	1323	0	1374	126	0
29	BH	1111	0	1148	102	0
29	DH	1111	0	1148	96	0
30	BI	1032	0	1088	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	DI	1032	0	1088	65	0
31	BJ	1129	0	1162	156	0
31	DJ	1129	0	1162	140	0
32	BK	939	0	1012	121	0
32	DK	939	0	1012	109	0
33	BL	1045	0	1117	130	1
33	DL	1045	0	1117	128	0
34	BM	1074	0	1157	90	0
34	DM	1074	0	1157	94	0
35	BN	961	0	1000	89	0
35	DN	961	0	1000	122	0
36	BO	892	0	923	74	0
36	DO	892	0	923	79	0
37	BP	917	0	965	141	0
37	DP	917	0	965	121	0
38	BQ	947	0	1022	127	0
38	DQ	947	0	1022	121	0
39	BR	816	0	839	116	0
39	DR	816	0	839	93	0
40	BS	857	0	922	74	0
40	DS	857	0	922	60	0
41	BT	739	0	807	112	0
41	DT	739	0	807	99	0
42	BU	780	0	834	54	0
42	DU	780	0	834	92	0
43	BV	753	0	780	66	0
43	DV	753	0	780	60	0
44	BW	596	0	610	204	0
44	DW	596	0	610	115	0
45	BX	625	0	655	56	0
45	DX	625	0	655	75	0
46	BY	509	0	543	50	0
46	DY	509	0	543	63	0
47	BZ	449	0	491	33	0
47	DZ	449	0	491	40	1
48	B0	444	0	461	30	0
48	D0	444	0	461	57	0
49	B1	410	0	440	33	0
49	D1	410	0	440	36	0
50	B2	377	0	418	35	0
50	D2	377	0	418	42	0
51	B3	504	0	574	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	D3	504	0	574	57	0
52	B4	302	0	340	30	0
52	D4	302	0	342	27	0
53	CA	32831	0	16521	1619	0
54	CG	1175	0	1230	131	0
55	CM	877	0	937	91	0
56	CP	639	0	656	61	0
57	DB	2507	0	1270	159	0
58	DF	1420	0	1460	184	0
59	AA	43	0	0	0	0
59	BA	134	0	0	0	0
59	BB	4	0	0	0	0
59	CA	41	0	0	0	0
59	CE	1	0	0	0	0
59	DA	133	0	0	0	0
59	DB	1	0	0	0	0
59	DC	2	0	0	0	0
59	DJ	1	0	0	0	0
60	BA	58	0	64	8	0
61	B4	1	0	0	0	0
61	D4	1	0	0	0	0
62	AA	198	0	0	5	0
62	AL	1	0	0	0	0
62	AN	6	0	0	1	0
62	AT	2	0	0	0	0
62	AU	1	0	0	0	0
62	B2	1	0	0	0	0
62	B3	3	0	0	0	0
62	B4	1	0	0	0	0
62	BA	598	0	0	29	0
62	BB	20	0	0	1	0
62	BC	10	0	0	0	0
62	BD	2	0	0	0	0
62	BE	1	0	0	0	0
62	BL	2	0	0	1	0
62	BN	3	0	0	1	0
62	BQ	1	0	0	0	0
62	BR	1	0	0	0	0
62	BT	1	0	0	1	0
62	CA	192	0	0	6	0
62	CE	5	0	0	1	0
62	CI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	CL	1	0	0	0	0
62	CN	3	0	0	0	0
62	CT	3	0	0	0	0
62	CU	2	0	0	0	0
62	D2	1	0	0	1	0
62	D3	1	0	0	0	0
62	D4	3	0	0	0	0
62	DA	595	0	0	28	0
62	DB	4	0	0	0	0
62	DC	13	0	0	1	0
62	DD	3	0	0	1	0
62	DE	3	0	0	0	0
62	DJ	6	0	0	0	0
62	DL	6	0	0	1	0
62	DN	2	0	0	0	0
62	DT	3	0	0	0	0
62	DU	2	0	0	0	0
62	DV	1	0	0	0	0
All	All	284525	0	190904	16341	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

The worst 5 of 16341 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)
53:CA:1157:A:H4'	53:CA:1158:C:O5'	1.38	1.20
22:DA:1808:A:H3'	22:DA:1809:A:H8	1.05	1.20
53:CA:120:A:C3'	53:CA:121:U:H5"	1.73	1.19
22:DA:2091:C:OP2	22:DA:2092:U:H3'	1.39	1.18
22:BA:900:A:C2'	22:BA:901:C:H5'	1.74	1.17

The worst 5 of 9 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)
22:BA:138:U:O4	22:DA:305:C:OP1[3_545]	1.58	0.62
22:BA:138:U:O4	22:DA:305:C:P[3_545]	1.90	0.30
1:AA:416:G:OP1	22:DA:2139:U:O4'[4_455]	1.91	0.29
25:BD:181:ASP:OD1	22:DA:2903:U:O4[2_454]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:138:U:C4	22:DA:304:U:O3'[3_545]	1.98	0.22

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	132 (61%)	52 (24%)	32 (15%)	0	1
2	CB	216/218 (99%)	155 (72%)	46 (21%)	15 (7%)	1	8
3	AC	204/206 (99%)	156 (76%)	32 (16%)	16 (8%)	1	6
3	CC	204/206 (99%)	147 (72%)	37 (18%)	20 (10%)	0	3
4	AD	203/205 (99%)	138 (68%)	37 (18%)	28 (14%)	0	1
4	CD	203/205 (99%)	140 (69%)	43 (21%)	20 (10%)	0	3
5	AE	148/150 (99%)	105 (71%)	23 (16%)	20 (14%)	0	1
5	CE	148/150 (99%)	112 (76%)	21 (14%)	15 (10%)	0	3
6	AF	98/100 (98%)	73 (74%)	13 (13%)	12 (12%)	0	2
6	CF	98/100 (98%)	65 (66%)	24 (24%)	9 (9%)	1	4
7	AG	149/151 (99%)	111 (74%)	32 (22%)	6 (4%)	3	17
8	AH	127/129 (98%)	92 (72%)	28 (22%)	7 (6%)	2	11
8	CH	127/129 (98%)	94 (74%)	22 (17%)	11 (9%)	1	5
9	AI	125/127 (98%)	89 (71%)	26 (21%)	10 (8%)	1	6
9	CI	125/127 (98%)	89 (71%)	25 (20%)	11 (9%)	1	5
10	AJ	96/98 (98%)	70 (73%)	13 (14%)	13 (14%)	0	1
10	CJ	96/98 (98%)	55 (57%)	28 (29%)	13 (14%)	0	1
11	AK	115/117 (98%)	85 (74%)	20 (17%)	10 (9%)	1	5
11	CK	115/117 (98%)	89 (77%)	19 (16%)	7 (6%)	1	10
12	AL	121/123 (98%)	88 (73%)	22 (18%)	11 (9%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	CL	121/123 (98%)	86 (71%)	27 (22%)	8 (7%)	1	9
13	AM	112/114 (98%)	88 (79%)	13 (12%)	11 (10%)	0	3
14	AN	92/100 (92%)	60 (65%)	20 (22%)	12 (13%)	0	2
14	CN	91/100 (91%)	59 (65%)	27 (30%)	5 (6%)	2	11
15	AO	86/88 (98%)	59 (69%)	23 (27%)	4 (5%)	2	14
15	CO	86/88 (98%)	67 (78%)	16 (19%)	3 (4%)	3	21
16	AP	80/82 (98%)	58 (72%)	14 (18%)	8 (10%)	0	3
17	AQ	78/80 (98%)	51 (65%)	15 (19%)	12 (15%)	0	1
17	CQ	78/80 (98%)	62 (80%)	8 (10%)	8 (10%)	0	3
18	AR	53/55 (96%)	46 (87%)	5 (9%)	2 (4%)	3	19
18	CR	53/55 (96%)	42 (79%)	11 (21%)	0	100	100
19	AS	77/79 (98%)	58 (75%)	10 (13%)	9 (12%)	0	2
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	4
20	AT	83/85 (98%)	58 (70%)	19 (23%)	6 (7%)	1	7
20	CT	83/85 (98%)	63 (76%)	12 (14%)	8 (10%)	0	4
21	AU	49/51 (96%)	25 (51%)	15 (31%)	9 (18%)	0	1
21	CU	49/51 (96%)	22 (45%)	8 (16%)	19 (39%)	0	0
24	BC	269/271 (99%)	203 (76%)	40 (15%)	26 (10%)	0	4
24	DC	269/271 (99%)	183 (68%)	54 (20%)	32 (12%)	0	2
25	BD	207/209 (99%)	148 (72%)	31 (15%)	28 (14%)	0	1
25	DD	207/209 (99%)	136 (66%)	40 (19%)	31 (15%)	0	1
26	BE	199/201 (99%)	149 (75%)	32 (16%)	18 (9%)	1	4
26	DE	199/201 (99%)	125 (63%)	46 (23%)	28 (14%)	0	1
27	BF	175/177 (99%)	130 (74%)	30 (17%)	15 (9%)	1	5
28	BG	174/176 (99%)	118 (68%)	32 (18%)	24 (14%)	0	1
28	DG	174/176 (99%)	102 (59%)	41 (24%)	31 (18%)	0	1
29	BH	147/149 (99%)	67 (46%)	52 (35%)	28 (19%)	0	1
29	DH	147/149 (99%)	76 (52%)	53 (36%)	18 (12%)	0	2
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	0	3
30	DI	139/141 (99%)	84 (60%)	38 (27%)	17 (12%)	0	2
31	BJ	140/142 (99%)	103 (74%)	26 (19%)	11 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DJ	140/142 (99%)	96 (69%)	29 (21%)	15 (11%)	0	3
32	BK	120/122 (98%)	88 (73%)	12 (10%)	20 (17%)	0	1
32	DK	120/122 (98%)	82 (68%)	18 (15%)	20 (17%)	0	1
33	BL	141/143 (99%)	103 (73%)	28 (20%)	10 (7%)	1	7
33	DL	141/143 (99%)	80 (57%)	41 (29%)	20 (14%)	0	1
34	BM	134/136 (98%)	100 (75%)	21 (16%)	13 (10%)	0	4
34	DM	134/136 (98%)	95 (71%)	27 (20%)	12 (9%)	1	4
35	BN	118/120 (98%)	92 (78%)	14 (12%)	12 (10%)	0	3
35	DN	118/120 (98%)	70 (59%)	36 (30%)	12 (10%)	0	3
36	BO	114/116 (98%)	88 (77%)	17 (15%)	9 (8%)	1	6
36	DO	114/116 (98%)	81 (71%)	26 (23%)	7 (6%)	1	10
37	BP	112/114 (98%)	74 (66%)	21 (19%)	17 (15%)	0	1
37	DP	112/114 (98%)	64 (57%)	29 (26%)	19 (17%)	0	1
38	BQ	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	1	7
38	DQ	115/117 (98%)	83 (72%)	20 (17%)	12 (10%)	0	3
39	BR	101/103 (98%)	80 (79%)	14 (14%)	7 (7%)	1	8
39	DR	101/103 (98%)	71 (70%)	18 (18%)	12 (12%)	0	2
40	BS	108/110 (98%)	84 (78%)	17 (16%)	7 (6%)	1	9
40	DS	108/110 (98%)	74 (68%)	25 (23%)	9 (8%)	1	5
41	BT	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	1
41	DT	91/93 (98%)	48 (53%)	28 (31%)	15 (16%)	0	1
42	BU	100/102 (98%)	67 (67%)	17 (17%)	16 (16%)	0	1
42	DU	100/102 (98%)	51 (51%)	28 (28%)	21 (21%)	0	0
43	BV	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	14	46
43	DV	92/94 (98%)	64 (70%)	21 (23%)	7 (8%)	1	6
44	BW	77/79 (98%)	28 (36%)	22 (29%)	27 (35%)	0	0
44	DW	77/79 (98%)	33 (43%)	23 (30%)	21 (27%)	0	0
45	BX	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	2	12
45	DX	75/77 (97%)	50 (67%)	17 (23%)	8 (11%)	0	3
46	BY	61/63 (97%)	44 (72%)	11 (18%)	6 (10%)	0	3
46	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	BZ	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	3	20
47	DZ	56/58 (97%)	34 (61%)	17 (30%)	5 (9%)	1	4
48	B0	54/56 (96%)	41 (76%)	9 (17%)	4 (7%)	1	7
48	D0	54/56 (96%)	40 (74%)	8 (15%)	6 (11%)	0	2
49	B1	48/50 (96%)	39 (81%)	5 (10%)	4 (8%)	1	5
49	D1	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	5
50	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	2	15
50	D2	44/46 (96%)	29 (66%)	11 (25%)	4 (9%)	1	4
51	B3	62/64 (97%)	50 (81%)	7 (11%)	5 (8%)	1	6
51	D3	62/64 (97%)	39 (63%)	18 (29%)	5 (8%)	1	6
52	B4	36/38 (95%)	29 (81%)	3 (8%)	4 (11%)	0	2
52	D4	36/38 (95%)	23 (64%)	8 (22%)	5 (14%)	0	1
54	CG	148/150 (99%)	100 (68%)	36 (24%)	12 (8%)	1	6
55	CM	111/113 (98%)	64 (58%)	35 (32%)	12 (11%)	0	3
56	CP	78/80 (98%)	50 (64%)	18 (23%)	10 (13%)	0	2
58	DF	176/178 (99%)	98 (56%)	46 (26%)	32 (18%)	0	1
All	All	11238/11447 (98%)	7713 (69%)	2283 (20%)	1242 (11%)	0	2

5 of 1242 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	18	GLN
2	AB	20	ARG
2	AB	33	ALA
2	AB	40	ILE
2	AB	72	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	141 (78%)	39 (22%)	1	4
2	CB	180/180 (100%)	152 (84%)	28 (16%)	2	11
3	AC	170/170 (100%)	142 (84%)	28 (16%)	2	10
3	CC	170/170 (100%)	151 (89%)	19 (11%)	6	23
4	AD	172/172 (100%)	145 (84%)	27 (16%)	2	11
4	CD	172/172 (100%)	135 (78%)	37 (22%)	1	4
5	AE	113/113 (100%)	86 (76%)	27 (24%)	0	2
5	CE	113/113 (100%)	90 (80%)	23 (20%)	1	4
6	AF	87/87 (100%)	73 (84%)	14 (16%)	2	10
6	CF	87/87 (100%)	74 (85%)	13 (15%)	3	12
7	AG	124/124 (100%)	106 (86%)	18 (14%)	3	14
8	AH	104/104 (100%)	89 (86%)	15 (14%)	3	14
8	CH	104/104 (100%)	91 (88%)	13 (12%)	4	19
9	AI	105/105 (100%)	83 (79%)	22 (21%)	1	4
9	CI	105/105 (100%)	91 (87%)	14 (13%)	4	16
10	AJ	86/86 (100%)	74 (86%)	12 (14%)	3	15
10	CJ	86/86 (100%)	75 (87%)	11 (13%)	4	18
11	AK	90/90 (100%)	75 (83%)	15 (17%)	2	9
11	CK	90/90 (100%)	78 (87%)	12 (13%)	4	16
12	AL	103/103 (100%)	85 (82%)	18 (18%)	2	8
12	CL	103/103 (100%)	86 (84%)	17 (16%)	2	10
13	AM	92/92 (100%)	87 (95%)	5 (5%)	22	53
14	AN	79/83 (95%)	75 (95%)	4 (5%)	24	54
14	CN	79/83 (95%)	69 (87%)	10 (13%)	4	18
15	AO	76/76 (100%)	70 (92%)	6 (8%)	12	37
15	CO	76/76 (100%)	70 (92%)	6 (8%)	12	37
16	AP	65/65 (100%)	58 (89%)	7 (11%)	6	24
17	AQ	74/74 (100%)	57 (77%)	17 (23%)	1	3
17	CQ	74/74 (100%)	60 (81%)	14 (19%)	1	6
18	AR	48/48 (100%)	45 (94%)	3 (6%)	18	47
18	CR	48/48 (100%)	43 (90%)	5 (10%)	7	25
19	AS	70/70 (100%)	62 (89%)	8 (11%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	CS	70/70 (100%)	63 (90%)	7 (10%)	7	27
20	AT	65/65 (100%)	49 (75%)	16 (25%)	0	2
20	CT	65/65 (100%)	51 (78%)	14 (22%)	1	4
21	AU	44/44 (100%)	34 (77%)	10 (23%)	1	3
21	CU	44/44 (100%)	36 (82%)	8 (18%)	1	7
24	BC	216/216 (100%)	167 (77%)	49 (23%)	1	3
24	DC	216/216 (100%)	189 (88%)	27 (12%)	4	19
25	BD	164/164 (100%)	134 (82%)	30 (18%)	1	7
25	DD	164/164 (100%)	144 (88%)	20 (12%)	5	20
26	BE	165/165 (100%)	122 (74%)	43 (26%)	0	1
26	DE	165/165 (100%)	147 (89%)	18 (11%)	6	24
27	BF	148/148 (100%)	130 (88%)	18 (12%)	5	20
28	BG	137/137 (100%)	105 (77%)	32 (23%)	1	3
28	DG	137/137 (100%)	119 (87%)	18 (13%)	4	17
29	BH	114/114 (100%)	96 (84%)	18 (16%)	2	11
29	DH	114/114 (100%)	96 (84%)	18 (16%)	2	11
30	BI	109/109 (100%)	91 (84%)	18 (16%)	2	10
30	DI	109/109 (100%)	102 (94%)	7 (6%)	17	47
31	BJ	116/116 (100%)	88 (76%)	28 (24%)	0	2
31	DJ	116/116 (100%)	100 (86%)	16 (14%)	3	16
32	BK	103/103 (100%)	81 (79%)	22 (21%)	1	4
32	DK	103/103 (100%)	83 (81%)	20 (19%)	1	5
33	BL	102/102 (100%)	76 (74%)	26 (26%)	0	1
33	DL	102/102 (100%)	85 (83%)	17 (17%)	2	9
34	BM	109/109 (100%)	87 (80%)	22 (20%)	1	5
34	DM	109/109 (100%)	96 (88%)	13 (12%)	5	20
35	BN	100/100 (100%)	82 (82%)	18 (18%)	1	7
35	DN	100/100 (100%)	85 (85%)	15 (15%)	3	12
36	BO	86/86 (100%)	69 (80%)	17 (20%)	1	5
36	DO	86/86 (100%)	77 (90%)	9 (10%)	7	25
37	BP	99/99 (100%)	73 (74%)	26 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DP	99/99 (100%)	89 (90%)	10 (10%)	7	27
38	BQ	89/89 (100%)	71 (80%)	18 (20%)	1	5
38	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	9
39	BR	84/84 (100%)	70 (83%)	14 (17%)	2	9
39	DR	84/84 (100%)	71 (84%)	13 (16%)	2	11
40	BS	93/93 (100%)	74 (80%)	19 (20%)	1	4
40	DS	93/93 (100%)	79 (85%)	14 (15%)	3	12
41	BT	80/80 (100%)	61 (76%)	19 (24%)	0	2
41	DT	80/80 (100%)	73 (91%)	7 (9%)	10	33
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	4
42	DU	83/83 (100%)	74 (89%)	9 (11%)	6	24
43	BV	78/78 (100%)	59 (76%)	19 (24%)	0	2
43	DV	78/78 (100%)	68 (87%)	10 (13%)	4	18
44	BW	59/59 (100%)	41 (70%)	18 (30%)	0	1
44	DW	59/59 (100%)	42 (71%)	17 (29%)	0	1
45	BX	67/67 (100%)	54 (81%)	13 (19%)	1	5
45	DX	67/67 (100%)	58 (87%)	9 (13%)	4	16
46	BY	55/55 (100%)	41 (74%)	14 (26%)	0	1
46	DY	55/55 (100%)	52 (94%)	3 (6%)	21	52
47	BZ	48/48 (100%)	33 (69%)	15 (31%)	0	1
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	2	9
48	B0	47/47 (100%)	39 (83%)	8 (17%)	2	9
48	D0	47/47 (100%)	39 (83%)	8 (17%)	2	9
49	B1	45/45 (100%)	37 (82%)	8 (18%)	2	7
49	D1	45/45 (100%)	41 (91%)	4 (9%)	9	32
50	B2	38/38 (100%)	29 (76%)	9 (24%)	1	2
50	D2	38/38 (100%)	33 (87%)	5 (13%)	4	17
51	B3	51/51 (100%)	44 (86%)	7 (14%)	3	16
51	D3	51/51 (100%)	40 (78%)	11 (22%)	1	4
52	B4	34/34 (100%)	28 (82%)	6 (18%)	2	8
52	D4	34/34 (100%)	29 (85%)	5 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
54	CG	123/123 (100%)	102 (83%)	21 (17%)	2 9
55	CM	91/91 (100%)	80 (88%)	11 (12%)	5 20
56	CP	65/65 (100%)	57 (88%)	8 (12%)	4 20
58	DF	149/149 (100%)	123 (83%)	26 (17%)	2 8
All	All	9331/9339 (100%)	7786 (83%)	1545 (17%)	2 9

5 of 1545 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CC	183	TYR
19	CS	11	ASP
4	CD	160	LEU
3	CC	182	ASP
9	CI	37	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
19	CS	51	HIS
37	DP	74	GLN
24	DC	57	HIS
28	DG	44	HIS
41	DT	15	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	363 (23%)	63 (4%)
22	BA	2850/2903 (98%)	554 (19%)	87 (3%)
22	DA	2837/2903 (97%)	869 (30%)	183 (6%)
23	BB	117/118 (99%)	19 (16%)	0
53	CA	1529/1530 (99%)	445 (29%)	81 (5%)
57	DB	116/117 (99%)	33 (28%)	7 (6%)
All	All	8981/9104 (98%)	2283 (25%)	421 (4%)

5 of 2283 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A

5 of 421 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	DA	14	A
22	DA	800	A
22	DA	2667	C
22	DA	103	A
22	DA	389	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 363 ligands modelled in this entry, 362 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	TEL	BA	3135	-	59,62,62	2.30	11 (18%)	77,92,92	3.45	30 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	TEL	BA	3135	-	1/1/19/19	10/73/108/108	0/4/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	3135	TEL	O16-C10	10.86	1.37	1.21
60	BA	3135	TEL	C10-N6	8.50	1.51	1.35
60	BA	3135	TEL	O5-C10	4.45	1.42	1.35
60	BA	3135	TEL	O9-C4	-4.21	1.39	1.46
60	BA	3135	TEL	O45-C50	-3.39	1.38	1.44

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	BA	3135	TEL	C3-N6-C10	-13.95	93.00	111.69
60	BA	3135	TEL	O5-C10-N6	-10.64	101.29	109.81
60	BA	3135	TEL	O5-C10-O16	-10.15	110.75	122.46
60	BA	3135	TEL	O16-C10-N6	-7.97	117.54	128.01
60	BA	3135	TEL	O5-C2-C3	-7.40	95.68	103.16

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
60	BA	3135	TEL	C3

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	BA	3135	TEL	C2-C3-C7-C12
60	BA	3135	TEL	C2-C3-C7-C13
60	BA	3135	TEL	O18-C13-C19-C23
60	BA	3135	TEL	N6-C11-C17-C22
60	BA	3135	TEL	C17-C22-C27-N31

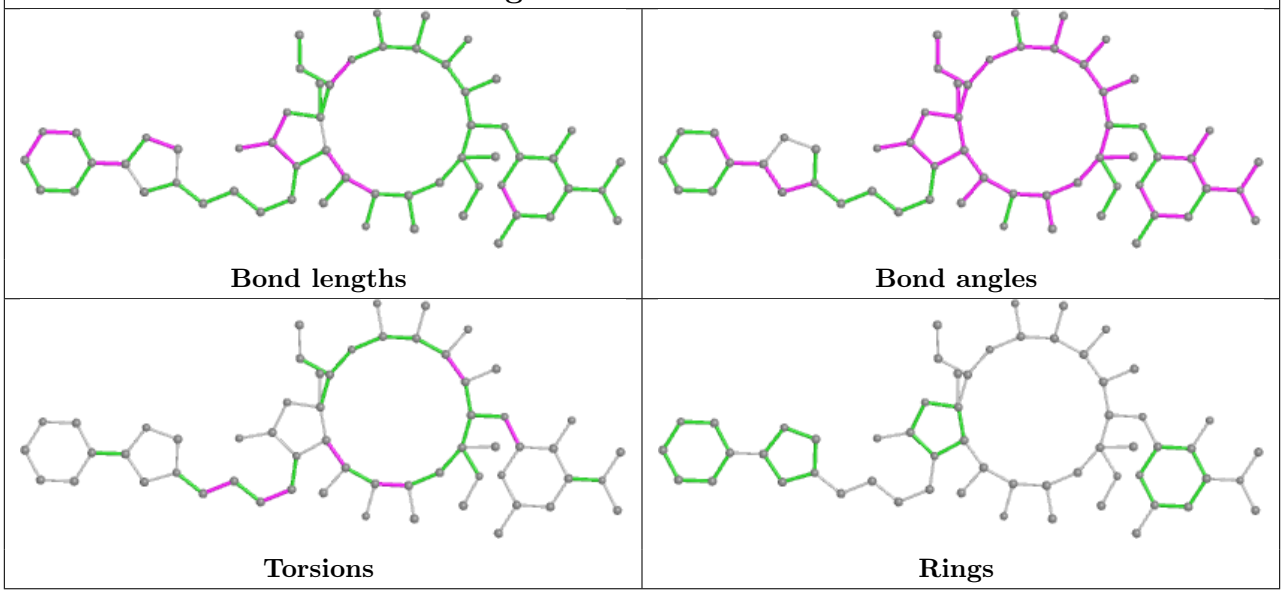
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BA	3135	TEL	8	0

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

Ligand TEL BA 3135



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	1533/1533 (100%)	-0.42	20 (1%)	77	75	31, 83, 185, 422	0
2	AB	218/218 (100%)	1.61	69 (31%)	0	0	67, 161, 222, 300	0
2	CB	218/218 (100%)	1.74	86 (39%)	0	0	76, 168, 231, 274	0
3	AC	206/206 (100%)	0.79	16 (7%)	13	12	53, 101, 156, 201	0
3	CC	206/206 (100%)	0.97	31 (15%)	2	2	76, 138, 202, 264	0
4	AD	205/205 (100%)	0.30	8 (3%)	39	36	48, 93, 168, 305	0
4	CD	205/205 (100%)	-0.16	1 (0%)	91	90	26, 60, 114, 257	0
5	AE	150/150 (100%)	0.14	2 (1%)	77	75	38, 76, 150, 231	0
5	CE	150/150 (100%)	0.24	2 (1%)	77	75	34, 85, 143, 282	0
6	AF	100/100 (100%)	0.20	4 (4%)	38	35	52, 100, 147, 188	0
6	CF	100/100 (100%)	0.25	4 (4%)	38	35	69, 109, 169, 214	0
7	AG	151/151 (100%)	0.67	16 (10%)	6	6	77, 131, 195, 217	0
8	AH	129/129 (100%)	0.37	5 (3%)	39	36	45, 82, 133, 191	0
8	CH	129/129 (100%)	0.66	13 (10%)	7	7	60, 101, 151, 212	0
9	AI	127/127 (100%)	1.06	25 (19%)	1	1	64, 137, 207, 266	0
9	CI	127/127 (100%)	1.51	39 (30%)	0	0	98, 168, 246, 283	0
10	AJ	98/98 (100%)	0.83	14 (14%)	2	2	65, 111, 196, 260	0
10	CJ	98/98 (100%)	2.69	50 (51%)	0	0	94, 178, 248, 272	0
11	AK	117/117 (100%)	0.91	20 (17%)	1	1	44, 108, 190, 238	0
11	CK	117/117 (100%)	0.78	14 (11%)	4	4	49, 112, 169, 192	0
12	AL	123/123 (100%)	-0.03	1 (0%)	86	86	24, 62, 106, 208	0
12	CL	123/123 (100%)	0.44	6 (4%)	29	27	37, 73, 124, 211	0
13	AM	114/114 (100%)	0.51	11 (9%)	8	8	86, 135, 206, 262	0
14	AN	96/100 (96%)	0.54	6 (6%)	20	19	58, 105, 187, 274	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
14	CN	95/100 (95%)	1.83	36 (37%) 0 0	95, 187, 280, 335	0
15	AO	88/88 (100%)	-0.21	1 (1%) 80 80	43, 81, 124, 170	0
15	CO	88/88 (100%)	0.16	2 (2%) 60 58	57, 107, 153, 265	0
16	AP	82/82 (100%)	0.77	12 (14%) 2 2	56, 80, 166, 241	0
17	AQ	80/80 (100%)	0.67	7 (8%) 10 10	44, 78, 145, 219	0
17	CQ	80/80 (100%)	1.01	11 (13%) 2 2	57, 106, 146, 163	0
18	AR	55/55 (100%)	0.42	5 (9%) 9 10	60, 88, 151, 212	0
18	CR	55/55 (100%)	0.05	0 100 100	55, 88, 179, 249	0
19	AS	79/79 (100%)	1.62	27 (34%) 0 0	96, 137, 193, 233	0
19	CS	79/79 (100%)	3.10	50 (63%) 0 0	183, 316, 391, 403	0
20	AT	85/85 (100%)	-0.02	1 (1%) 79 77	47, 84, 131, 157	0
20	CT	85/85 (100%)	1.30	19 (22%) 0 1	66, 115, 191, 210	0
21	AU	51/51 (100%)	2.20	29 (56%) 0 0	96, 152, 206, 217	0
21	CU	51/51 (100%)	0.78	6 (11%) 4 4	66, 117, 183, 253	0
22	BA	2854/2903 (98%)	-0.38	36 (1%) 77 75	5, 32, 160, 403	0
22	DA	2841/2903 (97%)	0.52	117 (4%) 37 34	53, 122, 250, 469	0
23	BB	118/118 (100%)	-0.41	0 100 100	13, 44, 74, 101	0
24	BC	271/271 (100%)	-0.15	9 (3%) 46 43	12, 42, 93, 209	0
24	DC	271/271 (100%)	0.72	24 (8%) 9 10	59, 93, 144, 185	0
25	BD	209/209 (100%)	-0.30	0 100 100	4, 26, 73, 178	0
25	DD	209/209 (100%)	1.17	39 (18%) 1 1	58, 109, 173, 246	0
26	BE	201/201 (100%)	-0.26	0 100 100	5, 43, 103, 156	0
26	DE	201/201 (100%)	2.12	84 (41%) 0 0	65, 192, 378, 459	0
27	BF	177/177 (100%)	0.48	19 (10%) 6 6	27, 75, 156, 242	0
28	BG	176/176 (100%)	0.15	4 (2%) 60 58	22, 62, 121, 186	0
28	DG	176/176 (100%)	1.79	70 (39%) 0 0	100, 185, 264, 328	0
29	BH	149/149 (100%)	3.03	69 (46%) 0 0	49, 179, 279, 375	0
29	DH	149/149 (100%)	2.64	67 (44%) 0 0	93, 184, 287, 326	0
30	BI	141/141 (100%)	2.93	78 (55%) 0 0	136, 253, 308, 367	0
30	DI	141/141 (100%)	3.80	106 (75%) 0 0	167, 294, 351, 377	0
31	BJ	142/142 (100%)	-0.43	0 100 100	7, 23, 64, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
31	DJ	142/142 (100%)	1.14	32 (22%) 0 1	52, 106, 159, 195	0
32	BK	122/122 (100%)	-0.26	0 100 100	10, 31, 80, 254	0
32	DK	122/122 (100%)	1.23	27 (22%) 0 1	57, 91, 150, 229	0
33	BL	143/143 (100%)	-0.24	0 100 100	7, 38, 74, 111	0
33	DL	143/143 (100%)	1.35	37 (25%) 0 0	69, 149, 262, 337	0
34	BM	136/136 (100%)	-0.34	0 100 100	6, 29, 76, 120	0
34	DM	136/136 (100%)	0.99	27 (19%) 1 1	46, 107, 161, 204	0
35	BN	120/120 (100%)	-0.49	0 100 100	9, 25, 46, 155	0
35	DN	120/120 (100%)	1.39	32 (26%) 0 0	73, 124, 194, 293	0
36	BO	116/116 (100%)	-0.02	0 100 100	24, 44, 83, 116	0
36	DO	116/116 (100%)	1.73	44 (37%) 0 0	113, 162, 224, 259	0
37	BP	114/114 (100%)	-0.13	1 (0%) 84 84	11, 41, 104, 161	0
37	DP	114/114 (100%)	0.98	18 (15%) 2 2	63, 105, 164, 195	0
38	BQ	117/117 (100%)	-0.52	1 (0%) 84 84	4, 20, 47, 206	0
38	DQ	117/117 (100%)	1.58	35 (29%) 0 0	67, 108, 191, 312	0
39	BR	103/103 (100%)	-0.35	1 (0%) 82 82	5, 30, 80, 109	0
39	DR	103/103 (100%)	2.45	54 (52%) 0 0	80, 138, 239, 291	0
40	BS	110/110 (100%)	-0.41	1 (0%) 84 84	6, 21, 61, 178	0
40	DS	110/110 (100%)	2.29	55 (50%) 0 0	70, 133, 241, 285	0
41	BT	93/93 (100%)	0.19	4 (4%) 35 33	23, 51, 121, 235	0
41	DT	93/93 (100%)	2.69	52 (55%) 0 0	110, 202, 299, 369	0
42	BU	102/102 (100%)	0.08	3 (2%) 51 50	19, 55, 136, 246	0
42	DU	102/102 (100%)	3.23	64 (62%) 0 0	122, 287, 418, 543	0
43	BV	94/94 (100%)	-0.05	0 100 100	13, 43, 85, 124	0
43	DV	94/94 (100%)	1.67	31 (32%) 0 0	100, 144, 196, 226	0
44	BW	79/79 (100%)	0.14	4 (5%) 28 26	10, 36, 110, 208	0
44	DW	79/79 (100%)	2.30	41 (51%) 0 0	87, 141, 230, 253	0
45	BX	77/77 (100%)	-0.25	0 100 100	15, 46, 88, 135	0
45	DX	77/77 (100%)	1.17	16 (20%) 1 1	67, 118, 172, 239	0
46	BY	63/63 (100%)	0.12	2 (3%) 47 45	34, 75, 134, 210	0
46	DY	63/63 (100%)	1.55	17 (26%) 0 0	130, 305, 419, 450	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
47	BZ	58/58 (100%)	-0.31	0	100	100	6, 24, 74, 116	0
47	DZ	58/58 (100%)	0.96	8 (13%)	2	2	86, 123, 190, 236	0
48	B0	56/56 (100%)	-0.56	0	100	100	3, 22, 75, 168	0
48	D0	56/56 (100%)	1.58	15 (26%)	0	0	66, 132, 242, 278	0
49	B1	50/50 (100%)	0.34	2 (4%)	38	35	30, 50, 98, 178	0
49	D1	50/50 (100%)	1.77	21 (42%)	0	0	98, 155, 211, 275	0
50	B2	46/46 (100%)	-0.47	0	100	100	13, 27, 51, 183	0
50	D2	46/46 (100%)	1.40	11 (23%)	0	0	78, 118, 155, 203	0
51	B3	64/64 (100%)	-0.31	0	100	100	9, 27, 46, 71	0
51	D3	64/64 (100%)	1.92	30 (46%)	0	0	90, 125, 198, 250	0
52	B4	38/38 (100%)	0.34	1 (2%)	56	52	28, 49, 87, 112	0
52	D4	38/38 (100%)	2.88	26 (68%)	0	0	78, 141, 210, 225	0
53	CA	1530/1530 (100%)	0.04	36 (2%)	59	55	38, 100, 272, 376	0
54	CG	150/150 (100%)	2.29	65 (43%)	0	0	118, 209, 283, 333	0
55	CM	113/113 (100%)	2.30	57 (50%)	0	0	196, 344, 437, 471	0
56	CP	80/80 (100%)	0.91	12 (15%)	2	2	59, 91, 145, 249	0
57	DB	117/117 (100%)	0.12	0	100	100	95, 167, 229, 249	0
58	DF	178/178 (100%)	2.30	98 (55%)	0	0	135, 220, 279, 350	0
All	All	20431/20551 (99%)	0.51	2372 (11%)	4	4	3, 97, 258, 543	0

The worst 5 of 2372 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	CS	29	PRO	18.4
29	DH	124	THR	17.9
29	DH	91	PHE	17.5
29	BH	118	PRO	15.2
29	DH	105	ALA	15.2

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DJ	201	1/1	-0.24	1.05	312,312,312,312	0
59	MG	DA	3002	1/1	-0.04	0.64	225,225,225,225	0
59	MG	DA	3005	1/1	-0.03	0.50	284,284,284,284	0
59	MG	DA	3016	1/1	0.07	1.14	214,214,214,214	0
59	MG	DA	3074	1/1	0.10	0.96	247,247,247,247	0
59	MG	DA	3018	1/1	0.16	0.17	125,125,125,125	0
59	MG	DA	3092	1/1	0.25	0.25	119,119,119,119	0
59	MG	DA	3091	1/1	0.30	0.37	154,154,154,154	0
59	MG	DA	3111	1/1	0.35	0.19	179,179,179,179	0
59	MG	DA	3004	1/1	0.35	0.17	122,122,122,122	0
59	MG	DA	3063	1/1	0.37	2.20	213,213,213,213	0
59	MG	DA	3130	1/1	0.41	3.18	280,280,280,280	0
59	MG	DA	3060	1/1	0.41	0.61	198,198,198,198	0
59	MG	DA	3133	1/1	0.43	0.38	198,198,198,198	0
59	MG	DA	3020	1/1	0.44	0.63	240,240,240,240	0
59	MG	CA	1618	1/1	0.45	0.30	146,146,146,146	0
59	MG	DA	3106	1/1	0.45	0.74	316,316,316,316	0
59	MG	DA	3039	1/1	0.45	0.17	79,79,79,79	0
59	MG	DA	3043	1/1	0.47	0.28	179,179,179,179	0
59	MG	DA	3110	1/1	0.48	0.38	146,146,146,146	0
59	MG	DA	3109	1/1	0.49	0.48	184,184,184,184	0
59	MG	DA	3045	1/1	0.50	0.25	160,160,160,160	0
59	MG	DA	3027	1/1	0.51	0.27	157,157,157,157	0
59	MG	DA	3047	1/1	0.51	0.21	142,142,142,142	0
59	MG	DA	3129	1/1	0.52	0.53	210,210,210,210	0
59	MG	CA	1619	1/1	0.53	0.34	210,210,210,210	0
59	MG	DA	3028	1/1	0.54	0.63	222,222,222,222	0
59	MG	DA	3084	1/1	0.55	0.17	201,201,201,201	0
59	MG	DA	3007	1/1	0.56	0.62	248,248,248,248	0
59	MG	DA	3090	1/1	0.56	0.11	78,78,78,78	0
59	MG	CA	1628	1/1	0.56	0.16	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3022	1/1	0.56	0.37	173,173,173,173	0
59	MG	DA	3097	1/1	0.57	0.39	137,137,137,137	0
59	MG	DA	3049	1/1	0.58	0.63	192,192,192,192	0
59	MG	DA	3127	1/1	0.58	0.87	228,228,228,228	0
59	MG	DA	3024	1/1	0.58	0.20	100,100,100,100	0
59	MG	AA	1629	1/1	0.59	0.11	84,84,84,84	0
59	MG	DA	3077	1/1	0.59	0.19	123,123,123,123	0
59	MG	DA	3120	1/1	0.60	0.20	91,91,91,91	0
59	MG	CA	1603	1/1	0.60	0.34	177,177,177,177	0
59	MG	DA	3019	1/1	0.61	0.18	192,192,192,192	0
59	MG	CA	1617	1/1	0.61	0.12	214,214,214,214	0
59	MG	DA	3026	1/1	0.62	0.91	258,258,258,258	0
59	MG	DA	3132	1/1	0.62	0.87	185,185,185,185	0
59	MG	DA	3015	1/1	0.63	0.74	176,176,176,176	0
59	MG	DA	3083	1/1	0.63	0.29	204,204,204,204	0
59	MG	DA	3010	1/1	0.63	0.57	195,195,195,195	0
59	MG	DA	3003	1/1	0.65	0.82	229,229,229,229	0
59	MG	DA	3079	1/1	0.66	0.89	200,200,200,200	0
59	MG	DA	3064	1/1	0.66	0.66	280,280,280,280	0
59	MG	DA	3014	1/1	0.66	0.37	133,133,133,133	0
59	MG	DA	3099	1/1	0.66	0.19	164,164,164,164	0
59	MG	DA	3001	1/1	0.66	0.09	149,149,149,149	0
59	MG	DA	3038	1/1	0.67	0.12	203,203,203,203	0
59	MG	DA	3082	1/1	0.67	0.19	132,132,132,132	0
59	MG	DA	3126	1/1	0.67	0.24	112,112,112,112	0
59	MG	DA	3088	1/1	0.68	0.17	170,170,170,170	0
59	MG	DA	3125	1/1	0.68	0.36	152,152,152,152	0
59	MG	AA	1616	1/1	0.68	0.14	106,106,106,106	0
59	MG	DA	3078	1/1	0.69	0.24	182,182,182,182	0
59	MG	CA	1615	1/1	0.70	0.30	170,170,170,170	0
59	MG	CA	1613	1/1	0.70	0.15	107,107,107,107	0
59	MG	DA	3006	1/1	0.70	0.10	176,176,176,176	0
59	MG	DA	3089	1/1	0.71	0.18	100,100,100,100	0
59	MG	DA	3123	1/1	0.71	0.30	183,183,183,183	0
59	MG	DA	3058	1/1	0.71	0.32	202,202,202,202	0
59	MG	BA	3117	1/1	0.71	0.26	173,173,173,173	0
59	MG	DA	3102	1/1	0.71	0.21	87,87,87,87	0
59	MG	DA	3062	1/1	0.72	0.56	213,213,213,213	0
59	MG	DA	3050	1/1	0.72	0.28	160,160,160,160	0
59	MG	CA	1610	1/1	0.72	0.06	151,151,151,151	0
59	MG	DA	3032	1/1	0.72	0.19	131,131,131,131	0
59	MG	CA	1620	1/1	0.73	0.15	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3044	1/1	0.73	0.17	92,92,92,92	0
59	MG	DA	3086	1/1	0.73	0.39	84,84,84,84	0
59	MG	DA	3098	1/1	0.73	0.33	151,151,151,151	0
59	MG	DA	3011	1/1	0.74	0.39	145,145,145,145	0
59	MG	DA	3008	1/1	0.74	0.17	112,112,112,112	0
59	MG	DA	3030	1/1	0.74	0.31	104,104,104,104	0
59	MG	DA	3071	1/1	0.75	0.18	74,74,74,74	0
59	MG	AA	1627	1/1	0.75	0.37	137,137,137,137	0
59	MG	DA	3035	1/1	0.75	0.14	79,79,79,79	0
59	MG	CA	1637	1/1	0.75	0.11	170,170,170,170	0
59	MG	DA	3041	1/1	0.76	0.15	110,110,110,110	0
59	MG	DA	3087	1/1	0.76	0.28	152,152,152,152	0
59	MG	DA	3059	1/1	0.76	0.39	197,197,197,197	0
59	MG	DA	3113	1/1	0.76	0.12	121,121,121,121	0
59	MG	DA	3116	1/1	0.76	0.12	54,54,54,54	0
59	MG	DA	3056	1/1	0.77	0.18	72,72,72,72	0
59	MG	DA	3033	1/1	0.77	0.32	132,132,132,132	0
59	MG	AA	1619	1/1	0.77	0.69	209,209,209,209	0
59	MG	DA	3036	1/1	0.77	0.58	222,222,222,222	0
59	MG	BA	3068	1/1	0.77	0.09	151,151,151,151	0
59	MG	DA	3053	1/1	0.77	0.25	98,98,98,98	0
61	ZN	D4	101	1/1	0.77	0.10	157,157,157,157	0
59	MG	DA	3040	1/1	0.78	0.15	65,65,65,65	0
59	MG	DA	3072	1/1	0.78	0.16	131,131,131,131	0
59	MG	DA	3104	1/1	0.78	0.16	33,33,33,33	0
59	MG	DA	3021	1/1	0.78	0.15	83,83,83,83	0
59	MG	AA	1626	1/1	0.79	0.10	52,52,52,52	0
59	MG	CA	1601	1/1	0.79	0.10	120,120,120,120	0
59	MG	DC	301	1/1	0.79	0.25	155,155,155,155	0
59	MG	AA	1617	1/1	0.79	0.16	147,147,147,147	0
59	MG	DA	3037	1/1	0.79	0.11	97,97,97,97	0
59	MG	DA	3115	1/1	0.80	0.21	126,126,126,126	0
59	MG	AA	1603	1/1	0.80	0.14	131,131,131,131	0
59	MG	CA	1623	1/1	0.80	0.17	121,121,121,121	0
59	MG	CA	1608	1/1	0.80	0.17	44,44,44,44	0
59	MG	BA	3007	1/1	0.80	0.15	104,104,104,104	0
59	MG	BA	3018	1/1	0.80	0.14	44,44,44,44	0
59	MG	DA	3048	1/1	0.80	0.15	95,95,95,95	0
59	MG	CA	1626	1/1	0.81	0.40	196,196,196,196	0
59	MG	CA	1607	1/1	0.81	0.23	134,134,134,134	0
59	MG	DA	3067	1/1	0.81	0.21	64,64,64,64	0
59	MG	CA	1602	1/1	0.81	0.16	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	1614	1/1	0.81	0.71	245,245,245,245	0
59	MG	DA	3108	1/1	0.81	0.67	212,212,212,212	0
59	MG	DA	3017	1/1	0.82	0.13	51,51,51,51	0
59	MG	CA	1612	1/1	0.82	0.41	113,113,113,113	0
59	MG	DB	201	1/1	0.82	0.10	88,88,88,88	0
59	MG	AA	1623	1/1	0.82	0.12	89,89,89,89	0
59	MG	DA	3031	1/1	0.82	0.18	76,76,76,76	0
59	MG	CA	1616	1/1	0.82	0.39	203,203,203,203	0
59	MG	DA	3124	1/1	0.83	0.18	70,70,70,70	0
59	MG	DA	3096	1/1	0.83	0.14	93,93,93,93	0
59	MG	BA	3089	1/1	0.83	0.13	95,95,95,95	0
59	MG	DA	3013	1/1	0.83	0.38	189,189,189,189	0
59	MG	DA	3122	1/1	0.83	0.15	94,94,94,94	0
59	MG	DA	3095	1/1	0.83	0.20	122,122,122,122	0
59	MG	AA	1630	1/1	0.84	0.37	189,189,189,189	0
59	MG	DA	3094	1/1	0.84	0.26	134,134,134,134	0
59	MG	DA	3076	1/1	0.84	0.25	149,149,149,149	0
59	MG	CE	201	1/1	0.84	0.27	132,132,132,132	0
59	MG	AA	1638	1/1	0.84	0.17	47,47,47,47	0
59	MG	DA	3069	1/1	0.84	0.57	233,233,233,233	0
59	MG	BA	3021	1/1	0.84	0.34	158,158,158,158	0
59	MG	CA	1635	1/1	0.84	0.14	201,201,201,201	0
59	MG	DA	3070	1/1	0.85	0.13	60,60,60,60	0
59	MG	CA	1625	1/1	0.85	0.17	48,48,48,48	0
59	MG	DA	3118	1/1	0.85	0.10	59,59,59,59	0
59	MG	BA	3085	1/1	0.85	0.20	124,124,124,124	0
59	MG	AA	1602	1/1	0.85	0.12	152,152,152,152	0
59	MG	AA	1639	1/1	0.85	0.12	109,109,109,109	0
59	MG	DA	3055	1/1	0.85	0.11	72,72,72,72	0
59	MG	DA	3046	1/1	0.85	0.24	125,125,125,125	0
59	MG	BB	201	1/1	0.85	0.28	228,228,228,228	0
59	MG	BA	3057	1/1	0.86	0.14	147,147,147,147	0
59	MG	DA	3128	1/1	0.86	0.31	116,116,116,116	0
59	MG	CA	1636	1/1	0.87	0.30	119,119,119,119	0
59	MG	BA	3004	1/1	0.87	0.24	156,156,156,156	0
59	MG	BA	3045	1/1	0.87	0.14	30,30,30,30	0
59	MG	DA	3042	1/1	0.87	0.20	99,99,99,99	0
59	MG	AA	1625	1/1	0.87	0.08	64,64,64,64	0
59	MG	BA	3003	1/1	0.87	0.10	58,58,58,58	0
59	MG	DA	3051	1/1	0.87	0.15	91,91,91,91	0
59	MG	DA	3073	1/1	0.87	0.08	148,148,148,148	0
59	MG	BA	3059	1/1	0.88	0.33	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1637	1/1	0.88	0.12	96,96,96,96	0
59	MG	DA	3121	1/1	0.88	0.13	122,122,122,122	0
59	MG	CA	1627	1/1	0.88	1.25	237,237,237,237	0
59	MG	DA	3075	1/1	0.88	0.41	172,172,172,172	0
59	MG	DA	3100	1/1	0.88	0.33	105,105,105,105	0
59	MG	CA	1631	1/1	0.89	0.10	160,160,160,160	0
59	MG	DA	3057	1/1	0.89	0.54	185,185,185,185	0
59	MG	BA	3025	1/1	0.89	0.56	165,165,165,165	0
59	MG	BA	3090	1/1	0.89	0.14	120,120,120,120	0
59	MG	BA	3055	1/1	0.89	0.35	215,215,215,215	0
59	MG	DA	3061	1/1	0.89	0.12	131,131,131,131	0
59	MG	DA	3085	1/1	0.89	0.44	132,132,132,132	0
59	MG	BB	202	1/1	0.90	0.06	64,64,64,64	0
59	MG	DA	3012	1/1	0.90	0.21	41,41,41,41	0
59	MG	AA	1628	1/1	0.90	0.35	136,136,136,136	0
59	MG	BA	3031	1/1	0.90	0.11	26,26,26,26	0
59	MG	AA	1614	1/1	0.90	0.17	156,156,156,156	0
59	MG	DA	3117	1/1	0.90	0.20	73,73,73,73	0
59	MG	CA	1606	1/1	0.90	0.16	54,54,54,54	0
59	MG	DA	3103	1/1	0.90	0.17	76,76,76,76	0
59	MG	DA	3081	1/1	0.90	0.28	78,78,78,78	0
59	MG	CA	1638	1/1	0.90	0.09	141,141,141,141	0
59	MG	BA	3131	1/1	0.90	0.40	184,184,184,184	0
59	MG	BA	3005	1/1	0.90	0.11	75,75,75,75	0
59	MG	BA	3070	1/1	0.91	0.21	135,135,135,135	0
59	MG	AA	1607	1/1	0.91	0.07	105,105,105,105	0
59	MG	DA	3009	1/1	0.91	0.14	100,100,100,100	0
59	MG	AA	1621	1/1	0.91	0.17	143,143,143,143	0
59	MG	BA	3034	1/1	0.91	0.28	197,197,197,197	0
59	MG	CA	1611	1/1	0.91	0.19	111,111,111,111	0
59	MG	CA	1629	1/1	0.91	0.24	126,126,126,126	0
59	MG	BA	3103	1/1	0.91	0.17	21,21,21,21	0
59	MG	DA	3119	1/1	0.91	0.11	67,67,67,67	0
59	MG	AA	1641	1/1	0.91	0.23	148,148,148,148	0
59	MG	CA	1621	1/1	0.91	0.18	50,50,50,50	0
59	MG	DC	302	1/1	0.91	0.31	159,159,159,159	0
59	MG	DA	3029	1/1	0.91	0.94	142,142,142,142	0
59	MG	DA	3080	1/1	0.91	0.11	152,152,152,152	0
59	MG	BA	3023	1/1	0.92	0.10	16,16,16,16	0
59	MG	AA	1620	1/1	0.92	0.10	126,126,126,126	0
59	MG	DA	3112	1/1	0.92	0.14	80,80,80,80	0
59	MG	BA	3028	1/1	0.92	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3114	1/1	0.92	0.10	147,147,147,147	0
59	MG	BA	3108	1/1	0.92	0.09	83,83,83,83	0
59	MG	DA	3052	1/1	0.92	0.12	56,56,56,56	0
59	MG	DA	3023	1/1	0.92	0.14	111,111,111,111	0
59	MG	CA	1639	1/1	0.92	0.22	161,161,161,161	0
59	MG	DA	3068	1/1	0.92	0.16	67,67,67,67	0
59	MG	BA	3114	1/1	0.92	0.15	8,8,8,8	0
59	MG	BA	3115	1/1	0.92	0.10	7,7,7,7	0
59	MG	DA	3093	1/1	0.92	0.17	234,234,234,234	0
59	MG	BA	3010	1/1	0.92	0.07	17,17,17,17	0
59	MG	BA	3067	1/1	0.93	0.12	17,17,17,17	0
59	MG	DA	3065	1/1	0.93	0.17	77,77,77,77	0
59	MG	BB	204	1/1	0.93	0.08	23,23,23,23	0
59	MG	BA	3077	1/1	0.93	0.13	38,38,38,38	0
59	MG	CA	1633	1/1	0.93	0.14	138,138,138,138	0
59	MG	BA	3118	1/1	0.93	0.14	23,23,23,23	0
59	MG	DA	3131	1/1	0.93	0.17	91,91,91,91	0
59	MG	DA	3105	1/1	0.93	0.20	61,61,61,61	0
59	MG	CA	1622	1/1	0.93	0.13	190,190,190,190	0
59	MG	DA	3107	1/1	0.93	0.24	91,91,91,91	0
59	MG	BA	3129	1/1	0.93	1.07	243,243,243,243	0
59	MG	BA	3001	1/1	0.93	0.09	117,117,117,117	0
59	MG	BA	3134	1/1	0.93	0.36	196,196,196,196	0
59	MG	BA	3069	1/1	0.93	0.25	136,136,136,136	0
59	MG	BA	3127	1/1	0.94	0.14	2,2,2,2	0
59	MG	BA	3073	1/1	0.94	0.17	17,17,17,17	0
59	MG	BA	3074	1/1	0.94	0.17	85,85,85,85	0
59	MG	BA	3133	1/1	0.94	0.26	146,146,146,146	0
59	MG	BA	3076	1/1	0.94	0.10	119,119,119,119	0
59	MG	BA	3047	1/1	0.94	0.09	151,151,151,151	0
59	MG	BA	3078	1/1	0.94	0.20	31,31,31,31	0
59	MG	BB	203	1/1	0.94	0.11	34,34,34,34	0
59	MG	DA	3101	1/1	0.94	0.13	75,75,75,75	0
59	MG	BA	3081	1/1	0.94	0.18	92,92,92,92	0
59	MG	BA	3048	1/1	0.94	0.17	101,101,101,101	0
59	MG	BA	3088	1/1	0.94	0.10	62,62,62,62	0
59	MG	AA	1618	1/1	0.94	0.18	87,87,87,87	0
59	MG	BA	3024	1/1	0.94	0.12	18,18,18,18	0
59	MG	CA	1630	1/1	0.94	0.27	126,126,126,126	0
59	MG	AA	1624	1/1	0.94	0.15	102,102,102,102	0
59	MG	BA	3060	1/1	0.94	0.30	188,188,188,188	0
59	MG	AA	1631	1/1	0.94	0.17	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1633	1/1	0.94	0.10	62,62,62,62	0
59	MG	AA	1635	1/1	0.94	0.14	73,73,73,73	0
59	MG	AA	1636	1/1	0.94	0.32	199,199,199,199	0
59	MG	BA	3121	1/1	0.94	0.13	35,35,35,35	0
59	MG	BA	3122	1/1	0.94	0.71	155,155,155,155	0
59	MG	BA	3095	1/1	0.95	0.19	117,117,117,117	0
59	MG	CA	1634	1/1	0.95	0.09	74,74,74,74	0
59	MG	CA	1604	1/1	0.95	0.05	57,57,57,57	0
59	MG	BA	3097	1/1	0.95	0.10	33,33,33,33	0
59	MG	BA	3101	1/1	0.95	0.09	18,18,18,18	0
59	MG	BA	3063	1/1	0.95	0.13	12,12,12,12	0
59	MG	AA	1610	1/1	0.95	0.11	201,201,201,201	0
59	MG	CA	1641	1/1	0.95	0.12	82,82,82,82	0
59	MG	BA	3110	1/1	0.95	0.16	89,89,89,89	0
59	MG	BA	3033	1/1	0.95	0.21	14,14,14,14	0
59	MG	AA	1640	1/1	0.95	0.04	84,84,84,84	0
59	MG	BA	3036	1/1	0.95	0.34	187,187,187,187	0
59	MG	BA	3071	1/1	0.95	0.11	7,7,7,7	0
59	MG	DA	3034	1/1	0.95	0.17	78,78,78,78	0
59	MG	BA	3037	1/1	0.95	0.17	24,24,24,24	0
59	MG	BA	3017	1/1	0.95	0.11	33,33,33,33	0
59	MG	BA	3124	1/1	0.95	0.14	33,33,33,33	0
59	MG	BA	3046	1/1	0.95	0.08	12,12,12,12	0
59	MG	AA	1612	1/1	0.95	0.10	85,85,85,85	0
59	MG	AA	1643	1/1	0.95	0.12	43,43,43,43	0
59	MG	BA	3132	1/1	0.95	0.13	1,1,1,1	0
59	MG	AA	1613	1/1	0.95	0.08	50,50,50,50	0
59	MG	BA	3083	1/1	0.95	0.17	37,37,37,37	0
59	MG	AA	1605	1/1	0.95	0.12	52,52,52,52	0
59	MG	BA	3086	1/1	0.95	0.12	134,134,134,134	0
59	MG	AA	1604	1/1	0.95	0.09	121,121,121,121	0
59	MG	AA	1609	1/1	0.95	0.12	54,54,54,54	0
59	MG	BA	3062	1/1	0.95	0.18	5,5,5,5	0
59	MG	BA	3091	1/1	0.95	0.07	49,49,49,49	0
59	MG	BA	3011	1/1	0.96	0.21	126,126,126,126	0
59	MG	BA	3032	1/1	0.96	0.12	25,25,25,25	0
59	MG	DA	3066	1/1	0.96	0.14	61,61,61,61	0
59	MG	BA	3015	1/1	0.96	0.17	95,95,95,95	0
59	MG	BA	3016	1/1	0.96	0.09	4,4,4,4	0
59	MG	AA	1615	1/1	0.96	0.10	128,128,128,128	0
59	MG	AA	1632	1/1	0.96	0.07	90,90,90,90	0
59	MG	CA	1640	1/1	0.96	0.16	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3043	1/1	0.96	0.06	18,18,18,18	0
59	MG	BA	3092	1/1	0.96	0.07	70,70,70,70	0
59	MG	AA	1601	1/1	0.96	0.10	77,77,77,77	0
59	MG	DA	3025	1/1	0.96	0.18	104,104,104,104	0
59	MG	BA	3096	1/1	0.96	0.14	93,93,93,93	0
59	MG	BA	3022	1/1	0.96	0.16	5,5,5,5	0
59	MG	AA	1606	1/1	0.96	0.08	72,72,72,72	0
59	MG	BA	3102	1/1	0.96	0.21	9,9,9,9	0
59	MG	BA	3008	1/1	0.96	0.16	12,12,12,12	0
59	MG	BA	3106	1/1	0.96	0.22	5,5,5,5	0
59	MG	BA	3049	1/1	0.96	0.13	6,6,6,6	0
59	MG	BA	3109	1/1	0.96	0.16	112,112,112,112	0
59	MG	BA	3051	1/1	0.96	0.17	24,24,24,24	0
59	MG	BA	3113	1/1	0.96	0.09	138,138,138,138	0
59	MG	BA	3009	1/1	0.96	0.17	38,38,38,38	0
59	MG	BA	3002	1/1	0.96	0.10	85,85,85,85	0
61	ZN	B4	101	1/1	0.96	0.07	118,118,118,118	0
59	MG	BA	3116	1/1	0.96	0.14	71,71,71,71	0
59	MG	BA	3027	1/1	0.97	0.17	119,119,119,119	0
59	MG	BA	3056	1/1	0.97	0.31	219,219,219,219	0
59	MG	BA	3012	1/1	0.97	0.13	1,1,1,1	0
59	MG	BA	3111	1/1	0.97	0.15	38,38,38,38	0
59	MG	BA	3058	1/1	0.97	0.04	47,47,47,47	0
59	MG	BA	3035	1/1	0.97	0.10	5,5,5,5	0
59	MG	BA	3072	1/1	0.97	0.21	97,97,97,97	0
59	MG	CA	1624	1/1	0.97	0.26	128,128,128,128	0
59	MG	BA	3029	1/1	0.97	0.10	52,52,52,52	0
59	MG	BA	3061	1/1	0.97	0.17	11,11,11,11	0
59	MG	DA	3054	1/1	0.97	0.14	70,70,70,70	0
59	MG	BA	3075	1/1	0.97	0.06	26,26,26,26	0
59	MG	BA	3119	1/1	0.97	0.07	47,47,47,47	0
59	MG	BA	3120	1/1	0.97	0.21	3,3,3,3	0
59	MG	AA	1634	1/1	0.97	0.08	62,62,62,62	0
59	MG	CA	1609	1/1	0.97	0.12	97,97,97,97	0
59	MG	CA	1632	1/1	0.97	0.09	65,65,65,65	0
59	MG	BA	3098	1/1	0.97	0.13	26,26,26,26	0
59	MG	BA	3026	1/1	0.97	0.08	32,32,32,32	0
59	MG	BA	3064	1/1	0.97	0.13	5,5,5,5	0
59	MG	BA	3065	1/1	0.97	0.11	20,20,20,20	0
59	MG	BA	3130	1/1	0.97	0.14	108,108,108,108	0
60	TEL	BA	3135	58/58	0.97	0.22	0,23,68,74	0
59	MG	BA	3066	1/1	0.97	0.10	21,21,21,21	0

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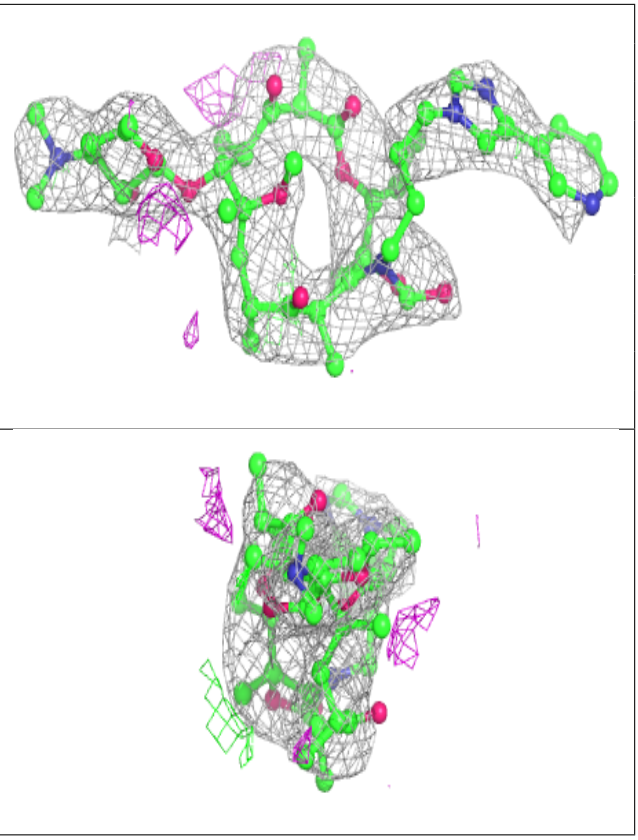
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3107	1/1	0.97	0.16	12,12,12,12	0
59	MG	BA	3052	1/1	0.98	0.16	46,46,46,46	0
59	MG	BA	3126	1/1	0.98	0.15	18,18,18,18	0
59	MG	BA	3100	1/1	0.98	0.13	85,85,85,85	0
59	MG	BA	3128	1/1	0.98	0.12	15,15,15,15	0
59	MG	BA	3079	1/1	0.98	0.17	11,11,11,11	0
59	MG	BA	3080	1/1	0.98	0.04	26,26,26,26	0
59	MG	BA	3053	1/1	0.98	0.15	6,6,6,6	0
59	MG	BA	3104	1/1	0.98	0.16	13,13,13,13	0
59	MG	BA	3105	1/1	0.98	0.17	27,27,27,27	0
59	MG	BA	3082	1/1	0.98	0.11	109,109,109,109	0
59	MG	BA	3054	1/1	0.98	0.09	58,58,58,58	0
59	MG	BA	3084	1/1	0.98	0.16	3,3,3,3	0
59	MG	BA	3040	1/1	0.98	0.18	13,13,13,13	0
59	MG	BA	3041	1/1	0.98	0.17	21,21,21,21	0
59	MG	BA	3087	1/1	0.98	0.12	36,36,36,36	0
59	MG	BA	3112	1/1	0.98	0.09	41,41,41,41	0
59	MG	BA	3006	1/1	0.98	0.07	31,31,31,31	0
59	MG	AA	1611	1/1	0.98	0.07	60,60,60,60	0
59	MG	CA	1605	1/1	0.98	0.14	32,32,32,32	0
59	MG	AA	1608	1/1	0.98	0.22	47,47,47,47	0
59	MG	BA	3013	1/1	0.98	0.19	1,1,1,1	0
59	MG	BA	3014	1/1	0.98	0.21	44,44,44,44	0
59	MG	BA	3093	1/1	0.98	0.07	35,35,35,35	0
59	MG	BA	3094	1/1	0.98	0.06	22,22,22,22	0
59	MG	AA	1642	1/1	0.98	0.14	36,36,36,36	0
59	MG	BA	3050	1/1	0.98	0.09	33,33,33,33	0
59	MG	BA	3030	1/1	0.98	0.17	9,9,9,9	0
59	MG	BA	3123	1/1	0.98	0.14	11,11,11,11	0
59	MG	BA	3039	1/1	0.99	0.16	8,8,8,8	0
59	MG	BA	3019	1/1	0.99	0.18	13,13,13,13	0
59	MG	AA	1622	1/1	0.99	0.19	40,40,40,40	0
59	MG	BA	3042	1/1	0.99	0.11	16,16,16,16	0
59	MG	BA	3125	1/1	0.99	0.14	16,16,16,16	0
59	MG	BA	3038	1/1	0.99	0.10	12,12,12,12	0
59	MG	BA	3044	1/1	0.99	0.06	43,43,43,43	0
59	MG	BA	3099	1/1	0.99	0.20	8,8,8,8	0
59	MG	BA	3020	1/1	1.00	0.12	11,11,11,11	0

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

Electron density around TEL BA 3135:

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



6.5 Other polymers (i)

There are no such residues in this entry.