wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 05:54 PM EDT

PDB ID	:	4V6E
Title	:	Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting
Authors	:	Zhang, W.; Dunkle, J.A.; Cate, J.H.D.
Deposited on	:	2009-06-28
Resolution	:	3.71 Å(reported)

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

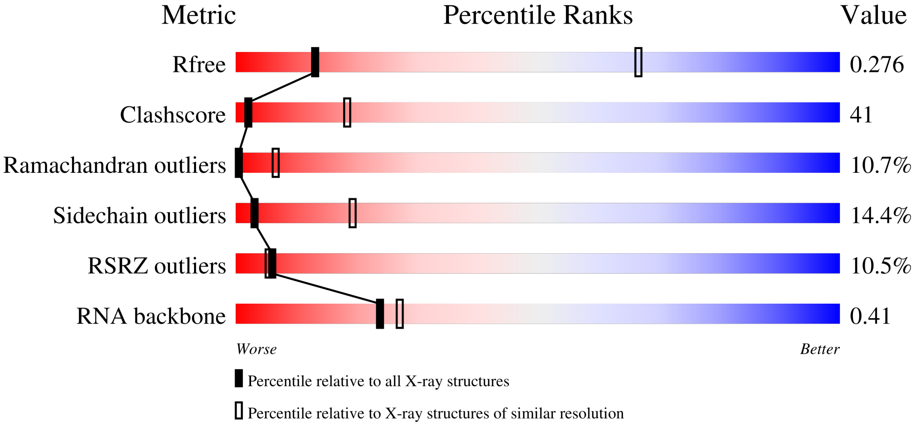
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

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

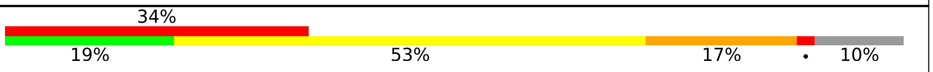
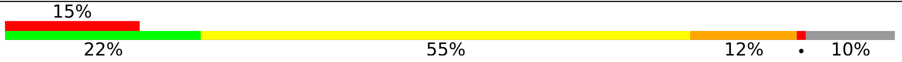
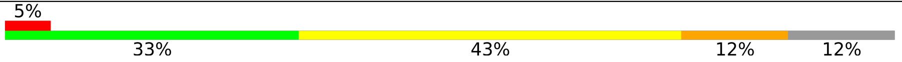
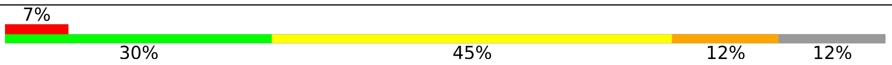
The reported resolution of this entry is 3.71 Å.

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	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)
RNA backbone	3102	1027 (4.40-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AB	241	
1	CB	241	
2	AC	233	
2	CC	233	

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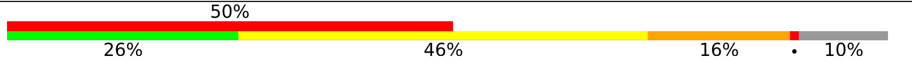
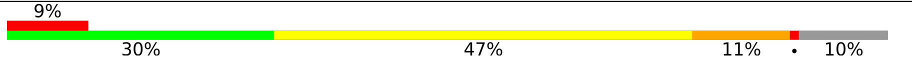
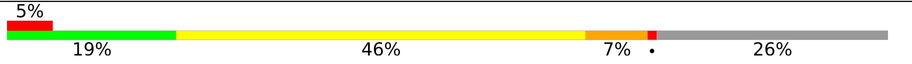
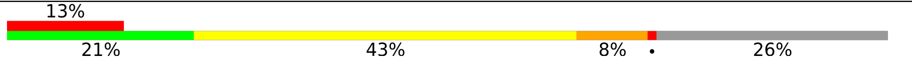
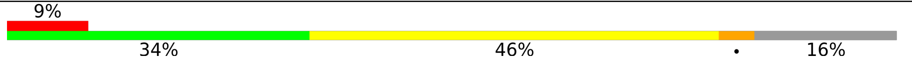
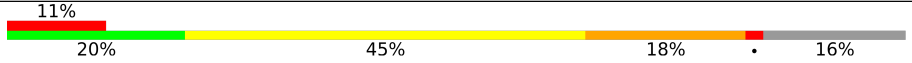
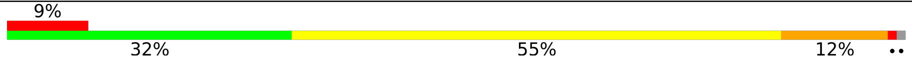
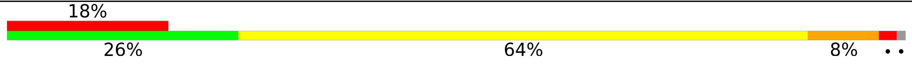
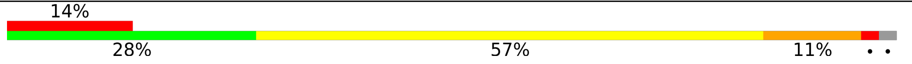
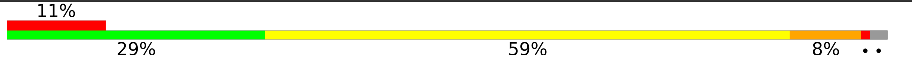
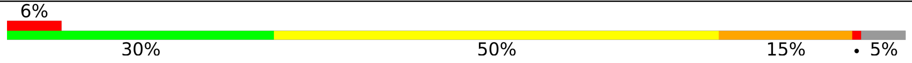
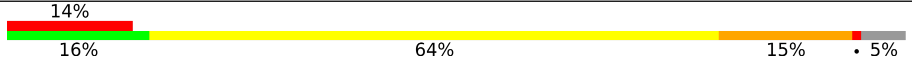
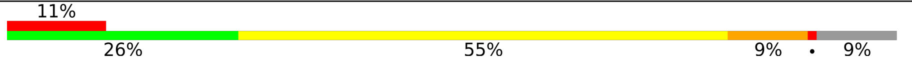
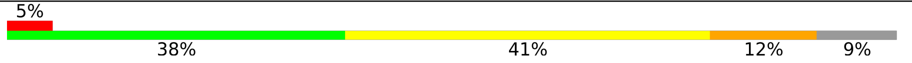
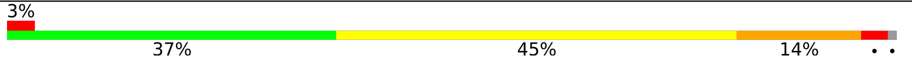
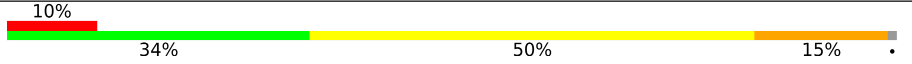
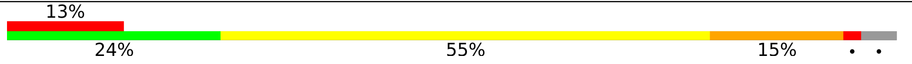
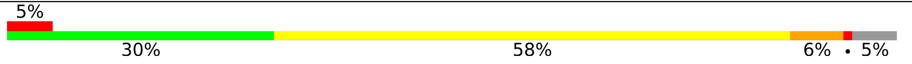
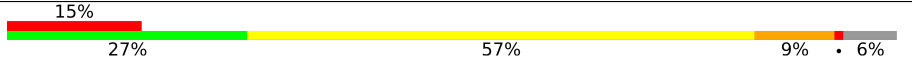
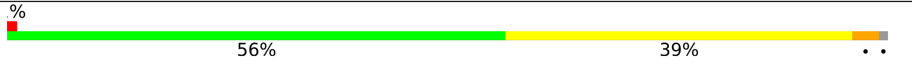
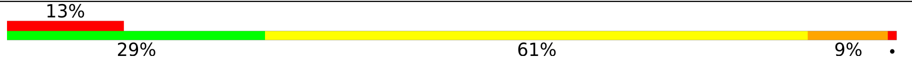
Mol	Chain	Length	Quality of chain
3	AD	206	
3	CD	206	
4	AE	167	
4	CE	167	
5	AF	135	
5	CF	135	
6	AG	179	
6	CG	179	
7	AH	130	
7	CH	130	
8	AI	130	
8	CI	130	
9	AJ	103	
9	CJ	103	
10	AK	129	
10	CK	129	
11	AL	124	
11	CL	124	
12	AM	118	
12	CM	118	
13	AN	101	
13	CN	101	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	28% 37% 48% 13% •
16	AQ	84	6% 30% 46% 18% • 5%
16	CQ	84	19% 31% 52% 12% 5%
17	AR	75	11% 31% 41% • 27%
17	CR	75	4% 24% 45% • • 27%
18	AS	92	29% 43% 37% 5% 14%
18	CS	92	28% 29% 42% 14% 14%
19	AT	87	3% 37% 51% 9% • •
19	CT	87	29% 45% 45% 7% • •
20	AU	71	8% 21% 37% 14% 28%
20	CU	71	3% 21% 30% 20% • 28%
21	AA	1533	% 17% 49% 16% 18%
22	AV	17	6% 24% 53% 24%
22	AX	17	6% 35% 53% 12%
22	CV	17	6% 18% 59% 24%
22	CX	17	47% 41% 47% 12%
23	AW	6	50% 33% 17%
23	CW	6	83% 17%
24	BA	2903	% 16% 43% 21% 19% •
24	DA	2903	5% 15% 45% 19% 20% •
25	BB	118	24% 42% 15% 19%
26	BC	273	% 38% 42% 16% • •
26	DC	273	9% 32% 56% 11% •
27	BD	209	% 36% 40% 21% •
27	DD	209	33% 35% 48% 16% •

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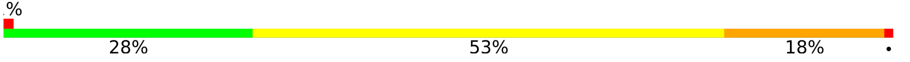
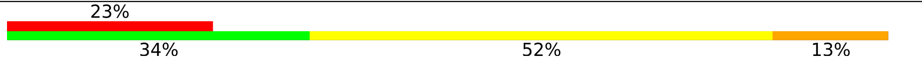
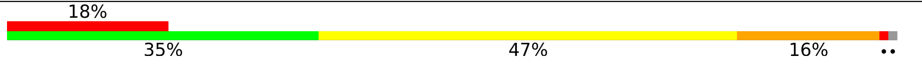
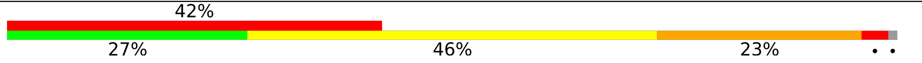
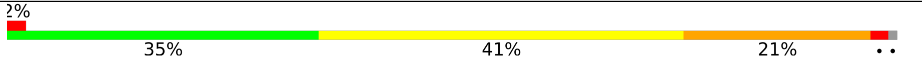
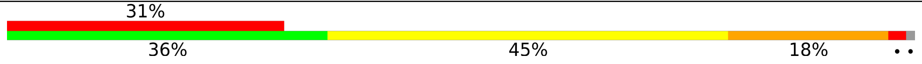
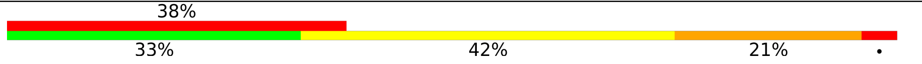
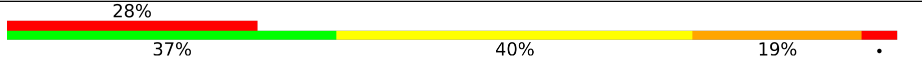
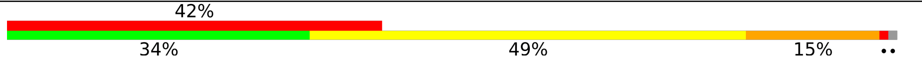
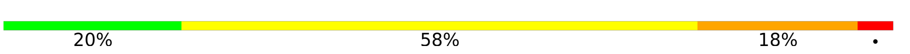
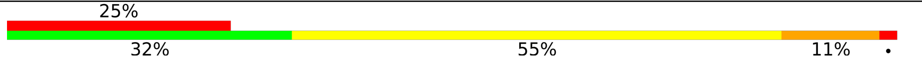
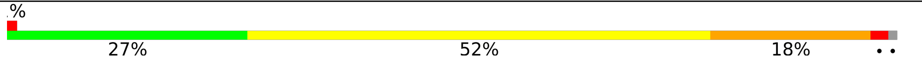
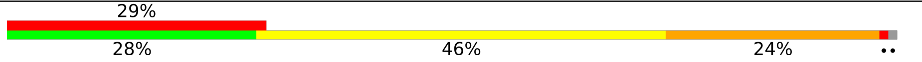
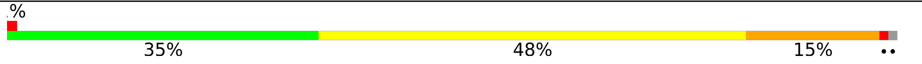
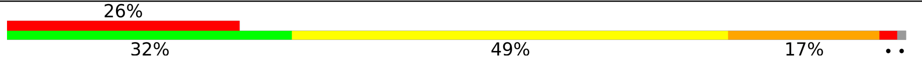
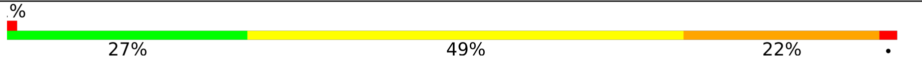
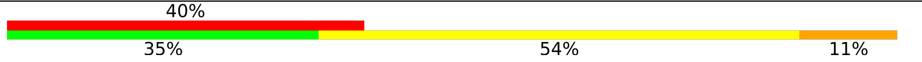
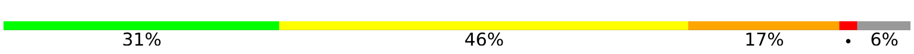
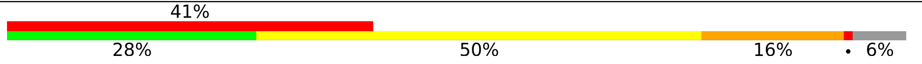
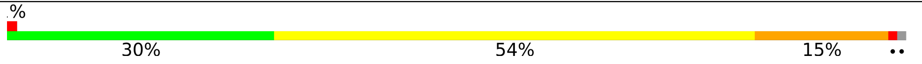
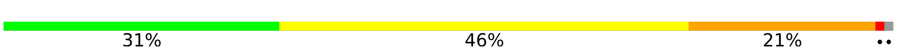
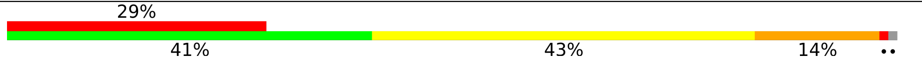
Mol	Chain	Length	Quality of chain
28	BE	201	 % 28% 53% 18% •
28	DE	201	 23% 34% 52% 13%
29	BF	179	 18% 35% 47% 16% ••
29	DF	179	 42% 27% 46% 23% • •
30	BG	177	 2% 35% 41% 21% • •
30	DG	177	 31% 36% 45% 18% • •
31	BH	149	 38% 33% 42% 21% •
31	DH	149	 28% 37% 40% 19% •
32	BI	142	 42% 34% 49% 15% ••
32	DI	142	 61% 42% 46% 10% • •
33	BJ	142	 20% 58% 18% •
33	DJ	142	 25% 32% 55% 11% •
34	BK	123	 % 27% 52% 18% • •
34	DK	123	 29% 28% 46% 24% ••
35	BL	144	 % 35% 48% 15% ••
35	DL	144	 26% 32% 49% 17% • •
36	BM	136	 % 27% 49% 22% •
36	DM	136	 40% 35% 54% 11%
37	BN	127	 31% 46% 17% • 6%
37	DN	127	 41% 28% 50% 16% • 6%
38	BO	117	 % 30% 54% 15% ••
38	DO	117	 48% 35% 56% 8% ••
39	BP	115	 31% 46% 21% ••
39	DP	115	 29% 41% 43% 14% ••
40	BQ	118	 31% 50% 18% •

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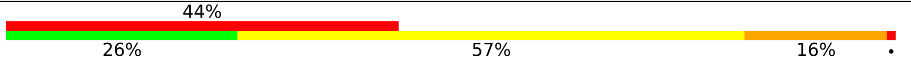
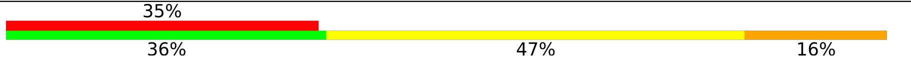
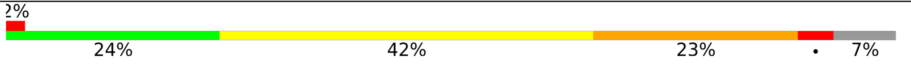
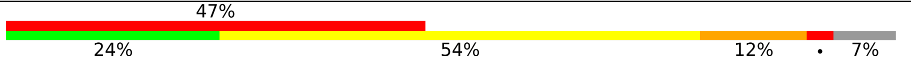
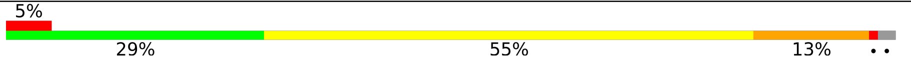
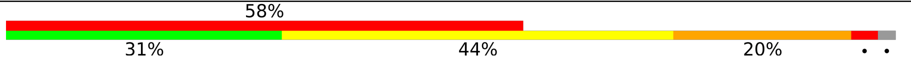
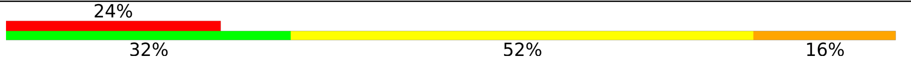
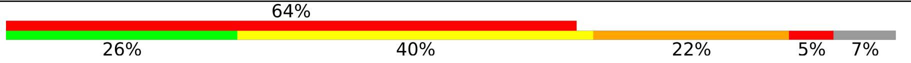
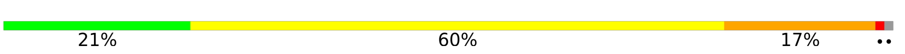
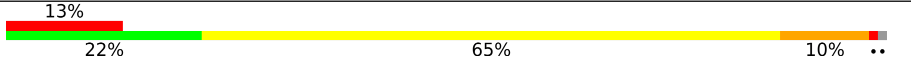
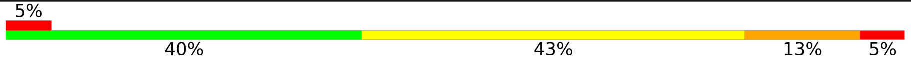
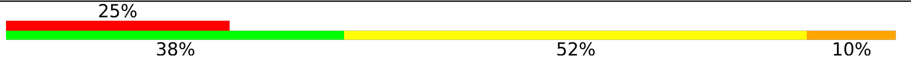
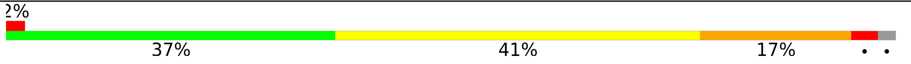
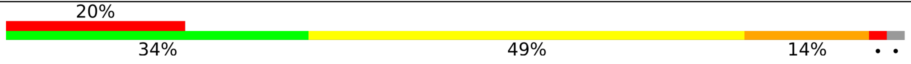
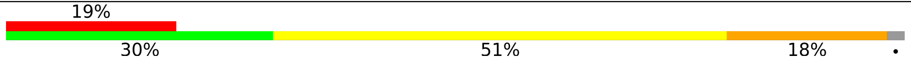
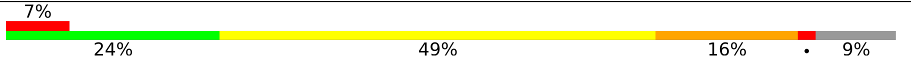
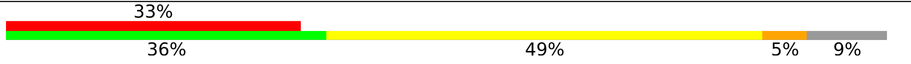
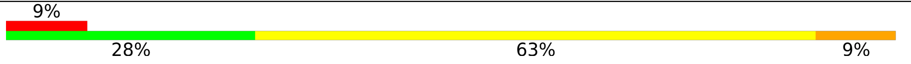
Mol	Chain	Length	Quality of chain
40	DQ	118	 21% 34% 53% 13% •
41	BR	103	 36% 42% 22%
41	DR	103	 44% 26% 57% 16% •
42	BS	110	 37% 43% 19% •
42	DS	110	 35% 36% 47% 16%
43	BT	100	 2% 24% 42% 23% • 7%
43	DT	100	 47% 24% 54% 12% • 7%
44	BU	104	 5% 29% 55% 13% • •
44	DU	104	 58% 31% 44% 20% • •
45	BV	94	 50% 38% 12%
45	DV	94	 24% 32% 52% 16%
46	BW	85	 2% 16% 34% 36% 6% 7%
46	DW	85	 64% 26% 40% 22% 5% 7%
47	BX	78	 21% 60% 17% ••
47	DX	78	 13% 22% 65% 10% ••
48	BY	63	 5% 40% 43% 13% 5%
48	DY	63	 25% 38% 52% 10%
49	BZ	59	 2% 37% 41% 17% • •
49	DZ	59	 20% 34% 49% 14% • •
50	B0	57	 42% 40% 16% •
50	D0	57	 19% 30% 51% 18% •
51	B1	55	 7% 24% 49% 16% • 9%
51	D1	55	 33% 36% 49% 5% 9%
52	B2	46	 46% 37% 17%
52	D2	46	 9% 28% 63% 9%

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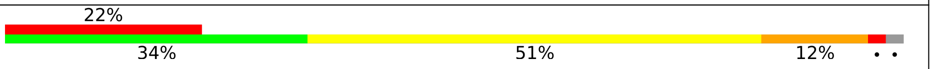
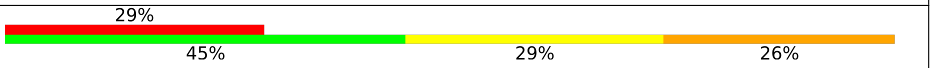
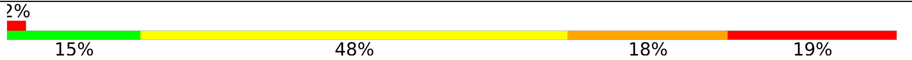
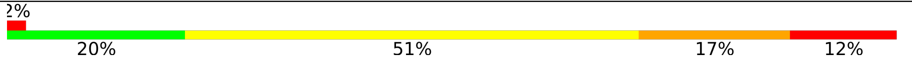
Mol	Chain	Length	Quality of chain
53	B3	65	
53	D3	65	
54	B4	38	
54	D4	38	
55	CA	1530	
56	DB	117	

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
57	MG	AA	1619	-	-	-	X
57	MG	AA	1637	-	-	-	X
57	MG	BA	3115	-	-	-	X
57	MG	CA	1614	-	-	-	X
57	MG	CA	1619	-	-	-	X
57	MG	CA	1620	-	-	-	X
57	MG	D4	101	-	-	-	X
57	MG	DA	3002	-	-	-	X
57	MG	DA	3003	-	-	-	X
57	MG	DA	3005	-	-	-	X
57	MG	DA	3015	-	-	-	X
57	MG	DA	3016	-	-	-	X
57	MG	DA	3020	-	-	-	X
57	MG	DA	3022	-	-	-	X
57	MG	DA	3029	-	-	-	X
57	MG	DA	3038	-	-	-	X
57	MG	DA	3041	-	-	-	X
57	MG	DA	3058	-	-	-	X
57	MG	DA	3060	-	-	-	X
57	MG	DA	3063	-	-	-	X
57	MG	DA	3064	-	-	-	X
57	MG	DA	3069	-	-	-	X
57	MG	DA	3072	-	-	-	X
57	MG	DA	3075	-	-	-	X
57	MG	DA	3078	-	-	-	X
57	MG	DA	3082	-	-	-	X
57	MG	DA	3094	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3108	-	-	-	X
57	MG	DA	3109	-	-	-	X
57	MG	DA	3121	-	-	-	X
57	MG	DA	3128	-	-	-	X
57	MG	DA	3129	-	-	-	X
57	MG	DJ	201	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 286150 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 protein called 30S ribosomal protein S2.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
6	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

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

- Molecule 21 is a RNA chain called 16S rRNA.

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

- Molecule 22 is a RNA chain called P-site tRNA ASL fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	AX	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	CV	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	CX	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			
23	CW	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
24	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
29	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
34	DK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

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

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is a RNA chain called 16S rRNA.

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

- Molecule 56 is a RNA chain called 5S rRNA.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	43	Total 43	Mg 43	0	0
57	BA	136	Total 136	Mg 136	0	0
57	BB	4	Total 4	Mg 4	0	0
57	BD	1	Total 1	Mg 1	0	0
57	CA	42	Total 42	Mg 42	0	0
57	DA	132	Total 132	Mg 132	0	0
57	DB	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	DC	2	Total Mg 2 2	0	0
57	DJ	1	Total Mg 1 1	0	0
57	D4	1	Total Mg 1 1	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AE	1	Total O 1 1	0	0
59	AL	3	Total O 3 3	0	0
59	AN	6	Total O 6 6	0	0
59	AT	1	Total O 1 1	0	0
59	AU	1	Total O 1 1	0	0
59	AA	196	Total O 196 196	0	0
59	BA	615	Total O 615 615	0	0
59	BB	20	Total O 20 20	0	0
59	BC	8	Total O 8 8	0	0
59	BD	3	Total O 3 3	0	0
59	BE	1	Total O 1 1	0	0
59	BL	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	BN	3	Total O 3 3	0	0
59	BT	1	Total O 1 1	0	0
59	B2	1	Total O 1 1	0	0
59	B3	3	Total O 3 3	0	0
59	B4	2	Total O 2 2	0	0
59	CE	4	Total O 4 4	0	0
59	CI	1	Total O 1 1	0	0
59	CL	1	Total O 1 1	0	0
59	CN	2	Total O 2 2	0	0
59	CT	2	Total O 2 2	0	0
59	CU	2	Total O 2 2	0	0
59	CA	195	Total O 195 195	0	0
59	DA	600	Total O 600 600	0	0
59	DB	4	Total O 4 4	0	0
59	DC	12	Total O 12 12	0	0
59	DD	2	Total O 2 2	0	0
59	DE	3	Total O 3 3	0	0
59	DJ	3	Total O 3 3	0	0
59	DL	6	Total O 6 6	0	0
59	DN	2	Total O 2 2	0	0
59	DT	2	Total O 2 2	0	0

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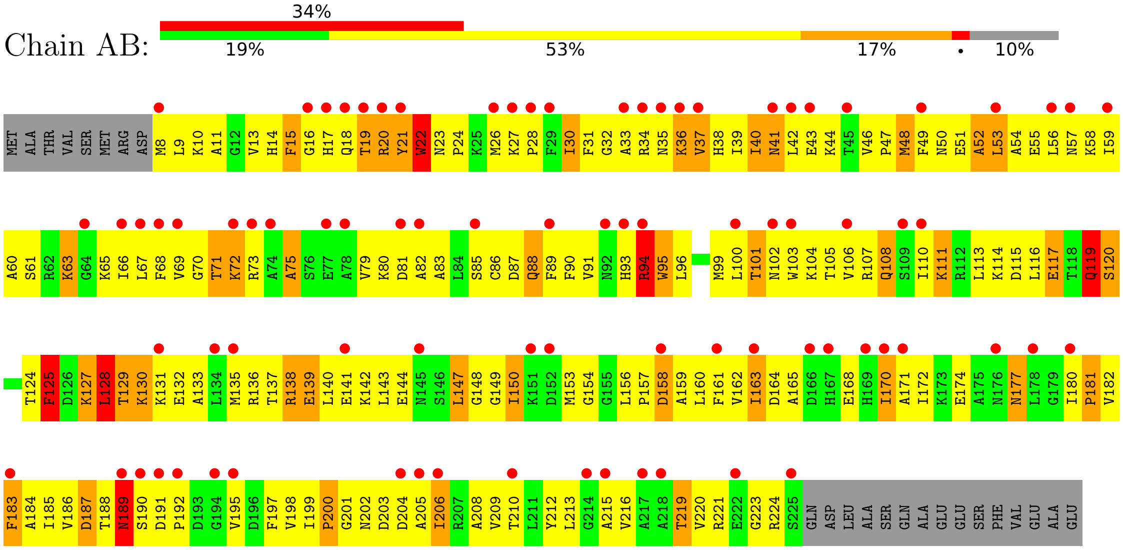
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	DU	1	Total O 1 1	0	0
59	DV	1	Total O 1 1	0	0
59	D2	1	Total O 1 1	0	0
59	D3	1	Total O 1 1	0	0
59	D4	5	Total O 5 5	0	0

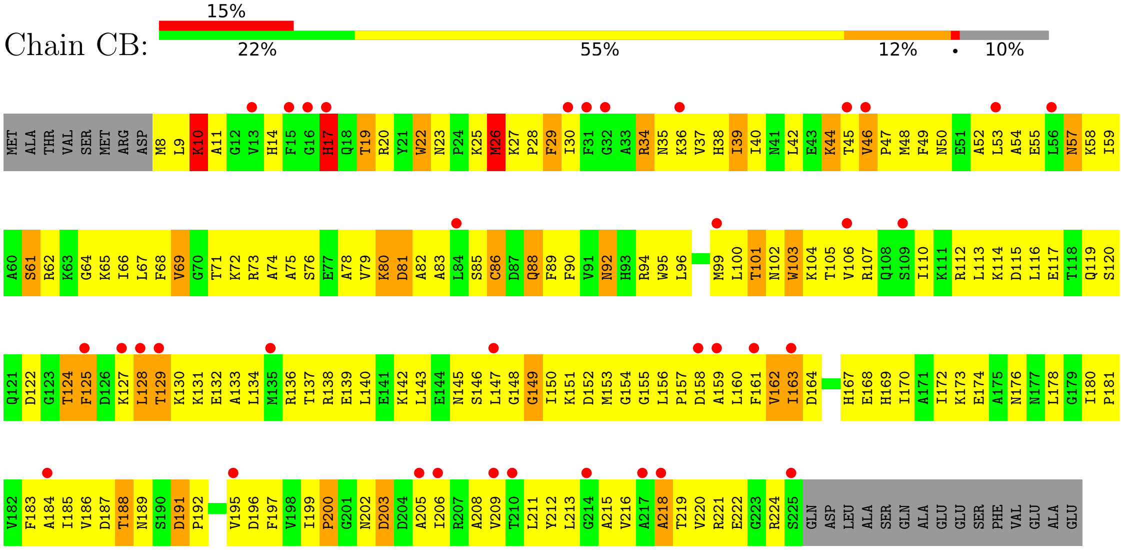
3 Residue-property plots ⓘ

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

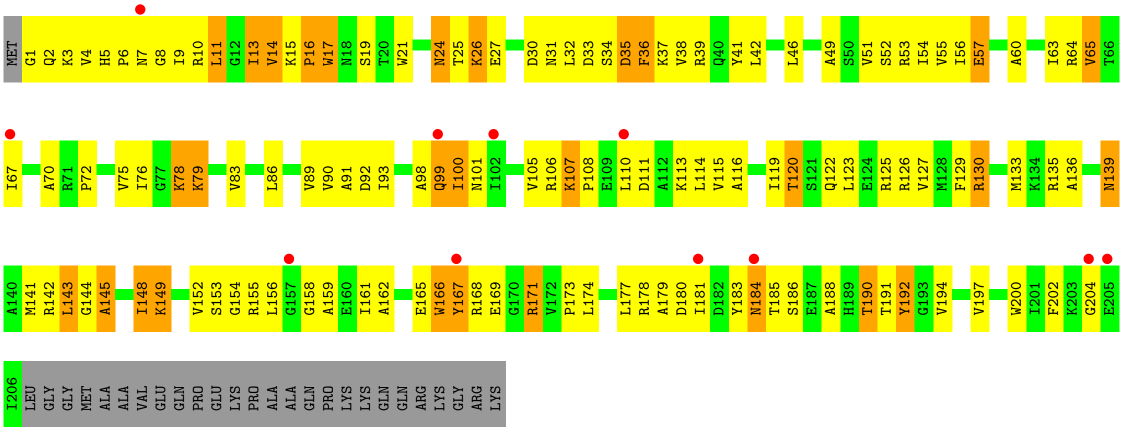
- Molecule 1: 30S ribosomal protein S2



- Molecule 1: 30S ribosomal protein S2

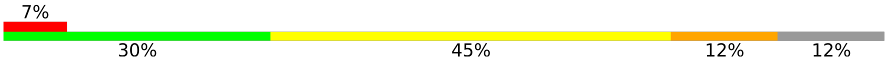


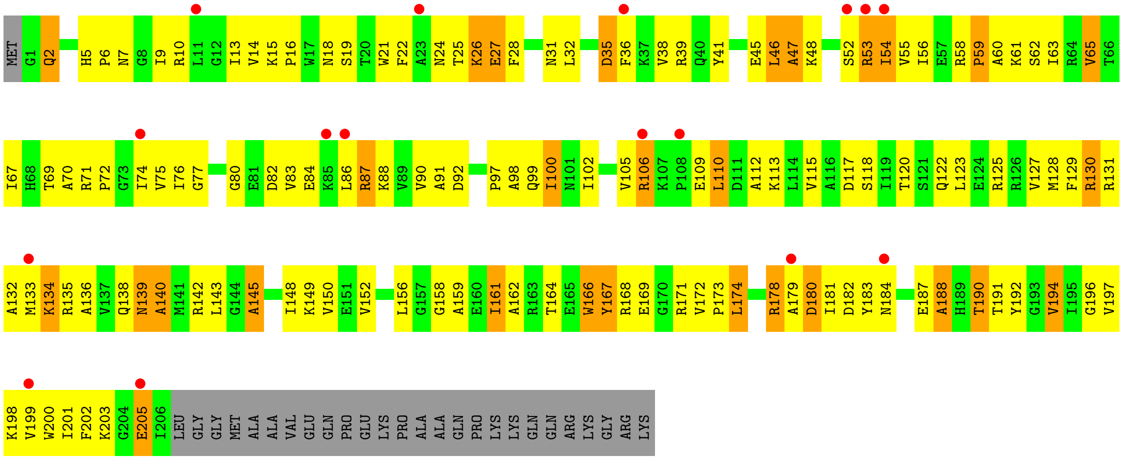
- Molecule 2: 30S ribosomal protein S3



- Molecule 2: 30S ribosomal protein S3

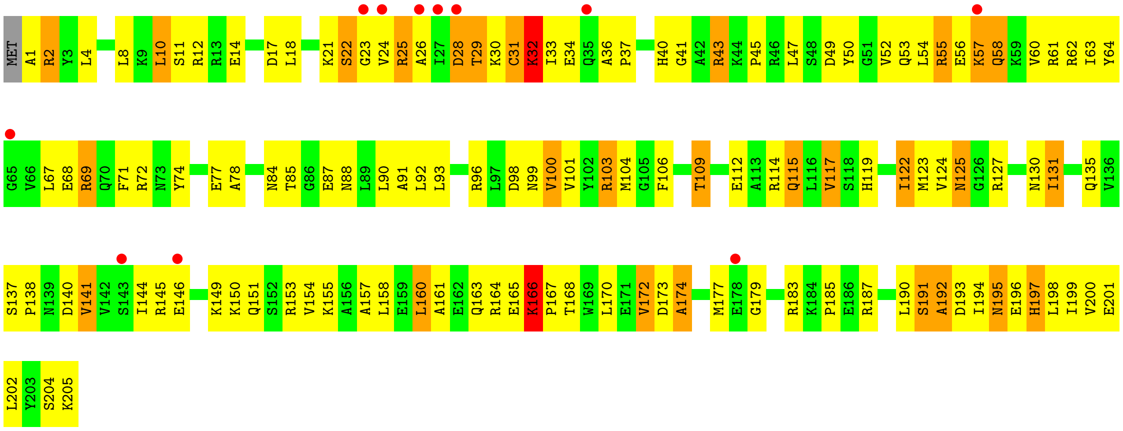
Chain CC:





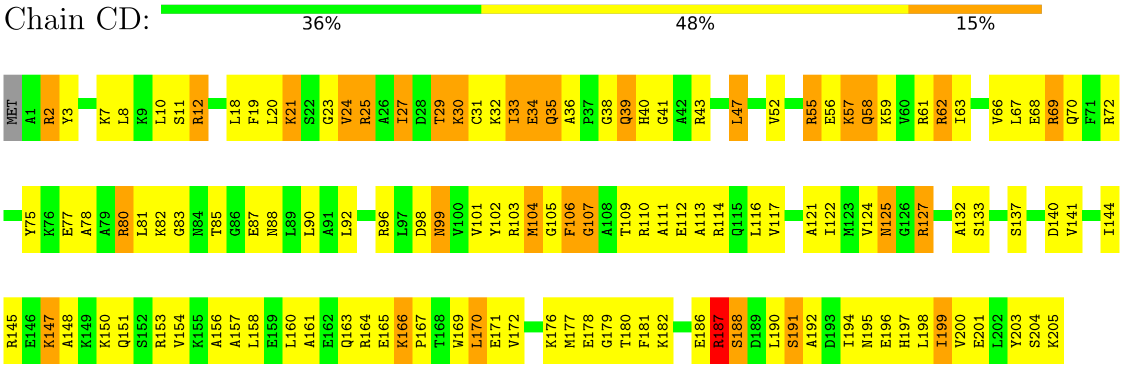
- Molecule 3: 30S ribosomal protein S4

Chain AD:



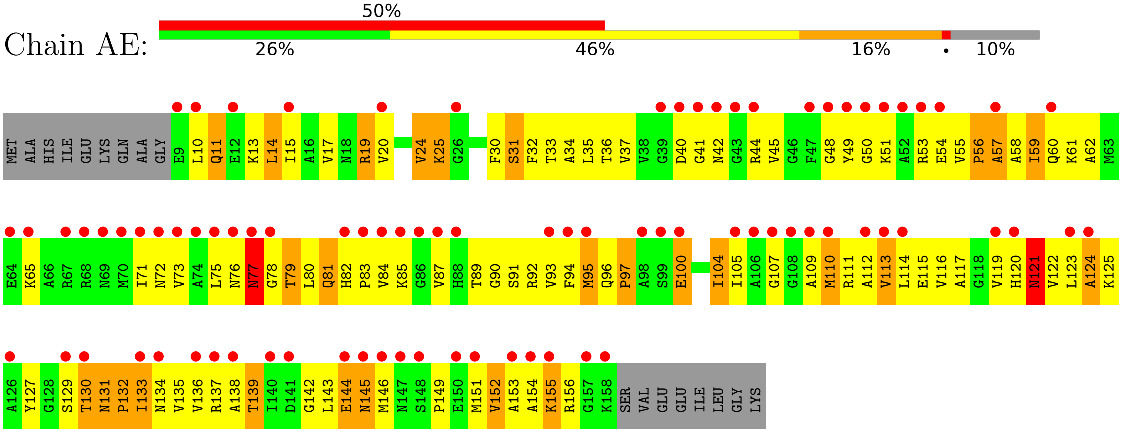
- Molecule 3: 30S ribosomal protein S4

Chain CD:



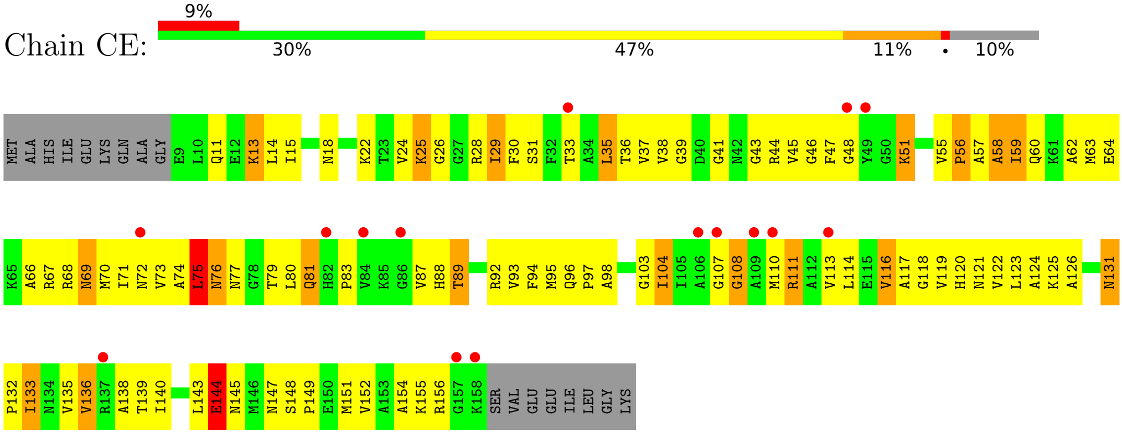
- Molecule 4: 30S ribosomal protein S5

Chain AE:



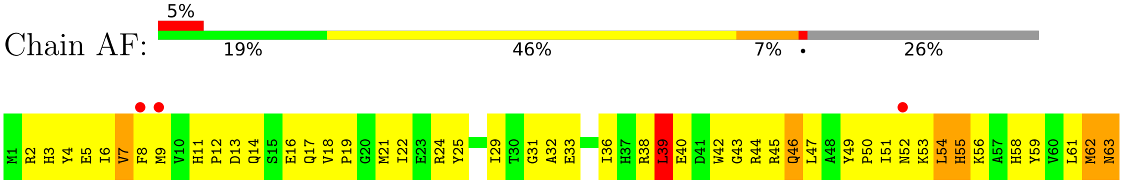
- Molecule 4: 30S ribosomal protein S5

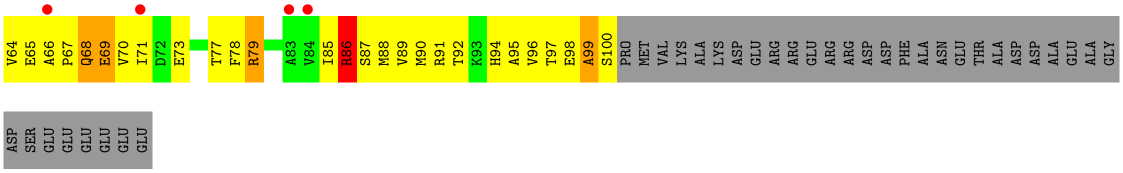
Chain CE:



- Molecule 5: 30S ribosomal protein S6

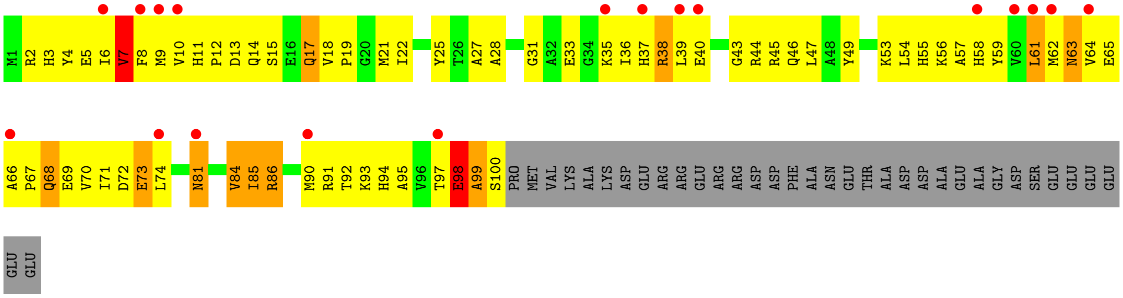
Chain AF:





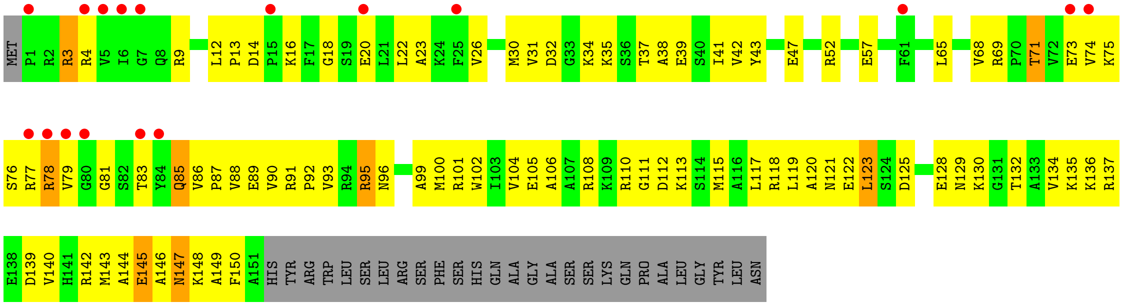
- Molecule 5: 30S ribosomal protein S6

Chain CF:



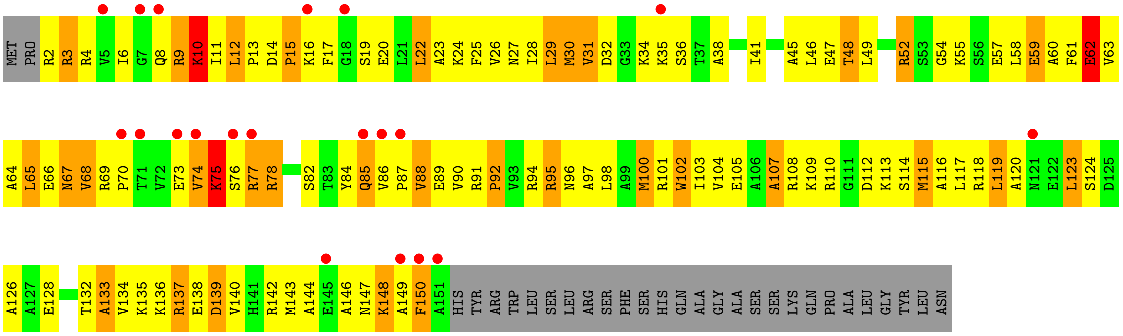
- Molecule 6: 30S ribosomal protein S7

Chain AG:



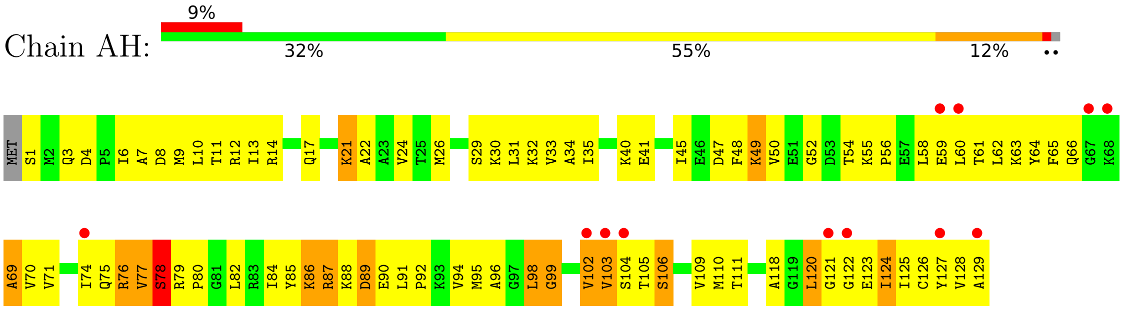
- Molecule 6: 30S ribosomal protein S7

Chain CG:



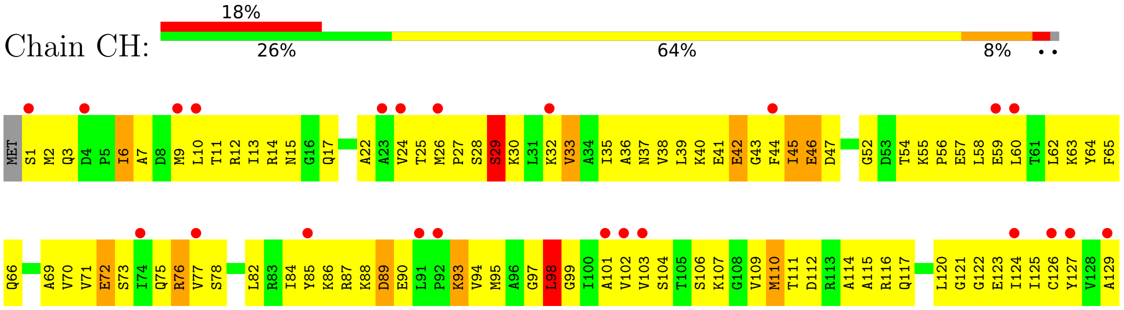
- Molecule 7: 30S ribosomal protein S8

Chain AH:



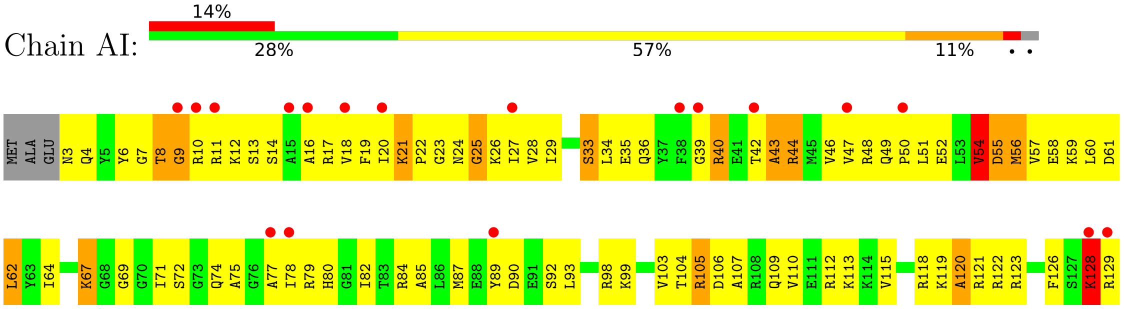
- Molecule 7: 30S ribosomal protein S8

Chain CH:



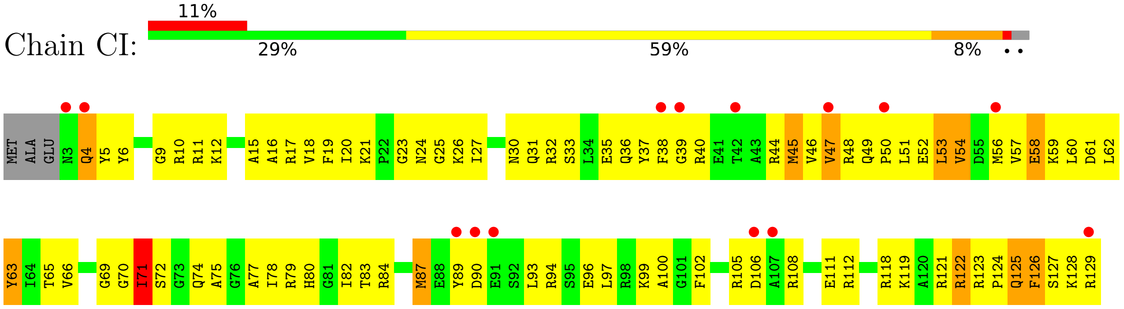
- Molecule 8: 30S ribosomal protein S9

Chain AI:



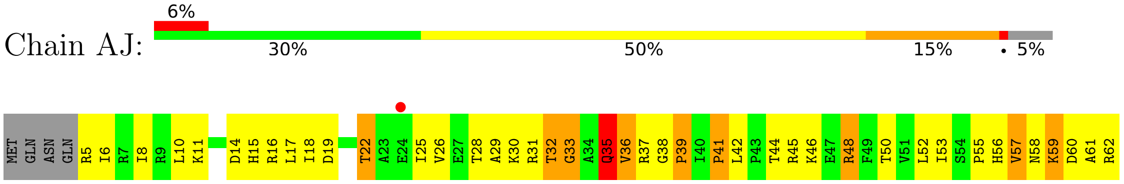
- Molecule 8: 30S ribosomal protein S9

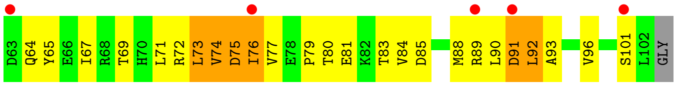
Chain CI:



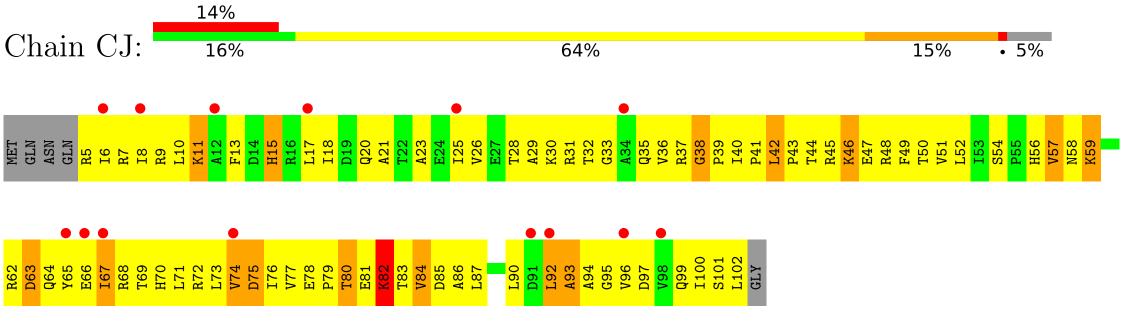
- Molecule 9: 30S ribosomal protein S10

Chain AJ:

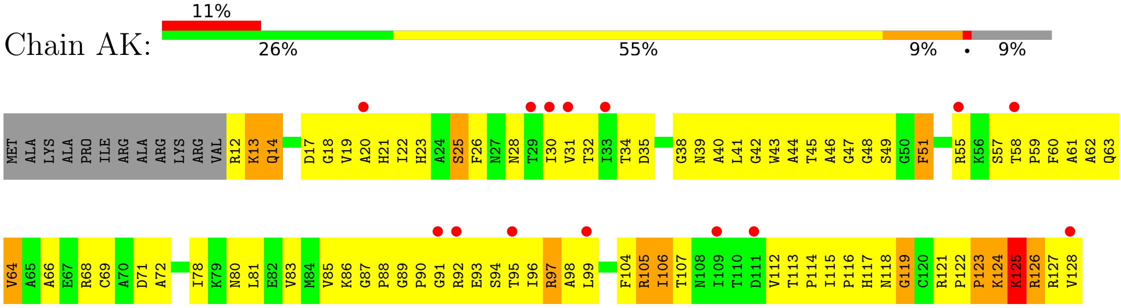




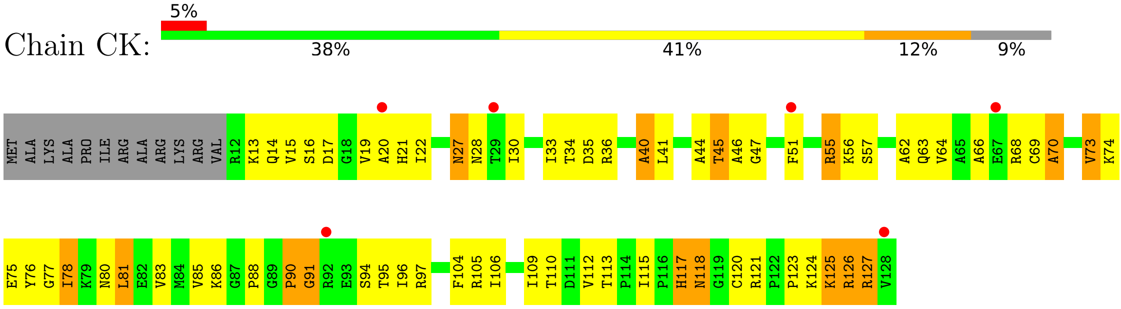
- Molecule 9: 30S ribosomal protein S10



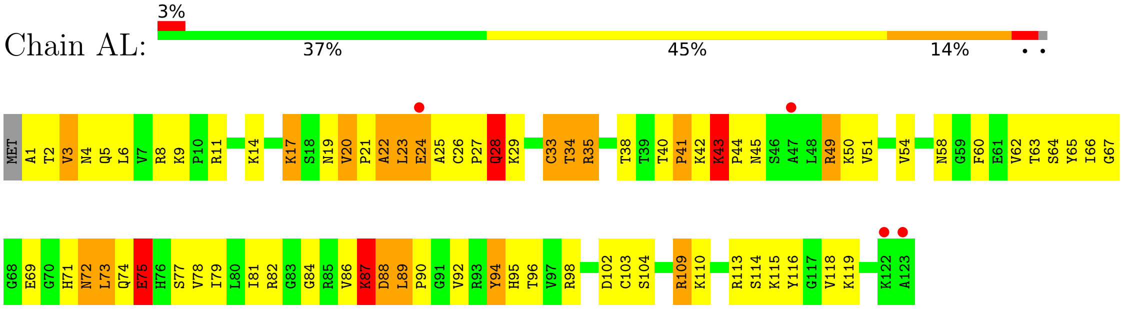
- Molecule 10: 30S ribosomal protein S11



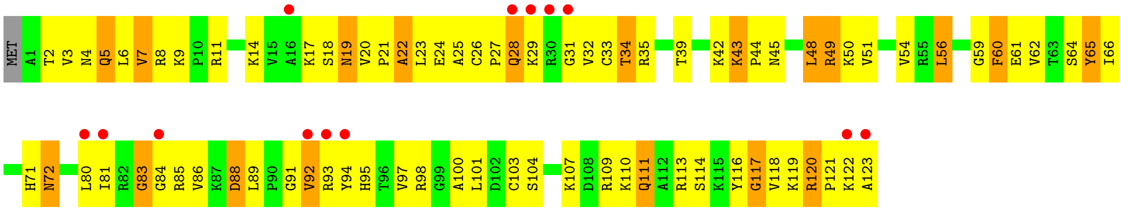
- Molecule 10: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S12

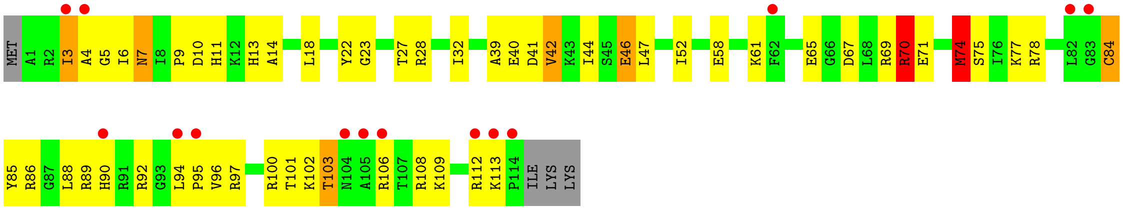


- Molecule 11: 30S ribosomal protein S12



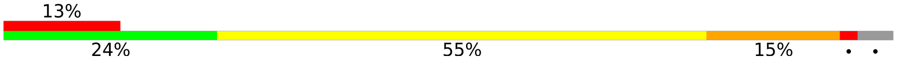
- Molecule 12: 30S ribosomal protein S13

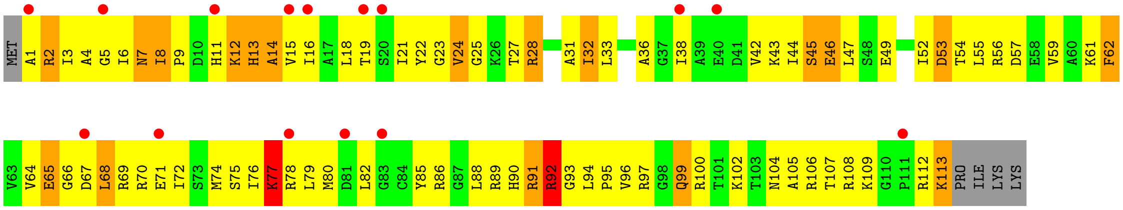
Chain AM:



- Molecule 12: 30S ribosomal protein S13

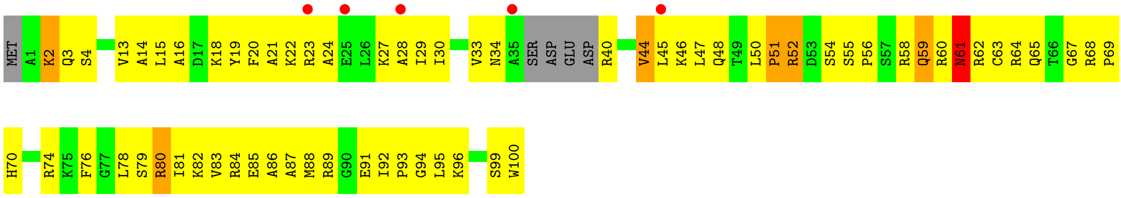
Chain CM:





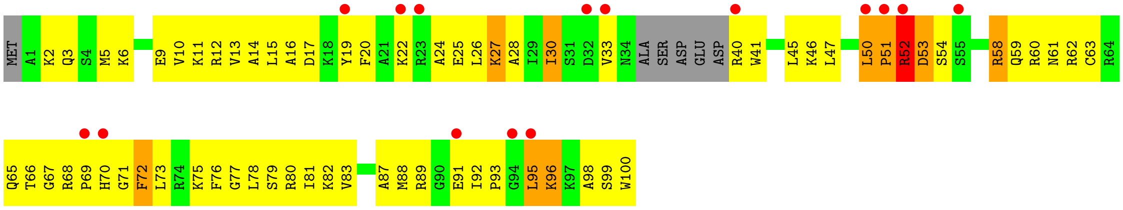
- Molecule 13: 30S ribosomal protein S14

Chain AN:



- Molecule 13: 30S ribosomal protein S14

Chain CN:

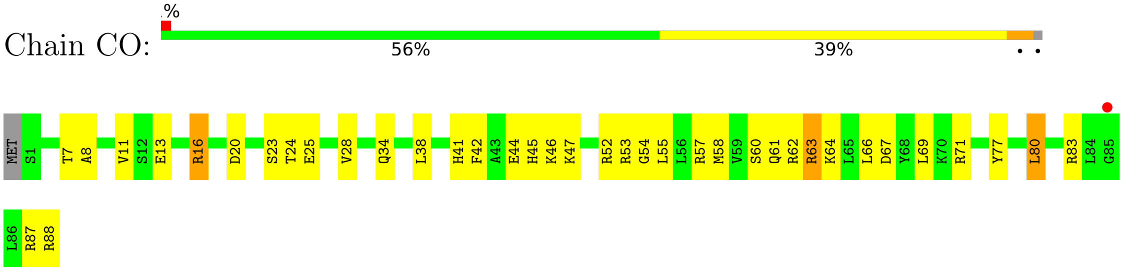


- Molecule 14: 30S ribosomal protein S15

Chain AO:

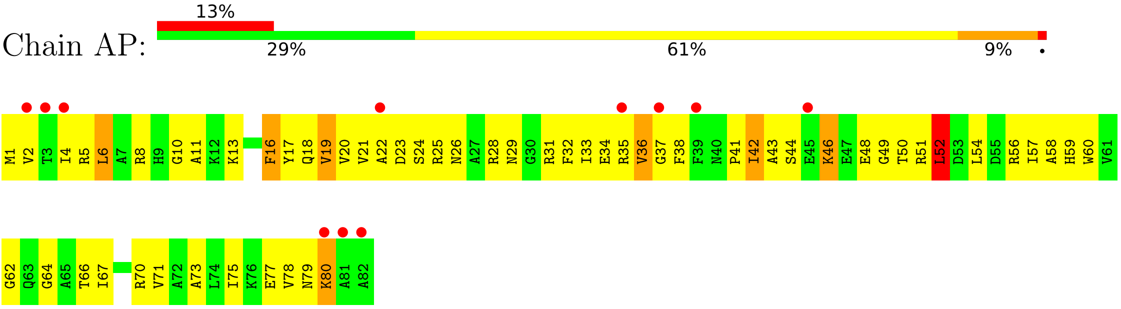
- Molecule 14: 30S ribosomal protein S15

Chain CO:



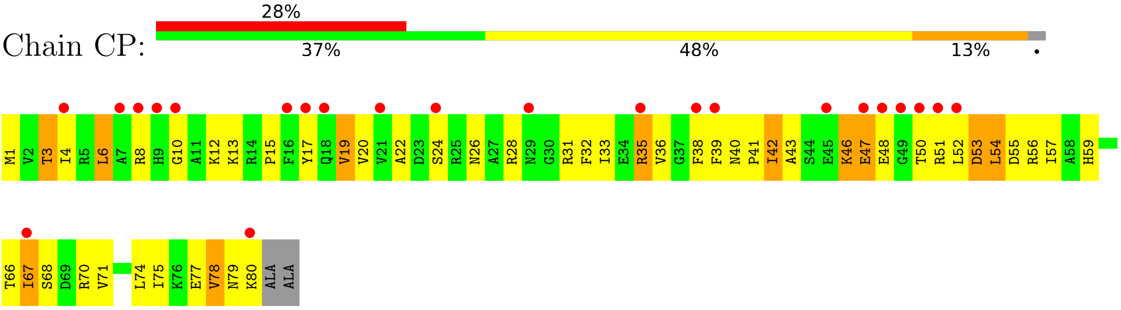
- Molecule 15: 30S ribosomal protein S16

Chain AP:



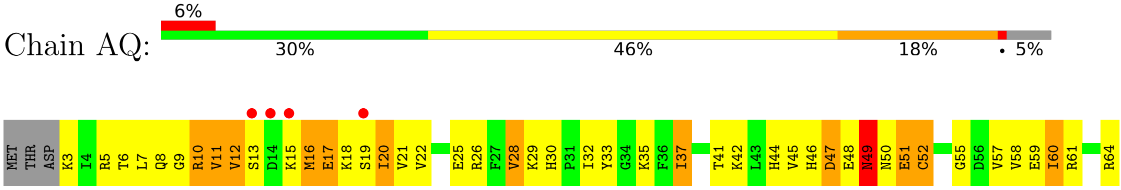
- Molecule 15: 30S ribosomal protein S16

Chain CP:



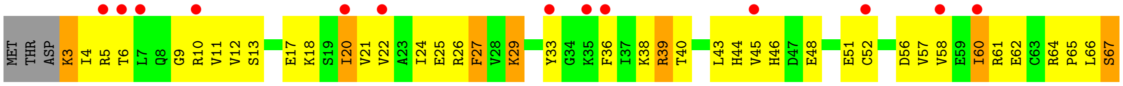
- Molecule 16: 30S ribosomal protein S17

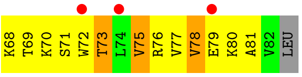
Chain AQ:



- Molecule 16: 30S ribosomal protein S17

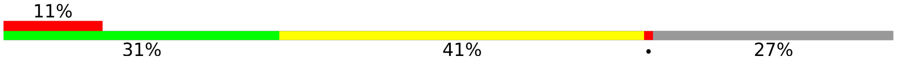
Chain CQ:

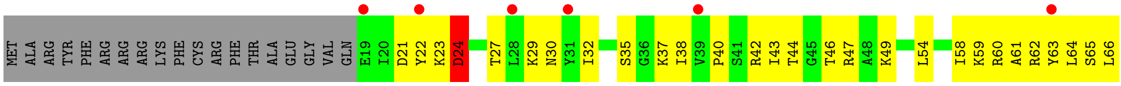


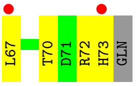


- Molecule 17: 30S ribosomal protein S18

Chain AR:

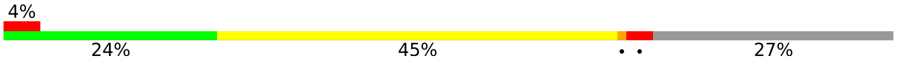


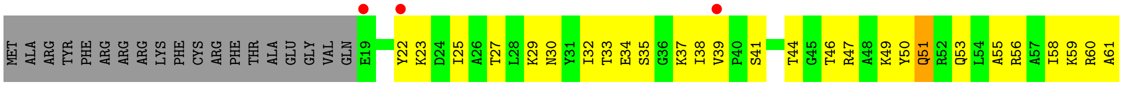




- Molecule 17: 30S ribosomal protein S18

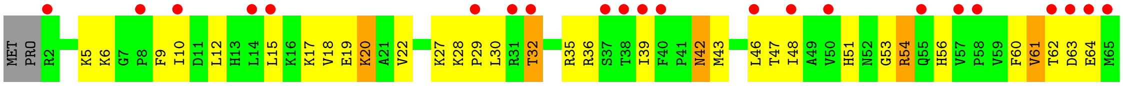
Chain CR:

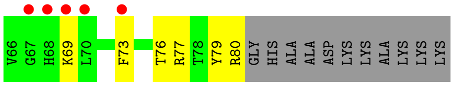




- Molecule 18: 30S ribosomal protein S19

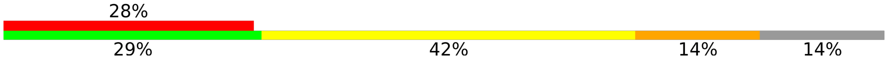
Chain AS:

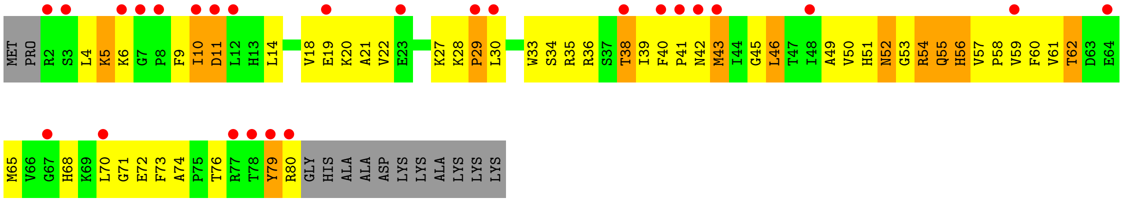




- Molecule 18: 30S ribosomal protein S19

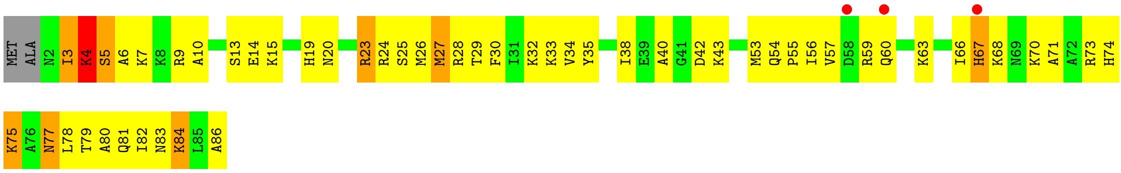
Chain CS:





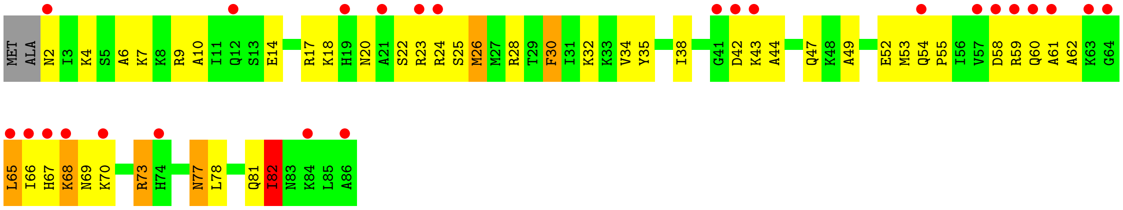
- Molecule 19: 30S ribosomal protein S20

Chain AT:



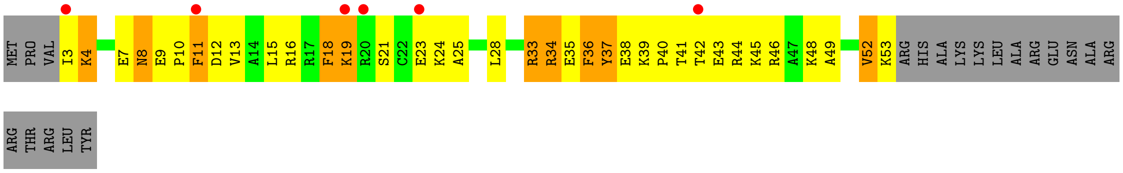
- Molecule 19: 30S ribosomal protein S20

Chain CT:



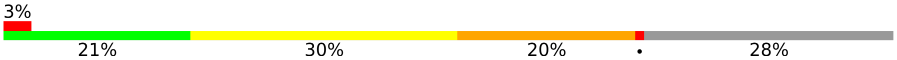
- Molecule 20: 30S ribosomal protein S21

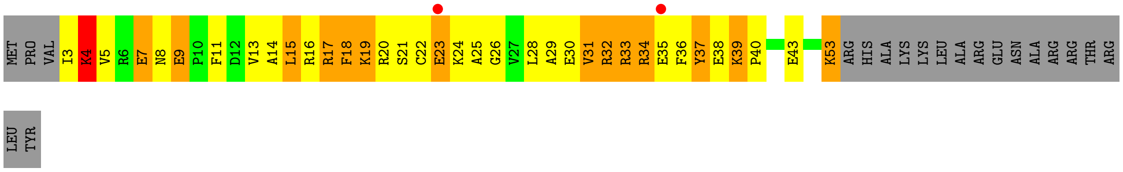
Chain AU:



- Molecule 20: 30S ribosomal protein S21

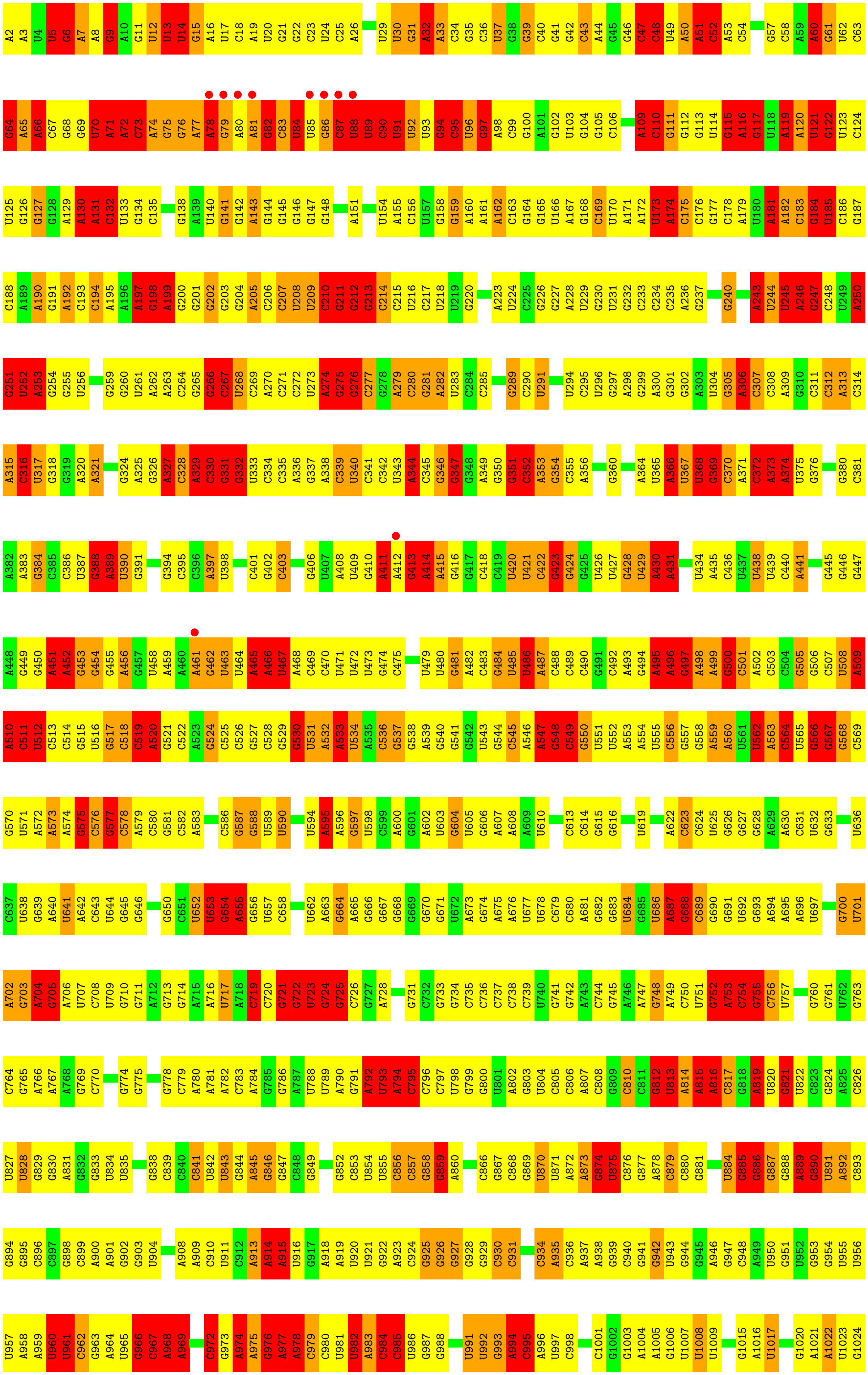
Chain CU:





- Molecule 21: 16S rRNA

Chain AA:


A2 A3 U4 U5 G6 A7 A8 G9 A10 G11 U12 U13 U14 G15 A16 U17 C18 A19 U20 G21 G22 C23 U24 C25 A26 U29 U30 G31 A32 A33 C34 G35 C36 U37 G38 G39 C40 G41 G42 C43 A44 G45 G46 C47 C48 U49 A50 A51 C52 A53 C54 G57 C58 A59 A60 G61 U62 C63
G64 A65 A66 C67 G68 G69 U70 A71 A72 C73 A74 G75 G76 A77 A78 G79 A80 A81 G82 C83 U84 U85 G86 C87 U88 U89 C90 U91 U92 U93 G94 C95 U96 G97 A98 C99 G100 A101 G102 U103 G104 G105 C106 A109 C110 G111 G112 G113 U114 G115 A116 G117 U118 A119 A120 U121 G122 U123 C124
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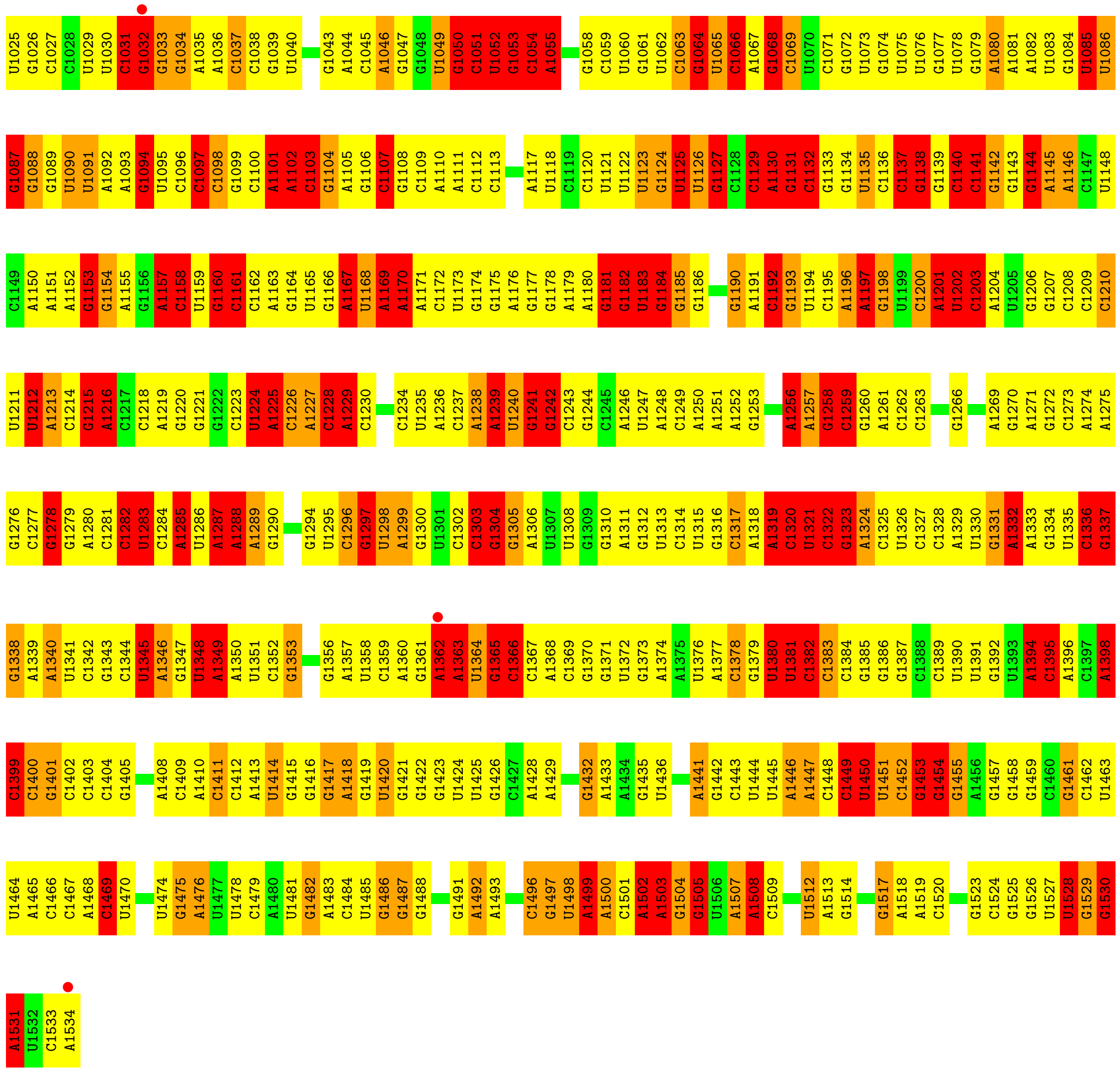

- Molecule 22: P-site tRNA ASL fragment

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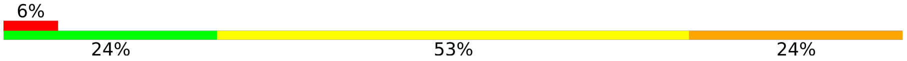

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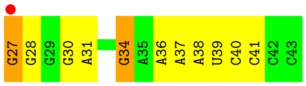

- Molecule 22: P-site tRNA ASL fragment

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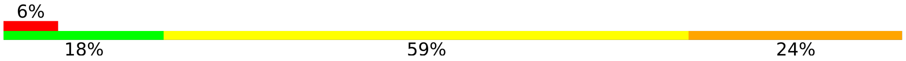

- Molecule 22: P-site tRNA ASL fragment

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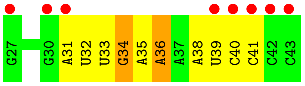

- Molecule 23: messenger RNA

Chain AW:

- Molecule 23: messenger RNA

Chain CW:

- Molecule 24: 23S rRNA

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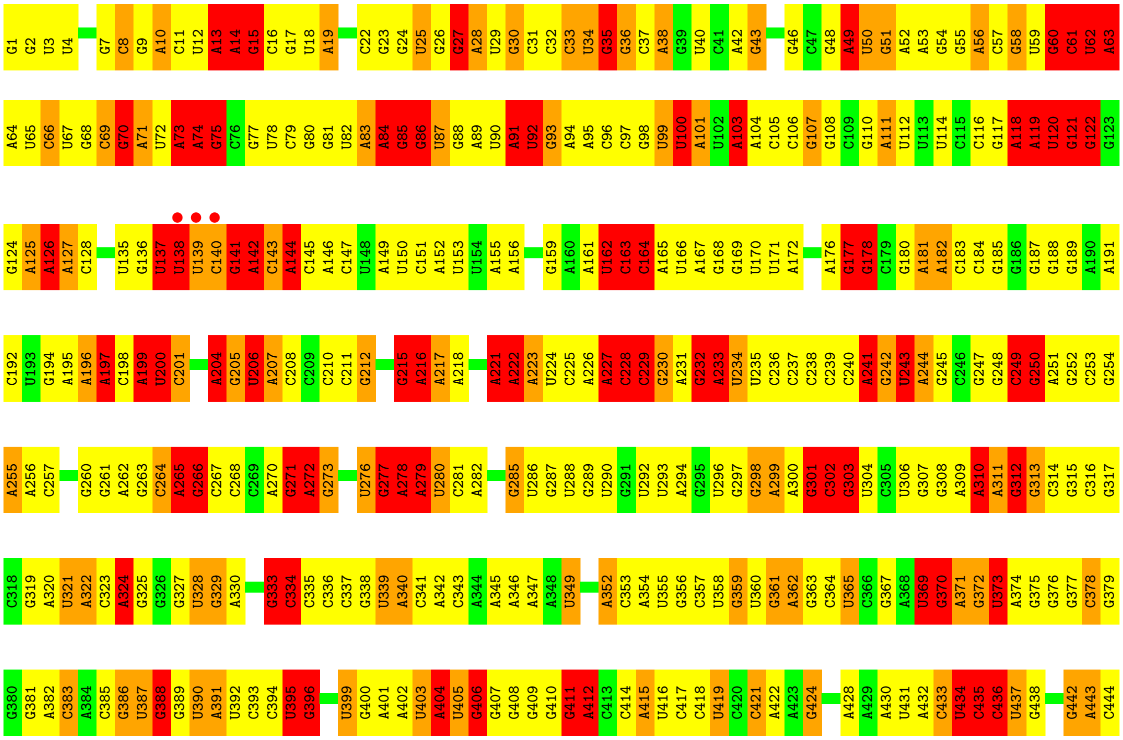

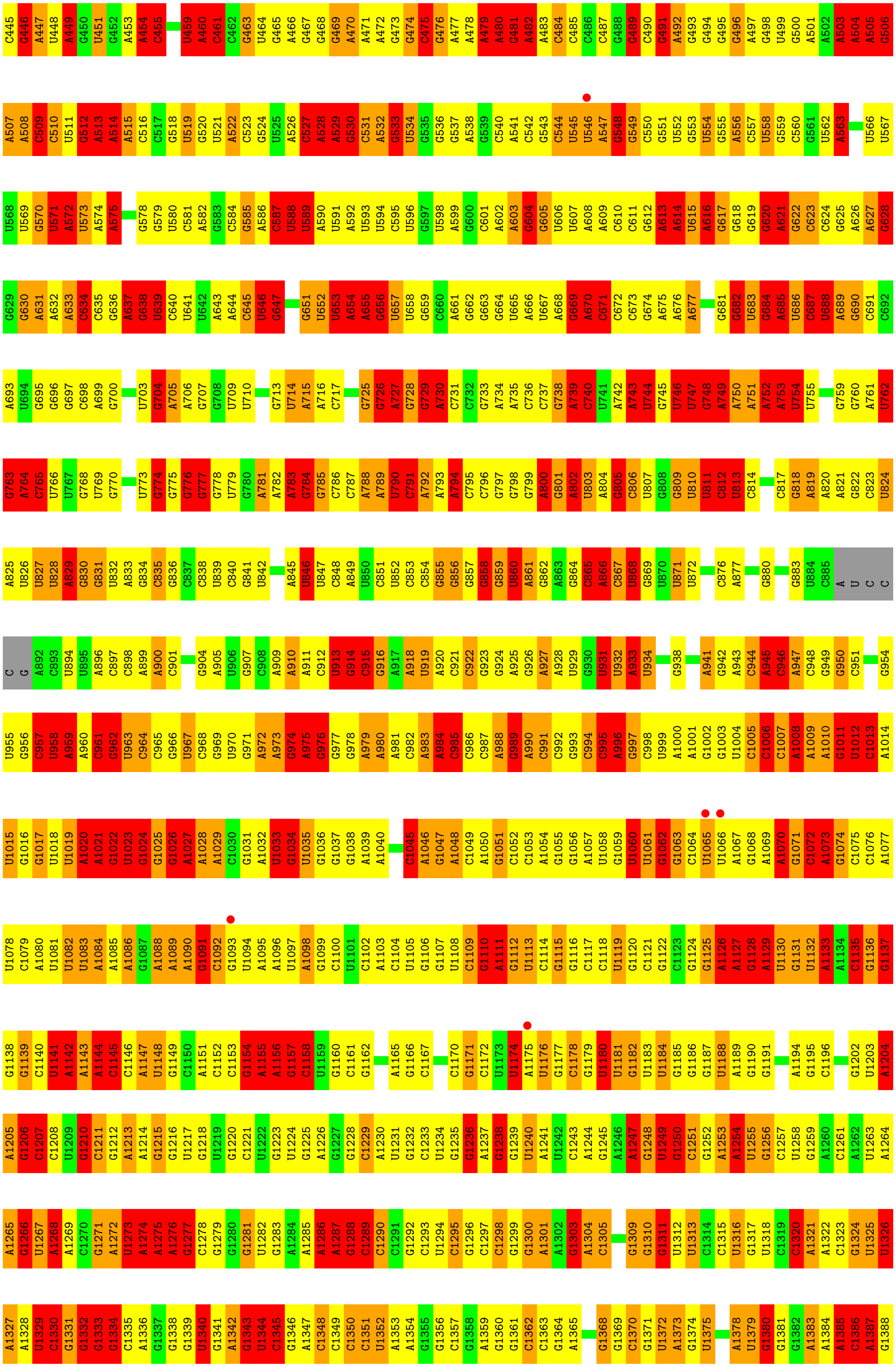
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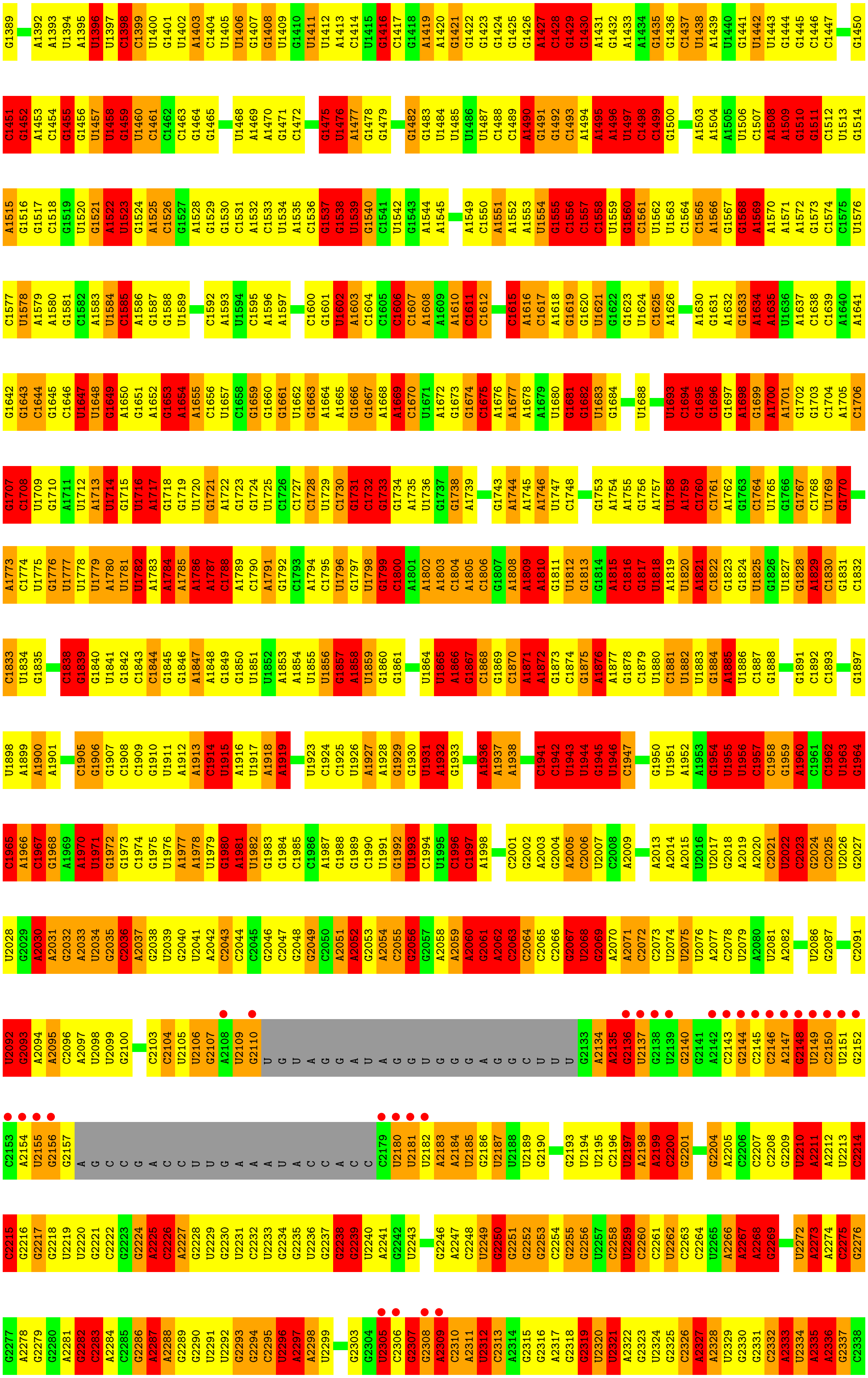
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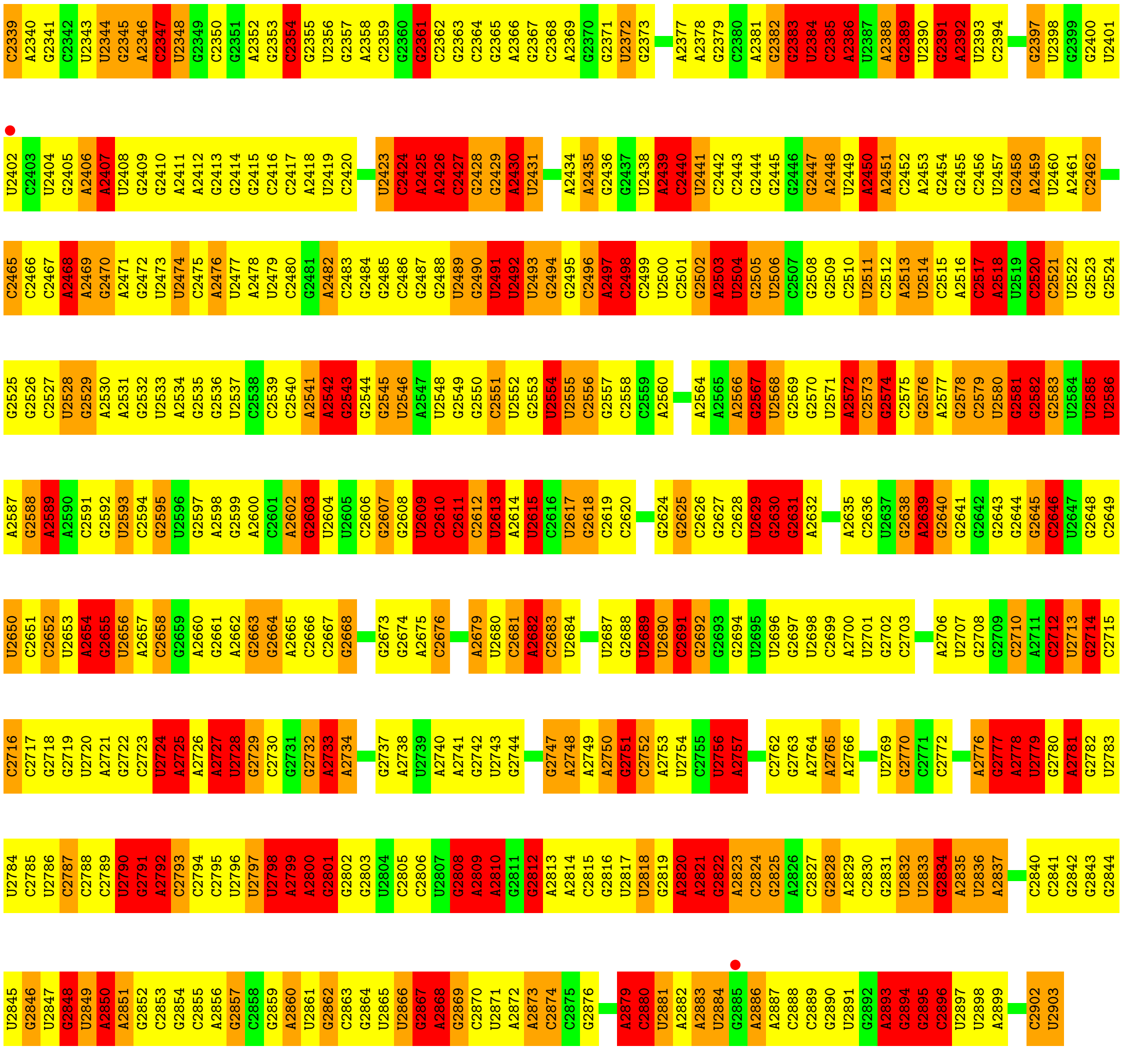

- Molecule 24: 23S rRNA

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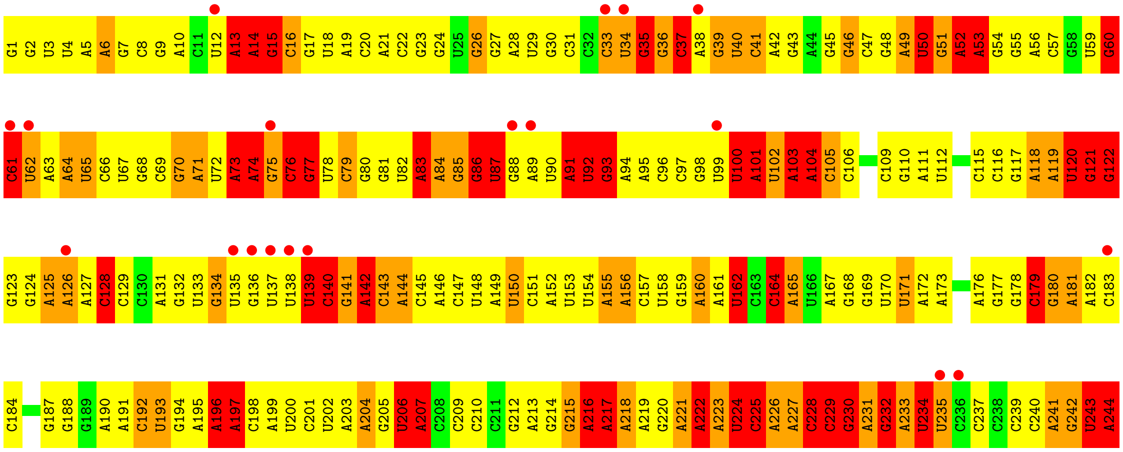

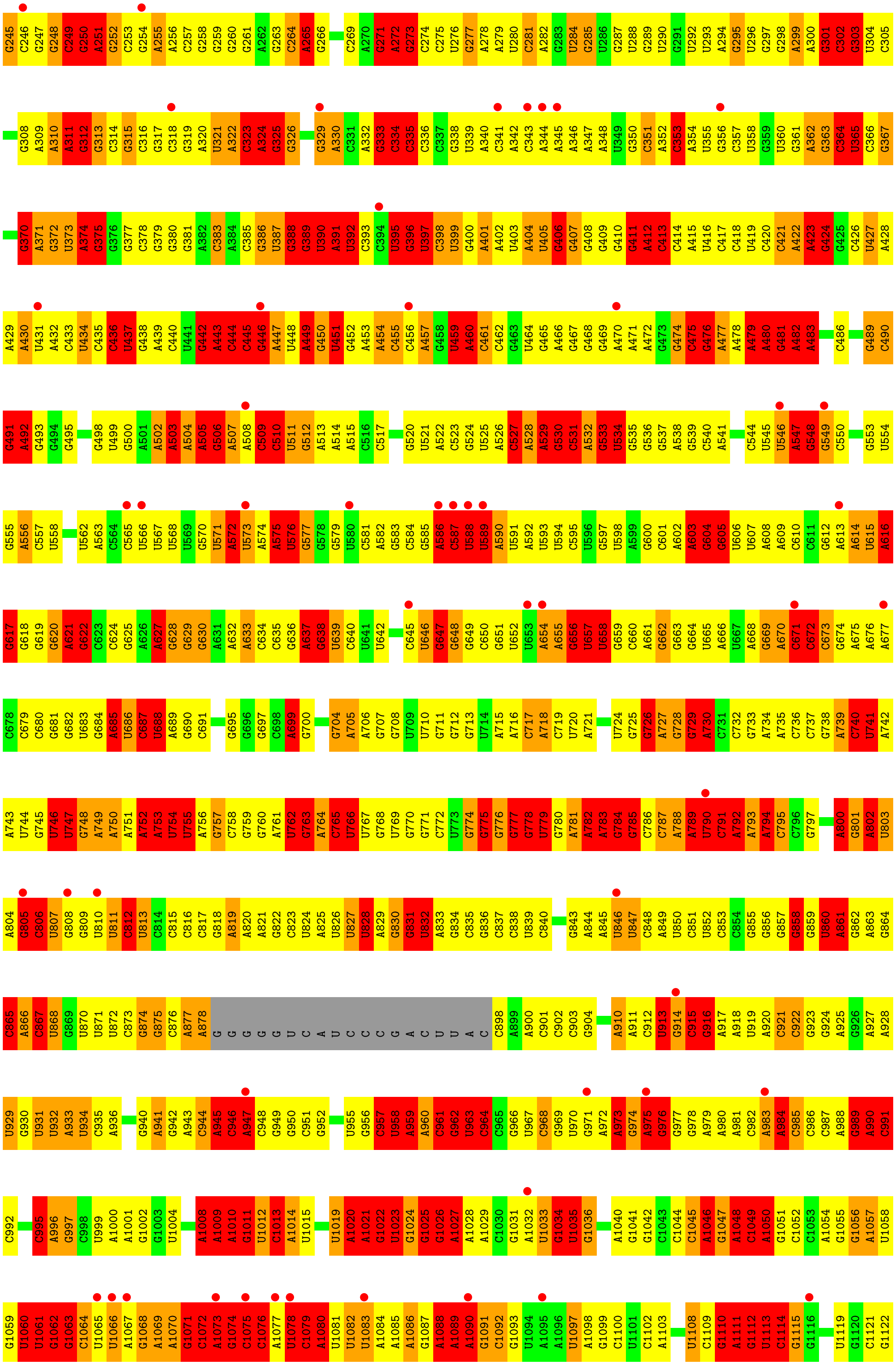
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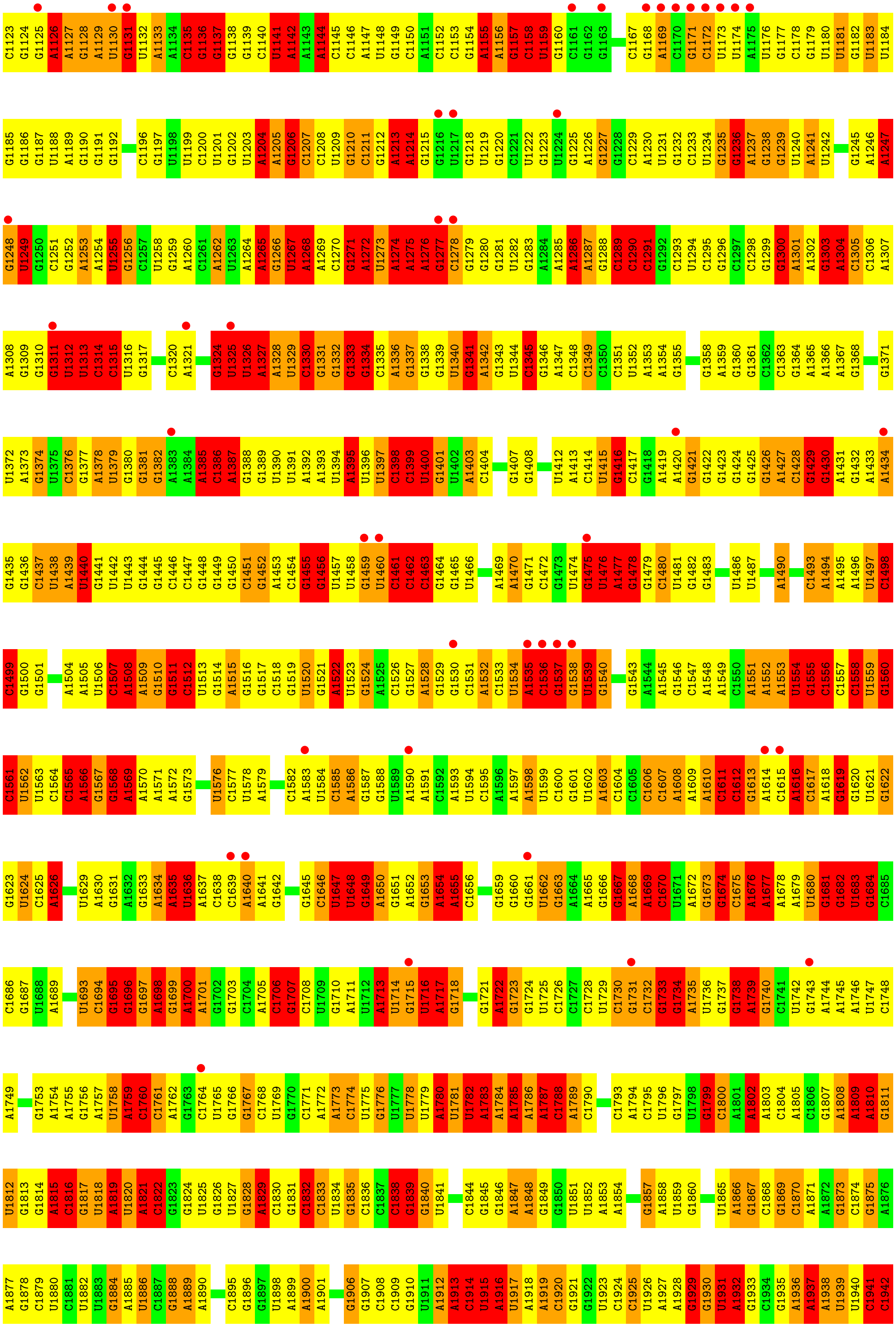
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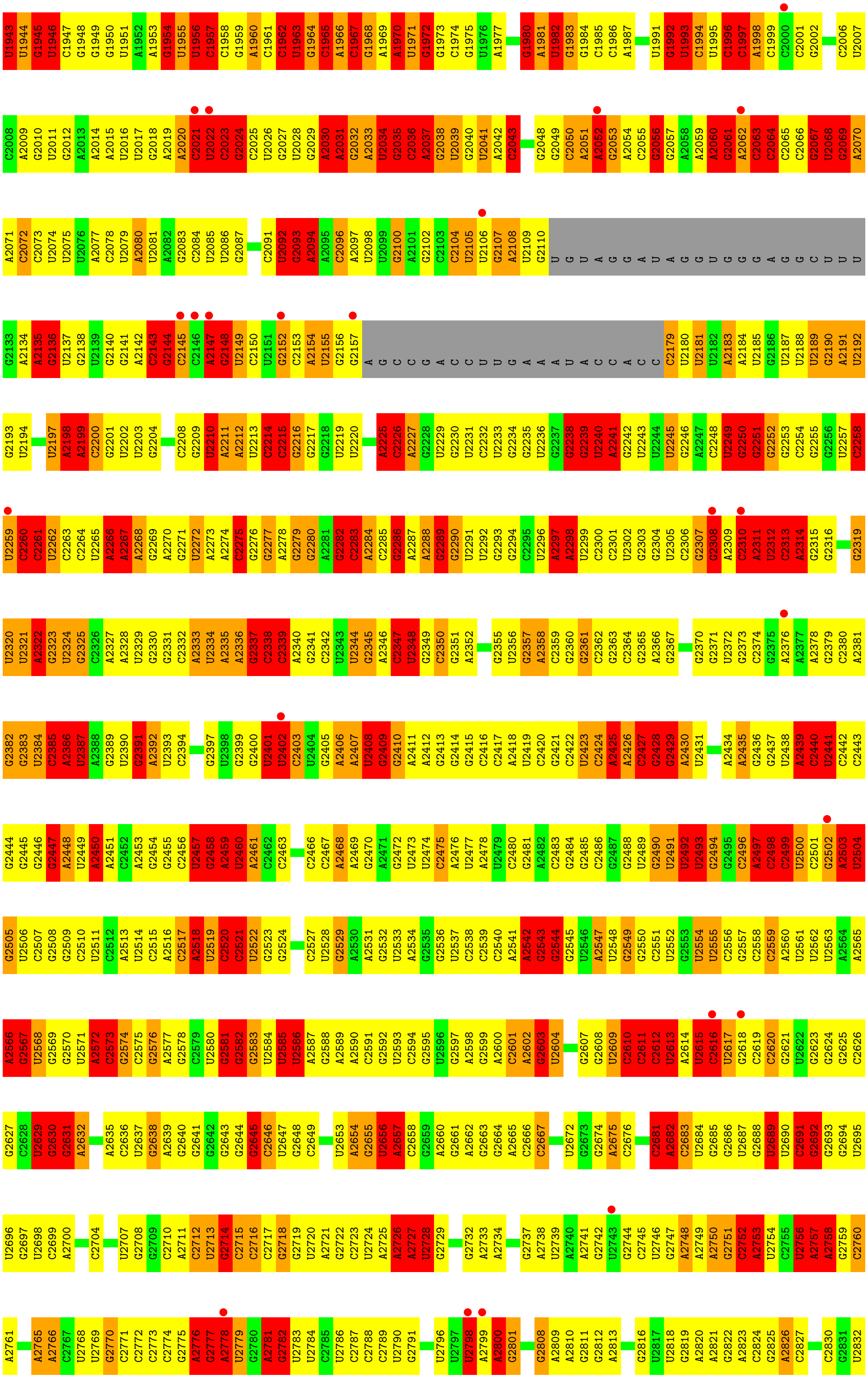
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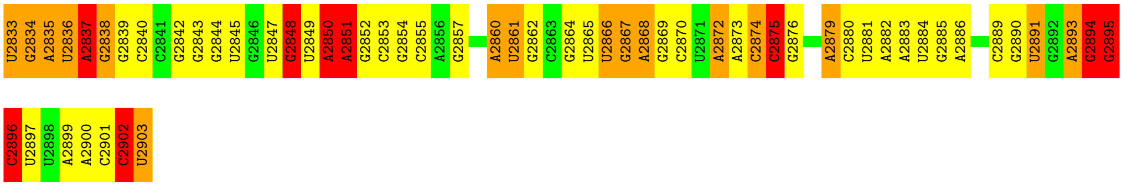

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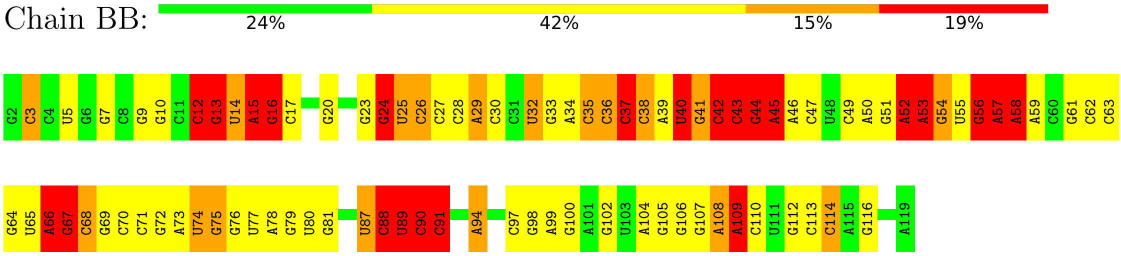
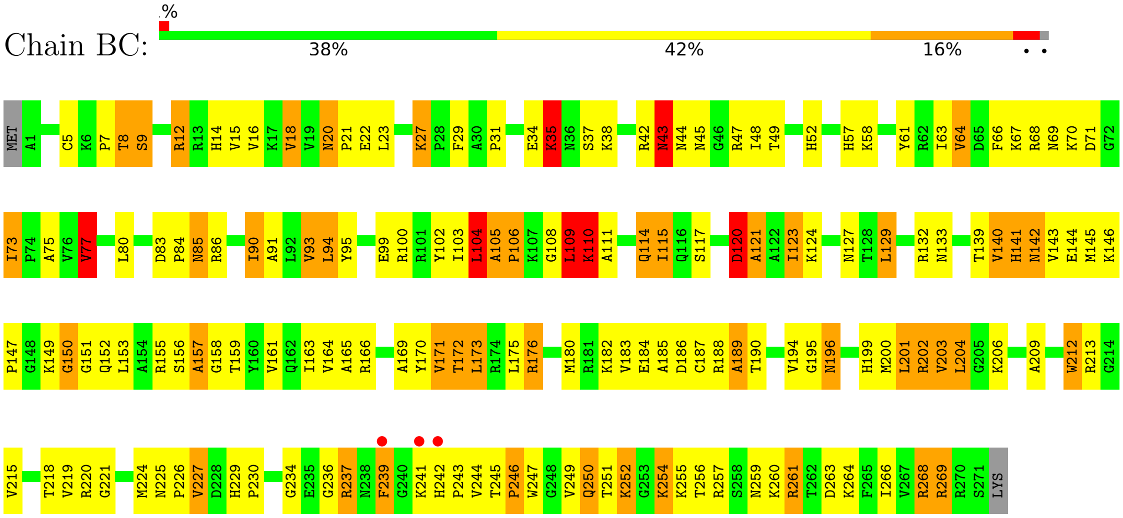


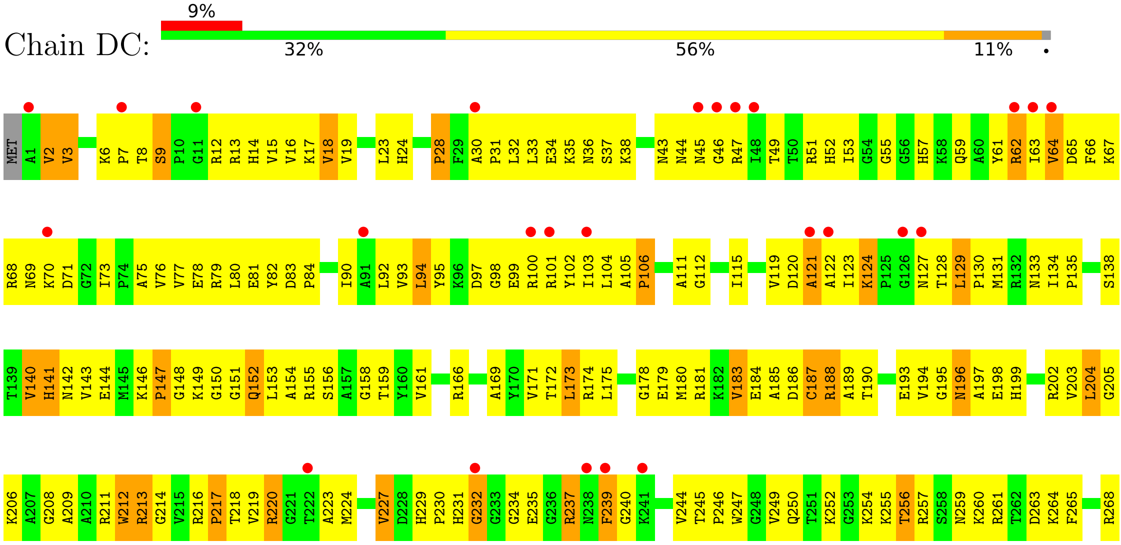
- Molecule 26: 50S ribosomal protein L2

Chain BC:



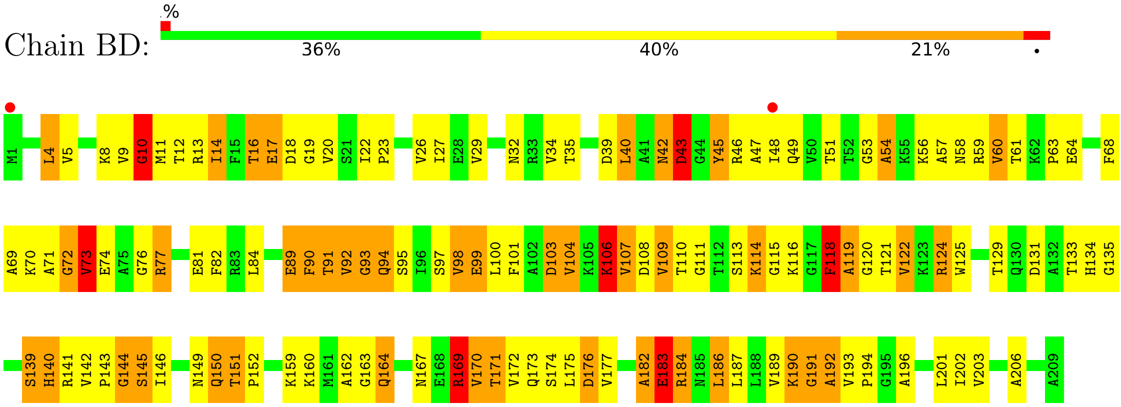
- Molecule 26: 50S ribosomal protein L2

Chain DC:



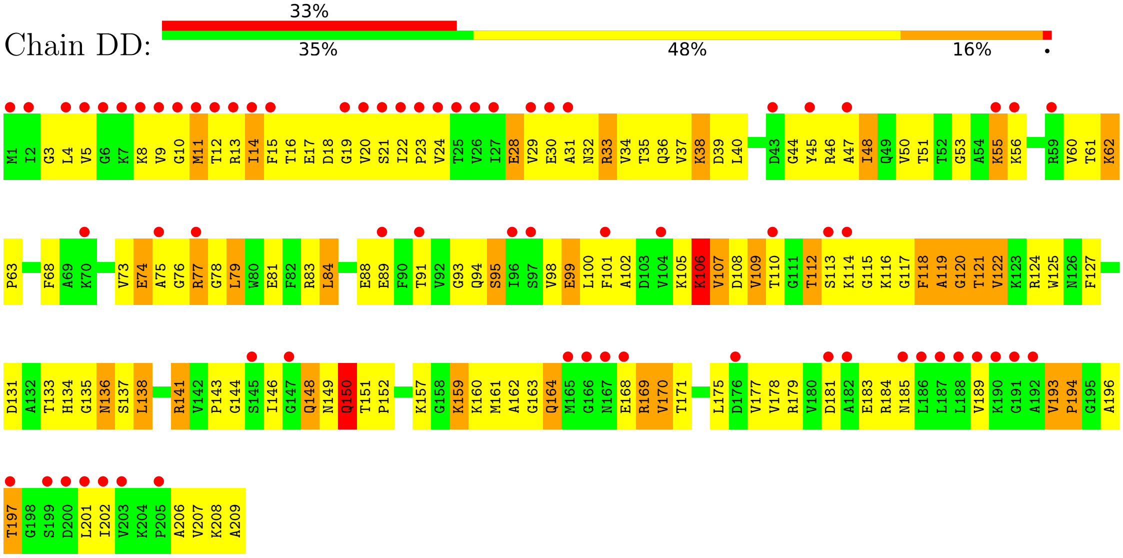
- Molecule 27: 50S ribosomal protein L3

Chain BD:



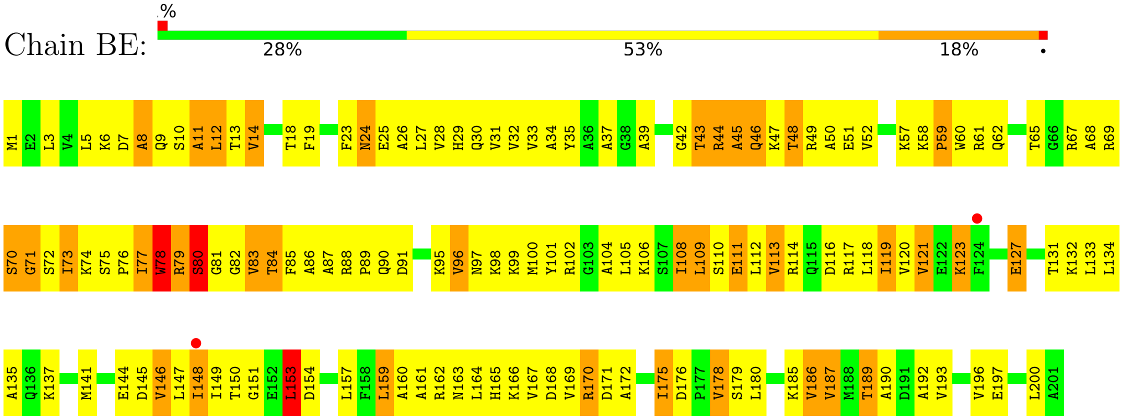
- Molecule 27: 50S ribosomal protein L3

Chain DD:

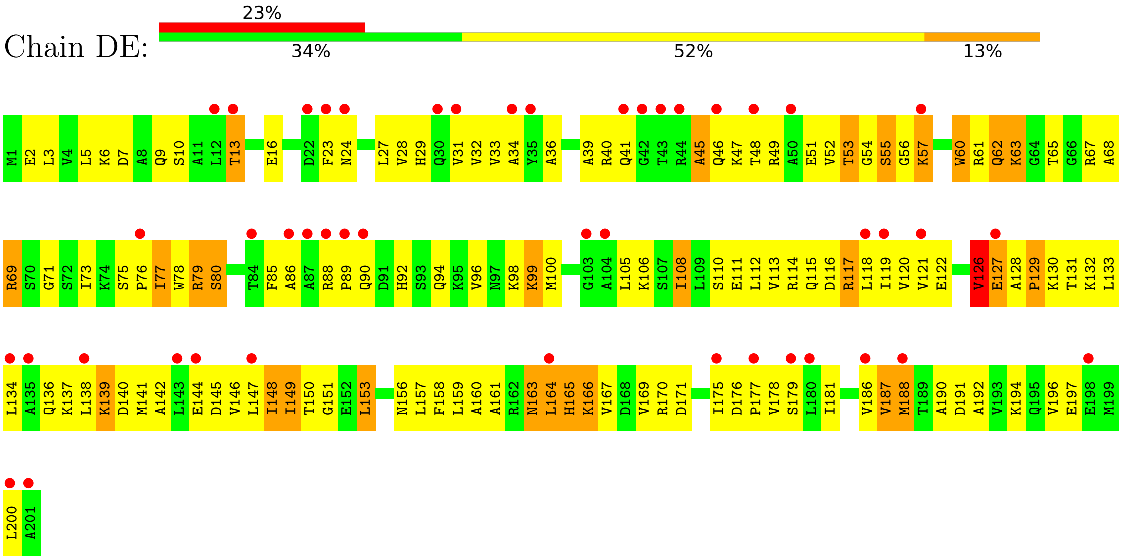


- Molecule 28: 50S ribosomal protein L4

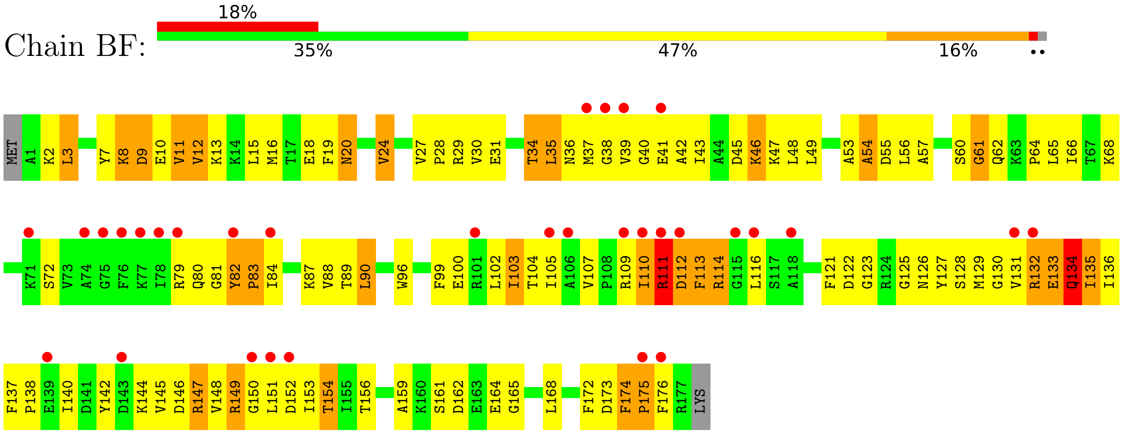
Chain BE:



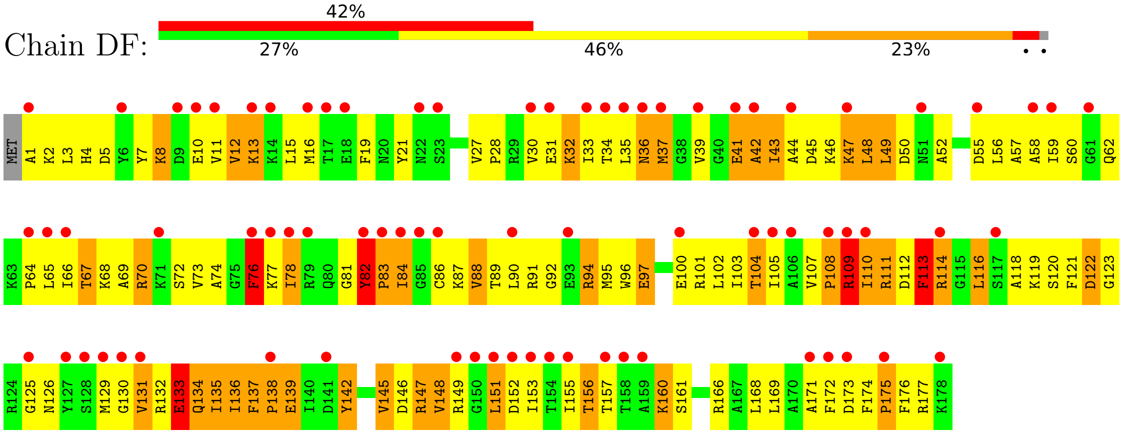
- Molecule 28: 50S ribosomal protein L4



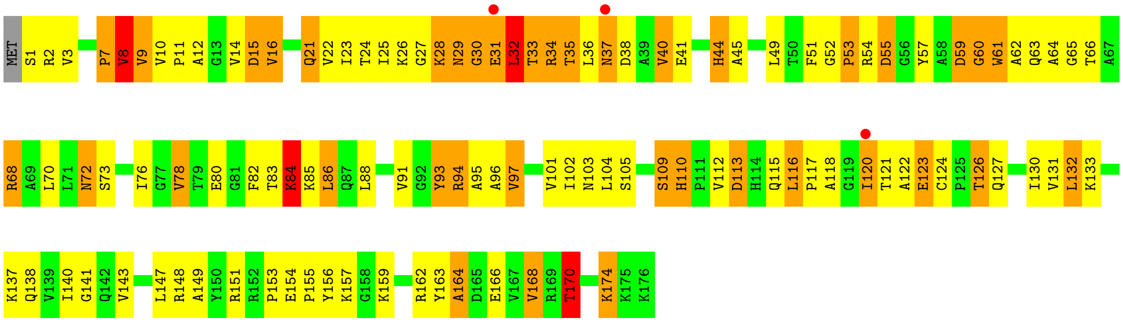
- Molecule 29: 50S ribosomal protein L5



- Molecule 29: 50S ribosomal protein L5

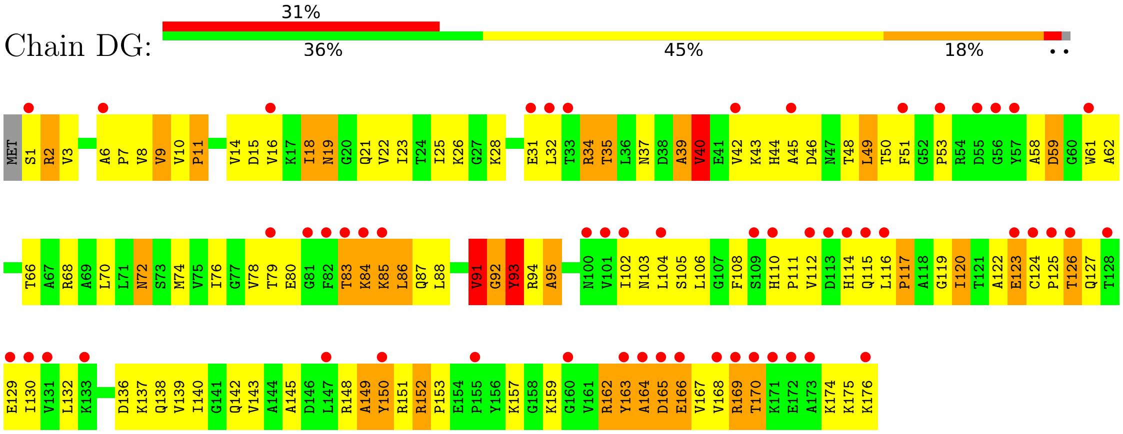


- Molecule 30: 50S ribosomal protein L6



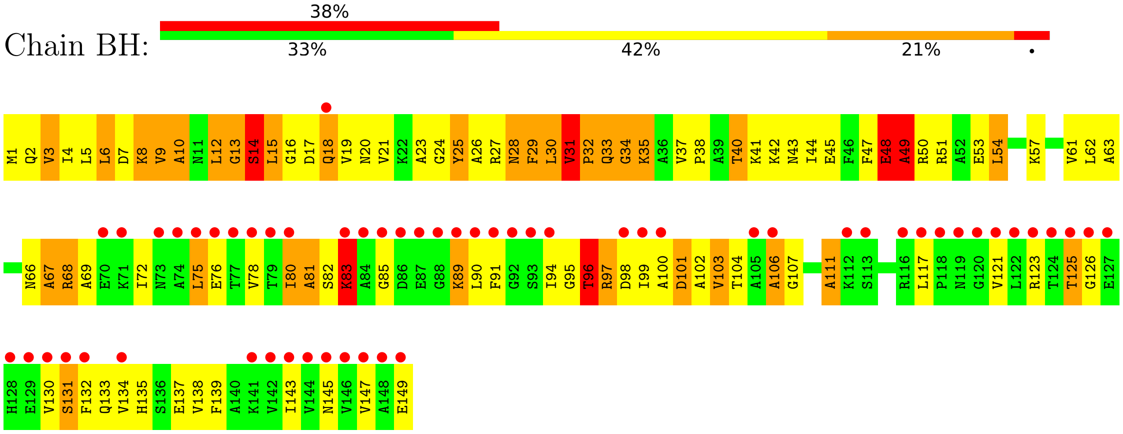
- Molecule 30: 50S ribosomal protein L6

Chain DG:



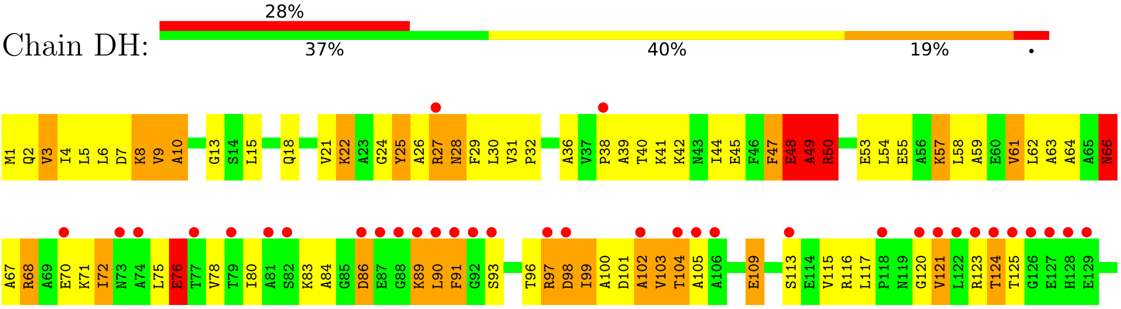
- Molecule 31: 50S ribosomal protein L9

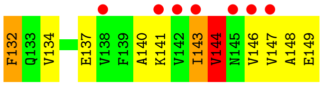
Chain BH:



- Molecule 31: 50S ribosomal protein L9

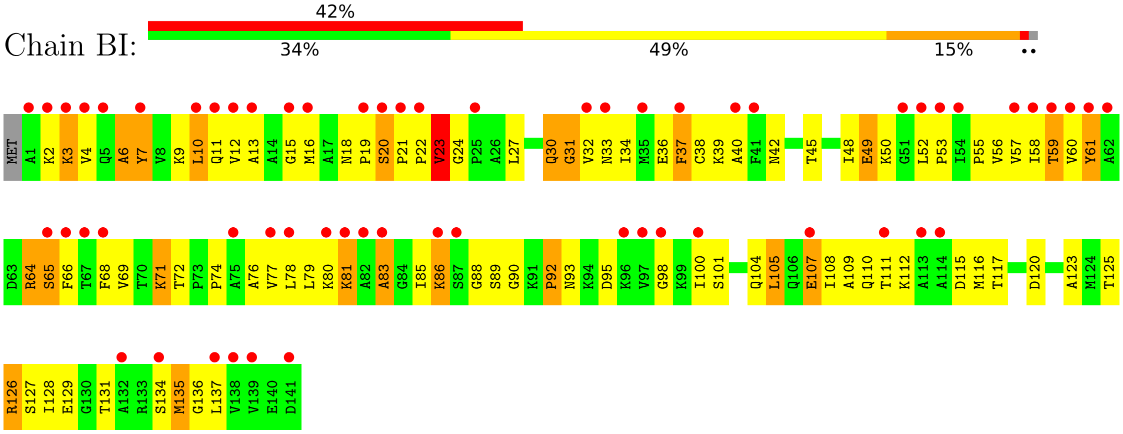
Chain DH:





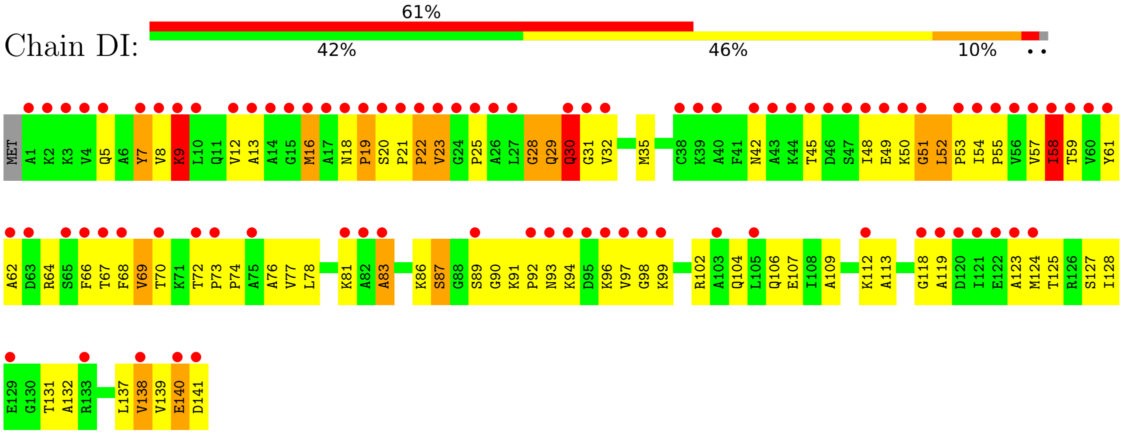
- Molecule 32: 50S ribosomal protein L11

Chain BI:



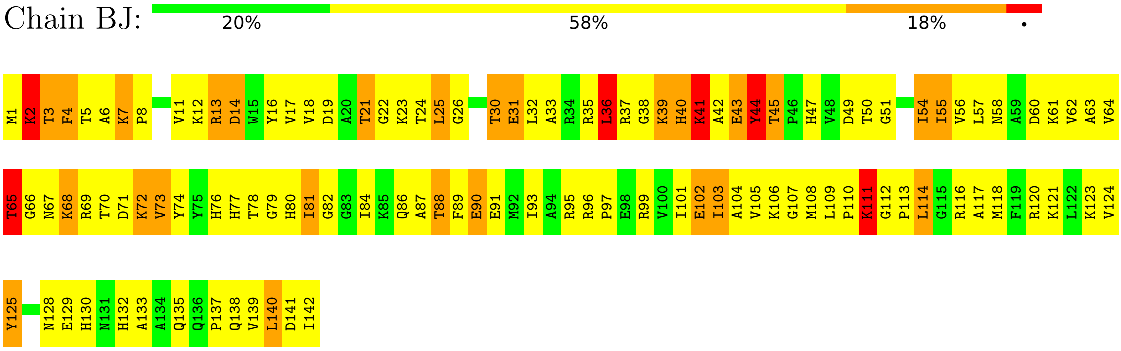
- Molecule 32: 50S ribosomal protein L11

Chain DI:



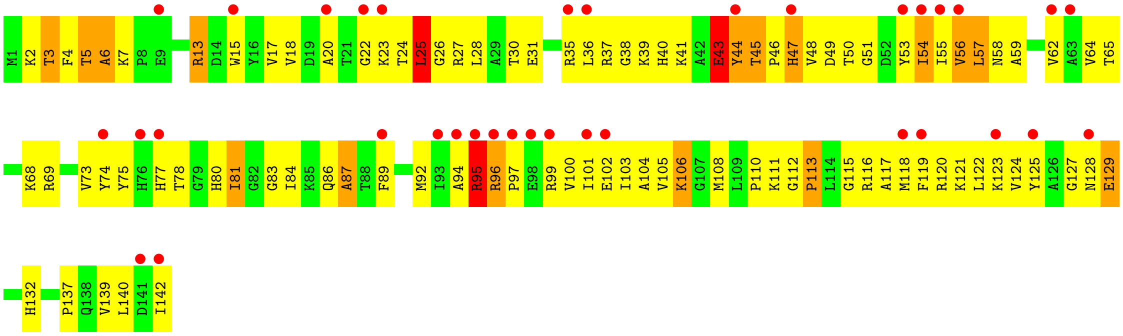
- Molecule 33: 50S ribosomal protein L13

Chain BJ:



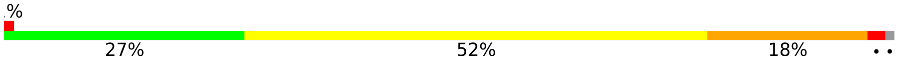
- Molecule 33: 50S ribosomal protein L13

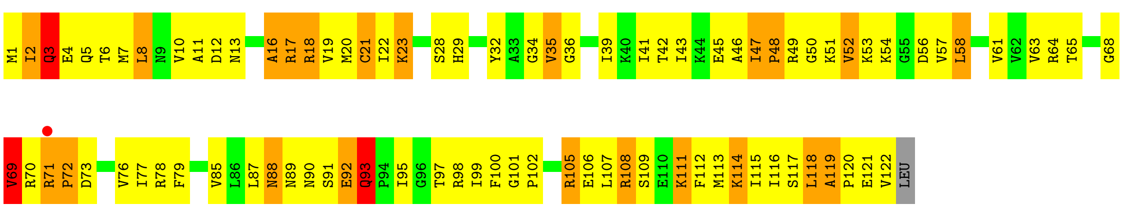
Chain DJ:



- Molecule 34: 50S ribosomal protein L14

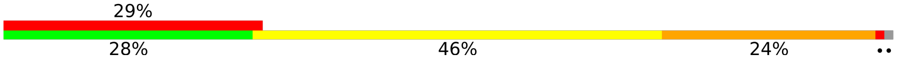
Chain BK:

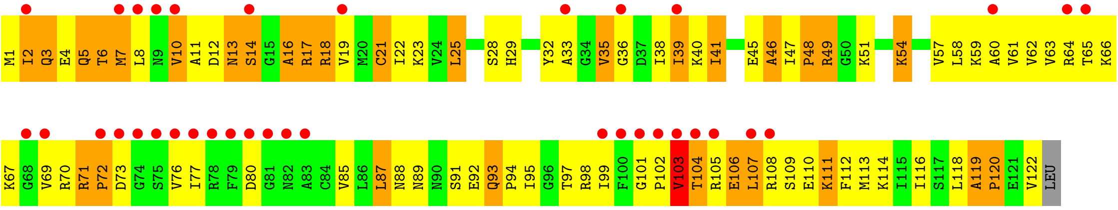




- Molecule 34: 50S ribosomal protein L14

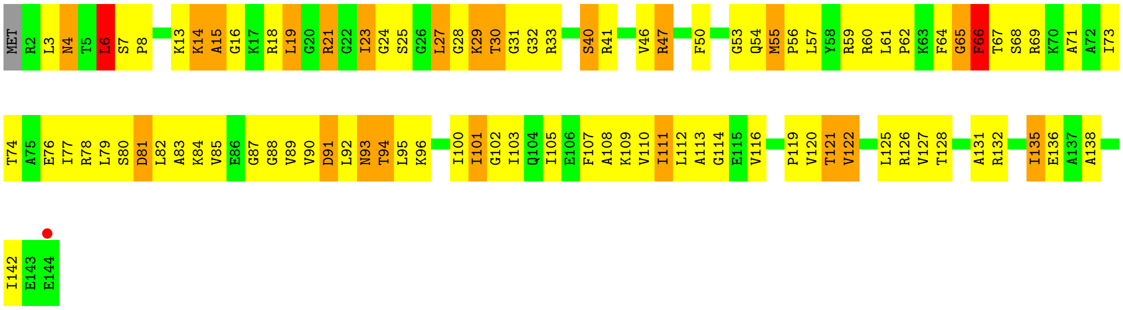
Chain DK:





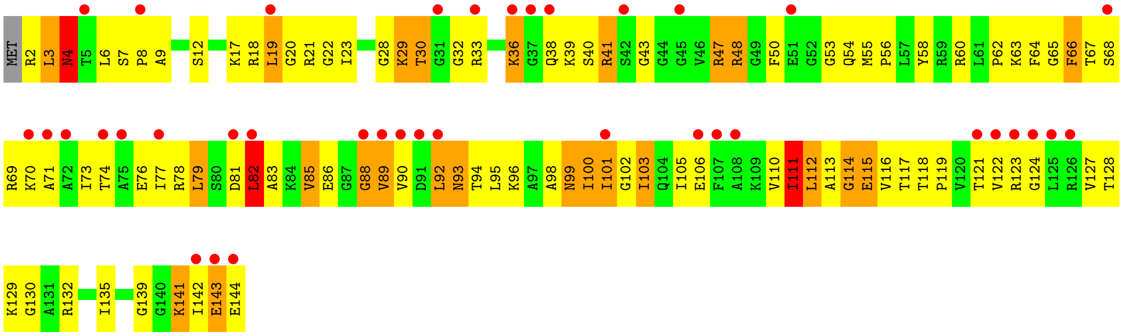
- Molecule 35: 50S ribosomal protein L15

Chain BL:



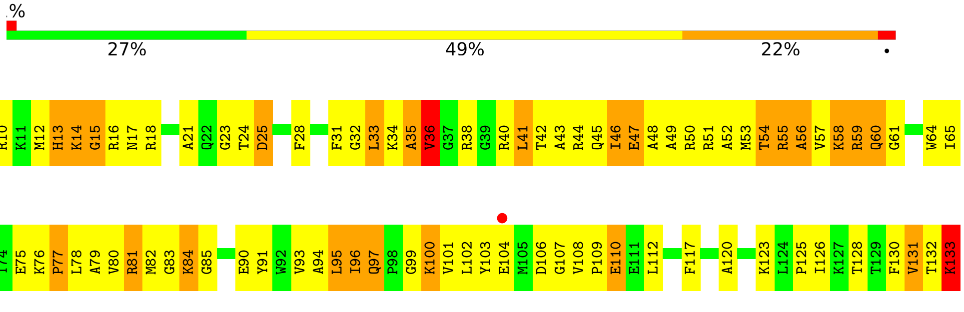
- Molecule 35: 50S ribosomal protein L15

Chain DL:



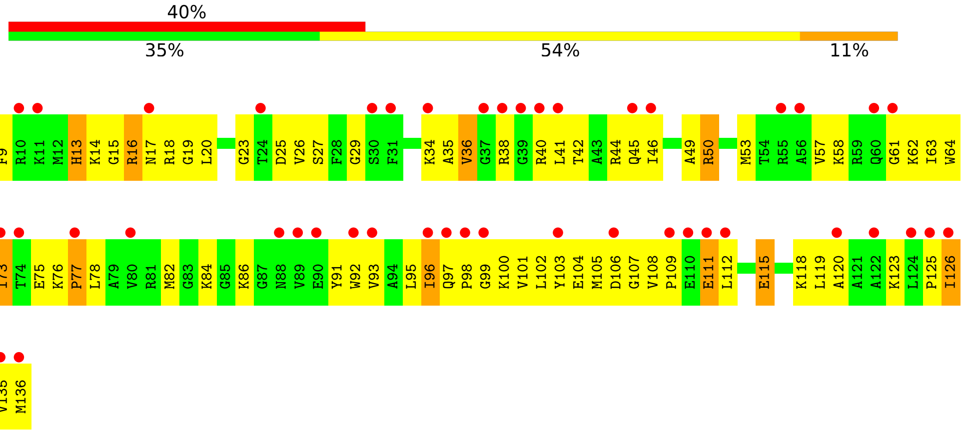
- Molecule 36: 50S ribosomal protein L16

Chain BM:



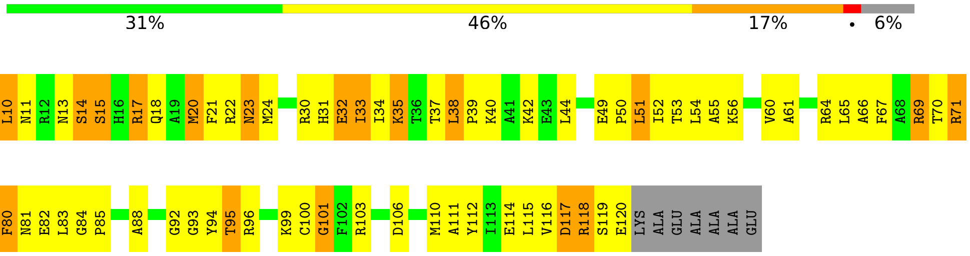
- Molecule 36: 50S ribosomal protein L16

Chain DM:



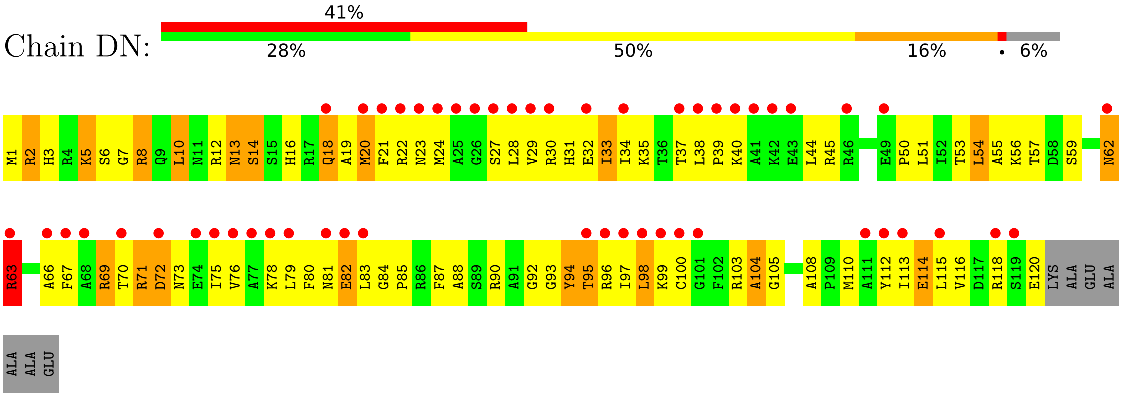
- Molecule 37: 50S ribosomal protein L17

Chain BN:



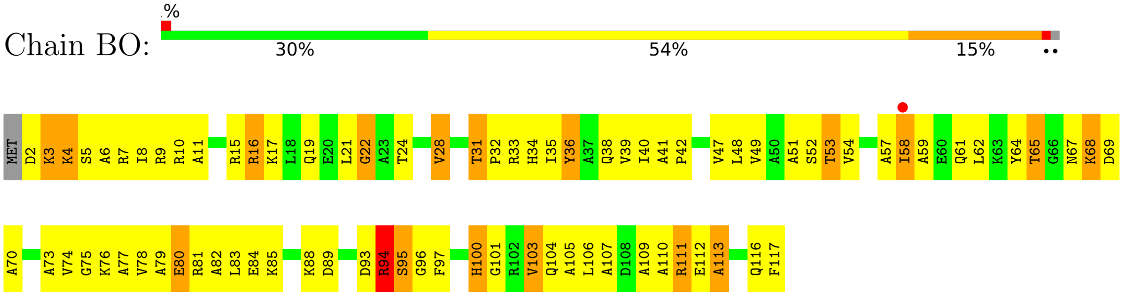
- Molecule 37: 50S ribosomal protein L17

Chain DN:



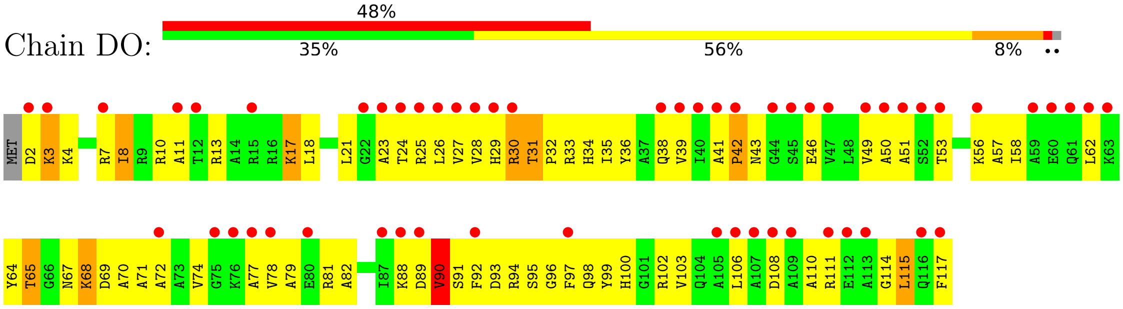
- Molecule 38: 50S ribosomal protein L18

Chain BO:



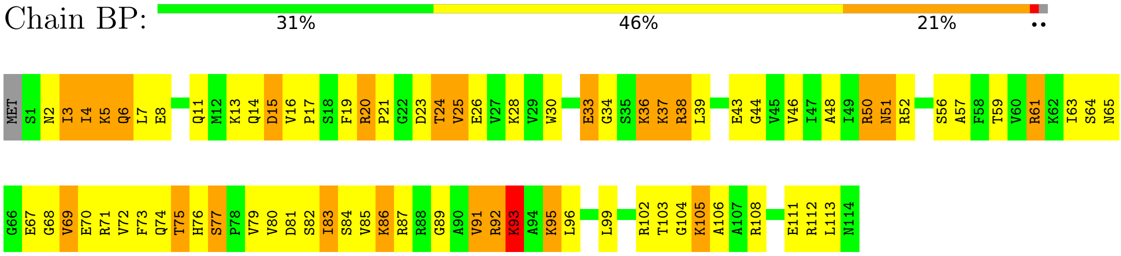
- Molecule 38: 50S ribosomal protein L18

Chain DO:



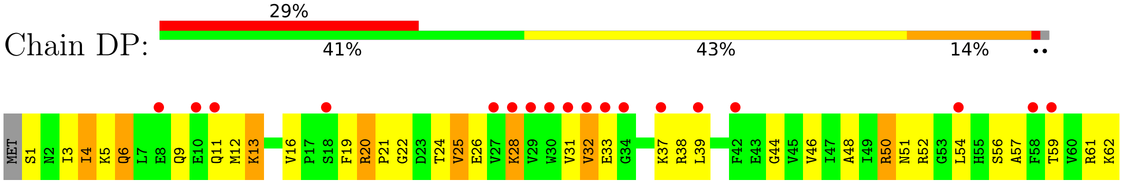
- Molecule 39: 50S ribosomal protein L19

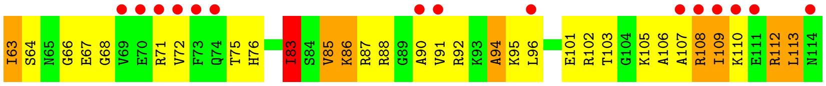
Chain BP:



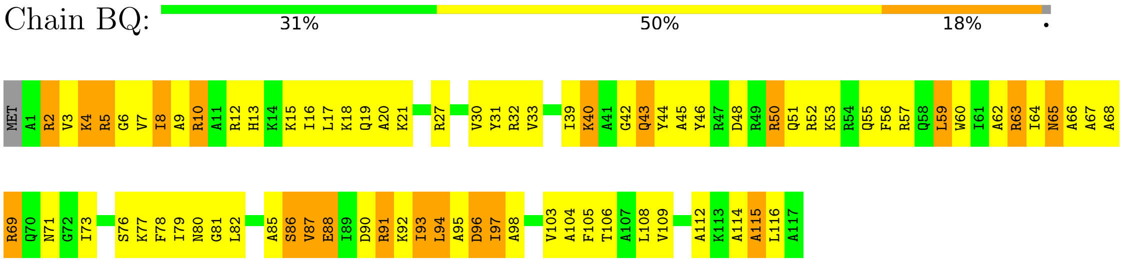
- Molecule 39: 50S ribosomal protein L19

Chain DP:

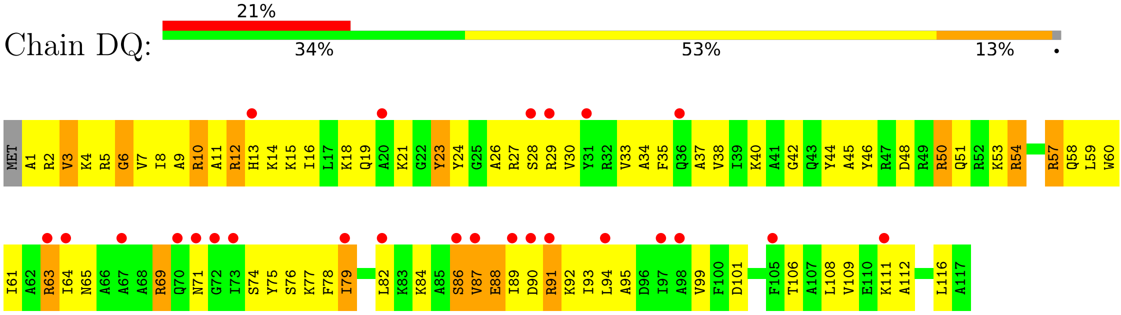




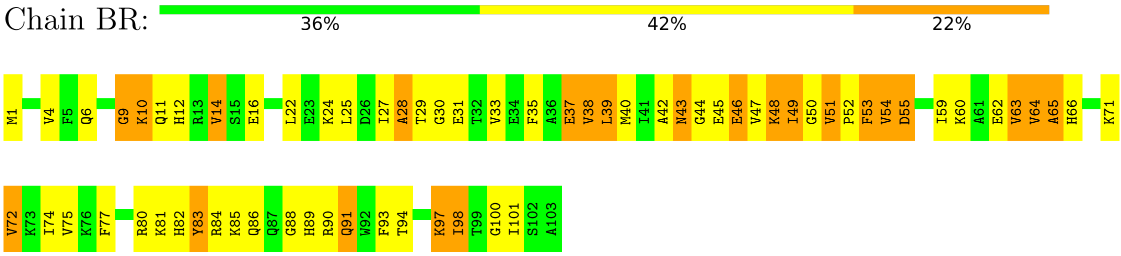
- Molecule 40: 50S ribosomal protein L20



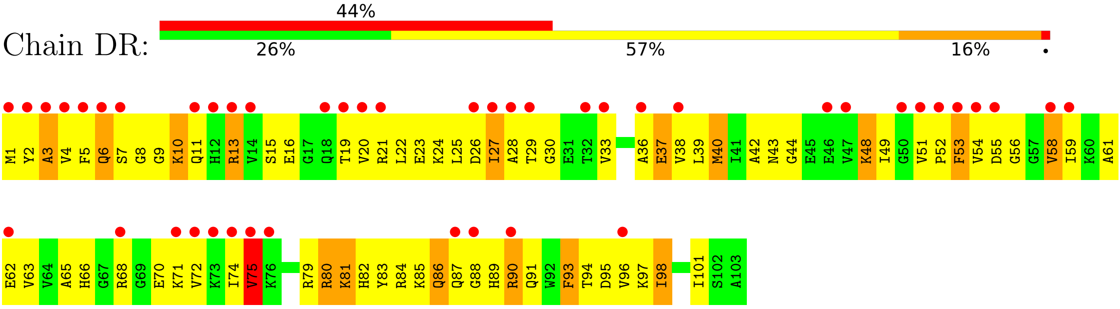
- Molecule 40: 50S ribosomal protein L20



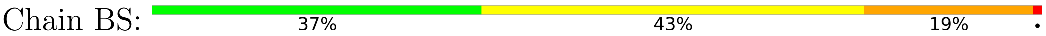
- Molecule 41: 50S ribosomal protein L21

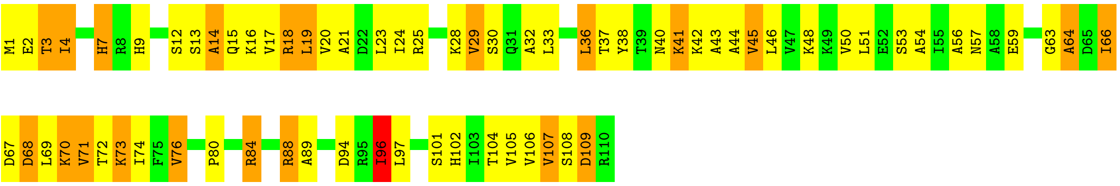


- Molecule 41: 50S ribosomal protein L21



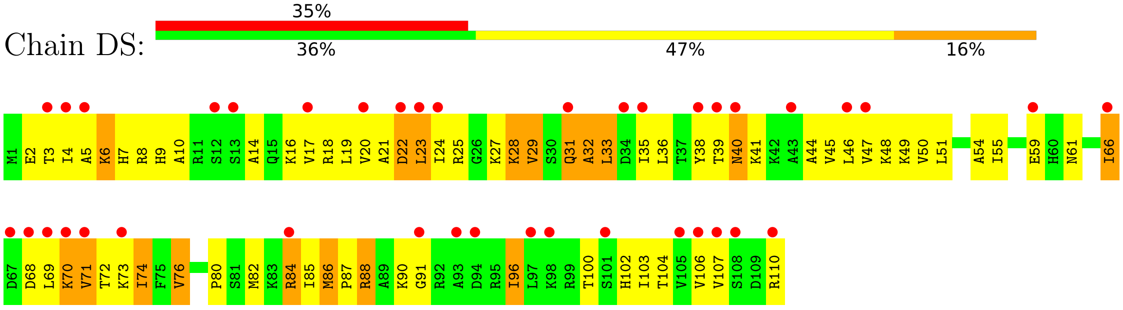
- Molecule 42: 50S ribosomal protein L22





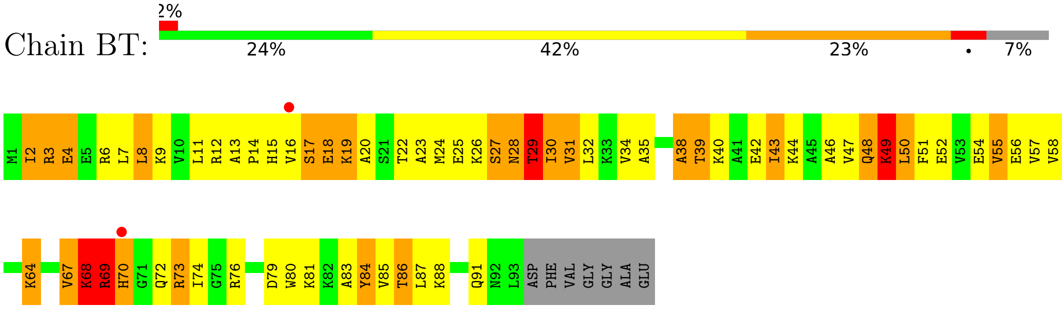
- Molecule 42: 50S ribosomal protein L22

Chain DS:



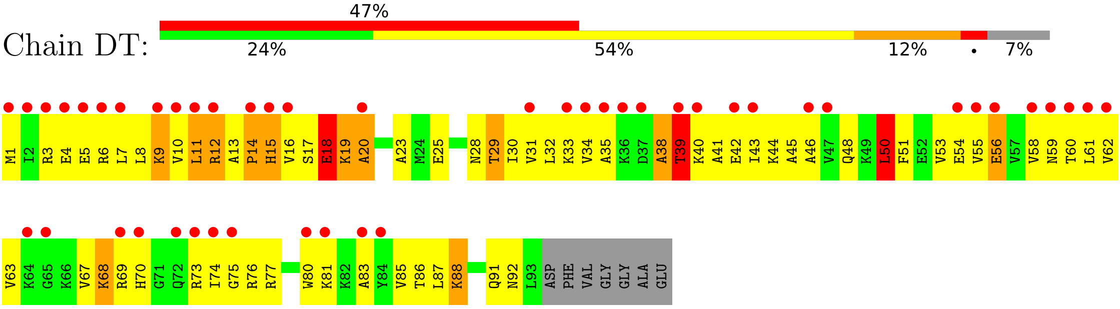
- Molecule 43: 50S ribosomal protein L23

Chain BT:



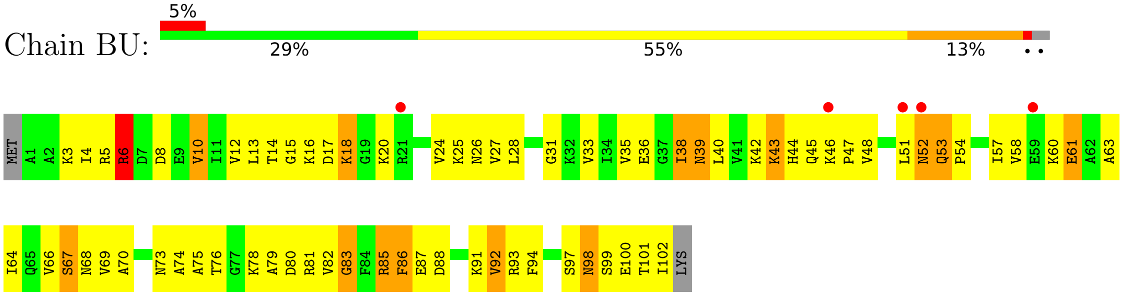
- Molecule 43: 50S ribosomal protein L23

Chain DT:

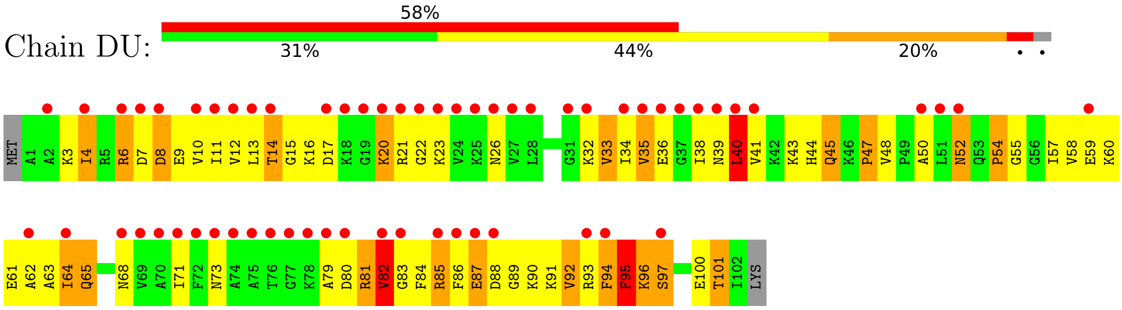


- Molecule 44: 50S ribosomal protein L24

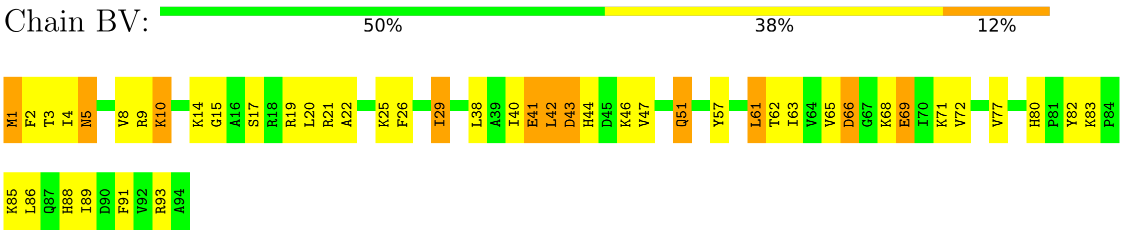
Chain BU:



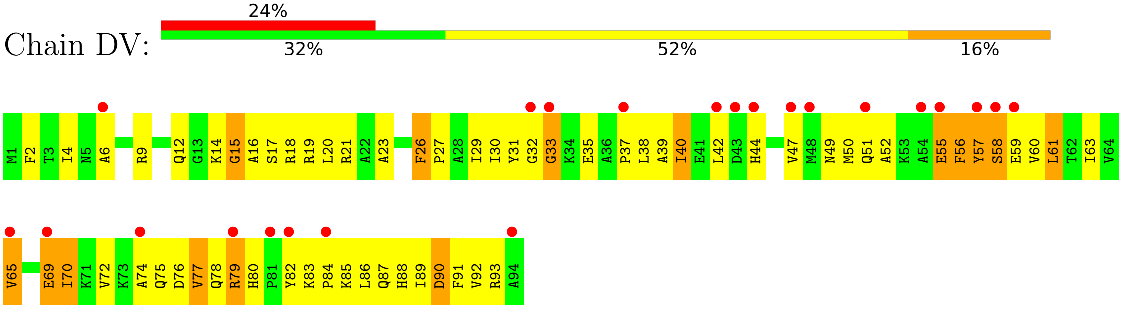
- Molecule 44: 50S ribosomal protein L24



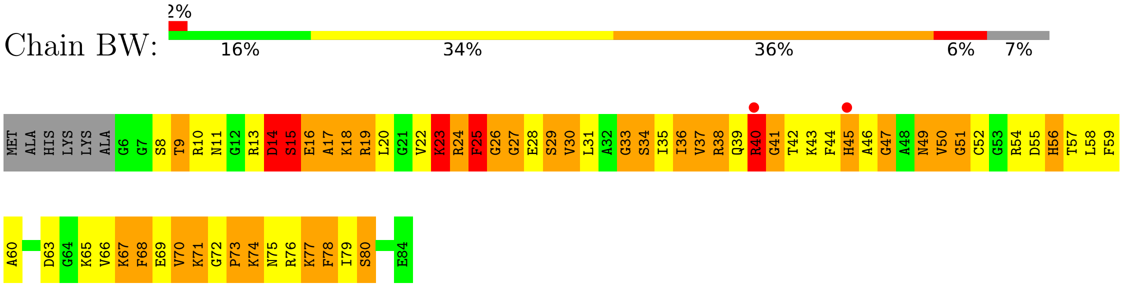
- Molecule 45: 50S ribosomal protein L25



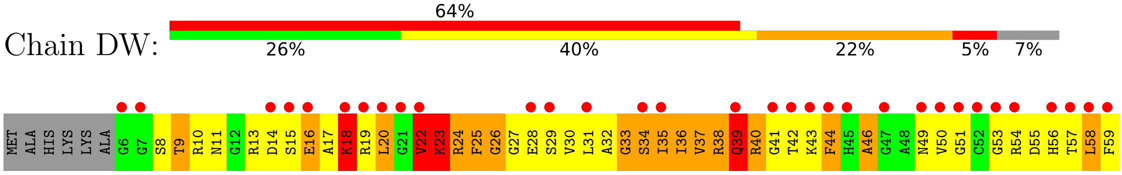
- Molecule 45: 50S ribosomal protein L25

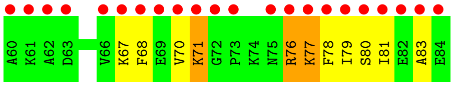


- Molecule 46: 50S ribosomal protein L27



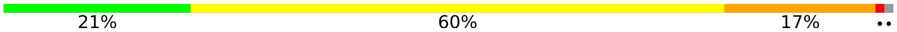
- Molecule 46: 50S ribosomal protein L27

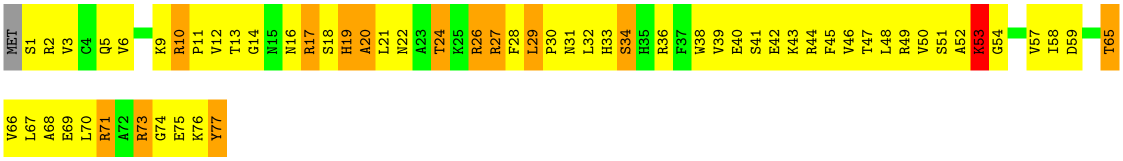




- Molecule 47: 50S ribosomal protein L28

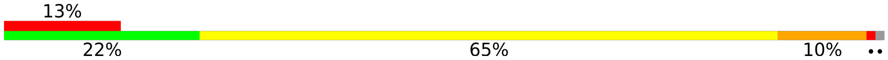
Chain BX:

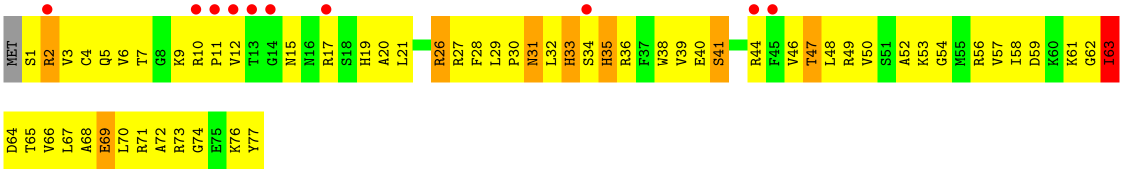




- Molecule 47: 50S ribosomal protein L28

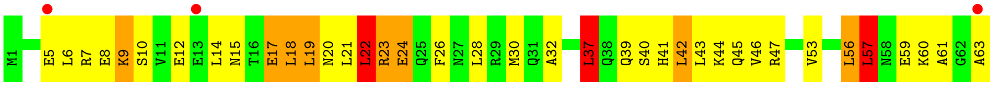
Chain DX:





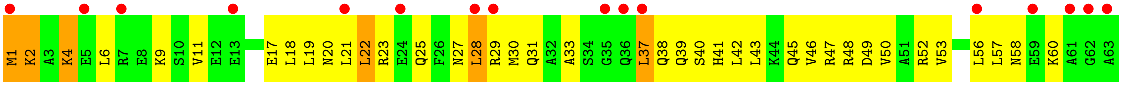
- Molecule 48: 50S ribosomal protein L29

Chain BY:



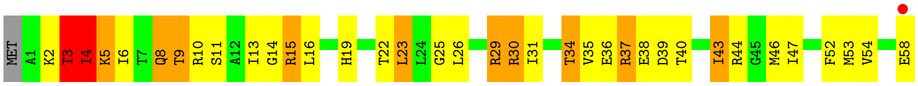
- Molecule 48: 50S ribosomal protein L29

Chain DY:



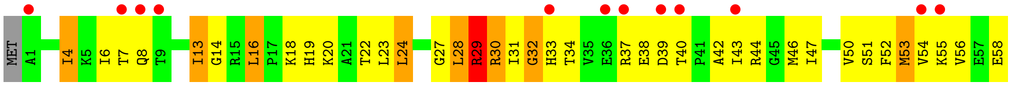
- Molecule 49: 50S ribosomal protein L30

Chain BZ:



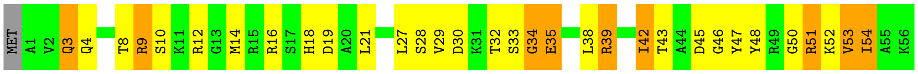
- Molecule 49: 50S ribosomal protein L30

Chain DZ:



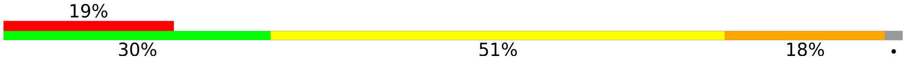
- Molecule 50: 50S ribosomal protein L32

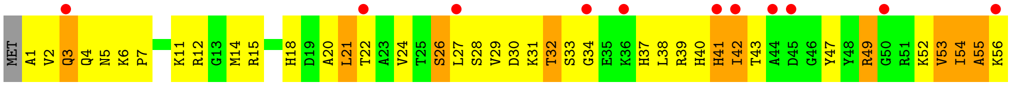
Chain B0:



- Molecule 50: 50S ribosomal protein L32

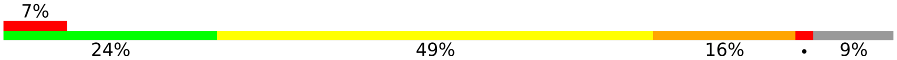
Chain D0:

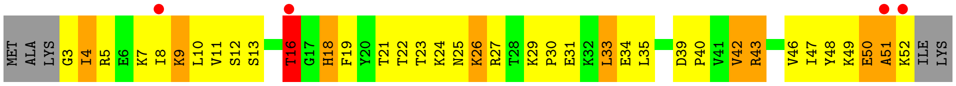




- Molecule 51: 50S ribosomal protein L33

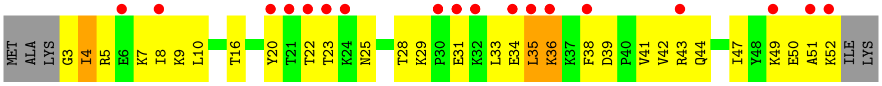
Chain B1:





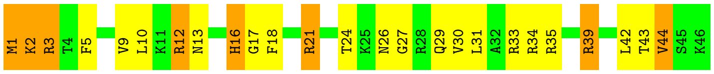
- Molecule 51: 50S ribosomal protein L33

Chain D1:



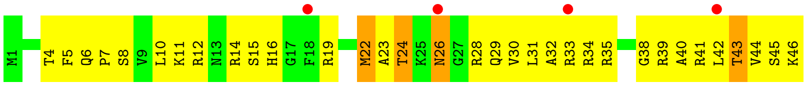
- Molecule 52: 50S ribosomal protein L34

Chain B2:



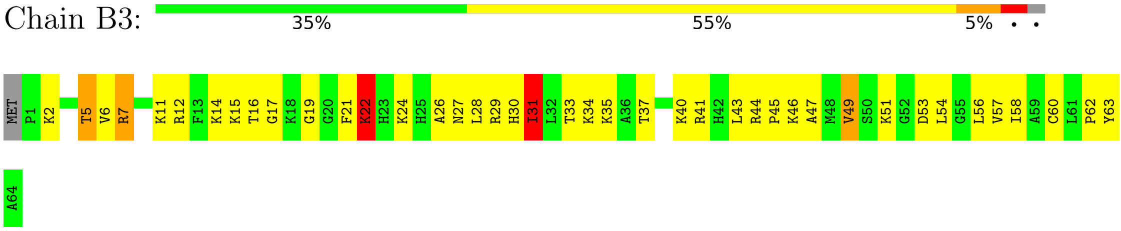
- Molecule 52: 50S ribosomal protein L34

Chain D2:



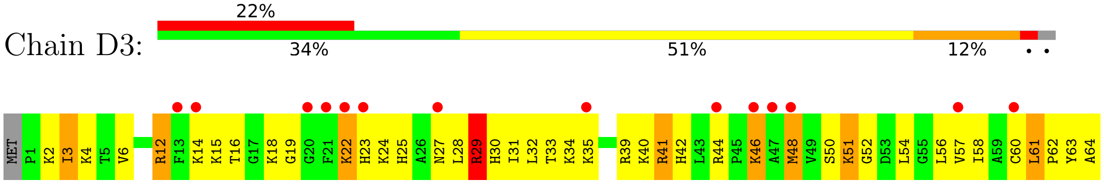
- Molecule 53: 50S ribosomal protein L35

Chain B3:



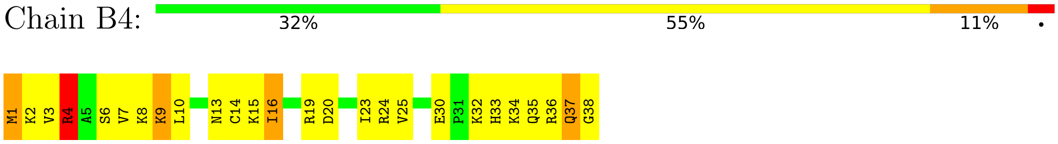
- Molecule 53: 50S ribosomal protein L35

Chain D3:



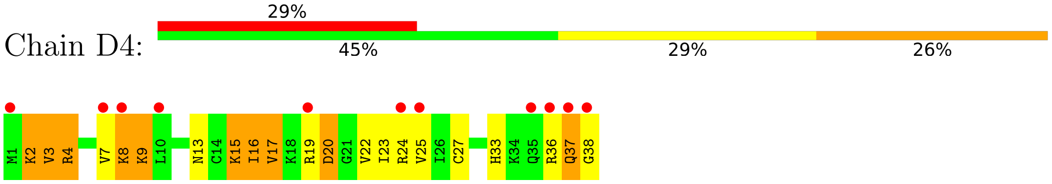
- Molecule 54: 50S ribosomal protein L36

Chain B4:



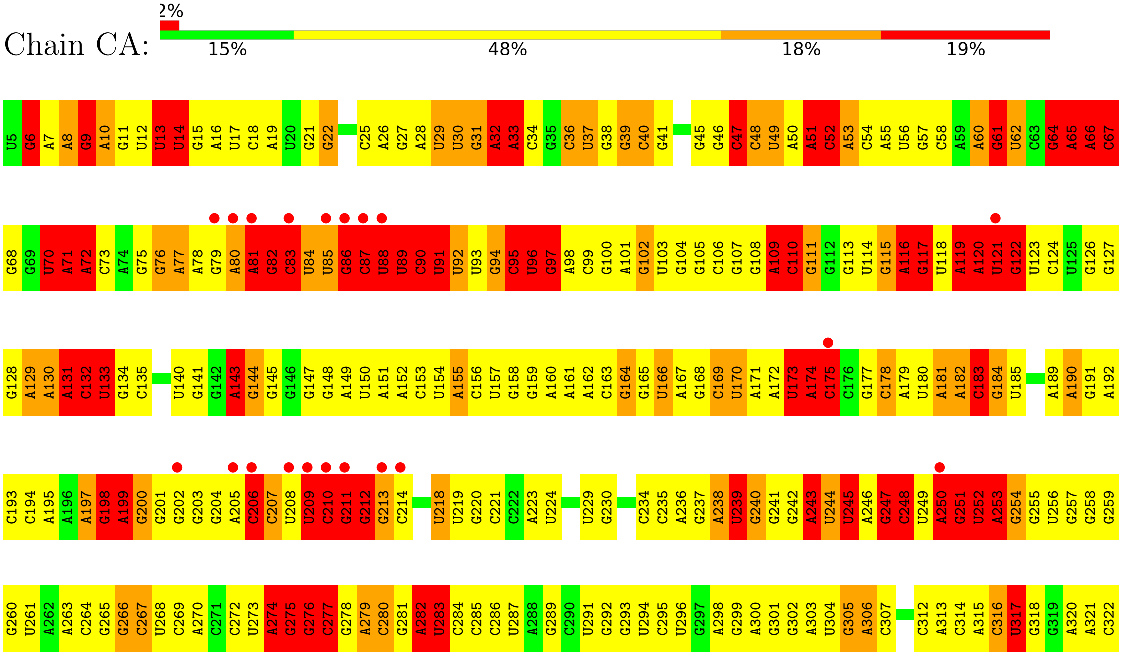
- Molecule 54: 50S ribosomal protein L36

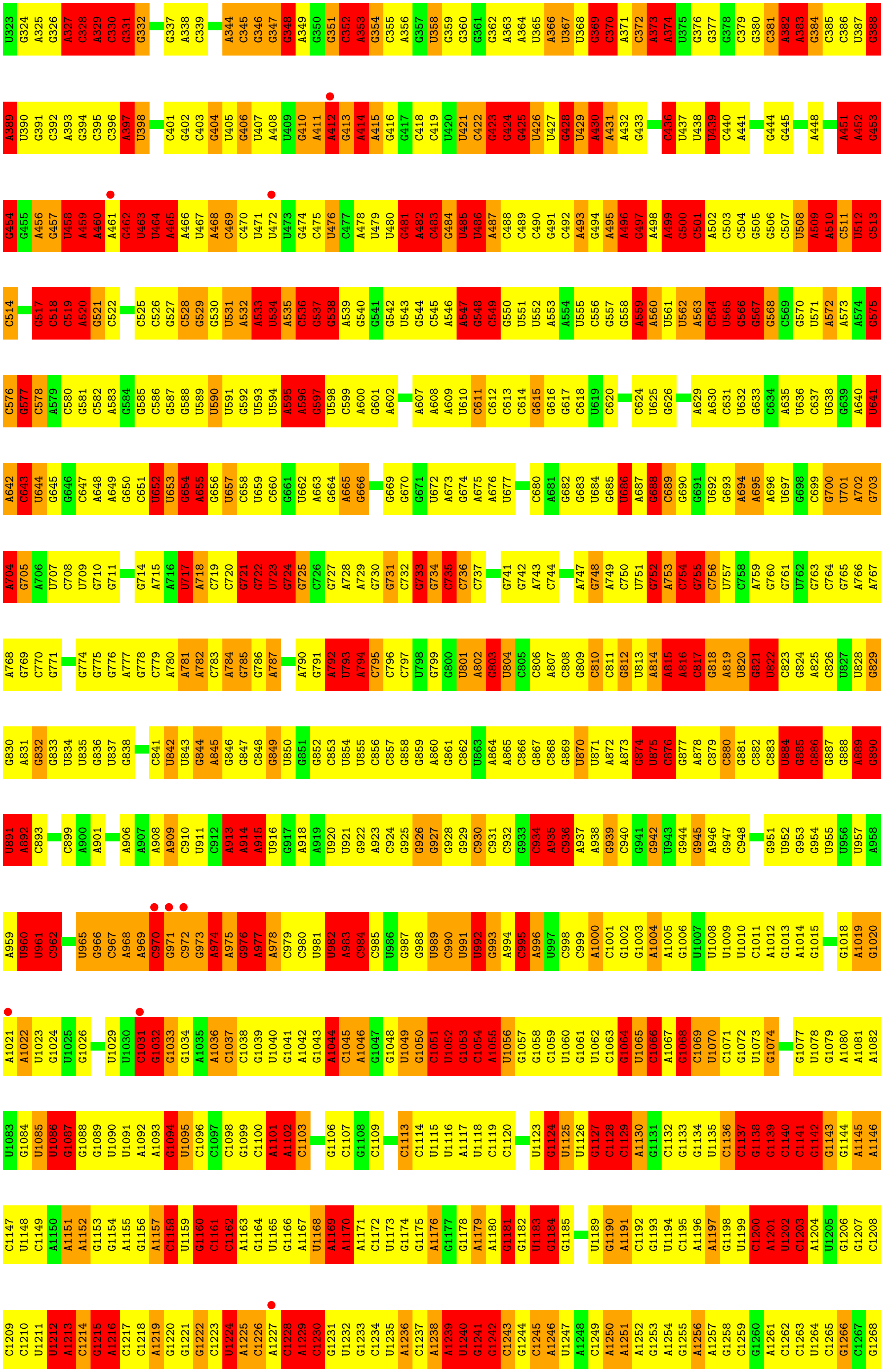
Chain D4:

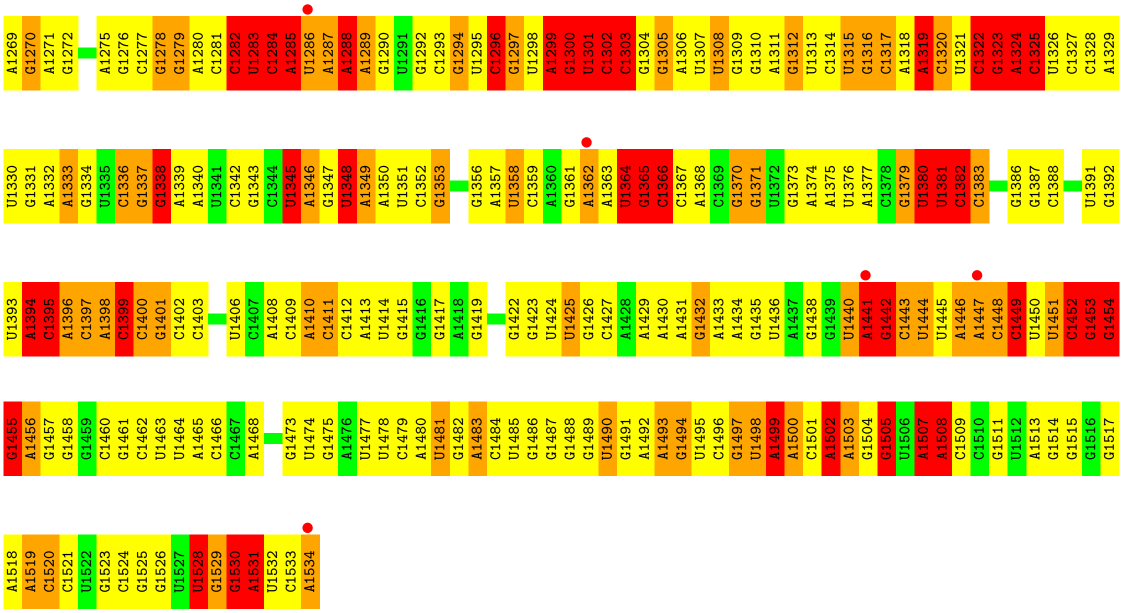


- Molecule 55: 16S rRNA

Chain CA:

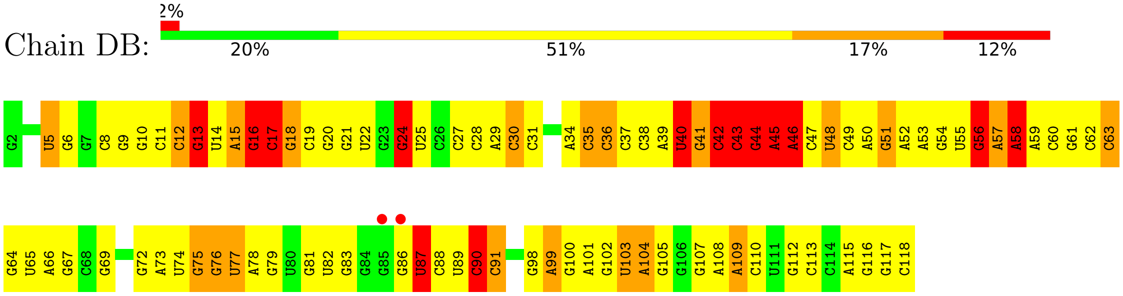



U323 G324 A325 G326 A327 C328 A329 C330 G331 G332 G337 A338 C339 A344 C345 G346 G347 G348 A349 G350 G351 C352 A353 G354 C355 A356 G357 U358 G359 G360 G361 G362 A363 A364 U365 A366 U367 U368 G369 C370 A371 C372 A373 A374 U375 G376 G377 G378 C379 G380 C381 A382 A383 G384 C385 C386 U387 G388
A389 U390 G391 C392 A393 G394 C395 C396 A397 U398 C401 G402 C403 G404 U405 G406 U407 A408 U409 G410 A411 A412 G413 A414 A415 G416 G417 C418 C419 U420 U421 C422 G423 G424 G425 U426 U427 G428 U429 A430 A431 A432 G433 C436 U437 U438 U439 C440 A441 G444 G445 A448 A451 A452 G453
G454 G455 A456 G457 U458 A459 A460 A461 G462 U463 U464 A465 A466 U467 A468 C469 C470 U471 U472 U473 G474 C475 U476 C477 A478 U479 U480 G481 A482 C483 G484 U485 U486 A487 C488 G489 C490 G491 C492 A493 G494 A495 A496 G497 A498 A499 G500 C501 A502 C503 C504 G505 G506 C507 U508 A509 A510 C511 U512 C513
C514 G517 C518 C519 A520 G521 C522 C525 C526 G527 C528 G529 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 G541 G542 U543 G544 C545 A546 A547 G548 C549 G550 U551 U552 A553 A554 U555 C556 G557 G558 A559 A560 U561 U562 A563 G564 U565 G566 G567 G568 C569 G570 U571 A572 A573 A574 G575
C576 G577 C578 A579 C580 G581 G582 A583 G584 G585 C586 G587 G588 U589 U590 U591 G592 U593 U594 A595 A596 G597 U598 C599 A600 G601 A602 A607 A608 A609 U610 C611 C612 C613 C614 G615 G616 G617 C618 U619 C620 C624 U625 G626 A629 A630 C631 U632 G633 C634 A635 U636 C637 U638 G639 A640 U641
A642 C643 U644 G645 G646 C647 A648 A649 G650 C651 U652 U653 G654 A655 G656 U657 C658 U659 C660 G661 U662 A663 G664 A665 G666 G669 G670 G671 U672 A673 G674 A675 A676 U677 C680 A681 G682 G683 U684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697 G698 C699 G700 U701 A702 G703
A704 G705 A706 U707 C708 U709 G710 G711 G714 A715 A716 U717 A718 C719 C720 G721 G722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 G733 G734 C735 C736 C737 G741 G742 A743 C744 A747 G748 A749 C750 U751 G752 A753 C754 G755 C756 U757 C758 A759 G760 G761 U762 G763 C764 G765 A766 A767
A768 G769 C770 G771 G774 G775 G776 A777 G778 C779 A780 A781 A782 C783 A784 G785 G786 A787 A790 G791 A792 U793 A794 C795 C796 C797 U798 G799 G800 U801 A802 G803 U804 C805 C806 A807 C808 G809 C810 C811 G812 U813 A814 A815 A816 C817 G818 A819 U820 G821 U822 C823 G824 A825 C826 U827 U828 G829
G830 A831 G832 G833 U834 U835 G836 U837 G838 C841 U842 U843 G844 A845 G846 G847 C848 G849 U850 G851 G852 C853 U854 U855 C856 C857 G858 G859 A860 G861 C862 U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 U875 C876 G877 A878 C879 C880 G881 C882 C883 U884 G885 G886 G887 G888 A889 G890
U891 A892 C893 C899 A900 A901 A906 A907 A908 A909 C910 U911 C912 A913 A914 A915 U916 G917 A918 A919 U920 U921 G922 A923 C924 G925 G926 G927 G928 G929 C930 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 G944 G945 A946 G947 C948 G951 U952 G953 G954 U955 U956 U957 A958
A959 U960 U961 C962 U965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 A976 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 A1005 G1006 U1007 U1008 U1009 U1010 C1011 A1012 G1013 A1014 G1015 G1018 A1019 G1020
A1021 A1022 U1023 G1024 U1025 G1026 U1029 U1030 C1031 G1032 G1033 G1034 A1035 A1036 C1037 C1038 G1039 U1040 G1041 A1042 G1043 A1044 C1045 A1046 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 U1060 G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 C1077 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 G1106 C1107 G1108 C1109 C1113 C1114 U1115 U1116 A1117 U1118 C1119 C1120 U1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 C1136 C1137 G1138 G1139 C1140 G1141 G1142 G1143 G1144 A1145 A1146
C1147 U1148 C1149 A1150 A1151 A1152 G1153 G1154 A1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 A1163 G1164 U1165 G1166 A1167 U1168 A1169 A1170 A1171 C1172 U1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 U1183 G1184 G1185 U1189 G1190 A1191 C1192 G1193 U1194 C1195 A1196 A1197 G1198 U1199 C1200 A1201 U1202 C1203 A1204 U1205 G1206 G1207 C1208
C1209 C1210 U1211 U1212 A1213 C1214 G1215 A1216 C1217 C1218 A1219 G1220 G1221 G1222 C1223 U1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240 G1241 G1242 C1243 G1244 C1245 A1246 U1247 A1248 C1249 A1250 A1251 A1252 G1253 A1254 G1255 A1256 A1257 G1258 C1259 G1260 A1261 C1262 C1263 U1264 C1265 G1266 C1267 G1268



• Molecule 56: 5S rRNA

Chain DB:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.95Å 433.08Å 624.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.44 – 3.71 73.44 – 3.71	Depositor EDS
% Data completeness (in resolution range)	75.7 (73.44-3.71) 75.7 (73.44-3.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 3.67Å)	Xtriage
Refinement program	PHENIX ?	Depositor
R, R_{free}	0.227 , 0.268 0.235 , 0.276	Depositor DCC
R_{free} test set	9161 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	109.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 85.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	286150	wwPDB-VP
Average B, all atoms (Å^2)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	AB	0.25	0/1735	0.47	0/2338
1	CB	0.25	0/1735	0.46	0/2338
2	AC	0.27	0/1651	0.48	0/2225
2	CC	0.26	0/1651	0.47	0/2225
3	AD	0.27	0/1665	0.48	0/2227
3	CD	0.30	0/1665	0.50	0/2227
4	AE	0.30	0/1118	0.54	0/1504
4	CE	0.29	0/1118	0.53	0/1504
5	AF	0.26	0/835	0.46	0/1128
5	CF	0.26	0/835	0.46	0/1128
6	AG	0.25	0/1195	0.43	0/1602
6	CG	0.27	0/1187	0.50	0/1591
7	AH	0.27	0/989	0.50	0/1326
7	CH	0.25	0/989	0.47	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.25	0/1034	0.47	0/1375
9	AJ	0.25	0/796	0.48	0/1077
9	CJ	0.24	0/796	0.47	0/1077
10	AK	0.26	0/893	0.48	0/1205
10	CK	0.26	0/893	0.50	0/1205
11	AL	0.33	0/969	0.62	0/1300
11	CL	0.31	0/969	0.53	0/1300
12	AM	0.36	0/892	0.64	3/1193 (0.3%)
12	CM	0.38	0/884	0.53	0/1181
13	AN	0.26	0/785	0.48	0/1043
13	CN	0.25	0/780	0.43	0/1036
14	AO	0.26	0/722	0.48	0/964
14	CO	0.24	0/722	0.46	0/964
15	AP	0.27	0/659	0.46	0/884
15	CP	0.27	0/648	0.47	0/870
16	AQ	0.33	0/657	0.55	0/881
16	CQ	0.26	0/657	0.46	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
17	AR	0.25	0/462	0.48	0/621
17	CR	0.27	0/462	0.49	0/621
18	AS	0.24	0/652	0.43	0/877
18	CS	0.23	0/652	0.46	0/877
19	AT	0.29	0/671	0.51	0/888
19	CT	0.24	0/671	0.44	0/888
20	AU	0.27	0/430	0.46	0/570
20	CU	0.29	0/430	0.54	0/570
21	AA	0.55	1/36834 (0.0%)	1.44	678/57462 (1.2%)
22	AV	0.59	0/408	1.14	1/634 (0.2%)
22	AX	0.52	0/408	1.04	0/634
22	CV	0.56	0/408	1.14	0/634
22	CX	0.41	0/408	0.82	0/634
23	AW	0.88	0/131	1.88	5/200 (2.5%)
23	CW	0.73	0/131	1.93	7/200 (3.5%)
24	BA	0.76	12/68626 (0.0%)	1.69	1758/107056 (1.6%)
24	DA	0.53	1/68314 (0.0%)	1.46	1365/106569 (1.3%)
25	BB	0.66	0/2828	1.67	74/4410 (1.7%)
26	BC	0.45	0/2121	0.72	1/2852 (0.0%)
26	DC	0.33	0/2121	0.54	0/2852
27	BD	0.50	0/1586	0.75	1/2134 (0.0%)
27	DD	0.31	0/1586	0.55	0/2134
28	BE	0.44	0/1571	0.67	0/2113
28	DE	0.25	0/1571	0.47	0/2113
29	BF	0.41	0/1434	0.68	3/1926 (0.2%)
29	DF	0.35	0/1444	0.73	5/1937 (0.3%)
30	BG	0.43	0/1343	0.65	0/1816
30	DG	0.23	0/1343	0.46	0/1816
31	BH	0.70	6/1122 (0.5%)	0.83	6/1515 (0.4%)
31	DH	0.53	3/1122 (0.3%)	0.67	3/1515 (0.2%)
32	BI	0.24	0/1046	0.50	0/1410
32	DI	0.23	0/1046	0.44	0/1410
33	BJ	0.55	0/1152	0.75	0/1551
33	DJ	0.28	0/1152	0.55	0/1551
34	BK	0.55	0/947	0.83	0/1268
34	DK	0.31	0/947	0.54	0/1268
35	BL	0.42	0/1054	0.77	1/1403 (0.1%)
35	DL	0.27	0/1054	0.51	0/1403
36	BM	0.51	0/1093	0.77	1/1460 (0.1%)
36	DM	0.31	0/1093	0.48	0/1460
37	BN	0.55	0/973	0.79	0/1301
37	DN	0.27	0/973	0.49	0/1301
38	BO	0.42	0/902	0.63	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DO	0.24	0/902	0.44	0/1209
39	BP	0.51	0/929	0.77	0/1242
39	DP	0.28	0/929	0.49	0/1242
40	BQ	0.60	0/960	0.71	0/1278
40	DQ	0.28	0/960	0.46	0/1278
41	BR	0.56	0/829	0.85	1/1107 (0.1%)
41	DR	0.28	0/829	0.50	0/1107
42	BS	0.50	0/864	0.75	0/1156
42	DS	0.29	0/864	0.54	0/1156
43	BT	0.48	0/744	0.70	0/994
43	DT	0.25	0/744	0.49	0/994
44	BU	0.41	0/787	0.70	0/1051
44	DU	0.25	0/787	0.47	0/1051
45	BV	0.48	0/766	0.66	0/1025
45	DV	0.38	0/766	0.54	0/1025
46	BW	0.51	0/603	0.76	0/797
46	DW	0.26	0/603	0.47	0/797
47	BX	0.42	0/635	0.67	0/848
47	DX	0.30	0/635	0.55	0/848
48	BY	0.40	0/510	0.66	0/677
48	DY	0.23	0/510	0.44	0/677
49	BZ	0.52	0/453	0.77	0/605
49	DZ	0.28	0/453	0.51	0/605
50	B0	0.45	0/450	0.79	0/599
50	D0	0.28	0/450	0.51	0/599
51	B1	0.40	0/416	0.63	0/554
51	D1	0.28	0/416	0.46	0/554
52	B2	0.47	0/380	0.73	0/498
52	D2	0.28	0/380	0.55	0/498
53	B3	0.51	0/513	0.76	0/676
53	D3	0.26	0/513	0.51	0/676
54	B4	0.47	0/303	0.76	0/397
54	D4	0.30	0/303	0.49	0/397
55	CA	0.53	0/36762	1.45	712/57350 (1.2%)
56	DB	0.52	0/2803	1.35	52/4371 (1.2%)
All	All	0.55	23/308631 (0.0%)	1.35	4677/461501 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	AM	0	1
27	BD	0	1
31	BH	0	2
31	DH	0	3
37	BN	0	1
All	All	0	8

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1142	A	N9-C4	-13.92	1.29	1.37
31	BH	48	GLU	C-O	9.51	1.41	1.23
24	BA	2451	A	C8-N7	9.03	1.37	1.31
31	DH	49	ALA	CA-CB	-7.88	1.35	1.52
31	BH	48	GLU	CA-CB	6.93	1.69	1.53

The worst 5 of 4677 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BA	2447	G	C6-N1-C2	-22.51	111.59	125.10
24	BA	2451	A	C5-N7-C8	-17.23	95.28	103.90
24	BA	2347	C	N1-C1'-C2'	-16.79	92.17	114.00
24	BA	790	U	P-O3'-C3'	-16.12	100.36	119.70
25	BB	88	C	O4'-C1'-N1	-15.24	96.01	108.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	AM	70	ARG	Peptide
27	BD	10	GLY	Peptide
31	BH	48	GLU	Mainchain
31	BH	49	ALA	Mainchain
37	BN	101	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1704	0	1732	253	0
1	CB	1704	0	1732	203	0
2	AC	1624	0	1699	133	0
2	CC	1624	0	1699	149	0
3	AD	1643	0	1710	139	0
3	CD	1643	0	1710	139	0
4	AE	1105	0	1148	196	0
4	CE	1105	0	1148	127	0
5	AF	817	0	808	91	0
5	CF	817	0	808	76	0
6	AG	1181	0	1240	100	0
6	CG	1174	0	1230	154	0
7	AH	979	0	1034	107	0
7	CH	979	0	1034	95	0
8	AI	1022	0	1070	122	0
8	CI	1022	0	1070	108	0
9	AJ	786	0	828	69	0
9	CJ	786	0	828	114	0
10	AK	877	0	887	103	0
10	CK	877	0	887	82	0
11	AL	955	0	1019	97	0
11	CL	955	0	1019	101	0
12	AM	883	0	944	69	0
12	CM	876	0	937	123	0
13	AN	774	0	827	72	0
13	CN	769	0	822	83	0
14	AO	714	0	737	50	0
14	CO	714	0	737	40	0
15	AP	649	0	666	63	0
15	CP	638	0	656	56	0
16	AQ	648	0	691	70	0
16	CQ	648	0	691	59	0
17	AR	455	0	478	36	0
17	CR	455	0	478	41	0
18	AS	637	0	665	42	0
18	CS	637	0	665	79	0
19	AT	665	0	714	56	0
19	CT	665	0	714	58	0
20	AU	425	0	449	65	0
20	CU	425	0	449	70	0
21	AA	32895	0	16553	1800	0
22	AV	365	0	185	24	0
22	AX	365	0	185	20	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	365	0	185	26	0
22	CX	365	0	185	11	0
23	AW	120	0	61	8	0
23	CW	120	0	61	4	0
24	BA	61274	0	30819	3133	0
24	DA	60995	0	30679	3843	0
25	BB	2529	0	1281	109	0
26	BC	2082	0	2157	226	0
26	DC	2082	0	2157	230	0
27	BD	1565	0	1616	200	0
27	DD	1565	0	1616	162	0
28	BE	1552	0	1619	158	0
28	DE	1552	0	1619	170	0
29	BF	1410	0	1447	144	0
29	DF	1420	0	1460	183	0
30	BG	1323	0	1374	149	0
30	DG	1323	0	1374	116	0
31	BH	1111	0	1148	108	0
31	DH	1111	0	1148	100	0
32	BI	1032	0	1088	116	0
32	DI	1032	0	1088	69	0
33	BJ	1129	0	1162	160	0
33	DJ	1129	0	1162	122	0
34	BK	938	0	1012	102	0
34	DK	938	0	1012	114	0
35	BL	1045	0	1117	133	0
35	DL	1045	0	1117	130	0
36	BM	1074	0	1157	129	0
36	DM	1074	0	1157	96	0
37	BN	960	0	1000	102	0
37	DN	960	0	1000	107	0
38	BO	892	0	923	82	0
38	DO	892	0	923	90	0
39	BP	917	0	965	120	0
39	DP	917	0	965	87	0
40	BQ	947	0	1022	147	0
40	DQ	947	0	1022	120	0
41	BR	816	0	839	102	0
41	DR	816	0	839	90	0
42	BS	857	0	922	89	0
42	DS	857	0	922	83	0
43	BT	738	0	807	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DT	738	0	807	96	0
44	BU	779	0	834	65	0
44	DU	779	0	834	93	0
45	BV	753	0	780	54	0
45	DV	753	0	780	98	0
46	BW	596	0	610	179	0
46	DW	596	0	610	105	0
47	BX	625	0	655	68	0
47	DX	625	0	655	76	0
48	BY	509	0	543	45	0
48	DY	509	0	543	55	0
49	BZ	449	0	491	41	0
49	DZ	449	0	491	40	0
50	B0	444	0	461	36	0
50	D0	444	0	461	63	0
51	B1	409	0	440	43	0
51	D1	409	0	440	33	0
52	B2	377	0	418	28	0
52	D2	377	0	418	42	0
53	B3	504	0	574	41	0
53	D3	504	0	574	54	0
54	B4	302	0	340	40	0
54	D4	302	0	340	27	0
55	CA	32831	0	16521	2003	0
56	DB	2507	0	1270	160	0
57	AA	43	0	0	0	0
57	BA	136	0	0	0	0
57	BB	4	0	0	0	0
57	BD	1	0	0	0	0
57	CA	42	0	0	0	0
57	D4	1	0	0	0	0
57	DA	132	0	0	0	0
57	DB	1	0	0	0	0
57	DC	2	0	0	0	0
57	DJ	1	0	0	0	0
58	B4	1	0	0	0	0
58	D4	1	0	0	0	0
59	AA	196	0	0	7	0
59	AE	1	0	0	0	0
59	AL	3	0	0	0	0
59	AN	6	0	0	1	0
59	AT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	AU	1	0	0	0	0
59	B2	1	0	0	0	0
59	B3	3	0	0	0	0
59	B4	2	0	0	0	0
59	BA	615	0	0	21	0
59	BB	20	0	0	1	0
59	BC	8	0	0	1	0
59	BD	3	0	0	4	0
59	BE	1	0	0	0	0
59	BL	3	0	0	0	0
59	BN	3	0	0	0	0
59	BT	1	0	0	1	0
59	CA	195	0	0	6	0
59	CE	4	0	0	0	0
59	CI	1	0	0	0	0
59	CL	1	0	0	0	0
59	CN	2	0	0	0	0
59	CT	2	0	0	0	0
59	CU	2	0	0	0	0
59	D2	1	0	0	0	0
59	D3	1	0	0	0	0
59	D4	5	0	0	0	0
59	DA	600	0	0	17	0
59	DB	4	0	0	0	0
59	DC	12	0	0	0	0
59	DD	2	0	0	0	0
59	DE	3	0	0	0	0
59	DJ	3	0	0	0	0
59	DL	6	0	0	0	0
59	DN	2	0	0	1	0
59	DT	2	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	286150	0	191700	19249	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

The worst 5 of 19249 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)
12:AM:67:ASP:O	12:AM:70:ARG:HD2	1.23	1.31
55:CA:1213:A:O2’	55:CA:1214:C:H5’	1.29	1.25
24:DA:604:G:O2’	24:DA:605:G:H5’	1.40	1.19
40:BQ:63:ARG:NH1	40:BQ:96:ASP:HA	1.56	1.18
24:DA:297:G:H5”	44:DU:84:PHE:HB2	1.26	1.18

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
1	AB	216/241 (90%)	119 (55%)	69 (32%)	28 (13%)	0	4
1	CB	216/241 (90%)	144 (67%)	50 (23%)	22 (10%)	0	8
2	AC	204/233 (88%)	140 (69%)	48 (24%)	16 (8%)	1	13
2	CC	204/233 (88%)	136 (67%)	52 (26%)	16 (8%)	1	13
3	AD	203/206 (98%)	143 (70%)	43 (21%)	17 (8%)	1	11
3	CD	203/206 (98%)	136 (67%)	46 (23%)	21 (10%)	0	7
4	AE	148/167 (89%)	105 (71%)	27 (18%)	16 (11%)	0	6
4	CE	148/167 (89%)	100 (68%)	34 (23%)	14 (10%)	0	9
5	AF	98/135 (73%)	68 (69%)	22 (22%)	8 (8%)	1	11
5	CF	98/135 (73%)	65 (66%)	27 (28%)	6 (6%)	1	18
6	AG	149/179 (83%)	103 (69%)	36 (24%)	10 (7%)	1	17
6	CG	148/179 (83%)	84 (57%)	44 (30%)	20 (14%)	0	4
7	AH	127/130 (98%)	90 (71%)	27 (21%)	10 (8%)	1	13
7	CH	127/130 (98%)	88 (69%)	30 (24%)	9 (7%)	1	15
8	AI	125/130 (96%)	81 (65%)	32 (26%)	12 (10%)	0	9
8	CI	125/130 (96%)	88 (70%)	33 (26%)	4 (3%)	4	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	96/103 (93%)	69 (72%)	16 (17%)	11 (12%)	0	5
9	CJ	96/103 (93%)	62 (65%)	22 (23%)	12 (12%)	0	5
10	AK	115/129 (89%)	84 (73%)	22 (19%)	9 (8%)	1	13
10	CK	115/129 (89%)	86 (75%)	19 (16%)	10 (9%)	1	11
11	AL	121/124 (98%)	82 (68%)	27 (22%)	12 (10%)	0	8
11	CL	121/124 (98%)	86 (71%)	26 (22%)	9 (7%)	1	14
12	AM	112/118 (95%)	89 (80%)	16 (14%)	7 (6%)	1	18
12	CM	111/118 (94%)	71 (64%)	28 (25%)	12 (11%)	0	6
13	AN	92/101 (91%)	63 (68%)	18 (20%)	11 (12%)	0	5
13	CN	91/101 (90%)	62 (68%)	24 (26%)	5 (6%)	2	21
14	AO	86/89 (97%)	64 (74%)	20 (23%)	2 (2%)	6	37
14	CO	86/89 (97%)	67 (78%)	19 (22%)	0	100	100
15	AP	80/82 (98%)	52 (65%)	22 (28%)	6 (8%)	1	14
15	CP	78/82 (95%)	52 (67%)	20 (26%)	6 (8%)	1	13
16	AQ	78/84 (93%)	47 (60%)	20 (26%)	11 (14%)	0	4
16	CQ	78/84 (93%)	57 (73%)	16 (20%)	5 (6%)	1	18
17	AR	53/75 (71%)	39 (74%)	11 (21%)	3 (6%)	1	20
17	CR	53/75 (71%)	39 (74%)	11 (21%)	3 (6%)	1	20
18	AS	77/92 (84%)	61 (79%)	13 (17%)	3 (4%)	3	27
18	CS	77/92 (84%)	55 (71%)	20 (26%)	2 (3%)	5	34
19	AT	83/87 (95%)	63 (76%)	14 (17%)	6 (7%)	1	15
19	CT	83/87 (95%)	59 (71%)	21 (25%)	3 (4%)	3	29
20	AU	49/71 (69%)	26 (53%)	16 (33%)	7 (14%)	0	3
20	CU	49/71 (69%)	23 (47%)	17 (35%)	9 (18%)	0	2
26	BC	269/273 (98%)	192 (71%)	48 (18%)	29 (11%)	0	6
26	DC	269/273 (98%)	169 (63%)	73 (27%)	27 (10%)	0	8
27	BD	207/209 (99%)	141 (68%)	35 (17%)	31 (15%)	0	3
27	DD	207/209 (99%)	129 (62%)	48 (23%)	30 (14%)	0	3
28	BE	199/201 (99%)	138 (69%)	41 (21%)	20 (10%)	0	8
28	DE	199/201 (99%)	129 (65%)	49 (25%)	21 (11%)	0	7
29	BF	175/179 (98%)	133 (76%)	26 (15%)	16 (9%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DF	176/179 (98%)	94 (53%)	43 (24%)	39 (22%)	0	1
30	BG	174/177 (98%)	114 (66%)	34 (20%)	26 (15%)	0	3
30	DG	174/177 (98%)	109 (63%)	36 (21%)	29 (17%)	0	3
31	BH	147/149 (99%)	63 (43%)	53 (36%)	31 (21%)	0	1
31	DH	147/149 (99%)	78 (53%)	48 (33%)	21 (14%)	0	3
32	BI	139/142 (98%)	84 (60%)	42 (30%)	13 (9%)	0	9
32	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	4
33	BJ	140/142 (99%)	100 (71%)	22 (16%)	18 (13%)	0	4
33	DJ	140/142 (99%)	95 (68%)	31 (22%)	14 (10%)	0	8
34	BK	120/123 (98%)	86 (72%)	17 (14%)	17 (14%)	0	3
34	DK	120/123 (98%)	79 (66%)	22 (18%)	19 (16%)	0	3
35	BL	141/144 (98%)	106 (75%)	23 (16%)	12 (8%)	1	11
35	DL	141/144 (98%)	80 (57%)	42 (30%)	19 (14%)	0	4
36	BM	134/136 (98%)	95 (71%)	16 (12%)	23 (17%)	0	2
36	DM	134/136 (98%)	89 (66%)	32 (24%)	13 (10%)	0	9
37	BN	118/127 (93%)	85 (72%)	23 (20%)	10 (8%)	1	11
37	DN	118/127 (93%)	73 (62%)	32 (27%)	13 (11%)	0	6
38	BO	114/117 (97%)	84 (74%)	20 (18%)	10 (9%)	1	10
38	DO	114/117 (97%)	80 (70%)	28 (25%)	6 (5%)	2	21
39	BP	112/115 (97%)	74 (66%)	23 (20%)	15 (13%)	0	4
39	DP	112/115 (97%)	67 (60%)	30 (27%)	15 (13%)	0	4
40	BQ	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	1	18
40	DQ	115/118 (98%)	85 (74%)	22 (19%)	8 (7%)	1	16
41	BR	101/103 (98%)	75 (74%)	14 (14%)	12 (12%)	0	5
41	DR	101/103 (98%)	71 (70%)	20 (20%)	10 (10%)	0	8
42	BS	108/110 (98%)	81 (75%)	20 (18%)	7 (6%)	1	18
42	DS	108/110 (98%)	80 (74%)	18 (17%)	10 (9%)	0	10
43	BT	91/100 (91%)	55 (60%)	20 (22%)	16 (18%)	0	2
43	DT	91/100 (91%)	47 (52%)	30 (33%)	14 (15%)	0	3
44	BU	100/104 (96%)	68 (68%)	16 (16%)	16 (16%)	0	3
44	DU	100/104 (96%)	49 (49%)	29 (29%)	22 (22%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BV	92/94 (98%)	76 (83%)	15 (16%)	1 (1%)	14	50
45	DV	92/94 (98%)	59 (64%)	25 (27%)	8 (9%)	1	11
46	BW	77/85 (91%)	32 (42%)	18 (23%)	27 (35%)	0	0
46	DW	77/85 (91%)	34 (44%)	25 (32%)	18 (23%)	0	0
47	BX	75/78 (96%)	58 (77%)	12 (16%)	5 (7%)	1	17
47	DX	75/78 (96%)	49 (65%)	19 (25%)	7 (9%)	0	10
48	BY	61/63 (97%)	39 (64%)	15 (25%)	7 (12%)	0	5
48	DY	61/63 (97%)	45 (74%)	11 (18%)	5 (8%)	1	11
49	BZ	56/59 (95%)	43 (77%)	10 (18%)	3 (5%)	2	21
49	DZ	56/59 (95%)	35 (62%)	14 (25%)	7 (12%)	0	5
50	B0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	4
50	D0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	4
51	B1	48/55 (87%)	32 (67%)	9 (19%)	7 (15%)	0	3
51	D1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	1	11
52	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	2	24
52	D2	44/46 (96%)	30 (68%)	9 (20%)	5 (11%)	0	5
53	B3	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	4	31
53	D3	62/65 (95%)	42 (68%)	15 (24%)	5 (8%)	1	12
54	B4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	1	11
54	D4	36/38 (95%)	22 (61%)	8 (22%)	6 (17%)	0	3
All	All	11238/11970 (94%)	7515 (67%)	2516 (22%)	1207 (11%)	0	6

5 of 1207 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	ARG
1	AB	22	TRP
1	AB	37	VAL
1	AB	71	THR
1	AB	125	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/199 (90%)	147 (82%)	33 (18%)	1	10
1	CB	180/199 (90%)	158 (88%)	22 (12%)	5	24
2	AC	170/190 (90%)	148 (87%)	22 (13%)	4	23
2	CC	170/190 (90%)	146 (86%)	24 (14%)	3	20
3	AD	172/173 (99%)	147 (86%)	25 (14%)	3	19
3	CD	172/173 (99%)	152 (88%)	20 (12%)	5	27
4	AE	113/126 (90%)	93 (82%)	20 (18%)	2	12
4	CE	113/126 (90%)	100 (88%)	13 (12%)	5	27
5	AF	87/116 (75%)	75 (86%)	12 (14%)	3	21
5	CF	87/116 (75%)	74 (85%)	13 (15%)	3	18
6	AG	124/147 (84%)	117 (94%)	7 (6%)	21	53
6	CG	123/147 (84%)	95 (77%)	28 (23%)	1	6
7	AH	104/105 (99%)	92 (88%)	12 (12%)	5	27
7	CH	104/105 (99%)	91 (88%)	13 (12%)	4	23
8	AI	105/107 (98%)	90 (86%)	15 (14%)	3	19
8	CI	105/107 (98%)	91 (87%)	14 (13%)	4	22
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	3	20
9	CJ	86/90 (96%)	77 (90%)	9 (10%)	7	30
10	AK	90/99 (91%)	80 (89%)	10 (11%)	6	29
10	CK	90/99 (91%)	80 (89%)	10 (11%)	6	29
11	AL	103/104 (99%)	85 (82%)	18 (18%)	2	12
11	CL	103/104 (99%)	88 (85%)	15 (15%)	3	18
12	AM	92/96 (96%)	87 (95%)	5 (5%)	22	54
12	CM	91/96 (95%)	74 (81%)	17 (19%)	1	10
13	AN	79/84 (94%)	73 (92%)	6 (8%)	13	43
13	CN	79/84 (94%)	68 (86%)	11 (14%)	3	21
14	AO	76/77 (99%)	72 (95%)	4 (5%)	22	54
14	CO	76/77 (99%)	72 (95%)	4 (5%)	22	54
15	AP	65/65 (100%)	60 (92%)	5 (8%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CP	65/65 (100%)	59 (91%)	6 (9%)	9	36
16	AQ	74/78 (95%)	60 (81%)	14 (19%)	1	9
16	CQ	74/78 (95%)	64 (86%)	10 (14%)	4	22
17	AR	48/65 (74%)	46 (96%)	2 (4%)	30	58
17	CR	48/65 (74%)	46 (96%)	2 (4%)	30	58
18	AS	70/79 (89%)	63 (90%)	7 (10%)	7	32
18	CS	70/79 (89%)	59 (84%)	11 (16%)	2	16
19	AT	65/66 (98%)	55 (85%)	10 (15%)	2	17
19	CT	65/66 (98%)	56 (86%)	9 (14%)	3	21
20	AU	44/61 (72%)	37 (84%)	7 (16%)	2	16
20	CU	44/61 (72%)	35 (80%)	9 (20%)	1	7
26	BC	216/218 (99%)	173 (80%)	43 (20%)	1	8
26	DC	216/218 (99%)	191 (88%)	25 (12%)	5	27
27	BD	164/164 (100%)	136 (83%)	28 (17%)	2	13
27	DD	164/164 (100%)	144 (88%)	20 (12%)	5	24
28	BE	165/165 (100%)	130 (79%)	35 (21%)	1	7
28	DE	165/165 (100%)	152 (92%)	13 (8%)	12	42
29	BF	148/150 (99%)	130 (88%)	18 (12%)	5	24
29	DF	149/150 (99%)	124 (83%)	25 (17%)	2	14
30	BG	137/138 (99%)	107 (78%)	30 (22%)	1	6
30	DG	137/138 (99%)	120 (88%)	17 (12%)	4	24
31	BH	114/114 (100%)	97 (85%)	17 (15%)	3	18
31	DH	114/114 (100%)	95 (83%)	19 (17%)	2	14
32	BI	109/110 (99%)	94 (86%)	15 (14%)	3	21
32	DI	109/110 (99%)	102 (94%)	7 (6%)	17	48
33	BJ	116/116 (100%)	90 (78%)	26 (22%)	1	6
33	DJ	116/116 (100%)	106 (91%)	10 (9%)	10	39
34	BK	103/104 (99%)	84 (82%)	19 (18%)	1	10
34	DK	103/104 (99%)	85 (82%)	18 (18%)	2	12
35	BL	102/103 (99%)	81 (79%)	21 (21%)	1	7
35	DL	102/103 (99%)	90 (88%)	12 (12%)	5	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BM	109/109 (100%)	90 (83%)	19 (17%)	2	12
36	DM	109/109 (100%)	100 (92%)	9 (8%)	11	40
37	BN	100/103 (97%)	81 (81%)	19 (19%)	1	9
37	DN	100/103 (97%)	85 (85%)	15 (15%)	3	18
38	BO	86/87 (99%)	69 (80%)	17 (20%)	1	8
38	DO	86/87 (99%)	78 (91%)	8 (9%)	9	35
39	BP	99/100 (99%)	79 (80%)	20 (20%)	1	8
39	DP	99/100 (99%)	91 (92%)	8 (8%)	11	41
40	BQ	89/90 (99%)	73 (82%)	16 (18%)	1	11
40	DQ	89/90 (99%)	79 (89%)	10 (11%)	6	28
41	BR	84/84 (100%)	69 (82%)	15 (18%)	2	11
41	DR	84/84 (100%)	70 (83%)	14 (17%)	2	14
42	BS	93/93 (100%)	73 (78%)	20 (22%)	1	7
42	DS	93/93 (100%)	79 (85%)	14 (15%)	3	18
43	BT	80/84 (95%)	61 (76%)	19 (24%)	0	5
43	DT	80/84 (95%)	74 (92%)	6 (8%)	13	44
44	BU	83/85 (98%)	69 (83%)	14 (17%)	2	13
44	DU	83/85 (98%)	72 (87%)	11 (13%)	4	22
45	BV	78/78 (100%)	64 (82%)	14 (18%)	2	11
45	DV	78/78 (100%)	68 (87%)	10 (13%)	4	23
46	BW	59/63 (94%)	43 (73%)	16 (27%)	0	3
46	DW	59/63 (94%)	44 (75%)	15 (25%)	0	4
47	BX	67/68 (98%)	53 (79%)	14 (21%)	1	7
47	DX	67/68 (98%)	58 (87%)	9 (13%)	4	22
48	BY	55/55 (100%)	44 (80%)	11 (20%)	1	8
48	DY	55/55 (100%)	52 (94%)	3 (6%)	21	53
49	BZ	48/49 (98%)	34 (71%)	14 (29%)	0	2
49	DZ	48/49 (98%)	41 (85%)	7 (15%)	3	18
50	B0	47/48 (98%)	42 (89%)	5 (11%)	6	30
50	D0	47/48 (98%)	42 (89%)	5 (11%)	6	30
51	B1	45/49 (92%)	37 (82%)	8 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	D1	45/49 (92%)	41 (91%)	4 (9%)	9	37
52	B2	38/38 (100%)	32 (84%)	6 (16%)	2	16
52	D2	38/38 (100%)	34 (90%)	4 (10%)	7	30
53	B3	51/52 (98%)	44 (86%)	7 (14%)	3	21
53	D3	51/52 (98%)	42 (82%)	9 (18%)	2	12
54	B4	34/34 (100%)	30 (88%)	4 (12%)	5	26
54	D4	34/34 (100%)	29 (85%)	5 (15%)	3	18
All	All	9331/9756 (96%)	7983 (86%)	1348 (14%)	3	19

5 of 1348 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	CL	28	GLN
33	DJ	54	ILE
12	CM	113	LYS
11	CL	19	ASN
26	DC	269	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 323 such sidechains are listed below:

Mol	Chain	Res	Type
26	DC	57	HIS
41	DR	86	GLN
27	DD	49	GLN
34	DK	3	GLN
45	DV	80	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	465 (30%)	230 (15%)
22	AV	17/17 (100%)	2 (11%)	1 (5%)
22	AX	17/17 (100%)	2 (11%)	1 (5%)
22	CV	17/17 (100%)	3 (17%)	1 (5%)
22	CX	16/17 (94%)	2 (12%)	0
23	AW	5/6 (83%)	3 (60%)	1 (20%)
23	CW	5/6 (83%)	1 (20%)	1 (20%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	BA	2850/2903 (98%)	925 (32%)	497 (17%)
24	DA	2838/2903 (97%)	1020 (35%)	505 (17%)
25	BB	117/118 (99%)	32 (27%)	22 (18%)
55	CA	1529/1530 (99%)	516 (33%)	245 (16%)
56	DB	116/117 (99%)	29 (25%)	13 (11%)
All	All	9059/9184 (98%)	3000 (33%)	1517 (16%)

5 of 3000 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	9	G
21	AA	13	U

5 of 1517 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	CA	1053	G
24	DA	778	G
55	CA	1213	A
55	CA	1051	C
24	DA	223	A

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 365 ligands modelled in this entry, 365 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AB	218/241 (90%)	1.99	83 (38%)	0	0	170, 274, 284, 290	0
1	CB	218/241 (90%)	0.79	36 (16%)	1	1	159, 222, 233, 241	0
2	AC	206/233 (88%)	0.43	11 (5%)	26	23	133, 162, 187, 202	0
2	CC	206/233 (88%)	0.59	16 (7%)	13	10	140, 172, 212, 228	0
3	AD	205/206 (99%)	0.25	11 (5%)	25	22	122, 157, 195, 218	0
3	CD	205/206 (99%)	-0.27	0	100	100	112, 131, 152, 165	0
4	AE	150/167 (89%)	2.91	84 (56%)	0	0	108, 211, 223, 227	0
4	CE	150/167 (89%)	0.50	15 (10%)	7	6	100, 156, 171, 176	0
5	AF	100/135 (74%)	0.30	7 (7%)	16	12	197, 229, 250, 260	0
5	CF	100/135 (74%)	0.85	18 (18%)	1	1	164, 186, 203, 209	0
6	AG	151/179 (84%)	0.34	17 (11%)	5	5	158, 192, 220, 237	0
6	CG	150/179 (83%)	0.34	20 (13%)	3	3	142, 194, 228, 244	0
7	AH	129/130 (99%)	0.34	12 (9%)	8	7	127, 155, 181, 193	0
7	CH	129/130 (99%)	0.81	23 (17%)	1	1	152, 177, 195, 203	0
8	AI	127/130 (97%)	0.71	18 (14%)	2	3	142, 193, 220, 233	0
8	CI	127/130 (97%)	0.52	14 (11%)	5	5	155, 195, 223, 232	0
9	AJ	98/103 (95%)	0.31	6 (6%)	21	16	135, 181, 216, 239	0
9	CJ	98/103 (95%)	0.83	14 (14%)	2	3	155, 196, 230, 240	0
10	AK	117/129 (90%)	0.74	14 (11%)	4	4	132, 195, 243, 254	0
10	CK	117/129 (90%)	0.31	6 (5%)	28	24	125, 155, 181, 196	0
11	AL	123/124 (99%)	0.15	4 (3%)	46	38	89, 106, 131, 150	0
11	CL	123/124 (99%)	0.67	13 (10%)	6	5	117, 139, 155, 161	0
12	AM	114/118 (96%)	0.61	14 (12%)	4	4	157, 219, 252, 264	0
12	CM	113/118 (95%)	0.71	15 (13%)	3	3	195, 269, 309, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AN	96/101 (95%)	0.28	5 (5%) 27 24	142, 165, 217, 227	0
13	CN	95/101 (94%)	1.05	15 (15%) 2 1	155, 207, 265, 284	0
14	AO	88/89 (98%)	-0.20	0 100 100	138, 168, 199, 219	0
14	CO	88/89 (98%)	-0.06	1 (1%) 80 76	142, 174, 193, 201	0
15	AP	82/82 (100%)	0.79	11 (13%) 3 3	117, 144, 178, 192	0
15	CP	80/82 (97%)	1.48	23 (28%) 0 0	151, 180, 203, 207	0
16	AQ	80/84 (95%)	0.64	5 (6%) 20 15	90, 113, 135, 144	0
16	CQ	80/84 (95%)	1.11	16 (20%) 1 1	99, 123, 145, 163	0
17	AR	55/75 (73%)	0.81	8 (14%) 2 2	175, 198, 219, 234	0
17	CR	55/75 (73%)	0.24	3 (5%) 25 21	148, 165, 180, 187	0
18	AS	79/92 (85%)	1.49	27 (34%) 0 0	171, 203, 244, 257	0
18	CS	79/92 (85%)	1.52	26 (32%) 0 0	223, 265, 319, 334	0
19	AT	85/87 (97%)	0.12	3 (3%) 44 36	114, 141, 164, 180	0
19	CT	85/87 (97%)	1.16	25 (29%) 0 0	194, 242, 275, 283	0
20	AU	51/71 (71%)	0.76	6 (11%) 4 4	133, 168, 248, 252	0
20	CU	51/71 (71%)	0.19	2 (3%) 39 32	126, 150, 183, 193	0
21	AA	1533/1533 (100%)	-0.47	13 (0%) 86 83	76, 150, 233, 282	0
22	AV	17/17 (100%)	0.19	1 (5%) 22 17	142, 154, 182, 203	0
22	AX	17/17 (100%)	-0.25	1 (5%) 22 17	139, 144, 186, 195	0
22	CV	17/17 (100%)	0.05	1 (5%) 22 17	158, 162, 193, 208	0
22	CX	17/17 (100%)	2.35	8 (47%) 0 0	187, 193, 221, 222	0
23	AW	6/6 (100%)	0.13	0 100 100	136, 138, 143, 152	0
23	CW	6/6 (100%)	0.47	0 100 100	160, 160, 168, 179	0
24	BA	2854/2903 (98%)	-0.38	39 (1%) 75 69	52, 81, 194, 355	0
24	DA	2841/2903 (97%)	0.27	139 (4%) 29 25	132, 200, 303, 402	0
25	BB	118/118 (100%)	-0.62	0 100 100	66, 101, 133, 171	0
26	BC	271/273 (99%)	-0.08	3 (1%) 80 76	60, 99, 129, 161	0
26	DC	271/273 (99%)	0.60	25 (9%) 9 7	133, 157, 179, 190	0
27	BD	209/209 (100%)	-0.18	2 (0%) 82 78	55, 75, 114, 129	0
27	DD	209/209 (100%)	1.42	68 (32%) 0 0	147, 200, 232, 242	0
28	BE	201/201 (100%)	-0.17	2 (0%) 82 78	56, 96, 129, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
28	DE	201/201 (100%)	1.26	46 (22%)	0	0	154, 282, 335, 351	0
29	BF	177/179 (98%)	1.04	32 (18%)	1	1	120, 166, 201, 215	0
29	DF	178/179 (99%)	2.08	76 (42%)	0	0	307, 314, 321, 323	0
30	BG	176/177 (99%)	0.09	3 (1%)	70	64	83, 108, 134, 152	0
30	DG	176/177 (99%)	1.59	55 (31%)	0	0	186, 221, 245, 259	0
31	BH	149/149 (100%)	2.05	57 (38%)	0	0	110, 239, 259, 264	0
31	DH	149/149 (100%)	1.54	42 (28%)	0	0	186, 240, 256, 260	0
32	BI	141/142 (99%)	2.13	60 (42%)	0	0	243, 307, 359, 366	0
32	DI	141/142 (99%)	3.16	87 (61%)	0	0	367, 394, 412, 419	0
33	BJ	142/142 (100%)	-0.30	0	100	100	59, 76, 102, 132	0
33	DJ	142/142 (100%)	1.24	35 (24%)	0	0	161, 201, 223, 233	0
34	BK	122/123 (99%)	-0.09	1 (0%)	86	83	55, 73, 113, 169	0
34	DK	122/123 (99%)	1.24	36 (29%)	0	0	151, 171, 189, 198	0
35	BL	143/144 (99%)	-0.27	1 (0%)	87	85	55, 93, 124, 136	0
35	DL	143/144 (99%)	1.19	38 (26%)	0	0	166, 240, 288, 297	0
36	BM	136/136 (100%)	-0.08	1 (0%)	87	85	58, 81, 111, 138	0
36	DM	136/136 (100%)	1.76	55 (40%)	0	0	144, 181, 210, 232	0
37	BN	120/127 (94%)	-0.07	0	100	100	61, 76, 96, 141	0
37	DN	120/127 (94%)	2.05	52 (43%)	0	0	183, 222, 252, 266	0
38	BO	116/117 (99%)	-0.05	1 (0%)	84	80	96, 105, 123, 147	0
38	DO	116/117 (99%)	2.44	56 (48%)	0	0	286, 293, 297, 303	0
39	BP	114/115 (99%)	-0.07	0	100	100	64, 81, 119, 134	0
39	DP	114/115 (99%)	1.41	33 (28%)	0	0	179, 203, 220, 230	0
40	BQ	117/118 (99%)	-0.47	0	100	100	56, 77, 99, 120	0
40	DQ	117/118 (99%)	1.13	25 (21%)	0	0	184, 211, 240, 247	0
41	BR	103/103 (100%)	-0.22	0	100	100	55, 87, 114, 131	0
41	DR	103/103 (100%)	2.21	45 (43%)	0	0	173, 249, 271, 277	0
42	BS	110/110 (100%)	-0.34	0	100	100	55, 70, 105, 159	0
42	DS	110/110 (100%)	1.74	39 (35%)	0	0	159, 223, 269, 278	0
43	BT	93/100 (93%)	0.11	2 (2%)	62	55	65, 105, 142, 151	0
43	DT	93/100 (93%)	2.27	47 (50%)	0	0	206, 253, 285, 294	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB($Å^2$)	Q<0.9
44	BU	102/104 (98%)	0.32	5 (4%)	29	25	89, 114, 136, 158	0
44	DU	102/104 (98%)	3.17	60 (58%)	0	0	272, 312, 355, 358	0
45	BV	94/94 (100%)	-0.15	0	100	100	71, 90, 116, 126	0
45	DV	94/94 (100%)	1.19	23 (24%)	0	0	228, 241, 252, 254	0
46	BW	79/85 (92%)	-0.02	2 (2%)	57	49	68, 86, 136, 156	0
46	DW	79/85 (92%)	3.13	54 (68%)	0	0	156, 216, 233, 252	0
47	BX	77/78 (98%)	-0.20	0	100	100	65, 101, 124, 137	0
47	DX	77/78 (98%)	0.78	10 (12%)	3	4	157, 185, 209, 224	0
48	BY	63/63 (100%)	-0.02	3 (4%)	30	26	101, 123, 149, 159	0
48	DY	63/63 (100%)	1.20	16 (25%)	0	0	264, 288, 316, 329	0
49	BZ	58/59 (98%)	0.14	1 (1%)	70	64	64, 74, 111, 141	0
49	DZ	58/59 (98%)	1.12	12 (20%)	1	1	188, 215, 238, 248	0
50	B0	56/57 (98%)	-0.52	0	100	100	54, 77, 113, 132	0
50	D0	56/57 (98%)	1.32	11 (19%)	1	1	157, 230, 260, 265	0
51	B1	50/55 (90%)	0.58	4 (8%)	12	10	76, 100, 118, 132	0
51	D1	50/55 (90%)	1.67	18 (36%)	0	0	174, 207, 228, 238	0
52	B2	46/46 (100%)	-0.27	0	100	100	62, 75, 103, 137	0
52	D2	46/46 (100%)	0.69	4 (8%)	10	8	155, 182, 198, 202	0
53	B3	64/65 (98%)	-0.30	0	100	100	58, 73, 96, 120	0
53	D3	64/65 (98%)	1.23	14 (21%)	0	0	180, 194, 211, 215	0
54	B4	38/38 (100%)	-0.03	0	100	100	69, 84, 110, 120	0
54	D4	38/38 (100%)	1.23	11 (28%)	0	0	171, 187, 198, 203	0
55	CA	1530/1530 (100%)	-0.14	34 (2%)	62	55	109, 171, 272, 362	0
56	DB	117/117 (100%)	0.07	2 (1%)	70	64	219, 294, 300, 302	0
All	All	20511/21154 (96%)	0.38	2158 (10%)	6	5	52, 166, 293, 419	0

The worst 5 of 2158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AB	194	GLY	17.7
31	BH	87	GLU	14.6
4	AE	145	ASN	14.0
24	BA	2179	C	13.7
29	DF	129	MET	13.7

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	DA	3002	1/1	-0.26	1.16	212,212,212,212	0
57	MG	DA	3073	1/1	-0.05	0.20	312,312,312,312	0
57	MG	DA	3020	1/1	0.16	2.42	229,229,229,229	0
57	MG	DA	3045	1/1	0.23	0.24	188,188,188,188	0
57	MG	DA	3132	1/1	0.24	0.26	198,198,198,198	0
57	MG	DA	3063	1/1	0.35	1.56	157,157,157,157	0
57	MG	DA	3003	1/1	0.36	1.42	229,229,229,229	0
57	MG	DA	3109	1/1	0.38	0.91	145,145,145,145	0
57	MG	CA	1610	1/1	0.39	0.22	181,181,181,181	0
57	MG	DA	3083	1/1	0.40	0.08	303,303,303,303	0
57	MG	DJ	201	1/1	0.40	0.55	183,183,183,183	0
57	MG	CA	1602	1/1	0.42	0.16	177,177,177,177	0
57	MG	CA	1627	1/1	0.44	0.35	136,136,136,136	0
57	MG	D4	101	1/1	0.45	1.38	183,183,183,183	0
57	MG	DA	3015	1/1	0.46	1.27	164,164,164,164	0
57	MG	DA	3108	1/1	0.46	0.65	172,172,172,172	0
57	MG	DA	3071	1/1	0.51	0.30	184,184,184,184	0
57	MG	BA	3070	1/1	0.51	0.17	158,158,158,158	0
57	MG	DA	3125	1/1	0.53	0.31	187,187,187,187	0
57	MG	DA	3064	1/1	0.55	0.51	157,157,157,157	0
57	MG	AA	1624	1/1	0.56	0.17	131,131,131,131	0
57	MG	AA	1619	1/1	0.57	0.48	162,162,162,162	0
57	MG	DA	3106	1/1	0.57	0.35	228,228,228,228	0
57	MG	DA	3006	1/1	0.58	0.17	296,296,296,296	0
57	MG	CA	1622	1/1	0.58	0.09	216,216,216,216	0
57	MG	DA	3049	1/1	0.58	0.11	249,249,249,249	0
57	MG	DA	3016	1/1	0.59	1.32	175,175,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3092	1/1	0.60	0.27	198,198,198,198	0
57	MG	DA	3128	1/1	0.61	0.65	132,132,132,132	0
57	MG	CA	1620	1/1	0.61	0.49	150,150,150,150	0
57	MG	CA	1607	1/1	0.62	0.22	134,134,134,134	0
57	MG	DA	3078	1/1	0.62	0.64	144,144,144,144	0
57	MG	CA	1619	1/1	0.62	0.92	135,135,135,135	0
57	MG	DA	3058	1/1	0.64	0.92	162,162,162,162	0
57	MG	DA	3018	1/1	0.64	0.40	248,248,248,248	0
57	MG	DA	3087	1/1	0.65	0.16	208,208,208,208	0
57	MG	CA	1606	1/1	0.66	0.14	124,124,124,124	0
57	MG	DA	3094	1/1	0.67	0.68	173,173,173,173	0
57	MG	DA	3044	1/1	0.67	0.24	210,210,210,210	0
57	MG	CA	1617	1/1	0.67	0.28	183,183,183,183	0
57	MG	DA	3069	1/1	0.68	0.52	139,139,139,139	0
57	MG	DA	3068	1/1	0.68	0.33	143,143,143,143	0
57	MG	AA	1617	1/1	0.69	0.29	150,150,150,150	0
57	MG	DA	3129	1/1	0.69	1.36	132,132,132,132	0
57	MG	DA	3059	1/1	0.69	0.28	136,136,136,136	0
57	MG	CA	1603	1/1	0.69	0.17	141,141,141,141	0
57	MG	DA	3082	1/1	0.69	0.42	220,220,220,220	0
57	MG	AA	1630	1/1	0.70	0.28	99,99,99,99	0
57	MG	DA	3029	1/1	0.71	0.62	179,179,179,179	0
57	MG	DA	3010	1/1	0.71	0.26	210,210,210,210	0
57	MG	DA	3095	1/1	0.71	0.19	152,152,152,152	0
57	MG	DA	3037	1/1	0.72	0.20	204,204,204,204	0
57	MG	DA	3121	1/1	0.72	0.45	206,206,206,206	0
57	MG	DA	3072	1/1	0.72	0.43	182,182,182,182	0
57	MG	AA	1636	1/1	0.72	0.36	154,154,154,154	0
57	MG	DA	3039	1/1	0.73	0.27	186,186,186,186	0
57	MG	DA	3022	1/1	0.73	0.77	152,152,152,152	0
57	MG	DA	3113	1/1	0.73	0.19	182,182,182,182	0
57	MG	DA	3097	1/1	0.73	0.34	156,156,156,156	0
57	MG	DA	3060	1/1	0.73	0.78	132,132,132,132	0
57	MG	DA	3013	1/1	0.74	0.29	165,165,165,165	0
57	MG	DA	3107	1/1	0.75	0.14	137,137,137,137	0
57	MG	CA	1616	1/1	0.75	0.33	199,199,199,199	0
57	MG	AA	1610	1/1	0.75	0.12	155,155,155,155	0
57	MG	DA	3110	1/1	0.75	0.17	219,219,219,219	0
57	MG	DA	3051	1/1	0.75	0.23	160,160,160,160	0
57	MG	DA	3093	1/1	0.75	0.14	208,208,208,208	0
57	MG	CA	1634	1/1	0.76	0.11	153,153,153,153	0
57	MG	DA	3070	1/1	0.76	0.09	147,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	DA	3033	1/1	0.76	0.14	162,162,162,162	0
57	MG	DA	3041	1/1	0.77	0.40	176,176,176,176	0
57	MG	DA	3005	1/1	0.77	1.13	197,197,197,197	0
57	MG	AA	1614	1/1	0.78	0.18	150,150,150,150	0
57	MG	BA	3098	1/1	0.78	0.37	72,72,72,72	0
57	MG	DA	3119	1/1	0.78	0.13	147,147,147,147	0
57	MG	DA	3075	1/1	0.78	0.96	155,155,155,155	0
57	MG	DA	3054	1/1	0.78	0.34	155,155,155,155	0
57	MG	DA	3081	1/1	0.78	0.23	182,182,182,182	0
57	MG	CA	1614	1/1	0.78	0.56	146,146,146,146	0
57	MG	BA	3115	1/1	0.78	0.53	65,65,65,65	0
57	MG	DB	201	1/1	0.78	0.15	224,224,224,224	0
57	MG	DA	3084	1/1	0.78	0.35	214,214,214,214	0
57	MG	CA	1624	1/1	0.78	0.29	99,99,99,99	0
57	MG	DA	3124	1/1	0.79	0.35	168,168,168,168	0
57	MG	DA	3048	1/1	0.79	0.14	203,203,203,203	0
57	MG	DA	3001	1/1	0.79	0.29	206,206,206,206	0
57	MG	DA	3038	1/1	0.79	0.43	197,197,197,197	0
57	MG	CA	1632	1/1	0.79	0.15	210,210,210,210	0
57	MG	DA	3008	1/1	0.79	0.13	198,198,198,198	0
57	MG	DA	3030	1/1	0.79	0.30	164,164,164,164	0
57	MG	AA	1637	1/1	0.79	0.57	118,118,118,118	0
57	MG	DA	3062	1/1	0.80	1.23	160,160,160,160	0
57	MG	CA	1629	1/1	0.80	0.23	157,157,157,157	0
57	MG	DA	3036	1/1	0.80	0.47	212,212,212,212	0
57	MG	DA	3096	1/1	0.80	0.31	190,190,190,190	0
57	MG	DA	3111	1/1	0.80	0.30	160,160,160,160	0
57	MG	DA	3079	1/1	0.80	0.22	148,148,148,148	0
57	MG	DC	301	1/1	0.80	0.18	135,135,135,135	0
57	MG	DA	3101	1/1	0.80	0.17	155,155,155,155	0
57	MG	CA	1611	1/1	0.80	0.29	132,132,132,132	0
57	MG	DA	3019	1/1	0.81	0.19	245,245,245,245	0
57	MG	BA	3101	1/1	0.81	0.14	54,54,54,54	0
57	MG	AA	1628	1/1	0.81	0.28	134,134,134,134	0
57	MG	DA	3025	1/1	0.81	0.09	135,135,135,135	0
57	MG	BA	3095	1/1	0.81	0.21	92,92,92,92	0
57	MG	CA	1642	1/1	0.81	0.12	170,170,170,170	0
57	MG	AA	1633	1/1	0.81	0.16	128,128,128,128	0
57	MG	AA	1641	1/1	0.82	0.43	108,108,108,108	0
57	MG	BA	3028	1/1	0.82	0.33	57,57,57,57	0
57	MG	DA	3076	1/1	0.82	1.13	145,145,145,145	0
57	MG	BA	3046	1/1	0.82	0.19	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	DA	3011	1/1	0.82	1.01	184,184,184,184	0
57	MG	DA	3047	1/1	0.82	0.25	208,208,208,208	0
57	MG	AA	1627	1/1	0.82	1.47	142,142,142,142	0
57	MG	DA	3131	1/1	0.82	0.44	181,181,181,181	0
57	MG	BA	3075	1/1	0.82	0.32	58,58,58,58	0
57	MG	BA	3092	1/1	0.82	0.08	127,127,127,127	0
57	MG	AA	1609	1/1	0.82	0.14	118,118,118,118	0
57	MG	DA	3088	1/1	0.82	0.30	180,180,180,180	0
57	MG	AA	1604	1/1	0.82	0.08	157,157,157,157	0
57	MG	CA	1636	1/1	0.83	1.56	120,120,120,120	0
57	MG	DA	3032	1/1	0.83	0.15	161,161,161,161	0
57	MG	CA	1639	1/1	0.83	0.12	266,266,266,266	0
57	MG	DA	3043	1/1	0.83	0.16	208,208,208,208	0
57	MG	CA	1633	1/1	0.83	0.14	123,123,123,123	0
57	MG	DA	3074	1/1	0.83	1.75	187,187,187,187	0
57	MG	AA	1625	1/1	0.83	0.32	114,114,114,114	0
57	MG	DA	3120	1/1	0.84	0.22	159,159,159,159	0
57	MG	AA	1635	1/1	0.84	0.17	148,148,148,148	0
57	MG	DA	3085	1/1	0.84	0.23	167,167,167,167	0
57	MG	BA	3133	1/1	0.84	0.58	73,73,73,73	0
57	MG	DA	3017	1/1	0.84	0.19	187,187,187,187	0
57	MG	DA	3091	1/1	0.84	0.93	174,174,174,174	0
57	MG	DA	3028	1/1	0.85	0.47	165,165,165,165	0
57	MG	BA	3026	1/1	0.85	0.44	59,59,59,59	0
57	MG	BA	3015	1/1	0.85	0.60	55,55,55,55	0
57	MG	DC	302	1/1	0.85	0.20	140,140,140,140	0
57	MG	CA	1625	1/1	0.85	0.49	127,127,127,127	0
57	MG	BA	3124	1/1	0.85	0.96	59,59,59,59	0
57	MG	DA	3050	1/1	0.86	0.22	180,180,180,180	0
57	MG	DA	3098	1/1	0.86	0.33	170,170,170,170	0
57	MG	BA	3032	1/1	0.86	0.13	57,57,57,57	0
57	MG	BA	3131	1/1	0.86	0.59	68,68,68,68	0
57	MG	AA	1632	1/1	0.86	0.10	117,117,117,117	0
57	MG	DA	3026	1/1	0.86	1.01	160,160,160,160	0
57	MG	DA	3014	1/1	0.86	0.28	162,162,162,162	0
57	MG	AA	1607	1/1	0.86	0.45	113,113,113,113	0
57	MG	BA	3007	1/1	0.86	0.17	111,111,111,111	0
57	MG	BA	3086	1/1	0.86	0.12	60,60,60,60	0
57	MG	DA	3007	1/1	0.86	0.47	250,250,250,250	0
57	MG	CA	1640	1/1	0.86	0.59	118,118,118,118	0
57	MG	DA	3040	1/1	0.87	0.26	171,171,171,171	0
57	MG	DA	3023	1/1	0.87	0.23	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3117	1/1	0.87	0.45	170,170,170,170	0
57	MG	CA	1641	1/1	0.87	0.17	151,151,151,151	0
57	MG	BA	3047	1/1	0.87	0.19	78,78,78,78	0
57	MG	BA	3011	1/1	0.87	0.30	62,62,62,62	0
57	MG	DA	3123	1/1	0.87	0.20	225,225,225,225	0
57	MG	AA	1601	1/1	0.87	0.12	133,133,133,133	0
57	MG	CA	1612	1/1	0.87	0.17	124,124,124,124	0
57	MG	AA	1634	1/1	0.88	0.12	121,121,121,121	0
57	MG	BA	3077	1/1	0.88	0.15	63,63,63,63	0
57	MG	DA	3099	1/1	0.88	0.19	211,211,211,211	0
57	MG	BA	3037	1/1	0.88	0.23	58,58,58,58	0
57	MG	DA	3102	1/1	0.88	0.15	141,141,141,141	0
57	MG	CA	1613	1/1	0.88	0.11	121,121,121,121	0
57	MG	BA	3090	1/1	0.88	0.11	63,63,63,63	0
57	MG	DA	3130	1/1	0.88	0.17	170,170,170,170	0
57	MG	BB	201	1/1	0.88	0.49	118,118,118,118	0
57	MG	BA	3019	1/1	0.88	0.12	86,86,86,86	0
57	MG	BA	3004	1/1	0.88	0.22	86,86,86,86	0
57	MG	BA	3056	1/1	0.88	0.30	64,64,64,64	0
57	MG	DA	3066	1/1	0.88	0.12	150,150,150,150	0
57	MG	DA	3080	1/1	0.88	0.12	134,134,134,134	0
57	MG	BA	3014	1/1	0.88	0.26	55,55,55,55	0
57	MG	AA	1620	1/1	0.89	0.17	186,186,186,186	0
57	MG	CA	1615	1/1	0.89	0.21	156,156,156,156	0
57	MG	CA	1635	1/1	0.89	0.10	142,142,142,142	0
57	MG	DA	3115	1/1	0.89	0.14	154,154,154,154	0
57	MG	CA	1608	1/1	0.89	0.19	121,121,121,121	0
57	MG	DA	3027	1/1	0.89	0.14	171,171,171,171	0
57	MG	BA	3079	1/1	0.89	0.06	110,110,110,110	0
57	MG	DA	3067	1/1	0.90	0.15	147,147,147,147	0
57	MG	BA	3062	1/1	0.90	0.68	55,55,55,55	0
57	MG	BA	3112	1/1	0.90	0.22	64,64,64,64	0
57	MG	BA	3030	1/1	0.90	0.40	58,58,58,58	0
57	MG	DA	3090	1/1	0.90	0.09	200,200,200,200	0
57	MG	DA	3100	1/1	0.90	0.32	150,150,150,150	0
57	MG	BA	3118	1/1	0.90	0.09	60,60,60,60	0
57	MG	DA	3118	1/1	0.90	0.25	181,181,181,181	0
57	MG	DA	3042	1/1	0.90	0.26	179,179,179,179	0
57	MG	DA	3103	1/1	0.90	0.15	150,150,150,150	0
57	MG	BA	3081	1/1	0.90	0.10	56,56,56,56	0
57	MG	AA	1605	1/1	0.90	0.20	124,124,124,124	0
57	MG	BA	3052	1/1	0.91	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	1621	1/1	0.91	0.27	80,80,80,80	0
57	MG	BA	3105	1/1	0.91	0.18	55,55,55,55	0
57	MG	AA	1611	1/1	0.91	0.23	126,126,126,126	0
57	MG	BB	202	1/1	0.91	0.14	127,127,127,127	0
57	MG	BA	3093	1/1	0.91	0.29	104,104,104,104	0
57	MG	BA	3051	1/1	0.91	0.14	57,57,57,57	0
57	MG	BA	3121	1/1	0.91	0.11	64,64,64,64	0
57	MG	DA	3055	1/1	0.91	0.13	136,136,136,136	0
57	MG	DA	3056	1/1	0.91	0.19	141,141,141,141	0
57	MG	CA	1628	1/1	0.91	1.01	99,99,99,99	0
57	MG	CA	1609	1/1	0.92	0.15	131,131,131,131	0
57	MG	BA	3103	1/1	0.92	0.07	81,81,81,81	0
57	MG	CA	1637	1/1	0.92	0.28	112,112,112,112	0
57	MG	BA	3044	1/1	0.92	0.08	88,88,88,88	0
57	MG	BA	3107	1/1	0.92	0.18	67,67,67,67	0
57	MG	AA	1629	1/1	0.92	0.21	161,161,161,161	0
57	MG	BA	3060	1/1	0.92	0.36	56,56,56,56	0
57	MG	DA	3031	1/1	0.92	0.16	159,159,159,159	0
57	MG	DA	3086	1/1	0.92	0.27	196,196,196,196	0
57	MG	AA	1603	1/1	0.92	0.09	93,93,93,93	0
57	MG	CA	1630	1/1	0.92	0.19	99,99,99,99	0
57	MG	DA	3034	1/1	0.92	0.14	158,158,158,158	0
57	MG	BA	3085	1/1	0.92	0.42	59,59,59,59	0
57	MG	DA	3004	1/1	0.92	0.21	206,206,206,206	0
57	MG	AA	1638	1/1	0.92	0.19	107,107,107,107	0
57	MG	DA	3057	1/1	0.92	0.28	133,133,133,133	0
57	MG	BA	3127	1/1	0.92	0.10	57,57,57,57	0
57	MG	DA	3035	1/1	0.93	0.11	155,155,155,155	0
57	MG	BB	204	1/1	0.93	0.09	74,74,74,74	0
57	MG	DA	3024	1/1	0.93	0.17	162,162,162,162	0
57	MG	DA	3052	1/1	0.93	0.12	144,144,144,144	0
57	MG	BA	3123	1/1	0.93	0.12	79,79,79,79	0
57	MG	BA	3035	1/1	0.93	0.28	72,72,72,72	0
57	MG	DA	3127	1/1	0.93	0.80	138,138,138,138	0
57	MG	AA	1602	1/1	0.93	0.37	97,97,97,97	0
57	MG	DA	3089	1/1	0.93	0.44	179,179,179,179	0
57	MG	AA	1623	1/1	0.93	0.11	129,129,129,129	0
57	MG	AA	1631	1/1	0.93	0.20	114,114,114,114	0
57	MG	BA	3088	1/1	0.93	0.12	77,77,77,77	0
57	MG	CA	1618	1/1	0.93	0.28	148,148,148,148	0
57	MG	DA	3009	1/1	0.93	0.22	199,199,199,199	0
57	MG	DA	3021	1/1	0.93	0.36	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3058	1/1	0.93	0.48	63,63,63,63	0
57	MG	DA	3065	1/1	0.93	0.37	152,152,152,152	0
57	MG	AA	1608	1/1	0.94	0.23	105,105,105,105	0
57	MG	AA	1642	1/1	0.94	0.26	90,90,90,90	0
57	MG	DA	3053	1/1	0.94	0.17	144,144,144,144	0
57	MG	BA	3036	1/1	0.94	0.09	65,65,65,65	0
57	MG	BA	3069	1/1	0.94	0.11	65,65,65,65	0
57	MG	BA	3099	1/1	0.94	0.09	58,58,58,58	0
57	MG	BD	301	1/1	0.94	0.20	55,55,55,55	0
57	MG	DA	3114	1/1	0.94	0.26	135,135,135,135	0
57	MG	CA	1601	1/1	0.94	0.13	224,224,224,224	0
57	MG	DA	3116	1/1	0.94	0.14	133,133,133,133	0
57	MG	AA	1643	1/1	0.94	0.11	101,101,101,101	0
57	MG	BA	3102	1/1	0.94	0.20	57,57,57,57	0
57	MG	CA	1604	1/1	0.94	0.04	117,117,117,117	0
57	MG	CA	1631	1/1	0.94	0.22	130,130,130,130	0
57	MG	BA	3071	1/1	0.94	0.33	55,55,55,55	0
57	MG	DA	3122	1/1	0.94	0.28	146,146,146,146	0
57	MG	BA	3104	1/1	0.94	0.18	55,55,55,55	0
57	MG	BA	3043	1/1	0.94	0.19	68,68,68,68	0
57	MG	BA	3018	1/1	0.94	0.08	80,80,80,80	0
57	MG	BA	3002	1/1	0.94	0.36	61,61,61,61	0
57	MG	BA	3024	1/1	0.94	0.15	60,60,60,60	0
57	MG	BA	3083	1/1	0.94	0.06	59,59,59,59	0
57	MG	BA	3048	1/1	0.94	0.22	91,91,91,91	0
57	MG	DA	3046	1/1	0.94	0.25	172,172,172,172	0
57	MG	BA	3122	1/1	0.94	0.22	57,57,57,57	0
57	MG	AA	1613	1/1	0.94	0.11	95,95,95,95	0
57	MG	BA	3005	1/1	0.94	0.15	91,91,91,91	0
57	MG	AA	1640	1/1	0.94	0.07	160,160,160,160	0
57	MG	DA	3077	1/1	0.94	0.12	162,162,162,162	0
57	MG	DA	3104	1/1	0.94	0.27	142,142,142,142	0
57	MG	BA	3135	1/1	0.95	0.34	60,60,60,60	0
57	MG	BA	3020	1/1	0.95	0.36	63,63,63,63	0
57	MG	BA	3053	1/1	0.95	0.08	57,57,57,57	0
57	MG	BA	3111	1/1	0.95	0.09	55,55,55,55	0
57	MG	DA	3012	1/1	0.95	0.32	168,168,168,168	0
57	MG	AA	1612	1/1	0.95	0.09	106,106,106,106	0
57	MG	BA	3114	1/1	0.95	0.11	88,88,88,88	0
57	MG	BA	3057	1/1	0.95	0.35	61,61,61,61	0
57	MG	BA	3094	1/1	0.95	0.12	92,92,92,92	0
57	MG	BA	3076	1/1	0.95	0.18	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	CA	1623	1/1	0.95	0.30	123,123,123,123	0
57	MG	BA	3009	1/1	0.95	0.09	61,61,61,61	0
57	MG	BA	3059	1/1	0.95	0.09	69,69,69,69	0
57	MG	BA	3010	1/1	0.95	0.13	64,64,64,64	0
57	MG	BA	3125	1/1	0.95	0.24	58,58,58,58	0
57	MG	BA	3061	1/1	0.95	0.38	56,56,56,56	0
57	MG	AA	1616	1/1	0.95	0.27	161,161,161,161	0
57	MG	BA	3063	1/1	0.95	0.12	54,54,54,54	0
57	MG	BA	3080	1/1	0.96	0.15	93,93,93,93	0
57	MG	BA	3029	1/1	0.96	0.07	54,54,54,54	0
57	MG	BA	3003	1/1	0.96	0.07	90,90,90,90	0
57	MG	BA	3084	1/1	0.96	0.22	61,61,61,61	0
57	MG	BA	3049	1/1	0.96	0.07	61,61,61,61	0
57	MG	AA	1639	1/1	0.96	0.08	143,143,143,143	0
57	MG	BA	3113	1/1	0.96	0.12	54,54,54,54	0
57	MG	BA	3064	1/1	0.96	0.07	55,55,55,55	0
57	MG	BA	3068	1/1	0.96	0.17	65,65,65,65	0
57	MG	AA	1606	1/1	0.96	0.12	119,119,119,119	0
57	MG	BA	3119	1/1	0.96	0.41	68,68,68,68	0
57	MG	BA	3120	1/1	0.96	0.17	59,59,59,59	0
57	MG	BA	3022	1/1	0.96	0.23	55,55,55,55	0
57	MG	BA	3055	1/1	0.96	0.11	62,62,62,62	0
57	MG	AA	1626	1/1	0.96	0.30	136,136,136,136	0
57	MG	BA	3008	1/1	0.96	0.13	59,59,59,59	0
57	MG	BA	3027	1/1	0.96	0.08	59,59,59,59	0
57	MG	BA	3126	1/1	0.96	0.24	70,70,70,70	0
57	MG	DA	3061	1/1	0.96	0.11	134,134,134,134	0
57	MG	BA	3078	1/1	0.96	0.07	100,100,100,100	0
57	MG	CA	1638	1/1	0.96	0.10	226,226,226,226	0
57	MG	BA	3016	1/1	0.96	0.26	56,56,56,56	0
57	MG	BA	3132	1/1	0.96	0.27	61,61,61,61	0
58	ZN	D4	102	1/1	0.96	0.07	99,99,99,99	0
57	MG	BA	3042	1/1	0.97	0.11	68,68,68,68	0
57	MG	BA	3065	1/1	0.97	0.06	55,55,55,55	0
57	MG	CA	1605	1/1	0.97	0.12	115,115,115,115	0
57	MG	BA	3089	1/1	0.97	0.18	66,66,66,66	0
57	MG	BA	3066	1/1	0.97	0.13	61,61,61,61	0
57	MG	BA	3091	1/1	0.97	0.13	88,88,88,88	0
57	MG	BA	3110	1/1	0.97	0.09	61,61,61,61	0
57	MG	BA	3128	1/1	0.97	0.14	64,64,64,64	0
57	MG	BA	3067	1/1	0.97	0.17	57,57,57,57	0
57	MG	DA	3126	1/1	0.97	0.17	199,199,199,199	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3105	1/1	0.97	0.12	159,159,159,159	0
57	MG	BA	3025	1/1	0.97	0.10	59,59,59,59	0
57	MG	BA	3013	1/1	0.97	0.17	55,55,55,55	0
57	MG	BA	3134	1/1	0.97	0.15	55,55,55,55	0
57	MG	BA	3045	1/1	0.97	0.32	80,80,80,80	0
57	MG	BA	3097	1/1	0.97	0.08	65,65,65,65	0
57	MG	BA	3116	1/1	0.97	0.17	55,55,55,55	0
57	MG	DA	3112	1/1	0.97	0.14	143,143,143,143	0
57	MG	BA	3040	1/1	0.97	0.17	58,58,58,58	0
57	MG	BA	3072	1/1	0.97	0.31	55,55,55,55	0
57	MG	BA	3100	1/1	0.97	0.15	74,74,74,74	0
57	MG	BA	3073	1/1	0.97	0.09	61,61,61,61	0
57	MG	AA	1622	1/1	0.98	0.10	113,113,113,113	0
57	MG	CA	1621	1/1	0.98	0.14	115,115,115,115	0
57	MG	BA	3082	1/1	0.98	0.12	55,55,55,55	0
57	MG	BA	3001	1/1	0.98	0.06	61,61,61,61	0
57	MG	BA	3017	1/1	0.98	0.12	56,56,56,56	0
57	MG	BA	3006	1/1	0.98	0.06	101,101,101,101	0
57	MG	CA	1626	1/1	0.98	0.31	139,139,139,139	0
57	MG	BA	3038	1/1	0.98	0.14	59,59,59,59	0
57	MG	BA	3087	1/1	0.98	0.14	61,61,61,61	0
57	MG	BA	3039	1/1	0.98	0.13	57,57,57,57	0
57	MG	BA	3074	1/1	0.98	0.16	54,54,54,54	0
57	MG	BA	3106	1/1	0.98	0.15	58,58,58,58	0
57	MG	BA	3050	1/1	0.98	0.14	56,56,56,56	0
57	MG	BA	3108	1/1	0.98	0.18	58,58,58,58	0
57	MG	BA	3130	1/1	0.98	0.16	68,68,68,68	0
57	MG	BA	3109	1/1	0.98	0.21	60,60,60,60	0
57	MG	BA	3012	1/1	0.98	0.13	54,54,54,54	0
57	MG	BA	3041	1/1	0.98	0.23	60,60,60,60	0
57	MG	AA	1618	1/1	0.98	0.16	131,131,131,131	0
57	MG	BA	3054	1/1	0.98	0.07	62,62,62,62	0
57	MG	BA	3136	1/1	0.98	0.37	64,64,64,64	0
57	MG	AA	1615	1/1	0.98	0.12	153,153,153,153	0
57	MG	BA	3096	1/1	0.98	0.22	61,61,61,61	0
57	MG	BA	3023	1/1	0.99	0.14	59,59,59,59	0
57	MG	BB	203	1/1	0.99	0.10	69,69,69,69	0
57	MG	BA	3033	1/1	0.99	0.17	56,56,56,56	0
57	MG	BA	3034	1/1	0.99	0.17	57,57,57,57	0
57	MG	BA	3021	1/1	0.99	0.31	59,59,59,59	0
57	MG	BA	3031	1/1	0.99	0.23	59,59,59,59	0
57	MG	BA	3129	1/1	0.99	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	ZN	B4	101	1/1	0.99	0.09	99,99,99,99	0
57	MG	BA	3117	1/1	0.99	0.15	67,67,67,67	0

6.5 Other polymers

There are no such residues in this entry.