wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 2, 2024 – 11:20 pm GMT

PDB ID	:	4WSD
Title	:	Complex of 70S ribosome with tRNA-Phe and mRNA with C-A mismatch in the second position in the A-site and with antibiotic paromomycin.
Authors	:	Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on	:	2014-10-27
Resolution	:	2.95 Å(reported)

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

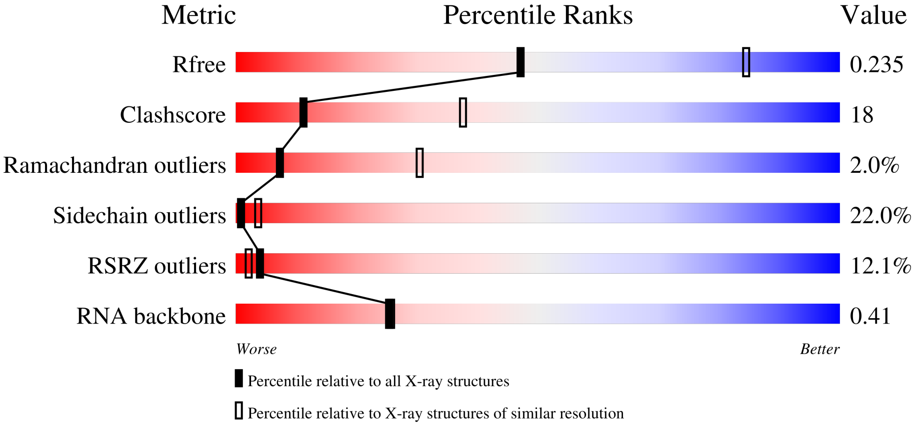
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

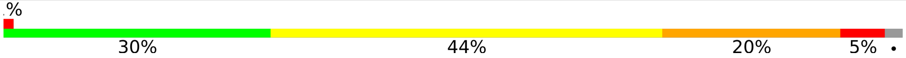
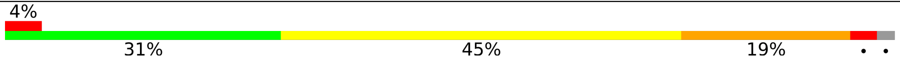
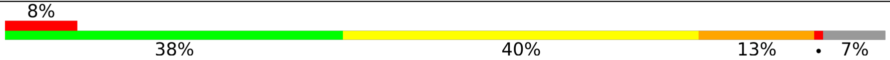
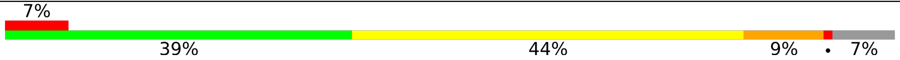
The reported resolution of this entry is 2.95 Å.

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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	13	1522	
1	1G	1522	
2	12	256	
2	1E	256	

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Mol	Chain	Length	Quality of chain
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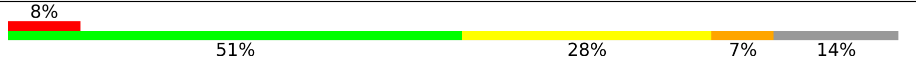
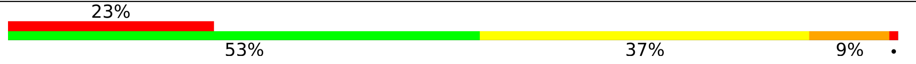
3	2E	239	
4	32	209	
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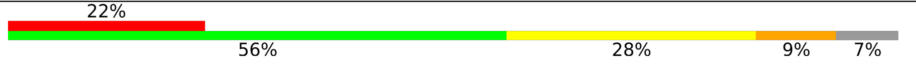
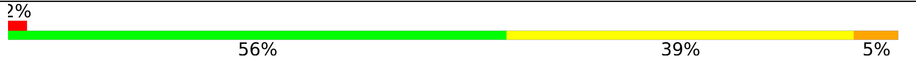
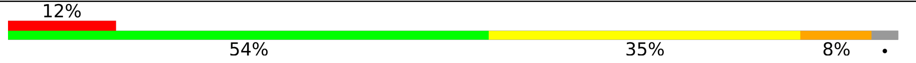
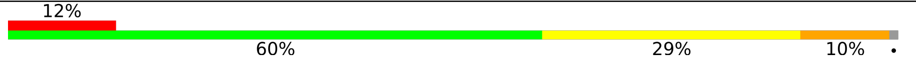
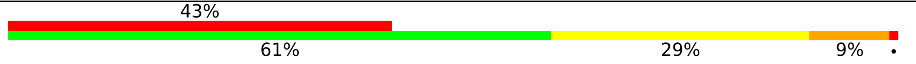
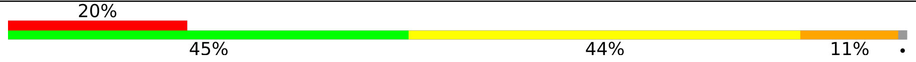
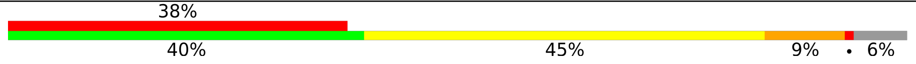
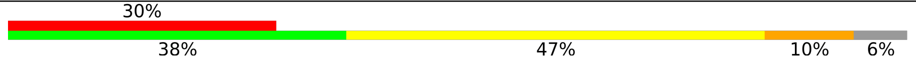
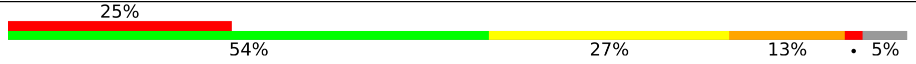
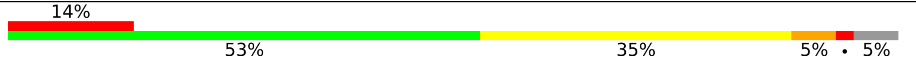
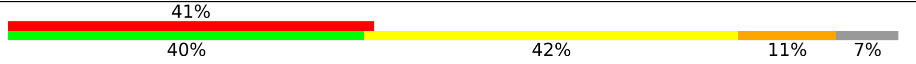
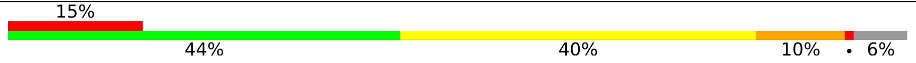
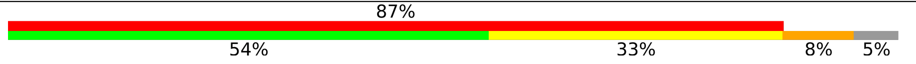
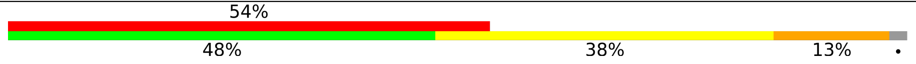
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	
15	6A	89	

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Mol	Chain	Length	Quality of chain
15	6I	89	11% 62% 29% 8% •
16	7A	88	39% 49% 43% • 5%
16	7I	88	48% 38% 48% 10% 5%
17	8A	105	39% 60% 30% 6% 5%
17	8I	105	21% 55% 30% 10% 5%
18	9A	88	6% 50% 28% • 18%
18	9I	88	44% 33% 5% 18%
19	AA	93	31% 31% 38% 15% 16%
19	AI	93	10% 42% 29% 15% • 13%
20	BA	106	40% 51% 35% 7% • 7%
20	BI	106	17% 46% 37% 10% 7%
21	1B	27	81% 33% 52% 7% 7%
21	1F	27	56% 63% 26% • 7%
22	1K	76	14% 25% 46% 22% 7%
23	2K	77	3% 30% 38% 26% 6%
23	2L	77	3% 31% 45% 16% 8%
24	3K	76	5% 17% 38% 34% 9% •
25	4K	30	7% 17% 20% 7% 57%
25	4L	30	3% 10% 13% 7% 7% 63%
26	14	2917	2% 27% 44% 23% 5%
26	1H	2917	% 21% 43% 29% 7%
27	16	122	31% 37% 25% 7%
27	1J	122	2% 26% 43% 26% 5%
28	11	276	4% 58% 31% 10% •
28	19	276	19% 55% 33% 8% • •

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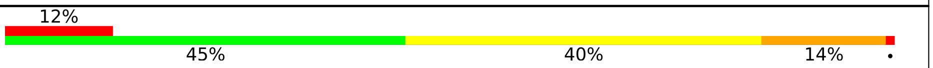
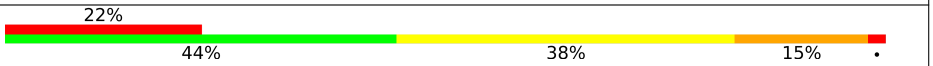
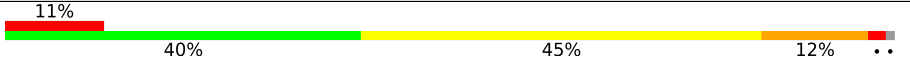
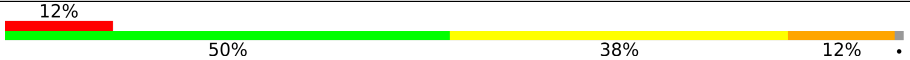
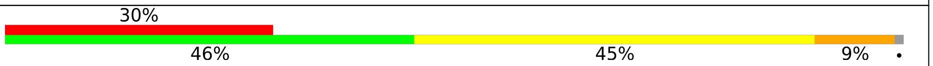
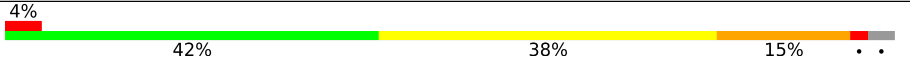
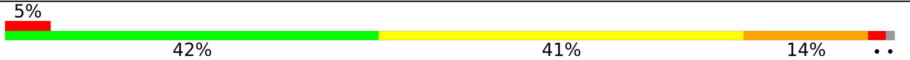
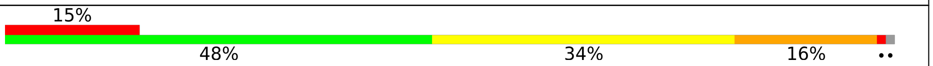
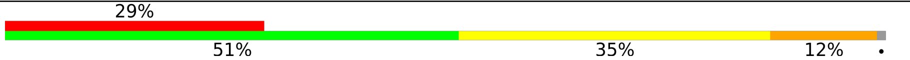
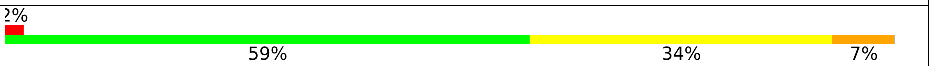
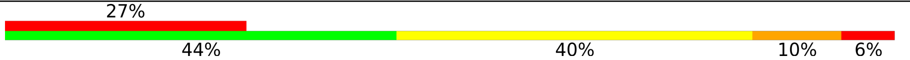
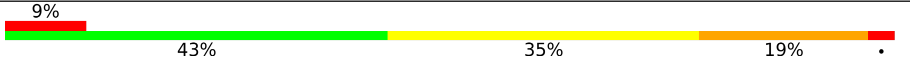
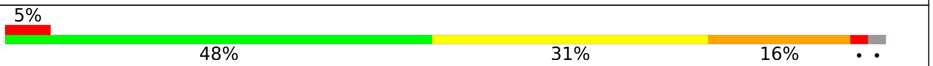
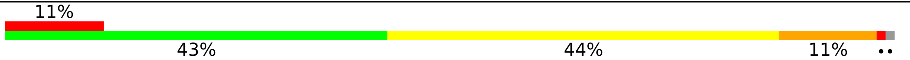
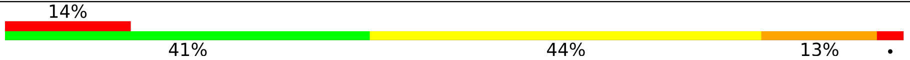
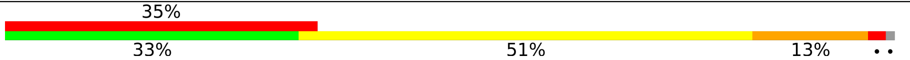
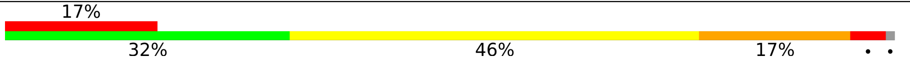
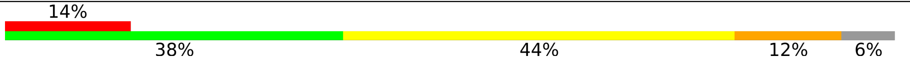
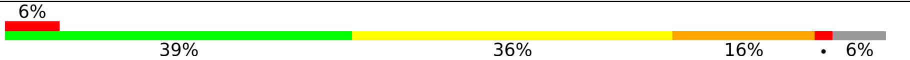
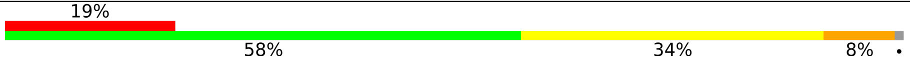
Mol	Chain	Length	Quality of chain
29	21	206	
29	29	206	
30	31	210	
30	39	210	
31	41	182	
31	49	182	
32	51	180	
32	59	180	
33	61	148	
33	69	148	
34	15	140	
34	58	140	
35	25	122	
35	68	122	
36	35	150	
36	78	150	
37	45	141	
37	88	141	
38	55	118	
38	98	118	
39	65	112	
39	A8	112	
40	75	146	
40	B8	146	
41	85	118	

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Mol	Chain	Length	Quality of chain
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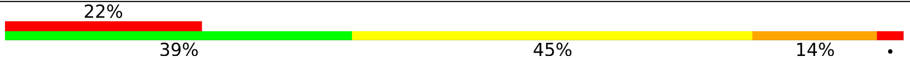
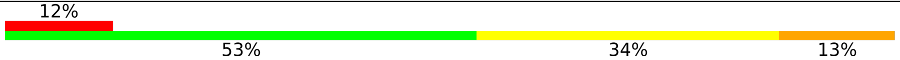
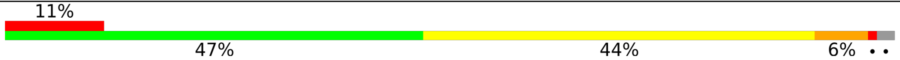
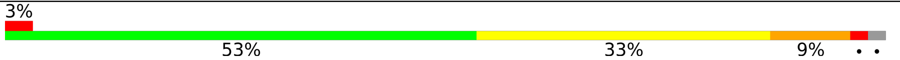
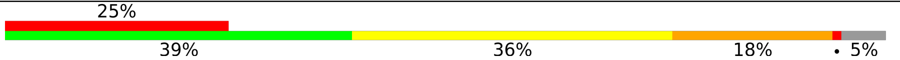
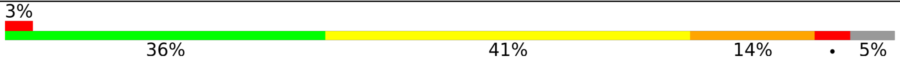
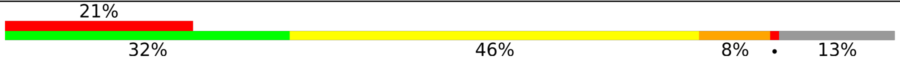
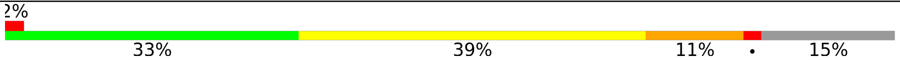
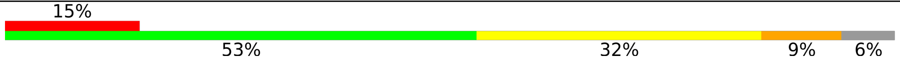
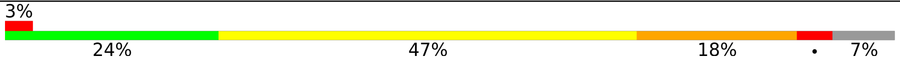
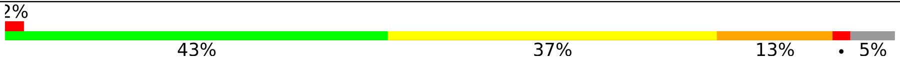
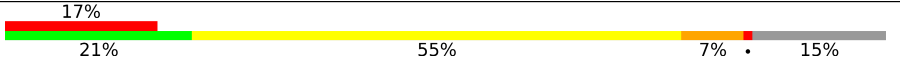
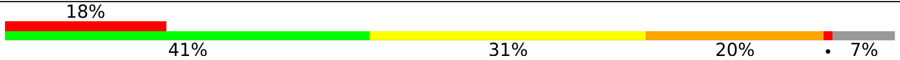
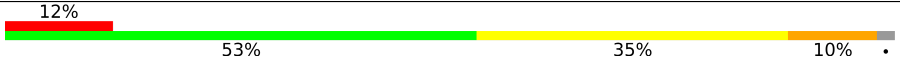
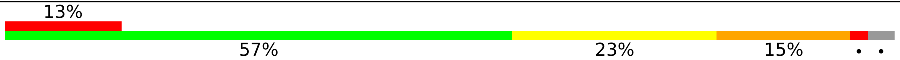
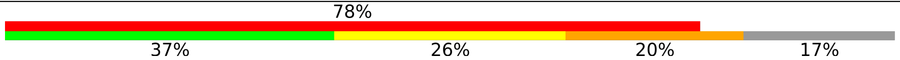
42	95	101	
42	D8	101	
43	A5	113	
43	E8	113	
44	B5	96	
44	F8	96	
45	C5	110	
45	G8	110	
46	D5	206	
46	H8	206	
47	E5	85	
47	I8	85	
48	F5	98	
48	J8	98	
49	G5	72	
49	K8	72	
50	H5	60	
50	L8	60	
51	I5	71	
51	M8	71	
52	J5	60	
52	N8	60	
53	K5	54	
53	O8	54	

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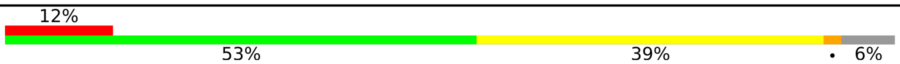
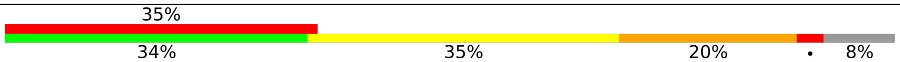
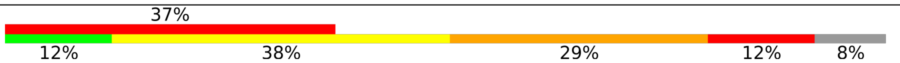
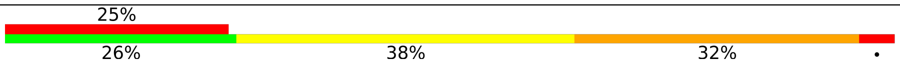
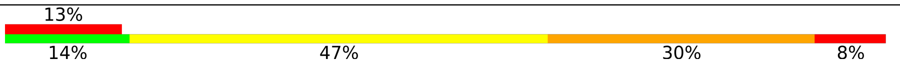
Mol	Chain	Length	Quality of chain
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	
56	1L	76	
57	3L	76	

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
58	MG	13	1710	-	-	-	X
58	MG	14	3143	-	-	-	X
58	MG	14	3158	-	-	-	X
58	MG	14	3193	-	-	-	X
58	MG	1H	3020	-	-	-	X
58	MG	1H	3056	-	-	-	X
58	MG	1H	3162	-	-	-	X
58	MG	1H	3247	-	-	-	X
58	MG	1H	3254	-	-	-	X
58	MG	1H	3262	-	-	-	X
58	MG	1H	3310	-	-	-	X
58	MG	1H	3334	-	-	-	X
58	MG	1H	3337	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300252 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	13	1498	Total C N O P 32207 14334 5973 10402 1498	0	0	0
1	1G	1498	Total C N O P 32204 14334 5973 10400 1497	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	1E	237	Total C N O S 1924 1228 344 347 5	0	0	0
2	12	237	Total C N O S 1924 1228 344 347 5	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	2E	205	Total C N O S 1605 1011 313 280 1	0	0	0
3	22	206	Total C N O S 1612 1016 314 281 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	3E	208	Total C N O S 1702 1066 339 290 7	0	0	0
4	32	208	Total C N O S 1702 1066 339 290 7	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	4E	151	Total C N O S 1155 729 218 204 4	0	0	0
5	42	151	Total C N O S 1155 729 218 204 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	5E	101	Total C N O S 842 531 155 153 3	0	0	0
6	52	101	Total C N O S 842 531 155 153 3	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	6E	155	Total C N O S 1256 781 252 217 6	0	0	0
7	62	152	Total C N O S 1243 774 249 214 6	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	7E	138	Total C N O S 1115 705 215 192 3	0	0	0
8	72	138	Total C N O S 1115 705 215 192 3	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	8E	127	Total C N O 1009 639 197 173	0	0	0
9	82	124	Total C N O 983 624 190 169	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	1I	99	Total C N O S 801 504 157 139 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1A	99	801	504	157	139	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	2I	116	864	537	164	160	3	0	0	0
11	2A	116	864	537	164	160	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	3I	125	975	614	196	164	1	0	0	0
12	3A	125	975	614	196	164	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	4I	118	938	580	193	163	2	0	0	0
13	4A	117	933	577	192	162	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4I	119	ALA	GLY	conflict	UNP P80377
4A	119	ALA	GLY	conflict	UNP P80377

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	5I	60	491	312	104	71	4	0	0	0
14	5A	58	475	303	99	69	4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	6I	88	Total C N O S 733 459 147 125 2	0	0	0
15	6A	88	Total C N O S 733 459 147 125 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	7I	84	Total C N O S 705 446 140 118 1	0	0	0
16	7A	84	Total C N O S 705 446 140 118 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	8I	100	Total C N O S 834 534 155 143 2	0	0	0
17	8A	100	Total C N O S 834 534 155 143 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	9I	72	Total C N O 590 376 117 97	0	0	0
18	9A	72	Total C N O 590 376 117 97	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	AI	81	Total C N O S 647 413 119 113 2	0	0	0
19	AA	78	Total C N O S 624 398 115 109 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	BI	99	Total C N O S 762 470 162 128 2	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	BA	99	Total C N O S 762 470 162 128 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	1F	25	Total C N O 217 134 52 31	0	0	0
21	1B	25	Total C N O 217 134 52 31	0	0	0

- Molecule 22 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	1K	76	Total C N O P S 1627 730 290 530 75 2	0	0	0

- Molecule 23 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	2K	77	Total C N O P S 1646 735 298 535 77 1	0	0	0
23	2L	77	Total C N O P S 1646 735 298 535 77 1	0	0	0

- Molecule 24 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	3K	75	Total C N O P S 1603 719 285 524 74 1	0	0	0

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	4K	13	Total C N O P 279 126 55 85 13	0	0	0
25	4L	11	Total C N O P 235 106 45 73 11	0	0	0

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2912	Total 62707	C 27911	N 11722	O 20163	P 2911	0	0	0
26	14	2909	Total 62647	C 27884	N 11716	O 20139	P 2908	0	0	0

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	16	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0
27	1J	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	11	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0
28	19	273	Total 2120	C 1338	N 421	O 358	S 3	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	21	205	Total 1568	C 991	N 300	O 271	S 6	0	0	0
29	29	205	Total 1568	C 991	N 300	O 271	S 6	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total 1585	C 1011	N 297	O 275	S 2	0	0	0
30	39	208	Total 1627	C 1037	N 304	O 283	S 3	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	181	Total 1473	C 942	N 268	O 259	S 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	49	181	Total C N O S 1473 942 268 259 4	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	51	174	Total C N O S 1336 848 251 236 1	0	0	0
32	59	170	Total C N O S 1307 829 245 232 1	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	61	146	Total C N O S 1136 726 201 208 1	0	0	0
33	69	146	Total C N O S 1136 726 201 208 1	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
34	58	138	Total C N O S 1104 712 206 182 4	0	0	0
34	15	138	Total C N O S 1104 712 206 182 4	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	68	122	Total C N O S 932 588 171 169 4	0	0	0
35	25	122	Total C N O S 932 588 171 169 4	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	78	150	Total C N O S 1144 712 232 197 3	0	0	0
36	35	150	Total C N O S 1144 712 232 197 3	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
37	88	138	Total C N O S 1086 693 208 179 6	0	0	0
37	45	141	Total C N O S 1121 715 212 187 7	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	98	118	Total C N O S 967 604 203 159 1	0	0	0
38	55	117	Total C N O 959 599 202 158	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
39	A8	111	Total C N O 881 556 176 149	0	0	0
39	65	111	Total C N O 881 556 176 149	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
40	B8	137	Total C N O S 1141 710 234 196 1	0	0	0
40	75	137	Total C N O S 1141 710 234 196 1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	C8	117	Total C N O S 963 610 202 150 1	0	0	0
41	85	117	Total C N O S 963 610 202 150 1	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	D8	101	Total C N O S 778 501 142 134 1	0	0	0
42	95	101	Total C N O S 778 501 142 134 1	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
43	E8	113	Total C N O S 899 566 177 154 2	0	0	0
43	A5	113	Total C N O S 899 566 177 154 2	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
44	F8	94	Total C N O S 742 482 134 125 1	0	0	0
44	B5	94	Total C N O 735 477 133 125	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	G8	104	Total C N O S 791 510 149 127 5	0	0	0
45	C5	104	Total C N O S 794 510 152 127 5	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
46	H8	175	Total C N O S 1397 892 251 251 3	0	0	0
46	D5	179	Total C N O S 1428 911 255 259 3	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	I8	80	Total C N O S 626 388 132 105 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	E5	77	612	379	129	103	1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I8	6	ALA	GLY	conflict	UNP P60493
I8	8	ALA	GLY	conflict	UNP P60493
E5	6	ALA	GLY	conflict	UNP P60493
E5	8	ALA	GLY	conflict	UNP P60493

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	J8	97	762	481	150	130	1	0	0	0
48	F5	94	737	463	146	127	1	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	K8	67	563	349	114	99	1	0	0	0
49	G5	67	563	349	114	99	1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
50	L8	57	452	288	88	76	0	0	0
50	H5	59	468	298	90	80	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	M8	66	533	335	96	97	5	0	0	0
51	I5	60	481	305	84	87	5	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	N8	58	Total C N O S 453 285 89 74 5	0	0	0
52	J5	59	Total C N O S 458 288 90 75 5	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
53	O8	45	Total C N O S 389 241 79 65 4	0	0	0
53	K5	45	Total C N O S 389 241 79 65 4	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
54	P8	45	Total C N O S 391 240 97 52 2	0	0	0
54	L5	46	Total C N O S 398 245 98 53 2	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
55	Q8	60	Total C N O S 480 306 98 74 2	0	0	0
55	M5	60	Total C N O S 477 303 98 74 2	0	0	0

- Molecule 56 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
56	1L	76	Total C N O P S 1627 730 290 531 75 1	0	0	0

- Molecule 57 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
57	3L	76	Total C N O P S 1624 725 290 532 76 1	0	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	13	148	Total Mg 148 148	0	0
58	3E	2	Total Mg 2 2	0	0
58	5E	1	Total Mg 1 1	0	0
58	2I	1	Total Mg 1 1	0	0
58	5I	2	Total Mg 2 2	0	0
58	1K	2	Total Mg 2 2	0	0
58	2K	5	Total Mg 5 5	0	0
58	3K	1	Total Mg 1 1	0	0
58	4K	1	Total Mg 1 1	0	0
58	1H	520	Total Mg 520 520	0	0
58	16	13	Total Mg 13 13	0	0
58	11	4	Total Mg 4 4	0	0
58	21	2	Total Mg 2 2	0	0
58	41	2	Total Mg 2 2	0	0
58	78	1	Total Mg 1 1	0	0
58	88	2	Total Mg 2 2	0	0
58	98	2	Total Mg 2 2	0	0
58	G8	1	Total Mg 1 1	0	0
58	I8	1	Total Mg 1 1	0	0
58	L8	1	Total Mg 1 1	0	0
58	P8	1	Total Mg 1 1	0	0

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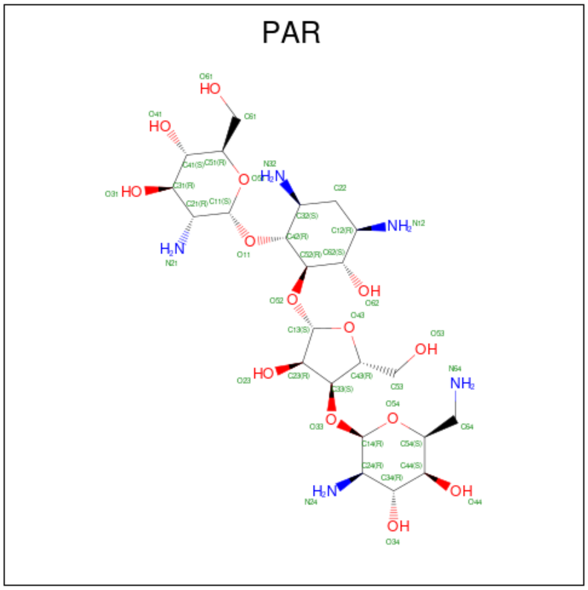
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1G	96	Total Mg 96 96	0	0
58	2A	2	Total Mg 2 2	0	0
58	7A	1	Total Mg 1 1	0	0
58	2L	3	Total Mg 3 3	0	0
58	3L	2	Total Mg 2 2	0	0
58	14	407	Total Mg 407 407	0	0
58	1J	5	Total Mg 5 5	0	0
58	29	4	Total Mg 4 4	0	0
58	49	1	Total Mg 1 1	0	0
58	25	1	Total Mg 1 1	0	0
58	55	1	Total Mg 1 1	0	0
58	C5	1	Total Mg 1 1	0	0
58	J5	1	Total Mg 1 1	0	0

- Molecule 59 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	13	1	Total C N O 42 23 5 14	0	0
59	1G	1	Total C N O 42 23 5 14	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	3E	1	Total Zn 1 1	0	0
60	5I	1	Total Zn 1 1	0	0
60	G8	1	Total Zn 1 1	0	0
60	32	1	Total Zn 1 1	0	0
60	5A	1	Total Zn 1 1	0	0
60	C5	1	Total Zn 1 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	13	197	Total O 197 197	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	3E	3	Total O 3 3	0	0
61	8E	2	Total O 2 2	0	0
61	1I	2	Total O 2 2	0	0
61	3I	1	Total O 1 1	0	0
61	5I	2	Total O 2 2	0	0
61	6I	1	Total O 1 1	0	0
61	7I	1	Total O 1 1	0	0
61	1K	5	Total O 5 5	0	0
61	2K	6	Total O 6 6	0	0
61	3K	1	Total O 1 1	0	0
61	4K	2	Total O 2 2	0	0
61	1H	999	Total O 999 999	0	0
61	16	21	Total O 21 21	0	0
61	11	13	Total O 13 13	0	0
61	21	4	Total O 4 4	0	0
61	31	4	Total O 4 4	0	0
61	58	2	Total O 2 2	0	0
61	78	5	Total O 5 5	0	0
61	B8	1	Total O 1 1	0	0
61	C8	3	Total O 3 3	0	0
61	D8	1	Total O 1 1	0	0

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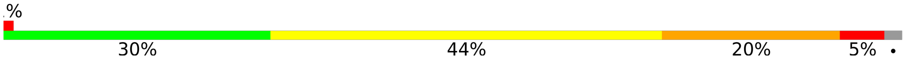
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	G8	4	Total O 4 4	0	0
61	I8	7	Total O 7 7	0	0
61	L8	1	Total O 1 1	0	0
61	P8	1	Total O 1 1	0	0
61	Q8	2	Total O 2 2	0	0
61	1G	82	Total O 82 82	0	0
61	7A	1	Total O 1 1	0	0
61	BA	1	Total O 1 1	0	0
61	3L	6	Total O 6 6	0	0
61	14	598	Total O 598 598	0	0
61	19	13	Total O 13 13	0	0
61	39	7	Total O 7 7	0	0
61	35	1	Total O 1 1	0	0
61	85	1	Total O 1 1	0	0
61	A5	1	Total O 1 1	0	0
61	G5	1	Total O 1 1	0	0
61	L5	1	Total O 1 1	0	0

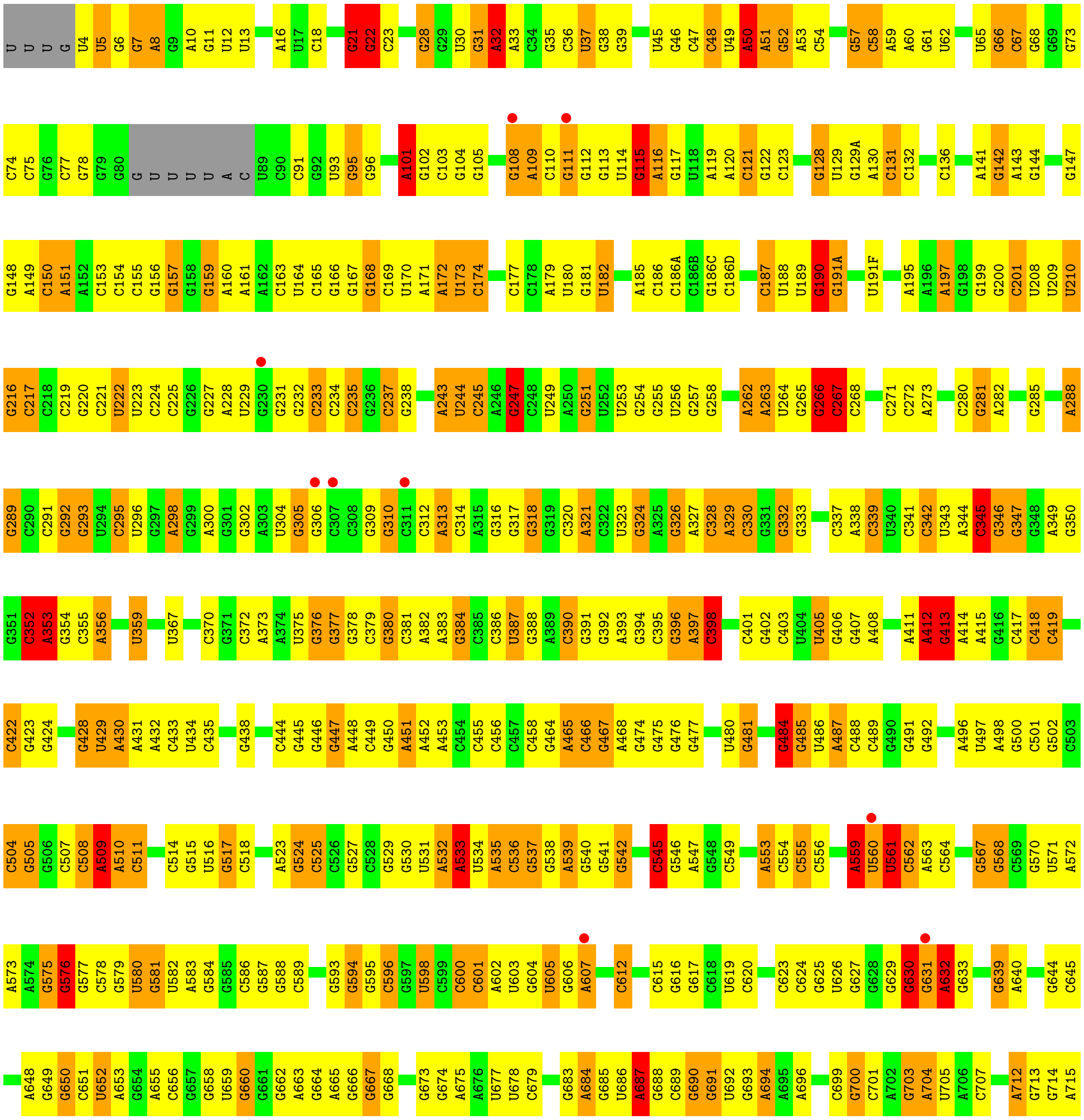
3 Residue-property plots ⓘ

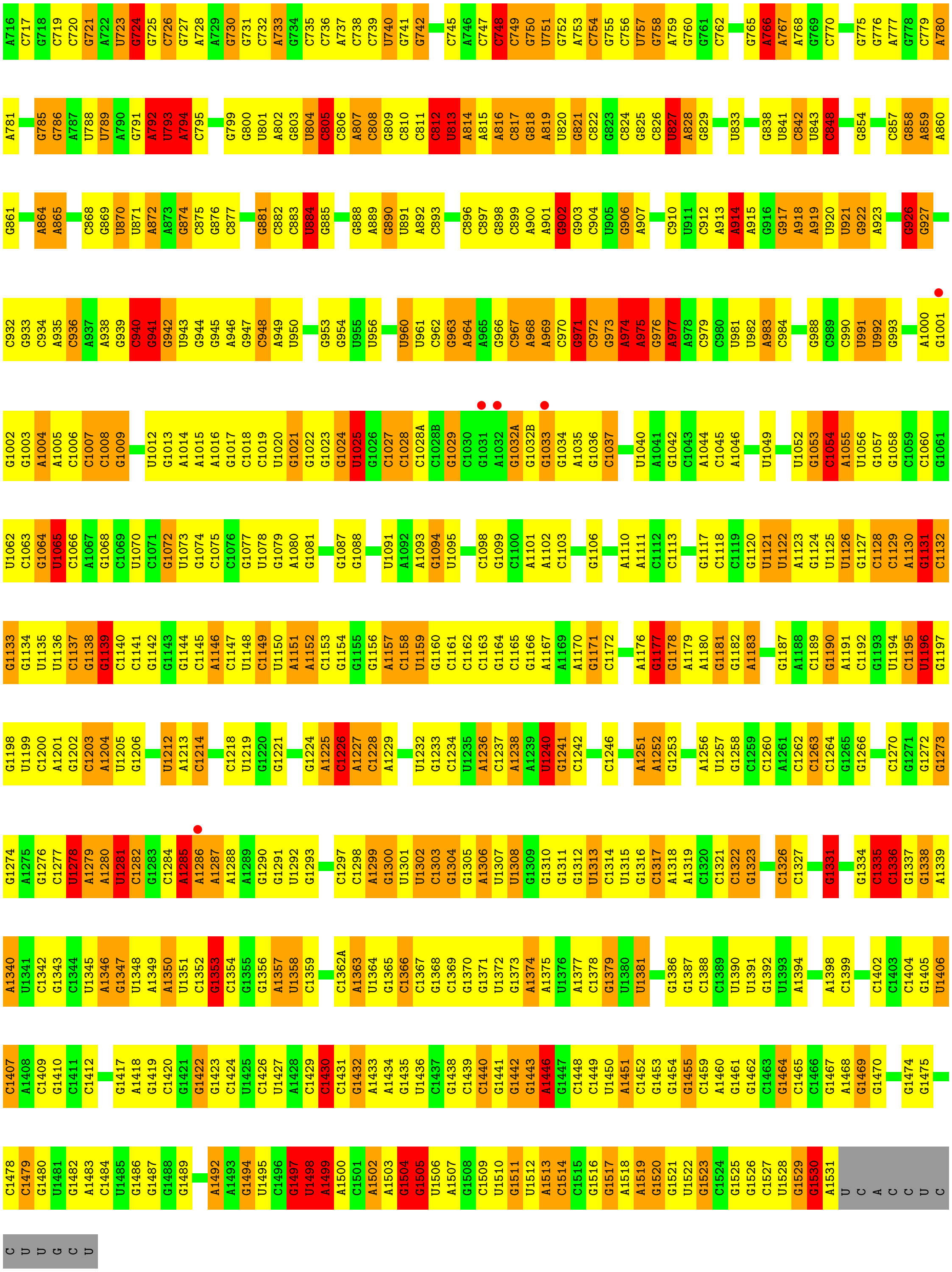
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S ribosomal RNA

Chain 13:

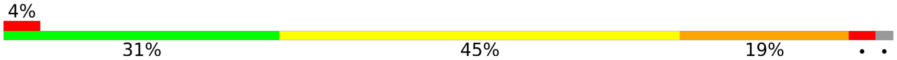


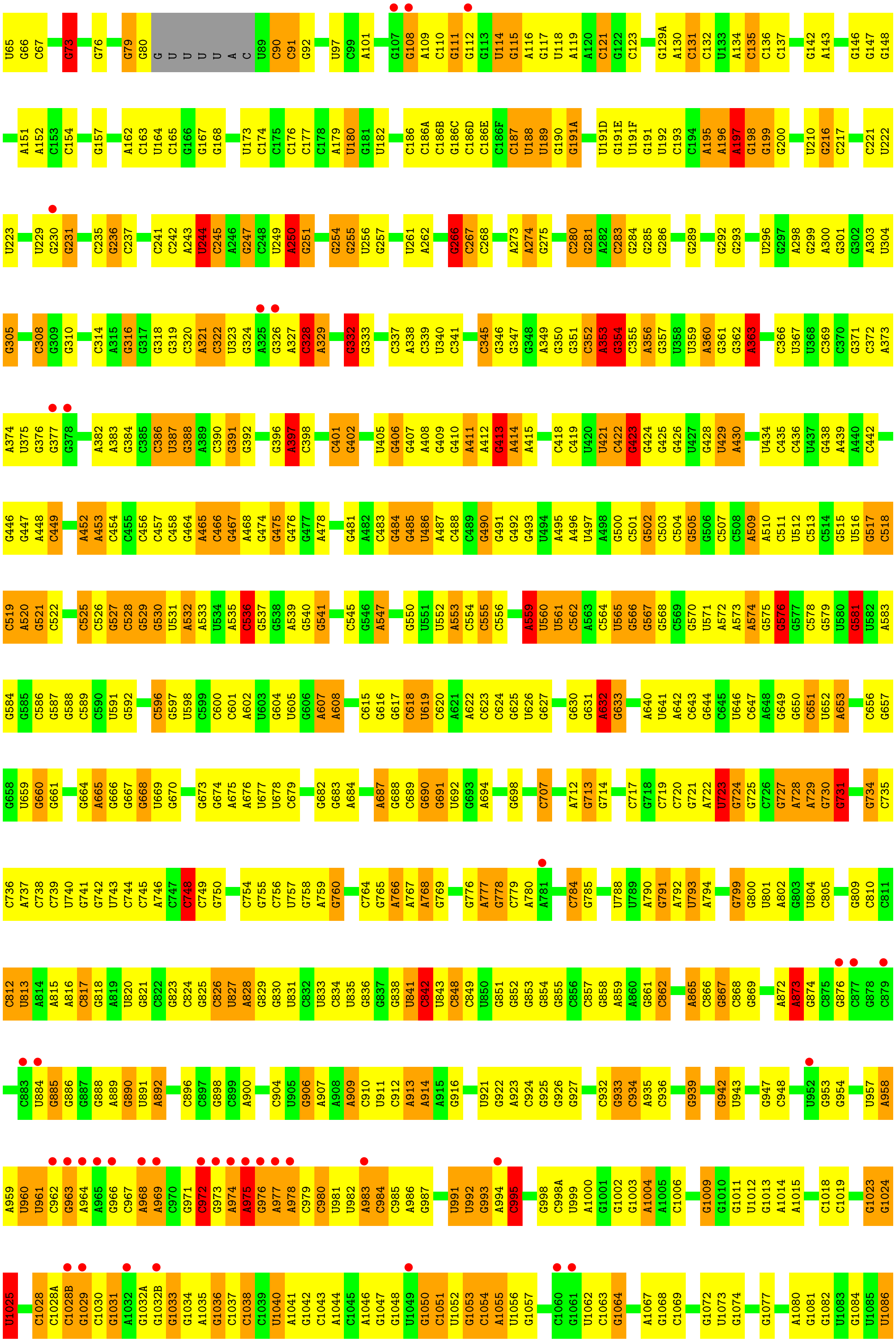




- Molecule 1: 16S ribosomal RNA

Chain 1G:

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A151 A152 C153 C154 G157 A162 C163 U164 C165 G166 G167 G168 U173 C174 C175 C176 C177 C178 A179 U180 G181 U182 C186 C186A C186B C186C C186D C186E C186F C187 U188 U189 G190 G191A U191D G191E U191F G191 U192 C193 C194 A195 A196 A197 G198 G199 G200 U210 G216 C217 C221 U222
U223 U229 G230 G231 C235 G236 C237 C241 C242 A243 U244 C245 A246 G247 C248 U249 A250 G251 G254 G255 U256 G257 U261 A262 G266 C267 C268 A273 A274 G275 C280 G281 A282 C283 G284 G285 G286 G289 G292 G293 U296 G297 A298 G299 A300 G301 G302 A303 U304
G305 C308 G309 G310 C314 A315 G316 G317 G318 C319 C320 A321 C322 U323 G324 A325 G326 A327 C328 A329 G332 C333 C337 A338 C339 U340 C341 C345 G346 G347 G348 A349 G350 C351 C352 A353 G354 C355 A356 G357 U358 U359 A360 G361 G362 A363 C366 U367 U368 C369 C370 G371 C372 A373
A374 U375 G376 G377 G378 A382 A383 G384 C385 C386 U387 G388 A389 C390 G391 G392 G396 A397 C398 C401 G402 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 C418 C419 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 U434 C435 C436 U437 G438 A439 A440 C442
G446 G447 A448 C449 A452 A453 C454 C455 C456 C457 C458 G464 A465 C466 G467 A468 G474 G475 G476 G477 A478 G481 A482 C483 G484 G485 U486 A487 C488 C489 G490 G491 G492 G493 U494 A495 A496 U497 A498 G500 C501 G502 C503 C504 G505 G506 C507 C508 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518
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G584 G585 C586 G587 G588 C589 C590 U591 G592 C596 G597 U598 C599 C600 C601 A602 U603 G604 U605 G606 A607 A608 C615 G616 G617 C618 U619 C620 A621 A622 C623 C624 G625 U626 G627 G630 G631 A632 G633 A640 U641 A642 C643 G644 C645 U646 C647 A648 G649 G650 C651 U652 A653 C656 G657
G658 U659 G660 G661 G664 A665 G666 G667 G668 U669 G670 G673 G674 A675 A676 U677 U678 C679 G682 G683 A684 A687 G688 C689 G690 G691 U692 G693 A694 G698 C707 A712 G713 G714 C717 G718 C719 C720 G721 A722 U723 G724 G725 C726 C727 A728 A729 G730 G731 G734 C735
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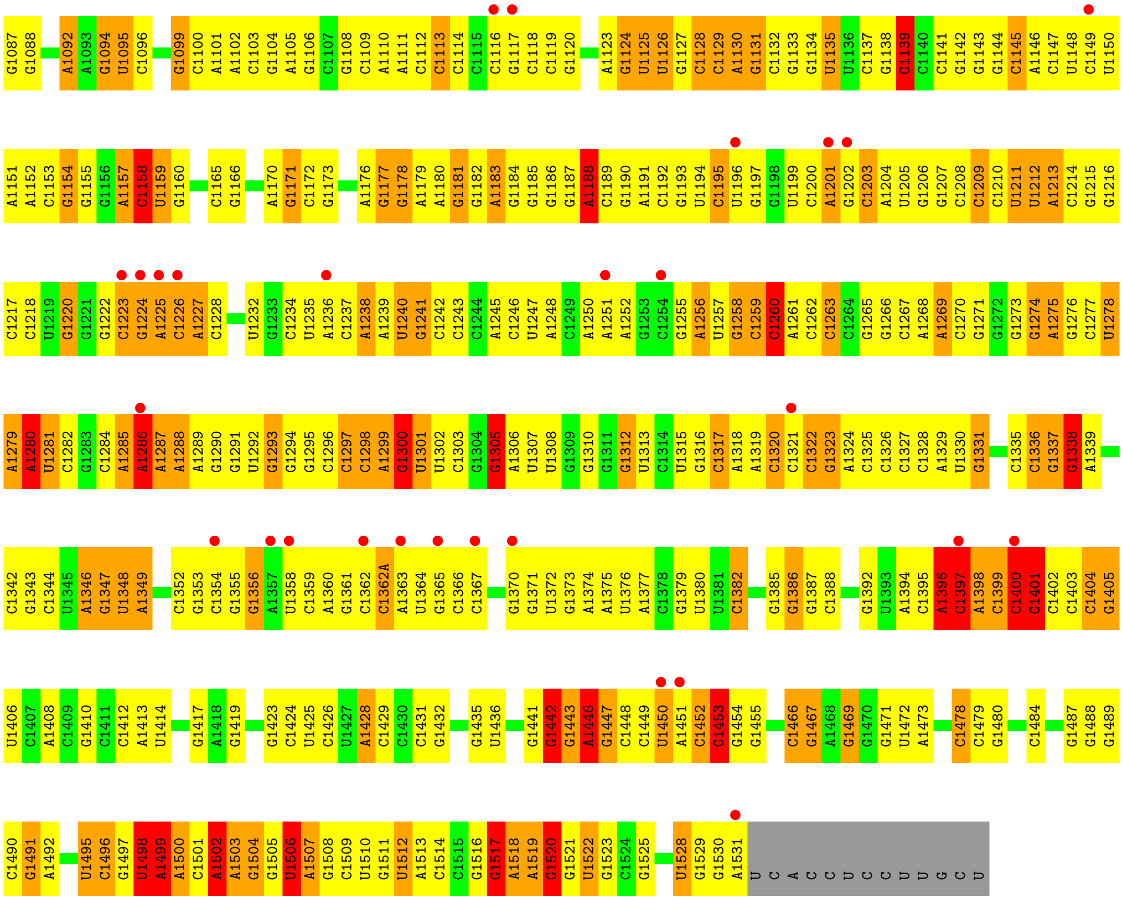
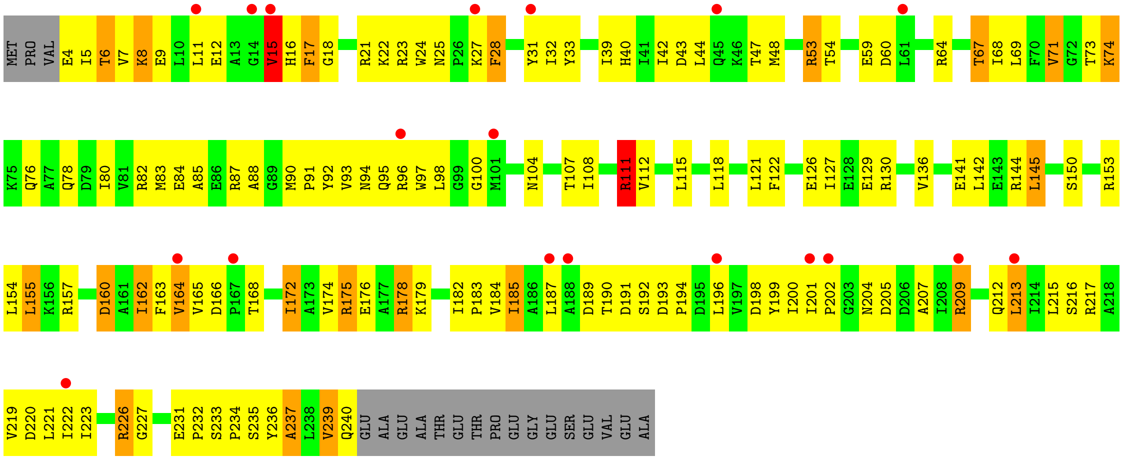
C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C822 C823 C824 G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 G838 U841 C842 U843 C848 C849 U850 G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862 A865 C866 G867 C868 G869 A872 A873 G874 C875 G876 C877 G878 C879
C883 U884 G885 G886 G887 G888 A889 G890 U891 A892 C896 C897 G898 C899 A900 C904 U905 G906 A907 A908 A909 C910 U911 C912 A913 A914 A915 G916 U921 G922 A923 C924 G925 G926 G927 C932 G933 C934 A935 C936 G939 G942 U943 G947 C948 U952 G953 G954 U957 A958
A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 G987 U991 U992 G993 A994 C995 G998 C998A U999 A1000 G1001 G1002 G1003 A1004 A1005 C1006 G1009 G1010 G1011 U1012 G1013 A1014 A1015 C1018 C1019 G1023 G1024
U1025 C1028 C1028A C1028B G1029 C1030 G1031 A1032 G1032A G1032B G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 C1060 G1061 U1062 C1063 G1064 A1067 G1068 C1069 G1072 U1073 G1074 G1077 A1080 G1081 G1082 U1083 G1084 U1085 U1086



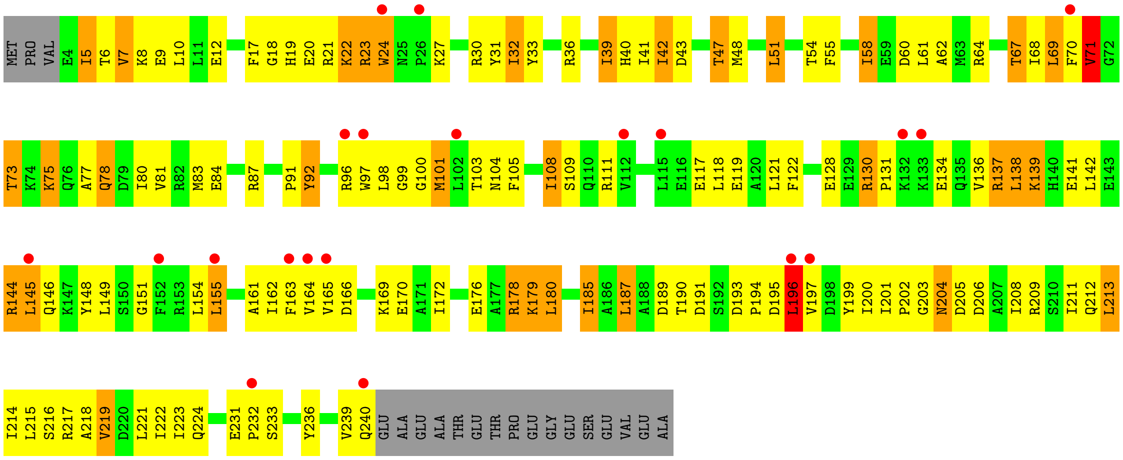
- Molecule 2: 30S ribosomal protein S2

Chain 1E:



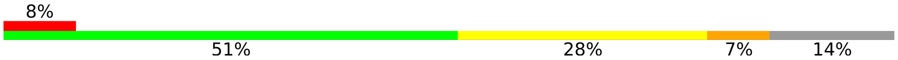
- Molecule 2: 30S ribosomal protein S2

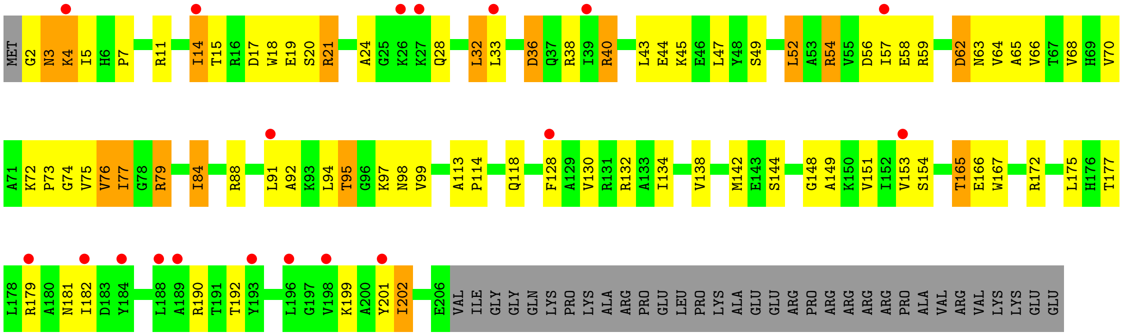
Chain 12:



- Molecule 3: 30S ribosomal protein S3

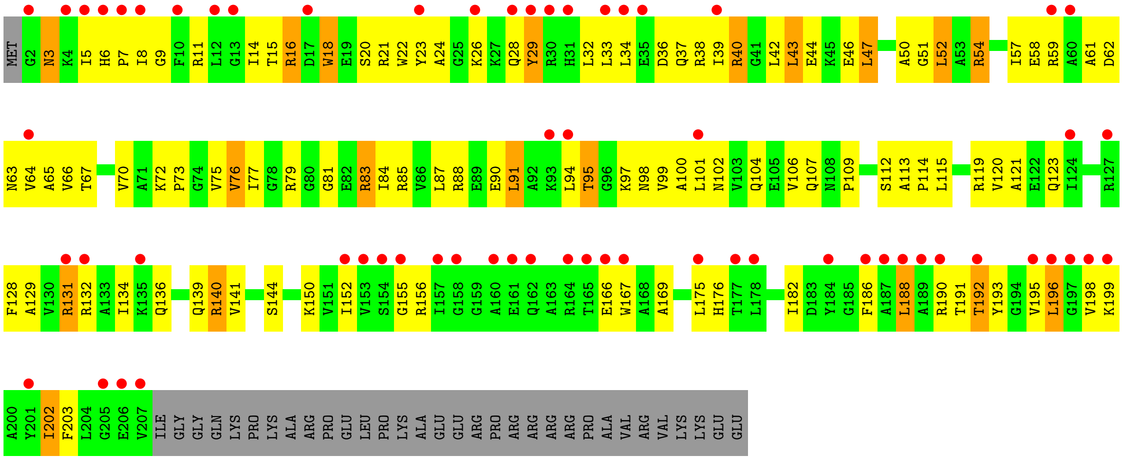
Chain 2E:





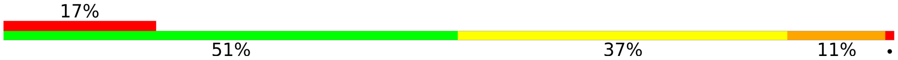
- Molecule 3: 30S ribosomal protein S3

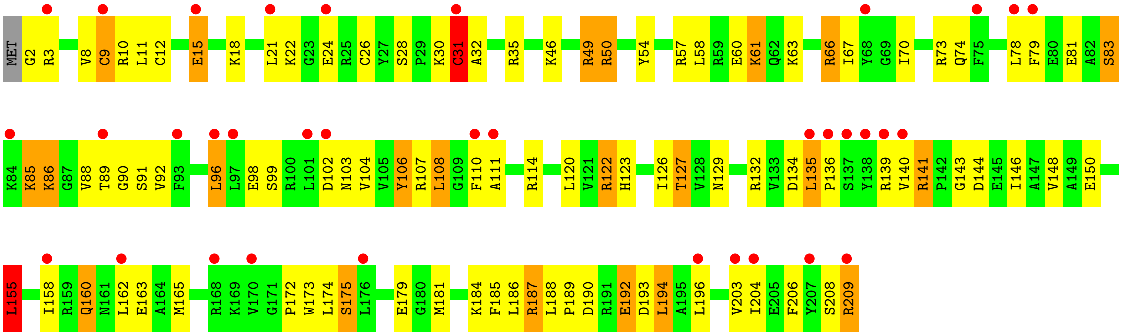
Chain 22:



- Molecule 4: 30S ribosomal protein S4

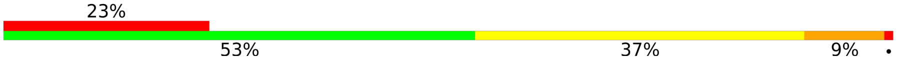
Chain 3E:

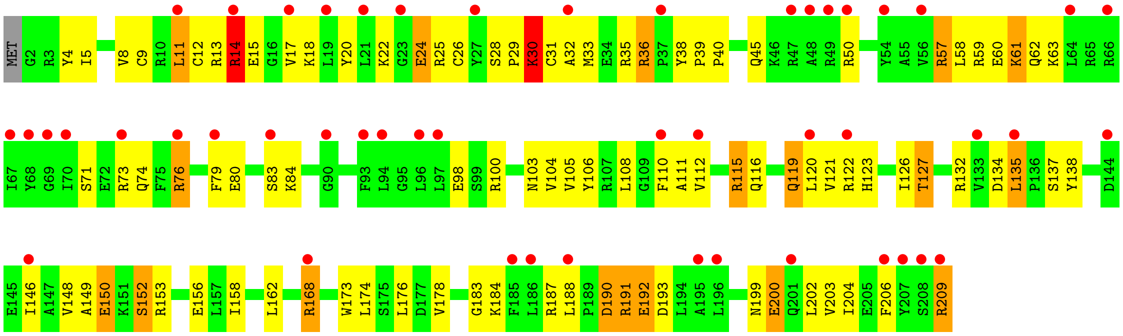




- Molecule 4: 30S ribosomal protein S4

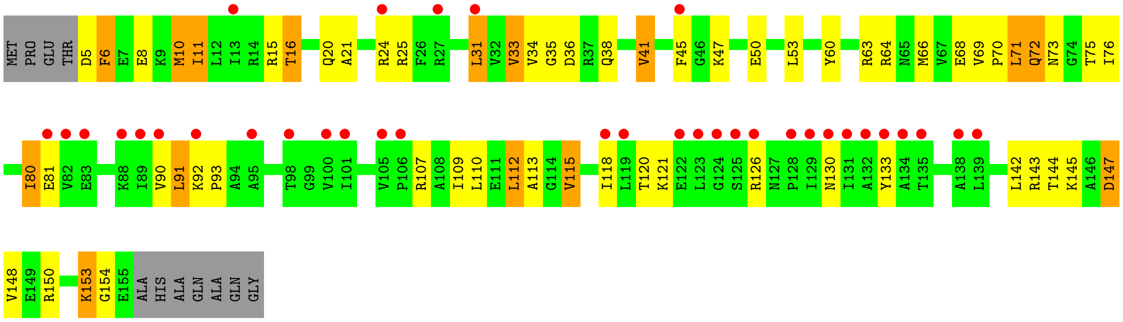
Chain 32:





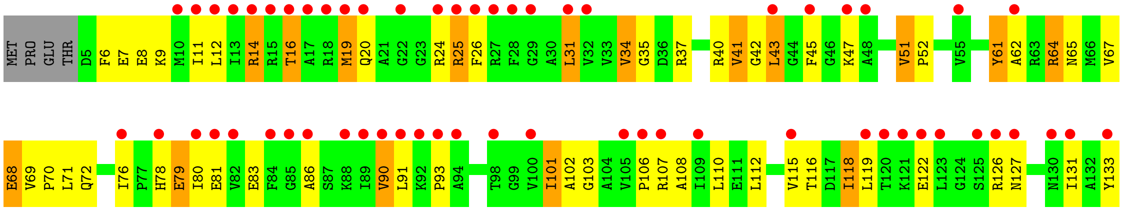
- Molecule 5: 30S ribosomal protein S5

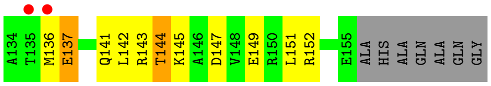
Chain 4E:



- Molecule 5: 30S ribosomal protein S5

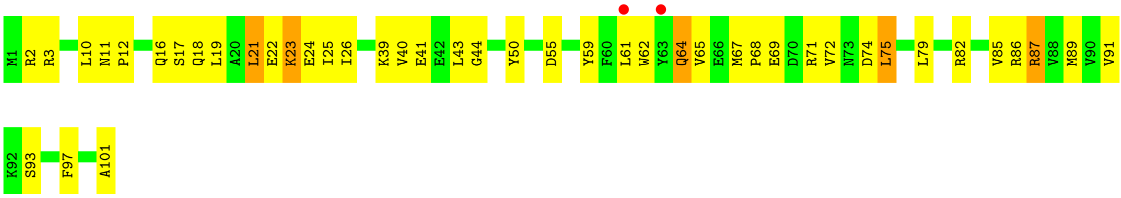
Chain 42:





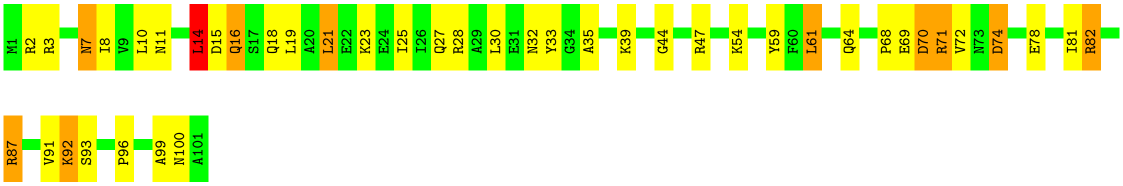
- Molecule 6: 30S ribosomal protein S6

Chain 5E:



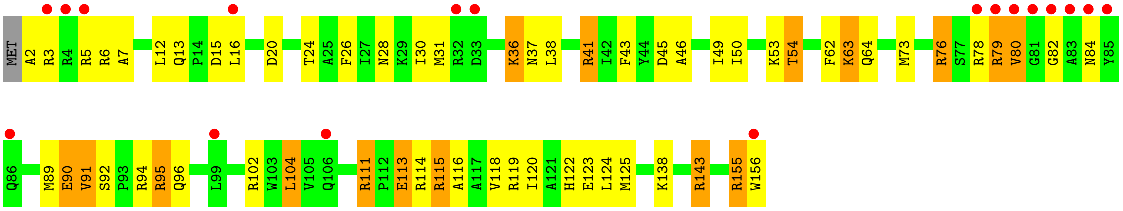
- Molecule 6: 30S ribosomal protein S6

Chain 52:



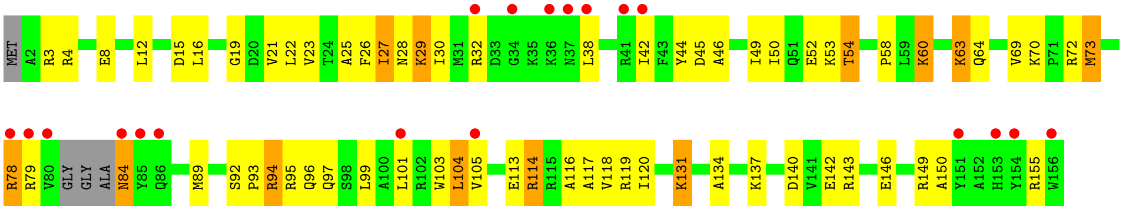
- Molecule 7: 30S ribosomal protein S7

Chain 6E:



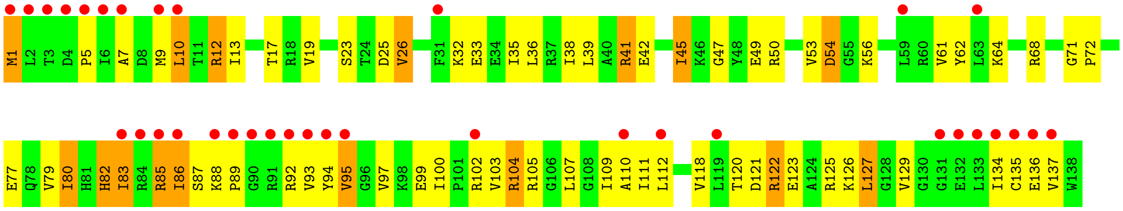
- Molecule 7: 30S ribosomal protein S7

Chain 62:



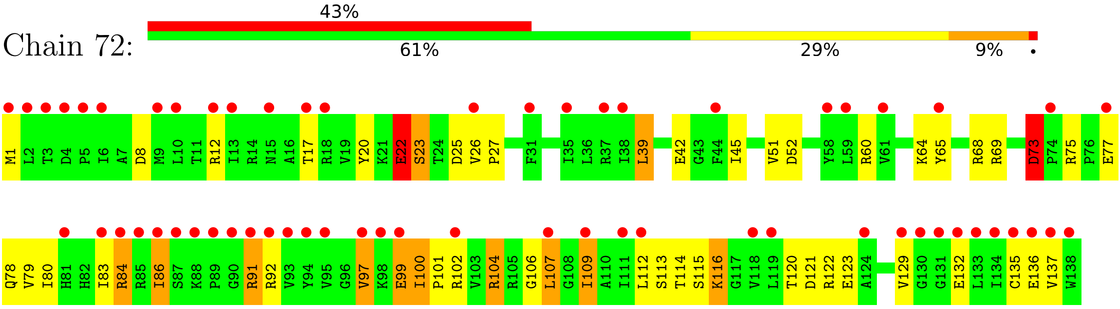
- Molecule 8: 30S ribosomal protein S8

Chain 7E:



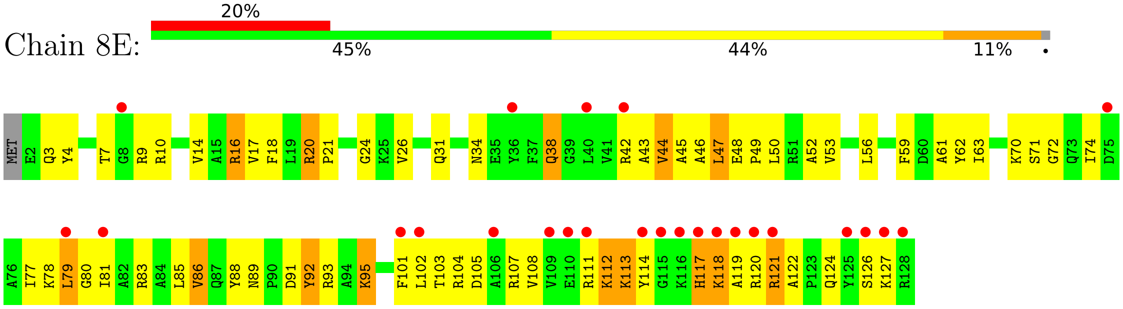
- Molecule 8: 30S ribosomal protein S8

Chain 72:



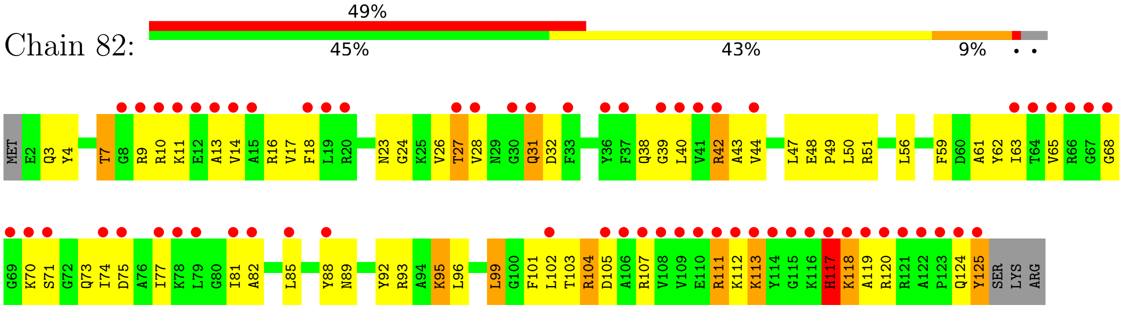
- Molecule 9: 30S ribosomal protein S9

Chain 8E:



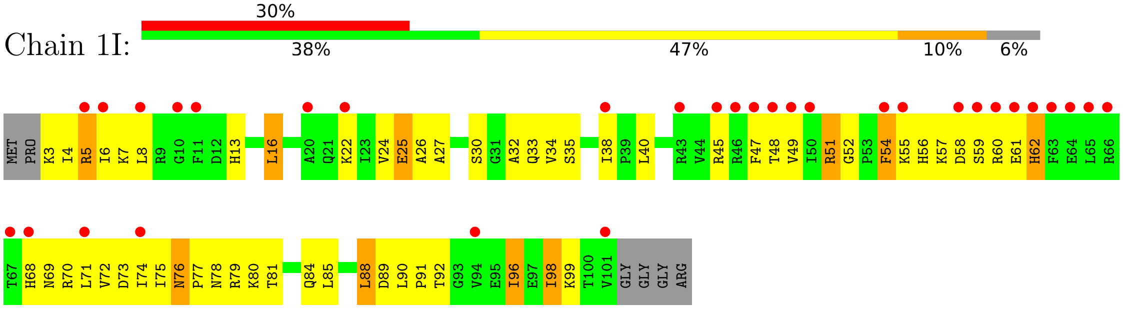
- Molecule 9: 30S ribosomal protein S9

Chain 82:

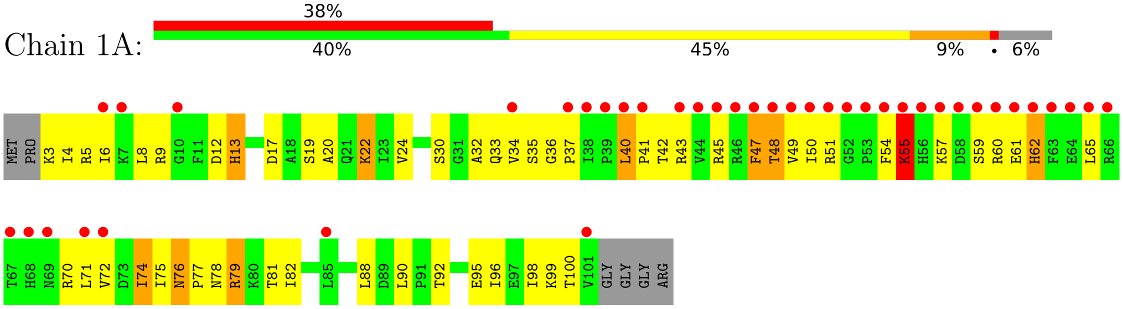


- Molecule 10: 30S ribosomal protein S10

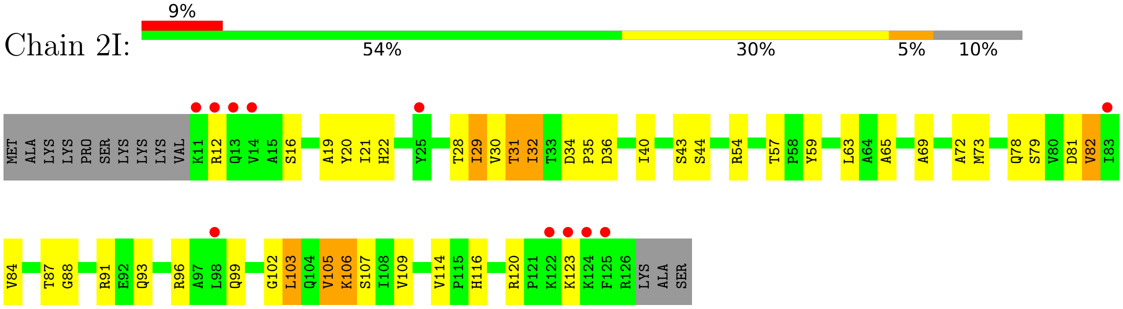
Chain 1I:



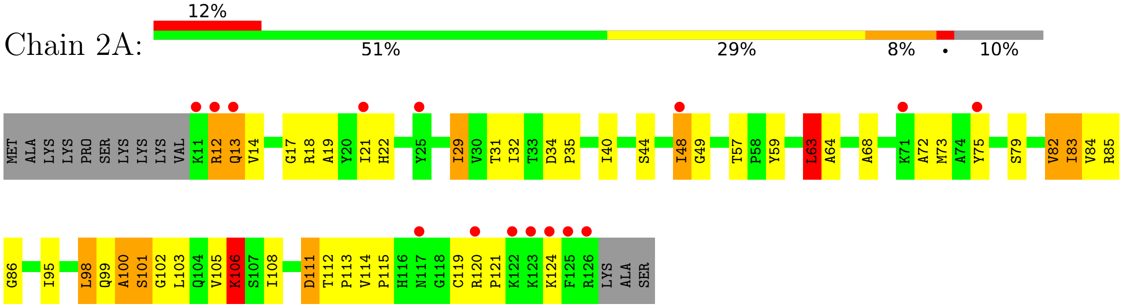
- Molecule 10: 30S ribosomal protein S10



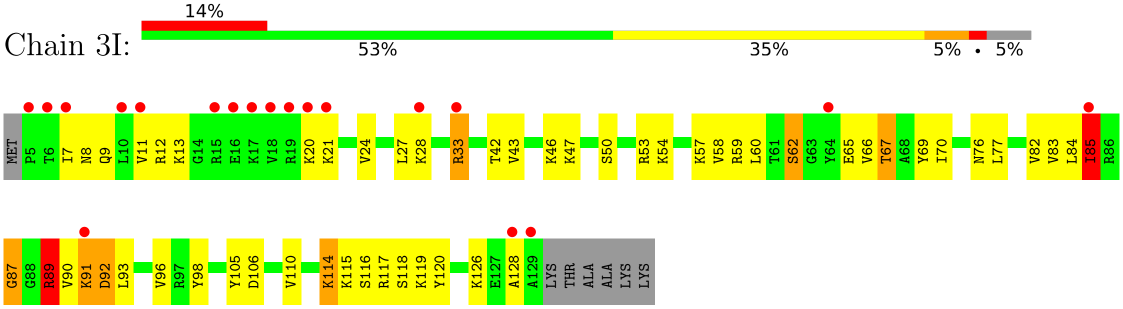
- Molecule 11: 30S ribosomal protein S11



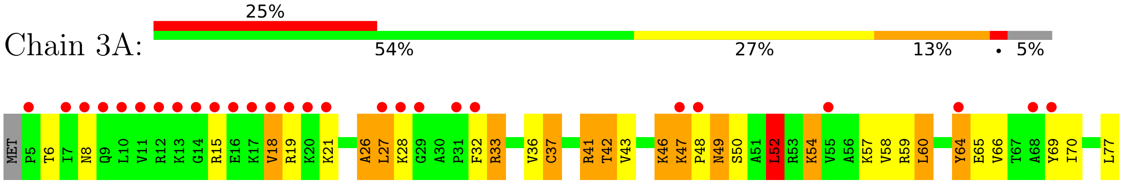
- Molecule 11: 30S ribosomal protein S11

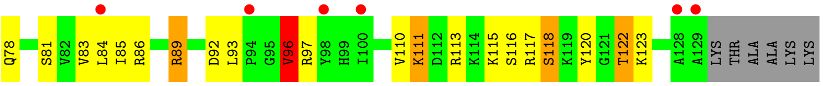


- Molecule 12: 30S ribosomal protein S12



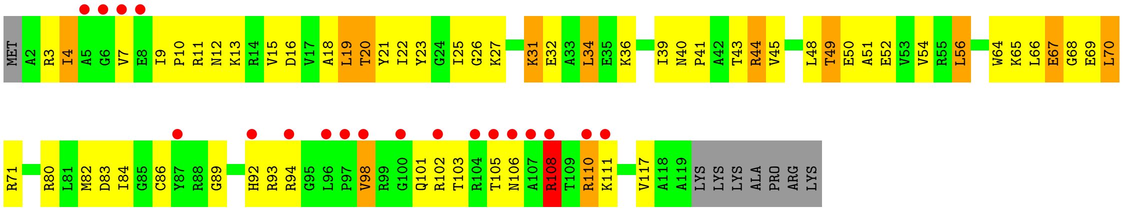
- Molecule 12: 30S ribosomal protein S12





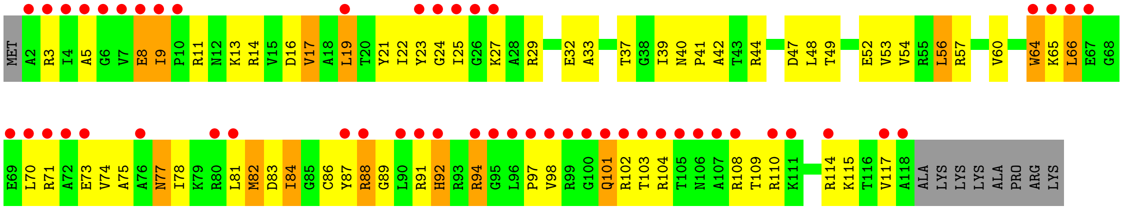
- Molecule 13: 30S ribosomal protein S13

Chain 4I:



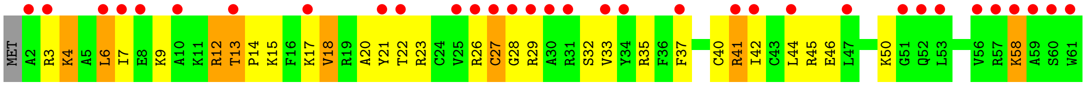
- Molecule 13: 30S ribosomal protein S13

Chain 4A:



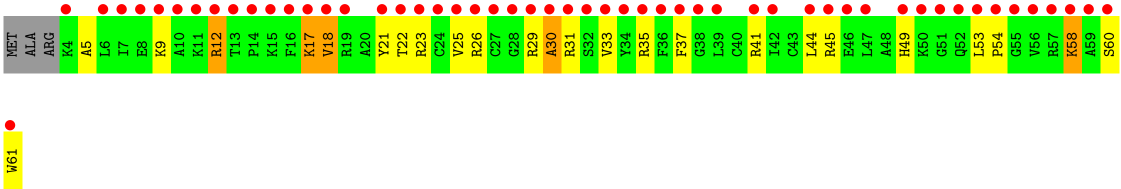
- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:



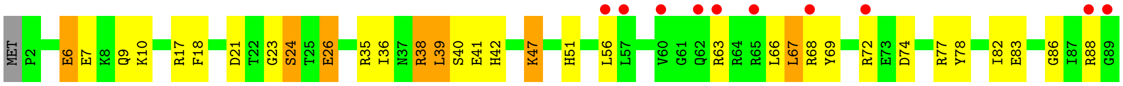
- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A:

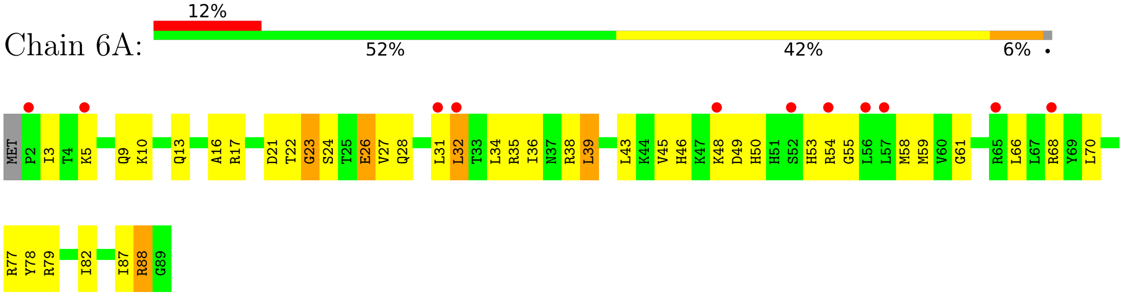


- Molecule 15: 30S ribosomal protein S15

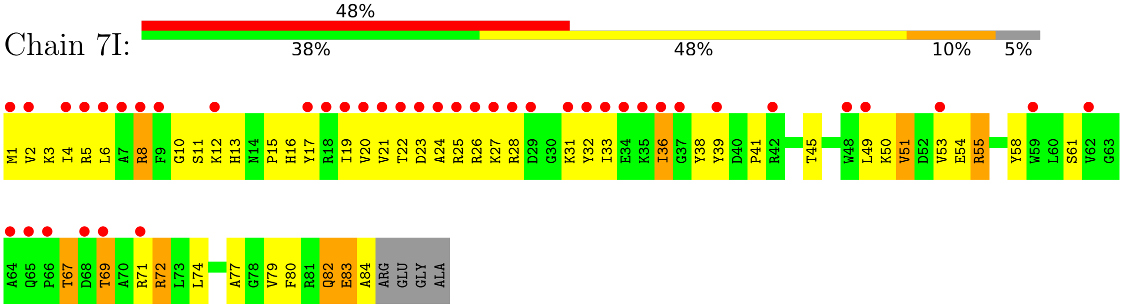
Chain 6I:



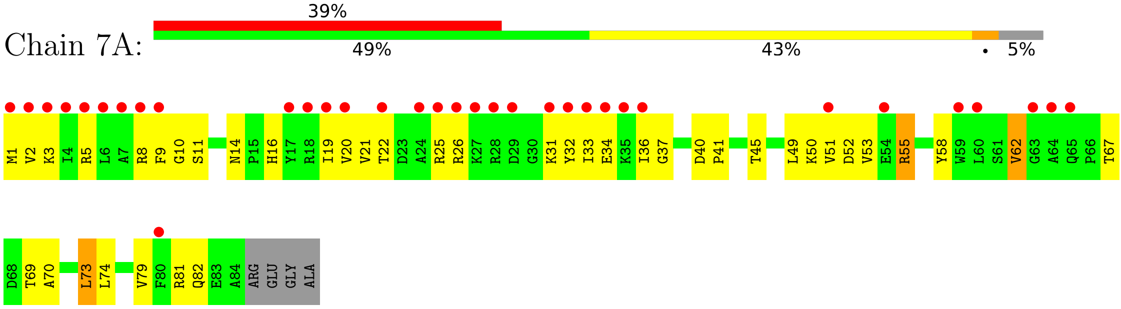
- Molecule 15: 30S ribosomal protein S15



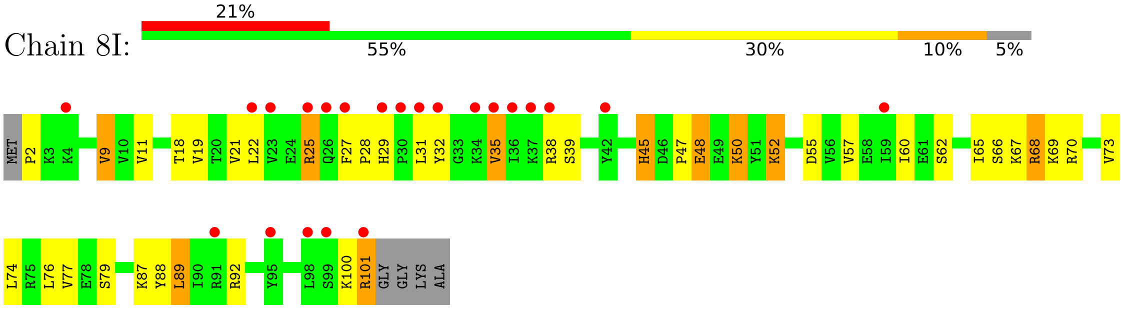
- Molecule 16: 30S ribosomal protein S16



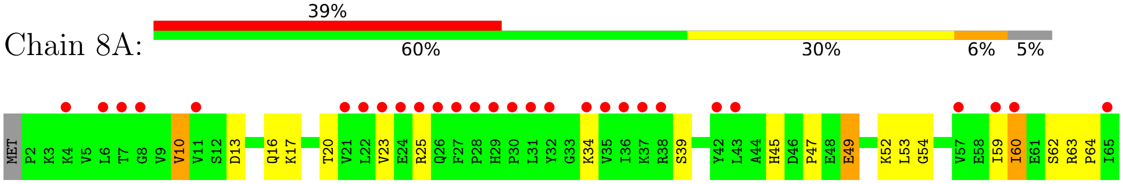
- Molecule 16: 30S ribosomal protein S16

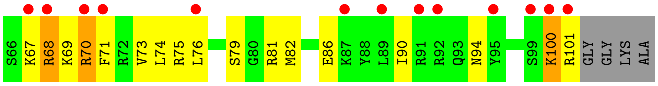


- Molecule 17: 30S ribosomal protein S17



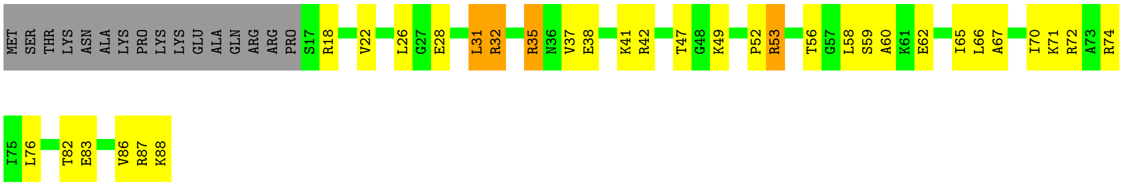
- Molecule 17: 30S ribosomal protein S17





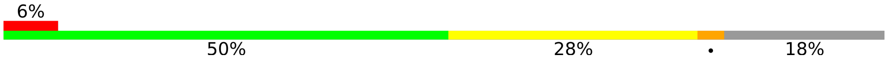
- Molecule 18: 30S ribosomal protein S18

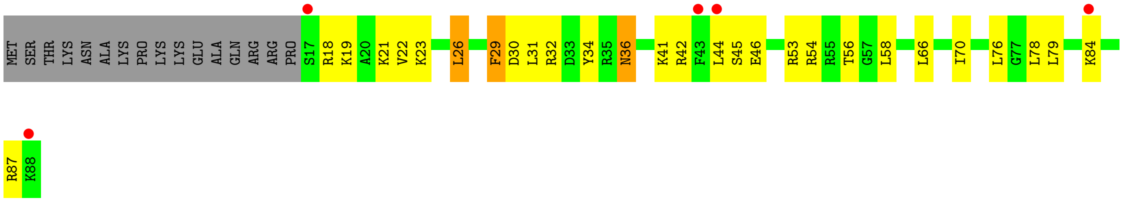
Chain 9I:



- Molecule 18: 30S ribosomal protein S18

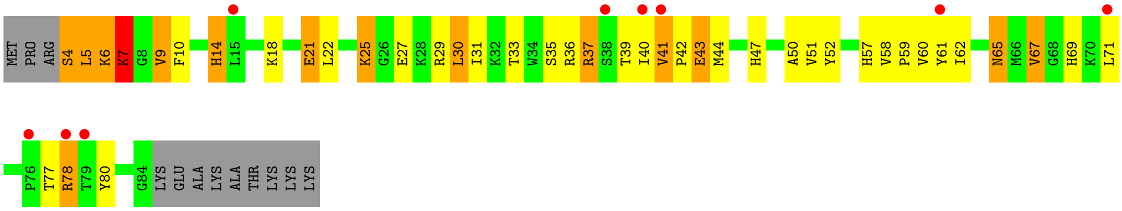
Chain 9A:





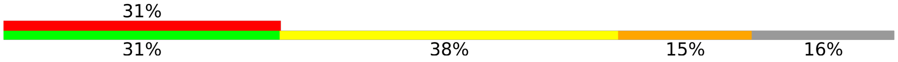
- Molecule 19: 30S ribosomal protein S19

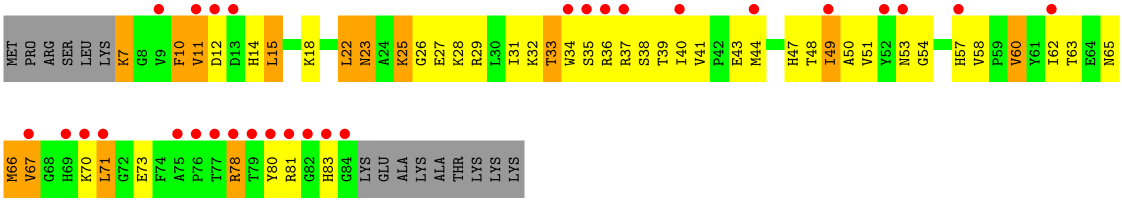
Chain AI:



- Molecule 19: 30S ribosomal protein S19

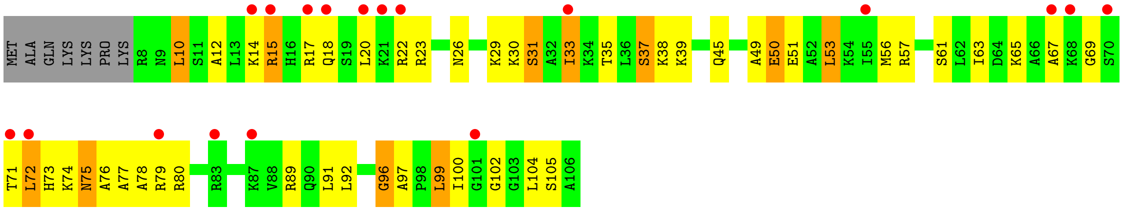
Chain AA:



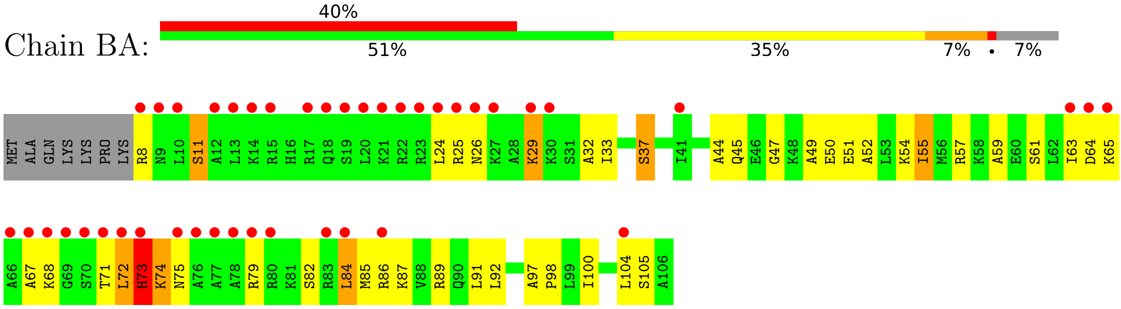


- Molecule 20: 30S ribosomal protein S20

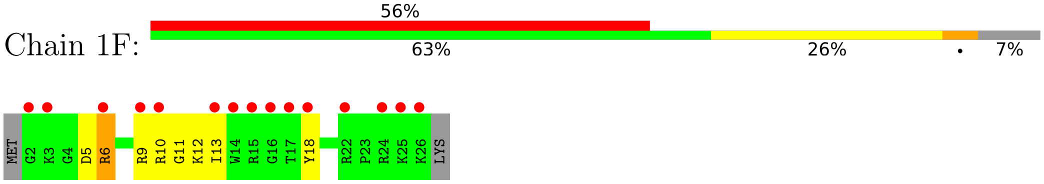
Chain BI:



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



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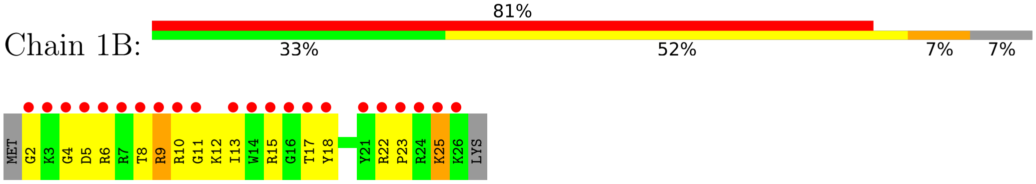

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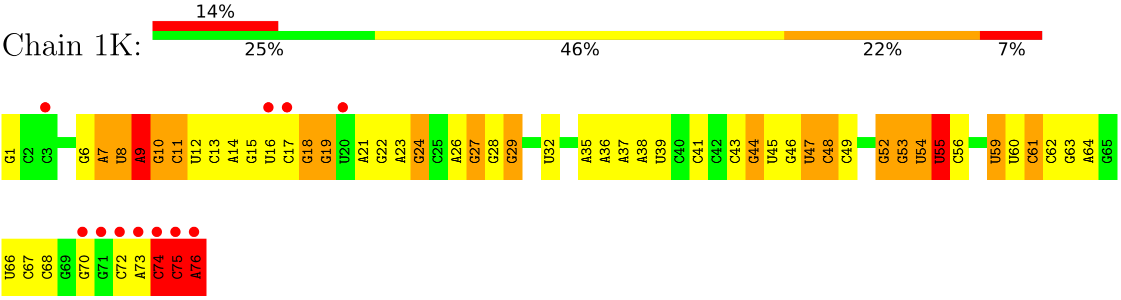

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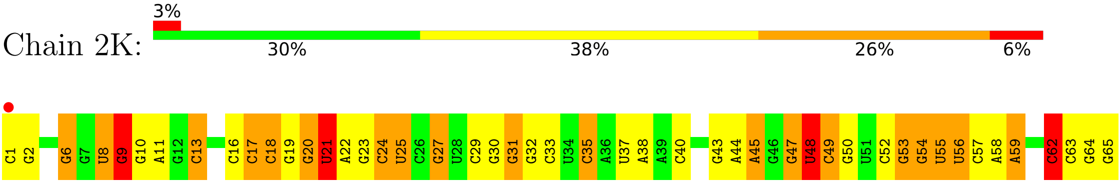

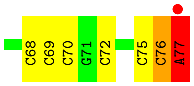

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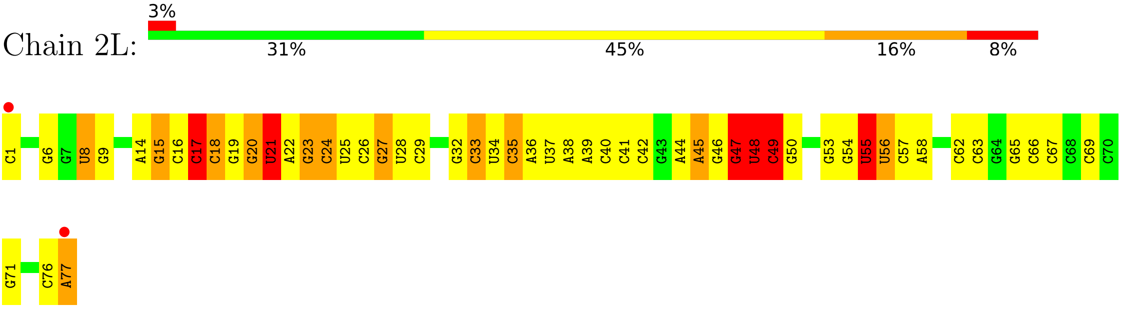

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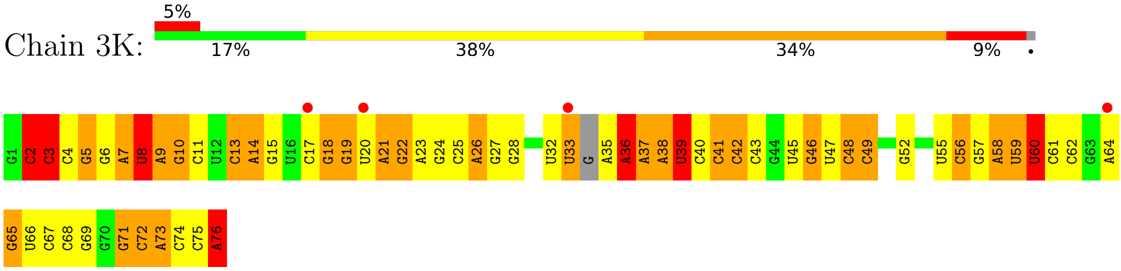

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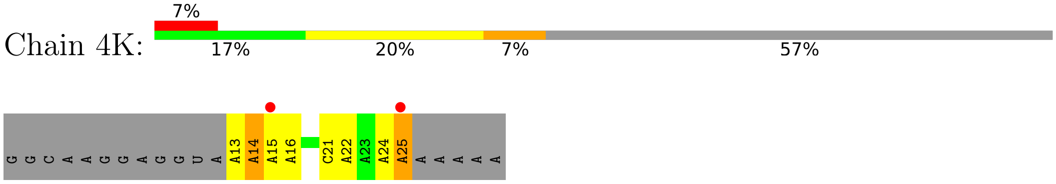

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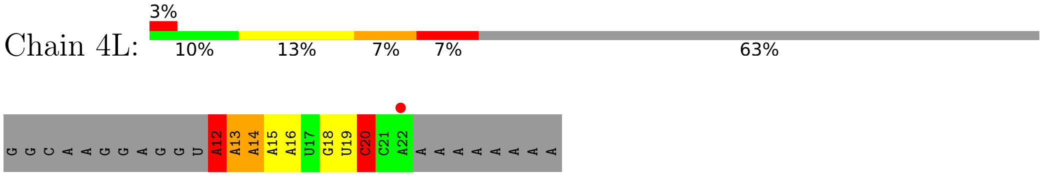

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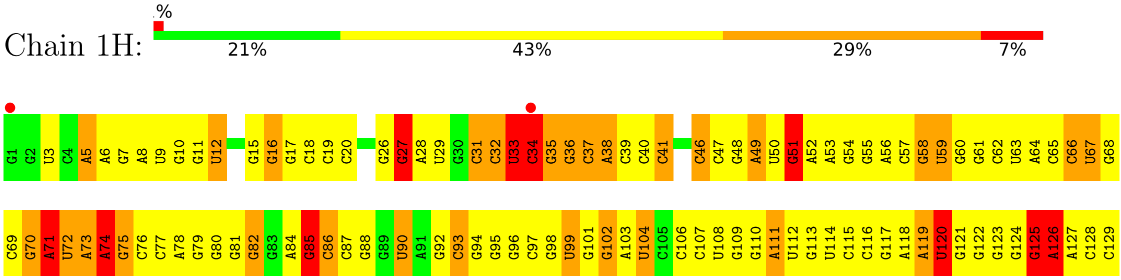

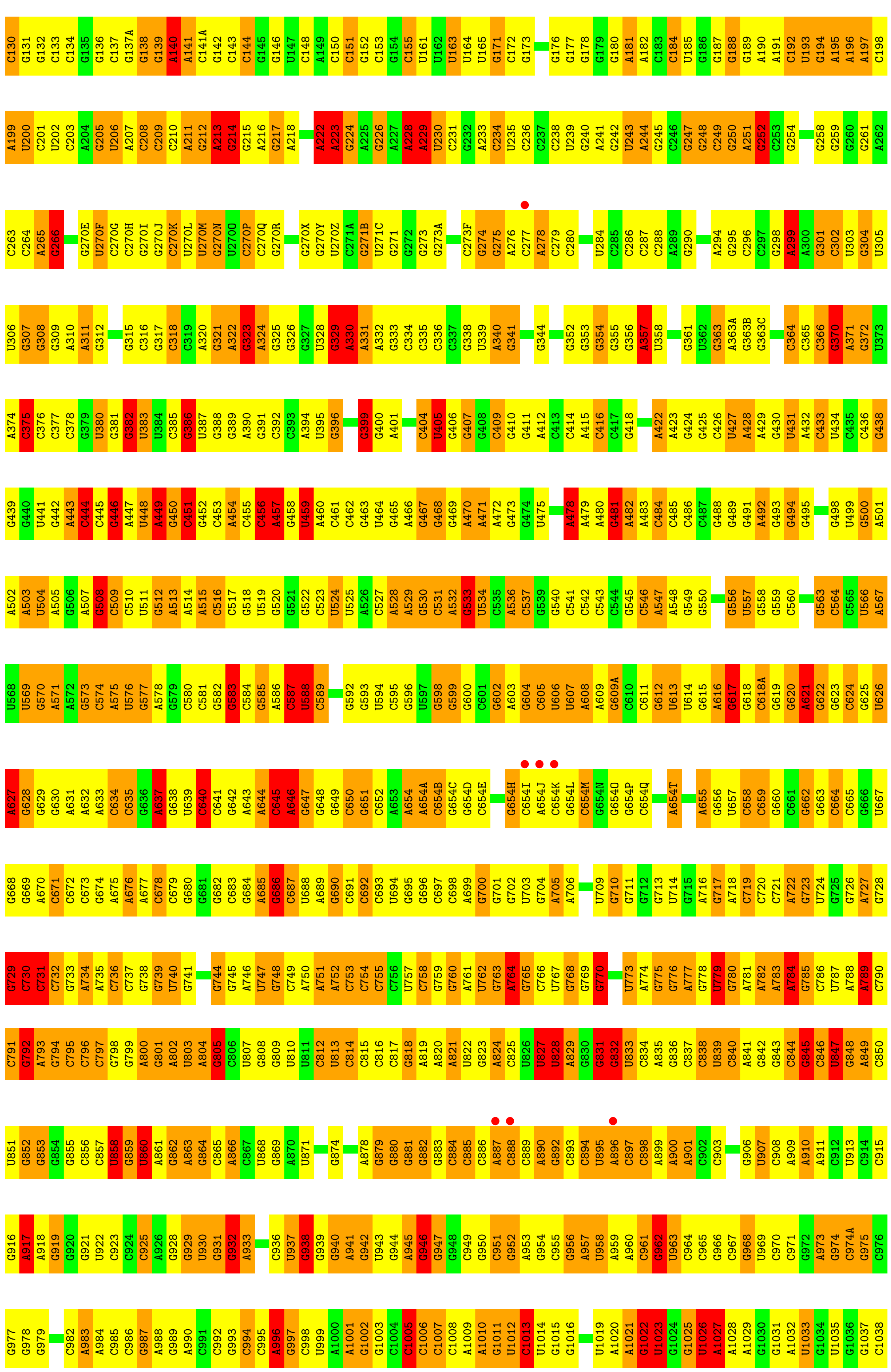
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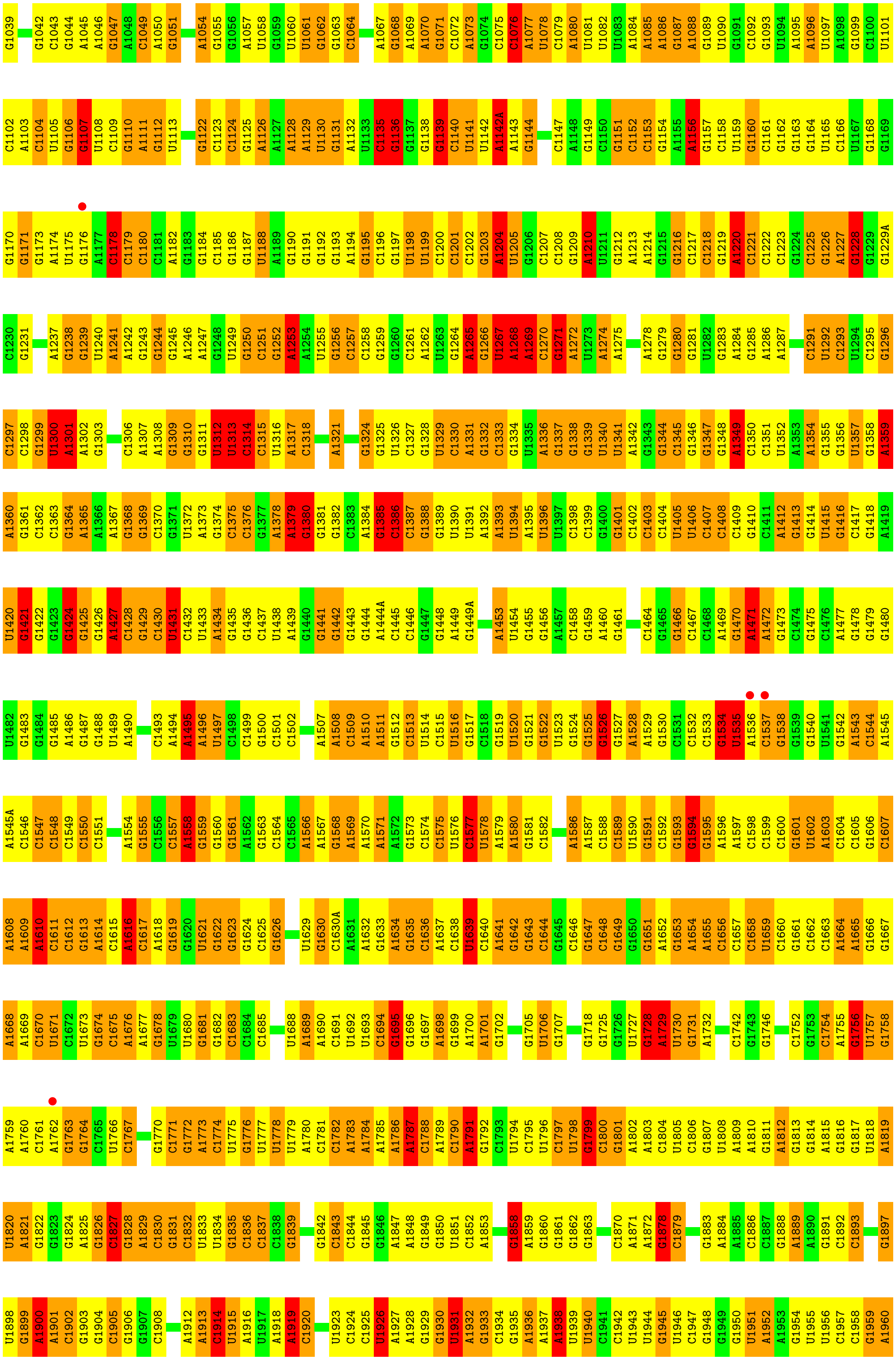
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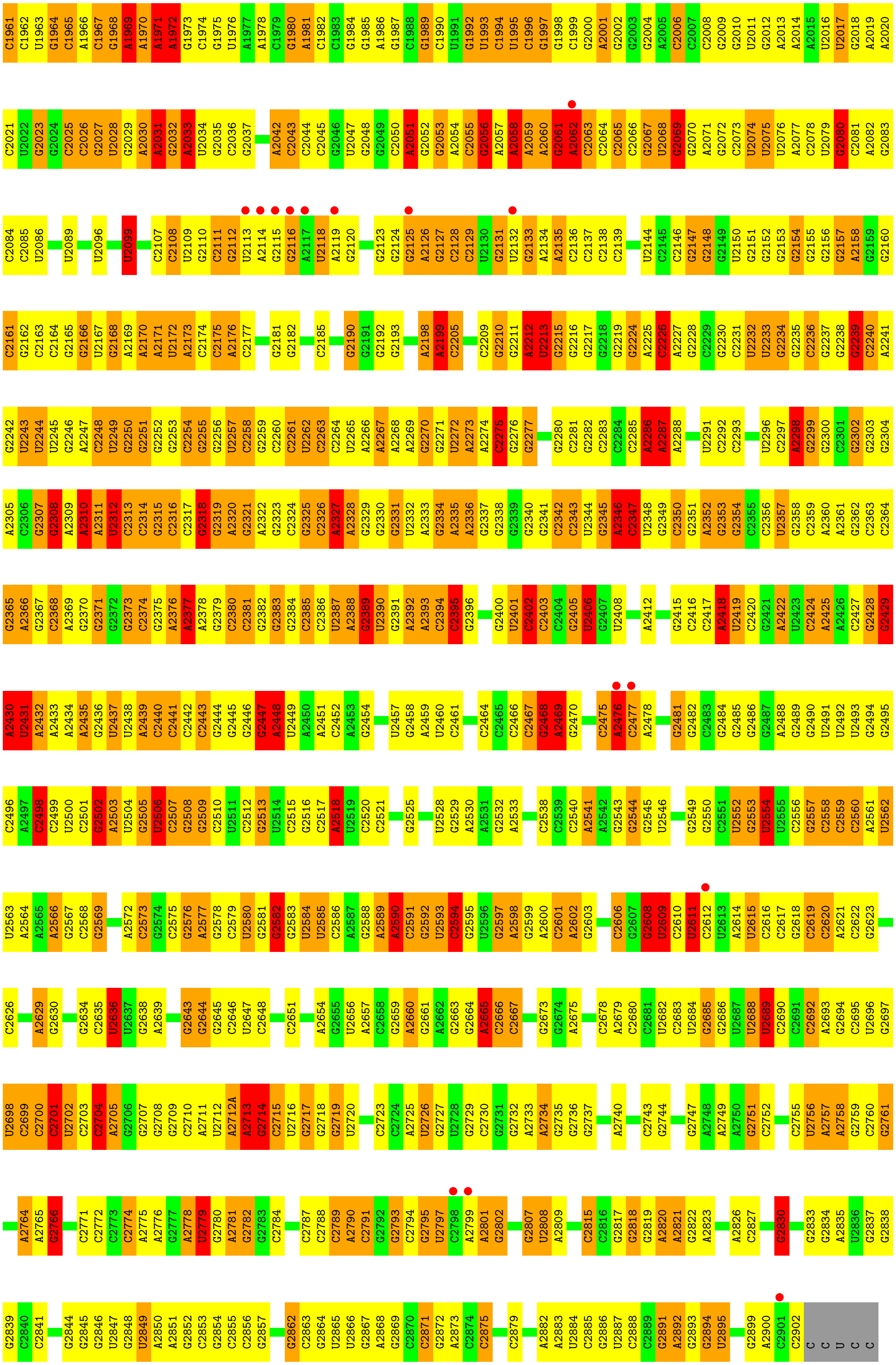

- Molecule 26: 23S ribosomal RNA

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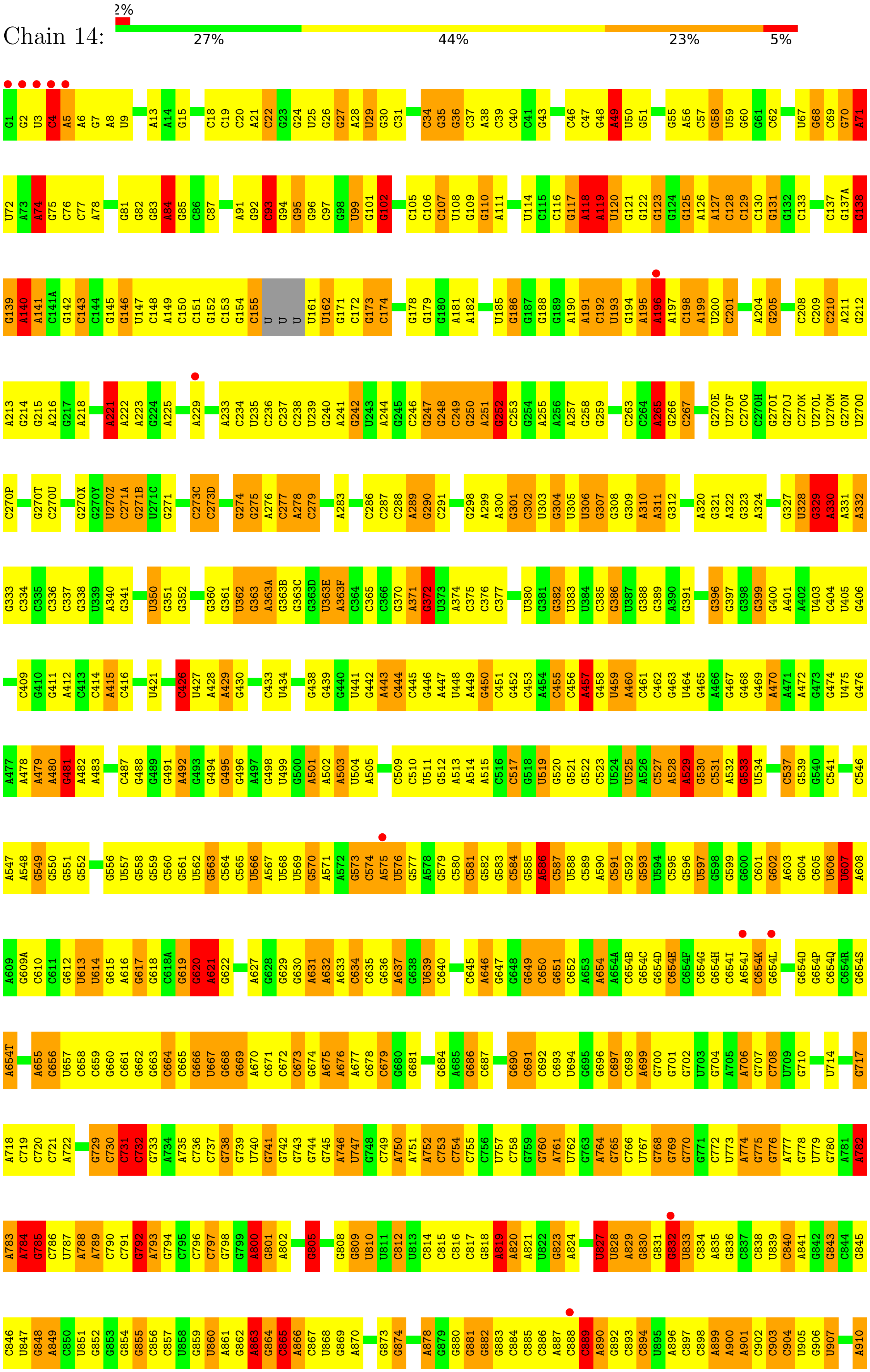

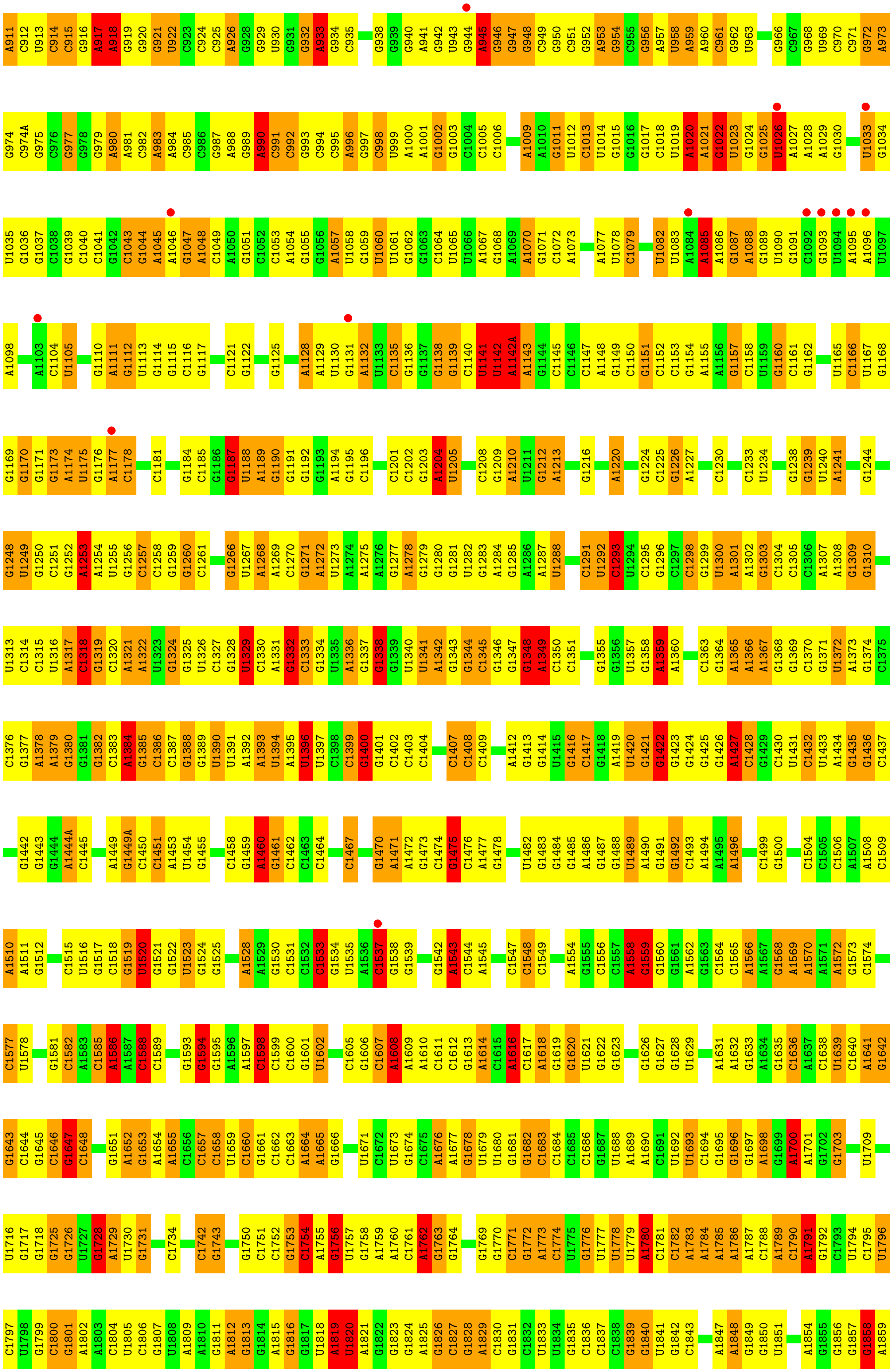
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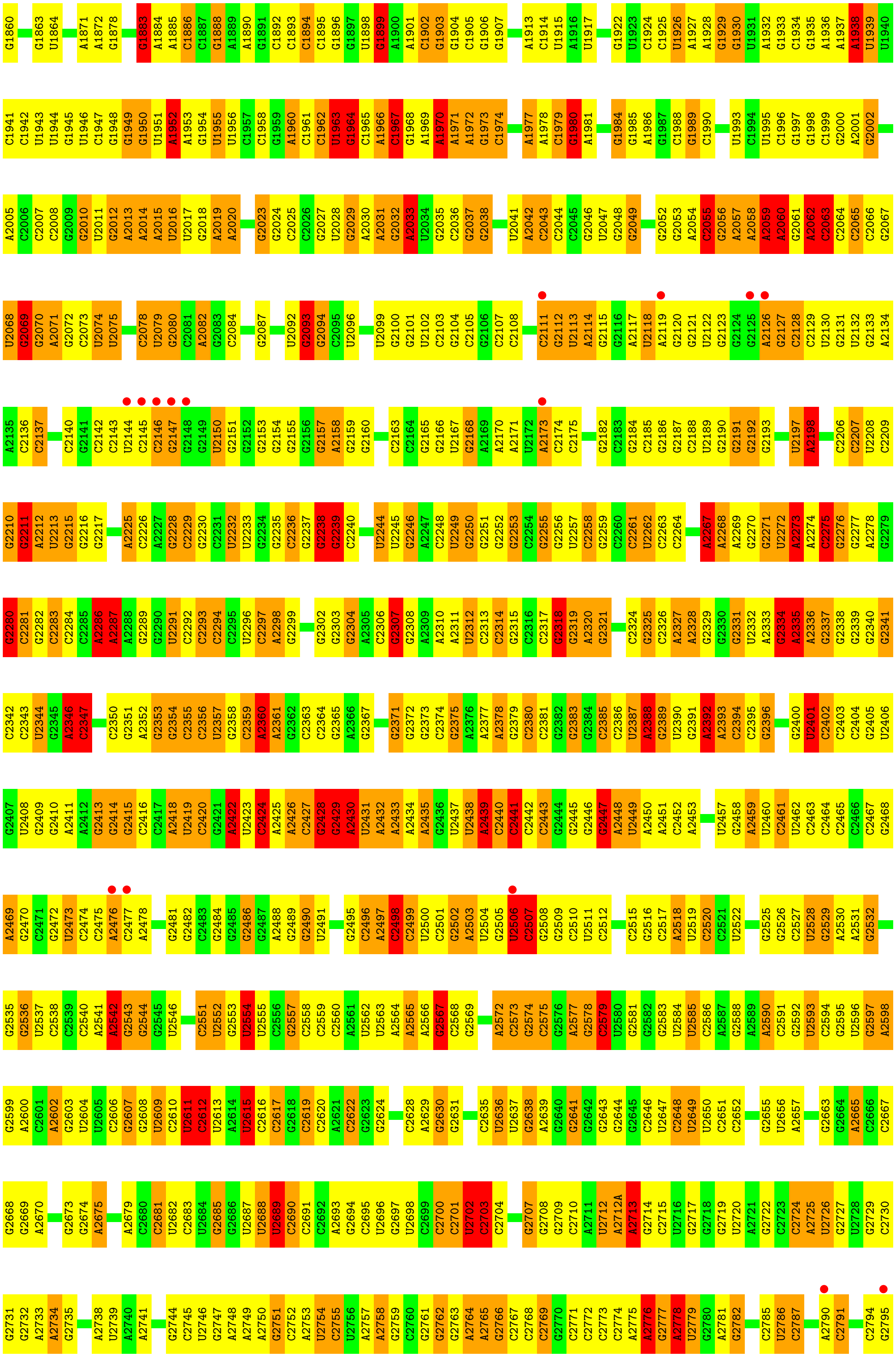
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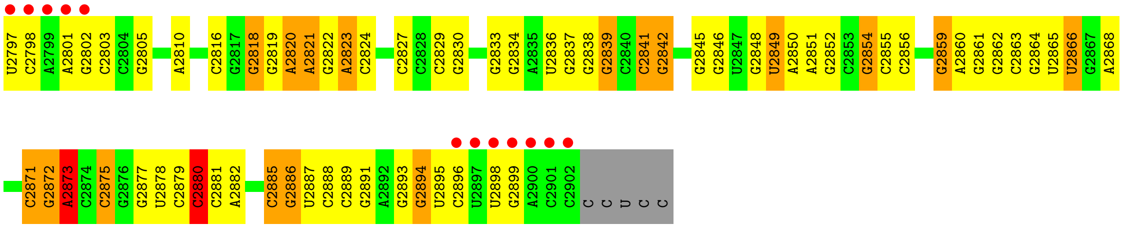
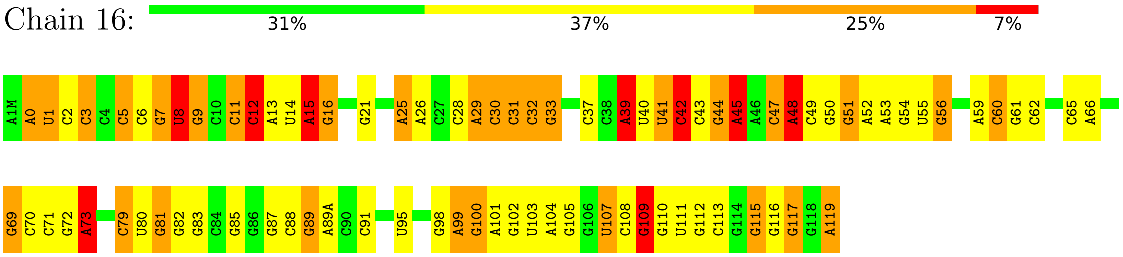
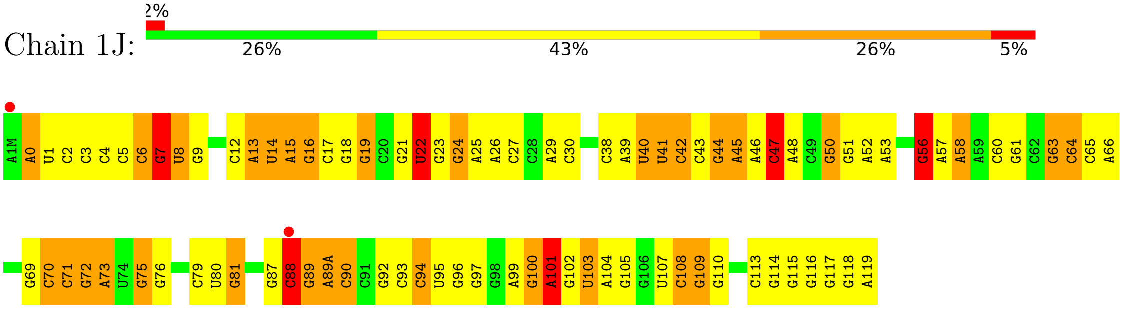


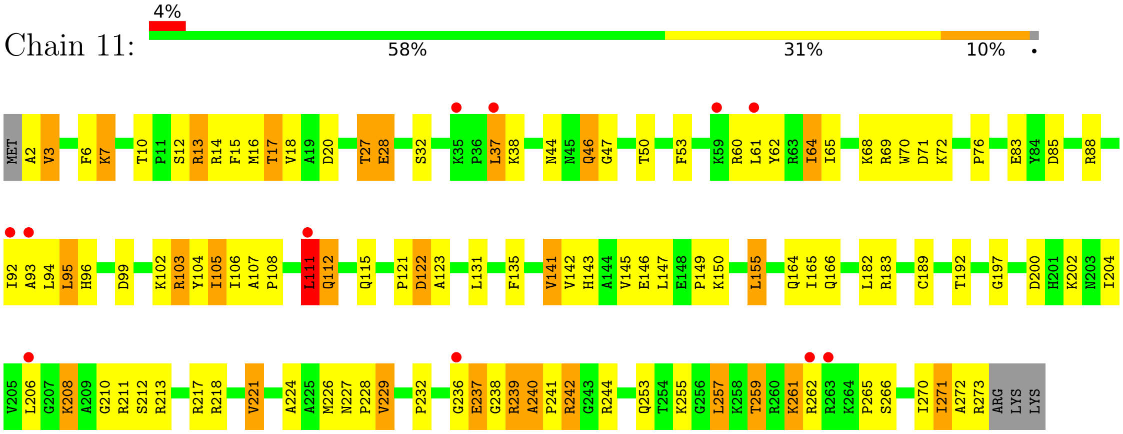
- Molecule 27: 5S ribosomal RNA



- Molecule 27: 5S ribosomal RNA



- Molecule 28: 50S ribosomal protein L2



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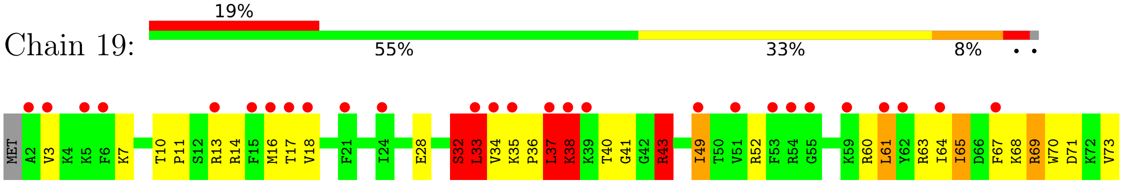

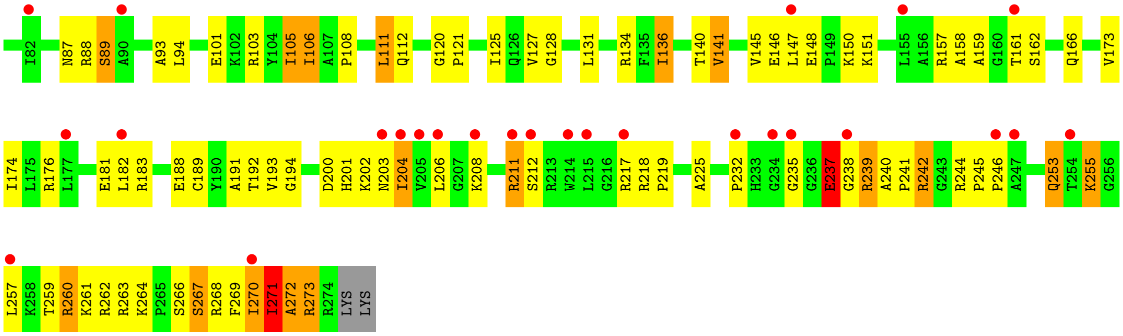

- Molecule 29: 50S ribosomal protein L3

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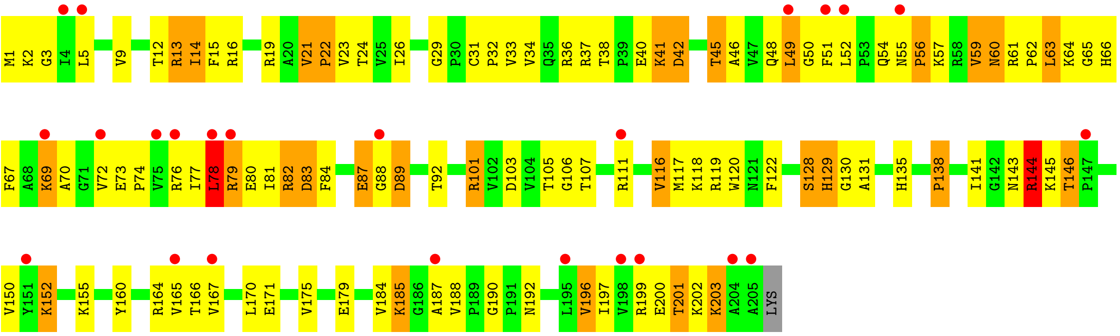

- Molecule 29: 50S ribosomal protein L3

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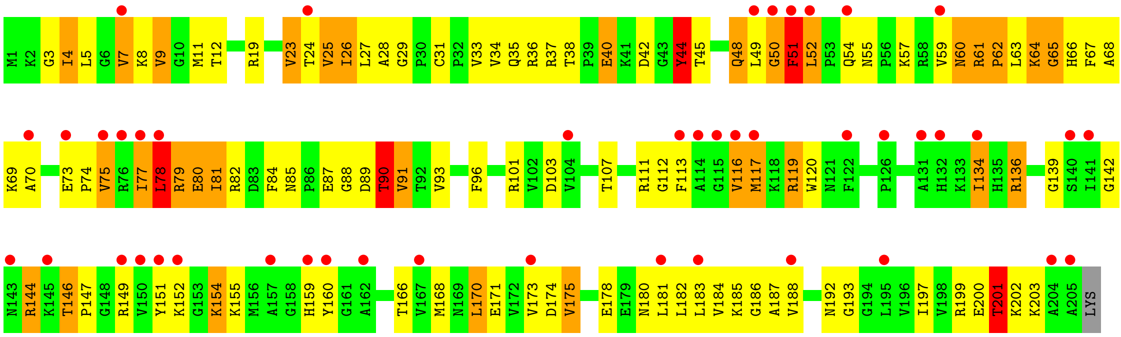
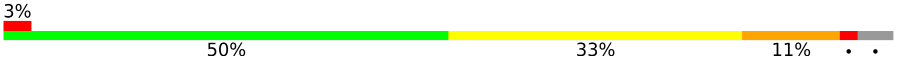
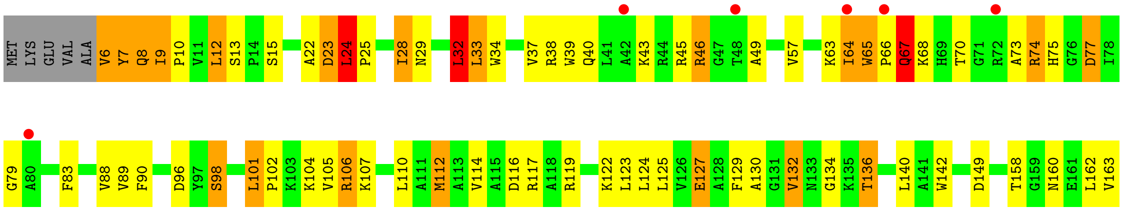
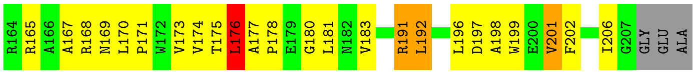


- Molecule 30: 50S ribosomal protein L4

Chain 31:







- Molecule 30: 50S ribosomal protein L4

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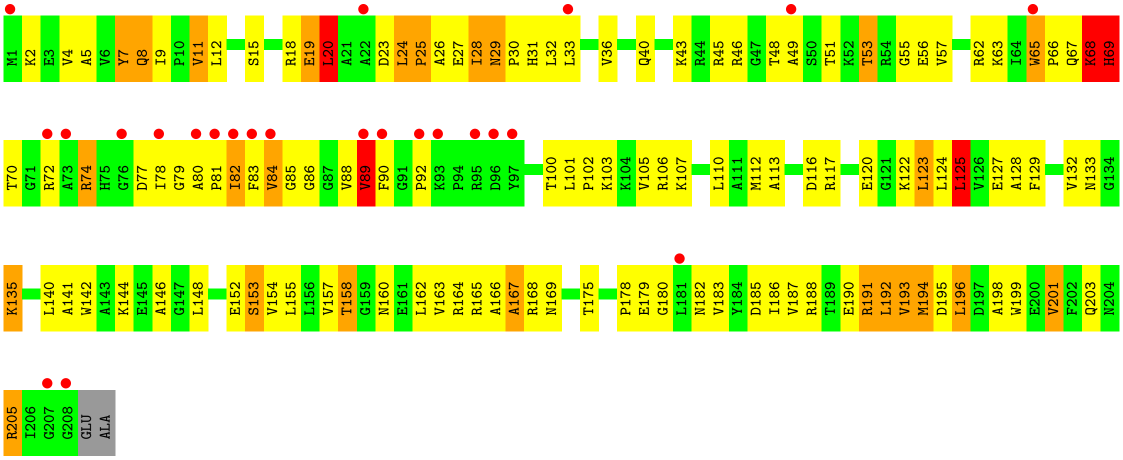
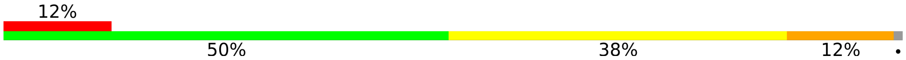
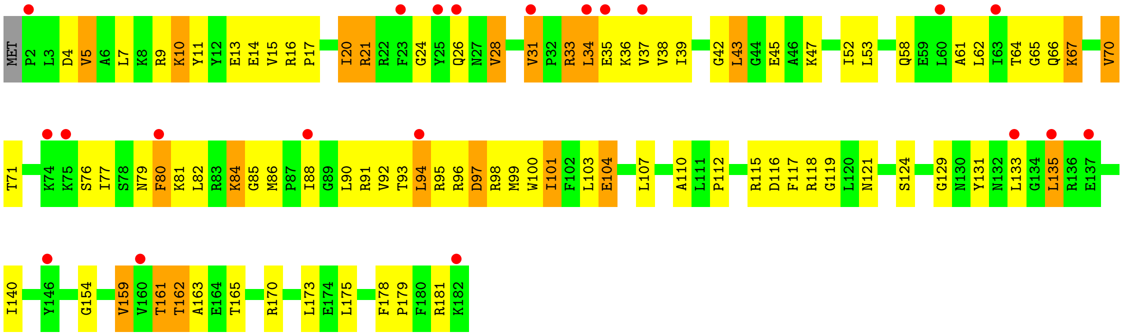


- Molecule 31: 50S ribosomal protein L5

Chain 41:





- Molecule 31: 50S ribosomal protein L5

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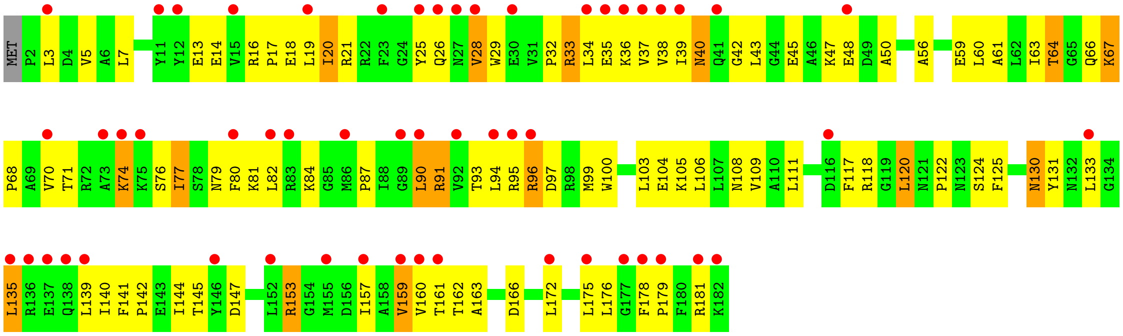

- Molecule 32: 50S ribosomal protein L6

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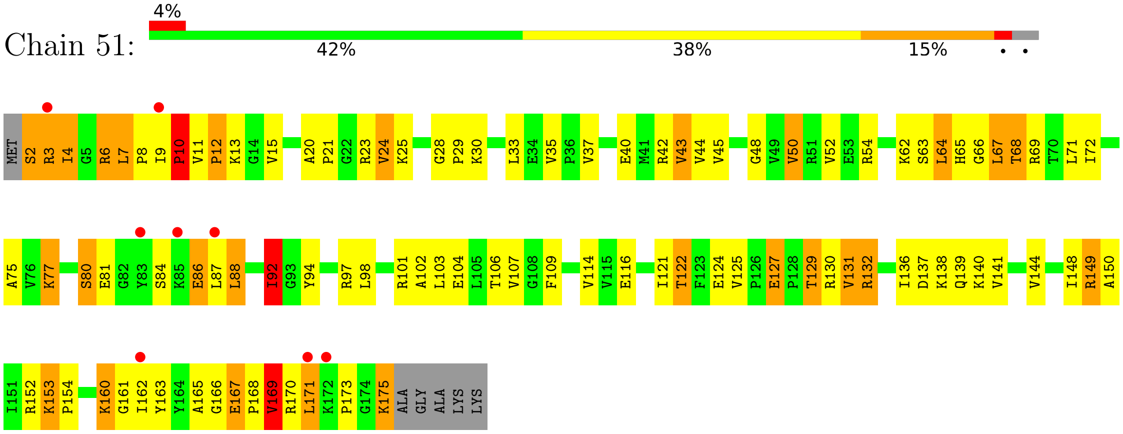

- Molecule 32: 50S ribosomal protein L6

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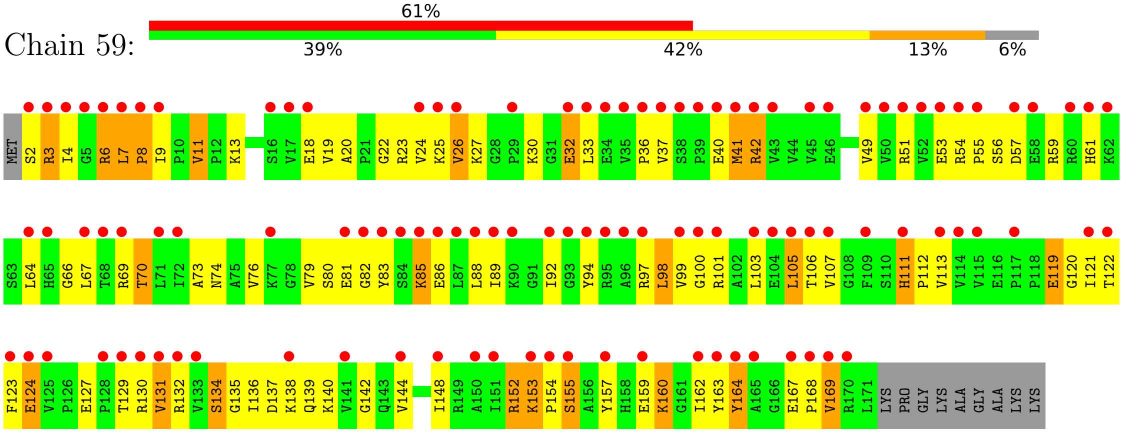

- Molecule 33: 50S ribosomal protein L9

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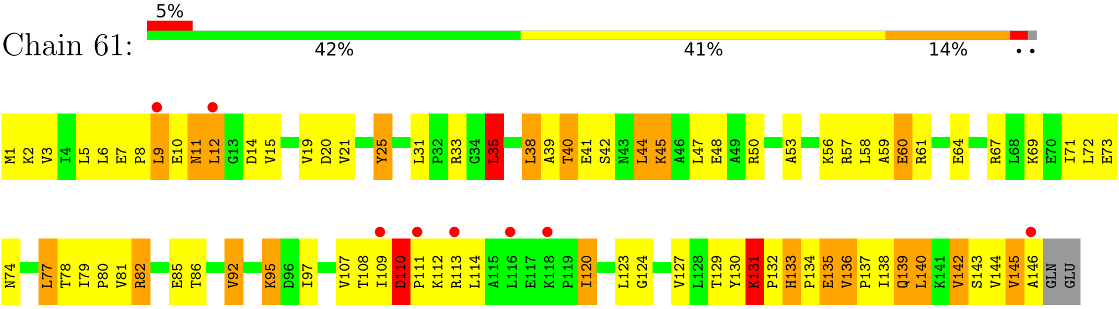

- Molecule 33: 50S ribosomal protein L9

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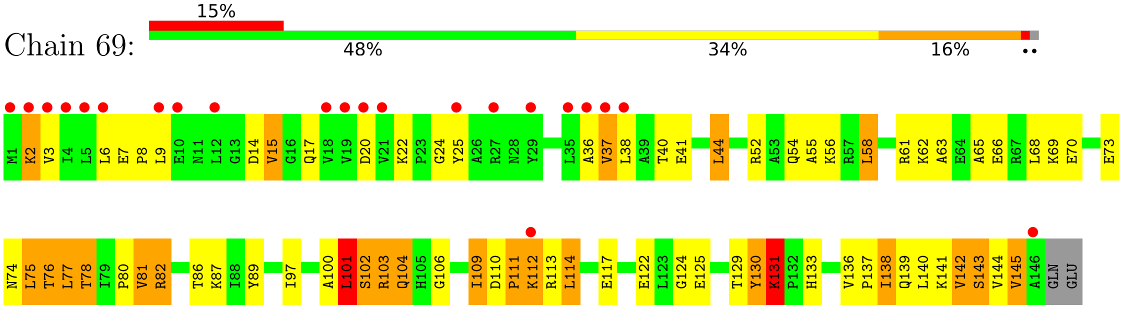
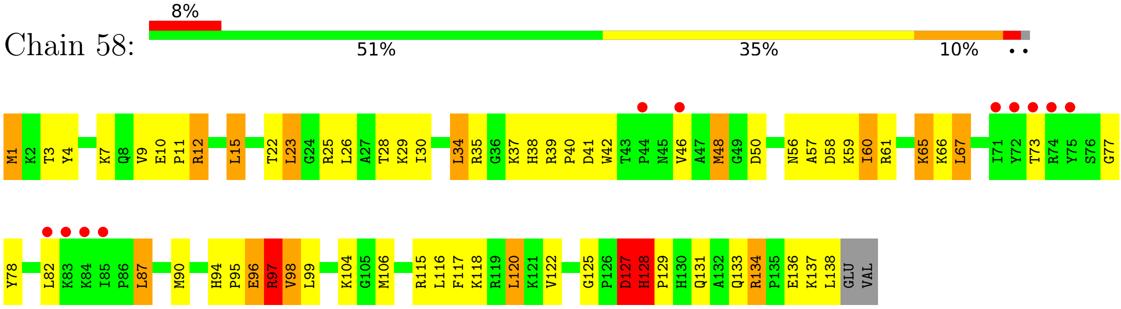
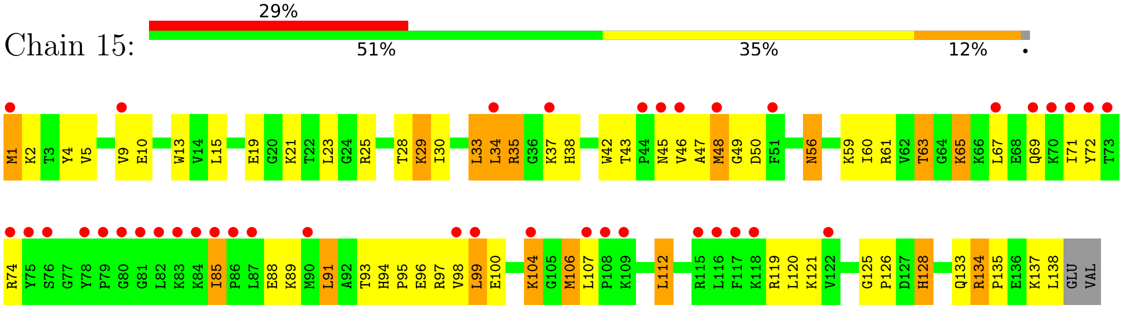


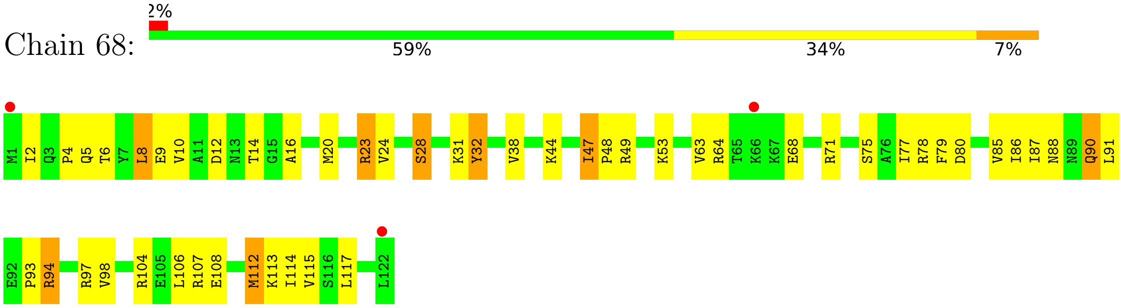
- Molecule 34: 50S ribosomal protein L13



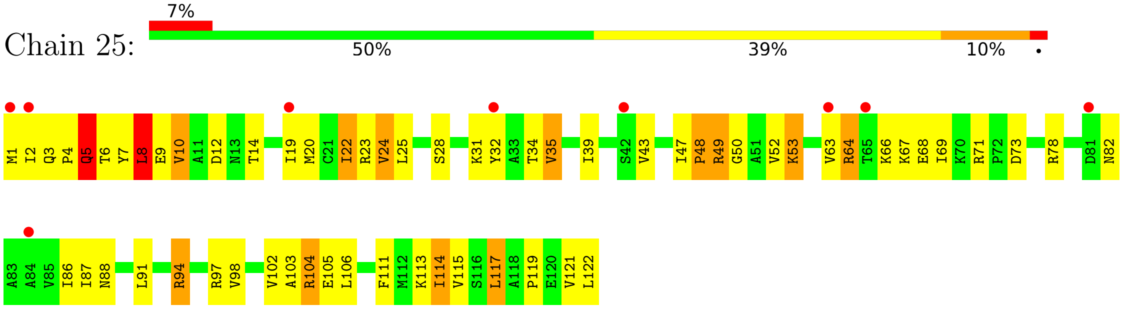
- Molecule 34: 50S ribosomal protein L13



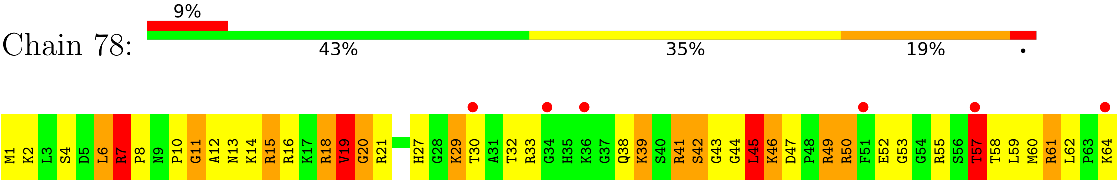
- Molecule 35: 50S ribosomal protein L14

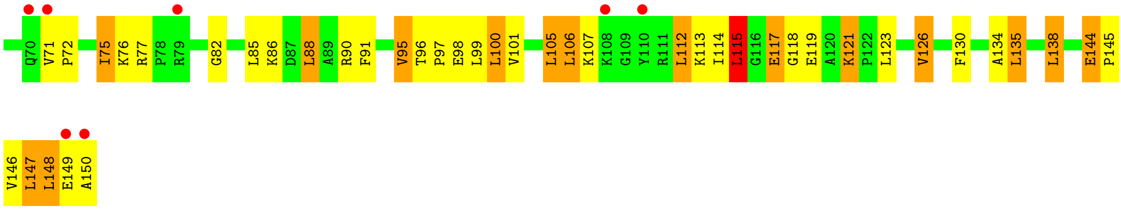


- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15





- Molecule 36: 50S ribosomal protein L15

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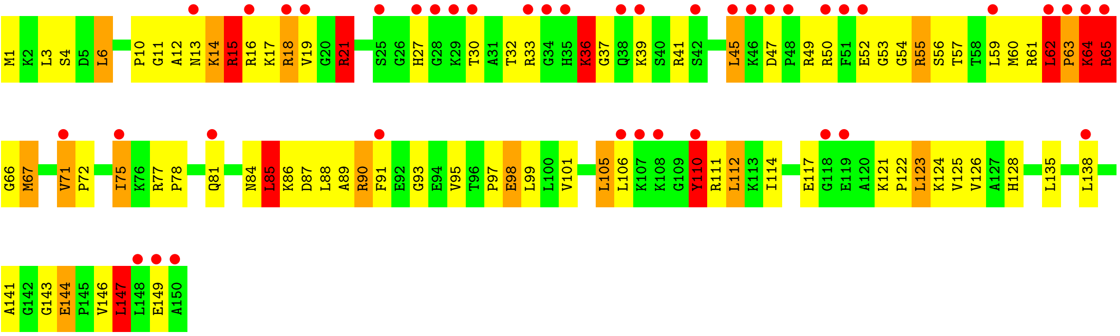
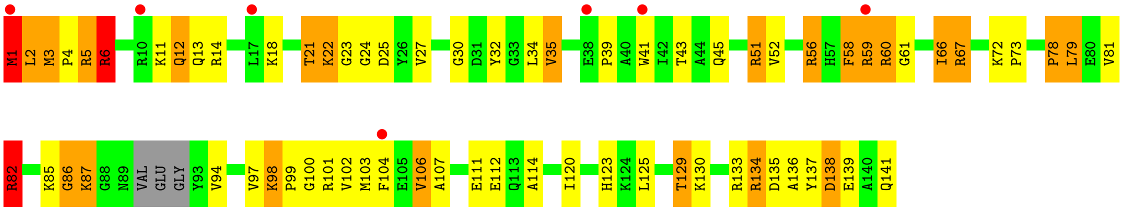


- Molecule 37: 50S ribosomal protein L16

Chain 88:



- Molecule 37: 50S ribosomal protein L16

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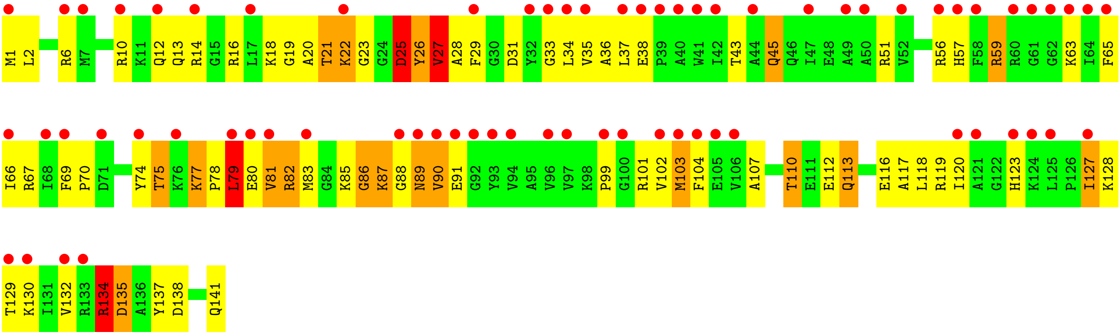
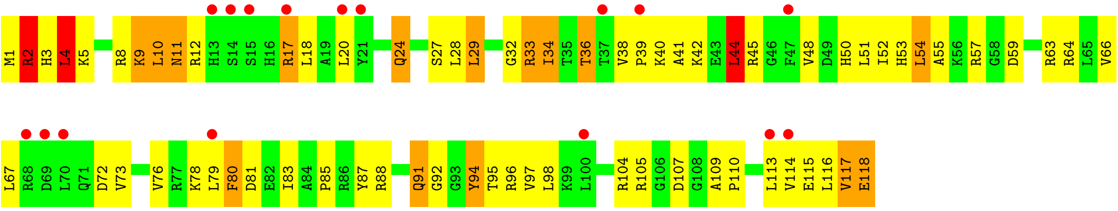


- Molecule 38: 50S ribosomal protein L17

Chain 98:



- Molecule 38: 50S ribosomal protein L17

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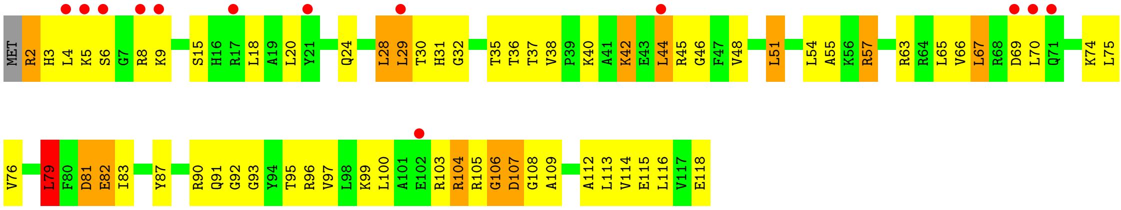
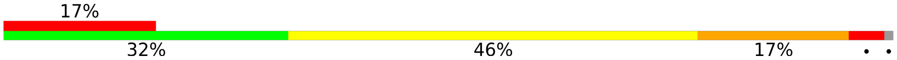
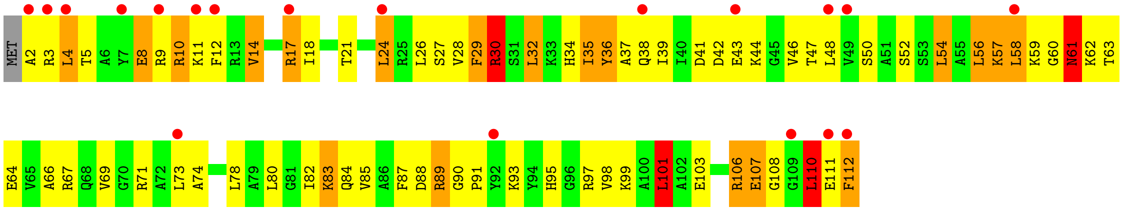


- Molecule 39: 50S ribosomal protein L18

Chain A8:





- Molecule 39: 50S ribosomal protein L18

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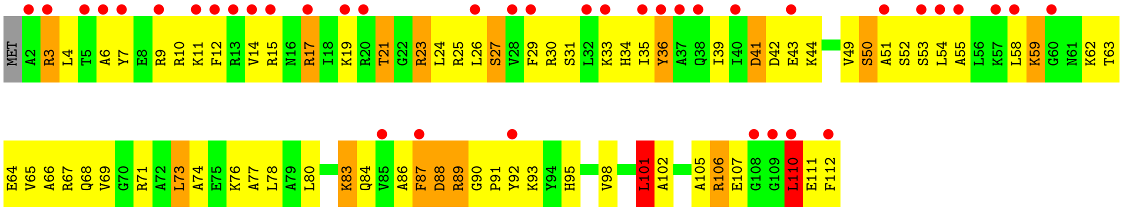
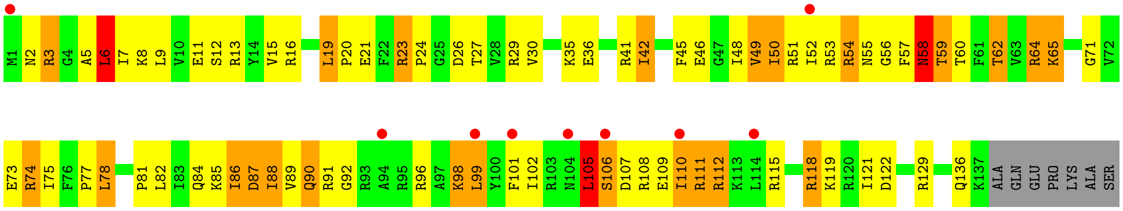
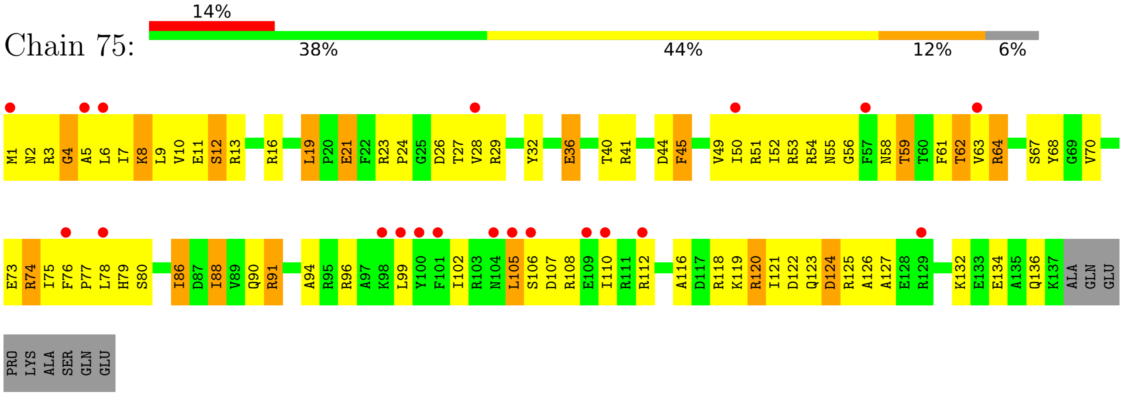


- Molecule 40: 50S ribosomal protein L19

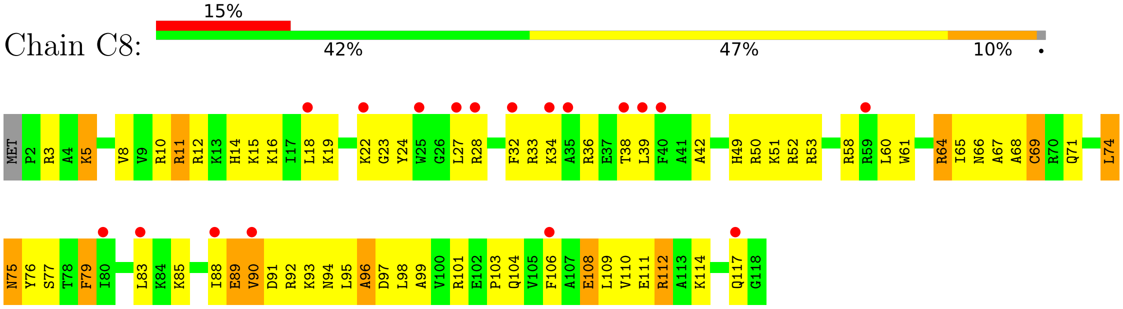
Chain B8:



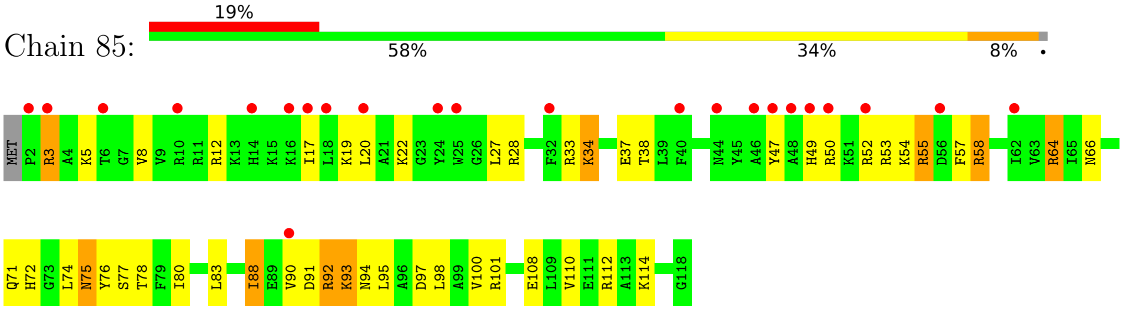
- Molecule 40: 50S ribosomal protein L19



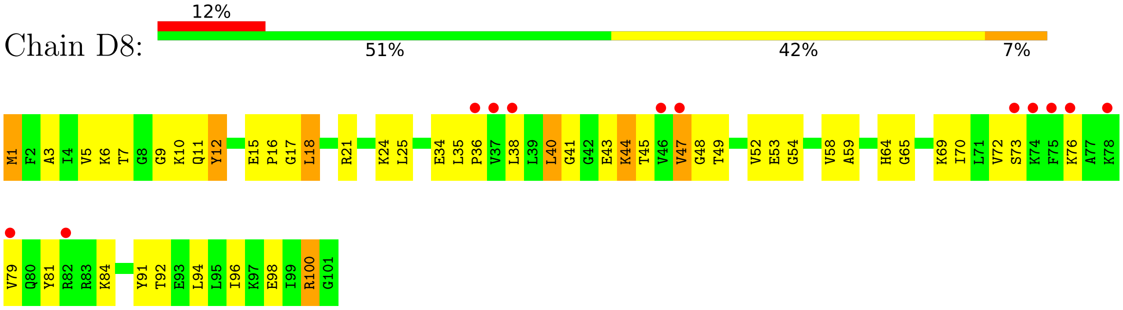
- Molecule 41: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L21

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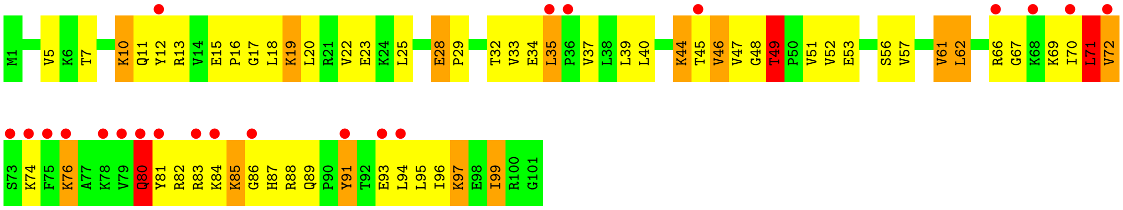
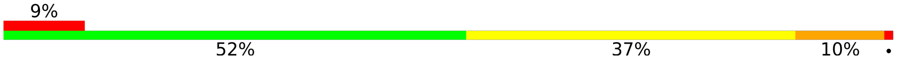
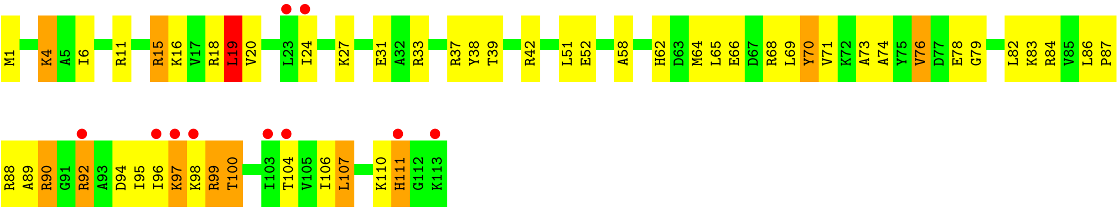


- Molecule 43: 50S ribosomal protein L22

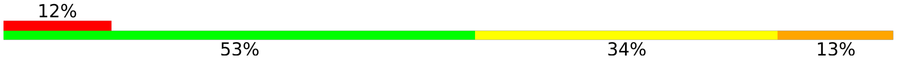
Chain E8:

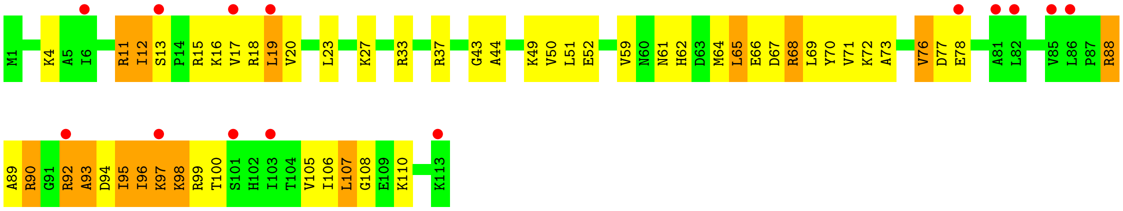




- Molecule 43: 50S ribosomal protein L22

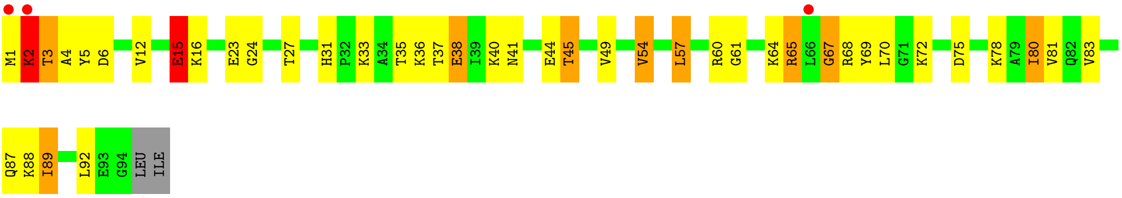
Chain A5:





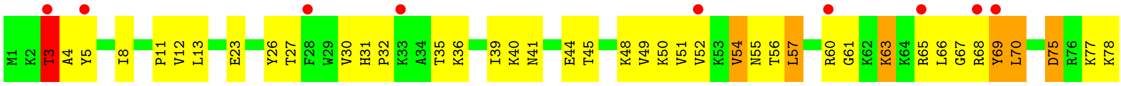
- Molecule 44: 50S ribosomal protein L23

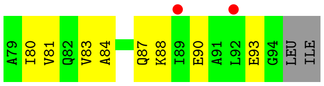
Chain F8:



- Molecule 44: 50S ribosomal protein L23

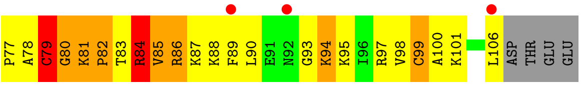
Chain B5:





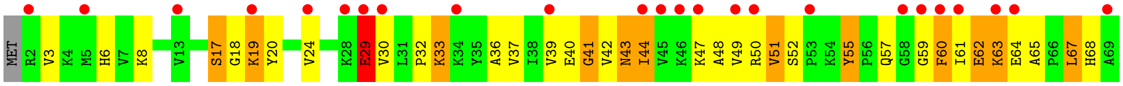
- Molecule 45: 50S ribosomal protein L24

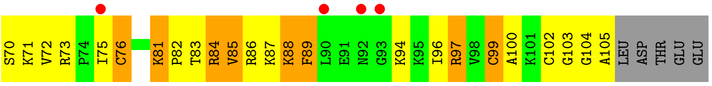
Chain G8:



- Molecule 45: 50S ribosomal protein L24

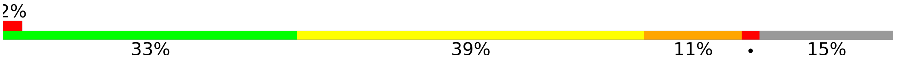
Chain C5:

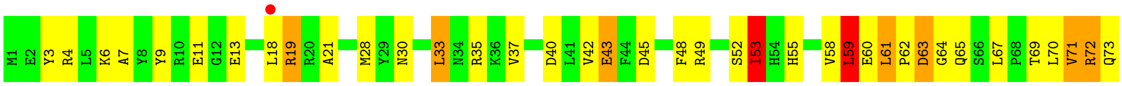


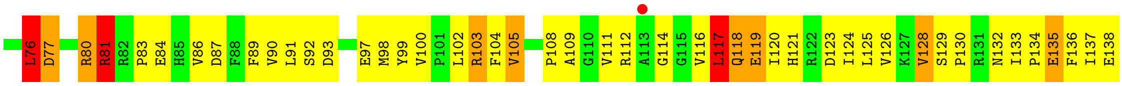


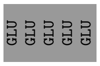
- Molecule 46: 50S ribosomal protein L25

Chain H8:



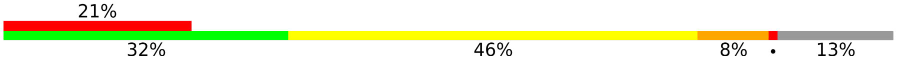


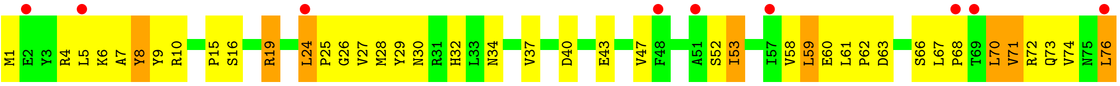


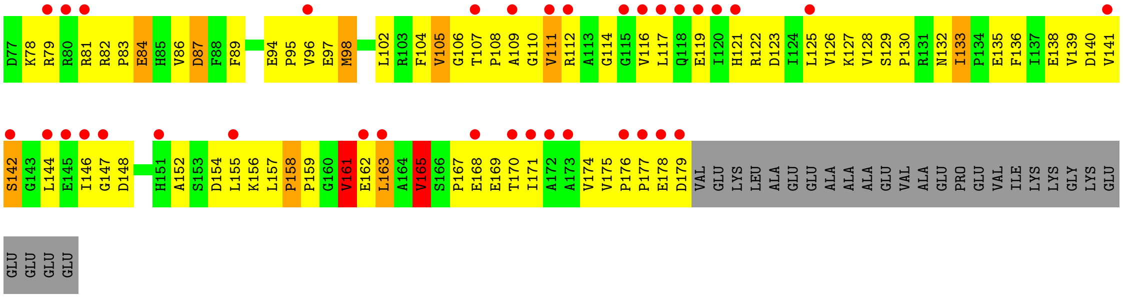


- Molecule 46: 50S ribosomal protein L25

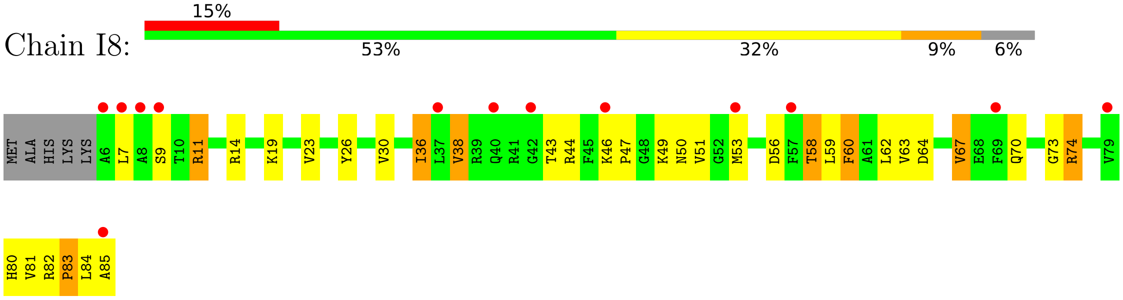
Chain D5:



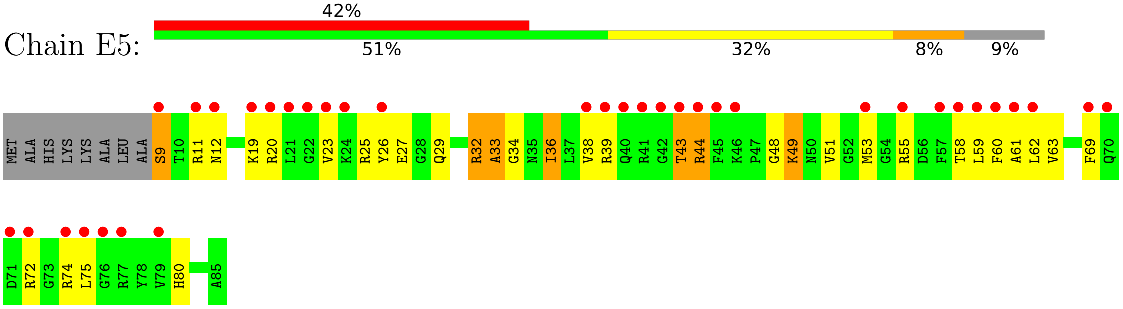




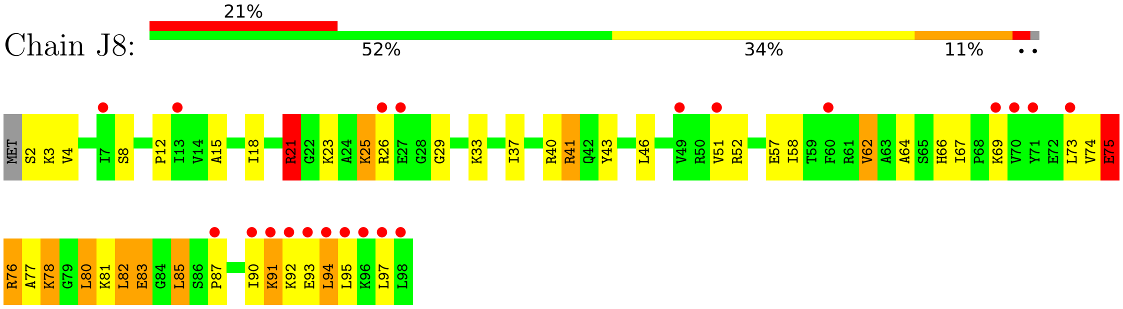
- Molecule 47: 50S ribosomal protein L27



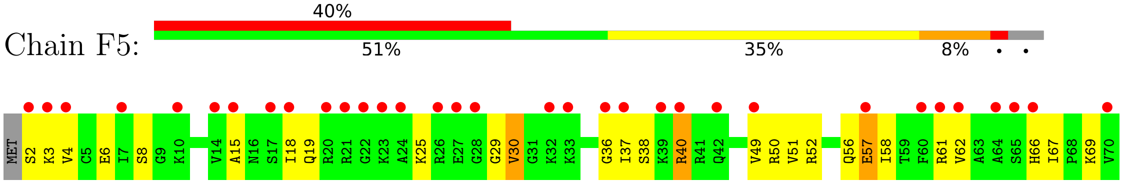
- Molecule 47: 50S ribosomal protein L27

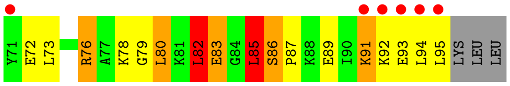


- Molecule 48: 50S ribosomal protein L28



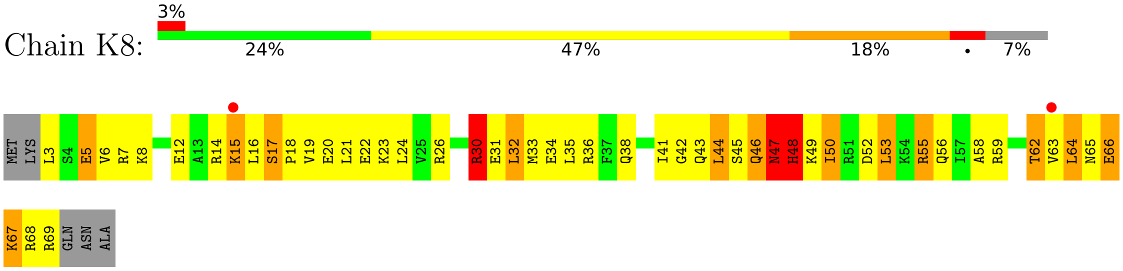
- Molecule 48: 50S ribosomal protein L28





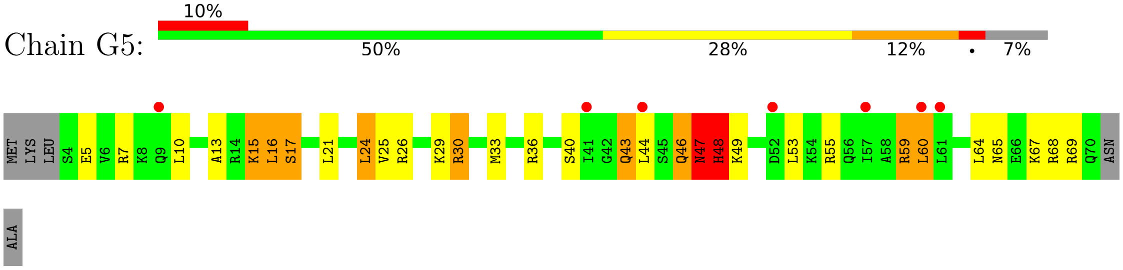
- Molecule 49: 50S ribosomal protein L29

Chain K8:



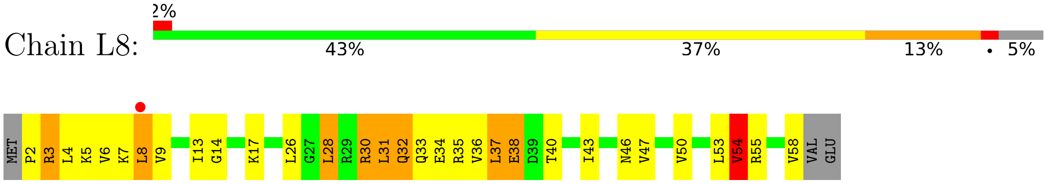
- Molecule 49: 50S ribosomal protein L29

Chain G5:



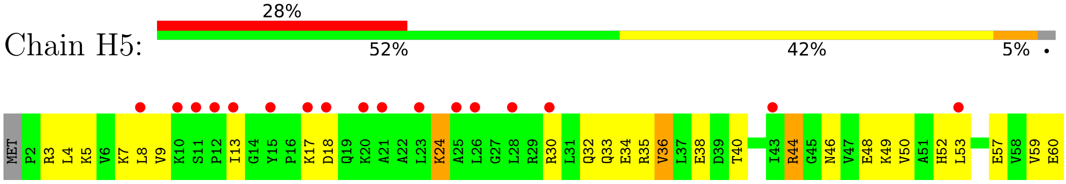
- Molecule 50: 50S ribosomal protein L30

Chain L8:



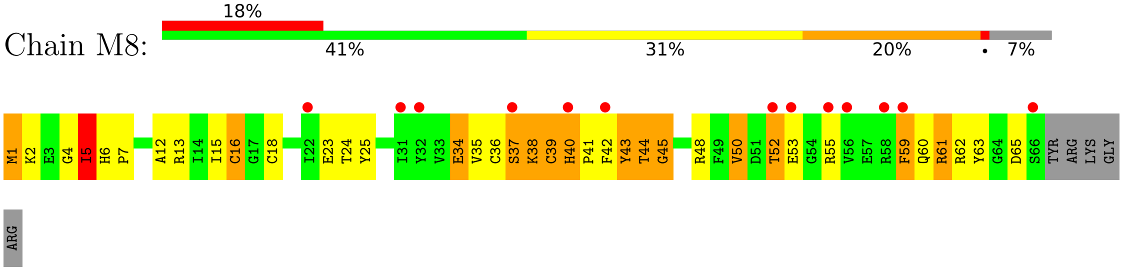
- Molecule 50: 50S ribosomal protein L30

Chain H5:



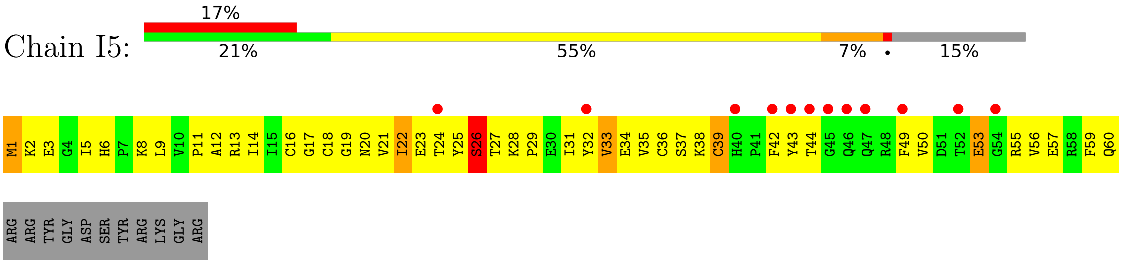
- Molecule 51: 50S ribosomal protein L31

Chain M8:



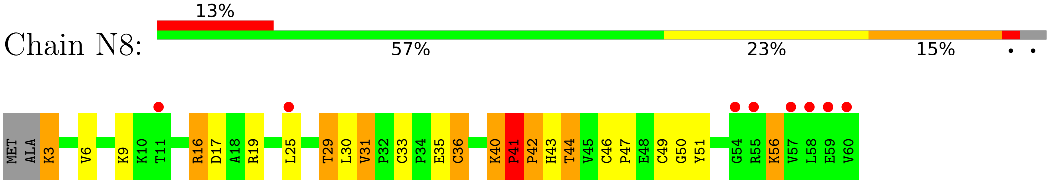
- Molecule 51: 50S ribosomal protein L31

Chain I5:



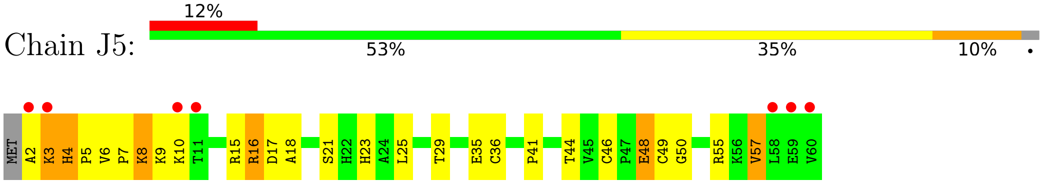
- Molecule 52: 50S ribosomal protein L32

Chain N8:



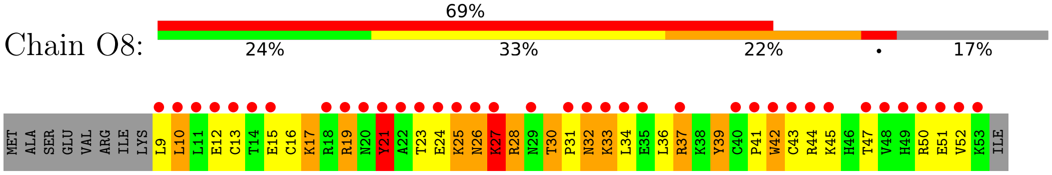
- Molecule 52: 50S ribosomal protein L32

Chain J5:



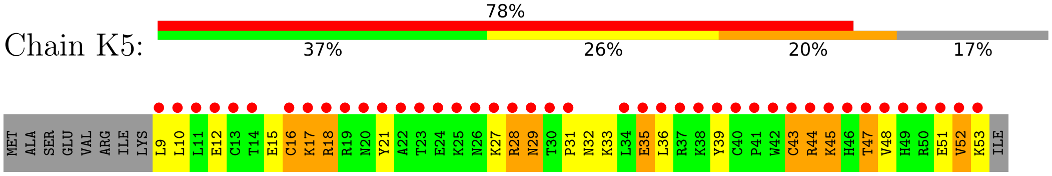
- Molecule 53: 50S ribosomal protein L33

Chain O8:



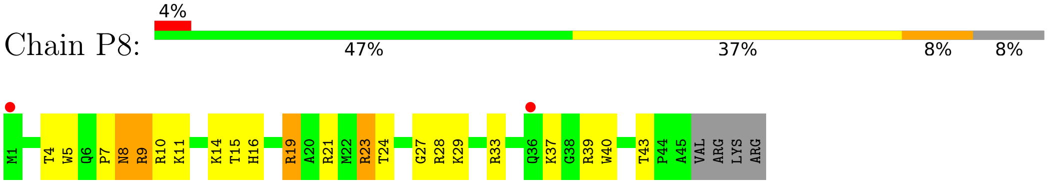
- Molecule 53: 50S ribosomal protein L33

Chain K5:



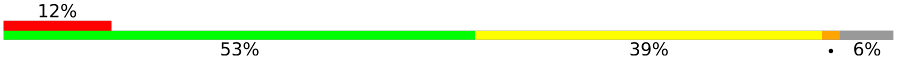
- Molecule 54: 50S ribosomal protein L34

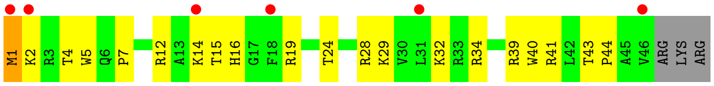
Chain P8:



- Molecule 54: 50S ribosomal protein L34

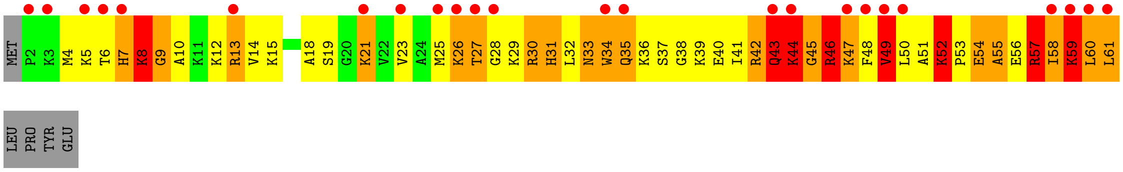
Chain L5:





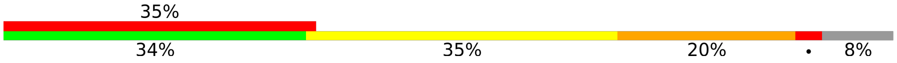
- Molecule 55: 50S ribosomal protein L35

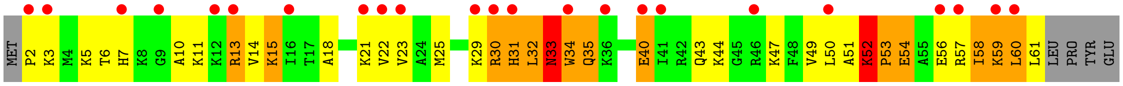
Chain Q8:



- Molecule 55: 50S ribosomal protein L35

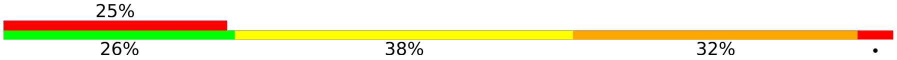
Chain M5:

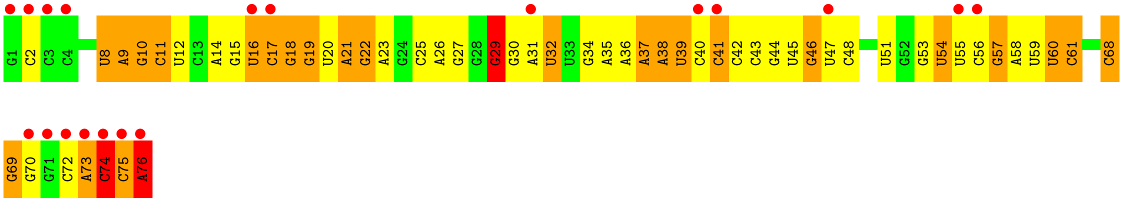




- Molecule 56: tRNA-Phe

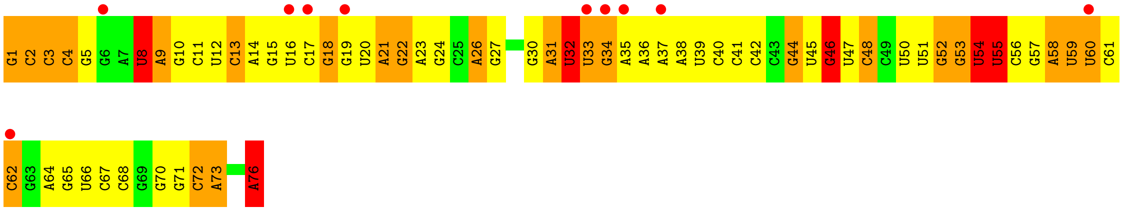
Chain 1L:





- Molecule 57: tRNA-Phe

Chain 3L:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.40Å 449.20Å 621.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	255.47 – 2.95 255.48 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (255.47-2.95) 94.1 (255.48-2.95)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.89 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.193 , 0.235 0.194 , 0.235	Depositor DCC
R_{free} test set	1999 reflections (0.16%)	wwPDB-VP
Wilson B-factor (Å^2)	78.0	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 77.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	300252	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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, 4SU, 5MU, PAR, PSU, ZN, MIA, 7MG, OMC

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	13	0.93	27/36052 (0.1%)	1.65	832/56266 (1.5%)
1	1G	0.76	3/36049 (0.0%)	1.45	463/56262 (0.8%)
2	12	0.40	0/1959	0.65	2/2642 (0.1%)
2	1E	0.46	0/1959	0.72	1/2642 (0.0%)
3	22	0.42	0/1636	0.65	1/2205 (0.0%)
3	2E	0.60	0/1629	0.76	0/2195
4	32	0.56	0/1732	0.76	0/2318
4	3E	0.75	2/1732 (0.1%)	0.83	1/2318 (0.0%)
5	42	0.50	0/1171	0.74	1/1576 (0.1%)
5	4E	0.65	0/1171	0.80	0/1576
6	52	0.61	0/855	0.77	1/1154 (0.1%)
6	5E	0.63	0/855	0.78	0/1154
7	62	0.49	0/1261	0.62	0/1689
7	6E	0.55	0/1275	0.68	0/1709
8	72	0.45	0/1135	0.64	0/1527
8	7E	0.62	0/1135	0.83	0/1527
9	82	0.47	0/1002	0.70	0/1346
9	8E	0.54	0/1028	0.75	1/1379 (0.1%)
10	1A	0.41	0/814	0.65	0/1095
10	1I	0.58	0/814	0.73	0/1095
11	2A	0.53	0/879	0.74	1/1187 (0.1%)
11	2I	0.61	0/879	0.80	1/1187 (0.1%)
12	3A	0.62	0/991	0.84	2/1327 (0.2%)
12	3I	0.82	0/991	1.02	3/1327 (0.2%)
13	4A	0.39	0/943	0.63	0/1265
13	4I	0.59	0/948	0.79	1/1272 (0.1%)
14	5A	0.42	0/484	0.69	0/643
14	5I	0.81	1/500 (0.2%)	0.83	0/664
15	6A	0.55	0/744	0.67	1/992 (0.1%)
15	6I	0.62	0/744	0.82	0/992
16	7A	0.59	0/721	0.73	0/970
16	7I	0.58	0/721	0.79	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
17	8A	0.60	1/847 (0.1%)	0.70	0/1131
17	8I	0.62	0/847	0.80	0/1131
18	9A	0.57	0/595	0.73	0/790
18	9I	0.61	0/595	0.87	1/790 (0.1%)
19	AA	0.40	0/638	0.64	0/860
19	AI	0.61	0/661	0.87	1/890 (0.1%)
20	BA	0.53	0/764	0.81	0/1007
20	BI	0.48	0/764	0.74	0/1007
21	1B	0.52	0/221	0.64	0/288
21	1F	0.57	0/221	0.81	0/288
22	1K	0.62	3/1673 (0.2%)	1.31	20/2606 (0.8%)
23	2K	1.06	5/1721 (0.3%)	1.71	46/2682 (1.7%)
23	2L	0.81	1/1721 (0.1%)	1.49	33/2682 (1.2%)
24	3K	0.64	1/1712 (0.1%)	1.32	18/2663 (0.7%)
25	4K	1.10	0/313	1.39	1/485 (0.2%)
25	4L	1.01	1/262 (0.4%)	1.64	6/403 (1.5%)
26	14	1.05	136/70167 (0.2%)	1.79	2340/109541 (2.1%)
26	1H	1.28	361/70233 (0.5%)	2.08	3902/109643 (3.6%)
27	16	1.03	6/2928 (0.2%)	1.88	107/4568 (2.3%)
27	1J	0.83	1/2928 (0.0%)	1.52	38/4568 (0.8%)
28	11	0.99	4/2165 (0.2%)	1.09	6/2919 (0.2%)
28	19	0.85	0/2170	1.02	5/2926 (0.2%)
29	21	0.79	0/1601	1.01	4/2160 (0.2%)
29	29	0.75	0/1601	1.02	6/2160 (0.3%)
30	31	0.90	1/1620 (0.1%)	1.05	6/2194 (0.3%)
30	39	0.71	1/1662 (0.1%)	0.96	3/2249 (0.1%)
31	41	0.65	0/1498	0.85	1/2016 (0.0%)
31	49	0.43	0/1498	0.68	0/2016
32	51	0.70	0/1362	0.92	2/1841 (0.1%)
32	59	0.43	0/1332	0.72	1/1802 (0.1%)
33	61	0.57	0/1151	0.83	3/1558 (0.2%)
33	69	0.54	0/1151	0.81	2/1558 (0.1%)
34	15	0.57	0/1131	0.77	0/1525
34	58	0.67	0/1131	0.89	2/1525 (0.1%)
35	25	0.71	0/942	0.88	2/1269 (0.2%)
35	68	0.79	0/942	0.88	1/1269 (0.1%)
36	35	0.76	0/1161	1.19	5/1544 (0.3%)
36	78	0.87	0/1161	1.12	3/1544 (0.2%)
37	45	0.74	1/1142 (0.1%)	0.99	2/1527 (0.1%)
37	88	0.97	3/1106 (0.3%)	1.20	5/1478 (0.3%)
38	55	0.78	0/973	1.02	2/1302 (0.2%)
38	98	0.70	0/981	0.99	1/1312 (0.1%)
39	65	0.61	0/891	0.94	2/1187 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	A8	0.76	0/891	1.01	3/1187 (0.3%)
40	75	0.67	0/1155	0.85	0/1542
40	B8	0.80	0/1155	0.96	2/1542 (0.1%)
41	85	0.66	0/981	0.82	0/1306
41	C8	0.84	1/981 (0.1%)	1.04	3/1306 (0.2%)
42	95	0.71	0/789	0.93	3/1057 (0.3%)
42	D8	0.75	0/789	0.94	1/1057 (0.1%)
43	A5	0.84	1/910 (0.1%)	0.91	0/1220
43	E8	0.78	0/910	0.97	2/1220 (0.2%)
44	B5	0.86	1/749 (0.1%)	0.88	0/1007
44	F8	1.00	1/756 (0.1%)	1.03	3/1014 (0.3%)
45	C5	0.74	0/807	0.97	2/1076 (0.2%)
45	G8	0.84	0/804	1.09	5/1073 (0.5%)
46	D5	0.47	0/1460	0.71	0/1982
46	H8	0.55	0/1427	0.86	3/1935 (0.2%)
47	E5	0.72	0/620	0.88	0/827
47	I8	0.88	0/634	0.97	1/847 (0.1%)
48	F5	0.77	0/744	1.03	2/989 (0.2%)
48	J8	0.87	0/769	0.98	3/1022 (0.3%)
49	G5	0.66	0/565	0.88	0/748
49	K8	1.00	2/565 (0.4%)	1.11	1/748 (0.1%)
50	H5	0.60	0/473	0.77	0/635
50	L8	0.72	0/457	0.99	2/613 (0.3%)
51	I5	0.47	0/492	0.80	0/663
51	M8	0.64	0/545	0.87	1/733 (0.1%)
52	J5	0.73	0/472	0.94	0/639
52	N8	0.74	0/467	0.98	1/632 (0.2%)
53	K5	0.74	0/396	0.98	1/529 (0.2%)
53	O8	0.82	1/396 (0.3%)	1.05	1/529 (0.2%)
54	L5	0.81	0/406	0.94	0/536
54	P8	1.07	0/399	1.26	5/526 (1.0%)
55	M5	1.07	2/483 (0.4%)	1.16	1/634 (0.2%)
55	Q8	1.43	2/486 (0.4%)	1.85	9/638 (1.4%)
56	1L	0.49	0/1717	1.05	5/2674 (0.2%)
57	3L	0.68	2/1698 (0.1%)	1.27	11/2646 (0.4%)
All	All	0.96	572/322340 (0.2%)	1.61	7960/482707 (1.6%)

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
2	1E	0	2
4	32	0	2
9	82	0	1
10	1A	0	1
11	2A	0	1
12	3I	0	1
13	4I	0	2
14	5A	0	1
19	AI	0	2
20	BA	0	2
20	BI	0	1
28	11	0	2
28	19	0	5
29	21	0	4
29	29	0	5
30	31	0	3
30	39	0	7
31	41	0	2
31	49	0	1
32	59	0	1
33	61	0	4
33	69	0	3
36	35	0	3
36	78	0	3
37	45	0	6
37	88	0	4
38	55	0	2
38	98	0	2
39	65	0	1
40	75	0	2
40	B8	0	2
41	85	0	2
41	C8	0	1
42	95	0	2
42	D8	0	1
43	A5	0	2
44	B5	0	1
45	C5	0	1
45	G8	0	3
46	D5	0	1
46	H8	0	3
47	I8	0	2
48	F5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
48	J8	0	2
49	G5	0	4
49	K8	0	2
51	I5	0	1
51	M8	0	2
52	N8	0	1
53	K5	0	4
53	O8	0	2
55	M5	0	3
55	Q8	0	8
All	All	0	127

The worst 5 of 572 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	2430	A	N9-C4	-14.70	1.29	1.37
26	14	783	A	N9-C4	-13.46	1.29	1.37
26	1H	774	A	N9-C4	-13.24	1.29	1.37
26	1H	676	A	N9-C4	-13.22	1.29	1.37
26	1H	783	A	N3-C4	-13.21	1.26	1.34

The worst 5 of 7960 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1H	783	A	C2-N3-C4	-29.75	95.72	110.60
26	1H	1899	G	N3-C4-N9	-29.71	108.17	126.00
26	1H	945	A	C6-C5-N7	-23.71	115.70	132.30
26	1H	676	A	C2-N3-C4	-23.41	98.89	110.60
26	1H	1899	G	N3-C4-C5	22.92	140.06	128.60

There are no chirality outliers.

5 of 127 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	237	ALA	Peptide
12	3I	87	GLY	Peptide
13	4I	105	THR	Peptide
13	4I	4	ILE	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	13	32207	0	16256	718	0
1	1G	32204	0	16255	829	0
2	12	1924	0	1975	99	0
2	1E	1924	0	1975	100	0
3	22	1612	0	1677	90	0
3	2E	1605	0	1668	52	0
4	32	1702	0	1763	86	0
4	3E	1702	0	1762	62	0
5	42	1155	0	1213	55	0
5	4E	1155	0	1213	53	0
6	52	842	0	857	31	0
6	5E	842	0	857	26	0
7	62	1243	0	1284	58	0
7	6E	1256	0	1296	42	0
8	72	1115	0	1177	41	0
8	7E	1115	0	1177	57	0
9	82	983	0	1006	61	0
9	8E	1009	0	1037	61	0
10	1A	801	0	849	45	0
10	1I	801	0	849	51	0
11	2A	864	0	881	32	0
11	2I	864	0	881	27	0
12	3A	975	0	1062	47	0
12	3I	975	0	1062	48	0
13	4A	933	0	992	64	0
13	4I	938	0	997	56	0
14	5A	475	0	511	29	0
14	5I	491	0	529	24	0
15	6A	733	0	771	33	0
15	6I	733	0	771	28	0
16	7A	705	0	725	29	0
16	7I	705	0	725	53	0
17	8A	834	0	904	22	0
17	8I	834	0	904	33	0
18	9A	590	0	662	18	0
18	9I	590	0	662	26	0
19	AA	624	0	636	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	647	0	665	53	0
20	BA	762	0	861	30	0
20	BI	762	0	861	48	0
21	1B	217	0	234	20	0
21	1F	217	0	234	8	0
22	1K	1627	0	836	35	0
23	2K	1646	0	845	27	0
23	2L	1646	0	845	32	0
24	3K	1603	0	824	57	0
25	4K	279	0	142	4	0
25	4L	235	0	121	14	0
26	14	62647	0	31578	1347	0
26	1H	62707	0	31600	1532	1
27	16	2617	0	1328	54	0
27	1J	2617	0	1328	106	0
28	11	2115	0	2195	85	0
28	19	2120	0	2197	88	0
29	21	1568	0	1634	89	0
29	29	1568	0	1634	92	0
30	31	1585	0	1632	93	0
30	39	1627	0	1680	104	0
31	41	1473	0	1535	80	0
31	49	1473	0	1535	62	0
32	51	1336	0	1418	71	0
32	59	1307	0	1382	63	0
33	61	1136	0	1223	54	0
33	69	1136	0	1223	54	0
34	15	1104	0	1180	53	0
34	58	1104	0	1180	54	0
35	25	932	0	996	48	0
35	68	932	0	996	35	0
36	35	1144	0	1228	101	0
36	78	1144	0	1228	98	0
37	45	1121	0	1179	74	0
37	88	1086	0	1129	64	0
38	55	959	0	1021	45	0
38	98	967	0	1033	53	0
39	65	881	0	943	70	0
39	A8	881	0	943	59	0
40	75	1141	0	1202	63	0
40	B8	1141	0	1202	70	0
41	85	963	0	1022	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	C8	963	0	1022	85	0
42	95	778	0	852	70	0
42	D8	778	0	852	34	0
43	A5	899	0	964	31	0
43	E8	899	0	964	33	0
44	B5	735	0	785	31	0
44	F8	742	0	803	42	0
45	C5	794	0	883	57	0
45	G8	791	0	882	59	0
46	D5	1428	0	1454	70	0
46	H8	1397	0	1430	84	0
47	E5	612	0	633	30	0
47	I8	626	0	642	26	0
48	F5	737	0	813	32	0
48	J8	762	0	848	37	0
49	G5	563	0	612	21	1
49	K8	563	0	612	36	0
50	H5	468	0	518	13	0
50	L8	452	0	503	21	0
51	I5	481	0	479	46	0
51	M8	533	0	526	43	0
52	J5	458	0	480	32	0
52	N8	453	0	475	28	0
53	K5	389	0	404	21	0
53	O8	389	0	404	28	0
54	L5	398	0	441	17	0
54	P8	391	0	432	17	0
55	M5	477	0	540	45	0
55	Q8	480	0	549	95	0
56	1L	1627	0	836	40	0
57	3L	1624	0	827	68	0
58	11	4	0	0	0	0
58	13	148	0	0	0	0
58	14	407	0	0	0	0
58	16	13	0	0	0	0
58	1G	96	0	0	0	0
58	1H	520	0	0	0	0
58	1J	5	0	0	0	0
58	1K	2	0	0	0	0
58	21	2	0	0	0	0
58	25	1	0	0	0	0
58	29	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2A	2	0	0	0	0
58	2I	1	0	0	0	0
58	2K	5	0	0	0	0
58	2L	3	0	0	0	0
58	3E	2	0	0	0	0
58	3K	1	0	0	0	0
58	3L	2	0	0	0	0
58	41	2	0	0	0	0
58	49	1	0	0	0	0
58	4K	1	0	0	0	0
58	55	1	0	0	0	0
58	5E	1	0	0	0	0
58	5I	2	0	0	0	0
58	78	1	0	0	0	0
58	7A	1	0	0	0	0
58	88	2	0	0	0	0
58	98	2	0	0	0	0
58	C5	1	0	0	0	0
58	G8	1	0	0	0	0
58	I8	1	0	0	0	0
58	J5	1	0	0	0	0
58	L8	1	0	0	0	0
58	P8	1	0	0	0	0
59	13	42	0	45	1	0
59	1G	42	0	45	2	0
60	32	1	0	0	0	0
60	3E	1	0	0	0	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	11	13	0	0	3	0
61	13	197	0	0	29	0
61	14	598	0	0	153	0
61	16	21	0	0	4	0
61	19	13	0	0	3	0
61	1G	82	0	0	18	0
61	1H	999	0	0	280	0
61	1I	2	0	0	1	0
61	1K	5	0	0	0	0
61	21	4	0	0	0	0
61	2K	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	31	4	0	0	0	0
61	35	1	0	0	0	0
61	39	7	0	0	1	0
61	3E	3	0	0	0	0
61	3I	1	0	0	0	0
61	3K	1	0	0	0	0
61	3L	6	0	0	1	0
61	4K	2	0	0	0	0
61	58	2	0	0	0	0
61	5I	2	0	0	1	0
61	6I	1	0	0	0	0
61	78	5	0	0	1	0
61	7A	1	0	0	0	0
61	7I	1	0	0	0	0
61	85	1	0	0	0	0
61	8E	2	0	0	0	0
61	A5	1	0	0	0	0
61	B8	1	0	0	0	0
61	BA	1	0	0	0	0
61	C8	3	0	0	0	0
61	D8	1	0	0	0	0
61	G5	1	0	0	0	0
61	G8	4	0	0	1	0
61	I8	7	0	0	0	0
61	L5	1	0	0	0	0
61	L8	1	0	0	1	0
61	P8	1	0	0	0	0
61	Q8	2	0	0	0	0
All	All	300252	0	200448	8632	1

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 18.

The worst 5 of 8632 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)
26:14:2701:C:H3’	26:14:2702:U:H5”	1.27	1.15
26:1H:2592:G:OP1	61:1H:4524:HOH:O	1.68	1.10
40:B8:50:ILE:HD11	40:B8:102:ILE:HD11	1.32	1.10
26:1H:1614:A:OP1	61:1H:3947:HOH:O	1.70	1.09
26:1H:945:A:OP1	61:1H:4167:HOH:O	1.70	1.09

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:277:C:O2’	49:G5:49:LYS:NZ[2_564]	2.14	0.06

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	
2	12	235/256 (92%)	192 (82%)	37 (16%)	6 (3%)	5	24
2	1E	235/256 (92%)	197 (84%)	37 (16%)	1 (0%)	34	69
3	22	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	29	64
3	2E	203/239 (85%)	184 (91%)	19 (9%)	0	100	100
4	32	206/209 (99%)	179 (87%)	25 (12%)	2 (1%)	15	48
4	3E	206/209 (99%)	192 (93%)	12 (6%)	2 (1%)	15	48
5	42	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	4E	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	56
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
7	62	148/156 (95%)	137 (93%)	11 (7%)	0	100	100
7	6E	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
8	72	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	10	38
8	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22	56
9	82	122/128 (95%)	113 (93%)	8 (7%)	1 (1%)	19	53
9	8E	125/128 (98%)	105 (84%)	19 (15%)	1 (1%)	19	53
10	1A	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	1I	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
11	2A	114/129 (88%)	102 (90%)	8 (7%)	4 (4%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2I	114/129 (88%)	99 (87%)	14 (12%)	1 (1%)	17	51
12	3A	123/132 (93%)	101 (82%)	18 (15%)	4 (3%)	4	18
12	3I	123/132 (93%)	103 (84%)	20 (16%)	0	100	100
13	4A	115/126 (91%)	96 (84%)	18 (16%)	1 (1%)	17	51
13	4I	116/126 (92%)	96 (83%)	19 (16%)	1 (1%)	17	51
14	5A	56/61 (92%)	46 (82%)	9 (16%)	1 (2%)	8	33
14	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	17
15	6A	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	6I	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	7A	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
16	7I	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
17	8A	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	8I	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
18	9A	70/88 (80%)	65 (93%)	5 (7%)	0	100	100
18	9I	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	11	39
19	AA	76/93 (82%)	59 (78%)	15 (20%)	2 (3%)	5	24
19	AI	79/93 (85%)	65 (82%)	11 (14%)	3 (4%)	3	15
20	BA	97/106 (92%)	84 (87%)	12 (12%)	1 (1%)	15	48
20	BI	97/106 (92%)	86 (89%)	10 (10%)	1 (1%)	15	48
21	1B	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	1F	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
28	11	270/276 (98%)	253 (94%)	12 (4%)	5 (2%)	8	32
28	19	271/276 (98%)	248 (92%)	16 (6%)	7 (3%)	5	24
29	21	203/206 (98%)	164 (81%)	30 (15%)	9 (4%)	2	12
29	29	203/206 (98%)	156 (77%)	35 (17%)	12 (6%)	1	7
30	31	200/210 (95%)	182 (91%)	15 (8%)	3 (2%)	10	38
30	39	206/210 (98%)	165 (80%)	34 (16%)	7 (3%)	3	17
31	41	179/182 (98%)	156 (87%)	21 (12%)	2 (1%)	14	46
31	49	179/182 (98%)	155 (87%)	22 (12%)	2 (1%)	14	46
32	51	172/180 (96%)	146 (85%)	18 (10%)	8 (5%)	2	11
32	59	168/180 (93%)	131 (78%)	30 (18%)	7 (4%)	3	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	61	144/148 (97%)	117 (81%)	23 (16%)	4 (3%)	5	22
33	69	144/148 (97%)	112 (78%)	29 (20%)	3 (2%)	7	29
34	15	136/140 (97%)	120 (88%)	15 (11%)	1 (1%)	22	56
34	58	136/140 (97%)	116 (85%)	16 (12%)	4 (3%)	4	21
35	25	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	9	34
35	68	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
36	35	148/150 (99%)	117 (79%)	27 (18%)	4 (3%)	5	23
36	78	148/150 (99%)	113 (76%)	29 (20%)	6 (4%)	3	13
37	45	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	22	56
37	88	134/141 (95%)	112 (84%)	15 (11%)	7 (5%)	2	9
38	55	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	9	34
38	98	116/118 (98%)	104 (90%)	10 (9%)	2 (2%)	9	34
39	65	109/112 (97%)	88 (81%)	18 (16%)	3 (3%)	5	22
39	A8	109/112 (97%)	91 (84%)	16 (15%)	2 (2%)	8	33
40	75	135/146 (92%)	115 (85%)	17 (13%)	3 (2%)	6	28
40	B8	135/146 (92%)	119 (88%)	15 (11%)	1 (1%)	22	56
41	85	115/118 (98%)	102 (89%)	12 (10%)	1 (1%)	17	51
41	C8	115/118 (98%)	104 (90%)	9 (8%)	2 (2%)	9	34
42	95	99/101 (98%)	77 (78%)	17 (17%)	5 (5%)	2	9
42	D8	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	48
43	A5	111/113 (98%)	102 (92%)	7 (6%)	2 (2%)	8	33
43	E8	111/113 (98%)	100 (90%)	11 (10%)	0	100	100
44	B5	92/96 (96%)	83 (90%)	5 (5%)	4 (4%)	2	12
44	F8	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	6	28
45	C5	102/110 (93%)	75 (74%)	21 (21%)	6 (6%)	1	7
45	G8	102/110 (93%)	80 (78%)	15 (15%)	7 (7%)	1	4
46	D5	177/206 (86%)	134 (76%)	33 (19%)	10 (6%)	2	8
46	H8	173/206 (84%)	142 (82%)	25 (14%)	6 (4%)	3	17
47	E5	75/85 (88%)	67 (89%)	6 (8%)	2 (3%)	5	23
47	I8	78/85 (92%)	68 (87%)	9 (12%)	1 (1%)	12	41
48	F5	92/98 (94%)	87 (95%)	4 (4%)	1 (1%)	14	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	J8	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	7	29
49	G5	65/72 (90%)	61 (94%)	2 (3%)	2 (3%)	4	19
49	K8	65/72 (90%)	58 (89%)	4 (6%)	3 (5%)	2	11
50	H5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	L8	55/60 (92%)	51 (93%)	3 (6%)	1 (2%)	8	33
51	I5	58/71 (82%)	29 (50%)	25 (43%)	4 (7%)	1	4
51	M8	64/71 (90%)	43 (67%)	18 (28%)	3 (5%)	2	11
52	J5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	8	33
52	N8	56/60 (93%)	48 (86%)	6 (11%)	2 (4%)	3	16
53	K5	43/54 (80%)	27 (63%)	14 (33%)	2 (5%)	2	11
53	O8	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	2	11
54	L5	44/49 (90%)	42 (96%)	2 (4%)	0	100	100
54	P8	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
55	M5	58/65 (89%)	49 (84%)	6 (10%)	3 (5%)	2	9
55	Q8	58/65 (89%)	30 (52%)	21 (36%)	7 (12%)	0	1
All	All	11318/12054 (94%)	9776 (86%)	1313 (12%)	229 (2%)	7	30

5 of 229 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	21	83	ASP
36	78	57	THR
41	C8	89	GLU
41	C8	90	VAL
45	G8	54	LYS

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	
2	12	205/220 (93%)	161 (78%)	44 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1E	205/220 (93%)	161 (78%)	44 (22%)	1	4
3	22	160/188 (85%)	128 (80%)	32 (20%)	1	5
3	2E	159/188 (85%)	128 (80%)	31 (20%)	1	6
4	32	180/181 (99%)	150 (83%)	30 (17%)	2	9
4	3E	180/181 (99%)	139 (77%)	41 (23%)	1	3
5	42	116/123 (94%)	90 (78%)	26 (22%)	1	3
5	4E	116/123 (94%)	94 (81%)	22 (19%)	1	6
6	52	90/90 (100%)	71 (79%)	19 (21%)	1	4
6	5E	90/90 (100%)	77 (86%)	13 (14%)	3	13
7	62	126/127 (99%)	106 (84%)	20 (16%)	2	10
7	6E	126/127 (99%)	101 (80%)	25 (20%)	1	6
8	72	119/119 (100%)	99 (83%)	20 (17%)	2	9
8	7E	119/119 (100%)	95 (80%)	24 (20%)	1	5
9	82	95/99 (96%)	79 (83%)	16 (17%)	2	9
9	8E	98/99 (99%)	73 (74%)	25 (26%)	0	2
10	1A	89/92 (97%)	70 (79%)	19 (21%)	1	4
10	1I	89/92 (97%)	72 (81%)	17 (19%)	1	6
11	2A	88/99 (89%)	72 (82%)	16 (18%)	1	7
11	2I	88/99 (89%)	72 (82%)	16 (18%)	1	7
12	3A	104/109 (95%)	81 (78%)	23 (22%)	1	3
12	3I	104/109 (95%)	89 (86%)	15 (14%)	3	13
13	4A	94/101 (93%)	70 (74%)	24 (26%)	0	2
13	4I	94/101 (93%)	73 (78%)	21 (22%)	1	3
14	5A	48/50 (96%)	40 (83%)	8 (17%)	2	9
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	2
15	6A	79/80 (99%)	66 (84%)	13 (16%)	2	9
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2	8
16	7A	72/74 (97%)	64 (89%)	8 (11%)	6	22
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	6
17	8A	95/97 (98%)	81 (85%)	14 (15%)	3	12
17	8I	95/97 (98%)	76 (80%)	19 (20%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	9A	63/77 (82%)	52 (82%)	11 (18%)	2	8
18	9I	63/77 (82%)	55 (87%)	8 (13%)	4	17
19	AA	67/80 (84%)	50 (75%)	17 (25%)	0	2
19	AI	70/80 (88%)	53 (76%)	17 (24%)	0	2
20	BA	76/82 (93%)	64 (84%)	12 (16%)	2	10
20	BI	76/82 (93%)	62 (82%)	14 (18%)	1	7
21	1B	20/22 (91%)	18 (90%)	2 (10%)	7	26
21	1F	20/22 (91%)	19 (95%)	1 (5%)	24	57
28	11	214/218 (98%)	173 (81%)	41 (19%)	1	6
28	19	214/218 (98%)	169 (79%)	45 (21%)	1	4
29	21	165/166 (99%)	124 (75%)	41 (25%)	0	2
29	29	165/166 (99%)	123 (74%)	42 (26%)	0	2
30	31	161/166 (97%)	128 (80%)	33 (20%)	1	5
30	39	165/166 (99%)	127 (77%)	38 (23%)	1	3
31	41	155/156 (99%)	120 (77%)	35 (23%)	1	3
31	49	155/156 (99%)	124 (80%)	31 (20%)	1	5
32	51	145/148 (98%)	108 (74%)	37 (26%)	0	2
32	59	142/148 (96%)	109 (77%)	33 (23%)	1	3
33	61	122/124 (98%)	88 (72%)	34 (28%)	0	1
33	69	122/124 (98%)	88 (72%)	34 (28%)	0	1
34	15	117/119 (98%)	91 (78%)	26 (22%)	1	3
34	58	117/119 (98%)	94 (80%)	23 (20%)	1	6
35	25	100/100 (100%)	79 (79%)	21 (21%)	1	4
35	68	100/100 (100%)	85 (85%)	15 (15%)	3	12
36	35	116/116 (100%)	84 (72%)	32 (28%)	0	1
36	78	116/116 (100%)	78 (67%)	38 (33%)	0	1
37	45	111/111 (100%)	86 (78%)	25 (22%)	1	3
37	88	104/111 (94%)	78 (75%)	26 (25%)	0	2
38	55	100/101 (99%)	79 (79%)	21 (21%)	1	4
38	98	101/101 (100%)	73 (72%)	28 (28%)	0	1
39	65	87/88 (99%)	64 (74%)	23 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	A8	87/88 (99%)	57 (66%)	30 (34%)	0	1
40	75	120/127 (94%)	87 (72%)	33 (28%)	0	1
40	B8	120/127 (94%)	82 (68%)	38 (32%)	0	1
41	85	93/94 (99%)	73 (78%)	20 (22%)	1	4
41	C8	93/94 (99%)	80 (86%)	13 (14%)	3	14
42	95	82/82 (100%)	58 (71%)	24 (29%)	0	1
42	D8	82/82 (100%)	68 (83%)	14 (17%)	2	8
43	A5	92/92 (100%)	71 (77%)	21 (23%)	1	3
43	E8	92/92 (100%)	68 (74%)	24 (26%)	0	2
44	B5	74/78 (95%)	58 (78%)	16 (22%)	1	4
44	F8	76/78 (97%)	60 (79%)	16 (21%)	1	4
45	C5	85/91 (93%)	63 (74%)	22 (26%)	0	2
45	G8	85/91 (93%)	62 (73%)	23 (27%)	0	1
46	D5	158/179 (88%)	123 (78%)	35 (22%)	1	3
46	H8	154/179 (86%)	121 (79%)	33 (21%)	1	4
47	E5	62/67 (92%)	53 (86%)	9 (14%)	3	13
47	I8	61/67 (91%)	48 (79%)	13 (21%)	1	4
48	F5	79/83 (95%)	62 (78%)	17 (22%)	1	4
48	J8	82/83 (99%)	65 (79%)	17 (21%)	1	4
49	G5	62/67 (92%)	44 (71%)	18 (29%)	0	1
49	K8	62/67 (92%)	37 (60%)	25 (40%)	0	0
50	H5	51/52 (98%)	37 (72%)	14 (28%)	0	1
50	L8	49/52 (94%)	35 (71%)	14 (29%)	0	1
51	I5	54/63 (86%)	44 (82%)	10 (18%)	1	7
51	M8	59/63 (94%)	42 (71%)	17 (29%)	0	1
52	J5	51/52 (98%)	39 (76%)	12 (24%)	1	3
52	N8	51/52 (98%)	39 (76%)	12 (24%)	1	3
53	K5	44/52 (85%)	36 (82%)	8 (18%)	1	7
53	O8	44/52 (85%)	29 (66%)	15 (34%)	0	1
54	L5	39/42 (93%)	33 (85%)	6 (15%)	2	11
54	P8	38/42 (90%)	32 (84%)	6 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	M5	49/55 (89%)	34 (69%)	15 (31%)	0 1
55	Q8	50/55 (91%)	32 (64%)	18 (36%)	0 1
All	All	9552/9998 (96%)	7454 (78%)	2098 (22%)	1 4

5 of 2098 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	85	5	LYS
43	A5	90	ARG
40	75	136	GLN
54	L5	14	LYS
40	B8	11	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
15	6A	53	HIS
34	15	128	HIS
33	69	104	GLN
37	45	89	ASN
41	C8	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1495/1522 (98%)	329 (22%)	34 (2%)
1	1G	1495/1522 (98%)	353 (23%)	37 (2%)
22	1K	74/76 (97%)	33 (44%)	3 (4%)
23	2K	76/77 (98%)	21 (27%)	2 (2%)
23	2L	76/77 (98%)	16 (21%)	1 (1%)
24	3K	72/76 (94%)	40 (55%)	6 (8%)
25	4K	12/30 (40%)	4 (33%)	0
25	4L	10/30 (33%)	3 (30%)	1 (10%)
26	14	2908/2917 (99%)	721 (24%)	52 (1%)
26	1H	2911/2917 (99%)	701 (24%)	51 (1%)
27	16	121/122 (99%)	27 (22%)	1 (0%)
27	1J	121/122 (99%)	35 (28%)	2 (1%)
56	1L	74/76 (97%)	34 (45%)	3 (4%)
57	3L	75/76 (98%)	37 (49%)	4 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9520/9640 (98%)	2354 (24%)	197 (2%)

5 of 2354 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	7	G
1	13	8	A
1	13	21	G

5 of 197 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	793	U
26	14	34	C
1	1G	992	U
1	1G	1346	A
26	14	503	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	PSU	1K	32	58,22	18,21,22	1.47	2 (11%)	22,30,33	1.72	4 (18%)
22	PSU	1K	55	22	18,21,22	1.39	2 (11%)	22,30,33	1.37	4 (18%)
23	4SU	2K	8	23	18,21,22	1.72	3 (16%)	26,30,33	3.12	5 (19%)
23	5MU	2K	55	58,23	19,22,23	3.98	5 (26%)	28,32,35	3.39	8 (28%)
23	PSU	2K	56	23	18,21,22	1.04	1 (5%)	22,30,33	2.02	4 (18%)
23	OMC	2L	33	23	19,22,23	1.82	3 (15%)	26,31,34	1.29	4 (15%)
22	5MU	1K	54	22	19,22,23	3.93	5 (26%)	28,32,35	3.19	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
57	7MG	3L	46	57	22,26,27	3.41	6 (27%)	29,39,42	2.82	12 (41%)
22	MIA	1K	37	22	24,31,32	2.49	4 (16%)	26,44,47	3.34	7 (26%)
22	4SU	1K	8	22	18,21,22	1.82	5 (27%)	26,30,33	2.15	5 (19%)
23	4SU	2L	8	23	18,21,22	1.97	5 (27%)	26,30,33	2.44	5 (19%)
57	PSU	3L	55	57	18,21,22	1.24	1 (5%)	22,30,33	1.46	4 (18%)
23	PSU	2L	56	23	18,21,22	1.43	2 (11%)	22,30,33	1.74	2 (9%)
24	MIA	3K	37	58,24	24,31,32	2.57	5 (20%)	26,44,47	2.48	8 (30%)
57	4SU	3L	8	57	18,21,22	2.05	5 (27%)	26,30,33	1.97	5 (19%)
24	PSU	3K	39	24	18,21,22	1.23	1 (5%)	22,30,33	1.47	3 (13%)
23	7MG	2L	47	23	22,26,27	3.24	5 (22%)	29,39,42	2.74	12 (41%)
56	PSU	1L	32	56	18,21,22	1.22	1 (5%)	22,30,33	1.73	5 (22%)
56	MIA	1L	37	56	24,31,32	2.41	4 (16%)	26,44,47	3.20	7 (26%)
56	PSU	1L	39	56	18,21,22	1.09	1 (5%)	22,30,33	1.46	3 (13%)
56	5MU	1L	54	56	19,22,23	4.04	5 (26%)	28,32,35	3.07	7 (25%)
24	PSU	3K	32	24	18,21,22	1.31	1 (5%)	22,30,33	1.72	4 (18%)
22	PSU	1K	39	22	18,21,22	1.16	1 (5%)	22,30,33	1.76	3 (13%)
23	OMC	2K	33	23	19,22,23	1.93	3 (15%)	26,31,34	1.14	2 (7%)
57	PSU	3L	32	57	18,21,22	1.28	2 (11%)	22,30,33	1.99	7 (31%)
23	5MU	2L	55	23	19,22,23	4.06	5 (26%)	28,32,35	3.41	11 (39%)
23	7MG	2K	47	23	22,26,27	3.10	6 (27%)	29,39,42	2.60	10 (34%)
57	5MU	3L	54	57	19,22,23	3.96	5 (26%)	28,32,35	3.03	11 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	1K	32	58,22	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	3/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	58,23	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
57	7MG	3L	46	57	-	0/7/37/38	0/3/3/3
22	MIA	1K	37	22	-	2/11/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	4SU	1K	8	22	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	2/7/25/26	0/2/2/2
57	PSU	3L	55	57	-	2/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
24	MIA	3K	37	58,24	-	6/11/33/34	0/3/3/3
57	4SU	3L	8	57	-	0/7/25/26	0/2/2/2
24	PSU	3K	39	24	-	4/7/25/26	0/2/2/2
23	7MG	2L	47	23	-	0/7/37/38	0/3/3/3
56	PSU	1L	32	56	-	1/7/25/26	0/2/2/2
56	MIA	1L	37	56	-	9/11/33/34	0/3/3/3
56	PSU	1L	39	56	-	0/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	0/7/25/26	0/2/2/2
24	PSU	3K	32	24	-	2/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
57	PSU	3L	32	57	-	1/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	3/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	2/7/37/38	0/3/3/3
57	5MU	3L	54	57	-	2/7/25/26	0/2/2/2

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	55	5MU	C2-N1	13.10	1.59	1.38
56	1L	54	5MU	C2-N1	13.08	1.59	1.38
23	2L	55	5MU	C2-N1	13.02	1.59	1.38
22	1K	54	5MU	C2-N1	12.17	1.58	1.38
57	3L	54	5MU	C2-N1	12.03	1.57	1.38

The worst 5 of 171 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1K	37	MIA	C11-S10-C2	11.81	111.09	102.27
22	1K	54	5MU	C5-C4-N3	11.34	124.99	115.31
23	2K	55	5MU	C5-C4-N3	11.22	124.89	115.31
56	1L	37	MIA	C11-S10-C2	11.02	110.49	102.27
56	1L	54	5MU	C5-C4-N3	10.39	124.18	115.31

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	3K	32	PSU	C2’-C1’-C5-C6
24	3K	37	MIA	C4’-C5’-O5’-P
24	3K	37	MIA	O4’-C4’-C5’-O5’
24	3K	37	MIA	C3’-C4’-C5’-O5’
24	3K	37	MIA	C5-C6-N6-C12

There are no ring outliers.

22 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	55	PSU	1	0
23	2K	8	4SU	1	0
23	2K	55	5MU	3	0
23	2K	56	PSU	2	0
23	2L	33	OMC	2	0
22	1K	54	5MU	1	0
57	3L	46	7MG	3	0
22	1K	8	4SU	1	0
23	2L	8	4SU	2	0
57	3L	55	PSU	2	0
23	2L	56	PSU	2	0
24	3K	37	MIA	2	0
57	3L	8	4SU	5	0
24	3K	39	PSU	2	0
23	2L	47	7MG	3	0
56	1L	37	MIA	1	0
56	1L	39	PSU	1	0
56	1L	54	5MU	2	0
57	3L	32	PSU	3	0
23	2L	55	5MU	2	0
23	2K	47	7MG	3	0
57	3L	54	5MU	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1246 ligands modelled in this entry, 1244 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	PAR	1G	1697	-	45,45,45	0.87	3 (6%)	64,67,67	1.64	15 (23%)
59	PAR	13	1749	-	45,45,45	0.71	1 (2%)	64,67,67	1.59	15 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PAR	1G	1697	-	-	5/18/94/94	0/4/4/4
59	PAR	13	1749	-	-	5/18/94/94	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1G	1697	PAR	C24-N24	-2.79	1.43	1.47
59	1G	1697	PAR	C34-C24	-2.37	1.50	1.53
59	1G	1697	PAR	C31-C21	-2.02	1.51	1.53
59	13	1749	PAR	C21-N21	-2.02	1.44	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	1G	1697	PAR	C13-O52-C52	-4.53	106.75	117.96
59	1G	1697	PAR	C14-O33-C33	-4.08	107.88	117.96
59	13	1749	PAR	C14-O54-C54	3.94	121.42	113.69
59	1G	1697	PAR	C34-C24-N24	-3.36	104.17	111.05
59	1G	1697	PAR	O11-C11-C21	-3.31	102.51	108.22

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	13	1749	PAR	C33-C43-C53-O53

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Mol	Chain	Res	Type	Atoms
59	13	1749	PAR	O43-C43-C53-O53
59	1G	1697	PAR	C44-C54-C64-N64
59	13	1749	PAR	O43-C13-O52-C52
59	1G	1697	PAR	O43-C43-C53-O53

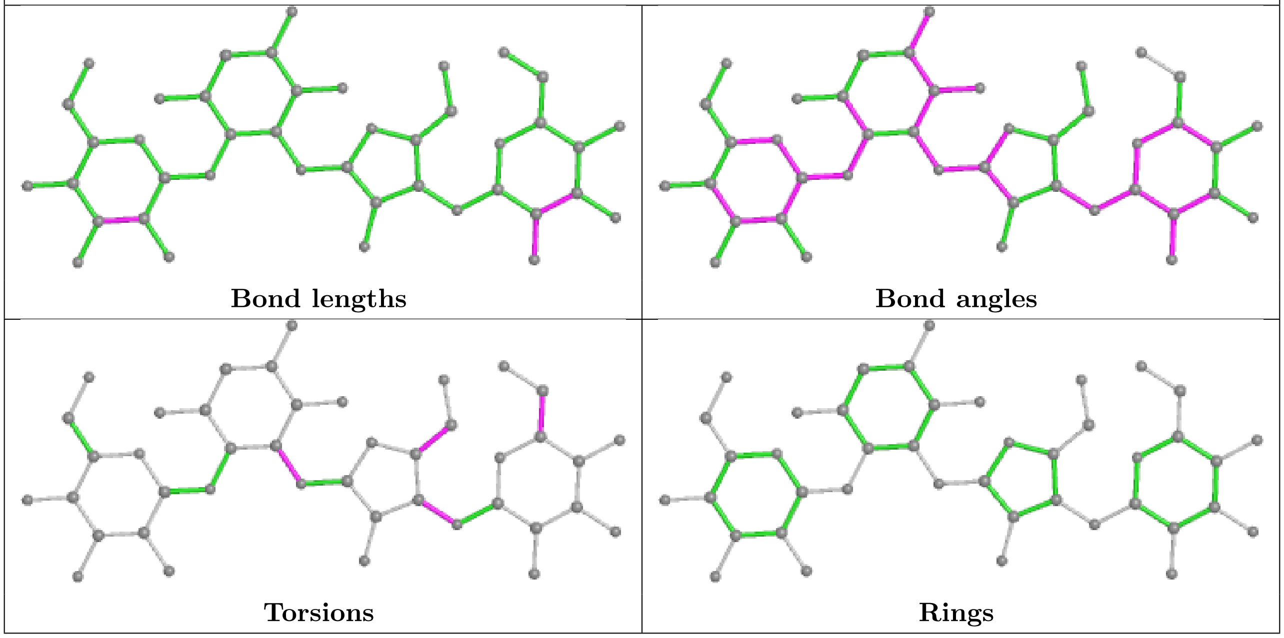
There are no ring outliers.

2 monomers are involved in 3 short contacts:

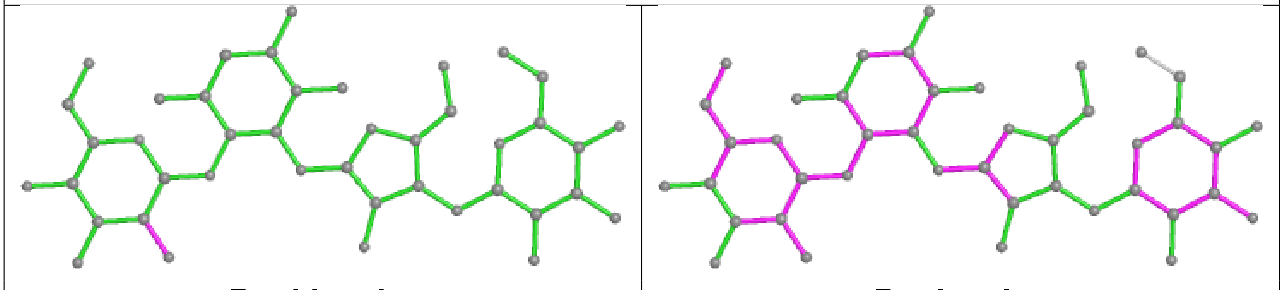
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1G	1697	PAR	2	0
59	13	1749	PAR	1	0

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

Ligand PAR 1G 1697

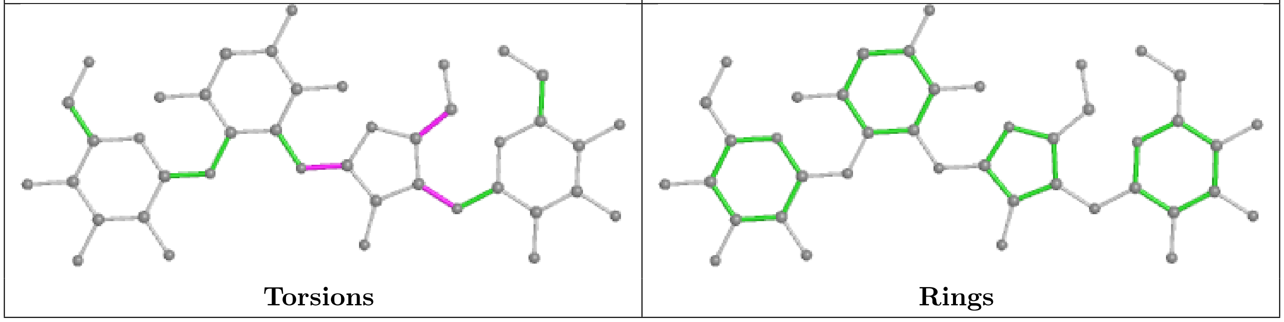


Ligand PAR 13 1749



Bond lengths

Bond angles



Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	13	1
1	1G	1
25	4L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	13	1530:G	O3'	1531:A	P	3.82
1	1G	1530:G	O3'	1531:A	P	3.28
1	4L	21:C	O3'	22:A	P	3.02

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	13	1498/1522 (98%)	0.27	14 (0%)	84	71	53, 93, 174, 276	0
1	1G	1498/1522 (98%)	0.40	67 (4%)	33	21	69, 116, 188, 285	0
2	12	237/256 (92%)	0.39	20 (8%)	11	6	141, 173, 195, 205	0
2	1E	237/256 (92%)	0.49	19 (8%)	12	7	105, 141, 169, 176	0
3	22	206/239 (86%)	1.37	63 (30%)	0	0	136, 162, 182, 190	0
3	2E	205/239 (85%)	0.72	19 (9%)	8	5	82, 102, 138, 147	0
4	32	208/209 (99%)	1.28	49 (23%)	0	0	93, 114, 138, 145	0
4	3E	208/209 (99%)	0.84	35 (16%)	1	1	75, 100, 123, 134	0
5	42	151/162 (93%)	1.85	61 (40%)	0	0	111, 135, 154, 184	0
5	4E	151/162 (93%)	1.15	35 (23%)	0	0	72, 93, 117, 160	0
6	52	101/101 (100%)	0.01	0	100	100	82, 100, 119, 142	0
6	5E	101/101 (100%)	0.33	2 (1%)	65	48	77, 96, 118, 141	0
7	62	152/156 (97%)	0.65	19 (12%)	3	2	112, 127, 147, 160	0
7	6E	155/156 (99%)	0.63	18 (11%)	4	2	92, 111, 146, 163	0
8	72	138/138 (100%)	2.12	60 (43%)	0	0	102, 132, 151, 155	0
8	7E	138/138 (100%)	1.25	35 (25%)	0	0	84, 101, 113, 121	0
9	82	124/128 (96%)	2.50	63 (50%)	0	0	115, 150, 165, 171	0
9	8E	127/128 (99%)	0.85	25 (19%)	1	0	80, 127, 148, 158	0
10	1A	99/105 (94%)	2.50	40 (40%)	0	0	131, 155, 176, 184	0
10	1I	99/105 (94%)	1.36	32 (32%)	0	0	73, 125, 159, 162	0
11	2A	116/129 (89%)	0.89	15 (12%)	3	2	85, 108, 130, 159	0
11	2I	116/129 (89%)	0.53	11 (9%)	8	5	69, 100, 127, 165	0
12	3A	125/132 (94%)	1.21	33 (26%)	0	0	83, 106, 134, 167	0
12	3I	125/132 (94%)	0.88	19 (15%)	2	1	60, 71, 107, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	117/126 (92%)	2.11	52 (44%) 0 0	118, 155, 179, 185	0
13	4I	118/126 (93%)	0.75	19 (16%) 1 1	74, 112, 132, 145	0
14	5A	58/61 (95%)	6.47	53 (91%) 0 0	134, 159, 174, 179	0
14	5I	60/61 (98%)	2.20	33 (55%) 0 0	80, 91, 106, 119	0
15	6A	88/89 (98%)	0.60	11 (12%) 3 2	87, 112, 127, 133	0
15	6I	88/89 (98%)	0.65	10 (11%) 5 3	69, 98, 116, 126	0
16	7A	84/88 (95%)	1.85	34 (40%) 0 0	87, 103, 126, 159	0
16	7I	84/88 (95%)	2.10	42 (50%) 0 0	93, 107, 141, 158	0
17	8A	100/105 (95%)	1.74	41 (41%) 0 0	93, 110, 128, 148	0
17	8I	100/105 (95%)	1.09	22 (22%) 0 0	83, 101, 113, 116	0
18	9A	72/88 (81%)	0.44	5 (6%) 16 10	92, 115, 144, 170	0
18	9I	72/88 (81%)	0.28	0 100 100	83, 100, 136, 168	0
19	AA	78/93 (83%)	1.81	29 (37%) 0 0	150, 182, 192, 196	0
19	AI	81/93 (87%)	0.56	9 (11%) 5 3	88, 113, 138, 146	0
20	BA	99/106 (93%)	1.65	42 (42%) 0 0	85, 111, 137, 149	0
20	BI	99/106 (93%)	0.96	18 (18%) 1 1	102, 117, 153, 161	0
21	1B	25/27 (92%)	5.51	22 (88%) 0 0	119, 140, 152, 167	0
21	1F	25/27 (92%)	2.57	15 (60%) 0 0	88, 97, 113, 142	0
22	1K	70/76 (92%)	0.76	11 (15%) 2 1	76, 203, 246, 250	0
23	2K	72/77 (93%)	0.16	2 (2%) 53 36	68, 91, 119, 138	0
23	2L	72/77 (93%)	-0.08	2 (2%) 53 36	80, 113, 149, 166	0
24	3K	72/76 (94%)	0.31	4 (5%) 24 15	71, 230, 258, 260	0
25	4K	13/30 (43%)	0.91	2 (15%) 2 1	64, 80, 130, 131	0
25	4L	11/30 (36%)	1.08	1 (9%) 9 5	93, 124, 136, 143	0
26	14	2909/2917 (99%)	0.35	53 (1%) 68 51	50, 84, 241, 338	0
26	1H	2912/2917 (99%)	0.38	28 (0%) 82 68	37, 70, 222, 303	0
27	16	122/122 (100%)	-0.03	0 100 100	63, 87, 110, 193	0
27	1J	122/122 (100%)	-0.16	2 (1%) 72 55	86, 120, 149, 192	0
28	11	272/276 (98%)	0.62	11 (4%) 38 25	38, 62, 78, 83	0
28	19	273/276 (98%)	1.21	53 (19%) 1 0	46, 71, 87, 97	0
29	21	205/206 (99%)	1.00	24 (11%) 4 2	50, 88, 129, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
29	29	205/206 (99%)	1.26	45 (21%)	0	0	61, 93, 141, 174	0
30	31	202/210 (96%)	0.47	6 (2%)	50	34	43, 73, 113, 131	0
30	39	208/210 (99%)	0.64	24 (11%)	4	3	56, 103, 167, 189	0
31	41	181/182 (99%)	0.71	21 (11%)	4	2	78, 98, 131, 148	0
31	49	181/182 (99%)	1.35	54 (29%)	0	0	120, 142, 168, 178	0
32	51	174/180 (96%)	0.54	8 (4%)	32	20	77, 102, 120, 135	0
32	59	170/180 (94%)	3.51	109 (64%)	0	0	142, 193, 215, 227	0
33	61	146/148 (98%)	0.41	8 (5%)	25	15	71, 129, 146, 151	0
33	69	146/148 (98%)	0.77	22 (15%)	2	1	81, 122, 150, 157	0
34	15	138/140 (98%)	1.44	40 (28%)	0	0	77, 106, 136, 163	0
34	58	138/140 (98%)	0.73	11 (7%)	12	7	62, 89, 128, 145	0
35	25	122/122 (100%)	0.72	9 (7%)	14	8	66, 87, 103, 109	0
35	68	122/122 (100%)	0.53	3 (2%)	57	40	57, 72, 89, 100	0
36	35	150/150 (100%)	1.45	41 (27%)	0	0	58, 106, 138, 169	0
36	78	150/150 (100%)	0.71	13 (8%)	10	6	43, 77, 104, 157	0
37	45	141/141 (100%)	2.47	69 (48%)	0	0	75, 107, 136, 152	0
37	88	138/141 (97%)	0.73	7 (5%)	28	17	50, 76, 98, 128	0
38	55	117/118 (99%)	0.82	13 (11%)	5	3	59, 76, 91, 110	0
38	98	118/118 (100%)	0.99	16 (13%)	3	1	61, 81, 102, 110	0
39	65	111/112 (99%)	1.46	39 (35%)	0	0	91, 114, 131, 139	0
39	A8	111/112 (99%)	1.00	19 (17%)	1	1	73, 84, 108, 123	0
40	75	137/146 (93%)	0.84	20 (14%)	2	1	78, 95, 150, 184	0
40	B8	137/146 (93%)	0.59	9 (6%)	18	10	69, 89, 145, 175	0
41	85	117/118 (99%)	0.92	23 (19%)	1	0	66, 94, 138, 155	0
41	C8	117/118 (99%)	0.93	18 (15%)	2	1	52, 79, 111, 129	0
42	95	101/101 (100%)	0.95	22 (21%)	0	0	66, 124, 140, 157	0
42	D8	101/101 (100%)	0.72	12 (11%)	4	2	54, 103, 129, 140	0
43	A5	113/113 (100%)	1.12	14 (12%)	4	2	60, 72, 105, 150	0
43	E8	113/113 (100%)	0.88	10 (8%)	10	5	56, 72, 105, 146	0
44	B5	94/96 (97%)	1.07	11 (11%)	4	2	68, 83, 109, 120	0
44	F8	94/96 (97%)	0.49	3 (3%)	47	31	55, 69, 90, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
45	C5	104/110 (94%)	1.55	28 (26%) 0 0	92, 115, 146, 153	0
45	G8	104/110 (94%)	0.46	3 (2%) 51 35	70, 90, 131, 142	0
46	D5	179/206 (86%)	1.27	44 (24%) 0 0	113, 151, 230, 237	0
46	H8	175/206 (84%)	0.30	4 (2%) 60 43	80, 119, 203, 216	0
47	E5	77/85 (90%)	2.07	36 (46%) 0 0	67, 88, 106, 145	0
47	I8	80/85 (94%)	1.11	13 (16%) 1 1	54, 67, 101, 108	0
48	F5	94/98 (95%)	1.74	39 (41%) 0 0	60, 79, 122, 132	0
48	J8	97/98 (98%)	1.39	21 (21%) 0 0	50, 69, 122, 149	0
49	G5	67/72 (93%)	0.69	7 (10%) 6 4	80, 100, 121, 144	0
49	K8	67/72 (93%)	0.68	2 (2%) 50 34	61, 77, 95, 125	0
50	H5	59/60 (98%)	1.48	17 (28%) 0 0	77, 100, 140, 153	0
50	L8	57/60 (95%)	0.53	1 (1%) 68 51	57, 78, 102, 109	0
51	I5	60/71 (84%)	1.03	12 (20%) 1 0	151, 187, 203, 206	0
51	M8	66/71 (92%)	0.88	13 (19%) 1 0	104, 144, 179, 189	0
52	J5	59/60 (98%)	1.06	7 (11%) 4 2	57, 81, 150, 183	0
52	N8	58/60 (96%)	1.28	8 (13%) 2 1	48, 97, 160, 163	0
53	K5	45/54 (83%)	7.57	42 (93%) 0 0	123, 152, 165, 172	0
53	O8	45/54 (83%)	4.33	37 (82%) 0 0	107, 137, 157, 161	0
54	L5	46/49 (93%)	1.25	6 (13%) 3 2	45, 58, 72, 85	0
54	P8	45/49 (91%)	0.69	2 (4%) 34 21	40, 48, 61, 75	0
55	M5	60/65 (92%)	1.93	23 (38%) 0 0	71, 79, 100, 124	0
55	Q8	60/65 (92%)	1.99	24 (40%) 0 0	56, 72, 98, 109	0
56	1L	72/76 (94%)	1.69	19 (26%) 0 0	122, 239, 257, 262	0
57	3L	71/76 (93%)	0.72	10 (14%) 2 1	82, 208, 243, 253	0
All	All	21028/21694 (96%)	0.79	2541 (12%) 4 2	37, 97, 186, 338	0

The worst 5 of 2541 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	59	100	GLY	23.3
32	59	4	ILE	21.1
53	K5	13	CYS	18.8
53	K5	50	ARG	17.1
53	K5	42	TRP	16.4

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

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
22	PSU	1K	55	20/21	0.76	0.16	112,129,148,149	0
56	5MU	1L	54	21/22	0.77	0.27	134,151,174,175	0
57	5MU	3L	54	21/22	0.78	0.18	115,149,174,177	0
57	PSU	3L	55	20/21	0.78	0.15	121,143,168,174	0
56	PSU	1L	32	20/21	0.80	0.32	124,129,142,152	0
57	4SU	3L	8	20/21	0.80	0.09	153,160,176,185	0
57	7MG	3L	46	24/25	0.83	0.10	147,158,169,181	0
24	MIA	3K	37	29/30	0.84	0.28	103,119,131,151	0
57	PSU	3L	32	20/21	0.86	0.18	119,134,142,142	0
56	PSU	1L	39	20/21	0.89	0.27	110,121,135,138	0
22	4SU	1K	8	20/21	0.89	0.10	129,144,162,164	0
23	PSU	2L	56	20/21	0.91	0.10	96,107,114,116	0
56	MIA	1L	37	29/30	0.91	0.35	102,116,122,128	0
23	5MU	2L	55	21/22	0.92	0.13	101,107,114,117	0
24	PSU	3K	39	20/21	0.93	0.14	113,120,126,127	0
24	PSU	3K	32	20/21	0.93	0.18	108,124,131,143	0
23	4SU	2L	8	20/21	0.93	0.11	94,105,113,115	0
23	PSU	2K	56	20/21	0.93	0.13	84,91,100,103	0
22	PSU	1K	32	20/21	0.94	0.23	89,96,103,114	0
22	5MU	1K	54	21/22	0.94	0.13	106,112,129,132	0
22	MIA	1K	37	29/30	0.95	0.25	70,75,87,93	0
22	PSU	1K	39	20/21	0.95	0.17	72,86,90,90	0
23	7MG	2K	47	24/25	0.95	0.14	82,93,103,108	0
23	4SU	2K	8	20/21	0.96	0.17	75,84,93,98	0
23	7MG	2L	47	24/25	0.96	0.10	107,115,120,123	0
23	5MU	2K	55	21/22	0.96	0.12	81,93,97,102	0
23	OMC	2L	33	21/22	0.97	0.21	87,93,96,103	0
23	OMC	2K	33	21/22	0.98	0.25	65,68,74,78	0

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
58	MG	1H	3491	1/1	0.32	0.13	105,105,105,105	0
60	ZN	G8	202	1/1	0.39	0.17	164,164,164,164	0
58	MG	1G	1607	1/1	0.46	0.26	85,85,85,85	0
58	MG	1G	1661	1/1	0.47	0.17	99,99,99,99	0
58	MG	1H	3292	1/1	0.47	0.38	84,84,84,84	0
58	MG	14	3266	1/1	0.51	0.26	84,84,84,84	0
58	MG	3K	101	1/1	0.52	0.23	80,80,80,80	0
58	MG	1H	3302	1/1	0.53	0.18	77,77,77,77	0
58	MG	14	3143	1/1	0.55	0.45	85,85,85,85	0
58	MG	14	3178	1/1	0.55	0.25	88,88,88,88	0
58	MG	14	3193	1/1	0.55	0.41	89,89,89,89	0
58	MG	1H	3334	1/1	0.55	0.46	95,95,95,95	0
58	MG	1H	3500	1/1	0.55	0.12	54,54,54,54	0
58	MG	14	3039	1/1	0.56	0.18	74,74,74,74	0
58	MG	29	304	1/1	0.56	0.28	95,95,95,95	0
58	MG	1H	3310	1/1	0.56	0.46	105,105,105,105	0
58	MG	14	3269	1/1	0.58	0.27	77,77,77,77	0
58	MG	1H	3214	1/1	0.58	0.26	67,67,67,67	0
58	MG	1H	3012	1/1	0.58	0.38	78,78,78,78	0
58	MG	1H	3392	1/1	0.59	0.09	94,94,94,94	0
58	MG	14	3035	1/1	0.59	0.21	72,72,72,72	0
60	ZN	C5	202	1/1	0.59	0.19	181,181,181,181	0
58	MG	1H	3045	1/1	0.60	0.29	72,72,72,72	0
58	MG	1H	3475	1/1	0.61	0.16	109,109,109,109	0
58	MG	1H	3027	1/1	0.62	0.24	76,76,76,76	0
58	MG	1H	3047	1/1	0.63	0.34	76,76,76,76	0
58	MG	1H	3262	1/1	0.64	0.43	96,96,96,96	0
58	MG	1H	3273	1/1	0.64	0.19	84,84,84,84	0
58	MG	1H	3025	1/1	0.65	0.30	90,90,90,90	0
58	MG	14	3272	1/1	0.66	0.21	85,85,85,85	0
58	MG	13	1666	1/1	0.66	0.32	82,82,82,82	0
58	MG	1H	3051	1/1	0.67	0.24	97,97,97,97	0
58	MG	1H	3314	1/1	0.67	0.34	84,84,84,84	0
58	MG	13	1622	1/1	0.67	0.30	66,66,66,66	0
58	MG	14	3298	1/1	0.67	0.13	93,93,93,93	0
58	MG	14	3337	1/1	0.67	0.10	73,73,73,73	0
58	MG	13	1684	1/1	0.67	0.33	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3185	1/1	0.67	0.18	81,81,81,81	0
58	MG	1H	3403	1/1	0.67	0.11	72,72,72,72	0
58	MG	1H	3205	1/1	0.68	0.18	68,68,68,68	0
58	MG	13	1710	1/1	0.68	0.43	148,148,148,148	0
58	MG	13	1664	1/1	0.68	0.16	74,74,74,74	0
58	MG	14	3049	1/1	0.69	0.22	86,86,86,86	0
58	MG	1H	3249	1/1	0.69	0.33	76,76,76,76	0
58	MG	14	3285	1/1	0.69	0.39	104,104,104,104	0
58	MG	1H	3019	1/1	0.69	0.25	85,85,85,85	0
58	MG	1H	3337	1/1	0.69	0.43	86,86,86,86	0
58	MG	1H	3248	1/1	0.69	0.36	75,75,75,75	0
58	MG	14	3265	1/1	0.69	0.21	90,90,90,90	0
58	MG	14	3048	1/1	0.69	0.23	76,76,76,76	0
58	MG	14	3186	1/1	0.70	0.22	85,85,85,85	0
58	MG	14	3029	1/1	0.70	0.15	87,87,87,87	0
58	MG	14	3077	1/1	0.70	0.14	77,77,77,77	0
58	MG	1H	3081	1/1	0.70	0.33	90,90,90,90	0
58	MG	1H	3345	1/1	0.70	0.26	81,81,81,81	0
58	MG	5I	101	1/1	0.70	0.21	81,81,81,81	0
58	MG	13	1665	1/1	0.71	0.25	88,88,88,88	0
58	MG	1H	3499	1/1	0.71	0.08	105,105,105,105	0
58	MG	1H	3454	1/1	0.72	0.23	67,67,67,67	0
58	MG	1G	1660	1/1	0.72	0.30	98,98,98,98	0
58	MG	1H	3161	1/1	0.72	0.13	89,89,89,89	0
58	MG	14	3010	1/1	0.72	0.23	78,78,78,78	0
58	MG	1H	3056	1/1	0.72	0.54	97,97,97,97	0
58	MG	13	1608	1/1	0.72	0.26	85,85,85,85	0
58	MG	14	3406	1/1	0.72	0.30	112,112,112,112	0
58	MG	1H	3092	1/1	0.72	0.31	57,57,57,57	0
58	MG	14	3255	1/1	0.72	0.32	92,92,92,92	0
58	MG	1H	3513	1/1	0.72	0.21	82,82,82,82	0
58	MG	1H	3275	1/1	0.73	0.35	82,82,82,82	0
58	MG	14	3289	1/1	0.73	0.16	78,78,78,78	0
58	MG	14	3158	1/1	0.73	0.45	95,95,95,95	0
58	MG	14	3160	1/1	0.73	0.14	82,82,82,82	0
58	MG	14	3361	1/1	0.73	0.05	76,76,76,76	0
58	MG	1H	3282	1/1	0.73	0.27	98,98,98,98	0
58	MG	1H	3218	1/1	0.73	0.28	55,55,55,55	0
58	MG	1H	3293	1/1	0.73	0.23	67,67,67,67	0
58	MG	14	3276	1/1	0.73	0.31	80,80,80,80	0
58	MG	13	1704	1/1	0.74	0.32	102,102,102,102	0
58	MG	1H	3254	1/1	0.74	0.43	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1694	1/1	0.74	0.23	78,78,78,78	0
58	MG	14	3038	1/1	0.74	0.35	86,86,86,86	0
58	MG	1H	3269	1/1	0.74	0.29	72,72,72,72	0
58	MG	1H	3247	1/1	0.74	0.54	92,92,92,92	0
58	MG	1G	1635	1/1	0.74	0.33	92,92,92,92	0
58	MG	1H	3208	1/1	0.74	0.22	70,70,70,70	0
58	MG	1H	3326	1/1	0.74	0.19	90,90,90,90	0
58	MG	7A	101	1/1	0.74	0.32	90,90,90,90	0
58	MG	1H	3267	1/1	0.75	0.17	71,71,71,71	0
58	MG	1H	3519	1/1	0.75	0.11	101,101,101,101	0
58	MG	16	203	1/1	0.75	0.22	81,81,81,81	0
58	MG	14	3045	1/1	0.75	0.27	70,70,70,70	0
58	MG	14	3381	1/1	0.75	0.09	91,91,91,91	0
58	MG	14	3271	1/1	0.75	0.19	86,86,86,86	0
58	MG	1J	204	1/1	0.75	0.30	94,94,94,94	0
58	MG	1H	3469	1/1	0.75	0.10	99,99,99,99	0
58	MG	14	3019	1/1	0.75	0.33	84,84,84,84	0
58	MG	1H	3024	1/1	0.75	0.30	77,77,77,77	0
58	MG	14	3051	1/1	0.76	0.33	102,102,102,102	0
58	MG	14	3293	1/1	0.76	0.34	94,94,94,94	0
58	MG	14	3211	1/1	0.76	0.15	81,81,81,81	0
58	MG	1H	3303	1/1	0.76	0.21	76,76,76,76	0
58	MG	1H	3258	1/1	0.76	0.23	64,64,64,64	0
58	MG	14	3144	1/1	0.76	0.34	81,81,81,81	0
58	MG	98	202	1/1	0.76	0.31	95,95,95,95	0
58	MG	1H	3180	1/1	0.76	0.32	77,77,77,77	0
58	MG	14	3015	1/1	0.76	0.21	80,80,80,80	0
58	MG	1H	3271	1/1	0.76	0.37	80,80,80,80	0
58	MG	14	3020	1/1	0.76	0.15	75,75,75,75	0
58	MG	14	3254	1/1	0.77	0.18	92,92,92,92	0
58	MG	1H	3137	1/1	0.77	0.31	71,71,71,71	0
58	MG	1H	3257	1/1	0.77	0.19	69,69,69,69	0
58	MG	1H	3281	1/1	0.77	0.39	98,98,98,98	0
58	MG	1H	3157	1/1	0.77	0.26	84,84,84,84	0
58	MG	14	3392	1/1	0.77	0.23	77,77,77,77	0
58	MG	14	3397	1/1	0.77	0.10	52,52,52,52	0
58	MG	1H	3290	1/1	0.77	0.24	84,84,84,84	0
58	MG	13	1609	1/1	0.77	0.16	81,81,81,81	0
58	MG	1H	3049	1/1	0.77	0.32	69,69,69,69	0
58	MG	1H	3198	1/1	0.77	0.22	70,70,70,70	0
58	MG	1H	3010	1/1	0.77	0.40	87,87,87,87	0
58	MG	11	304	1/1	0.78	0.26	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3220	1/1	0.78	0.17	74,74,74,74	0
58	MG	1H	3177	1/1	0.78	0.39	86,86,86,86	0
58	MG	1H	3021	1/1	0.78	0.34	68,68,68,68	0
58	MG	1H	3196	1/1	0.78	0.38	102,102,102,102	0
58	MG	1H	3484	1/1	0.78	0.12	73,73,73,73	0
58	MG	1H	3316	1/1	0.78	0.28	81,81,81,81	0
58	MG	3L	101	1/1	0.78	0.25	99,99,99,99	0
58	MG	13	1745	1/1	0.78	0.14	107,107,107,107	0
58	MG	13	1708	1/1	0.78	0.29	90,90,90,90	0
58	MG	1H	3020	1/1	0.78	0.49	90,90,90,90	0
58	MG	1H	3052	1/1	0.78	0.33	83,83,83,83	0
58	MG	1H	3054	1/1	0.78	0.32	92,92,92,92	0
58	MG	1H	3389	1/1	0.79	0.07	74,74,74,74	0
58	MG	3L	102	1/1	0.79	0.11	151,151,151,151	0
58	MG	1H	3321	1/1	0.79	0.25	72,72,72,72	0
58	MG	1H	3162	1/1	0.79	0.43	89,89,89,89	0
58	MG	1H	3426	1/1	0.79	0.12	88,88,88,88	0
58	MG	14	3082	1/1	0.79	0.23	63,63,63,63	0
58	MG	14	3372	1/1	0.79	0.11	76,76,76,76	0
58	MG	14	3379	1/1	0.79	0.07	106,106,106,106	0
58	MG	14	3263	1/1	0.79	0.29	76,76,76,76	0
58	MG	13	1675	1/1	0.79	0.14	78,78,78,78	0
58	MG	1H	3035	1/1	0.79	0.37	89,89,89,89	0
58	MG	14	3268	1/1	0.79	0.14	87,87,87,87	0
58	MG	1G	1675	1/1	0.79	0.18	90,90,90,90	0
58	MG	1G	1688	1/1	0.79	0.10	102,102,102,102	0
58	MG	14	3166	1/1	0.79	0.35	81,81,81,81	0
58	MG	1H	3287	1/1	0.79	0.34	77,77,77,77	0
58	MG	1G	1601	1/1	0.80	0.29	90,90,90,90	0
58	MG	1H	3259	1/1	0.80	0.33	82,82,82,82	0
58	MG	1H	3283	1/1	0.80	0.24	73,73,73,73	0
58	MG	1H	3240	1/1	0.80	0.18	77,77,77,77	0
58	MG	1H	3133	1/1	0.80	0.23	53,53,53,53	0
58	MG	1H	3331	1/1	0.80	0.15	67,67,67,67	0
58	MG	1H	3184	1/1	0.80	0.33	78,78,78,78	0
58	MG	1H	3195	1/1	0.80	0.38	81,81,81,81	0
58	MG	1H	3295	1/1	0.80	0.40	87,87,87,87	0
58	MG	14	3389	1/1	0.80	0.13	75,75,75,75	0
58	MG	1H	3301	1/1	0.80	0.31	59,59,59,59	0
58	MG	14	3116	1/1	0.80	0.26	80,80,80,80	0
58	MG	13	1615	1/1	0.80	0.34	84,84,84,84	0
58	MG	13	1699	1/1	0.80	0.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	41	202	1/1	0.80	0.34	81,81,81,81	0
58	MG	14	3159	1/1	0.80	0.11	73,73,73,73	0
58	MG	1H	3234	1/1	0.80	0.32	67,67,67,67	0
58	MG	13	1701	1/1	0.81	0.21	99,99,99,99	0
58	MG	14	3151	1/1	0.81	0.53	91,91,91,91	0
58	MG	14	3274	1/1	0.81	0.23	88,88,88,88	0
58	MG	1H	3339	1/1	0.81	0.33	75,75,75,75	0
58	MG	1G	1606	1/1	0.81	0.17	83,83,83,83	0
58	MG	14	3023	1/1	0.81	0.26	90,90,90,90	0
58	MG	14	3292	1/1	0.81	0.26	84,84,84,84	0
58	MG	1H	3268	1/1	0.81	0.25	71,71,71,71	0
58	MG	14	3172	1/1	0.81	0.13	72,72,72,72	0
58	MG	1H	3492	1/1	0.81	0.28	82,82,82,82	0
58	MG	14	3338	1/1	0.81	0.12	74,74,74,74	0
58	MG	1G	1636	1/1	0.81	0.38	106,106,106,106	0
58	MG	14	3370	1/1	0.81	0.10	106,106,106,106	0
58	MG	1G	1647	1/1	0.81	0.16	94,94,94,94	0
58	MG	14	3376	1/1	0.81	0.06	119,119,119,119	0
58	MG	13	1736	1/1	0.81	0.08	116,116,116,116	0
58	MG	1H	3040	1/1	0.81	0.47	76,76,76,76	0
58	MG	14	3385	1/1	0.81	0.12	91,91,91,91	0
58	MG	14	3229	1/1	0.81	0.34	91,91,91,91	0
58	MG	1H	3155	1/1	0.81	0.10	58,58,58,58	0
58	MG	14	3050	1/1	0.81	0.39	94,94,94,94	0
58	MG	1H	3043	1/1	0.81	0.22	77,77,77,77	0
58	MG	1H	3431	1/1	0.81	0.10	94,94,94,94	0
58	MG	16	206	1/1	0.81	0.21	74,74,74,74	0
58	MG	13	1652	1/1	0.81	0.16	85,85,85,85	0
58	MG	13	1700	1/1	0.81	0.30	92,92,92,92	0
58	MG	1G	1680	1/1	0.82	0.38	101,101,101,101	0
58	MG	13	1712	1/1	0.82	0.14	80,80,80,80	0
58	MG	1H	3308	1/1	0.82	0.26	75,75,75,75	0
58	MG	2L	102	1/1	0.82	0.20	85,85,85,85	0
58	MG	1H	3340	1/1	0.82	0.35	82,82,82,82	0
58	MG	1H	3192	1/1	0.82	0.17	71,71,71,71	0
58	MG	1H	3023	1/1	0.82	0.53	88,88,88,88	0
58	MG	1H	3315	1/1	0.82	0.32	80,80,80,80	0
58	MG	1H	3272	1/1	0.82	0.24	68,68,68,68	0
58	MG	13	1651	1/1	0.82	0.23	79,79,79,79	0
58	MG	14	3220	1/1	0.82	0.30	66,66,66,66	0
58	MG	14	3407	1/1	0.82	0.09	117,117,117,117	0
58	MG	1J	202	1/1	0.82	0.34	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3174	1/1	0.82	0.25	70,70,70,70	0
58	MG	13	1606	1/1	0.82	0.43	88,88,88,88	0
58	MG	14	3147	1/1	0.82	0.16	81,81,81,81	0
58	MG	1H	3156	1/1	0.82	0.17	78,78,78,78	0
58	MG	14	3148	1/1	0.83	0.19	65,65,65,65	0
58	MG	1H	3077	1/1	0.83	0.18	54,54,54,54	0
58	MG	1H	3457	1/1	0.83	0.15	82,82,82,82	0
58	MG	1H	3246	1/1	0.83	0.27	75,75,75,75	0
58	MG	1H	3474	1/1	0.83	0.10	100,100,100,100	0
58	MG	14	3034	1/1	0.83	0.27	82,82,82,82	0
58	MG	14	3169	1/1	0.83	0.22	92,92,92,92	0
58	MG	14	3300	1/1	0.83	0.20	63,63,63,63	0
58	MG	13	1705	1/1	0.83	0.44	91,91,91,91	0
58	MG	1H	3030	1/1	0.83	0.21	67,67,67,67	0
58	MG	1H	3159	1/1	0.83	0.28	73,73,73,73	0
58	MG	14	3367	1/1	0.83	0.07	103,103,103,103	0
58	MG	1H	3346	1/1	0.83	0.16	80,80,80,80	0
58	MG	14	3047	1/1	0.83	0.15	92,92,92,92	0
58	MG	1H	3348	1/1	0.83	0.33	73,73,73,73	0
58	MG	1H	3187	1/1	0.83	0.17	78,78,78,78	0
58	MG	1H	3188	1/1	0.83	0.31	73,73,73,73	0
58	MG	14	3234	1/1	0.83	0.16	80,80,80,80	0
58	MG	14	3244	1/1	0.83	0.13	68,68,68,68	0
58	MG	13	1723	1/1	0.83	0.13	70,70,70,70	0
58	MG	1H	3421	1/1	0.83	0.15	46,46,46,46	0
58	MG	16	204	1/1	0.83	0.19	67,67,67,67	0
58	MG	1H	3422	1/1	0.83	0.15	66,66,66,66	0
58	MG	14	3121	1/1	0.83	0.30	75,75,75,75	0
58	MG	14	3126	1/1	0.83	0.21	79,79,79,79	0
58	MG	11	301	1/1	0.83	0.26	50,50,50,50	0
58	MG	1H	3327	1/1	0.83	0.35	77,77,77,77	0
58	MG	1H	3075	1/1	0.83	0.19	76,76,76,76	0
58	MG	14	3123	1/1	0.84	0.24	78,78,78,78	0
58	MG	14	3299	1/1	0.84	0.17	76,76,76,76	0
58	MG	14	3227	1/1	0.84	0.11	84,84,84,84	0
58	MG	1G	1646	1/1	0.84	0.37	95,95,95,95	0
58	MG	14	3140	1/1	0.84	0.23	69,69,69,69	0
58	MG	14	3242	1/1	0.84	0.20	78,78,78,78	0
58	MG	14	3025	1/1	0.84	0.21	81,81,81,81	0
58	MG	1H	3333	1/1	0.84	0.28	71,71,71,71	0
58	MG	1G	1649	1/1	0.84	0.23	101,101,101,101	0
58	MG	13	1636	1/1	0.84	0.27	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1692	1/1	0.84	0.18	79,79,79,79	0
58	MG	16	205	1/1	0.84	0.20	81,81,81,81	0
58	MG	13	1680	1/1	0.84	0.18	97,97,97,97	0
58	MG	1H	3277	1/1	0.84	0.27	70,70,70,70	0
58	MG	1H	3224	1/1	0.84	0.49	92,92,92,92	0
58	MG	1H	3136	1/1	0.84	0.18	73,73,73,73	0
58	MG	13	1683	1/1	0.84	0.12	76,76,76,76	0
58	MG	1H	3266	1/1	0.84	0.24	91,91,91,91	0
58	MG	1H	3242	1/1	0.84	0.33	77,77,77,77	0
58	MG	14	3286	1/1	0.84	0.14	71,71,71,71	0
58	MG	1H	3153	1/1	0.84	0.29	72,72,72,72	0
58	MG	1H	3007	1/1	0.84	0.36	64,64,64,64	0
58	MG	1H	3033	1/1	0.84	0.37	78,78,78,78	0
58	MG	13	1706	1/1	0.85	0.38	81,81,81,81	0
58	MG	14	3076	1/1	0.85	0.13	73,73,73,73	0
58	MG	88	202	1/1	0.85	0.22	64,64,64,64	0
58	MG	14	3296	1/1	0.85	0.16	74,74,74,74	0
58	MG	1H	3241	1/1	0.85	0.29	71,71,71,71	0
58	MG	1H	3098	1/1	0.85	0.41	71,71,71,71	0
58	MG	14	3118	1/1	0.85	0.15	72,72,72,72	0
58	MG	1H	3183	1/1	0.85	0.18	60,60,60,60	0
58	MG	1H	3138	1/1	0.85	0.14	65,65,65,65	0
58	MG	1G	1625	1/1	0.85	0.12	129,129,129,129	0
58	MG	14	3236	1/1	0.85	0.21	86,86,86,86	0
58	MG	1G	1630	1/1	0.85	0.14	78,78,78,78	0
58	MG	1H	3322	1/1	0.85	0.22	88,88,88,88	0
58	MG	14	3248	1/1	0.85	0.20	79,79,79,79	0
58	MG	1H	3185	1/1	0.85	0.27	72,72,72,72	0
58	MG	1H	3119	1/1	0.85	0.33	91,91,91,91	0
58	MG	1H	3514	1/1	0.85	0.09	77,77,77,77	0
58	MG	14	3386	1/1	0.85	0.12	94,94,94,94	0
58	MG	1H	3330	1/1	0.85	0.23	75,75,75,75	0
58	MG	1H	3297	1/1	0.85	0.31	78,78,78,78	0
58	MG	1H	3154	1/1	0.85	0.19	59,59,59,59	0
58	MG	14	3404	1/1	0.85	0.12	66,66,66,66	0
58	MG	1H	3440	1/1	0.85	0.09	52,52,52,52	0
58	MG	14	3164	1/1	0.85	0.34	78,78,78,78	0
58	MG	1H	3026	1/1	0.85	0.32	80,80,80,80	0
58	MG	14	3167	1/1	0.85	0.19	86,86,86,86	0
58	MG	1J	205	1/1	0.85	0.20	78,78,78,78	0
58	MG	14	3168	1/1	0.85	0.32	92,92,92,92	0
58	MG	1H	3228	1/1	0.85	0.22	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3175	1/1	0.85	0.19	65,65,65,65	0
58	MG	1H	3250	1/1	0.86	0.46	86,86,86,86	0
58	MG	1G	1685	1/1	0.86	0.11	88,88,88,88	0
58	MG	14	3231	1/1	0.86	0.21	70,70,70,70	0
58	MG	14	3145	1/1	0.86	0.33	87,87,87,87	0
58	MG	1H	3335	1/1	0.86	0.22	59,59,59,59	0
58	MG	1H	3509	1/1	0.86	0.12	68,68,68,68	0
58	MG	1H	3252	1/1	0.86	0.15	60,60,60,60	0
58	MG	1H	3031	1/1	0.86	0.41	90,90,90,90	0
58	MG	14	3369	1/1	0.86	0.07	102,102,102,102	0
58	MG	1H	3217	1/1	0.86	0.25	54,54,54,54	0
58	MG	1G	1633	1/1	0.86	0.31	82,82,82,82	0
58	MG	14	3258	1/1	0.86	0.12	82,82,82,82	0
58	MG	14	3060	1/1	0.86	0.17	58,58,58,58	0
58	MG	14	3075	1/1	0.86	0.13	89,89,89,89	0
58	MG	14	3012	1/1	0.86	0.13	69,69,69,69	0
58	MG	1H	3341	1/1	0.86	0.16	96,96,96,96	0
58	MG	14	3387	1/1	0.86	0.17	93,93,93,93	0
58	MG	1H	3343	1/1	0.86	0.54	99,99,99,99	0
58	MG	14	3090	1/1	0.86	0.15	68,68,68,68	0
58	MG	1H	3042	1/1	0.86	0.17	64,64,64,64	0
58	MG	14	3273	1/1	0.86	0.12	62,62,62,62	0
58	MG	14	3180	1/1	0.86	0.15	74,74,74,74	0
58	MG	1H	3243	1/1	0.86	0.27	81,81,81,81	0
58	MG	14	3282	1/1	0.86	0.45	88,88,88,88	0
58	MG	1H	3165	1/1	0.86	0.24	60,60,60,60	0
58	MG	14	3190	1/1	0.86	0.14	53,53,53,53	0
58	MG	13	1647	1/1	0.86	0.13	87,87,87,87	0
58	MG	1H	3113	1/1	0.86	0.21	68,68,68,68	0
58	MG	3E	301	1/1	0.86	0.14	109,109,109,109	0
58	MG	14	3281	1/1	0.87	0.30	84,84,84,84	0
58	MG	5I	102	1/1	0.87	0.26	90,90,90,90	0
58	MG	1H	3354	1/1	0.87	0.13	49,49,49,49	0
58	MG	1H	3376	1/1	0.87	0.18	67,67,67,67	0
58	MG	1G	1671	1/1	0.87	0.18	82,82,82,82	0
58	MG	1H	3221	1/1	0.87	0.26	63,63,63,63	0
58	MG	1H	3520	1/1	0.87	0.51	97,97,97,97	0
58	MG	14	3294	1/1	0.87	0.15	94,94,94,94	0
58	MG	14	3201	1/1	0.87	0.19	69,69,69,69	0
58	MG	1H	3284	1/1	0.87	0.25	74,74,74,74	0
58	MG	1H	3285	1/1	0.87	0.12	80,80,80,80	0
58	MG	14	3223	1/1	0.87	0.10	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2K	103	1/1	0.87	0.31	88,88,88,88	0
58	MG	1H	3329	1/1	0.87	0.33	85,85,85,85	0
58	MG	16	209	1/1	0.87	0.26	65,65,65,65	0
58	MG	13	1677	1/1	0.87	0.29	74,74,74,74	0
58	MG	14	3001	1/1	0.87	0.28	89,89,89,89	0
58	MG	14	3239	1/1	0.87	0.37	98,98,98,98	0
58	MG	1H	3430	1/1	0.87	0.09	73,73,73,73	0
58	MG	13	1644	1/1	0.87	0.36	78,78,78,78	0
58	MG	78	201	1/1	0.87	0.25	80,80,80,80	0
58	MG	14	3250	1/1	0.87	0.22	72,72,72,72	0
58	MG	14	3253	1/1	0.87	0.18	151,151,151,151	0
58	MG	13	1630	1/1	0.87	0.16	67,67,67,67	0
58	MG	1H	3044	1/1	0.87	0.21	61,61,61,61	0
58	MG	1H	3199	1/1	0.87	0.19	44,44,44,44	0
58	MG	1H	3200	1/1	0.87	0.17	35,35,35,35	0
58	MG	1H	3338	1/1	0.87	0.34	80,80,80,80	0
58	MG	14	3400	1/1	0.87	0.09	65,65,65,65	0
58	MG	1H	3202	1/1	0.87	0.23	58,58,58,58	0
58	MG	1H	3478	1/1	0.87	0.13	91,91,91,91	0
58	MG	1G	1631	1/1	0.87	0.25	82,82,82,82	0
58	MG	1H	3078	1/1	0.87	0.21	67,67,67,67	0
58	MG	1H	3080	1/1	0.87	0.14	56,56,56,56	0
58	MG	13	1707	1/1	0.87	0.45	80,80,80,80	0
58	MG	13	1648	1/1	0.87	0.36	78,78,78,78	0
58	MG	13	1687	1/1	0.87	0.21	98,98,98,98	0
58	MG	14	3277	1/1	0.87	0.13	104,104,104,104	0
58	MG	1G	1678	1/1	0.88	0.29	108,108,108,108	0
58	MG	1G	1679	1/1	0.88	0.39	120,120,120,120	0
58	MG	13	1738	1/1	0.88	0.07	84,84,84,84	0
58	MG	14	3122	1/1	0.88	0.36	79,79,79,79	0
58	MG	1H	3311	1/1	0.88	0.31	81,81,81,81	0
58	MG	1H	3434	1/1	0.88	0.09	63,63,63,63	0
58	MG	2A	201	1/1	0.88	0.13	91,91,91,91	0
58	MG	2A	202	1/1	0.88	0.27	98,98,98,98	0
58	MG	13	1739	1/1	0.88	0.07	85,85,85,85	0
58	MG	13	1627	1/1	0.88	0.31	90,90,90,90	0
58	MG	2L	103	1/1	0.88	0.21	93,93,93,93	0
58	MG	1H	3342	1/1	0.88	0.30	89,89,89,89	0
58	MG	14	3275	1/1	0.88	0.18	86,86,86,86	0
58	MG	1H	3460	1/1	0.88	0.16	81,81,81,81	0
58	MG	13	1646	1/1	0.88	0.26	61,61,61,61	0
58	MG	1H	3204	1/1	0.88	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	1H	3034	1/1	0.88	0.38	73,73,73,73	0
58	MG	14	3163	1/1	0.88	0.17	71,71,71,71	0
58	MG	13	1643	1/1	0.88	0.35	78,78,78,78	0
58	MG	14	3165	1/1	0.88	0.21	83,83,83,83	0
58	MG	14	3016	1/1	0.88	0.32	91,91,91,91	0
58	MG	1H	3186	1/1	0.88	0.17	74,74,74,74	0
58	MG	1H	3485	1/1	0.88	0.09	87,87,87,87	0
58	MG	1H	3373	1/1	0.88	0.08	75,75,75,75	0
58	MG	1G	1626	1/1	0.88	0.35	99,99,99,99	0
58	MG	14	3176	1/1	0.88	0.19	58,58,58,58	0
58	MG	13	1721	1/1	0.88	0.09	83,83,83,83	0
58	MG	1H	3497	1/1	0.88	0.14	42,42,42,42	0
58	MG	14	3181	1/1	0.88	0.28	79,79,79,79	0
58	MG	1H	3383	1/1	0.88	0.12	61,61,61,61	0
58	MG	13	1669	1/1	0.88	0.11	68,68,68,68	0
58	MG	1H	3503	1/1	0.88	0.28	73,73,73,73	0
58	MG	14	3042	1/1	0.88	0.24	87,87,87,87	0
58	MG	14	3044	1/1	0.88	0.16	57,57,57,57	0
58	MG	13	1725	1/1	0.88	0.08	77,77,77,77	0
58	MG	14	3215	1/1	0.88	0.09	73,73,73,73	0
58	MG	14	3216	1/1	0.88	0.08	63,63,63,63	0
58	MG	14	3046	1/1	0.88	0.24	68,68,68,68	0
58	MG	1H	3398	1/1	0.88	0.10	57,57,57,57	0
58	MG	1H	3169	1/1	0.88	0.37	85,85,85,85	0
58	MG	1H	3515	1/1	0.88	0.05	83,83,83,83	0
58	MG	14	3390	1/1	0.88	0.12	109,109,109,109	0
58	MG	1H	3253	1/1	0.88	0.23	76,76,76,76	0
58	MG	1G	1665	1/1	0.88	0.52	127,127,127,127	0
58	MG	1G	1668	1/1	0.88	0.12	84,84,84,84	0
58	MG	1G	1670	1/1	0.88	0.12	88,88,88,88	0
58	MG	13	1671	1/1	0.88	0.22	95,95,95,95	0
58	MG	14	3243	1/1	0.88	0.35	70,70,70,70	0
58	MG	1H	3309	1/1	0.88	0.17	70,70,70,70	0
58	MG	14	3245	1/1	0.88	0.29	77,77,77,77	0
58	MG	1G	1676	1/1	0.88	0.35	95,95,95,95	0
58	MG	29	303	1/1	0.88	0.19	73,73,73,73	0
58	MG	14	3087	1/1	0.88	0.16	48,48,48,48	0
58	MG	14	3251	1/1	0.88	0.30	84,84,84,84	0
58	MG	1G	1677	1/1	0.88	0.14	97,97,97,97	0
58	MG	14	3196	1/1	0.89	0.12	65,65,65,65	0
58	MG	14	3283	1/1	0.89	0.23	82,82,82,82	0
58	MG	13	1673	1/1	0.89	0.22	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1688	1/1	0.89	0.35	97,97,97,97	0
58	MG	1H	3147	1/1	0.89	0.27	63,63,63,63	0
58	MG	14	3290	1/1	0.89	0.20	79,79,79,79	0
58	MG	1G	1655	1/1	0.89	0.24	86,86,86,86	0
58	MG	1G	1658	1/1	0.89	0.11	92,92,92,92	0
58	MG	13	1654	1/1	0.89	0.15	76,76,76,76	0
58	MG	1H	3453	1/1	0.89	0.08	105,105,105,105	0
58	MG	14	3026	1/1	0.89	0.15	71,71,71,71	0
58	MG	1G	1662	1/1	0.89	0.34	83,83,83,83	0
58	MG	14	3146	1/1	0.89	0.10	64,64,64,64	0
58	MG	14	3334	1/1	0.89	0.09	49,49,49,49	0
58	MG	14	3032	1/1	0.89	0.23	82,82,82,82	0
58	MG	13	1633	1/1	0.89	0.15	49,49,49,49	0
58	MG	14	3352	1/1	0.89	0.18	99,99,99,99	0
58	MG	1H	3209	1/1	0.89	0.10	57,57,57,57	0
58	MG	1H	3211	1/1	0.89	0.39	78,78,78,78	0
58	MG	1H	3279	1/1	0.89	0.25	67,67,67,67	0
58	MG	13	1670	1/1	0.89	0.33	91,91,91,91	0
58	MG	14	3162	1/1	0.89	0.24	81,81,81,81	0
58	MG	13	1709	1/1	0.89	0.32	84,84,84,84	0
58	MG	1H	3015	1/1	0.89	0.16	73,73,73,73	0
58	MG	1H	3480	1/1	0.89	0.11	88,88,88,88	0
58	MG	98	201	1/1	0.89	0.21	56,56,56,56	0
58	MG	1H	3318	1/1	0.89	0.27	85,85,85,85	0
58	MG	1H	3320	1/1	0.89	0.27	71,71,71,71	0
58	MG	13	1634	1/1	0.89	0.17	47,47,47,47	0
58	MG	13	1672	1/1	0.89	0.10	72,72,72,72	0
58	MG	14	3173	1/1	0.89	0.17	79,79,79,79	0
58	MG	1G	1610	1/1	0.89	0.10	88,88,88,88	0
58	MG	1H	3130	1/1	0.89	0.12	59,59,59,59	0
58	MG	1H	3289	1/1	0.89	0.47	89,89,89,89	0
58	MG	13	1713	1/1	0.89	0.40	88,88,88,88	0
58	MG	14	3183	1/1	0.89	0.14	66,66,66,66	0
58	MG	1H	3135	1/1	0.89	0.28	61,61,61,61	0
58	MG	1H	3235	1/1	0.89	0.34	83,83,83,83	0
58	MG	1H	3294	1/1	0.89	0.68	61,61,61,61	0
58	MG	1H	3038	1/1	0.89	0.45	73,73,73,73	0
58	MG	14	3278	1/1	0.89	0.14	89,89,89,89	0
58	MG	14	3279	1/1	0.89	0.15	74,74,74,74	0
58	MG	14	3195	1/1	0.89	0.24	70,70,70,70	0
58	MG	1G	1674	1/1	0.90	0.23	98,98,98,98	0
58	MG	1H	3270	1/1	0.90	0.38	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3471	1/1	0.90	0.08	63,63,63,63	0
58	MG	1H	3018	1/1	0.90	0.37	73,73,73,73	0
58	MG	14	3184	1/1	0.90	0.26	91,91,91,91	0
58	MG	13	1655	1/1	0.90	0.08	77,77,77,77	0
58	MG	1H	3100	1/1	0.90	0.25	64,64,64,64	0
58	MG	1H	3109	1/1	0.90	0.10	46,46,46,46	0
58	MG	1G	1681	1/1	0.90	0.22	75,75,75,75	0
58	MG	1G	1682	1/1	0.90	0.19	103,103,103,103	0
58	MG	P8	101	1/1	0.90	0.29	73,73,73,73	0
58	MG	1G	1687	1/1	0.90	0.09	104,104,104,104	0
58	MG	1H	3110	1/1	0.90	0.13	45,45,45,45	0
58	MG	1G	1692	1/1	0.90	0.09	83,83,83,83	0
58	MG	14	3115	1/1	0.90	0.27	66,66,66,66	0
58	MG	14	3297	1/1	0.90	0.09	75,75,75,75	0
58	MG	1G	1602	1/1	0.90	0.20	93,93,93,93	0
58	MG	1G	1605	1/1	0.90	0.36	83,83,83,83	0
58	MG	1H	3332	1/1	0.90	0.26	74,74,74,74	0
58	MG	1H	3488	1/1	0.90	0.10	69,69,69,69	0
58	MG	1H	3046	1/1	0.90	0.25	84,84,84,84	0
58	MG	14	3232	1/1	0.90	0.58	52,52,52,52	0
58	MG	1H	3306	1/1	0.90	0.45	78,78,78,78	0
58	MG	14	3358	1/1	0.90	0.08	82,82,82,82	0
58	MG	1H	3493	1/1	0.90	0.22	79,79,79,79	0
58	MG	14	3237	1/1	0.90	0.15	79,79,79,79	0
58	MG	1H	3280	1/1	0.90	0.45	82,82,82,82	0
58	MG	14	3240	1/1	0.90	0.11	83,83,83,83	0
58	MG	1H	3230	1/1	0.90	0.52	91,91,91,91	0
58	MG	1H	3423	1/1	0.90	0.11	59,59,59,59	0
58	MG	1H	3009	1/1	0.90	0.49	73,73,73,73	0
58	MG	1H	3428	1/1	0.90	0.15	74,74,74,74	0
58	MG	1G	1637	1/1	0.90	0.23	79,79,79,79	0
58	MG	1H	3127	1/1	0.90	0.12	50,50,50,50	0
58	MG	1H	3207	1/1	0.90	0.17	56,56,56,56	0
58	MG	14	3024	1/1	0.90	0.27	82,82,82,82	0
58	MG	1G	1648	1/1	0.90	0.20	79,79,79,79	0
58	MG	14	3391	1/1	0.90	0.09	97,97,97,97	0
58	MG	13	1682	1/1	0.90	0.22	73,73,73,73	0
58	MG	13	1662	1/1	0.90	0.29	115,115,115,115	0
58	MG	14	3398	1/1	0.90	0.09	70,70,70,70	0
58	MG	14	3261	1/1	0.90	0.13	84,84,84,84	0
58	MG	1H	3448	1/1	0.90	0.09	51,51,51,51	0
58	MG	14	3033	1/1	0.90	0.21	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1653	1/1	0.90	0.28	87,87,87,87	0
58	MG	1H	3344	1/1	0.90	0.28	70,70,70,70	0
58	MG	1H	3245	1/1	0.90	0.32	81,81,81,81	0
58	MG	1H	3459	1/1	0.90	0.21	73,73,73,73	0
58	MG	1H	3091	1/1	0.90	0.23	77,77,77,77	0
58	MG	16	210	1/1	0.90	0.15	73,73,73,73	0
58	MG	25	201	1/1	0.90	0.48	102,102,102,102	0
58	MG	14	3175	1/1	0.90	0.20	87,87,87,87	0
58	MG	1H	3466	1/1	0.90	0.06	67,67,67,67	0
58	MG	11	303	1/1	0.91	0.12	41,41,41,41	0
58	MG	1H	3325	1/1	0.91	0.37	92,92,92,92	0
58	MG	1H	3378	1/1	0.91	0.09	79,79,79,79	0
58	MG	14	3182	1/1	0.91	0.24	86,86,86,86	0
58	MG	14	3280	1/1	0.91	0.40	87,87,87,87	0
58	MG	1G	1672	1/1	0.91	0.26	88,88,88,88	0
58	MG	1H	3120	1/1	0.91	0.36	70,70,70,70	0
58	MG	1H	3265	1/1	0.91	0.22	79,79,79,79	0
58	MG	13	1661	1/1	0.91	0.22	97,97,97,97	0
58	MG	2K	102	1/1	0.91	0.15	80,80,80,80	0
58	MG	14	3191	1/1	0.91	0.12	70,70,70,70	0
58	MG	L8	101	1/1	0.91	0.42	79,79,79,79	0
58	MG	14	3070	1/1	0.91	0.11	79,79,79,79	0
58	MG	14	3074	1/1	0.91	0.16	73,73,73,73	0
58	MG	1H	3236	1/1	0.91	0.26	79,79,79,79	0
58	MG	14	3206	1/1	0.91	0.14	50,50,50,50	0
58	MG	1H	3016	1/1	0.91	0.41	97,97,97,97	0
58	MG	1H	3017	1/1	0.91	0.41	66,66,66,66	0
58	MG	1G	1604	1/1	0.91	0.17	98,98,98,98	0
58	MG	13	1702	1/1	0.91	0.38	81,81,81,81	0
58	MG	14	3326	1/1	0.91	0.16	61,61,61,61	0
58	MG	1H	3494	1/1	0.91	0.11	82,82,82,82	0
58	MG	1H	3206	1/1	0.91	0.13	54,54,54,54	0
58	MG	1H	3305	1/1	0.91	0.21	75,75,75,75	0
58	MG	1G	1613	1/1	0.91	0.08	87,87,87,87	0
58	MG	1G	1614	1/1	0.91	0.24	91,91,91,91	0
58	MG	1G	1618	1/1	0.91	0.17	78,78,78,78	0
58	MG	14	3365	1/1	0.91	0.19	83,83,83,83	0
58	MG	14	3366	1/1	0.91	0.10	94,94,94,94	0
58	MG	1G	1624	1/1	0.91	0.14	85,85,85,85	0
58	MG	1H	3178	1/1	0.91	0.10	63,63,63,63	0
58	MG	13	1703	1/1	0.91	0.15	89,89,89,89	0
58	MG	1G	1628	1/1	0.91	0.37	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3508	1/1	0.91	0.12	55,55,55,55	0
58	MG	1H	3048	1/1	0.91	0.42	81,81,81,81	0
58	MG	14	3011	1/1	0.91	0.24	70,70,70,70	0
58	MG	1H	3510	1/1	0.91	0.25	51,51,51,51	0
58	MG	14	3246	1/1	0.91	0.16	85,85,85,85	0
58	MG	13	1733	1/1	0.91	0.10	104,104,104,104	0
58	MG	3E	302	1/1	0.91	0.25	108,108,108,108	0
58	MG	14	3154	1/1	0.91	0.12	68,68,68,68	0
58	MG	1H	3105	1/1	0.91	0.22	71,71,71,71	0
58	MG	13	1696	1/1	0.91	0.10	70,70,70,70	0
58	MG	1H	3039	1/1	0.91	0.39	75,75,75,75	0
58	MG	16	202	1/1	0.91	0.29	81,81,81,81	0
58	MG	14	3259	1/1	0.91	0.17	102,102,102,102	0
58	MG	14	3402	1/1	0.91	0.11	76,76,76,76	0
58	MG	14	3403	1/1	0.91	0.08	66,66,66,66	0
58	MG	1H	3011	1/1	0.91	0.13	72,72,72,72	0
58	MG	1G	1650	1/1	0.91	0.33	81,81,81,81	0
58	MG	1H	3223	1/1	0.91	0.26	60,60,60,60	0
58	MG	14	3031	1/1	0.91	0.20	78,78,78,78	0
58	MG	1G	1657	1/1	0.91	0.22	107,107,107,107	0
58	MG	1H	3464	1/1	0.91	0.11	84,84,84,84	0
58	MG	1H	3118	1/1	0.91	0.17	53,53,53,53	0
58	MG	1H	3371	1/1	0.91	0.09	45,45,45,45	0
58	MG	1H	3059	1/1	0.91	0.26	56,56,56,56	0
58	MG	1H	3472	1/1	0.91	0.07	72,72,72,72	0
60	ZN	5A	101	1/1	0.91	0.12	143,143,143,143	0
58	MG	1G	1667	1/1	0.91	0.21	92,92,92,92	0
58	MG	1H	3288	1/1	0.92	0.18	58,58,58,58	0
58	MG	13	1642	1/1	0.92	0.24	64,64,64,64	0
58	MG	13	1657	1/1	0.92	0.28	89,89,89,89	0
58	MG	14	3171	1/1	0.92	0.26	80,80,80,80	0
58	MG	1G	1643	1/1	0.92	0.28	74,74,74,74	0
58	MG	1H	3146	1/1	0.92	0.32	67,67,67,67	0
58	MG	1H	3261	1/1	0.92	0.21	64,64,64,64	0
58	MG	1H	3101	1/1	0.92	0.28	72,72,72,72	0
58	MG	1H	3436	1/1	0.92	0.09	67,67,67,67	0
58	MG	1H	3264	1/1	0.92	0.18	67,67,67,67	0
58	MG	1G	1651	1/1	0.92	0.17	77,77,77,77	0
58	MG	1H	3447	1/1	0.92	0.14	55,55,55,55	0
58	MG	1G	1656	1/1	0.92	0.14	140,140,140,140	0
58	MG	1H	3150	1/1	0.92	0.35	69,69,69,69	0
58	MG	1H	3449	1/1	0.92	0.08	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1659	1/1	0.92	0.20	95,95,95,95	0
58	MG	1H	3298	1/1	0.92	0.22	68,68,68,68	0
58	MG	1H	3299	1/1	0.92	0.56	98,98,98,98	0
58	MG	16	208	1/1	0.92	0.29	77,77,77,77	0
58	MG	13	1698	1/1	0.92	0.15	80,80,80,80	0
58	MG	1H	3233	1/1	0.92	0.25	70,70,70,70	0
58	MG	1H	3041	1/1	0.92	0.19	88,88,88,88	0
58	MG	14	3321	1/1	0.92	0.11	55,55,55,55	0
58	MG	14	3204	1/1	0.92	0.23	63,63,63,63	0
58	MG	1H	3463	1/1	0.92	0.15	66,66,66,66	0
58	MG	13	1691	1/1	0.92	0.26	75,75,75,75	0
58	MG	41	201	1/1	0.92	0.15	67,67,67,67	0
58	MG	1H	3112	1/1	0.92	0.22	71,71,71,71	0
58	MG	14	3353	1/1	0.92	0.12	82,82,82,82	0
58	MG	13	1737	1/1	0.92	0.06	93,93,93,93	0
58	MG	14	3221	1/1	0.92	0.27	72,72,72,72	0
58	MG	88	201	1/1	0.92	0.16	84,84,84,84	0
58	MG	1H	3470	1/1	0.92	0.06	73,73,73,73	0
58	MG	14	3084	1/1	0.92	0.10	81,81,81,81	0
58	MG	13	1686	1/1	0.92	0.19	80,80,80,80	0
58	MG	13	1693	1/1	0.92	0.42	94,94,94,94	0
58	MG	14	3371	1/1	0.92	0.08	79,79,79,79	0
58	MG	14	3106	1/1	0.92	0.19	62,62,62,62	0
58	MG	14	3235	1/1	0.92	0.19	80,80,80,80	0
58	MG	I8	101	1/1	0.92	0.08	56,56,56,56	0
58	MG	1H	3473	1/1	0.92	0.07	85,85,85,85	0
58	MG	14	3383	1/1	0.92	0.09	66,66,66,66	0
58	MG	1H	3352	1/1	0.92	0.13	45,45,45,45	0
58	MG	1H	3274	1/1	0.92	0.28	83,83,83,83	0
58	MG	1H	3313	1/1	0.92	0.30	78,78,78,78	0
58	MG	1H	3079	1/1	0.92	0.15	53,53,53,53	0
58	MG	1H	3481	1/1	0.92	0.09	132,132,132,132	0
58	MG	14	3129	1/1	0.92	0.25	69,69,69,69	0
58	MG	1H	3164	1/1	0.92	0.30	58,58,58,58	0
58	MG	14	3394	1/1	0.92	0.12	53,53,53,53	0
58	MG	14	3395	1/1	0.92	0.24	75,75,75,75	0
58	MG	1H	3121	1/1	0.92	0.23	35,35,35,35	0
58	MG	1H	3487	1/1	0.92	0.12	100,100,100,100	0
58	MG	1H	3122	1/1	0.92	0.20	68,68,68,68	0
58	MG	2K	105	1/1	0.92	0.06	81,81,81,81	0
58	MG	1G	1616	1/1	0.92	0.29	86,86,86,86	0
58	MG	13	1742	1/1	0.92	0.21	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1620	1/1	0.92	0.18	77,77,77,77	0
58	MG	14	3004	1/1	0.92	0.23	78,78,78,78	0
58	MG	14	3156	1/1	0.92	0.21	63,63,63,63	0
58	MG	1H	3131	1/1	0.92	0.28	57,57,57,57	0
58	MG	1H	3400	1/1	0.92	0.20	54,54,54,54	0
58	MG	1H	3496	1/1	0.92	0.12	59,59,59,59	0
58	MG	1H	3082	1/1	0.92	0.17	61,61,61,61	0
58	MG	1H	3417	1/1	0.92	0.11	66,66,66,66	0
58	MG	C5	201	1/1	0.92	0.32	105,105,105,105	0
58	MG	14	3018	1/1	0.92	0.16	50,50,50,50	0
58	MG	4K	101	1/1	0.92	0.21	73,73,73,73	0
58	MG	1H	3006	1/1	0.92	0.23	57,57,57,57	0
58	MG	1G	1609	1/1	0.93	0.11	81,81,81,81	0
58	MG	1H	3149	1/1	0.93	0.22	61,61,61,61	0
58	MG	14	3179	1/1	0.93	0.27	72,72,72,72	0
58	MG	1H	3439	1/1	0.93	0.13	51,51,51,51	0
58	MG	1H	3222	1/1	0.93	0.11	58,58,58,58	0
58	MG	1H	3443	1/1	0.93	0.11	66,66,66,66	0
58	MG	14	3284	1/1	0.93	0.43	94,94,94,94	0
58	MG	13	1676	1/1	0.93	0.09	88,88,88,88	0
58	MG	13	1660	1/1	0.93	0.30	86,86,86,86	0
58	MG	13	1678	1/1	0.93	0.11	89,89,89,89	0
58	MG	1H	3191	1/1	0.93	0.45	70,70,70,70	0
58	MG	13	1610	1/1	0.93	0.20	66,66,66,66	0
58	MG	1G	1627	1/1	0.93	0.18	88,88,88,88	0
58	MG	1G	1695	1/1	0.93	0.08	96,96,96,96	0
58	MG	1G	1696	1/1	0.93	0.04	109,109,109,109	0
58	MG	1H	3193	1/1	0.93	0.14	60,60,60,60	0
58	MG	14	3197	1/1	0.93	0.19	73,73,73,73	0
58	MG	14	3083	1/1	0.93	0.18	88,88,88,88	0
58	MG	13	1612	1/1	0.93	0.29	89,89,89,89	0
58	MG	14	3307	1/1	0.93	0.12	49,49,49,49	0
58	MG	13	1728	1/1	0.93	0.13	95,95,95,95	0
58	MG	1H	3237	1/1	0.93	0.28	72,72,72,72	0
58	MG	14	3333	1/1	0.93	0.13	67,67,67,67	0
58	MG	14	3213	1/1	0.93	0.19	75,75,75,75	0
58	MG	14	3097	1/1	0.93	0.21	77,77,77,77	0
58	MG	14	3098	1/1	0.93	0.16	71,71,71,71	0
58	MG	14	3217	1/1	0.93	0.17	101,101,101,101	0
58	MG	14	3219	1/1	0.93	0.18	51,51,51,51	0
58	MG	14	3354	1/1	0.93	0.15	56,56,56,56	0
58	MG	14	3104	1/1	0.93	0.15	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3089	1/1	0.93	0.31	72,72,72,72	0
58	MG	14	3362	1/1	0.93	0.06	56,56,56,56	0
58	MG	14	3363	1/1	0.93	0.12	54,54,54,54	0
58	MG	14	3110	1/1	0.93	0.10	55,55,55,55	0
58	MG	1H	3465	1/1	0.93	0.14	76,76,76,76	0
58	MG	16	207	1/1	0.93	0.25	88,88,88,88	0
58	MG	14	3368	1/1	0.93	0.06	89,89,89,89	0
58	MG	14	3230	1/1	0.93	0.60	82,82,82,82	0
58	MG	1H	3359	1/1	0.93	0.13	60,60,60,60	0
58	MG	13	1695	1/1	0.93	0.19	83,83,83,83	0
58	MG	14	3007	1/1	0.93	0.33	68,68,68,68	0
58	MG	14	3373	1/1	0.93	0.06	64,64,64,64	0
58	MG	14	3375	1/1	0.93	0.11	89,89,89,89	0
58	MG	14	3009	1/1	0.93	0.15	66,66,66,66	0
58	MG	14	3124	1/1	0.93	0.23	76,76,76,76	0
58	MG	1H	3128	1/1	0.93	0.20	66,66,66,66	0
58	MG	16	212	1/1	0.93	0.04	81,81,81,81	0
58	MG	14	3138	1/1	0.93	0.11	94,94,94,94	0
58	MG	1H	3163	1/1	0.93	0.28	65,65,65,65	0
58	MG	14	3014	1/1	0.93	0.17	77,77,77,77	0
58	MG	13	1607	1/1	0.93	0.28	71,71,71,71	0
58	MG	1H	3319	1/1	0.93	0.22	83,83,83,83	0
58	MG	1H	3094	1/1	0.93	0.21	54,54,54,54	0
58	MG	1H	3095	1/1	0.93	0.18	49,49,49,49	0
58	MG	14	3393	1/1	0.93	0.17	76,76,76,76	0
58	MG	13	1656	1/1	0.93	0.25	79,79,79,79	0
58	MG	14	3022	1/1	0.93	0.20	78,78,78,78	0
58	MG	1H	3036	1/1	0.93	0.30	65,65,65,65	0
58	MG	13	1674	1/1	0.93	0.16	77,77,77,77	0
58	MG	1H	3413	1/1	0.93	0.09	50,50,50,50	0
58	MG	1H	3414	1/1	0.93	0.28	64,64,64,64	0
58	MG	14	3027	1/1	0.93	0.31	81,81,81,81	0
58	MG	14	3161	1/1	0.93	0.21	74,74,74,74	0
58	MG	14	3028	1/1	0.93	0.17	99,99,99,99	0
58	MG	1H	3251	1/1	0.93	0.28	79,79,79,79	0
58	MG	14	3030	1/1	0.93	0.16	70,70,70,70	0
58	MG	1G	1663	1/1	0.93	0.14	112,112,112,112	0
58	MG	13	1641	1/1	0.93	0.11	69,69,69,69	0
58	MG	1H	3212	1/1	0.93	0.29	70,70,70,70	0
58	MG	1H	3179	1/1	0.93	0.39	67,67,67,67	0
58	MG	1H	3255	1/1	0.93	0.34	83,83,83,83	0
58	MG	1H	3215	1/1	0.93	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3022	1/1	0.93	0.12	88,88,88,88	0
60	ZN	32	301	1/1	0.93	0.38	112,112,112,112	0
58	MG	13	1711	1/1	0.93	0.26	76,76,76,76	0
58	MG	1H	3148	1/1	0.93	0.24	78,78,78,78	0
58	MG	1H	3381	1/1	0.94	0.16	62,62,62,62	0
58	MG	1H	3382	1/1	0.94	0.09	71,71,71,71	0
58	MG	1G	1632	1/1	0.94	0.30	83,83,83,83	0
58	MG	13	1679	1/1	0.94	0.15	75,75,75,75	0
58	MG	1H	3387	1/1	0.94	0.14	65,65,65,65	0
58	MG	1H	3076	1/1	0.94	0.24	51,51,51,51	0
58	MG	14	3086	1/1	0.94	0.17	67,67,67,67	0
58	MG	14	3287	1/1	0.94	0.15	96,96,96,96	0
58	MG	1H	3468	1/1	0.94	0.11	63,63,63,63	0
58	MG	14	3089	1/1	0.94	0.24	81,81,81,81	0
58	MG	14	3003	1/1	0.94	0.24	77,77,77,77	0
58	MG	14	3091	1/1	0.94	0.12	57,57,57,57	0
58	MG	14	3096	1/1	0.94	0.24	73,73,73,73	0
58	MG	14	3295	1/1	0.94	0.18	79,79,79,79	0
58	MG	1G	1642	1/1	0.94	0.18	92,92,92,92	0
58	MG	14	3198	1/1	0.94	0.26	94,94,94,94	0
58	MG	1H	3210	1/1	0.94	0.34	67,67,67,67	0
58	MG	14	3202	1/1	0.94	0.25	64,64,64,64	0
58	MG	1H	3393	1/1	0.94	0.10	58,58,58,58	0
58	MG	14	3301	1/1	0.94	0.15	87,87,87,87	0
58	MG	14	3305	1/1	0.94	0.09	69,69,69,69	0
58	MG	14	3205	1/1	0.94	0.16	58,58,58,58	0
58	MG	14	3312	1/1	0.94	0.12	88,88,88,88	0
58	MG	14	3317	1/1	0.94	0.12	48,48,48,48	0
58	MG	1H	3394	1/1	0.94	0.15	70,70,70,70	0
58	MG	14	3208	1/1	0.94	0.14	83,83,83,83	0
58	MG	14	3332	1/1	0.94	0.16	64,64,64,64	0
58	MG	14	3209	1/1	0.94	0.17	81,81,81,81	0
58	MG	13	1616	1/1	0.94	0.22	65,65,65,65	0
58	MG	14	3335	1/1	0.94	0.16	80,80,80,80	0
58	MG	14	3111	1/1	0.94	0.18	92,92,92,92	0
58	MG	14	3214	1/1	0.94	0.25	75,75,75,75	0
58	MG	14	3344	1/1	0.94	0.13	64,64,64,64	0
58	MG	14	3346	1/1	0.94	0.10	74,74,74,74	0
58	MG	14	3348	1/1	0.94	0.08	76,76,76,76	0
58	MG	13	1690	1/1	0.94	0.28	90,90,90,90	0
58	MG	2K	101	1/1	0.94	0.22	66,66,66,66	0
58	MG	1H	3406	1/1	0.94	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3355	1/1	0.94	0.09	64,64,64,64	0
58	MG	14	3218	1/1	0.94	0.15	71,71,71,71	0
58	MG	21	302	1/1	0.94	0.17	68,68,68,68	0
58	MG	13	1618	1/1	0.94	0.20	63,63,63,63	0
58	MG	1H	3216	1/1	0.94	0.27	71,71,71,71	0
58	MG	13	1717	1/1	0.94	0.07	76,76,76,76	0
58	MG	1H	3420	1/1	0.94	0.14	50,50,50,50	0
58	MG	14	3127	1/1	0.94	0.14	54,54,54,54	0
58	MG	1H	3141	1/1	0.94	0.14	40,40,40,40	0
58	MG	14	3134	1/1	0.94	0.17	62,62,62,62	0
58	MG	14	3137	1/1	0.94	0.20	78,78,78,78	0
58	MG	14	3233	1/1	0.94	0.10	63,63,63,63	0
58	MG	1H	3219	1/1	0.94	0.12	70,70,70,70	0
58	MG	1H	3144	1/1	0.94	0.30	49,49,49,49	0
58	MG	14	3141	1/1	0.94	0.11	46,46,46,46	0
58	MG	1H	3197	1/1	0.94	0.21	63,63,63,63	0
58	MG	14	3377	1/1	0.94	0.14	107,107,107,107	0
58	MG	14	3378	1/1	0.94	0.07	71,71,71,71	0
58	MG	1H	3312	1/1	0.94	0.13	73,73,73,73	0
58	MG	14	3380	1/1	0.94	0.07	76,76,76,76	0
58	MG	1H	3114	1/1	0.94	0.16	66,66,66,66	0
58	MG	13	1605	1/1	0.94	0.31	76,76,76,76	0
58	MG	1H	3495	1/1	0.94	0.09	47,47,47,47	0
58	MG	13	1722	1/1	0.94	0.10	76,76,76,76	0
58	MG	13	1743	1/1	0.94	0.07	60,60,60,60	0
58	MG	14	3153	1/1	0.94	0.34	60,60,60,60	0
58	MG	1H	3347	1/1	0.94	0.45	78,78,78,78	0
58	MG	1H	3317	1/1	0.94	0.22	84,84,84,84	0
58	MG	14	3157	1/1	0.94	0.15	71,71,71,71	0
58	MG	14	3252	1/1	0.94	0.34	91,91,91,91	0
58	MG	1H	3229	1/1	0.94	0.20	50,50,50,50	0
58	MG	1H	3203	1/1	0.94	0.38	79,79,79,79	0
58	MG	14	3396	1/1	0.94	0.11	53,53,53,53	0
58	MG	1G	1611	1/1	0.94	0.10	91,91,91,91	0
58	MG	14	3256	1/1	0.94	0.42	57,57,57,57	0
58	MG	1H	3231	1/1	0.94	0.26	74,74,74,74	0
58	MG	14	3043	1/1	0.94	0.25	76,76,76,76	0
58	MG	1H	3367	1/1	0.94	0.10	54,54,54,54	0
58	MG	1H	3511	1/1	0.94	0.11	82,82,82,82	0
58	MG	1H	3005	1/1	0.94	0.31	53,53,53,53	0
58	MG	1G	1619	1/1	0.94	0.24	92,92,92,92	0
58	MG	13	1624	1/1	0.94	0.29	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1747	1/1	0.94	0.07	96,96,96,96	0
58	MG	1G	1691	1/1	0.94	0.19	89,89,89,89	0
58	MG	1H	3518	1/1	0.94	0.13	94,94,94,94	0
58	MG	14	3053	1/1	0.94	0.19	45,45,45,45	0
58	MG	49	201	1/1	0.94	0.22	128,128,128,128	0
58	MG	1H	3458	1/1	0.94	0.12	45,45,45,45	0
58	MG	14	3062	1/1	0.94	0.35	75,75,75,75	0
58	MG	13	1625	1/1	0.94	0.15	82,82,82,82	0
58	MG	14	3177	1/1	0.94	0.20	84,84,84,84	0
58	MG	14	3073	1/1	0.94	0.25	91,91,91,91	0
58	MG	16	201	1/1	0.94	0.41	79,79,79,79	0
58	MG	13	1716	1/1	0.95	0.08	73,73,73,73	0
58	MG	14	3152	1/1	0.95	0.21	75,75,75,75	0
58	MG	1H	3369	1/1	0.95	0.18	55,55,55,55	0
58	MG	1H	3476	1/1	0.95	0.11	70,70,70,70	0
58	MG	14	3017	1/1	0.95	0.20	63,63,63,63	0
58	MG	1H	3300	1/1	0.95	0.31	72,72,72,72	0
58	MG	1H	3479	1/1	0.95	0.09	79,79,79,79	0
58	MG	13	1628	1/1	0.95	0.18	58,58,58,58	0
58	MG	1H	3375	1/1	0.95	0.05	81,81,81,81	0
58	MG	13	1740	1/1	0.95	0.10	70,70,70,70	0
58	MG	1H	3151	1/1	0.95	0.28	73,73,73,73	0
58	MG	1H	3380	1/1	0.95	0.12	77,77,77,77	0
58	MG	13	1635	1/1	0.95	0.19	48,48,48,48	0
58	MG	13	1649	1/1	0.95	0.17	79,79,79,79	0
58	MG	1H	3307	1/1	0.95	0.24	60,60,60,60	0
58	MG	1H	3028	1/1	0.95	0.32	64,64,64,64	0
58	MG	1G	1634	1/1	0.95	0.15	84,84,84,84	0
58	MG	1H	3106	1/1	0.95	0.17	49,49,49,49	0
58	MG	1H	3390	1/1	0.95	0.12	56,56,56,56	0
58	MG	1H	3256	1/1	0.95	0.15	58,58,58,58	0
58	MG	1G	1638	1/1	0.95	0.30	84,84,84,84	0
58	MG	1H	3029	1/1	0.95	0.31	72,72,72,72	0
58	MG	14	3036	1/1	0.95	0.19	67,67,67,67	0
58	MG	1H	3158	1/1	0.95	0.11	44,44,44,44	0
58	MG	1G	1644	1/1	0.95	0.21	110,110,110,110	0
58	MG	1H	3053	1/1	0.95	0.37	66,66,66,66	0
58	MG	13	1744	1/1	0.95	0.08	89,89,89,89	0
58	MG	1H	3504	1/1	0.95	0.12	66,66,66,66	0
58	MG	14	3303	1/1	0.95	0.14	53,53,53,53	0
58	MG	1H	3505	1/1	0.95	0.09	41,41,41,41	0
58	MG	1H	3506	1/1	0.95	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3507	1/1	0.95	0.10	43,43,43,43	0
58	MG	1G	1653	1/1	0.95	0.29	78,78,78,78	0
58	MG	1H	3213	1/1	0.95	0.15	43,43,43,43	0
58	MG	13	1689	1/1	0.95	0.20	118,118,118,118	0
58	MG	14	3329	1/1	0.95	0.09	54,54,54,54	0
58	MG	14	3330	1/1	0.95	0.11	53,53,53,53	0
58	MG	13	1746	1/1	0.95	0.07	84,84,84,84	0
58	MG	1H	3066	1/1	0.95	0.25	48,48,48,48	0
58	MG	14	3194	1/1	0.95	0.13	61,61,61,61	0
58	MG	14	3057	1/1	0.95	0.21	62,62,62,62	0
58	MG	14	3059	1/1	0.95	0.13	55,55,55,55	0
58	MG	1H	3415	1/1	0.95	0.12	63,63,63,63	0
58	MG	14	3339	1/1	0.95	0.09	62,62,62,62	0
58	MG	14	3340	1/1	0.95	0.09	67,67,67,67	0
58	MG	1H	3068	1/1	0.95	0.17	50,50,50,50	0
58	MG	14	3063	1/1	0.95	0.22	70,70,70,70	0
58	MG	1H	3418	1/1	0.95	0.10	70,70,70,70	0
58	MG	14	3203	1/1	0.95	0.28	83,83,83,83	0
58	MG	14	3071	1/1	0.95	0.15	42,42,42,42	0
58	MG	1H	3071	1/1	0.95	0.18	39,39,39,39	0
58	MG	1H	3170	1/1	0.95	0.41	77,77,77,77	0
58	MG	1H	3173	1/1	0.95	0.24	65,65,65,65	0
58	MG	14	3360	1/1	0.95	0.07	69,69,69,69	0
58	MG	1H	3323	1/1	0.95	0.34	78,78,78,78	0
58	MG	1H	3324	1/1	0.95	0.18	76,76,76,76	0
58	MG	14	3081	1/1	0.95	0.21	80,80,80,80	0
58	MG	14	3364	1/1	0.95	0.08	75,75,75,75	0
58	MG	1G	1669	1/1	0.95	0.12	80,80,80,80	0
58	MG	1H	3073	1/1	0.95	0.24	73,73,73,73	0
58	MG	1H	3074	1/1	0.95	0.40	88,88,88,88	0
58	MG	1H	3124	1/1	0.95	0.18	39,39,39,39	0
58	MG	13	1650	1/1	0.95	0.27	72,72,72,72	0
58	MG	1H	3226	1/1	0.95	0.17	89,89,89,89	0
58	MG	1H	3276	1/1	0.95	0.12	55,55,55,55	0
58	MG	13	1727	1/1	0.95	0.09	55,55,55,55	0
58	MG	14	3094	1/1	0.95	0.12	76,76,76,76	0
58	MG	14	3224	1/1	0.95	0.19	77,77,77,77	0
58	MG	14	3225	1/1	0.95	0.20	57,57,57,57	0
58	MG	13	1681	1/1	0.95	0.11	66,66,66,66	0
58	MG	1H	3444	1/1	0.95	0.09	82,82,82,82	0
58	MG	1H	3037	1/1	0.95	0.30	62,62,62,62	0
58	MG	14	3099	1/1	0.95	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3102	1/1	0.95	0.19	73,73,73,73	0
58	MG	14	3382	1/1	0.95	0.09	81,81,81,81	0
58	MG	14	3103	1/1	0.95	0.32	78,78,78,78	0
58	MG	11	302	1/1	0.95	0.12	35,35,35,35	0
58	MG	2I	201	1/1	0.95	0.17	77,77,77,77	0
58	MG	1H	3232	1/1	0.95	0.11	72,72,72,72	0
58	MG	1H	3452	1/1	0.95	0.08	74,74,74,74	0
58	MG	1H	3134	1/1	0.95	0.22	50,50,50,50	0
58	MG	13	1730	1/1	0.95	0.07	67,67,67,67	0
58	MG	1H	3455	1/1	0.95	0.15	66,66,66,66	0
58	MG	1H	3456	1/1	0.95	0.08	80,80,80,80	0
58	MG	13	1613	1/1	0.95	0.27	83,83,83,83	0
58	MG	13	1734	1/1	0.95	0.07	100,100,100,100	0
58	MG	1H	3083	1/1	0.95	0.30	68,68,68,68	0
58	MG	14	3247	1/1	0.95	0.26	85,85,85,85	0
58	MG	1H	3139	1/1	0.95	0.25	52,52,52,52	0
58	MG	14	3249	1/1	0.95	0.23	65,65,65,65	0
58	MG	1H	3462	1/1	0.95	0.09	79,79,79,79	0
58	MG	1H	3085	1/1	0.95	0.13	69,69,69,69	0
58	MG	14	3130	1/1	0.95	0.29	85,85,85,85	0
58	MG	14	3405	1/1	0.95	0.17	75,75,75,75	0
58	MG	1H	3142	1/1	0.95	0.21	39,39,39,39	0
58	MG	1H	3143	1/1	0.95	0.22	50,50,50,50	0
58	MG	1H	3244	1/1	0.95	0.38	98,98,98,98	0
58	MG	14	3002	1/1	0.95	0.23	64,64,64,64	0
58	MG	1H	3467	1/1	0.95	0.18	69,69,69,69	0
58	MG	14	3142	1/1	0.95	0.36	88,88,88,88	0
58	MG	13	1667	1/1	0.95	0.22	82,82,82,82	0
58	MG	1H	3351	1/1	0.95	0.15	53,53,53,53	0
58	MG	1H	3296	1/1	0.95	0.22	72,72,72,72	0
58	MG	13	1611	1/1	0.95	0.28	71,71,71,71	0
58	MG	14	3267	1/1	0.95	0.13	79,79,79,79	0
58	MG	2K	104	1/1	0.95	0.12	80,80,80,80	0
58	MG	1H	3361	1/1	0.95	0.09	64,64,64,64	0
58	MG	14	3150	1/1	0.95	0.18	50,50,50,50	0
58	MG	14	3041	1/1	0.96	0.18	66,66,66,66	0
58	MG	1G	1654	1/1	0.96	0.23	85,85,85,85	0
58	MG	1H	3168	1/1	0.96	0.20	64,64,64,64	0
58	MG	1H	3450	1/1	0.96	0.10	62,62,62,62	0
58	MG	1H	3357	1/1	0.96	0.10	35,35,35,35	0
58	MG	1H	3129	1/1	0.96	0.09	63,63,63,63	0
58	MG	1H	3088	1/1	0.96	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3174	1/1	0.96	0.17	84,84,84,84	0
58	MG	1H	3364	1/1	0.96	0.14	47,47,47,47	0
58	MG	1H	3171	1/1	0.96	0.15	58,58,58,58	0
58	MG	1H	3172	1/1	0.96	0.35	79,79,79,79	0
58	MG	13	1639	1/1	0.96	0.16	55,55,55,55	0
58	MG	1G	1664	1/1	0.96	0.14	92,92,92,92	0
58	MG	13	1729	1/1	0.96	0.12	86,86,86,86	0
58	MG	1G	1666	1/1	0.96	0.15	84,84,84,84	0
58	MG	1H	3374	1/1	0.96	0.07	90,90,90,90	0
58	MG	1H	3461	1/1	0.96	0.13	51,51,51,51	0
58	MG	1H	3055	1/1	0.96	0.31	85,85,85,85	0
58	MG	14	3068	1/1	0.96	0.16	60,60,60,60	0
58	MG	14	3069	1/1	0.96	0.18	60,60,60,60	0
58	MG	14	3187	1/1	0.96	0.14	47,47,47,47	0
58	MG	13	1626	1/1	0.96	0.33	90,90,90,90	0
58	MG	1H	3377	1/1	0.96	0.09	61,61,61,61	0
58	MG	14	3310	1/1	0.96	0.07	56,56,56,56	0
58	MG	14	3192	1/1	0.96	0.11	59,59,59,59	0
58	MG	14	3313	1/1	0.96	0.08	48,48,48,48	0
58	MG	13	1629	1/1	0.96	0.24	69,69,69,69	0
58	MG	14	3318	1/1	0.96	0.10	47,47,47,47	0
58	MG	14	3319	1/1	0.96	0.16	65,65,65,65	0
58	MG	1H	3096	1/1	0.96	0.21	50,50,50,50	0
58	MG	1H	3064	1/1	0.96	0.18	43,43,43,43	0
58	MG	14	3327	1/1	0.96	0.06	58,58,58,58	0
58	MG	1H	3181	1/1	0.96	0.23	63,63,63,63	0
58	MG	1H	3182	1/1	0.96	0.34	61,61,61,61	0
58	MG	14	3331	1/1	0.96	0.09	56,56,56,56	0
58	MG	14	3078	1/1	0.96	0.18	63,63,63,63	0
58	MG	14	3199	1/1	0.96	0.35	96,96,96,96	0
58	MG	1H	3386	1/1	0.96	0.14	50,50,50,50	0
58	MG	1H	3225	1/1	0.96	0.19	79,79,79,79	0
58	MG	13	1614	1/1	0.96	0.23	86,86,86,86	0
58	MG	1H	3227	1/1	0.96	0.35	87,87,87,87	0
58	MG	14	3085	1/1	0.96	0.21	52,52,52,52	0
58	MG	13	1735	1/1	0.96	0.12	84,84,84,84	0
58	MG	14	3207	1/1	0.96	0.12	68,68,68,68	0
58	MG	1G	1683	1/1	0.96	0.07	61,61,61,61	0
58	MG	1H	3102	1/1	0.96	0.24	60,60,60,60	0
58	MG	1G	1686	1/1	0.96	0.10	84,84,84,84	0
58	MG	14	3212	1/1	0.96	0.17	75,75,75,75	0
58	MG	1H	3104	1/1	0.96	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1603	1/1	0.96	0.18	87,87,87,87	0
58	MG	14	3357	1/1	0.96	0.10	69,69,69,69	0
58	MG	14	3095	1/1	0.96	0.13	83,83,83,83	0
58	MG	1G	1690	1/1	0.96	0.12	104,104,104,104	0
58	MG	1H	3396	1/1	0.96	0.07	69,69,69,69	0
58	MG	1H	3070	1/1	0.96	0.31	68,68,68,68	0
58	MG	13	1748	1/1	0.96	0.10	82,82,82,82	0
58	MG	1H	3402	1/1	0.96	0.09	53,53,53,53	0
58	MG	1G	1608	1/1	0.96	0.16	72,72,72,72	0
58	MG	1H	3189	1/1	0.96	0.14	61,61,61,61	0
58	MG	1H	3107	1/1	0.96	0.18	52,52,52,52	0
58	MG	14	3107	1/1	0.96	0.20	58,58,58,58	0
58	MG	1H	3486	1/1	0.96	0.14	50,50,50,50	0
58	MG	1H	3408	1/1	0.96	0.14	49,49,49,49	0
58	MG	14	3114	1/1	0.96	0.36	79,79,79,79	0
58	MG	1H	3410	1/1	0.96	0.10	33,33,33,33	0
58	MG	1G	1615	1/1	0.96	0.17	85,85,85,85	0
58	MG	14	3374	1/1	0.96	0.10	86,86,86,86	0
58	MG	1H	3412	1/1	0.96	0.09	50,50,50,50	0
58	MG	14	3120	1/1	0.96	0.07	54,54,54,54	0
58	MG	1H	3108	1/1	0.96	0.12	50,50,50,50	0
58	MG	1H	3072	1/1	0.96	0.26	61,61,61,61	0
58	MG	1H	3004	1/1	0.96	0.35	68,68,68,68	0
58	MG	1G	1622	1/1	0.96	0.21	81,81,81,81	0
58	MG	14	3125	1/1	0.96	0.20	70,70,70,70	0
58	MG	14	3008	1/1	0.96	0.19	65,65,65,65	0
58	MG	1H	3416	1/1	0.96	0.11	67,67,67,67	0
58	MG	1H	3238	1/1	0.96	0.65	52,52,52,52	0
58	MG	1H	3239	1/1	0.96	0.10	67,67,67,67	0
58	MG	14	3132	1/1	0.96	0.15	44,44,44,44	0
58	MG	14	3388	1/1	0.96	0.10	79,79,79,79	0
58	MG	1H	3498	1/1	0.96	0.11	47,47,47,47	0
58	MG	14	3136	1/1	0.96	0.25	49,49,49,49	0
58	MG	1H	3111	1/1	0.96	0.27	44,44,44,44	0
58	MG	1G	1629	1/1	0.96	0.28	96,96,96,96	0
58	MG	1H	3152	1/1	0.96	0.27	71,71,71,71	0
58	MG	13	1658	1/1	0.96	0.26	92,92,92,92	0
58	MG	13	1659	1/1	0.96	0.36	68,68,68,68	0
58	MG	1H	3425	1/1	0.96	0.16	49,49,49,49	0
58	MG	5E	201	1/1	0.96	0.21	67,67,67,67	0
58	MG	1H	3201	1/1	0.96	0.16	41,41,41,41	0
58	MG	1H	3115	1/1	0.96	0.21	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1632	1/1	0.96	0.24	71,71,71,71	0
58	MG	13	1645	1/1	0.96	0.26	69,69,69,69	0
58	MG	1G	1640	1/1	0.96	0.14	83,83,83,83	0
58	MG	1H	3435	1/1	0.96	0.08	82,82,82,82	0
58	MG	13	1637	1/1	0.96	0.12	66,66,66,66	0
58	MG	1K	101	1/1	0.96	0.08	85,85,85,85	0
58	MG	1J	201	1/1	0.96	0.40	76,76,76,76	0
58	MG	1G	1645	1/1	0.96	0.19	142,142,142,142	0
58	MG	1H	3013	1/1	0.96	0.23	52,52,52,52	0
58	MG	14	3270	1/1	0.96	0.20	95,95,95,95	0
58	MG	1H	3516	1/1	0.96	0.07	86,86,86,86	0
58	MG	1H	3517	1/1	0.96	0.13	57,57,57,57	0
58	MG	1H	3050	1/1	0.96	0.27	63,63,63,63	0
58	MG	1H	3349	1/1	0.96	0.14	40,40,40,40	0
58	MG	1H	3032	1/1	0.96	0.23	82,82,82,82	0
58	MG	J5	101	1/1	0.96	0.11	52,52,52,52	0
59	PAR	1G	1697	42/42	0.96	0.19	75,80,88,91	0
60	ZN	5I	103	1/1	0.96	0.18	91,91,91,91	0
58	MG	14	3037	1/1	0.96	0.16	82,82,82,82	0
58	MG	1G	1652	1/1	0.96	0.19	81,81,81,81	0
58	MG	1K	102	1/1	0.96	0.21	72,72,72,72	0
58	MG	14	3040	1/1	0.96	0.15	82,82,82,82	0
58	MG	1H	3362	1/1	0.97	0.15	41,41,41,41	0
58	MG	1H	3363	1/1	0.97	0.14	40,40,40,40	0
58	MG	16	211	1/1	0.97	0.09	70,70,70,70	0
58	MG	13	1724	1/1	0.97	0.11	96,96,96,96	0
58	MG	14	3072	1/1	0.97	0.22	74,74,74,74	0
58	MG	1H	3366	1/1	0.97	0.14	56,56,56,56	0
58	MG	14	3238	1/1	0.97	0.11	86,86,86,86	0
58	MG	1H	3116	1/1	0.97	0.37	51,51,51,51	0
58	MG	1H	3145	1/1	0.97	0.38	76,76,76,76	0
58	MG	14	3241	1/1	0.97	0.28	80,80,80,80	0
58	MG	1H	3482	1/1	0.97	0.10	54,54,54,54	0
58	MG	14	3342	1/1	0.97	0.09	49,49,49,49	0
58	MG	14	3005	1/1	0.97	0.28	60,60,60,60	0
58	MG	21	301	1/1	0.97	0.27	54,54,54,54	0
58	MG	14	3080	1/1	0.97	0.21	62,62,62,62	0
58	MG	14	3351	1/1	0.97	0.18	87,87,87,87	0
58	MG	1H	3483	1/1	0.97	0.07	90,90,90,90	0
58	MG	1H	3370	1/1	0.97	0.07	55,55,55,55	0
58	MG	13	1638	1/1	0.97	0.25	62,62,62,62	0
58	MG	1H	3069	1/1	0.97	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3432	1/1	0.97	0.10	70,70,70,70	0
58	MG	1H	3260	1/1	0.97	0.22	35,35,35,35	0
58	MG	1H	3490	1/1	0.97	0.10	64,64,64,64	0
58	MG	13	1621	1/1	0.97	0.14	74,74,74,74	0
58	MG	1H	3328	1/1	0.97	0.25	56,56,56,56	0
58	MG	1H	3437	1/1	0.97	0.18	54,54,54,54	0
58	MG	14	3093	1/1	0.97	0.18	63,63,63,63	0
58	MG	1H	3014	1/1	0.97	0.15	58,58,58,58	0
58	MG	1H	3263	1/1	0.97	0.49	56,56,56,56	0
58	MG	14	3260	1/1	0.97	0.20	100,100,100,100	0
58	MG	14	3021	1/1	0.97	0.23	73,73,73,73	0
58	MG	13	1603	1/1	0.97	0.34	50,50,50,50	0
58	MG	14	3264	1/1	0.97	0.19	77,77,77,77	0
58	MG	13	1663	1/1	0.97	0.34	62,62,62,62	0
58	MG	13	1623	1/1	0.97	0.23	62,62,62,62	0
58	MG	14	3101	1/1	0.97	0.15	65,65,65,65	0
58	MG	13	1714	1/1	0.97	0.12	45,45,45,45	0
58	MG	1H	3103	1/1	0.97	0.20	58,58,58,58	0
58	MG	1H	3501	1/1	0.97	0.09	42,42,42,42	0
58	MG	1H	3336	1/1	0.97	0.13	62,62,62,62	0
58	MG	14	3189	1/1	0.97	0.15	46,46,46,46	0
58	MG	1H	3451	1/1	0.97	0.10	55,55,55,55	0
58	MG	14	3108	1/1	0.97	0.23	50,50,50,50	0
58	MG	13	1602	1/1	0.97	0.27	49,49,49,49	0
58	MG	1H	3003	1/1	0.97	0.24	49,49,49,49	0
58	MG	14	3113	1/1	0.97	0.23	62,62,62,62	0
58	MG	1G	1612	1/1	0.97	0.22	83,83,83,83	0
58	MG	1H	3391	1/1	0.97	0.05	60,60,60,60	0
58	MG	1G	1673	1/1	0.97	0.09	92,92,92,92	0
58	MG	1H	3304	1/1	0.97	0.12	71,71,71,71	0
58	MG	13	1620	1/1	0.97	0.30	72,72,72,72	0
58	MG	13	1719	1/1	0.97	0.10	67,67,67,67	0
58	MG	1G	1617	1/1	0.97	0.12	74,74,74,74	0
58	MG	1H	3395	1/1	0.97	0.14	36,36,36,36	0
58	MG	1H	3512	1/1	0.97	0.09	44,44,44,44	0
58	MG	13	1720	1/1	0.97	0.12	82,82,82,82	0
58	MG	1H	3397	1/1	0.97	0.08	49,49,49,49	0
58	MG	1H	3160	1/1	0.97	0.35	79,79,79,79	0
58	MG	13	1685	1/1	0.97	0.18	74,74,74,74	0
58	MG	1H	3190	1/1	0.97	0.25	69,69,69,69	0
58	MG	14	3210	1/1	0.97	0.14	51,51,51,51	0
58	MG	14	3131	1/1	0.97	0.28	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3058	1/1	0.97	0.24	36,36,36,36	0
58	MG	1H	3278	1/1	0.97	0.21	106,106,106,106	0
58	MG	14	3135	1/1	0.97	0.12	54,54,54,54	0
58	MG	13	1631	1/1	0.97	0.22	82,82,82,82	0
58	MG	1G	1689	1/1	0.97	0.10	84,84,84,84	0
58	MG	1H	3060	1/1	0.97	0.30	52,52,52,52	0
58	MG	1H	3350	1/1	0.97	0.09	51,51,51,51	0
58	MG	1J	203	1/1	0.97	0.18	100,100,100,100	0
58	MG	1H	3194	1/1	0.97	0.15	40,40,40,40	0
58	MG	1H	3140	1/1	0.97	0.30	69,69,69,69	0
58	MG	29	301	1/1	0.97	0.21	64,64,64,64	0
58	MG	29	302	1/1	0.97	0.19	57,57,57,57	0
58	MG	1H	3166	1/1	0.97	0.24	64,64,64,64	0
58	MG	1H	3061	1/1	0.97	0.28	56,56,56,56	0
58	MG	13	1668	1/1	0.97	0.18	66,66,66,66	0
58	MG	14	3315	1/1	0.97	0.16	57,57,57,57	0
58	MG	55	201	1/1	0.97	0.18	58,58,58,58	0
58	MG	1H	3286	1/1	0.97	0.15	71,71,71,71	0
58	MG	14	3226	1/1	0.97	0.20	67,67,67,67	0
59	PAR	13	1749	42/42	0.97	0.23	52,62,69,75	0
58	MG	14	3064	1/1	0.97	0.20	86,86,86,86	0
58	MG	14	3065	1/1	0.97	0.17	62,62,62,62	0
58	MG	14	3323	1/1	0.97	0.10	65,65,65,65	0
58	MG	14	3066	1/1	0.97	0.20	59,59,59,59	0
58	MG	14	3067	1/1	0.97	0.15	81,81,81,81	0
58	MG	14	3328	1/1	0.97	0.11	49,49,49,49	0
58	MG	1H	3065	1/1	0.98	0.21	43,43,43,43	0
58	MG	1H	3409	1/1	0.98	0.11	41,41,41,41	0
58	MG	14	3336	1/1	0.98	0.10	60,60,60,60	0
58	MG	G8	201	1/1	0.98	0.21	73,73,73,73	0
58	MG	1H	3502	1/1	0.98	0.11	66,66,66,66	0
58	MG	14	3112	1/1	0.98	0.19	65,65,65,65	0
58	MG	13	1715	1/1	0.98	0.12	89,89,89,89	0
58	MG	14	3341	1/1	0.98	0.14	41,41,41,41	0
58	MG	1H	3411	1/1	0.98	0.12	46,46,46,46	0
58	MG	1H	3067	1/1	0.98	0.25	46,46,46,46	0
58	MG	14	3052	1/1	0.98	0.23	59,59,59,59	0
58	MG	14	3347	1/1	0.98	0.11	48,48,48,48	0
58	MG	14	3117	1/1	0.98	0.22	57,57,57,57	0
58	MG	14	3349	1/1	0.98	0.14	62,62,62,62	0
58	MG	14	3350	1/1	0.98	0.08	92,92,92,92	0
58	MG	1H	3372	1/1	0.98	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3119	1/1	0.98	0.14	49,49,49,49	0
58	MG	14	3188	1/1	0.98	0.11	53,53,53,53	0
58	MG	14	3054	1/1	0.98	0.15	51,51,51,51	0
58	MG	14	3262	1/1	0.98	0.07	78,78,78,78	0
58	MG	14	3356	1/1	0.98	0.08	65,65,65,65	0
58	MG	14	3055	1/1	0.98	0.21	54,54,54,54	0
58	MG	1H	3008	1/1	0.98	0.33	68,68,68,68	0
58	MG	14	3359	1/1	0.98	0.08	73,73,73,73	0
58	MG	1H	3084	1/1	0.98	0.33	69,69,69,69	0
58	MG	1H	3132	1/1	0.98	0.27	62,62,62,62	0
58	MG	14	3061	1/1	0.98	0.20	58,58,58,58	0
58	MG	13	1732	1/1	0.98	0.07	78,78,78,78	0
58	MG	1H	3086	1/1	0.98	0.19	54,54,54,54	0
58	MG	14	3128	1/1	0.98	0.16	58,58,58,58	0
58	MG	14	3006	1/1	0.98	0.21	62,62,62,62	0
58	MG	1H	3087	1/1	0.98	0.22	75,75,75,75	0
58	MG	14	3200	1/1	0.98	0.22	94,94,94,94	0
58	MG	1H	3379	1/1	0.98	0.04	72,72,72,72	0
58	MG	13	1604	1/1	0.98	0.41	81,81,81,81	0
58	MG	1H	3291	1/1	0.98	0.14	86,86,86,86	0
58	MG	13	1640	1/1	0.98	0.10	64,64,64,64	0
58	MG	13	1718	1/1	0.98	0.09	69,69,69,69	0
58	MG	1H	3384	1/1	0.98	0.12	34,34,34,34	0
58	MG	1H	3429	1/1	0.98	0.05	72,72,72,72	0
58	MG	14	3139	1/1	0.98	0.22	63,63,63,63	0
58	MG	1H	3385	1/1	0.98	0.12	45,45,45,45	0
58	MG	1H	3057	1/1	0.98	0.18	44,44,44,44	0
58	MG	1H	3093	1/1	0.98	0.20	53,53,53,53	0
58	MG	1H	3433	1/1	0.98	0.04	73,73,73,73	0
58	MG	1H	3001	1/1	0.98	0.38	53,53,53,53	0
58	MG	1G	1621	1/1	0.98	0.10	90,90,90,90	0
58	MG	14	3079	1/1	0.98	0.20	73,73,73,73	0
58	MG	14	3384	1/1	0.98	0.07	68,68,68,68	0
58	MG	13	1726	1/1	0.98	0.08	93,93,93,93	0
58	MG	14	3291	1/1	0.98	0.18	70,70,70,70	0
58	MG	1H	3167	1/1	0.98	0.20	56,56,56,56	0
58	MG	14	3149	1/1	0.98	0.10	62,62,62,62	0
58	MG	1H	3353	1/1	0.98	0.15	40,40,40,40	0
58	MG	1H	3438	1/1	0.98	0.14	55,55,55,55	0
58	MG	1H	3117	1/1	0.98	0.14	43,43,43,43	0
58	MG	14	3222	1/1	0.98	0.21	75,75,75,75	0
58	MG	1H	3355	1/1	0.98	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1697	1/1	0.98	0.13	73,73,73,73	0
58	MG	14	3155	1/1	0.98	0.22	65,65,65,65	0
58	MG	1H	3097	1/1	0.98	0.33	69,69,69,69	0
58	MG	14	3302	1/1	0.98	0.24	83,83,83,83	0
58	MG	16	213	1/1	0.98	0.12	66,66,66,66	0
58	MG	14	3399	1/1	0.98	0.11	77,77,77,77	0
58	MG	14	3304	1/1	0.98	0.11	50,50,50,50	0
58	MG	14	3401	1/1	0.98	0.08	45,45,45,45	0
58	MG	14	3228	1/1	0.98	0.26	85,85,85,85	0
58	MG	1H	3489	1/1	0.98	0.17	53,53,53,53	0
58	MG	14	3308	1/1	0.98	0.07	46,46,46,46	0
58	MG	14	3309	1/1	0.98	0.14	59,59,59,59	0
58	MG	1H	3446	1/1	0.98	0.09	59,59,59,59	0
58	MG	14	3311	1/1	0.98	0.09	65,65,65,65	0
58	MG	14	3092	1/1	0.98	0.16	48,48,48,48	0
58	MG	13	1619	1/1	0.98	0.15	75,75,75,75	0
58	MG	14	3314	1/1	0.98	0.12	58,58,58,58	0
58	MG	1G	1684	1/1	0.98	0.09	70,70,70,70	0
58	MG	14	3316	1/1	0.98	0.10	62,62,62,62	0
58	MG	1H	3099	1/1	0.98	0.33	63,63,63,63	0
58	MG	1H	3062	1/1	0.98	0.17	44,44,44,44	0
58	MG	1H	3401	1/1	0.98	0.18	47,47,47,47	0
58	MG	14	3320	1/1	0.98	0.10	42,42,42,42	0
58	MG	13	1617	1/1	0.98	0.17	60,60,60,60	0
58	MG	14	3322	1/1	0.98	0.06	72,72,72,72	0
58	MG	1G	1639	1/1	0.98	0.16	80,80,80,80	0
58	MG	14	3325	1/1	0.98	0.09	76,76,76,76	0
58	MG	14	3100	1/1	0.98	0.23	66,66,66,66	0
58	MG	1H	3125	1/1	0.98	0.19	47,47,47,47	0
58	MG	14	3170	1/1	0.98	0.10	84,84,84,84	0
60	ZN	3E	303	1/1	0.98	0.44	97,97,97,97	0
58	MG	1H	3404	1/1	0.98	0.15	48,48,48,48	0
58	MG	1H	3176	1/1	0.98	0.30	82,82,82,82	0
58	MG	1G	1693	1/1	0.98	0.12	82,82,82,82	0
58	MG	14	3105	1/1	0.98	0.27	45,45,45,45	0
58	MG	1H	3407	1/1	0.98	0.12	43,43,43,43	0
58	MG	1H	3360	1/1	0.99	0.12	46,46,46,46	0
58	MG	1H	3126	1/1	0.99	0.28	60,60,60,60	0
58	MG	1H	3399	1/1	0.99	0.10	52,52,52,52	0
58	MG	13	1741	1/1	0.99	0.14	82,82,82,82	0
58	MG	1H	3090	1/1	0.99	0.11	37,37,37,37	0
58	MG	1H	3477	1/1	0.99	0.17	62,62,62,62	0

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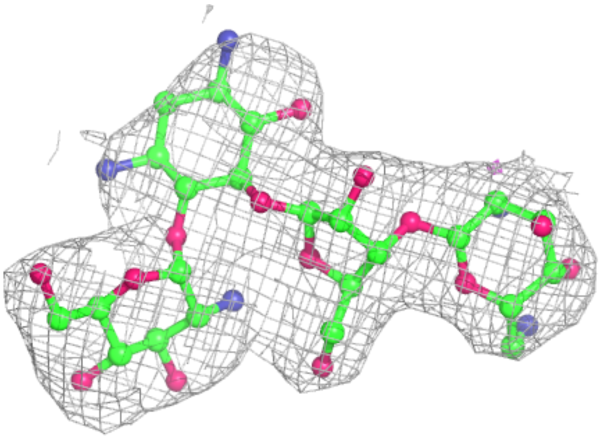
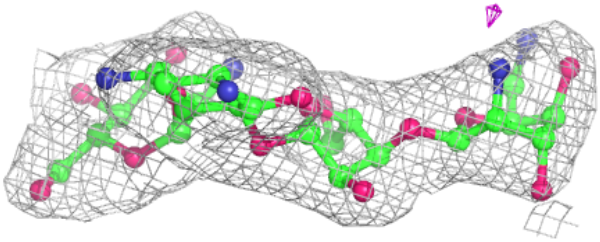
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3388	1/1	0.99	0.08	59,59,59,59	0
58	MG	14	3288	1/1	0.99	0.13	78,78,78,78	0
58	MG	14	3324	1/1	0.99	0.14	62,62,62,62	0
58	MG	13	1731	1/1	0.99	0.10	68,68,68,68	0
58	MG	1G	1641	1/1	0.99	0.13	98,98,98,98	0
58	MG	14	3257	1/1	0.99	0.17	58,58,58,58	0
58	MG	1H	3419	1/1	0.99	0.10	47,47,47,47	0
58	MG	14	3013	1/1	0.99	0.25	56,56,56,56	0
58	MG	1H	3365	1/1	0.99	0.10	44,44,44,44	0
58	MG	1H	3405	1/1	0.99	0.11	43,43,43,43	0
58	MG	14	3133	1/1	0.99	0.21	77,77,77,77	0
58	MG	13	1601	1/1	0.99	0.20	52,52,52,52	0
58	MG	1G	1694	1/1	0.99	0.12	67,67,67,67	0
58	MG	1H	3441	1/1	0.99	0.08	51,51,51,51	0
58	MG	1G	1623	1/1	0.99	0.22	91,91,91,91	0
58	MG	1H	3442	1/1	0.99	0.14	54,54,54,54	0
58	MG	1H	3123	1/1	0.99	0.29	49,49,49,49	0
58	MG	1H	3424	1/1	0.99	0.15	73,73,73,73	0
58	MG	14	3109	1/1	0.99	0.19	62,62,62,62	0
58	MG	2L	101	1/1	0.99	0.15	88,88,88,88	0
58	MG	14	3306	1/1	0.99	0.12	52,52,52,52	0
58	MG	14	3343	1/1	0.99	0.08	47,47,47,47	0
58	MG	1H	3445	1/1	0.99	0.11	44,44,44,44	0
58	MG	14	3345	1/1	0.99	0.14	51,51,51,51	0
58	MG	1H	3368	1/1	0.99	0.14	56,56,56,56	0
58	MG	1H	3356	1/1	0.99	0.12	52,52,52,52	0
58	MG	1H	3427	1/1	0.99	0.12	41,41,41,41	0
58	MG	1H	3002	1/1	0.99	0.22	60,60,60,60	0
58	MG	14	3056	1/1	0.99	0.26	58,58,58,58	0
58	MG	1H	3063	1/1	0.99	0.17	64,64,64,64	0
58	MG	14	3058	1/1	0.99	0.22	58,58,58,58	0
58	MG	14	3088	1/1	0.99	0.20	45,45,45,45	0
58	MG	1H	3358	1/1	1.00	0.09	43,43,43,43	0

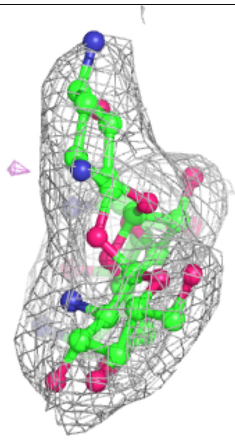
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR 1G 1697:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

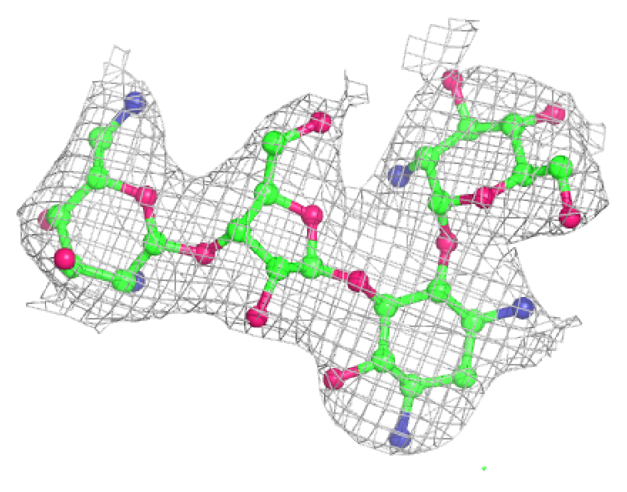


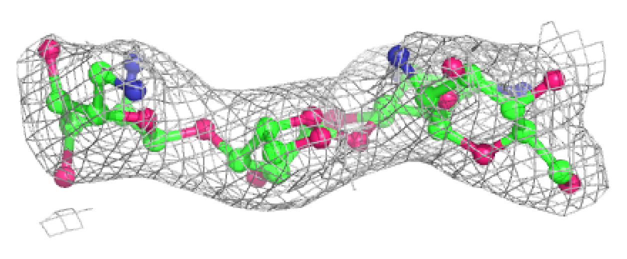


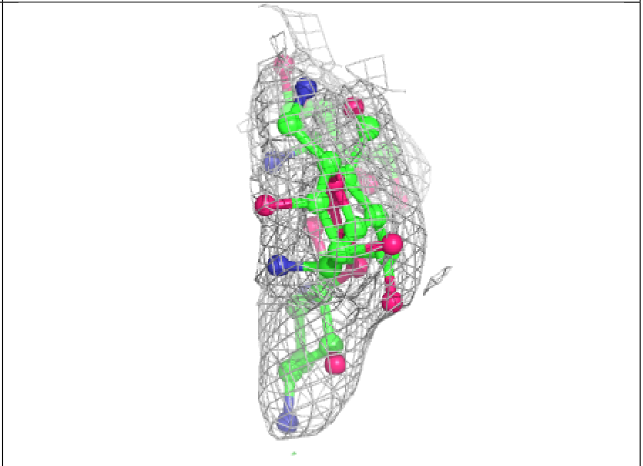


Electron density around PAR 13 1749:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers

There are no such residues in this entry.