wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2023 – 10:47 PM EDT

PDB ID	:	4TUB
Title	:	Crystal structure of tRNA-Thr bound to Codon ACC-C on the Ribosome
Authors	:	Fagan, C.E.; Dunham, C.M.
Deposited on	:	2014-06-24
Resolution	:	3.60 Å(reported)

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

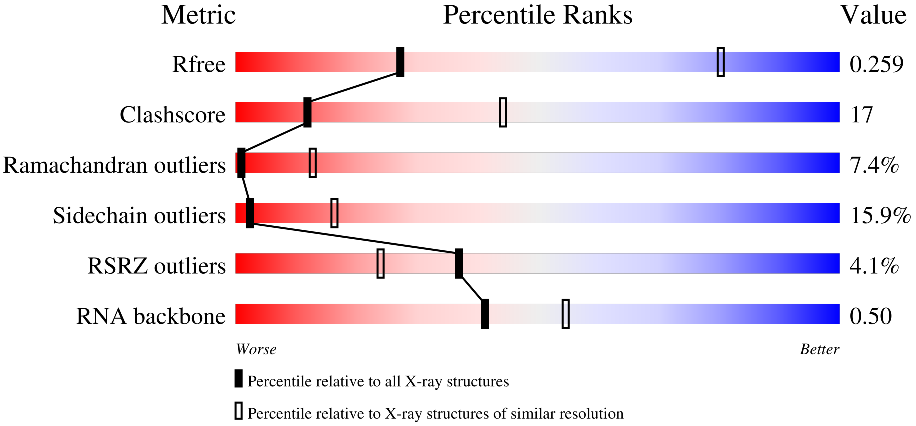
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance ⓘ

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

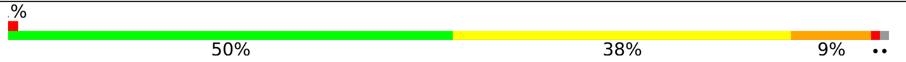
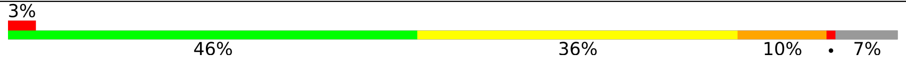
The reported resolution of this entry is 3.60 Å.

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.



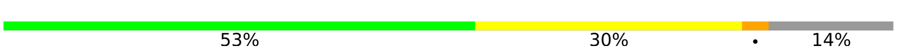
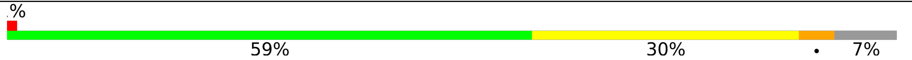
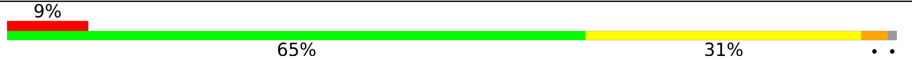
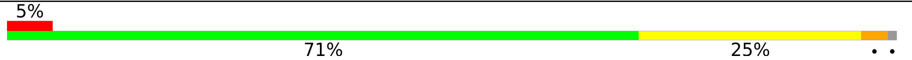
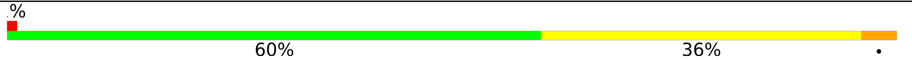
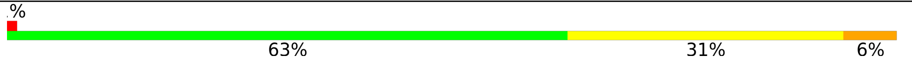
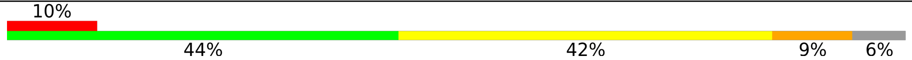
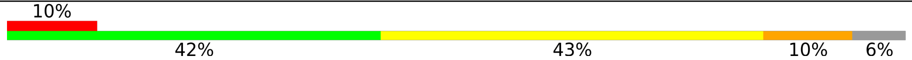
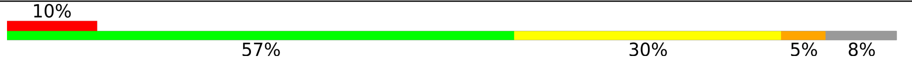
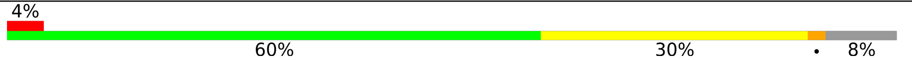
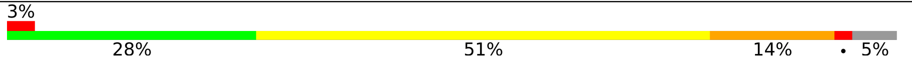
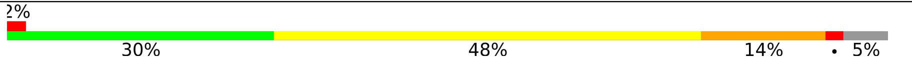
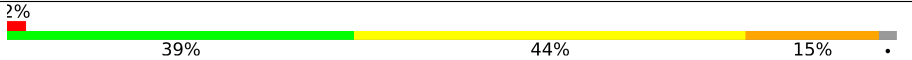
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	
1	XA	1522	
2	QB	256	
2	XB	256	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

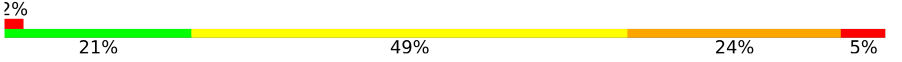
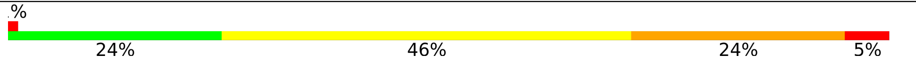
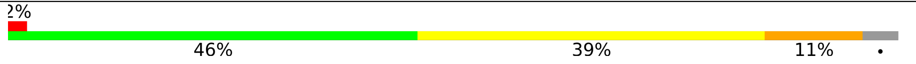
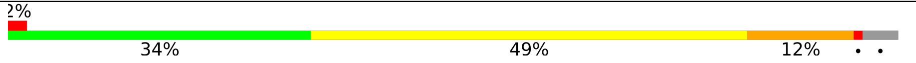
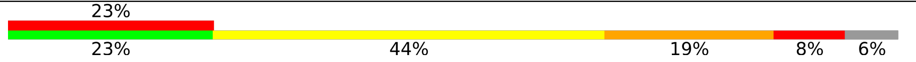
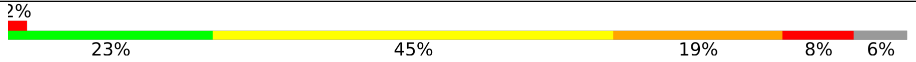
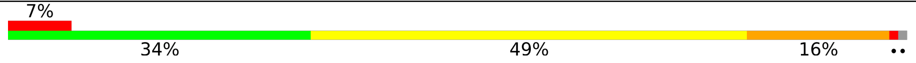
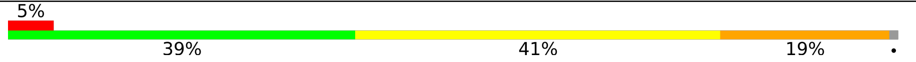
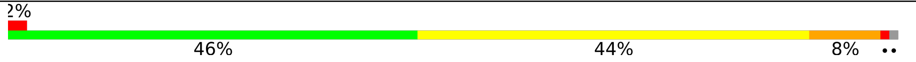
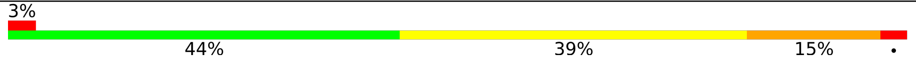
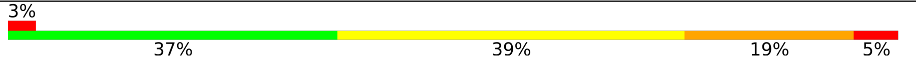
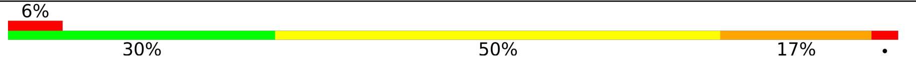
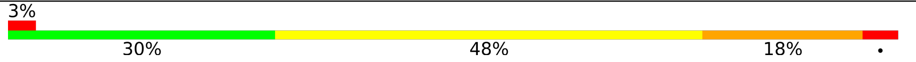
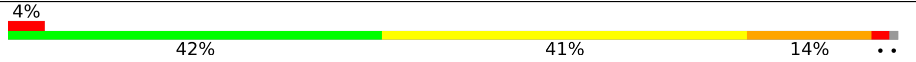
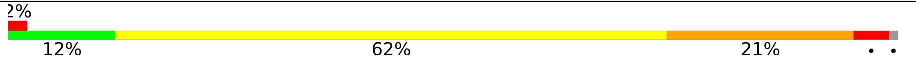
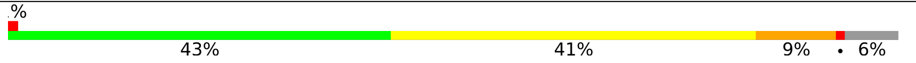
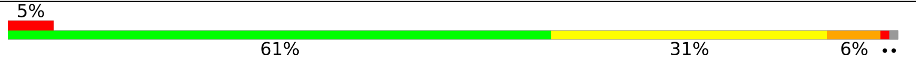
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	XO	89	% 66% 25% 8% •
16	QP	88	% 67% 24% 5% 5%
16	XP	88	% 53% 39% • 5%
17	QQ	105	59% 33% •• 5%
17	XQ	105	71% 20% • 5%
18	QR	88	5% 55% 18% 5% • 20%
18	XR	88	% 43% 33% • 20%
19	QS	93	5% 37% 34% 18% • 10%
19	XS	93	2% 33% 42% 12% • 10%
20	QT	106	2% 54% 34% 6% 7%
20	XT	106	8% 38% 47% 8% 7%
21	QU	27	7% 44% 48% 7%
21	XU	27	4% 67% 26% 7%
22	QV	77	% 48% 40% 12%
22	XV	77	% 64% 25% 12%
23	QX	25	24% 8% • 64%
23	XX	25	4% 28% 8% • 60%
24	QY	17	6% 71% 18% 6% 6%
24	XY	17	47% 47% 6%
25	RA	2915	4% 51% 36% 11% ••
25	YA	2915	4% 50% 38% 10% ••
26	RB	122	% 42% 43% 13% ••
26	YB	122	34% 44% 18% ••
27	RD	276	52% 37% 9% •
27	YD	276	29% 54% 14% ••

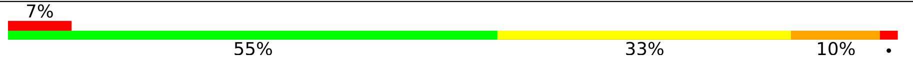
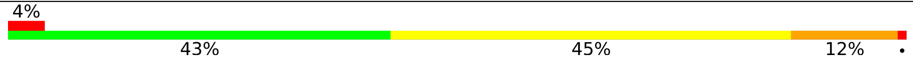
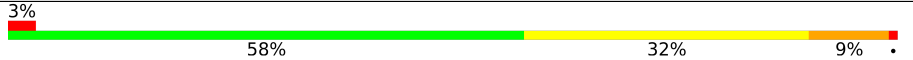
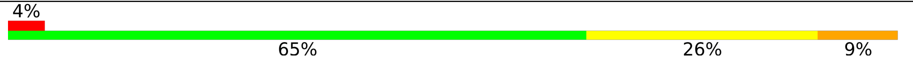
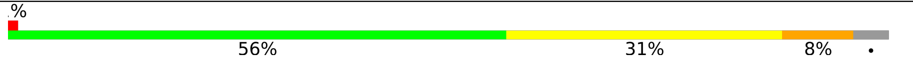
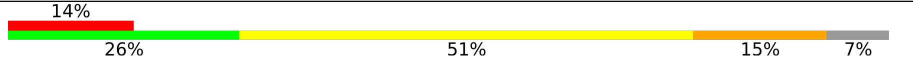
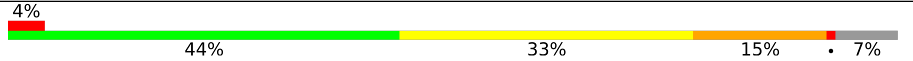
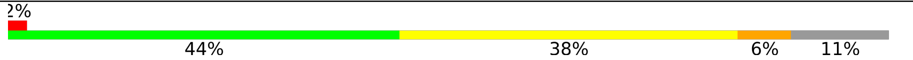
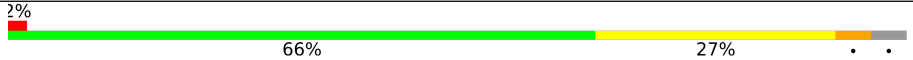
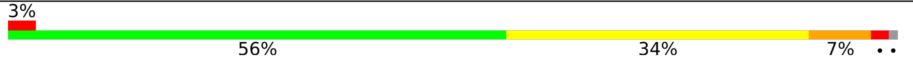
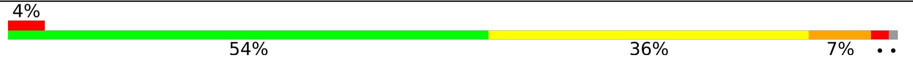
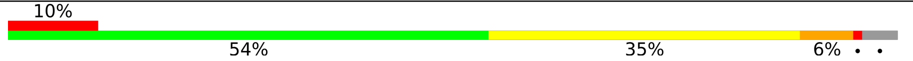
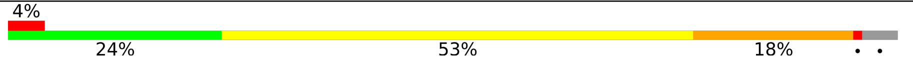
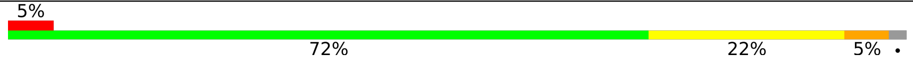
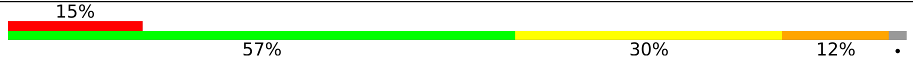
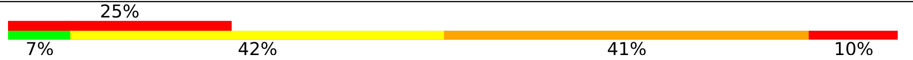
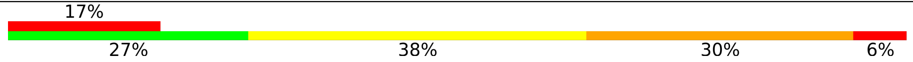
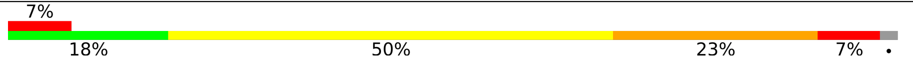
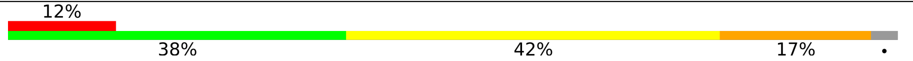
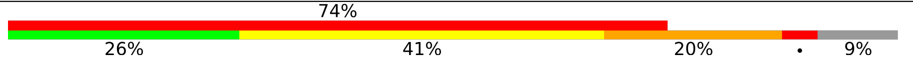
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	

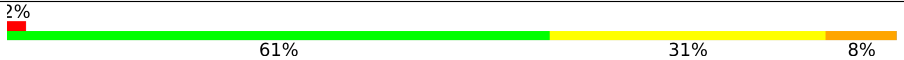
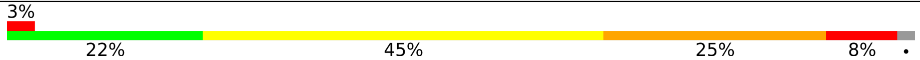
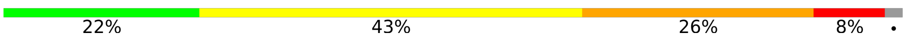
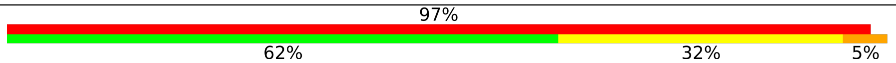
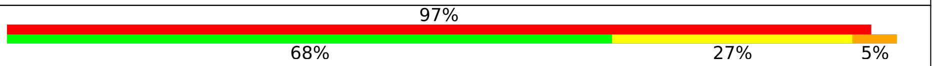
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z5	3	
56	Z6	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1603	-	-	-	X
57	MG	QA	1640	-	-	-	X
57	MG	QA	1656	-	-	-	X
57	MG	QA	1658	-	-	-	X
57	MG	QA	1661	-	-	-	X
57	MG	QA	1668	-	-	-	X
57	MG	QA	1673	-	-	-	X
57	MG	RA	3170	-	-	-	X
57	MG	RA	3197	-	-	-	X
57	MG	RA	3201	-	-	-	X
57	MG	RA	3209	-	-	-	X
57	MG	RA	3213	-	-	-	X
57	MG	RA	3251	-	-	-	X
57	MG	RA	3256	-	-	-	X
57	MG	RA	3264	-	-	-	X
57	MG	RA	3270	-	-	-	X
57	MG	RA	3271	-	-	-	X
57	MG	RA	3274	-	-	-	X
57	MG	RA	3280	-	-	-	X
57	MG	RA	3303	-	-	-	X
57	MG	RA	3308	-	-	-	X
57	MG	RA	3313	-	-	-	X
57	MG	RR	201	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	XA	1649	-	-	-	X
57	MG	XA	1662	-	-	-	X
57	MG	XA	1675	-	-	-	X
57	MG	XA	1706	-	-	-	X
57	MG	YA	3113	-	-	-	X
57	MG	YA	3117	-	-	-	X
57	MG	YA	3174	-	-	-	X
57	MG	YA	3175	-	-	-	X
57	MG	YA	3191	-	-	-	X
57	MG	YA	3194	-	-	-	X
57	MG	YA	3208	-	-	-	X
57	MG	YA	3216	-	-	-	X
57	MG	YA	3226	-	-	-	X
57	MG	YA	3227	-	-	-	X
57	MG	YA	3257	-	-	-	X
57	MG	YA	3283	-	-	-	X
57	MG	YA	3292	-	-	-	X
57	MG	YA	3295	-	-	-	X
57	MG	YA	3298	-	-	-	X
57	MG	YA	3302	-	-	-	X
57	MG	YA	3321	-	-	-	X
57	MG	YA	3333	-	-	-	X
57	MG	YA	3337	-	-	-	X
57	MG	YA	3339	-	-	-	X
57	MG	YA	3355	-	-	-	X
57	MG	YP	201	-	-	-	X

2 Entry composition ⓘ

There are 59 unique types of molecules in this entry. The entry contains 292320 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	QA	1500	32247	14353	5981	10414	1499	0	0	0
1	XA	1500	32249	14354	5984	10412	1499	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	QB	237	1924	1228	344	347	5	0	0	0
2	XB	237	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
			Total	C	N	O	S			
3	QC	205	1605	1011	313	280	1	0	0	0
3	XC	205	1605	1011	313	280	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	QD	208	1703	1066	339	291	7	0	0	0
4	XD	208	1703	1066	339	291	7	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	QE	151	Total C N O S 1155 729 218 204 4	0	0	0
5	XE	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	QF	101	Total C N O S 843 531 155 154 3	0	0	0
6	XF	101	Total C N O S 843 531 155 154 3	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	QG	155	Total C N O S 1257 781 252 218 6	0	0	0
7	XG	155	Total C N O S 1257 781 252 218 6	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	QH	138	Total C N O S 1116 705 215 193 3	0	0	0
8	XH	138	Total C N O S 1116 705 215 193 3	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	QI	127	Total C N O 1010 639 197 174	0	0	0
9	XI	127	Total C N O 1010 639 197 174	0	0	0

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total 885	C 549	N 168	O 165	S 3	0	0	0
11	XK	119	Total 885	C 549	N 168	O 165	S 3	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	121	Total 964	C 597	N 199	O 166	S 2	0	0	0
13	XM	121	Total 964	C 597	N 199	O 166	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	QN	60	Total 492	C 312	N 104	O 72	S 4	0	0	0
14	XN	60	Total 492	C 312	N 104	O 72	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total 734	C 459	N 147	O 126	S 2	0	0	0
15	XO	88	Total 734	C 459	N 147	O 126	S 2	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	QU	25	217	134	52	31	0	0	0
21	XU	25	217	134	52	31	0	0	0

- Molecule 22 is a RNA chain called P-site tRNA f-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	QV	77	1644	732	297	538	77	0	0	0
22	XV	77	1644	732	297	538	77	0	0	0

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	QX	9	191	86	36	60	9	0	0	0
23	XX	10	213	96	41	66	10	0	0	0

- Molecule 24 is a RNA chain called A-site tRNA Thr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	QY	16	344	153	62	113	16	0	0	0
24	XY	16	344	153	62	113	16	0	0	0

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	RA	2882	62071	27627	11611	19952	2881	0	0	0
25	YA	2882	62071	27627	11611	19952	2881	0	0	0

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	RB	120	2573	1146	476	832	119	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	YB	120	Total C N O P 2573 1146 476 832 119	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	RD	272	Total C N O S 2115 1335 420 357 3	0	0	0
27	YD	272	Total C N O S 2115 1335 420 357 3	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	RE	205	Total C N O S 1568 991 300 271 6	0	0	0
28	YE	205	Total C N O S 1568 991 300 271 6	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	RF	202	Total C N O S 1585 1011 297 275 2	0	0	0
29	YF	202	Total C N O S 1585 1011 297 275 2	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	RG	181	Total C N O S 1474 942 268 260 4	0	0	0
30	YG	181	Total C N O S 1474 942 268 260 4	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	RH	170	Total C N O S 1307 829 245 232 1	0	0	0
31	YH	170	Total C N O S 1307 829 245 232 1	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
32	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
33	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
35	YP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RR	118	Total 968	C 604	N 203	O 160	S 1	0	0	0
37	YR	118	Total 968	C 604	N 203	O 160	S 1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	RS	111	Total 882	C 556	N 176	O 150	0	0	0
38	YS	111	Total 882	C 556	N 176	O 150	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RT	137	Total 1141	C 710	N 234	O 196	S 1	0	0	0
39	YT	137	Total 1141	C 710	N 234	O 196	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0
40	YU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RV	101	Total 779	C 501	N 142	O 135	S 1	0	0	0
41	YV	101	Total 779	C 501	N 142	O 135	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RW	113	Total 900	C 566	N 177	O 155	S 2	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			
43	YX	92	Total	C	N	O	0	0	0
			725	471	131	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
44	YY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
45	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			
46	Y0	82	Total	C	N	O	S	0	0	0
			647	401	137	108	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
47	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	R2	69	Total C N O S 581 358 118 104 1	0	0	0
48	Y2	69	Total C N O S 581 358 118 104 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	R3	59	Total C N O 469 298 90 81	0	0	0
49	Y3	59	Total C N O 469 298 90 81	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
50	R4	71	Total C N O S 581 364 108 104 5	0	0	0
50	Y4	71	Total C N O S 581 364 108 104 5	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
51	R5	59	Total C N O S 459 288 90 76 5	0	0	0
51	Y5	58	Total C N O S 454 285 89 75 5	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	R6	49	Total C N O S 424 264 87 69 4	0	0	0
52	Y6	49	Total C N O S 424 264 87 69 4	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
53	R7	49	Total C N O S 430 263 108 57 2	0	0	0
53	Y7	49	Total C N O S 430 263 108 57 2	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
54	R8	64	Total C N O S 517 331 102 82 2	0	0	0
54	Y8	64	Total C N O S 517 331 102 82 2	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
55	R9	37	Total C N O S 307 188 68 47 4	0	0	0
55	Y9	37	Total C N O S 307 188 68 47 4	0	0	0

- Molecule 56 is a RNA chain called CC-Puro.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
56	Z5	3	Total C N O P 74 40 13 19 2	0	0	0
56	Z6	3	Total C N O P 74 40 13 19 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QA	80	Total Mg 80 80	0	0
57	QE	1	Total Mg 1 1	0	0
57	QF	1	Total Mg 1 1	0	0
57	QM	1	Total Mg 1 1	0	0
57	QV	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

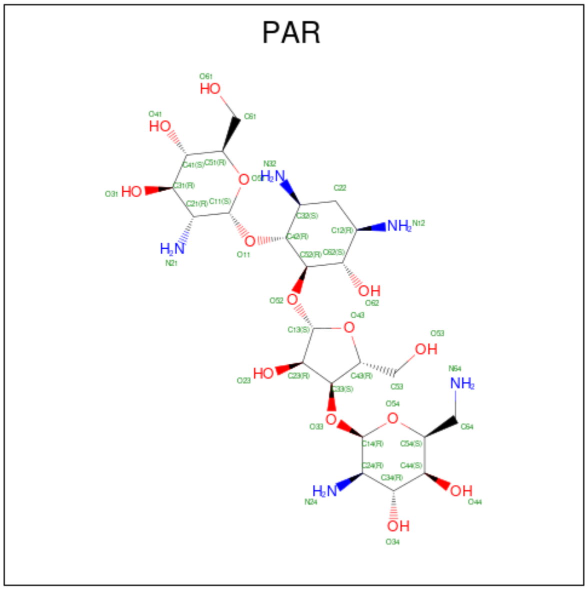
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QX	2	Total 2	Mg 2	0	0
57	QY	1	Total 1	Mg 1	0	0
57	RA	326	Total 326	Mg 326	0	0
57	RB	5	Total 5	Mg 5	0	0
57	RE	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	XA	110	Total 110	Mg 110	0	0
57	XB	1	Total 1	Mg 1	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XV	2	Total 2	Mg 2	0	0
57	XX	1	Total 1	Mg 1	0	0
57	YA	356	Total 356	Mg 356	0	0
57	YB	4	Total 4	Mg 4	0	0
57	YD	1	Total 1	Mg 1	0	0
57	YE	2	Total 2	Mg 2	0	0
57	YP	3	Total 3	Mg 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	YQ	1	Total Mg 1 1	0	0
57	YU	1	Total Mg 1 1	0	0
57	YY	1	Total Mg 1 1	0	0
57	Y0	3	Total Mg 3 3	0	0
57	Y1	1	Total Mg 1 1	0	0
57	Y3	1	Total Mg 1 1	0	0
57	Y5	1	Total Mg 1 1	0	0
57	Y7	1	Total Mg 1 1	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	QA	1	Total C N O 42 23 5 14	0	0
58	XA	1	Total C N O 42 23 5 14	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

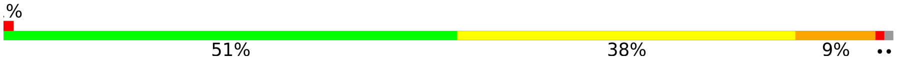
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	QD	1	Total Zn 1 1	0	0
59	QN	1	Total Zn 1 1	0	0
59	XD	1	Total Zn 1 1	0	0
59	XN	1	Total Zn 1 1	0	0

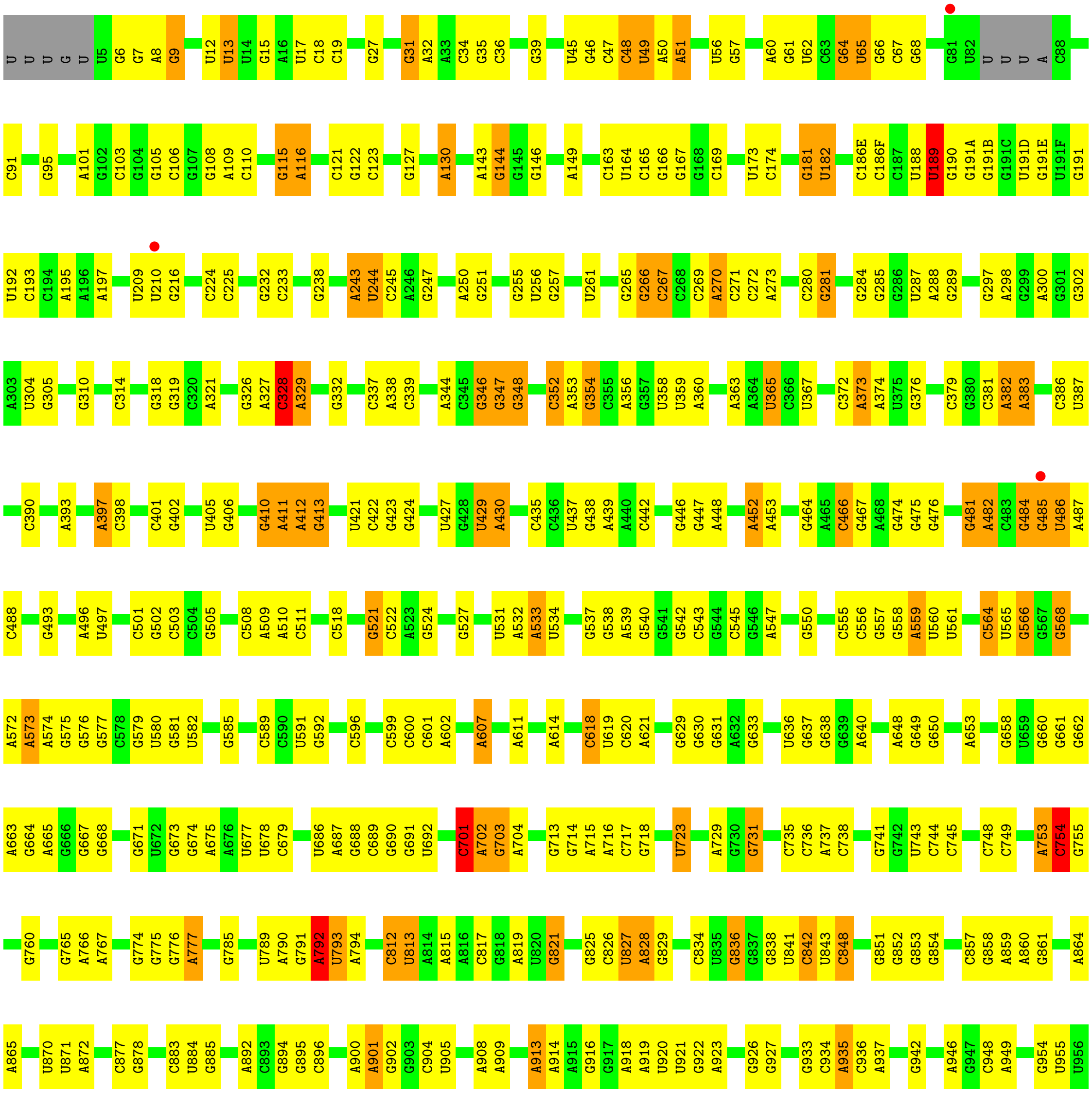
3 Residue-property plots ⓘ

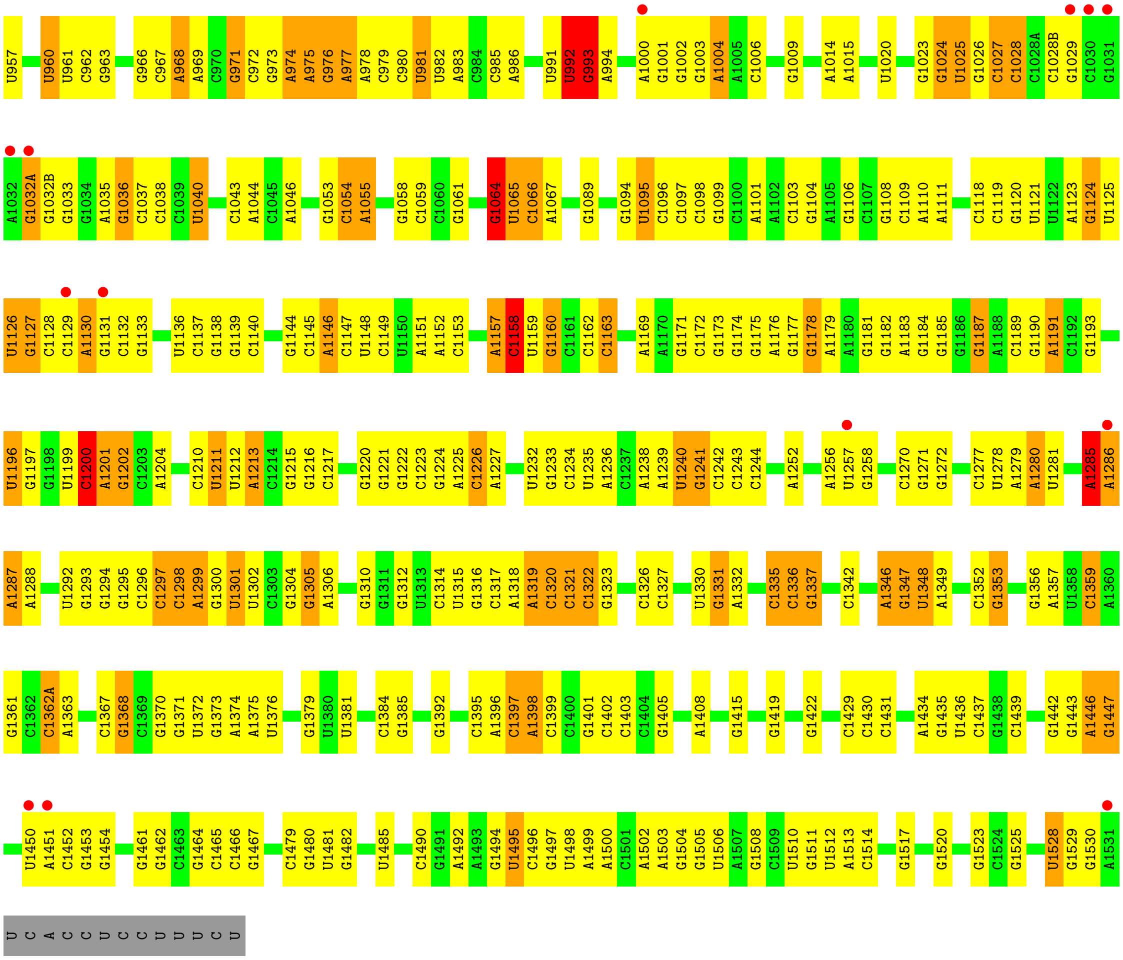
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S rRNA

Chain QA:

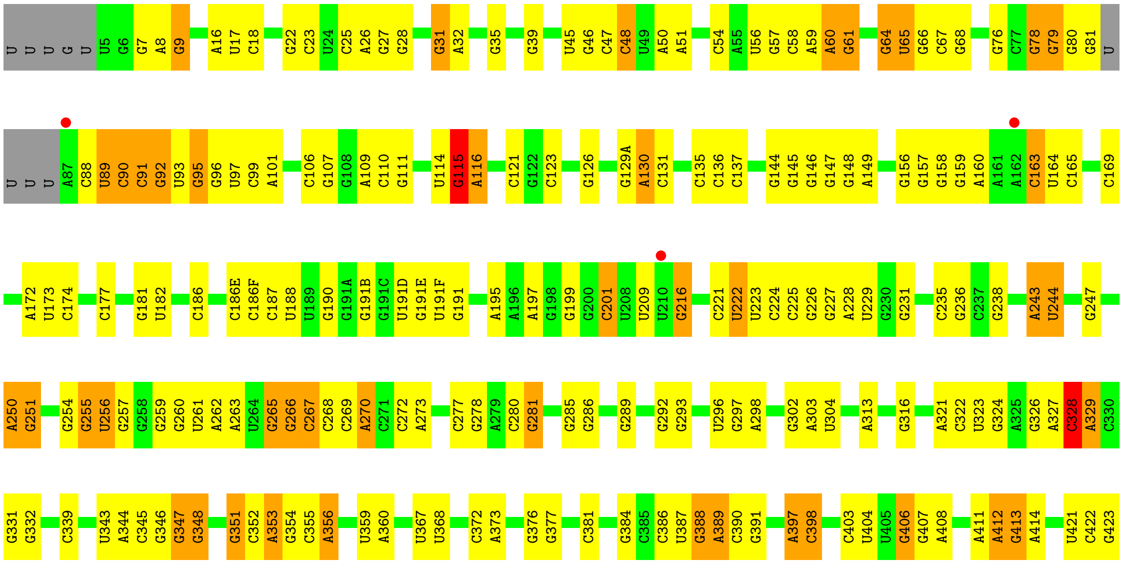


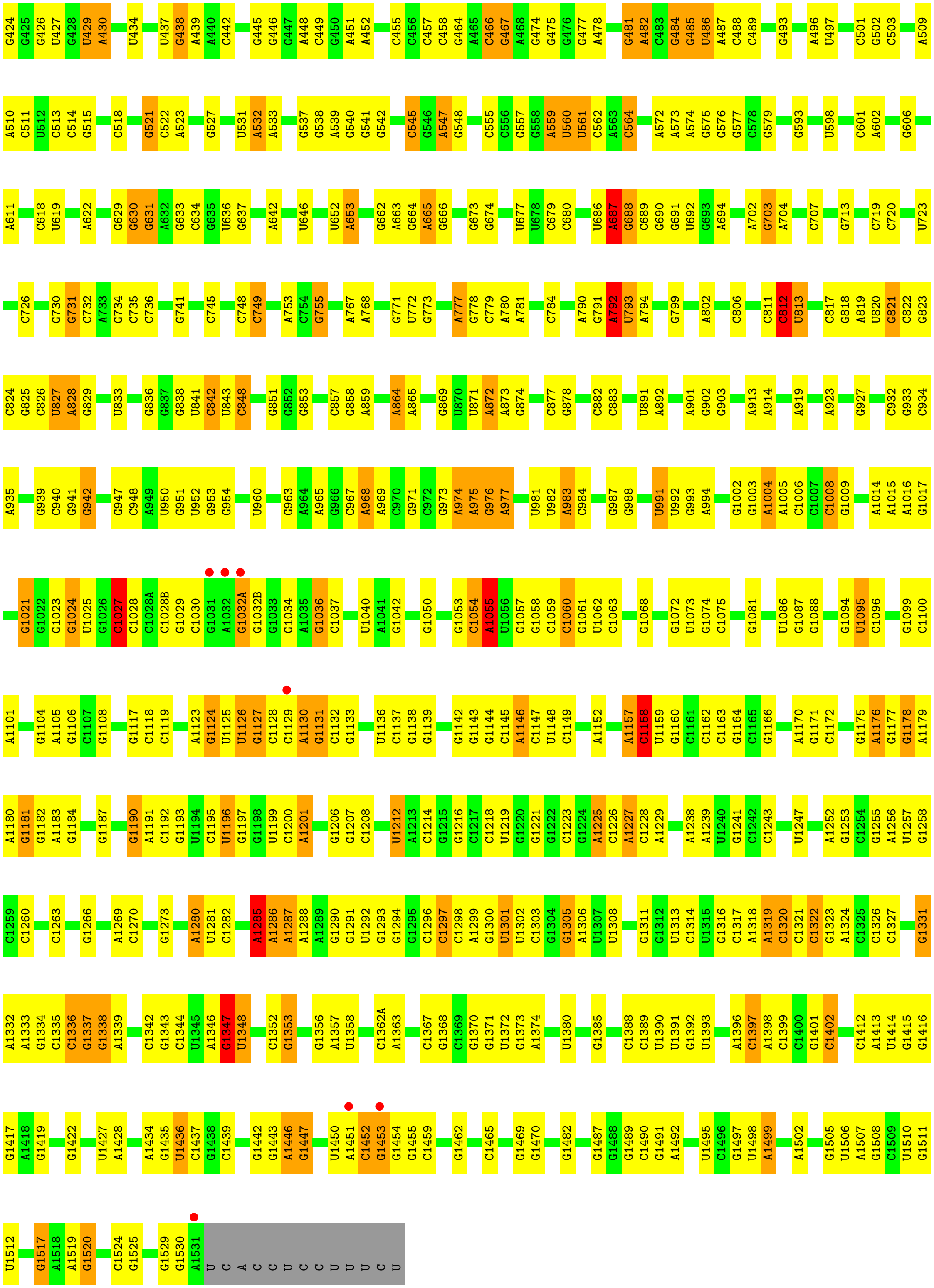




- Molecule 1: 16S rRNA

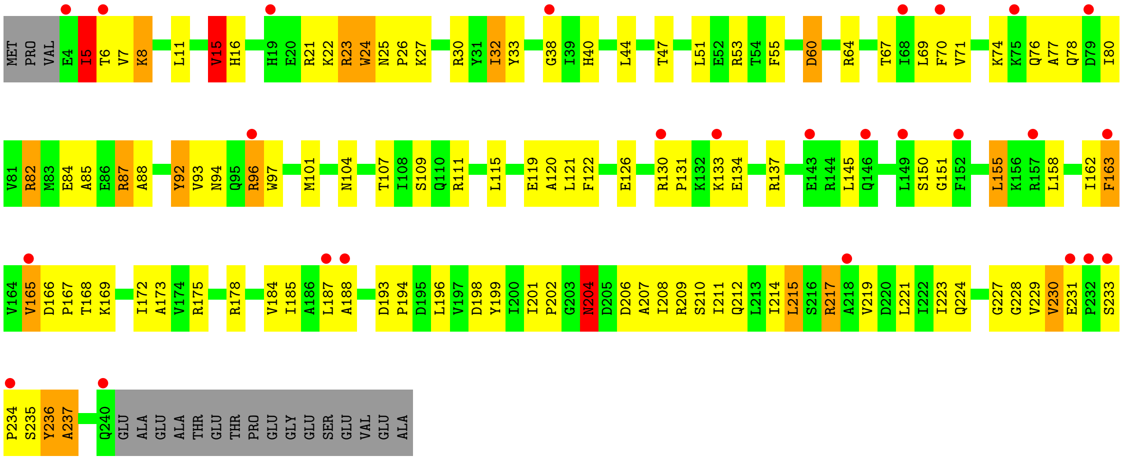
Chain XA:





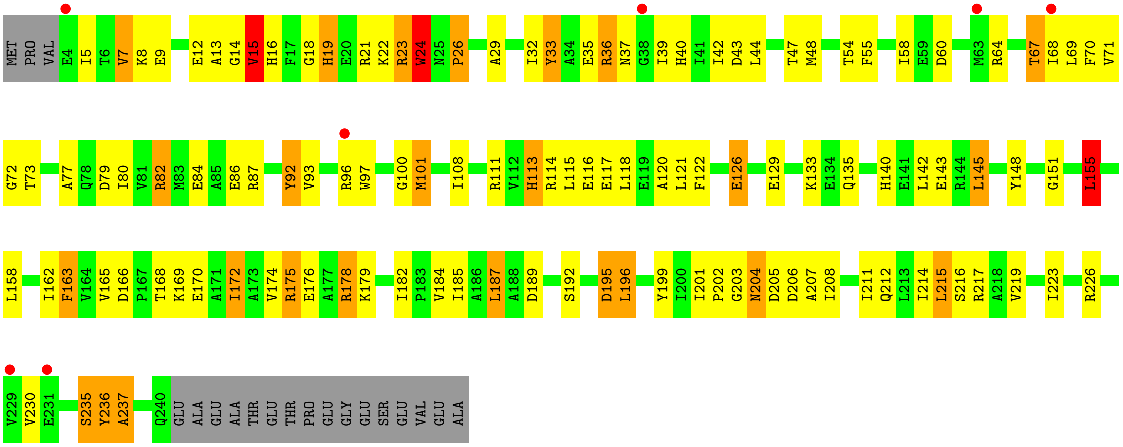
- Molecule 2: 30S ribosomal protein S2

Chain QB:



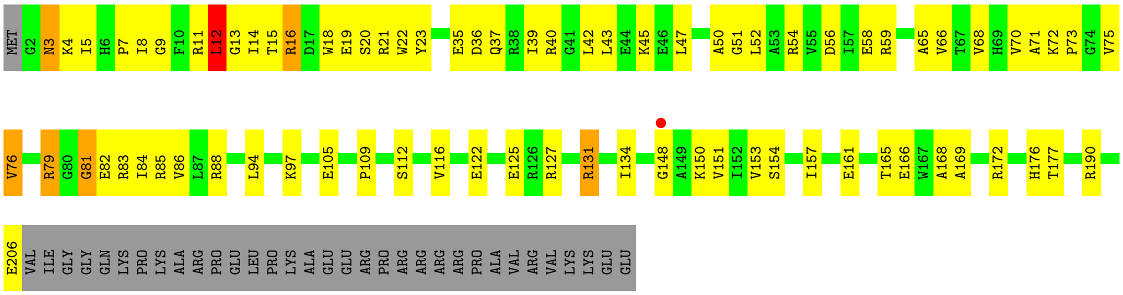
- Molecule 2: 30S ribosomal protein S2

Chain XB:



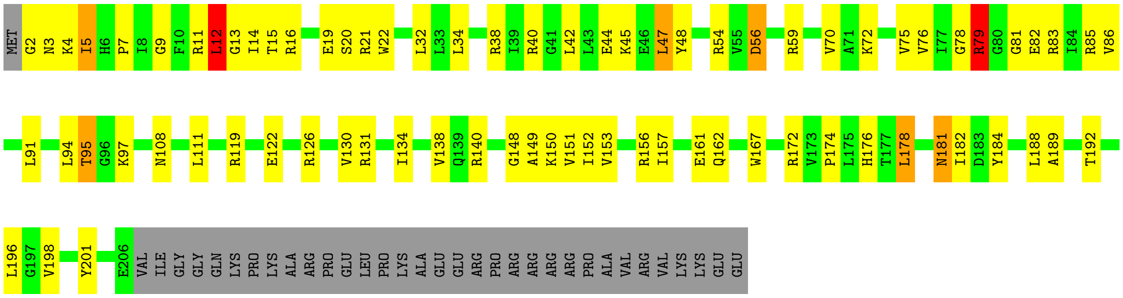
- Molecule 3: 30S ribosomal protein S3

Chain QC:



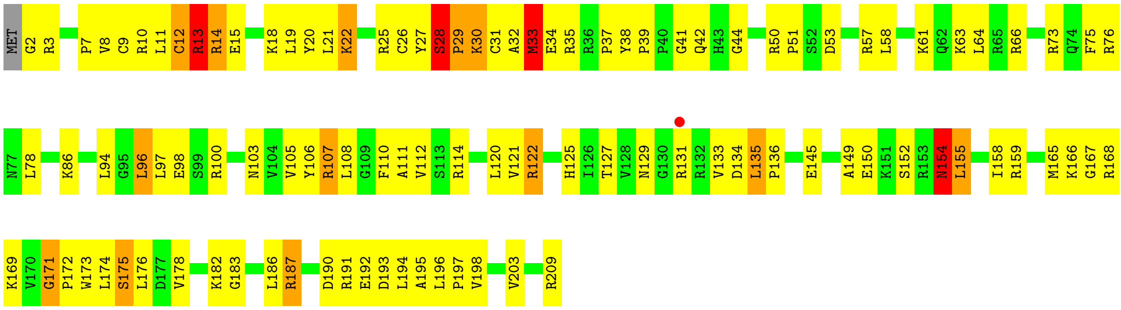
- Molecule 3: 30S ribosomal protein S3

Chain XC:



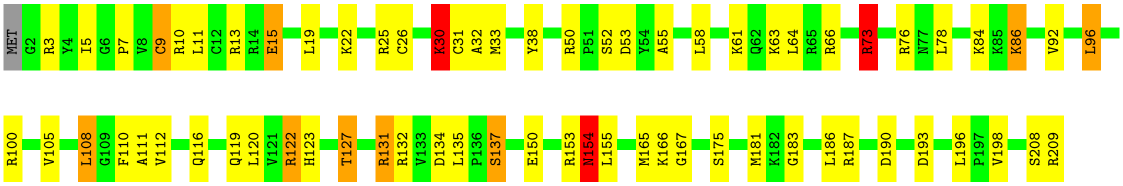
- Molecule 4: 30S ribosomal protein S4

Chain QD:



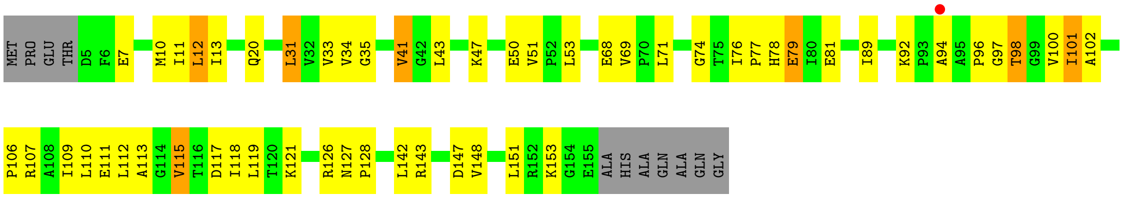
- Molecule 4: 30S ribosomal protein S4

Chain XD:



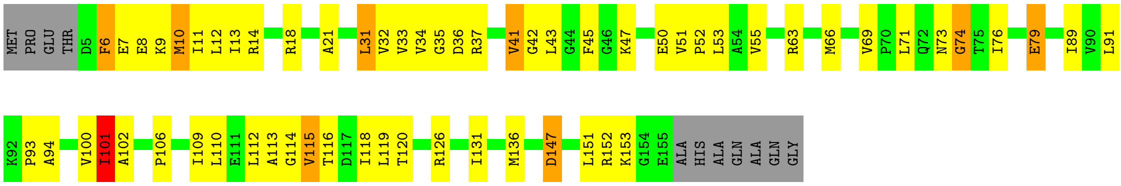
- Molecule 5: 30S ribosomal protein S5

Chain QE:



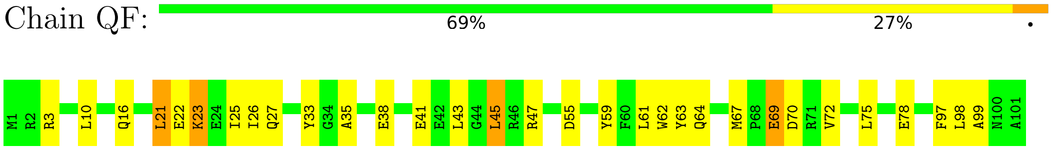
- Molecule 5: 30S ribosomal protein S5

Chain XE:



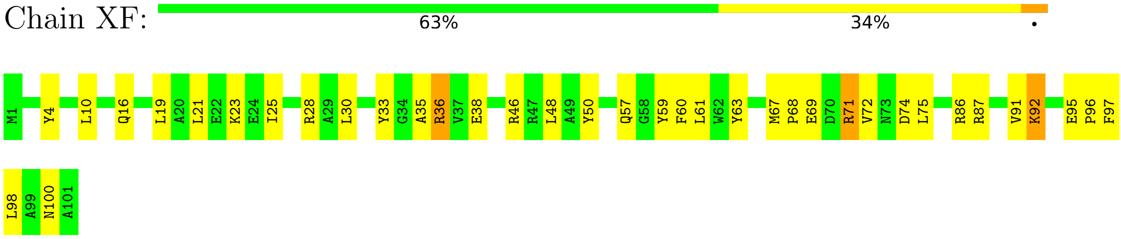
- Molecule 6: 30S ribosomal protein S6

Chain QF:



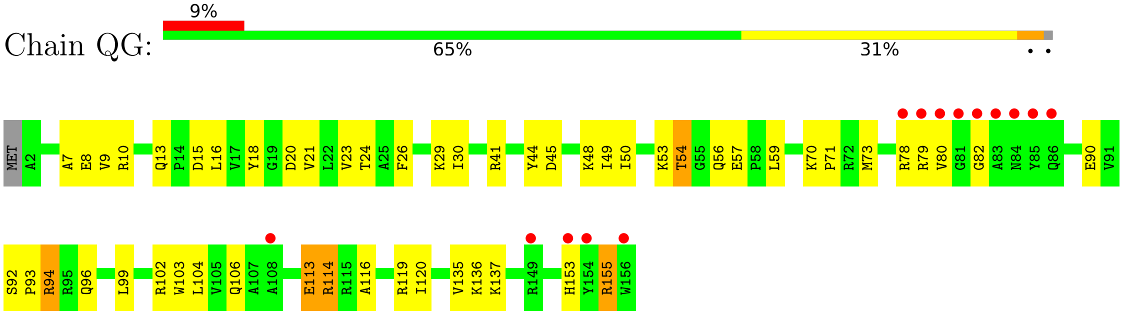
- Molecule 6: 30S ribosomal protein S6

Chain XF:



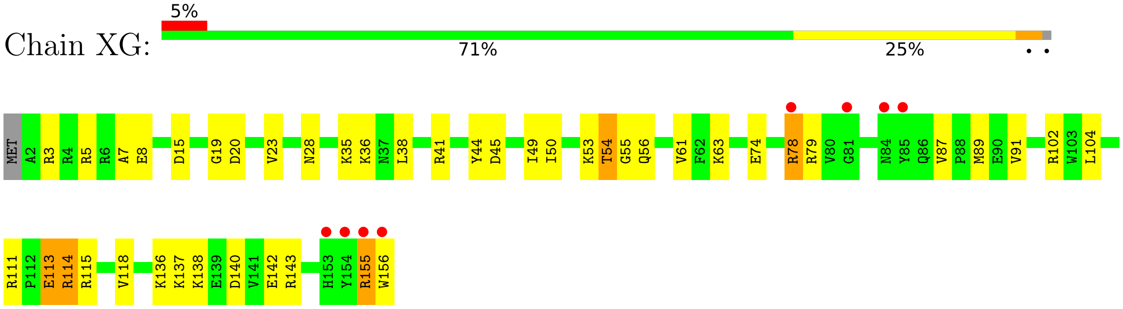
- Molecule 7: 30S ribosomal protein S7

Chain QG:



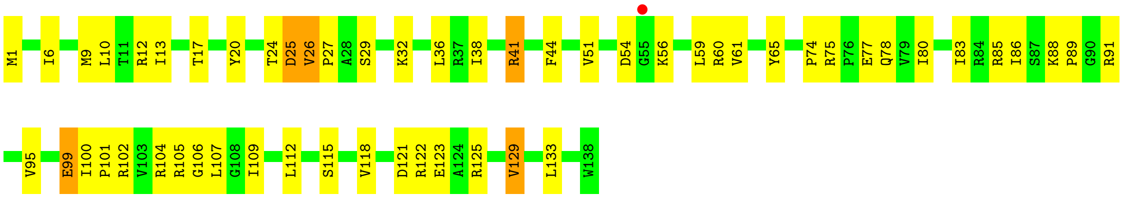
- Molecule 7: 30S ribosomal protein S7

Chain XG:



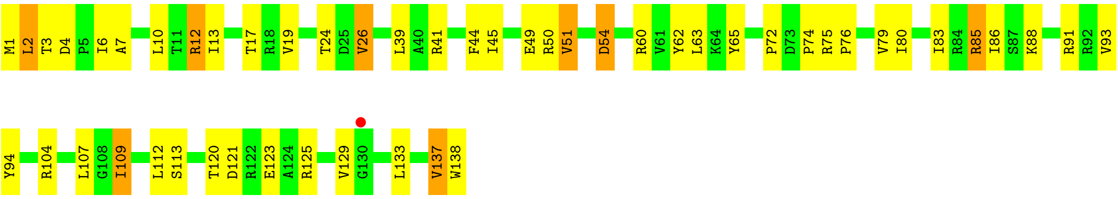
- Molecule 8: 30S ribosomal protein S8

Chain QH:



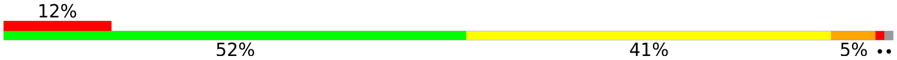
- Molecule 8: 30S ribosomal protein S8

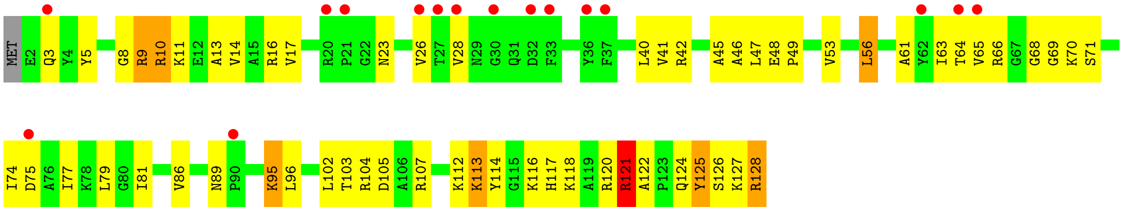
Chain XH:



- Molecule 9: 30S ribosomal protein S9

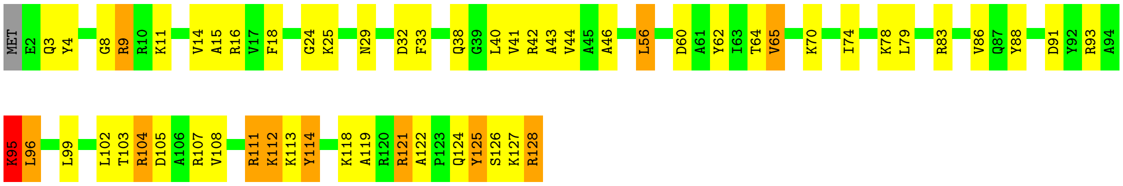
Chain QI:





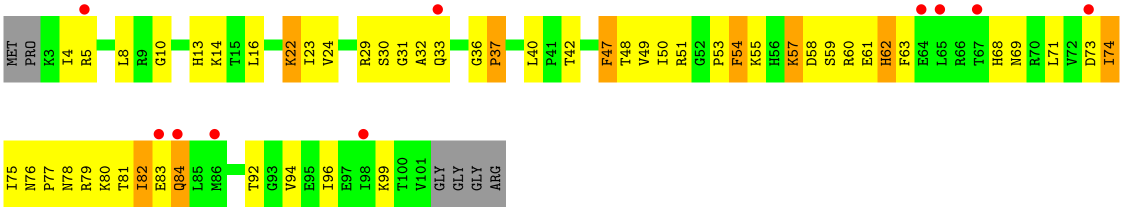
- Molecule 9: 30S ribosomal protein S9

Chain XI:

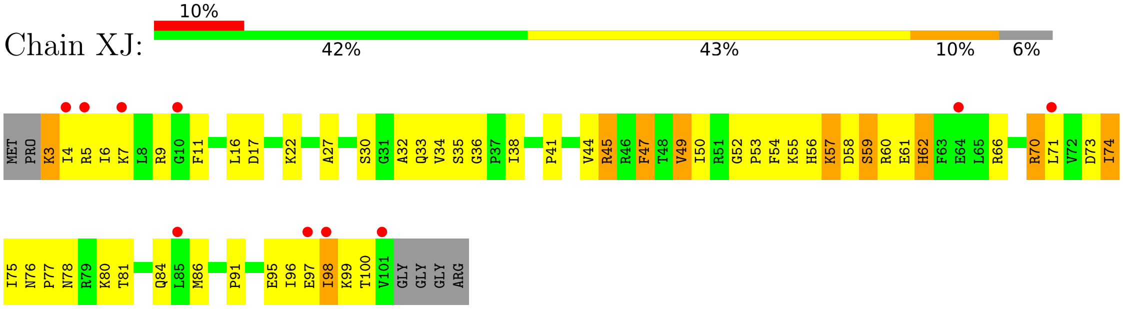


- Molecule 10: 30S ribosomal protein S10

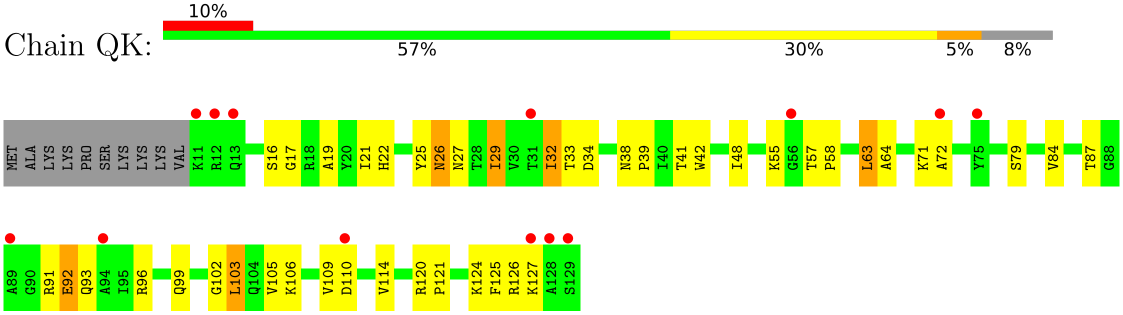
Chain QJ:



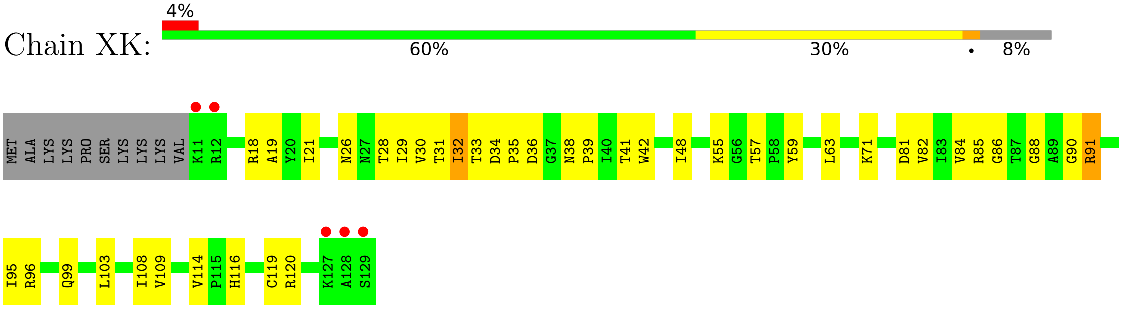
- Molecule 10: 30S ribosomal protein S10



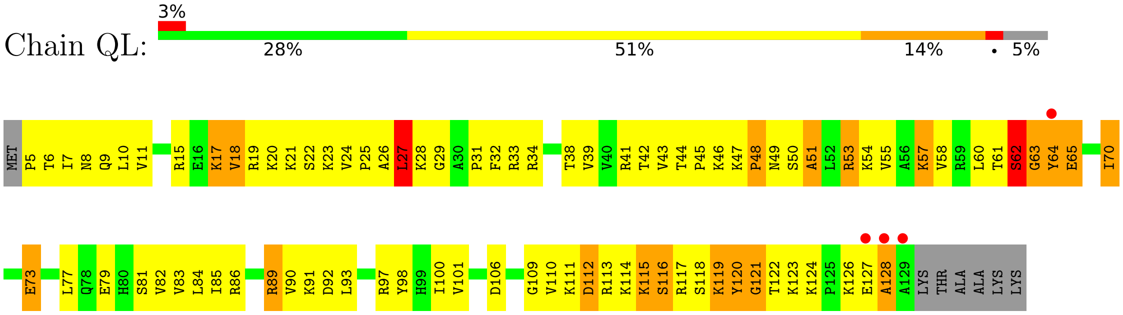
- Molecule 11: 30S ribosomal protein S11



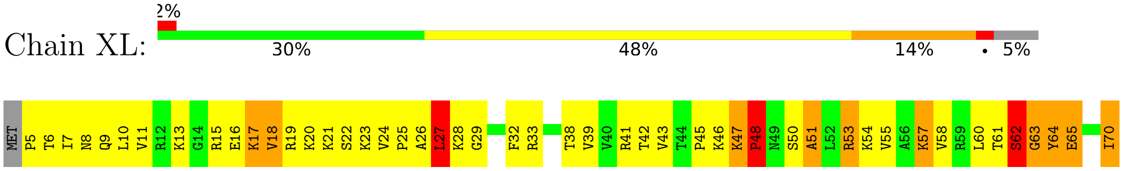
- Molecule 11: 30S ribosomal protein S11

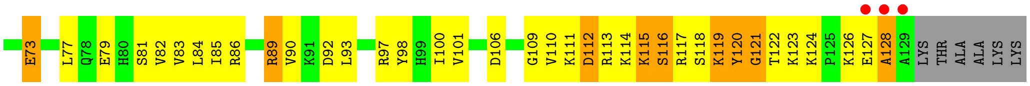


- Molecule 12: 30S ribosomal protein S12

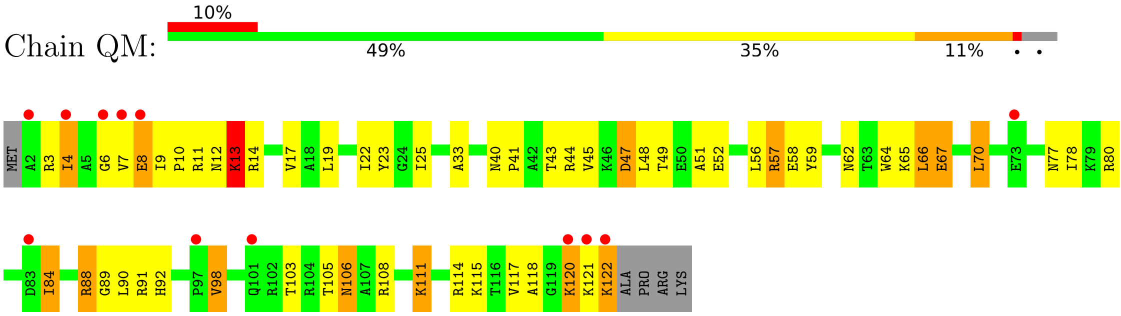


- Molecule 12: 30S ribosomal protein S12

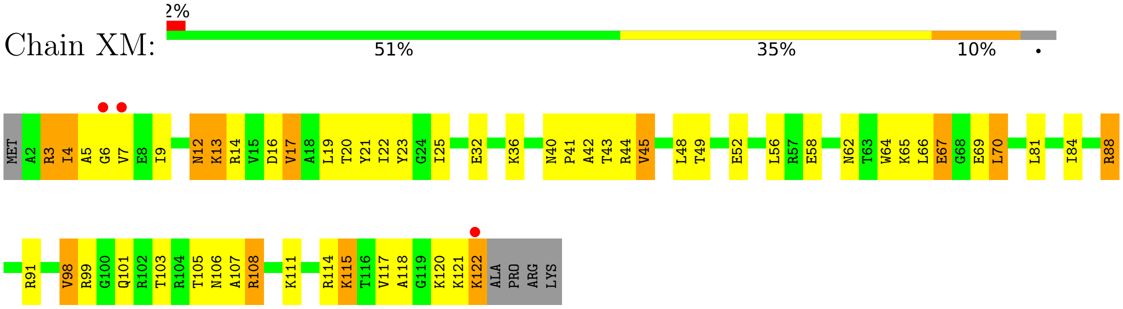




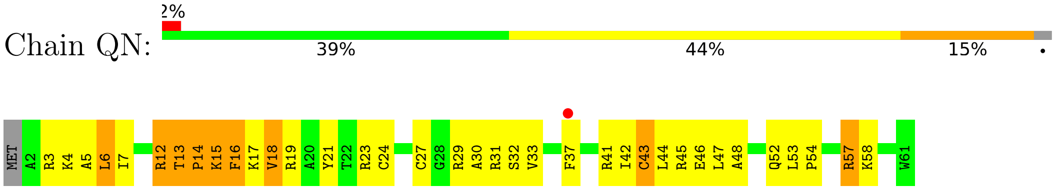
- Molecule 13: 30S ribosomal protein S13



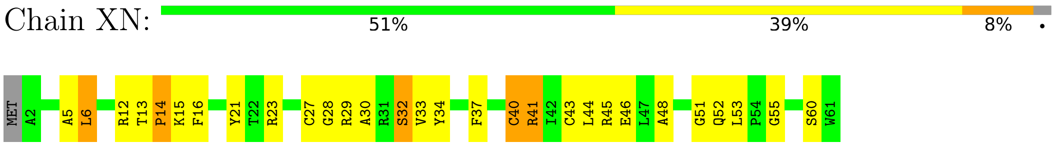
- Molecule 13: 30S ribosomal protein S13



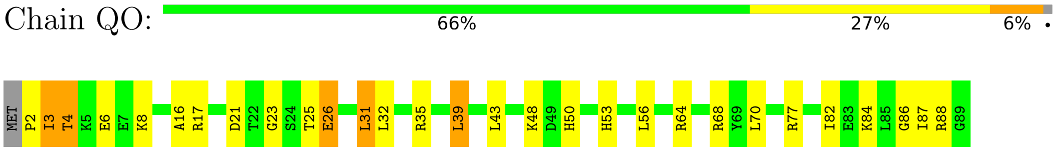
- Molecule 14: 30S ribosomal protein S14 type Z



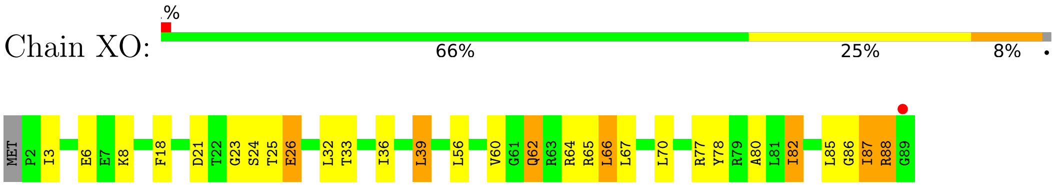
- Molecule 14: 30S ribosomal protein S14 type Z



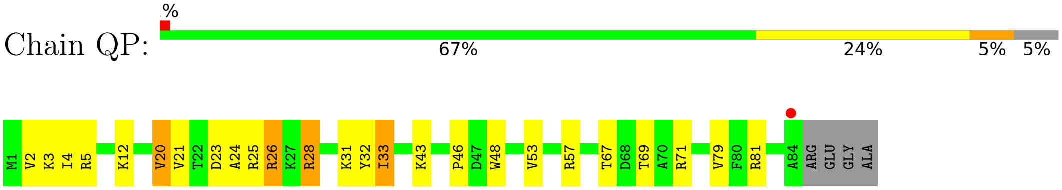
- Molecule 15: 30S ribosomal protein S15



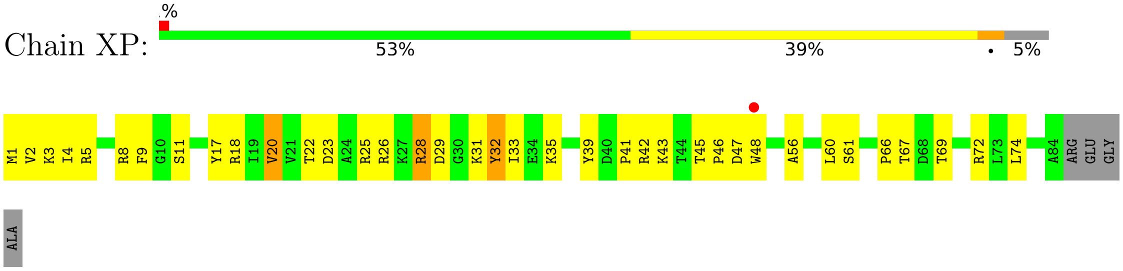
- Molecule 15: 30S ribosomal protein S15



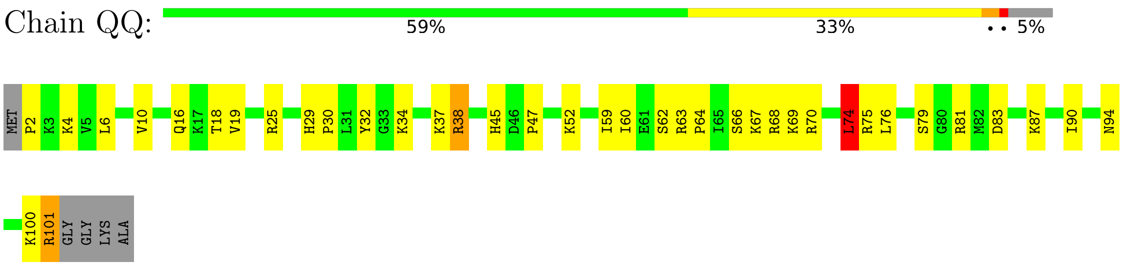
- Molecule 16: 30S ribosomal protein S16



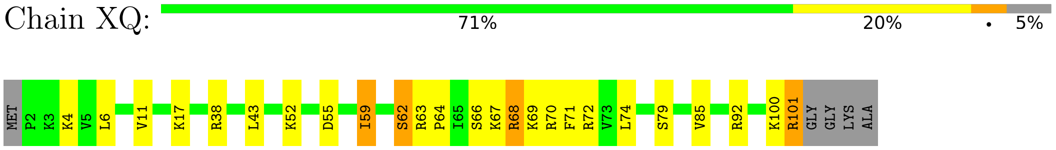
- Molecule 16: 30S ribosomal protein S16



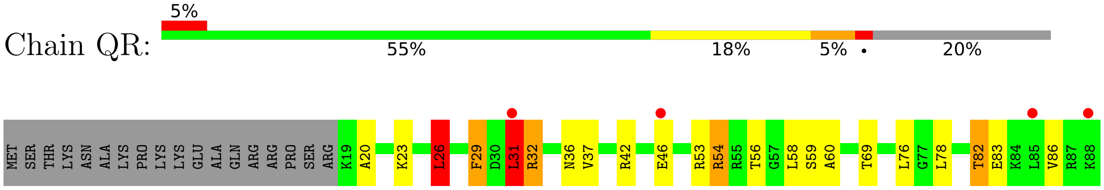
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

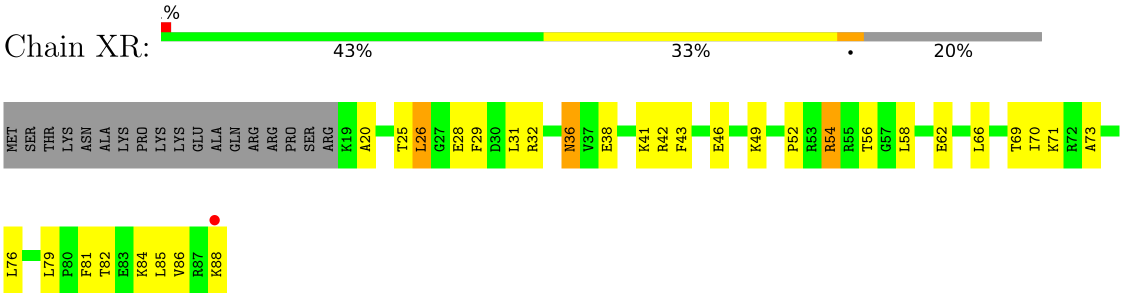


- Molecule 18: 30S ribosomal protein S18



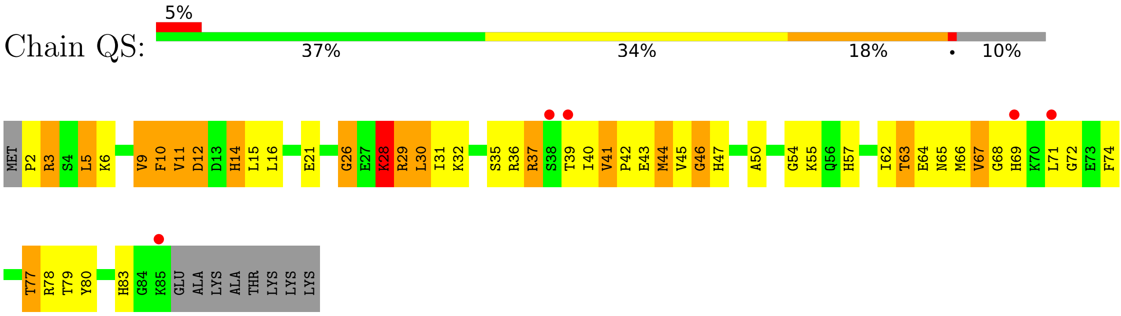
- Molecule 18: 30S ribosomal protein S18

Chain XR:



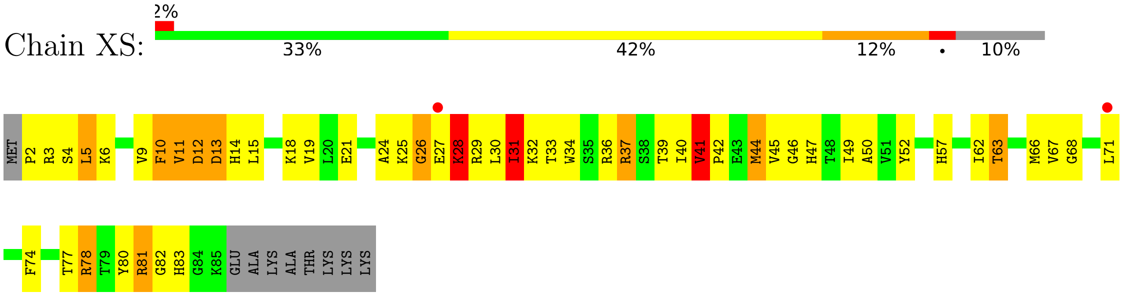
- Molecule 19: 30S ribosomal protein S19

Chain QS:



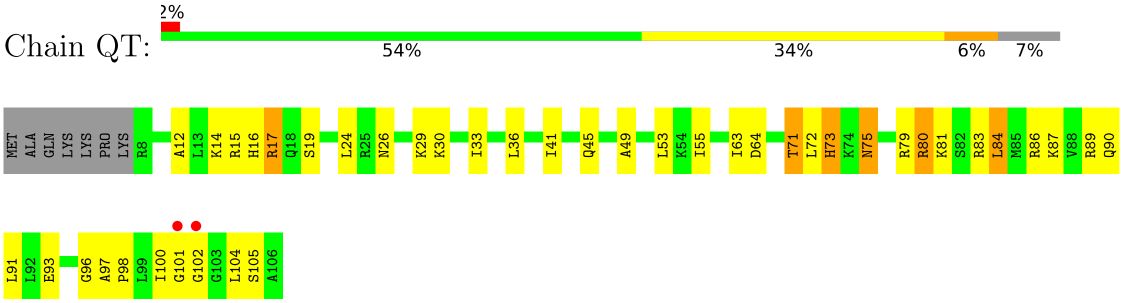
- Molecule 19: 30S ribosomal protein S19

Chain XS:



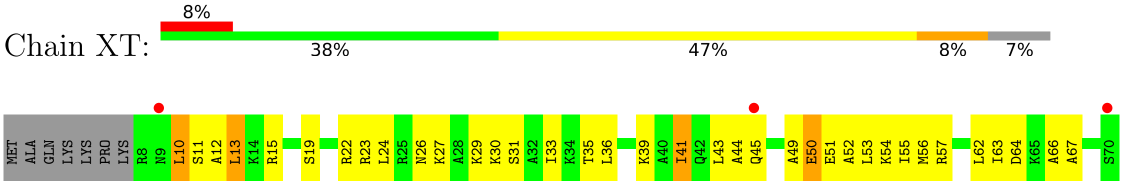
- Molecule 20: 30S ribosomal protein S20

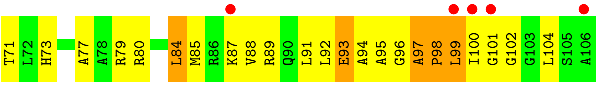
Chain QT:



- Molecule 20: 30S ribosomal protein S20

Chain XT:



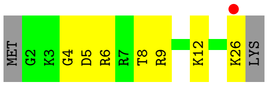


- Molecule 21: 30S ribosomal protein Thx

Chain QU:

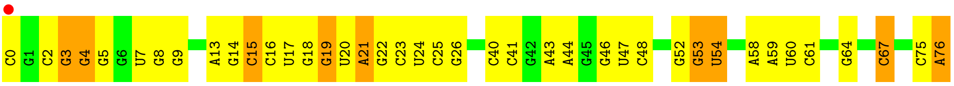
- Molecule 21: 30S ribosomal protein Thx

Chain XU:



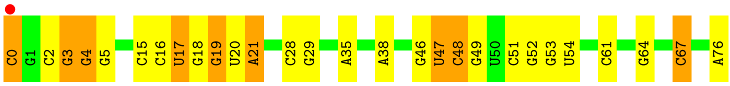
- Molecule 22: P-site tRNA f-Met

Chain QV:



- Molecule 22: P-site tRNA f-Met

Chain XV:



- Molecule 23: messenger RNA

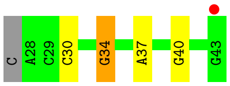
Chain QX:

- Molecule 23: messenger RNA

Chain XX:

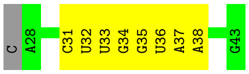
- Molecule 24: A-site tRNA Thr

Chain QY:



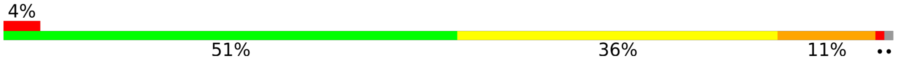
- Molecule 24: A-site tRNA Thr

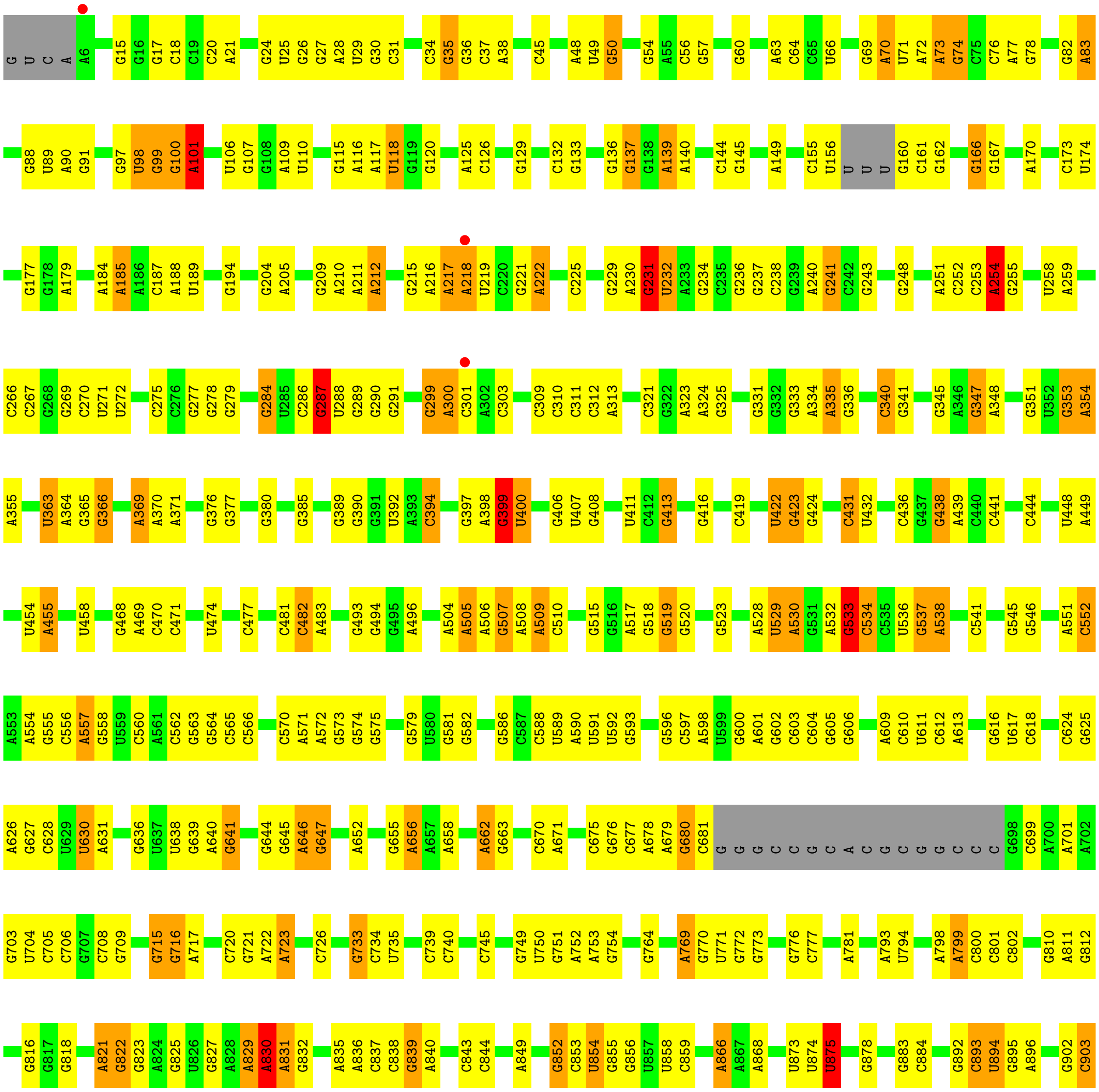
Chain XY:

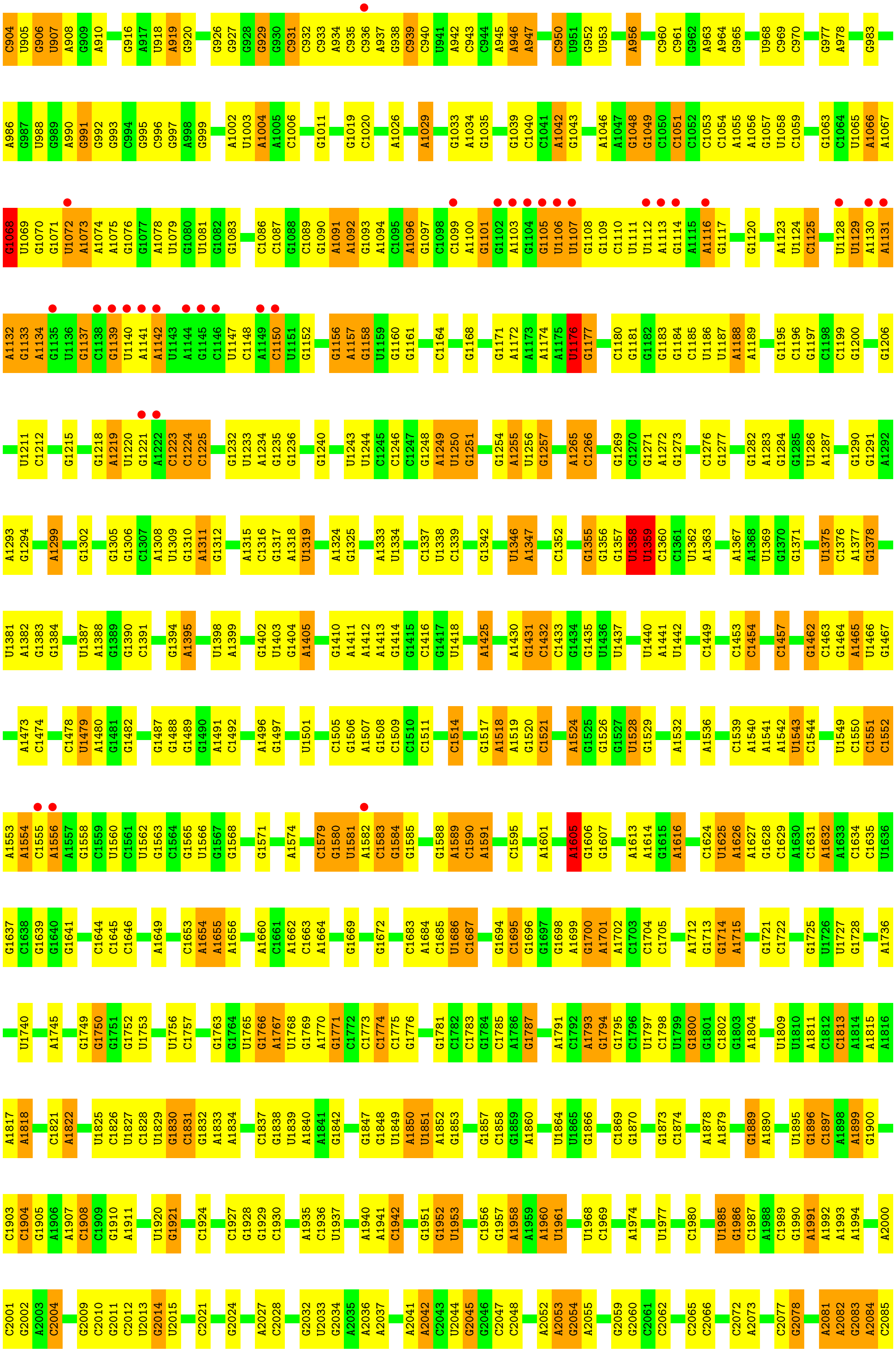


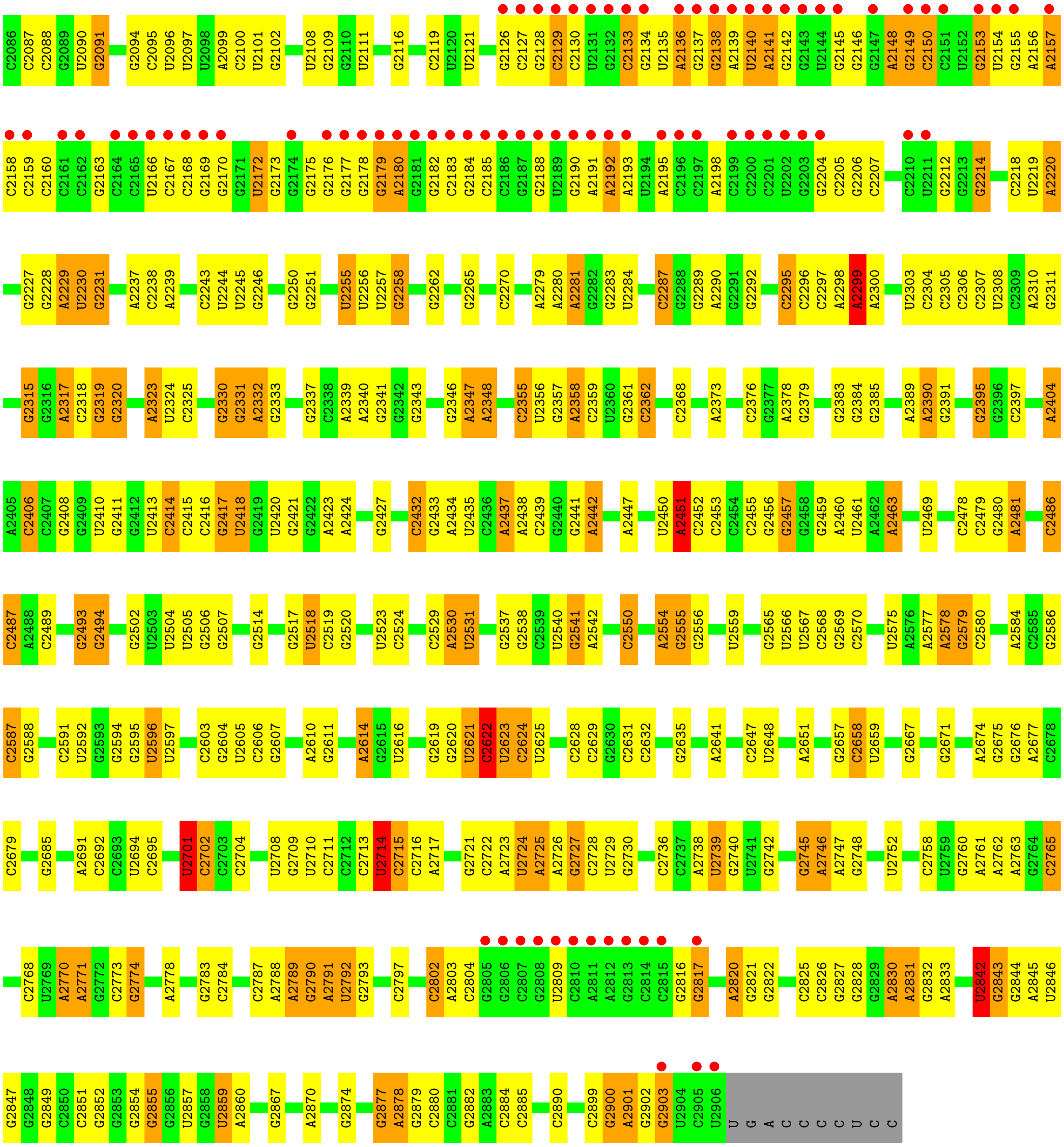
- Molecule 25: 23S rRNA

Chain RA:



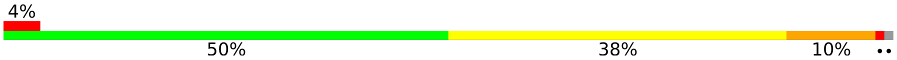


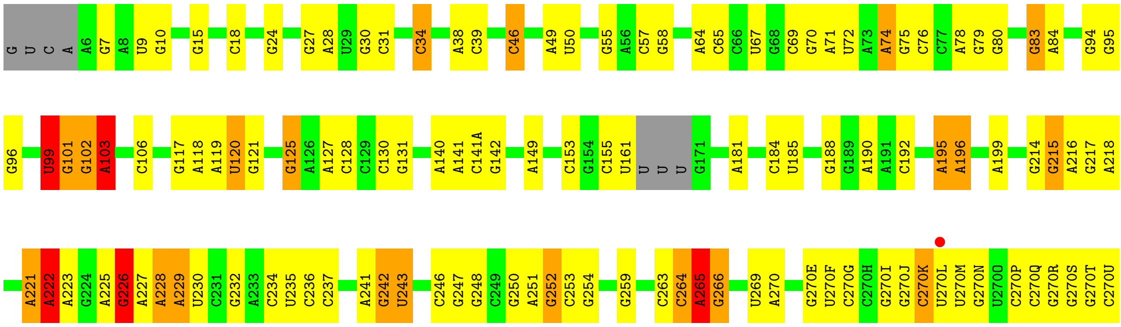

C904 U905 G906 U907 A908 G909 A910 G916 A917 U918 A919 G920 G926 G927 G928 G929 G930 C931 C932 G933 A934 C935 C936 A937 G938 C939 C940 U941 A942 C943 C944 A945 A946 A947 C950 U951 G952 U953 A956 C960 C961 G962 A963 A964 G965 U968 C969 C970 G977 A978 G983
A986 G987 U988 G989 A990 G991 G992 G993 C994 G995 C996 G997 A998 G999 A1002 U1003 A1004 A1005 C1006 G1011 G1019 C1020 A1026 A1029 G1033 A1034 G1035 G1039 C1040 C1041 A1042 G1043 A1046 A1047 G1048 G1049 C1050 C1051 C1052 C1053 C1054 A1055 A1056 G1057 U1058 C1059 G1063 C1064 U1065 A1066 A1067
G1068 U1069 G1070 G1071 U1072 A1073 A1074 A1075 G1076 G1077 A1078 U1079 G1080 U1081 G1082 G1083 C1086 C1087 G1088 C1089 G1090 A1091 A1092 G1093 A1094 C1095 A1096 G1097 C1098 C1099 A1100 G1101 G1102 A1103 G1104 G1105 U1106 U1107 G1108 G1109 C1110 U1111 U1112 A1113 G1114 A1115 A1116 G1117 G1120 A1123 U1124 C1125 U1128 U1129 A1130 A1131
A1132 G1133 A1134 G1135 U1136 G1137 C1138 G1139 U1140 A1141 A1142 U1143 A1144 G1145 C1146 U1147 C1148 A1149 C1150 U1151 G1152 G1156 A1157 G1158 U1159 G1160 G1161 C1164 G1168 G1171 A1172 A1173 A1174 A1175 U1176 G1177 C1180 G1181 G1182 G1183 G1184 C1185 U1186 U1187 A1188 A1189 G1195 C1196 G1197 C1198 C1199 G1200 G1206
U1211 C1212 G1215 G1218 A1219 U1220 G1221 A1222 C1223 C1224 C1225 G1232 U1233 A1234 G1235 G1236 G1240 U1243 U1244 C1245 C1246 C1247 G1248 A1249 U1250 G1251 G1254 A1255 U1256 G1257 A1265 C1266 G1269 C1270 G1271 A1272 G1273 C1276 G1277 G1282 A1283 G1284 G1285 U1286 A1287 G1290 G1291 A1292
A1293 G1294 A1299 G1302 G1305 G1306 C1307 A1308 U1309 G1310 A1311 G1312 A1315 C1316 G1317 A1318 U1319 A1324 G1325 A1333 U1334 C1337 U1338 C1339 G1342 U1346 A1347 C1352 G1355 G1356 G1357 U1358 U1359 C1360 C1361 U1362 A1363 A1367 A1368 U1369 G1370 G1371 U1375 C1376 A1377 G1378
U1381 A1382 G1383 G1384 U1387 A1388 G1389 G1390 C1391 G1394 A1395 U1398 A1399 G1402 U1403 G1404 A1405 G1410 A1411 A1412 A1413 G1414 G1415 C1416 G1417 U1418 A1425 A1430 G1431 C1432 C1433 G1434 G1435 U1436 U1437 U1440 A1441 U1442 C1449 C1453 C1454 C1457 G1462 C1463 G1464 A1465 U1466 G1467
A1473 C1474 C1478 U1479 A1480 G1481 G1482 G1487 G1488 G1489 G1490 A1491 C1492 A1496 G1497 U1501 C1505 G1506 A1507 G1508 C1509 C1510 C1511 C1514 G1517 A1518 A1519 G1520 C1521 A1524 G1525 G1526 G1527 U1528 G1529 A1532 A1536 C1539 A1540 A1541 A1542 U1543 C1544 U1549 C1550 C1551 C1552
A1553 A1554 C1555 A1556 A1557 G1558 C1559 U1560 C1561 U1562 G1563 C1564 G1565 U1566 G1567 G1568 G1571 A1574 C1579 G1580 U1581 A1582 C1583 G1584 G1585 G1588 A1589 C1590 A1591 C1595 A1601 A1605 G1606 G1607 A1613 A1614 G1615 A1616 C1624 U1625 A1626 A1627 G1628 C1629 A1630 C1631 A1632 A1633 C1634 C1635 U1636
G1637 C1638 G1639 G1640 G1641 C1644 C1645 C1646 A1649 C1653 A1654 A1655 A1656 A1660 C1661 A1662 C1663 A1664 G1669 G1672 C1683 A1684 C1685 U1686 C1687 G1694 C1695 G1696 G1697 G1698 A1699 G1700 A1701 A1702 C1703 C1704 C1705 A1712 G1713 G1714 A1715 G1721 C1722 G1725 U1726 U1727 G1728 A1736
U1740 A1745 G1749 G1750 G1751 G1752 U1753 U1756 C1757 G1763 G1764 U1765 G1766 A1767 U1768 G1769 A1770 C1771 C1772 C1773 C1774 C1775 G1776 G1781 C1782 C1783 G1784 C1785 A1786 G1787 A1791 C1792 A1793 G1794 G1795 C1796 U1797 C1798 U1799 G1800 G1801 C1802 G1803 A1804 U1809 U1810 A1811 C1812 C1813 A1814 A1815 A1816
A1817 A1818 C1821 A1822 U1825 C1826 U1827 C1828 U1829 G1830 C1831 G1832 A1833 A1834 C1837 G1838 U1839 A1840 A1841 G1842 G1847 G1848 U1849 A1850 U1851 A1852 G1853 G1857 C1858 G1859 A1860 U1864 U1865 G1866 C1869 G1870 G1873 C1874 A1878 A1879 G1889 A1890 U1895 G1896 C1897 A1898 A1899 G1900
C1903 C1904 G1905 A1906 A1907 C1908 C1909 G1910 A1911 U1920 G1921 C1924 C1927 G1928 G1929 C1930 A1935 C1936 U1937 A1940 A1941 C1942 G1951 G1952 U1953 C1956 G1957 A1958 A1959 A1960 U1961 U1968 C1969 A1974 U1977 C1980 U1985 G1986 C1987 A1988 C1989 G1990 A1991 A1992 A1993 A1994 A2000
C2001 G2002 A2003 C2004 G2009 C2010 G2011 C2012 U2013 G2014 U2015 C2021 G2024 A2027 C2028 G2032 U2033 G2034 A2035 A2036 A2037 A2041 A2042 C2043 U2044 G2045 G2046 C2047 C2048 A2052 A2053 G2054 A2055 G2059 G2060 C2061 C2062 C2065 C2066 C2072 A2073 C2077 G2078 A2081 A2082 G2083 A2084 C2085

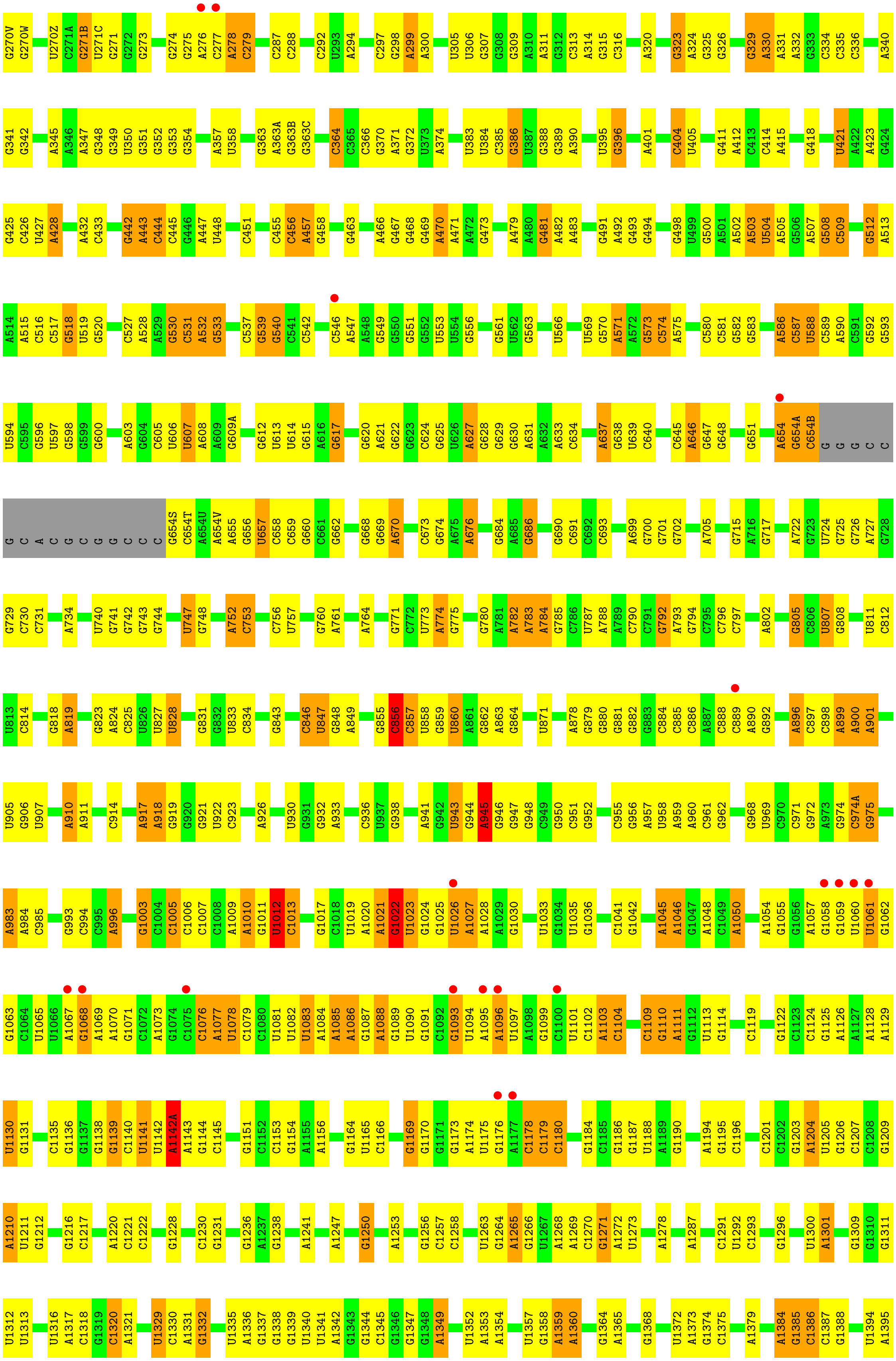


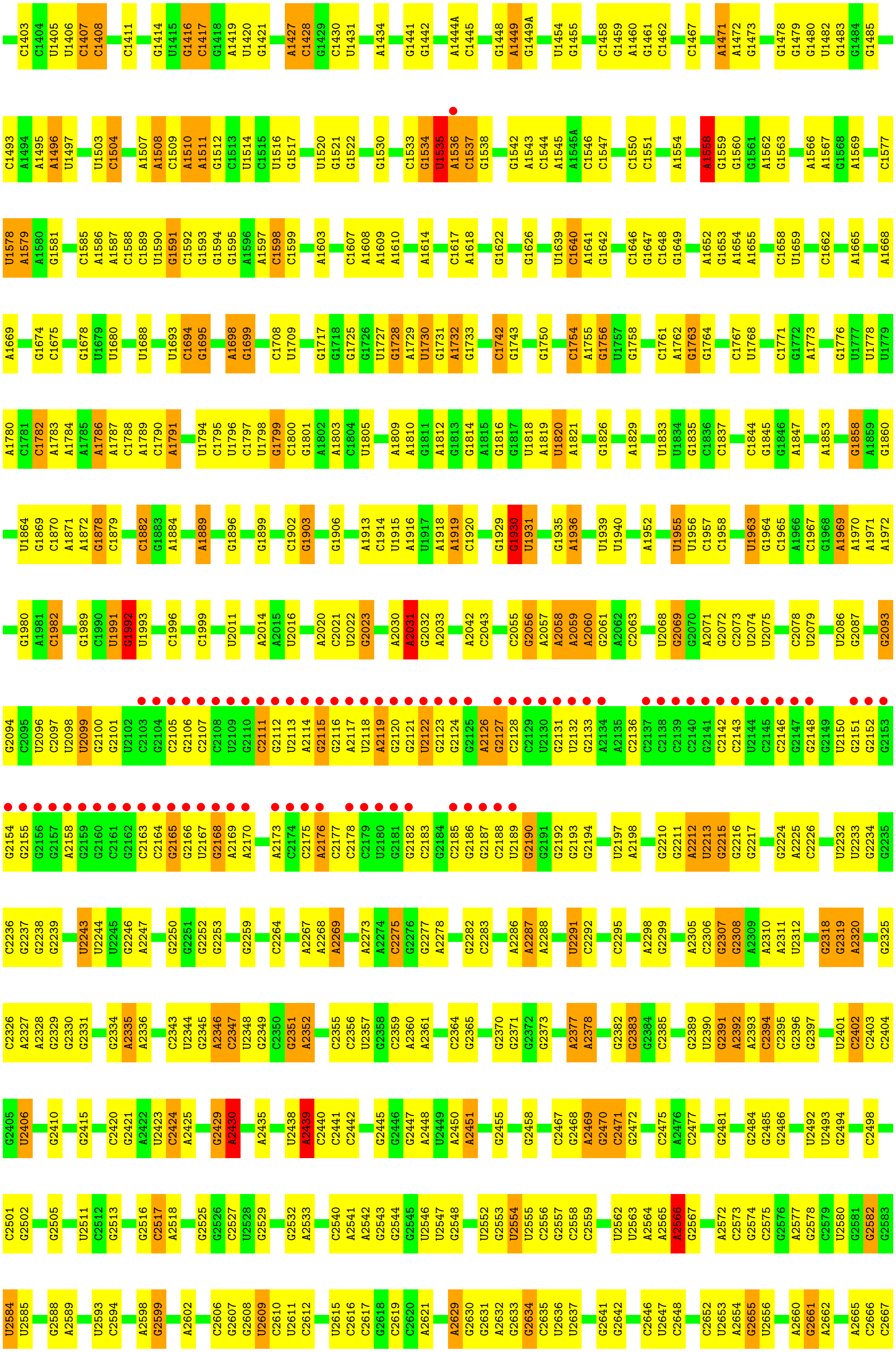
- Molecule 25: 23S rRNA

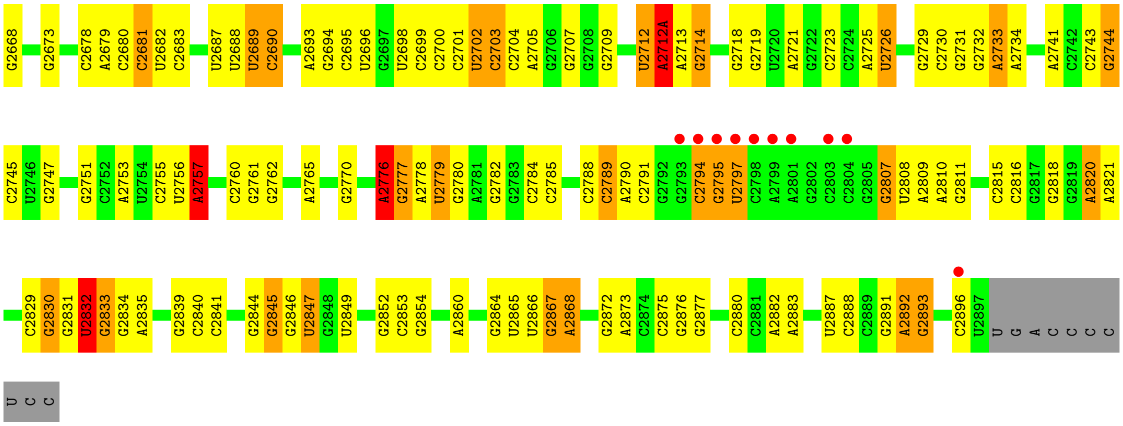
Chain YA:



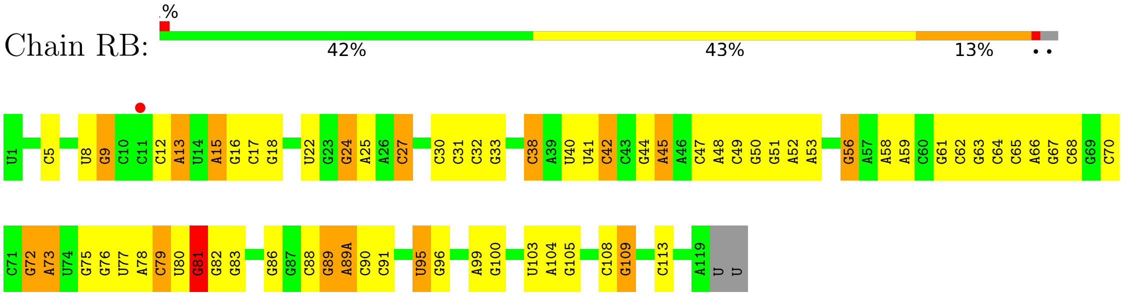



G270V G270W U270Z C271A G271B U271C G271 G272 G273 G274 G275 A276 C277 A278 C279 C287 C288 C292 U293 A294 C297 G298 A299 A300 U305 U306 G307 G308 G309 A310 A311 G312 C313 A314 G315 C316 A320 G323 A324 G325 G326 G329 A330 A331 A332 G333 C334 C335 C336 A340
G341 G342 A345 A346 A347 G348 G349 U350 G351 G352 G353 G354 A357 U358 G363 A363A G363B G363C C364 C365 C366 G370 A371 G372 U373 A374 U383 U384 C385 G386 U387 G388 G389 A390 U395 G396 A401 C404 U405 G411 A412 C413 C414 A415 G418 U421 A422 A423 G424
G425 C426 U427 A428 A432 C433 G442 A443 C444 C445 G446 A447 U448 C451 C455 C456 A457 G458 G463 A466 G467 G468 G469 A470 A471 A472 G473 A479 A480 G481 A482 A483 G491 A492 G493 G494 G498 U499 G500 A501 A502 A503 U504 A505 G506 A507 G508 C509 G512 A513
A514 A515 C516 C517 G518 U519 G520 C527 A528 A529 G530 C531 A532 G533 C537 G539 G540 C541 C542 C546 A547 A548 G549 G550 G551 G552 U553 U554 G556 G561 U562 G563 U566 U569 G570 A571 A572 G573 C574 A575 C580 C581 G582 G583 A586 C587 U588 C589 A590 C591 G592 G593
U594 C595 G596 U597 G598 G599 G600 A603 G604 C605 U606 U607 A608 A609 G609A G612 U613 U614 G615 A616 G617 G620 A621 G622 G623 C624 G625 U626 A627 G628 G629 G630 A631 A632 A633 C634 A637 G638 U639 C640 C645 A646 G647 G648 G651 A654 G654A C654B G G G C C
G C A C G C G G C C C G654S C654T A654U A654V A655 G656 U657 C658 C659 G660 C661 G662 G668 G669 A670 C673 G674 A675 A676 G684 A685 G686 G690 C691 C692 C693 A699 G700 G701 G702 A705 G715 A716 G717 A722 G723 U724 G725 G726 A727 G728
G729 C730 C731 A734 U740 G741 G742 G743 G744 U747 G748 A752 C753 C756 U757 G760 A761 A764 G771 C772 U773 A774 G775 G780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795 C796 C797 A802 G805 C806 U807 G808 U811 C812
U813 C814 G818 A819 G823 A824 C825 U826 U827 U828 G831 G832 U833 C834 G843 C846 U847 G848 A849 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 U871 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 A896 C897 C898 A899 A900 A901
U905 G906 U907 A910 A911 C914 A917 A918 G919 G920 G921 U922 C923 A926 U930 G931 G932 A933 C936 U937 G938 A941 G942 U943 G944 A945 G946 G947 G948 C949 G950 C951 G952 C955 G956 A957 U958 A959 A960 C961 G962 G968 U969 C970 C971 G972 A973 G974 C974A G975
A983 A984 C985 G993 C994 C995 A996 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 U1033 G1034 U1035 G1036 C1041 G1042 A1045 A1046 G1047 A1048 C1049 A1050 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U1061 G1062
G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 C1109 G1110 A1111 G1112 U1113 G1114 C1119 G1122 C1123 C1124 G1125 A1126 A1127 A1128 A1129
U1130 G1131 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 G1144 C1145 G1151 C1152 C1153 G1154 A1155 A1156 G1164 U1165 C1166 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 G1184 C1185 G1186 G1187 U1188 A1189 G1190 A1194 G1195 C1196 C1201 C1202 G1203 A1204 U1205 G1206 C1207 C1208 G1209
A1210 U1211 G1212 G1216 C1217 A1220 C1221 C1222 G1228 C1230 G1231 G1236 A1237 G1238 A1241 A1247 G1250 A1253 G1256 C1257 C1258 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1278 A1287 C1291 U1292 C1293 G1296 U1300 A1301 G1309 G1310 G1311
U1312 U1313 U1316 A1317 C1318 G1319 C1320 A1321 U1329 C1330 A1331 G1332 U1335 A1336 G1337 G1338 G1339 U1340 U1341 A1342 G1343 G1344 C1345 G1346 G1347 G1348 A1349 U1352 A1353 A1354 U1357 G1358 A1359 A1360 G1364 A1365 G1368 U1372 A1373 G1374 C1375 A1379 A1384 G1385 C1386 C1387 G1388 U1394 A1395

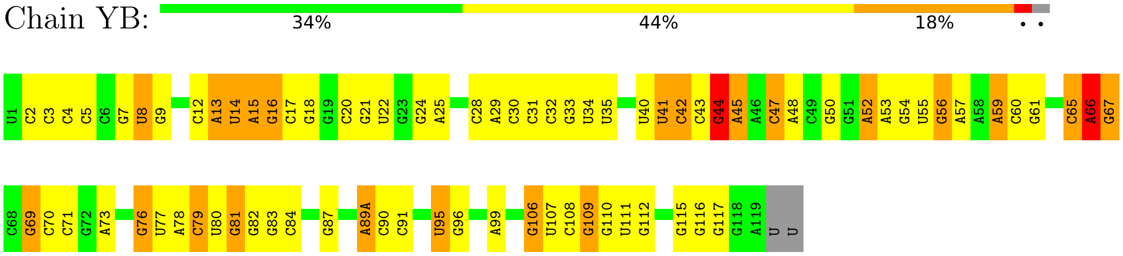

C1403 C1404 U1405 U1406 C1407 C1408 C1411 G1414 U1415 G1416 C1417 G1418 A1419 U1420 G1421 A1427 C1428 G1429 C1430 U1431 A1434 G1441 G1442 A1444A C1445 G1448 A1449 G1449A U1454 G1455 C1458 G1459 A1460 G1461 C1462 C1467 A1471 A1472 G1473 G1478 G1479 G1480 U1482 G1483 G1484 G1485
C1493 A1494 A1495 A1496 U1497 U1503 C1504 A1507 A1508 C1509 A1510 A1511 G1512 C1513 U1514 C1515 U1516 G1517 U1520 G1521 G1522 G1530 C1533 G1534 U1535 A1536 C1537 G1538 G1542 A1543 C1544 A1545 A1545A C1546 C1547 C1550 C1551 A1554 A1558 G1559 G1560 G1561 A1562 G1563 A1566 A1567 G1568 A1569 C1577
U1578 A1579 A1580 G1581 C1585 A1586 A1587 C1588 C1589 U1590 G1591 C1592 G1593 G1594 G1595 A1596 A1597 C1598 C1599 A1603 C1607 A1608 A1609 A1610 A1614 C1617 A1618 G1622 G1626 U1639 C1640 A1641 G1642 C1646 G1647 C1648 G1649 A1652 G1653 A1654 A1655 C1658 U1659 C1662 A1665 A1668
A1669 G1674 C1675 G1678 U1679 U1680 U1688 U1693 C1694 G1695 A1698 G1699 C1708 U1709 G1717 G1718 G1725 G1726 U1727 G1728 A1729 U1730 G1731 A1732 G1733 C1742 G1743 G1750 C1754 A1755 G1756 U1757 G1758 C1761 A1762 G1763 G1764 C1767 U1768 C1771 G1772 A1773 G1776 U1777 U1778 U1779
A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 A1809 A1810 G1811 A1812 G1813 G1814 A1815 G1816 G1817 U1818 A1819 U1820 A1821 G1826 A1829 U1833 U1834 G1835 C1836 C1837 C1844 G1845 G1846 A1847 A1853 G1858 A1859 G1860
U1864 G1869 C1870 A1871 A1872 G1878 C1879 C1882 G1883 A1884 A1889 G1896 G1899 C1902 G1903 G1906 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1929 G1930 U1931 G1935 A1936 U1939 U1940 A1952 U1955 U1956 C1957 C1958 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972
G1980 A1981 C1982 G1989 C1990 U1991 G1992 U1993 C1996 C1999 U2011 A2014 A2015 U2016 A2020 C2021 U2022 G2023 A2030 A2031 G2032 A2033 A2042 C2043 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 U2068 G2069 G2070 A2071 G2072 C2073 U2074 U2075 C2078 U2079 U2086 G2087 G2093
G2094 C2095 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153
G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 G2193 G2194 U2197 A2198 G2210 G2211 A2212 U2213 G2215 G2216 G2217 G2224 A2225 C2226 U2232 U2233 G2234 G2235
C2236 G2237 G2238 G2239 U2243 U2244 U2245 G2246 A2247 G2250 G2251 G2252 G2253 G2259 C2264 A2267 A2268 A2269 A2273 A2274 C2275 G2276 G2277 A2278 G2282 C2283 A2286 A2287 A2288 U2291 C2292 C2295 A2298 G2299 A2305 C2306 G2307 G2308 A2309 A2310 A2311 U2312 G2318 G2319 A2320 G2325
C2326 A2327 A2328 G2329 G2330 G2331 G2334 A2335 A2336 C2343 U2344 G2345 A2346 C2347 U2348 G2349 C2350 G2351 A2352 C2355 C2356 U2357 G2358 C2359 A2360 A2361 C2364 G2365 C2370 G2371 G2372 G2373 A2377 A2378 G2382 G2383 G2384 C2385 G2389 U2390 G2391 A2392 A2393 C2394 C2395 G2396 G2397 U2401 C2402 C2403 C2404
G2405 U2406 G2410 G2415 C2420 G2421 A2422 U2423 C2424 A2425 G2429 A2430 A2435 U2438 A2439 C2440 C2441 C2442 G2445 G2446 G2447 A2448 U2449 A2450 A2451 G2455 G2458 C2467 G2468 A2469 G2470 C2471 G2472 C2475 A2476 C2477 G2481 G2484 G2485 G2486 U2492 U2493 G2494 C2498
C2501 G2502 G2505 U2511 C2512 G2513 G2516 C2517 A2518 G2525 G2526 C2527 U2528 G2529 G2532 A2533 C2540 A2541 A2542 G2543 G2544 G2545 U2546 U2547 G2548 U2552 G2553 U2554 U2555 C2556 G2557 G2558 C2559 U2562 U2563 A2564 A2565 A2566 G2567 A2572 C2573 G2574 C2575 G2576 A2577 G2578 C2579 U2580 G2581 G2582 G2583
U2584 U2585 G2588 A2589 U2593 C2594 A2598 G2599 A2602 C2606 G2607 G2608 U2609 C2610 U2611 C2612 U2615 C2616 C2617 G2618 C2619 C2620 A2621 A2629 G2630 G2631 A2632 G2633 G2634 C2635 U2636 U2637 G2641 G2642 C2646 U2647 C2648 C2652 U2653 A2654 G2655 U2656 A2660 G2661 A2662 A2665 C2666 C2667



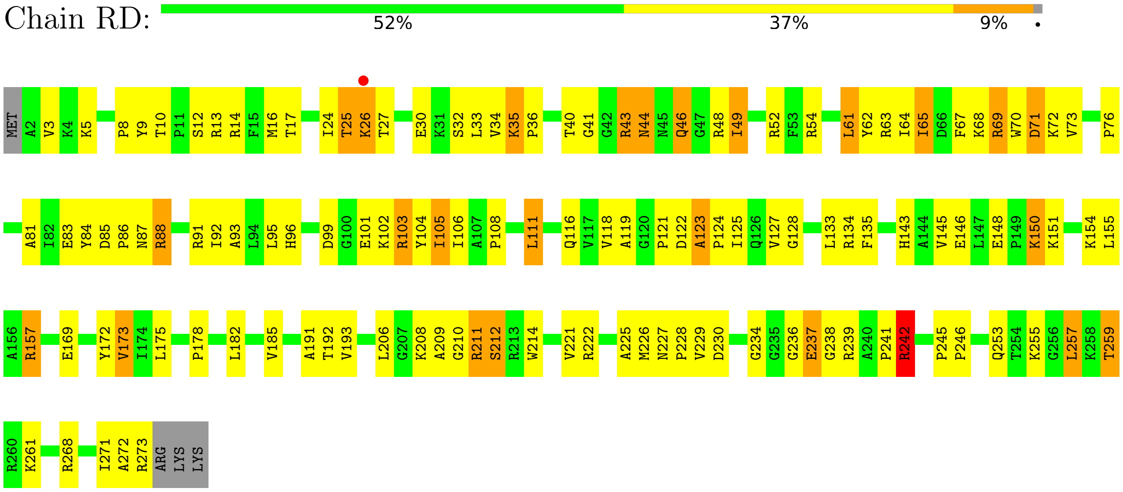
- Molecule 26: 5S rRNA



- Molecule 26: 5S rRNA

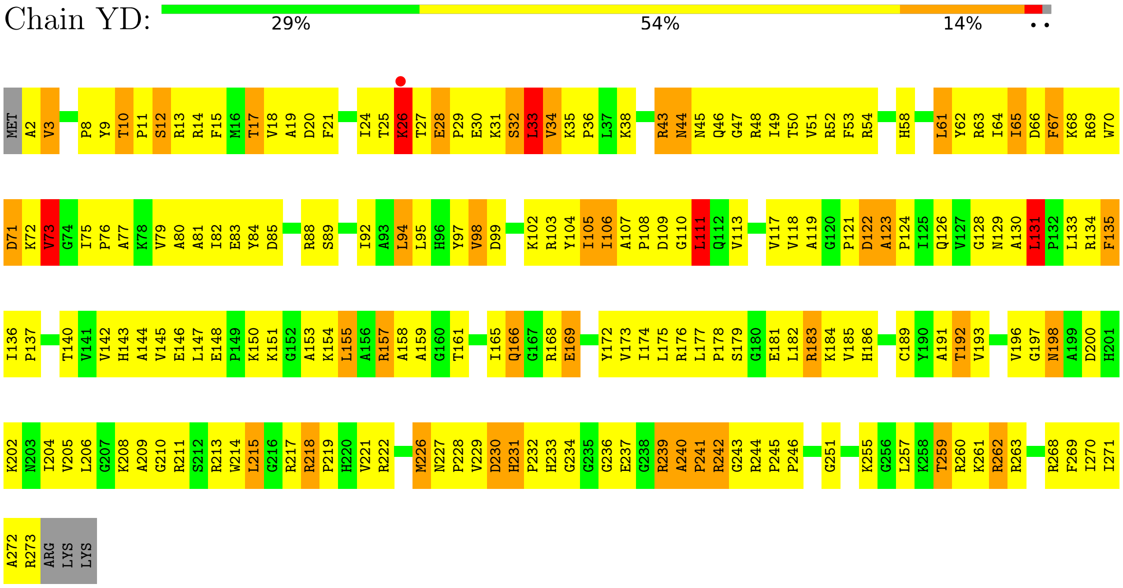


- Molecule 27: 50S ribosomal protein L2



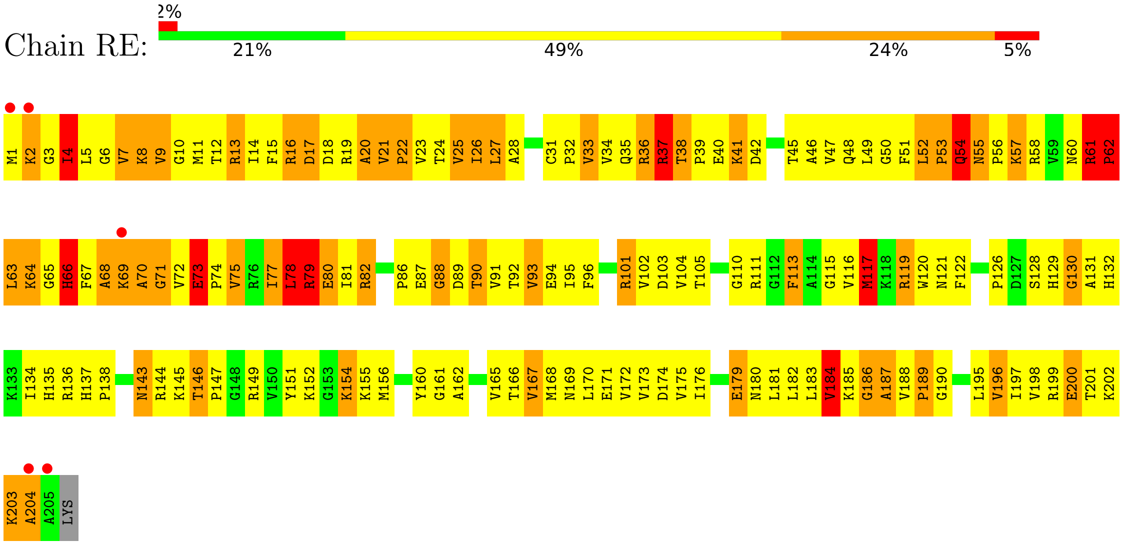
- Molecule 27: 50S ribosomal protein L2

Chain YD:



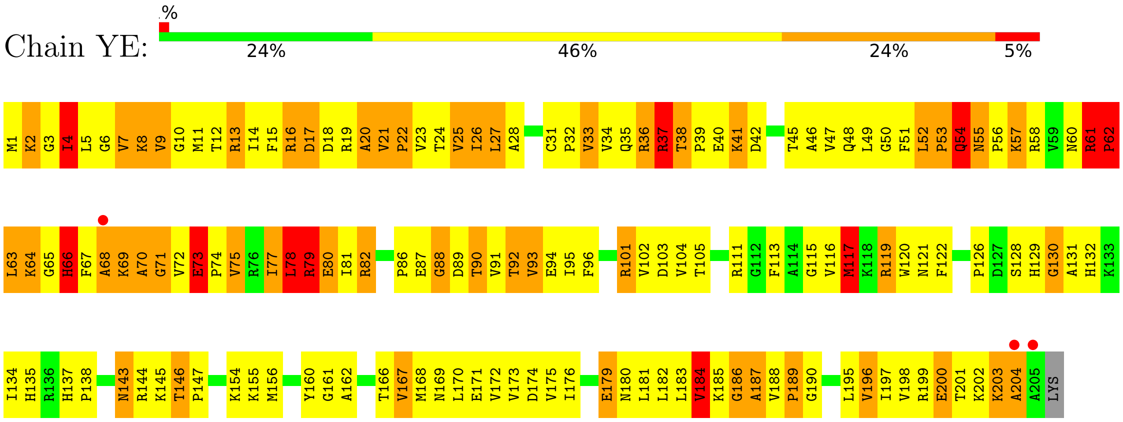
- Molecule 28: 50S ribosomal protein L3

Chain RE:



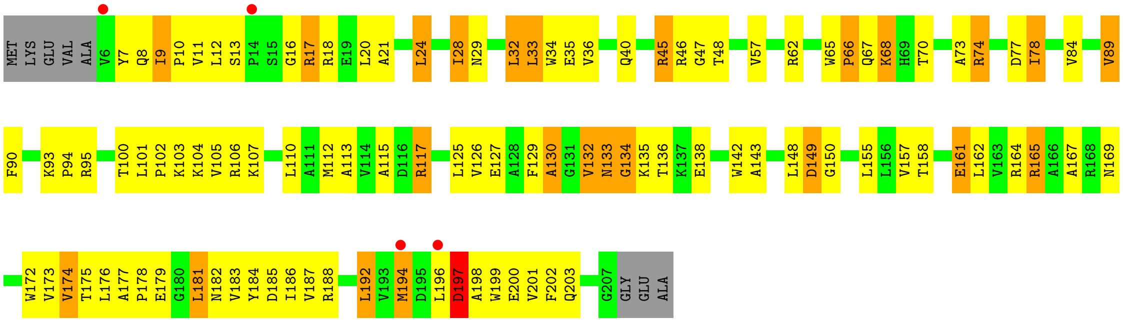
- Molecule 28: 50S ribosomal protein L3

Chain YE:



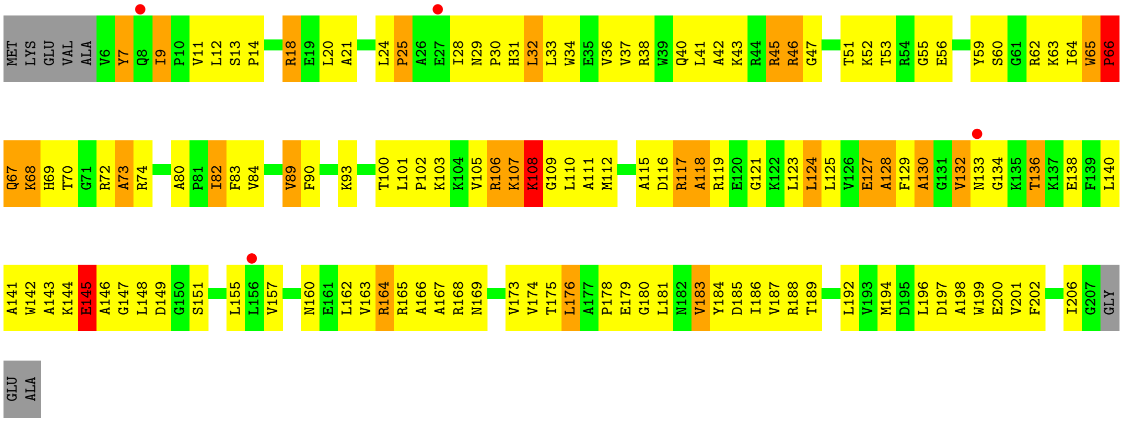
- Molecule 29: 50S ribosomal protein L4

Chain RF:



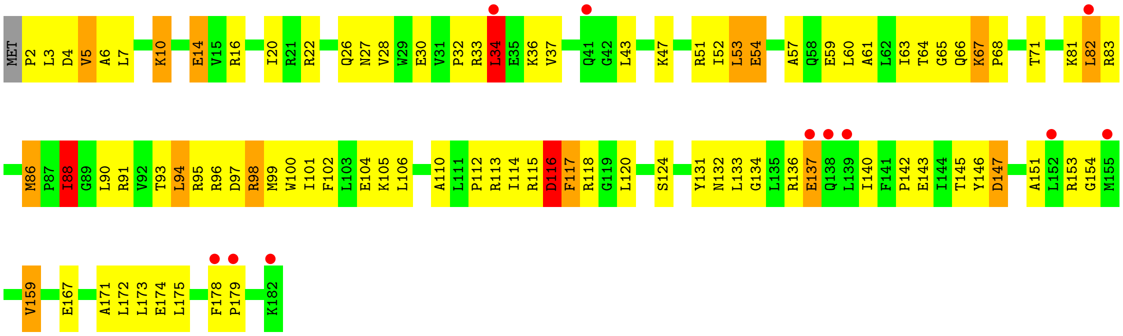
- Molecule 29: 50S ribosomal protein L4

Chain YF:



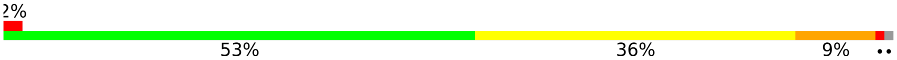
- Molecule 30: 50S ribosomal protein L5

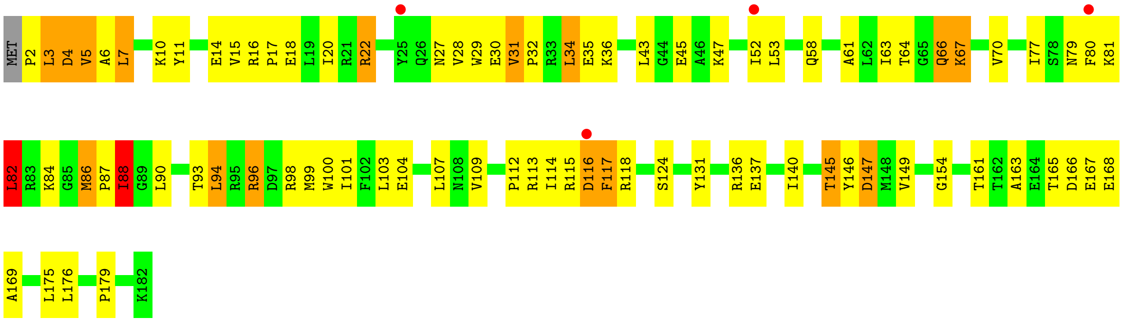
Chain RG:



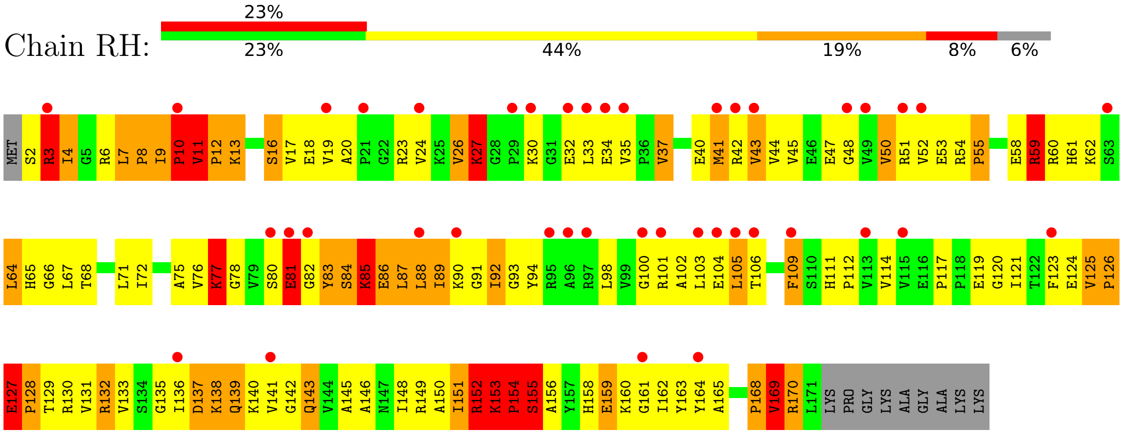
- Molecule 30: 50S ribosomal protein L5

Chain YG:

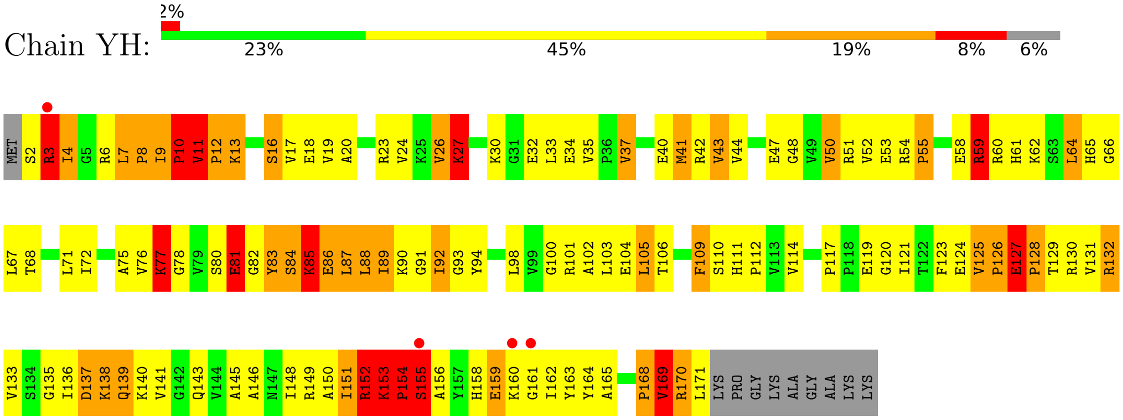




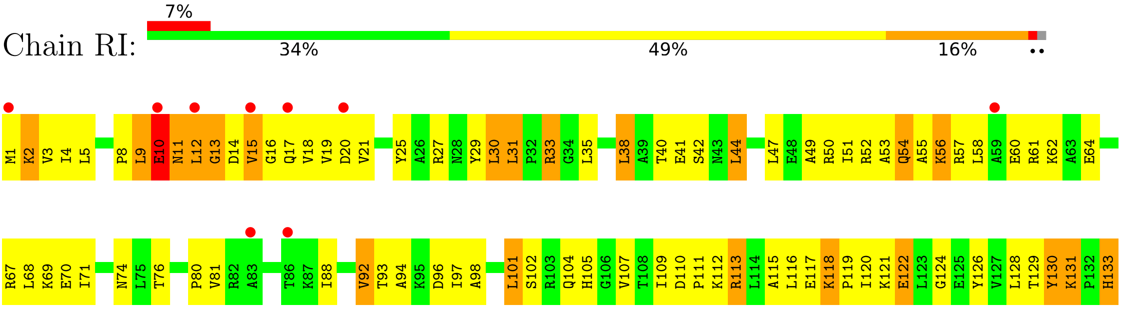
- Molecule 31: 50S ribosomal protein L6

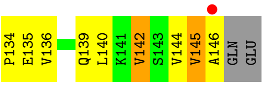


- Molecule 31: 50S ribosomal protein L6

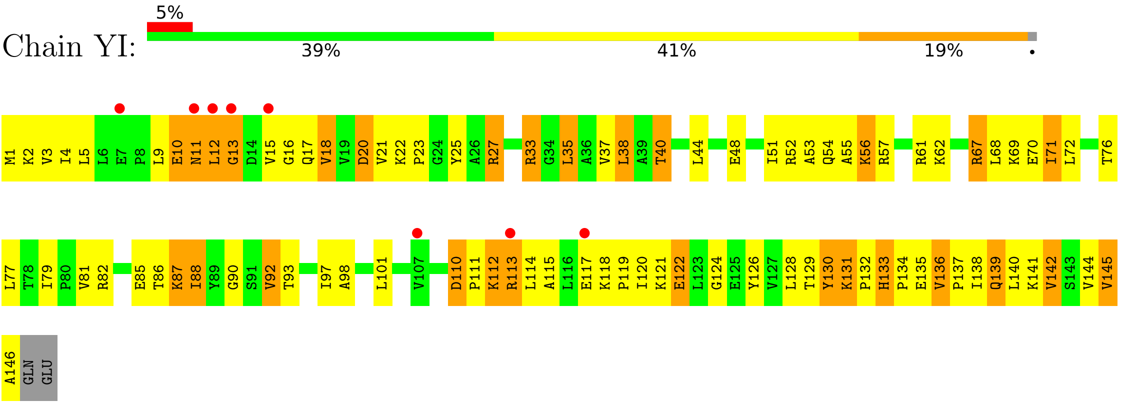


- Molecule 32: 50S ribosomal protein L9

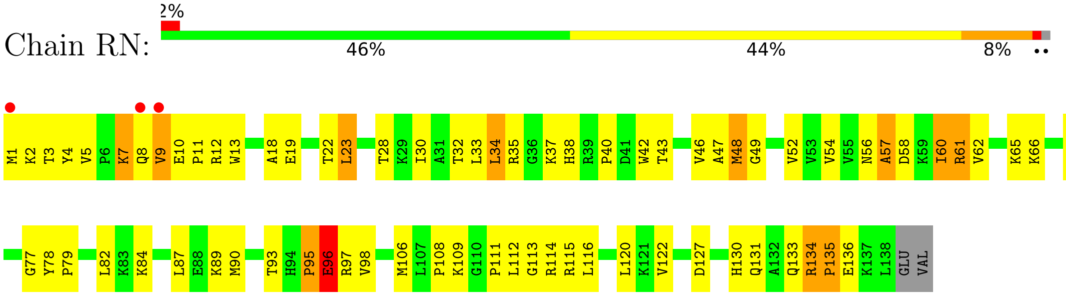




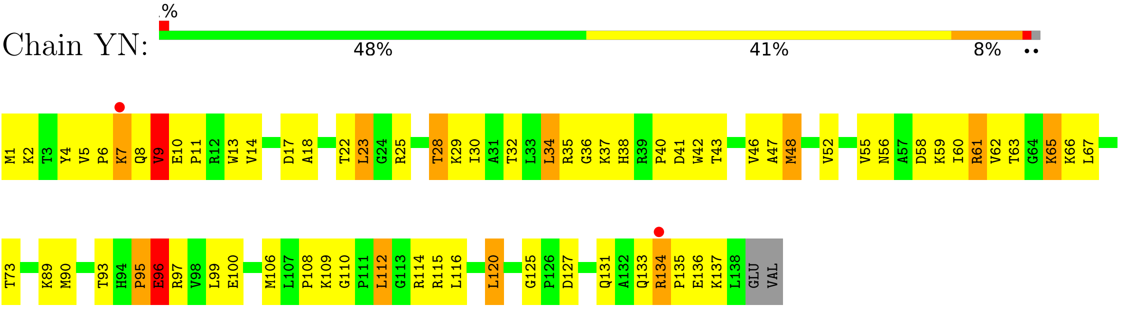
- Molecule 32: 50S ribosomal protein L9



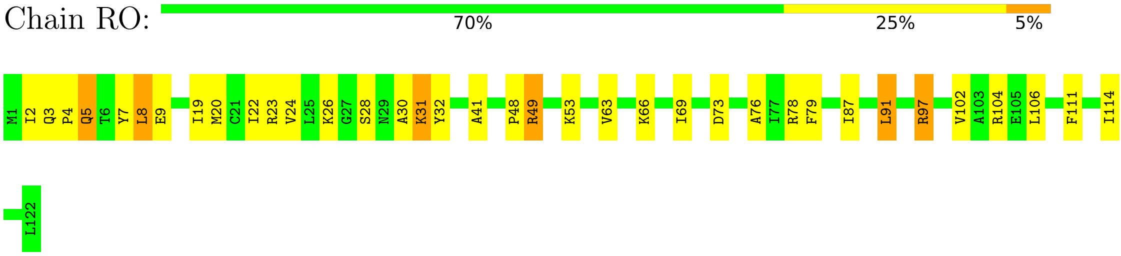
- Molecule 33: 50S ribosomal protein L13



- Molecule 33: 50S ribosomal protein L13

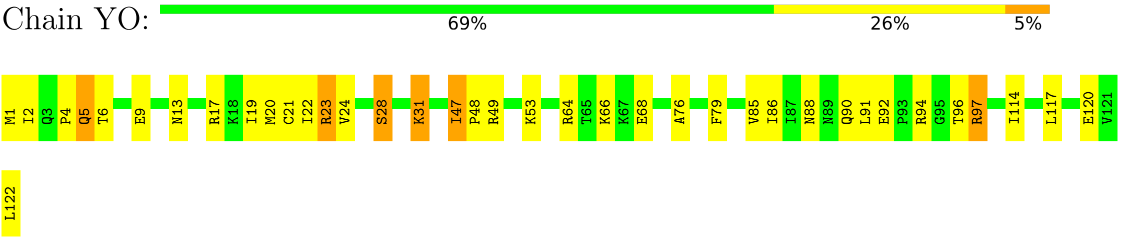


- Molecule 34: 50S ribosomal protein L14



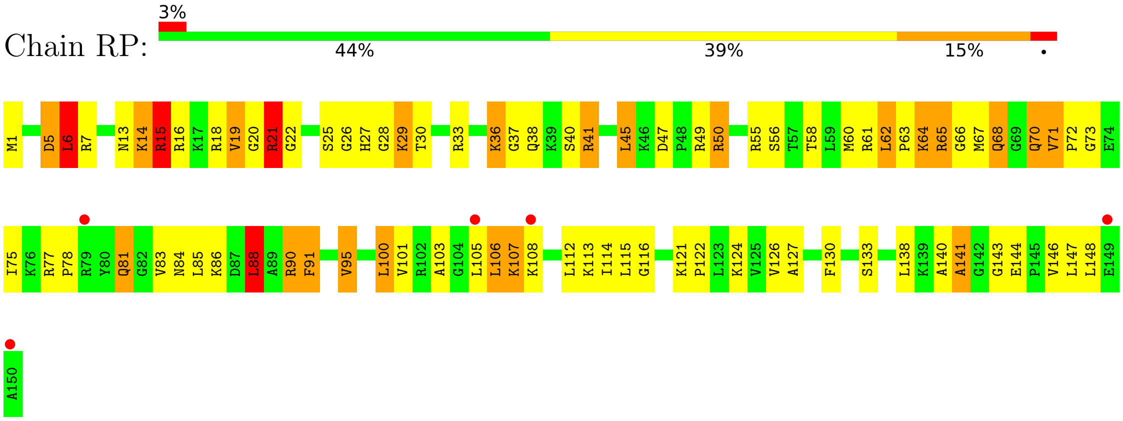
- Molecule 34: 50S ribosomal protein L14

Chain YO:



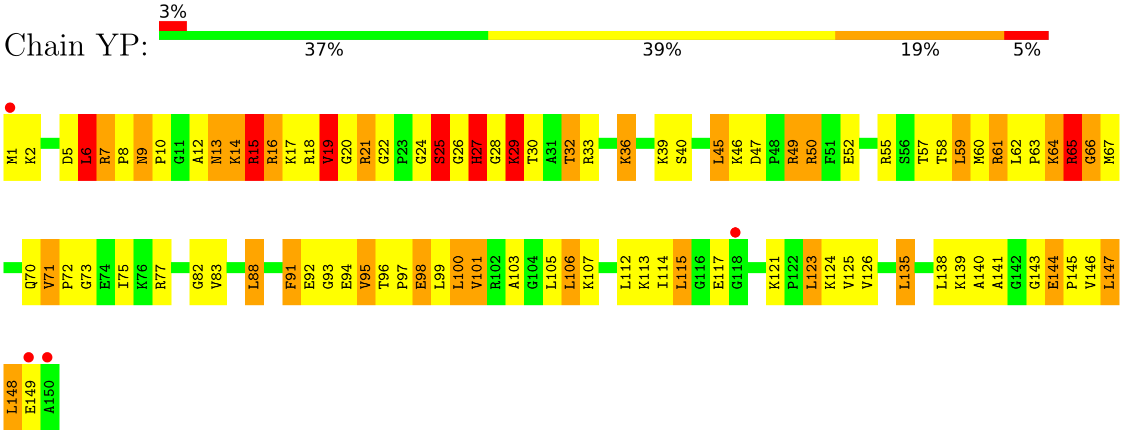
- Molecule 35: 50S ribosomal protein L15

Chain RP:



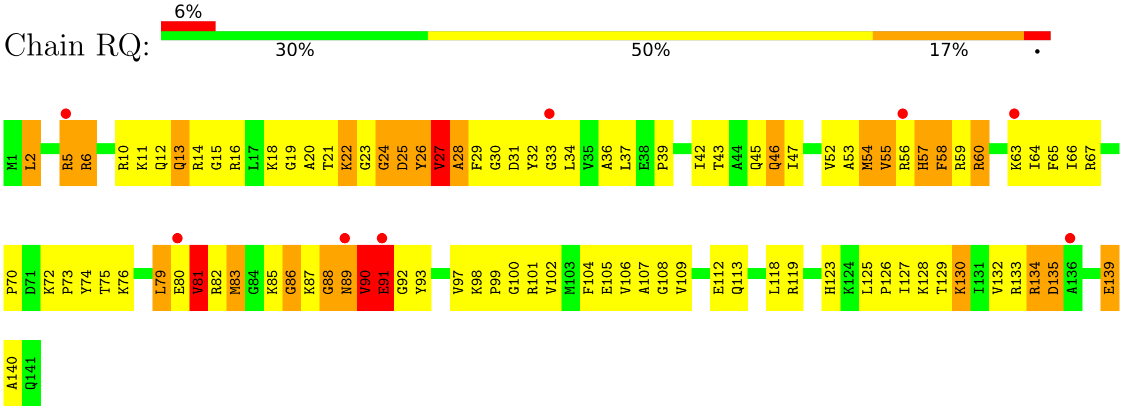
- Molecule 35: 50S ribosomal protein L15

Chain YP:



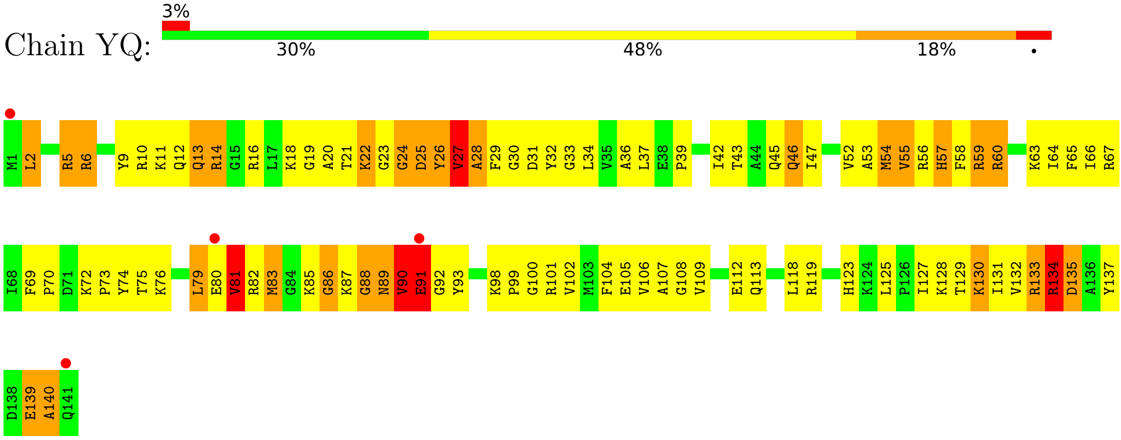
- Molecule 36: 50S ribosomal protein L16

Chain RQ:



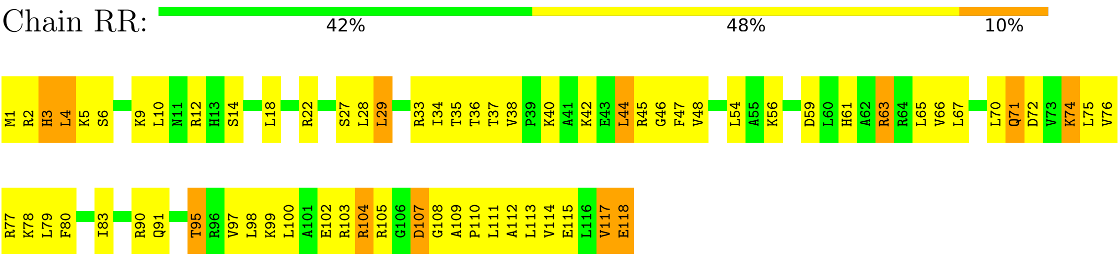
- Molecule 36: 50S ribosomal protein L16

Chain YQ:



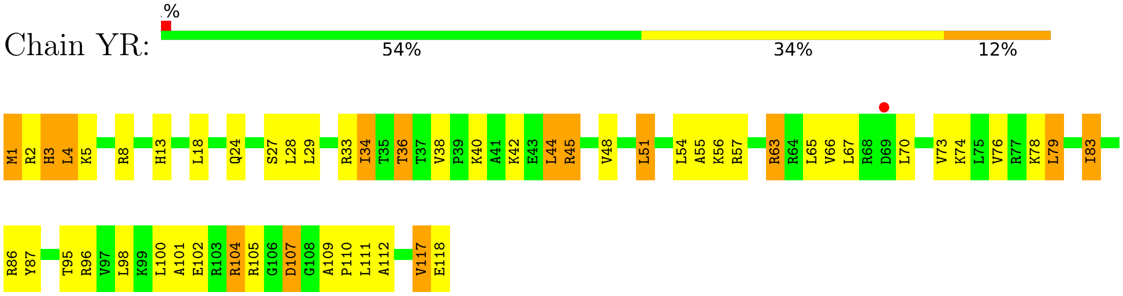
- Molecule 37: 50S ribosomal protein L17

Chain RR:



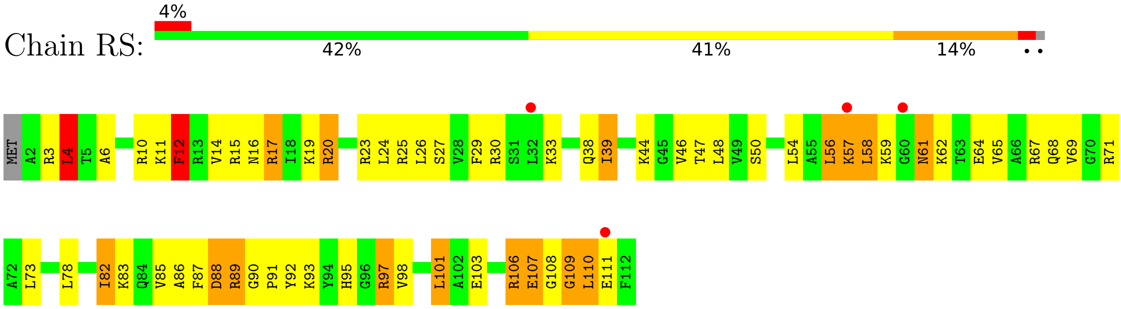
- Molecule 37: 50S ribosomal protein L17

Chain YR:



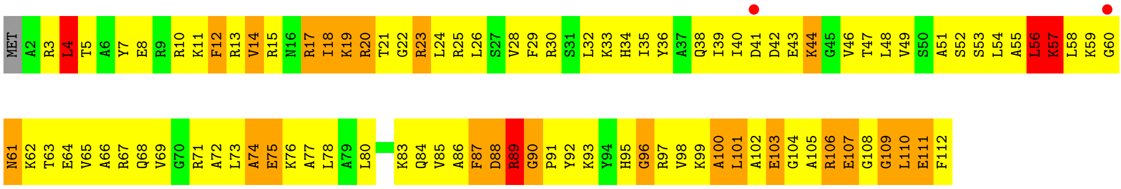
- Molecule 38: 50S ribosomal protein L18

Chain RS:



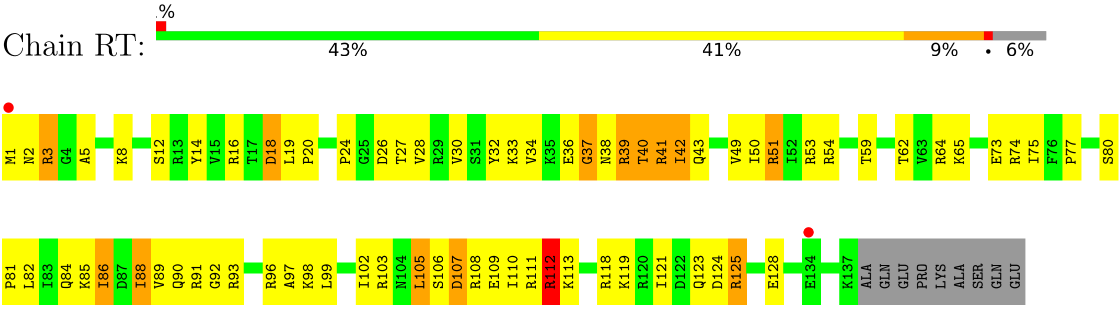
- Molecule 38: 50S ribosomal protein L18

Chain YS:



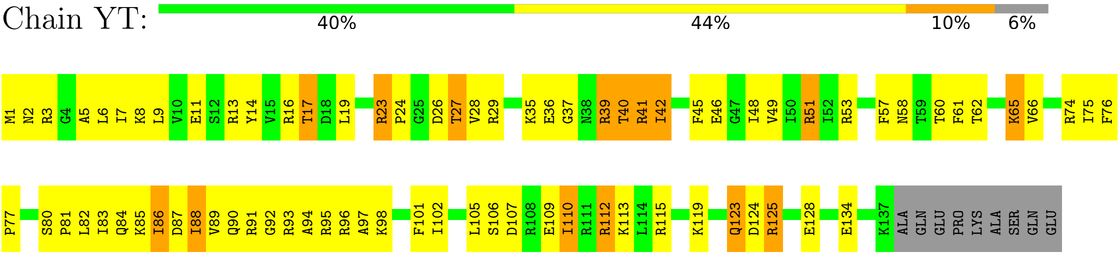
- Molecule 39: 50S ribosomal protein L19

Chain RT:



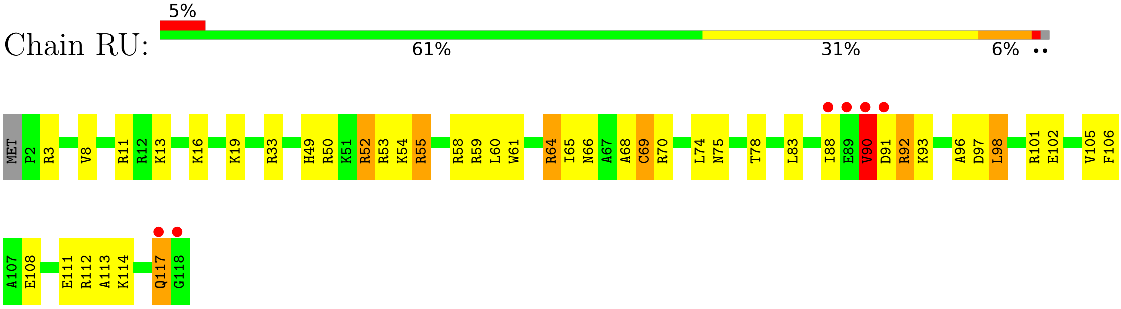
- Molecule 39: 50S ribosomal protein L19

Chain YT:



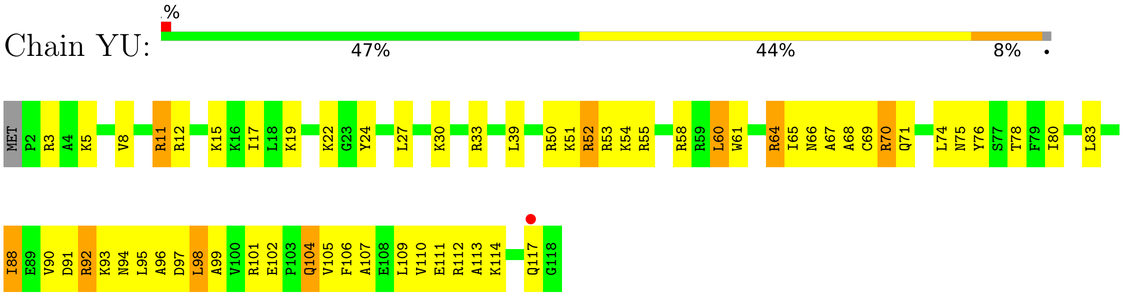
- Molecule 40: 50S ribosomal protein L20

Chain RU:

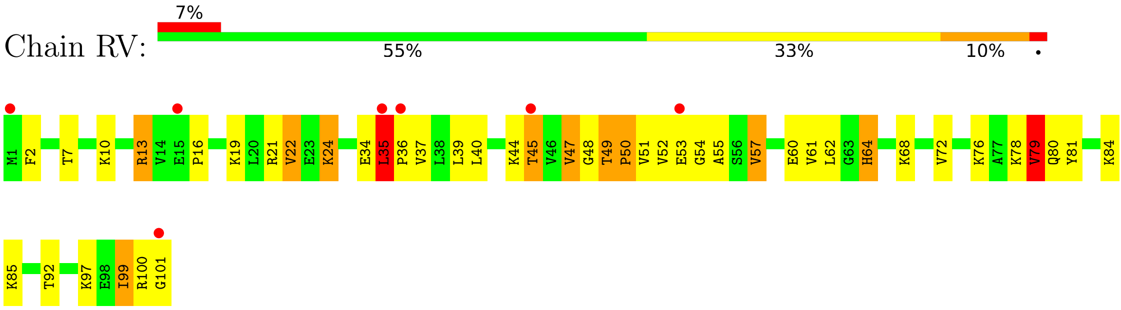


- Molecule 40: 50S ribosomal protein L20

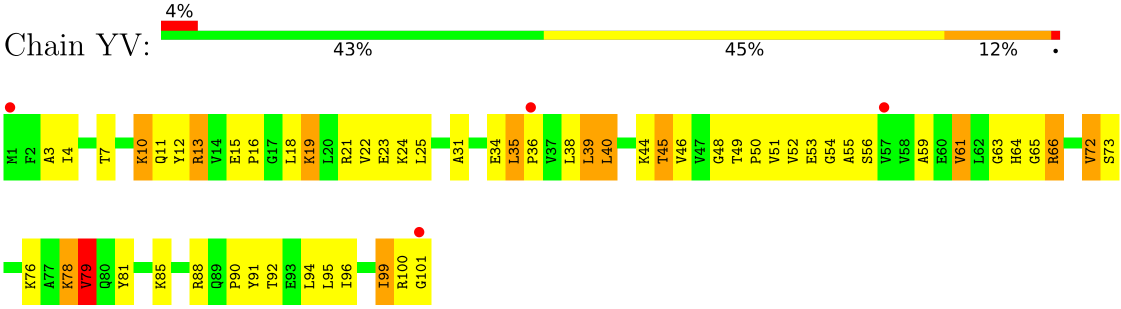
Chain YU:



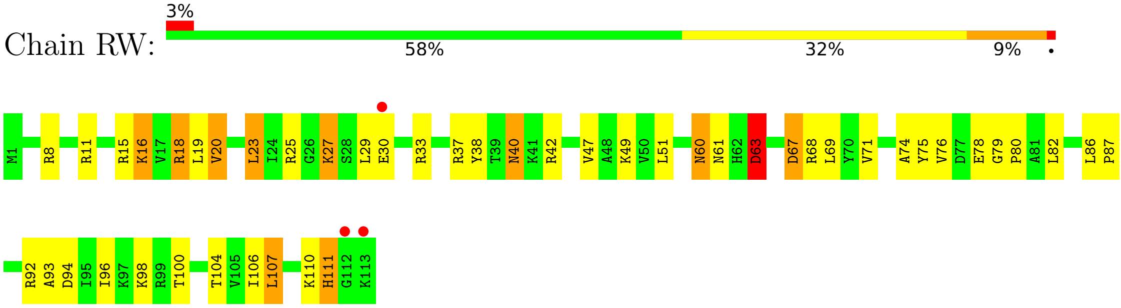
- Molecule 41: 50S ribosomal protein L21



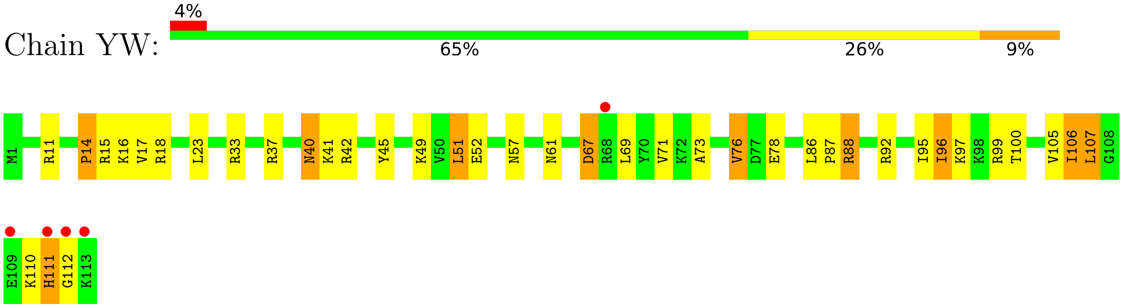
- Molecule 41: 50S ribosomal protein L21



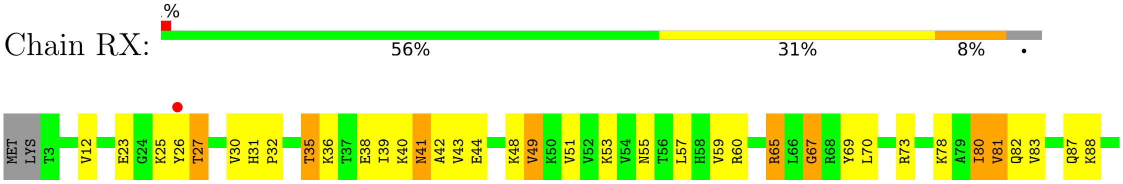
- Molecule 42: 50S ribosomal protein L22

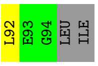


- Molecule 42: 50S ribosomal protein L22



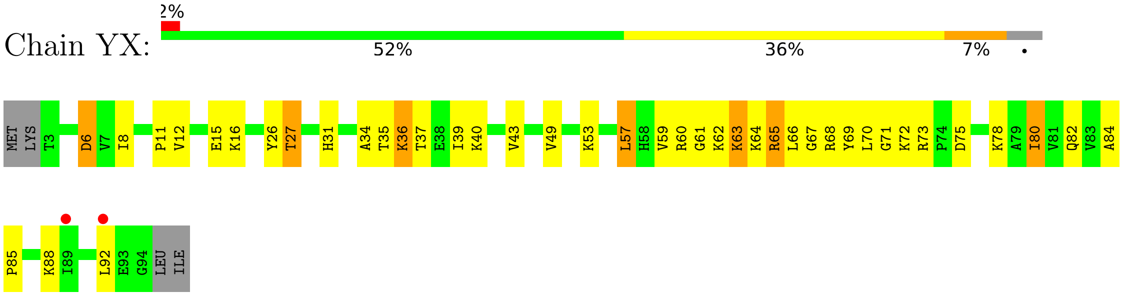
- Molecule 43: 50S ribosomal protein L23





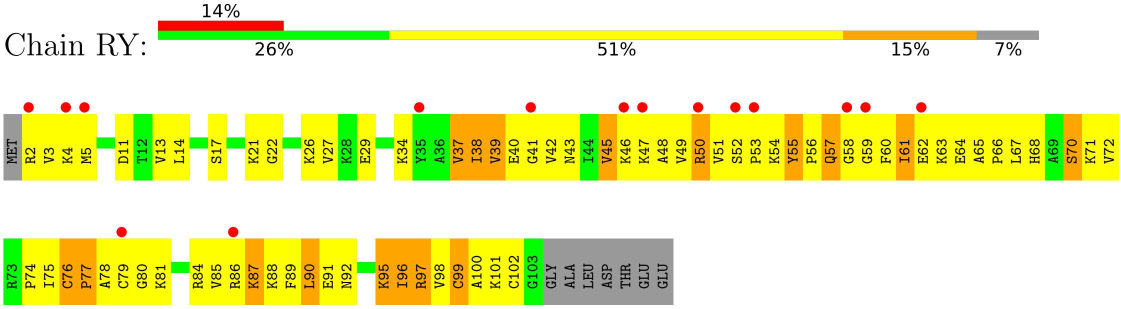
- Molecule 43: 50S ribosomal protein L23

Chain YX:



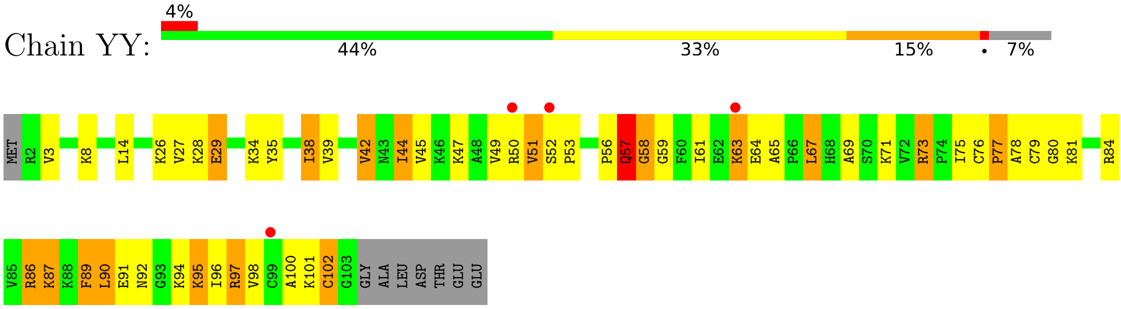
- Molecule 44: 50S ribosomal protein L24

Chain RY:



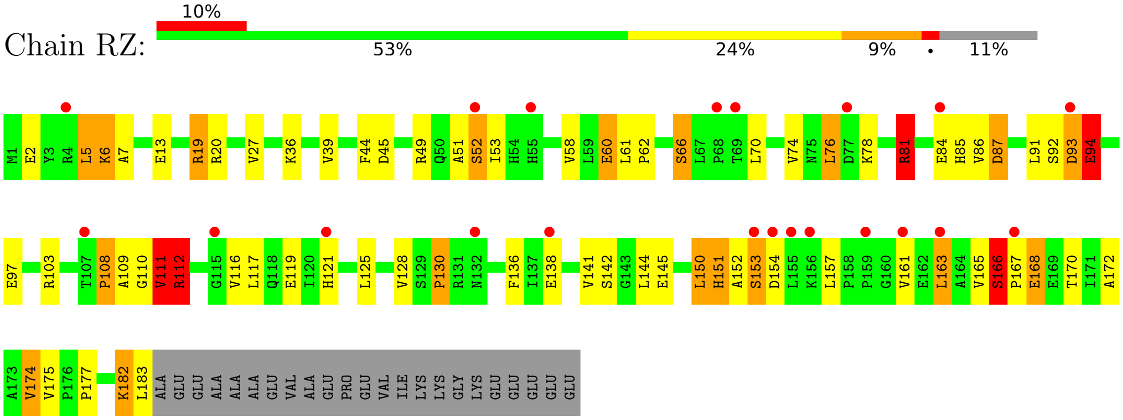
- Molecule 44: 50S ribosomal protein L24

Chain YY:

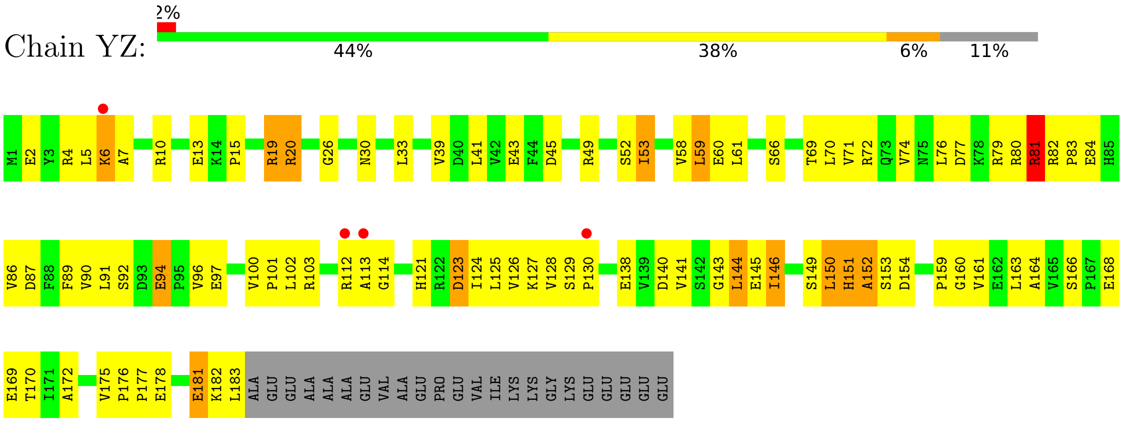


- Molecule 45: 50S ribosomal protein L25

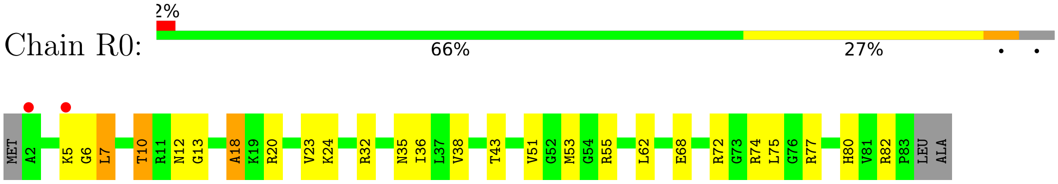
Chain RZ:



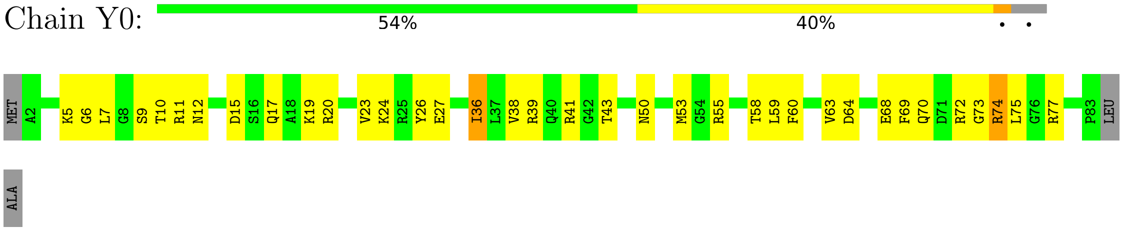
- Molecule 45: 50S ribosomal protein L25



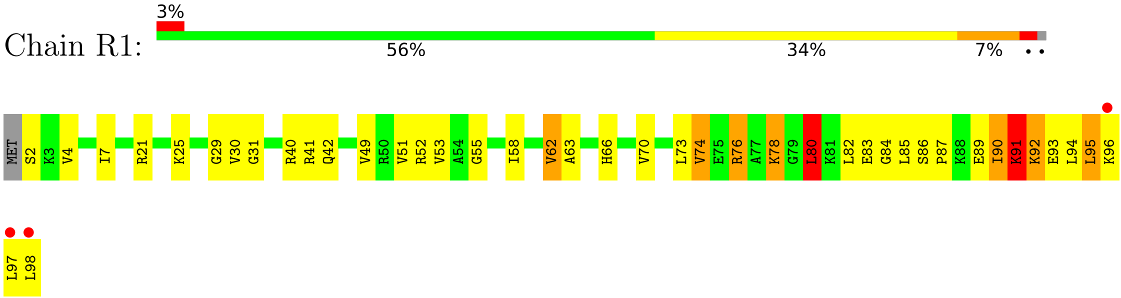
- Molecule 46: 50S ribosomal protein L27



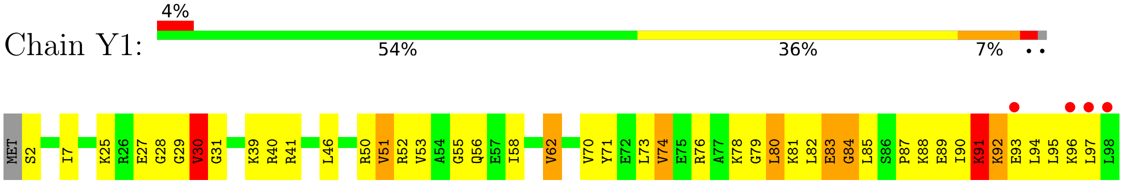
- Molecule 46: 50S ribosomal protein L27



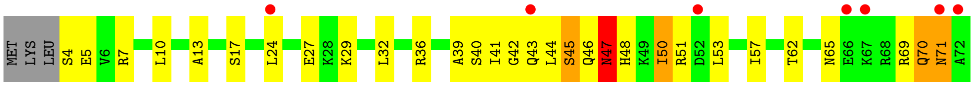
- Molecule 47: 50S ribosomal protein L28



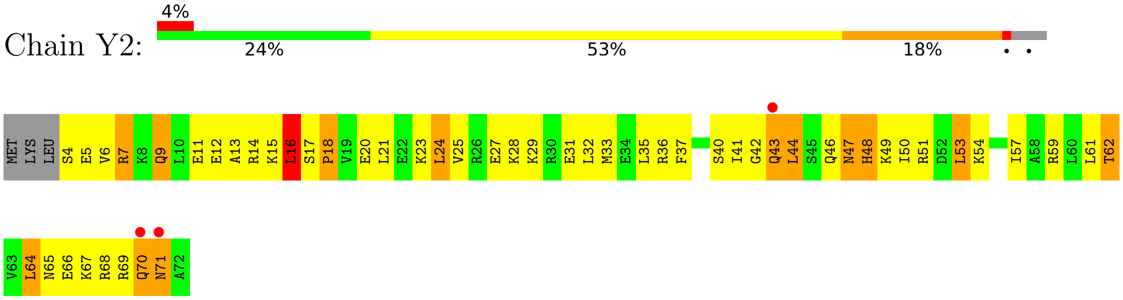
- Molecule 47: 50S ribosomal protein L28



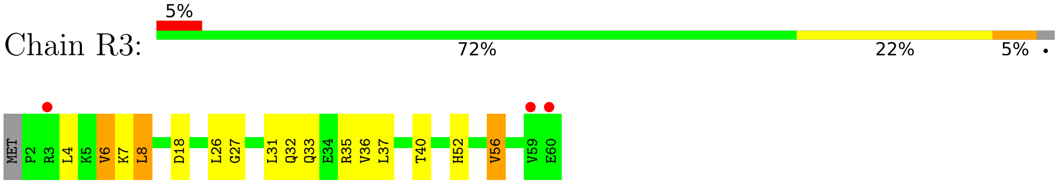
- Molecule 48: 50S ribosomal protein L29



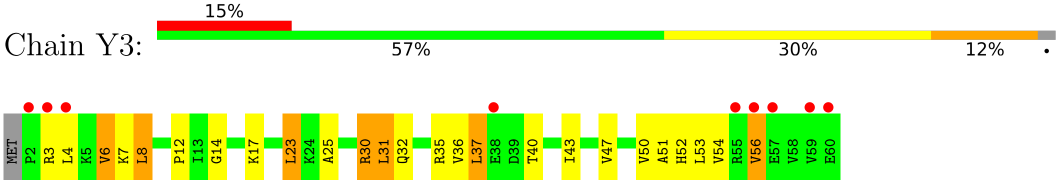
- Molecule 48: 50S ribosomal protein L29



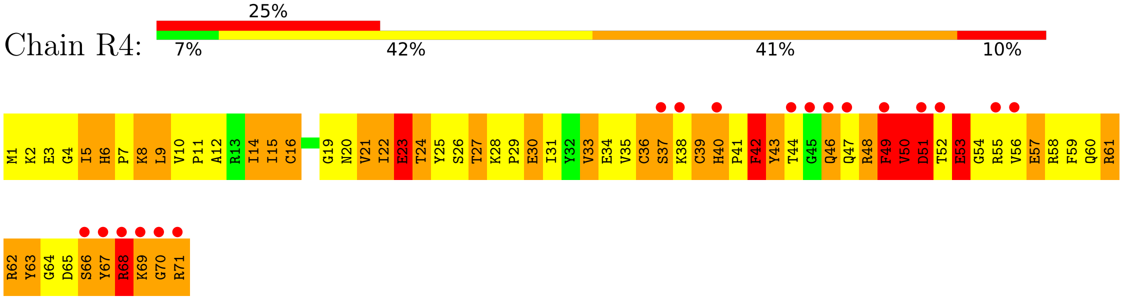
- Molecule 49: 50S ribosomal protein L30



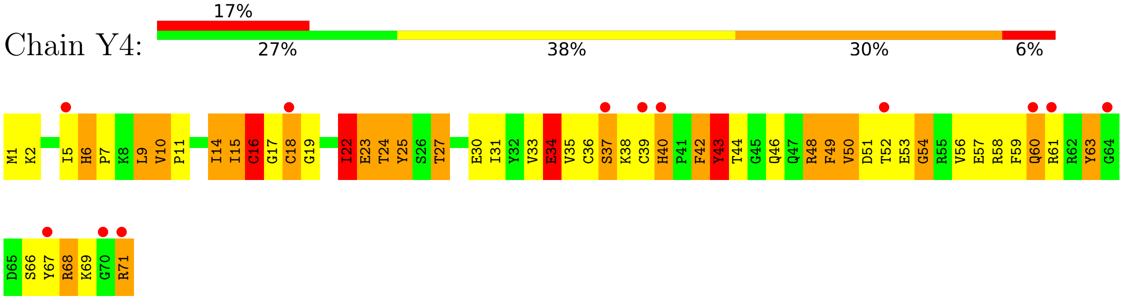
- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L31

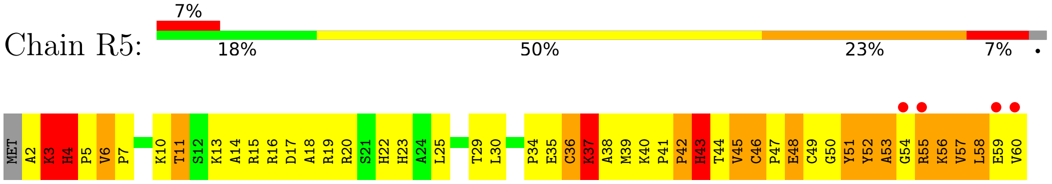


- Molecule 50: 50S ribosomal protein L31



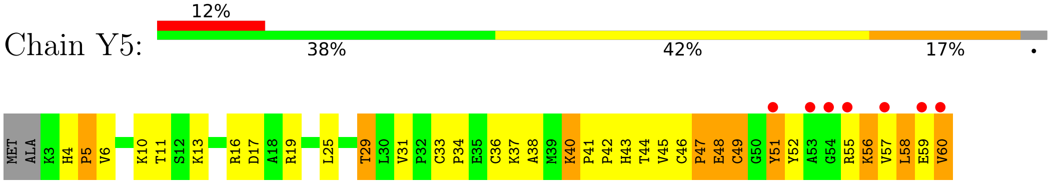
- Molecule 51: 50S ribosomal protein L32

Chain R5:



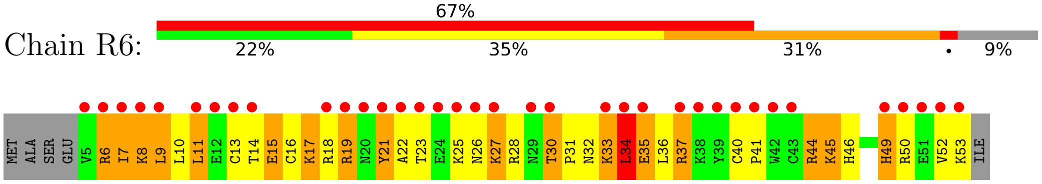
- Molecule 51: 50S ribosomal protein L32

Chain Y5:



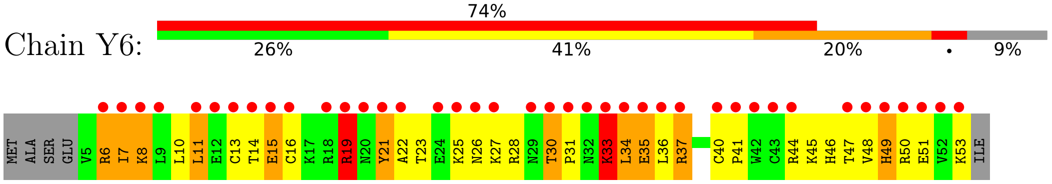
- Molecule 52: 50S ribosomal protein L33

Chain R6:



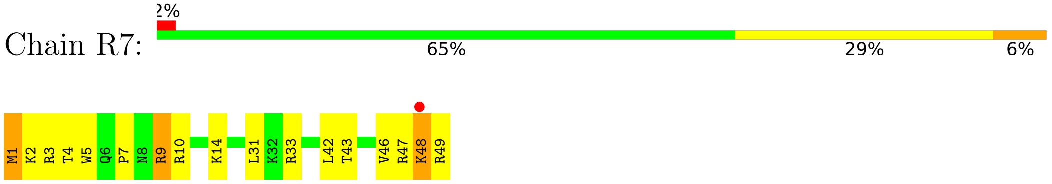
- Molecule 52: 50S ribosomal protein L33

Chain Y6:



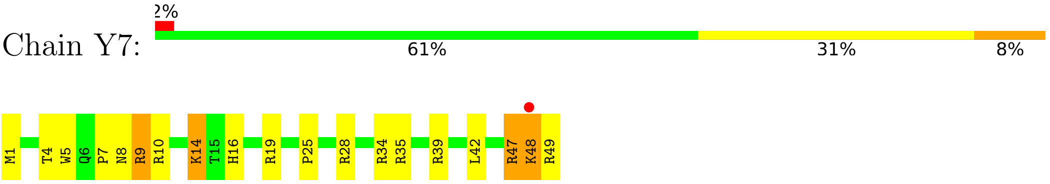
- Molecule 53: 50S ribosomal protein L34

Chain R7:



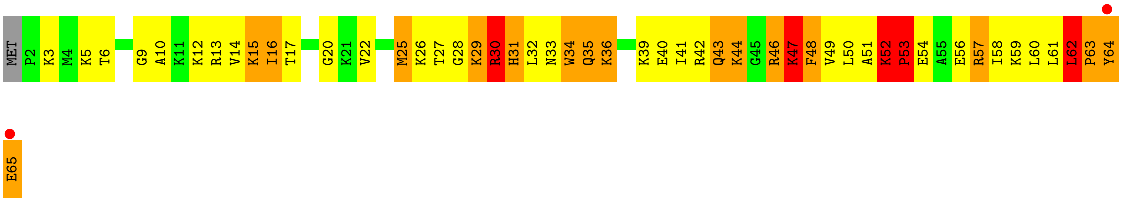
- Molecule 53: 50S ribosomal protein L34

Chain Y7:

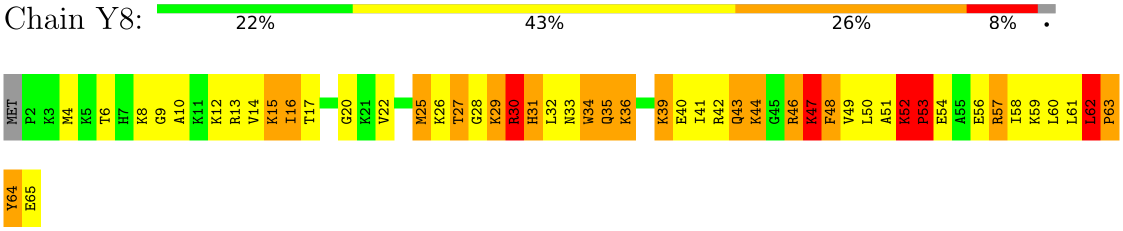


- Molecule 54: 50S ribosomal protein L35

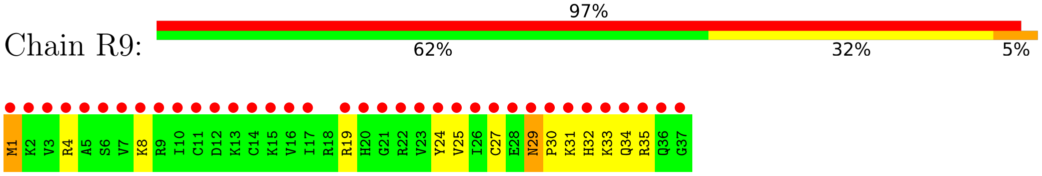
Chain R8:



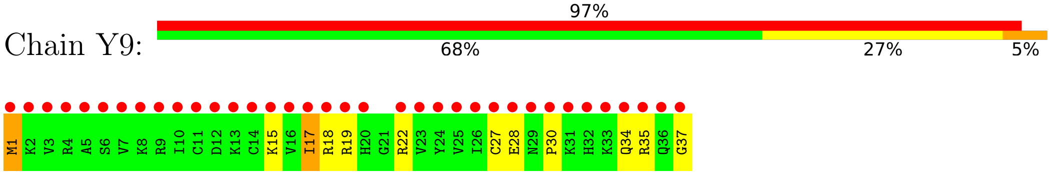
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: CC-Puro

- Molecule 56: CC-Puro

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.99Å 444.57Å 616.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.39 – 3.60 69.39 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (69.39-3.60) 97.2 (69.39-3.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.217 , 0.259 0.217 , 0.259	Depositor DCC
R_{free} test set	34831 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å^2)	87.0	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 95.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	292320	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	QA	0.32	0/36098	0.87	44/56341 (0.1%)
1	XA	0.36	0/36101	0.88	26/56346 (0.0%)
2	QB	0.32	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.32	0/1629	0.54	0/2195
3	XC	0.37	0/1629	0.56	0/2195
4	QD	0.41	0/1733	0.60	2/2318 (0.1%)
4	XD	0.40	0/1733	0.59	0/2318
5	QE	0.38	0/1171	0.60	0/1576
5	XE	0.43	1/1171 (0.1%)	0.63	2/1576 (0.1%)
6	QF	0.38	0/856	0.55	0/1154
6	XF	0.39	0/856	0.58	0/1154
7	QG	0.34	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.51	0/1709
8	QH	0.34	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.56	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.33	0/814	0.54	0/1095
10	XJ	0.39	1/814 (0.1%)	0.63	1/1095 (0.1%)
11	QK	0.38	0/900	0.59	1/1213 (0.1%)
11	XK	0.39	0/900	0.59	0/1213
12	QL	0.49	1/991 (0.1%)	0.80	1/1327 (0.1%)
12	XL	0.50	0/991	0.85	3/1327 (0.2%)
13	QM	0.32	0/974	0.58	0/1303
13	XM	0.37	0/974	0.62	0/1303
14	QN	0.37	0/501	0.62	0/664
14	XN	0.43	0/501	0.66	0/664
15	QO	0.35	0/745	0.54	0/992
15	XO	0.40	0/745	0.54	0/992
16	QP	0.36	0/721	0.57	0/970
16	XP	0.35	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\lvert Z\rvert>5$	RMSZ	#$\lvert Z\rvert>5$
17	QQ	0.35	0/847	0.54	0/1131
17	XQ	0.36	0/847	0.54	0/1131
18	QR	0.36	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.59	0/768
19	QS	0.34	0/689	0.61	0/926
19	XS	0.38	0/689	0.69	1/926 (0.1%)
20	QT	0.35	0/765	0.65	0/1007
20	XT	0.32	0/765	0.61	0/1007
21	QU	0.30	0/221	0.55	0/288
21	XU	0.31	0/221	0.62	0/288
22	QV	0.38	1/1836 (0.1%)	0.80	0/2859
22	XV	0.41	1/1836 (0.1%)	0.83	0/2859
23	QX	0.33	0/213	0.81	0/329
23	XX	0.67	0/238	0.86	0/368
24	QY	0.43	0/384	0.83	0/597
24	XY	0.36	0/384	0.85	0/597
25	RA	0.39	2/69521 (0.0%)	0.91	59/108529 (0.1%)
25	YA	0.42	1/69521 (0.0%)	0.94	81/108529 (0.1%)
26	RB	0.51	0/2878	1.17	11/4490 (0.2%)
26	YB	0.62	1/2878 (0.0%)	1.28	24/4490 (0.5%)
27	RD	0.51	0/2165	0.70	0/2919
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.44	0/1620	0.70	3/2194 (0.1%)
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.32	0/1499	0.57	1/2016 (0.0%)
30	YG	0.40	0/1499	0.60	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.38	0/1151	0.67	0/1558
32	YI	0.38	0/1151	0.65	0/1558
33	RN	0.41	0/1131	0.62	0/1525
33	YN	0.46	0/1131	0.66	1/1525 (0.1%)
34	RO	0.41	0/943	0.63	1/1269 (0.1%)
34	YO	0.49	0/943	0.65	0/1269
35	RP	0.41	0/1162	0.79	1/1544 (0.1%)
35	YP	0.53	0/1162	0.89	2/1544 (0.1%)
36	RQ	0.54	0/1143	0.90	3/1527 (0.2%)
36	YQ	0.53	0/1143	0.87	3/1527 (0.2%)
37	RR	0.42	0/982	0.69	0/1312
37	YR	0.44	0/982	0.73	0/1312
38	RS	0.36	0/892	0.65	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YS	0.46	0/892	0.83	1/1187 (0.1%)
39	RT	0.42	0/1155	0.63	0/1542
39	YT	0.43	0/1155	0.66	0/1542
40	RU	0.39	0/982	0.65	0/1306
40	YU	0.51	0/982	0.70	0/1306
41	RV	0.38	0/790	0.61	1/1057 (0.1%)
41	YV	0.46	0/790	0.73	1/1057 (0.1%)
42	RW	0.49	0/911	0.67	0/1220
42	YW	0.45	0/911	0.68	0/1220
43	RX	0.47	0/739	0.62	0/993
43	YX	0.48	0/739	0.65	0/993
44	RY	0.44	0/798	0.68	0/1064
44	YY	0.46	0/798	0.70	0/1064
45	RZ	0.30	0/1493	0.52	0/2026
45	YZ	0.29	0/1493	0.55	0/2026
46	R0	0.45	0/657	0.65	0/874
46	Y0	0.49	0/656	0.70	0/872
47	R1	0.44	0/770	0.66	0/1022
47	Y1	0.46	0/770	0.69	0/1022
48	R2	0.39	0/583	0.64	0/771
48	Y2	0.51	0/583	0.83	1/771 (0.1%)
49	R3	0.35	0/474	0.57	0/635
49	Y3	0.42	0/474	0.59	0/635
50	R4	0.39	0/594	0.78	1/795 (0.1%)
50	Y4	0.37	0/594	0.68	0/795
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.50	0/468	0.72	0/632
52	R6	0.34	0/431	0.69	0/575
52	Y6	0.37	0/431	0.67	0/575
53	R7	0.49	0/438	0.68	0/575
53	Y7	0.56	0/438	0.71	0/575
54	R8	0.61	0/525	0.92	1/691 (0.1%)
54	Y8	0.62	0/525	0.92	1/691 (0.1%)
55	R9	0.26	0/310	0.45	0/407
55	Y9	0.33	0/310	0.48	0/407
56	Z5	0.80	0/40	1.79	1/60 (1.7%)
56	Z6	0.79	0/40	1.79	1/60 (1.7%)
All	All	0.40	9/316522 (0.0%)	0.86	296/473223 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	0	C	OP3-P	-10.63	1.48	1.61
22	XV	0	C	OP3-P	-10.58	1.48	1.61
5	XE	101	ILE	C-N	5.68	1.47	1.34
25	RA	2299	A	N9-C4	-5.68	1.34	1.37
25	YA	1021	A	N9-C4	-5.59	1.34	1.37

The worst 5 of 296 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	YE	21	VAL	C-N-CD	-10.10	98.37	120.60
28	RE	21	VAL	C-N-CD	-10.10	98.39	120.60
1	XA	1054	C	C6-N1-C2	-9.78	116.39	120.30
1	XA	1495	U	N1-C2-O2	9.30	129.31	122.80
25	RA	2432	C	O5'-P-OP1	-9.29	97.34	105.70

There are no chirality outliers.

There are no planarity outliers.

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	QA	32247	0	16278	544	0
1	XA	32249	0	16279	566	0
2	QB	1924	0	1975	64	0
2	XB	1924	0	1975	88	0
3	QC	1605	0	1668	51	0
3	XC	1605	0	1668	63	0
4	QD	1703	0	1765	106	0
4	XD	1703	0	1762	47	0
5	QE	1155	0	1213	48	0
5	XE	1155	0	1213	52	0
6	QF	843	0	857	17	0
6	XF	843	0	857	33	0
7	QG	1257	0	1296	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	27	0
8	QH	1116	0	1177	42	0
8	XH	1116	0	1177	33	0
9	QI	1010	0	1037	49	0
9	XI	1010	0	1037	51	0
10	QJ	801	0	849	52	0
10	XJ	801	0	849	63	0
11	QK	885	0	904	32	0
11	XK	885	0	904	29	0
12	QL	975	0	1062	98	0
12	XL	975	0	1062	95	0
13	QM	964	0	1034	66	0
13	XM	964	0	1034	47	0
14	QN	492	0	529	33	0
14	XN	492	0	529	20	0
15	QO	734	0	771	19	0
15	XO	734	0	771	18	0
16	QP	705	0	725	17	0
16	XP	705	0	725	24	0
17	QQ	834	0	904	25	0
17	XQ	834	0	904	17	0
18	QR	574	0	644	11	0
18	XR	574	0	644	23	0
19	QS	674	0	699	95	0
19	XS	674	0	699	43	0
20	QT	763	0	861	31	0
20	XT	763	0	861	68	0
21	QU	217	0	234	13	0
21	XU	217	0	234	5	0
22	QV	1644	0	835	20	0
22	XV	1644	0	836	18	0
23	QX	191	0	99	1	0
23	XX	213	0	110	3	0
24	QY	344	0	173	3	0
24	XY	344	0	173	14	0
25	RA	62071	0	31290	1016	0
25	YA	62071	0	31290	988	0
26	RB	2573	0	1306	57	0
26	YB	2573	0	1306	79	0
27	RD	2115	0	2195	104	0
27	YD	2115	0	2195	327	0
28	RE	1568	0	1634	282	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	273	0
29	RF	1585	0	1632	78	0
29	YF	1585	0	1632	179	0
30	RG	1474	0	1535	111	0
30	YG	1474	0	1535	69	0
31	RH	1307	0	1382	228	0
31	YH	1307	0	1382	227	0
32	RI	1136	0	1223	106	0
32	YI	1136	0	1223	68	0
33	RN	1104	0	1180	45	0
33	YN	1104	0	1180	53	0
34	RO	933	0	996	26	0
34	YO	933	0	996	27	0
35	RP	1145	0	1228	117	0
35	YP	1145	0	1227	113	0
36	RQ	1122	0	1179	168	0
36	YQ	1122	0	1179	176	0
37	RR	968	0	1033	53	0
37	YR	968	0	1033	41	0
38	RS	882	0	943	54	0
38	YS	882	0	943	164	0
39	RT	1141	0	1202	72	0
39	YT	1141	0	1202	59	0
40	RU	964	0	1022	38	0
40	YU	964	0	1021	59	0
41	RV	779	0	852	26	0
41	YV	779	0	852	45	0
42	RW	900	0	964	29	0
42	YW	900	0	964	27	0
43	RX	725	0	778	31	0
43	YX	725	0	778	26	0
44	RY	785	0	878	53	0
44	YY	785	0	878	39	0
45	RZ	1461	0	1493	43	0
45	YZ	1461	0	1493	63	0
46	R0	648	0	672	26	0
46	Y0	647	0	668	41	0
47	R1	763	0	848	33	0
47	Y1	763	0	848	36	0
48	R2	581	0	629	24	0
48	Y2	581	0	629	73	0
49	R3	469	0	518	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	16	0
50	R4	581	0	575	230	0
50	Y4	581	0	577	63	0
51	R5	459	0	480	76	0
51	Y5	454	0	475	40	0
52	R6	424	0	450	41	0
52	Y6	424	0	450	38	0
53	R7	430	0	480	18	0
53	Y7	430	0	480	22	0
54	R8	517	0	582	132	0
54	Y8	517	0	582	103	0
55	R9	307	0	338	11	0
55	Y9	307	0	338	17	0
56	Z5	74	0	51	13	0
56	Z6	74	0	51	9	0
57	QA	80	0	0	0	0
57	QE	1	0	0	0	0
57	QF	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	2	0	0	0	0
57	QX	2	0	0	0	0
57	QY	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	RA	326	0	0	0	0
57	RB	5	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	1	0	0	0	0
57	RR	1	0	0	0	0
57	XA	110	0	0	0	0
57	XB	1	0	0	0	0
57	XD	1	0	0	0	0
57	XF	1	0	0	0	0
57	XV	2	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	3	0	0	0	0
57	Y1	1	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	356	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YB	4	0	0	0	0
57	YD	1	0	0	0	0
57	YE	2	0	0	0	0
57	YP	3	0	0	0	0
57	YQ	1	0	0	0	0
57	YU	1	0	0	0	0
57	YY	1	0	0	0	0
58	QA	42	0	45	4	0
58	XA	42	0	45	2	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	292320	0	198405	8425	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 8425 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)
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52
32:RI:144:VAL:O	32:RI:145:VAL:HG12	1.22	1.36
4:QD:9:CYS:SG	4:QD:22:LYS:CE	2.22	1.28
32:YI:144:VAL:O	32:YI:145:VAL:HG22	1.22	1.28

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	174 (74%)	44 (19%)	17 (7%)	1	13
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1	17
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	4	33
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	10	47
4	QD	206/209 (99%)	178 (86%)	19 (9%)	9 (4%)	2	23
4	XD	206/209 (99%)	176 (85%)	25 (12%)	5 (2%)	6	37
5	QE	149/162 (92%)	136 (91%)	9 (6%)	4 (3%)	5	35
5	XE	149/162 (92%)	134 (90%)	13 (9%)	2 (1%)	12	50
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	136 (89%)	15 (10%)	2 (1%)	12	50
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	12	50
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	22	61
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	4	33
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3	26
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	4	31
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	4	32
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	20
11	QK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	9	45
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	9	45
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	6
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	6
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	12
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	12
14	QN	58/61 (95%)	50 (86%)	4 (7%)	4 (7%)	1	14
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	7
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	51
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	38
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	13	51
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	13	51
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	7	41
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	23
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	10	47
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	4
19	XS	82/93 (88%)	54 (66%)	18 (22%)	10 (12%)	0	5
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1	17
20	XT	97/106 (92%)	75 (77%)	17 (18%)	5 (5%)	2	20
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	24
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	24
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	23
27	YD	270/276 (98%)	205 (76%)	46 (17%)	19 (7%)	1	14
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
29	RF	200/210 (95%)	171 (86%)	19 (10%)	10 (5%)	2	21
29	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	0	8
30	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	11
30	YG	179/182 (98%)	143 (80%)	24 (13%)	12 (7%)	1	15
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	99 (69%)	31 (22%)	14 (10%)	0	8
32	YI	144/148 (97%)	106 (74%)	21 (15%)	17 (12%)	0	5
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	9
33	YN	136/140 (97%)	109 (80%)	16 (12%)	11 (8%)	1	11
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9	45
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	9	45
35	RP	148/150 (99%)	112 (76%)	25 (17%)	11 (7%)	1	13
35	YP	148/150 (99%)	111 (75%)	22 (15%)	15 (10%)	0	7
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	7
36	YQ	139/141 (99%)	98 (70%)	25 (18%)	16 (12%)	0	6
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	24
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2	20
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	62 (57%)	29 (27%)	18 (16%)	0	3
39	RT	135/146 (92%)	107 (79%)	16 (12%)	12 (9%)	1	9
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	13
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	30
40	YU	115/118 (98%)	101 (88%)	12 (10%)	2 (2%)	9	45
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	17
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	11
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	3	29
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	8	43
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6	39
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	6	39
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	3
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	5
45	RZ	181/206 (88%)	128 (71%)	33 (18%)	20 (11%)	0	6
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	0	8
46	R0	80/85 (94%)	65 (81%)	14 (18%)	1 (1%)	12	50
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	8
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	17
48	R2	67/72 (93%)	54 (81%)	9 (13%)	4 (6%)	1	17
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	4
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	30
49	Y3	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	43
50	R4	69/71 (97%)	22 (32%)	21 (30%)	26 (38%)	0	0
50	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
51	Y5	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	3	29
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	0
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	2
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	7	40
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	7	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	R8	62/65 (95%)	36 (58%)	14 (23%)	12 (19%)	0	2
54	Y8	62/65 (95%)	36 (58%)	14 (23%)	12 (19%)	0	2
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11469/12128 (95%)	9009 (79%)	1610 (14%)	850 (7%)	1	13

5 of 850 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	28	SER
4	QD	33	MET

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	QB	205/220 (93%)	172 (84%)	33 (16%)	2	16
2	XB	205/220 (93%)	180 (88%)	25 (12%)	5	26
3	QC	159/188 (85%)	145 (91%)	14 (9%)	10	40
3	XC	159/188 (85%)	145 (91%)	14 (9%)	10	40
4	QD	180/181 (99%)	155 (86%)	25 (14%)	3	22
4	XD	180/181 (99%)	154 (86%)	26 (14%)	3	20
5	QE	116/123 (94%)	104 (90%)	12 (10%)	7	34
5	XE	116/123 (94%)	104 (90%)	12 (10%)	7	34
6	QF	90/90 (100%)	78 (87%)	12 (13%)	4	23
6	XF	90/90 (100%)	82 (91%)	8 (9%)	9	40
7	QG	126/127 (99%)	114 (90%)	12 (10%)	8	37
7	XG	126/127 (99%)	114 (90%)	12 (10%)	8	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	109 (92%)	10 (8%)	11	42
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	32
9	QI	98/99 (99%)	80 (82%)	18 (18%)	1	10
9	XI	98/99 (99%)	79 (81%)	19 (19%)	1	9
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4	23
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	2	17
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	35
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	35
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	23
12	XL	104/109 (95%)	89 (86%)	15 (14%)	3	20
13	QM	97/101 (96%)	73 (75%)	24 (25%)	0	4
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	8
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	10
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	21
15	QO	79/80 (99%)	72 (91%)	7 (9%)	9	40
15	XO	79/80 (99%)	69 (87%)	10 (13%)	4	24
16	QP	72/74 (97%)	64 (89%)	8 (11%)	6	31
16	XP	72/74 (97%)	64 (89%)	8 (11%)	6	31
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	11	42
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	53
18	QR	61/77 (79%)	50 (82%)	11 (18%)	1	11
18	XR	61/77 (79%)	52 (85%)	9 (15%)	3	19
19	QS	73/80 (91%)	59 (81%)	14 (19%)	1	9
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	6
20	QT	76/82 (93%)	67 (88%)	9 (12%)	5	28
20	XT	76/82 (93%)	67 (88%)	9 (12%)	5	28
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	59
27	RD	214/218 (98%)	174 (81%)	40 (19%)	1	10
27	YD	214/218 (98%)	178 (83%)	36 (17%)	2	14
28	RE	165/166 (99%)	127 (77%)	38 (23%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	5
29	RF	161/166 (97%)	131 (81%)	30 (19%)	1	10
29	YF	161/166 (97%)	140 (87%)	21 (13%)	4	24
30	RG	155/156 (99%)	134 (86%)	21 (14%)	4	23
30	YG	155/156 (99%)	133 (86%)	22 (14%)	3	21
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	8
31	YH	142/148 (96%)	115 (81%)	27 (19%)	1	9
32	RI	122/124 (98%)	100 (82%)	22 (18%)	1	11
32	YI	122/124 (98%)	92 (75%)	30 (25%)	0	4
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2	13
33	YN	117/119 (98%)	94 (80%)	23 (20%)	1	8
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7	35
34	YO	100/100 (100%)	88 (88%)	12 (12%)	5	27
35	RP	116/116 (100%)	86 (74%)	30 (26%)	0	4
35	YP	116/116 (100%)	79 (68%)	37 (32%)	0	2
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	15
36	YQ	111/111 (100%)	91 (82%)	20 (18%)	1	11
37	RR	101/101 (100%)	83 (82%)	18 (18%)	2	11
37	YR	101/101 (100%)	81 (80%)	20 (20%)	1	8
38	RS	87/88 (99%)	69 (79%)	18 (21%)	1	7
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	19
39	RT	120/127 (94%)	102 (85%)	18 (15%)	3	19
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2	12
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3	19
40	YU	93/94 (99%)	77 (83%)	16 (17%)	2	13
41	RV	82/82 (100%)	66 (80%)	16 (20%)	1	9
41	YV	82/82 (100%)	67 (82%)	15 (18%)	1	10
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1	7
42	YW	92/92 (100%)	76 (83%)	16 (17%)	2	12
43	RX	74/78 (95%)	64 (86%)	10 (14%)	4	23
43	YX	74/78 (95%)	60 (81%)	14 (19%)	1	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	4
44	YY	85/91 (93%)	64 (75%)	21 (25%)	0	4
45	RZ	162/179 (90%)	138 (85%)	24 (15%)	3	19
45	YZ	162/179 (90%)	145 (90%)	17 (10%)	7	33
46	R0	65/67 (97%)	60 (92%)	5 (8%)	13	45
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	9	39
47	R1	82/83 (99%)	73 (89%)	9 (11%)	6	31
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	3	20
48	R2	64/67 (96%)	55 (86%)	9 (14%)	3	21
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	32
49	R3	51/52 (98%)	45 (88%)	6 (12%)	5	28
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	2	17
50	R4	63/63 (100%)	46 (73%)	17 (27%)	0	3
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	5
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	5
52	R6	48/52 (92%)	35 (73%)	13 (27%)	0	3
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	7
53	R7	42/42 (100%)	34 (81%)	8 (19%)	1	9
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	14
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	3
54	Y8	54/55 (98%)	38 (70%)	16 (30%)	0	2
55	R9	34/34 (100%)	32 (94%)	2 (6%)	19	55
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	55
All	All	9702/10066 (96%)	8159 (84%)	1543 (16%)	2	16

5 of 1543 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	XL	20	LYS
31	YH	11	VAL
13	XM	98	VAL
12	XL	17	LYS
27	YD	131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
55	R9	29	ASN
39	YT	58	ASN
2	XB	204	ASN
27	YD	166	GLN
2	XB	19	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	279 (18%)	43 (2%)
1	XA	1498/1522 (98%)	282 (18%)	37 (2%)
22	QV	76/77 (98%)	21 (27%)	1 (1%)
22	XV	76/77 (98%)	13 (17%)	1 (1%)
23	QX	8/25 (32%)	2 (25%)	0
23	XX	9/25 (36%)	1 (11%)	0
24	QY	15/17 (88%)	2 (13%)	0
24	XY	15/17 (88%)	1 (6%)	0
25	RA	2879/2915 (98%)	606 (21%)	50 (1%)
25	YA	2879/2915 (98%)	607 (21%)	56 (1%)
26	RB	119/122 (97%)	22 (18%)	2 (1%)
26	YB	119/122 (97%)	27 (22%)	1 (0%)
56	Z5	1/3 (33%)	0	0
56	Z6	1/3 (33%)	0	0
All	All	9193/9362 (98%)	1863 (20%)	191 (2%)

5 of 1863 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C

5 of 191 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	485	G
25	YA	271(B)	G
1	XA	687	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1397	C
25	YA	637	A

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

2 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	$\#\|Z\| > 2$
56	PPU	Z5	101	56,25	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)
56	PPU	Z6	101	56,25	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)

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
56	PPU	Z5	101	56,25	-	2/21/43/44	0/4/4/4
56	PPU	Z6	101	56,25	-	2/21/43/44	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z5	101	PPU	O-C	9.30	1.41	1.23
56	Z6	101	PPU	O-C	9.27	1.41	1.23
56	Z6	101	PPU	C9-N6	-5.95	1.31	1.45
56	Z5	101	PPU	C9-N6	-5.95	1.32	1.45
56	Z5	101	PPU	C-N3'	5.72	1.46	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Z5	101	PPU	C3'-N3'-C	-8.61	110.23	123.21
56	Z6	101	PPU	C3'-N3'-C	-8.59	110.26	123.21
56	Z5	101	PPU	N3-C2-N1	-4.65	121.42	128.68
56	Z6	101	PPU	N3-C2-N1	-4.62	121.45	128.68
56	Z5	101	PPU	CA-C-N3'	4.05	121.76	116.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Z5	101	PPU	O-C-CA-N
56	Z6	101	PPU	O-C-CA-N
56	Z5	101	PPU	N3'-C-CA-N
56	Z6	101	PPU	N3'-C-CA-N

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z5	101	PPU	12	0
56	Z6	101	PPU	7	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 924 ligands modelled in this entry, 922 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	$\#\|Z\| > 2$
58	PAR	QA	1681	-	45,45,45	1.59	8 (17%)	64,67,67	1.37	7 (10%)
58	PAR	XA	1710	-	45,45,45	1.60	7 (15%)	64,67,67	1.29	5 (7%)

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
58	PAR	QA	1681	-	-	7/18/94/94	0/4/4/4
58	PAR	XA	1710	-	-	8/18/94/94	0/4/4/4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	XA	1710	PAR	C64-C54	5.12	1.59	1.52
58	QA	1681	PAR	C64-C54	5.00	1.58	1.52
58	QA	1681	PAR	C52-C42	3.19	1.58	1.52
58	QA	1681	PAR	O54-C14	3.13	1.49	1.41
58	XA	1710	PAR	C52-C42	3.11	1.58	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	QA	1681	PAR	C14-O54-C54	5.16	123.82	113.69
58	XA	1710	PAR	O33-C14-C24	4.62	116.17	108.22
58	XA	1710	PAR	C14-O54-C54	3.81	121.17	113.69
58	XA	1710	PAR	O52-C13-C23	3.55	115.33	107.96
58	QA	1681	PAR	O54-C54-C64	3.52	112.56	106.01

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	QA	1681	PAR	C44-C54-C64-N64
58	QA	1681	PAR	O54-C54-C64-N64
58	XA	1710	PAR	C44-C54-C64-N64
58	XA	1710	PAR	O43-C43-C53-O53
58	XA	1710	PAR	C33-C43-C53-O53

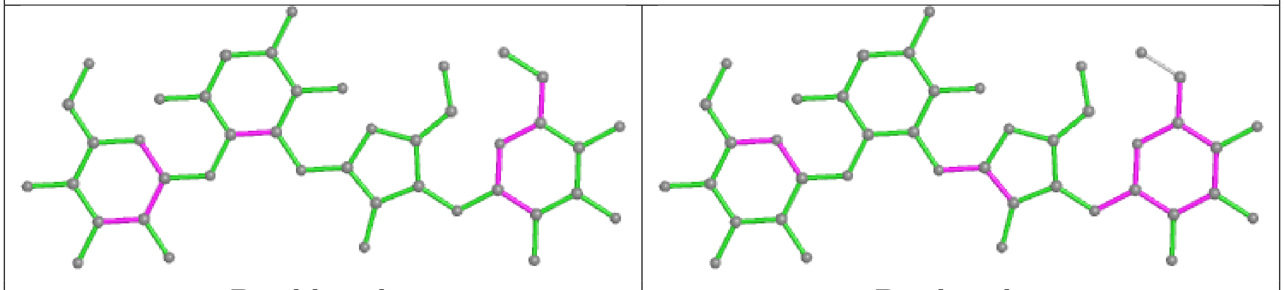
There are no ring outliers.

2 monomers are involved in 6 short contacts:

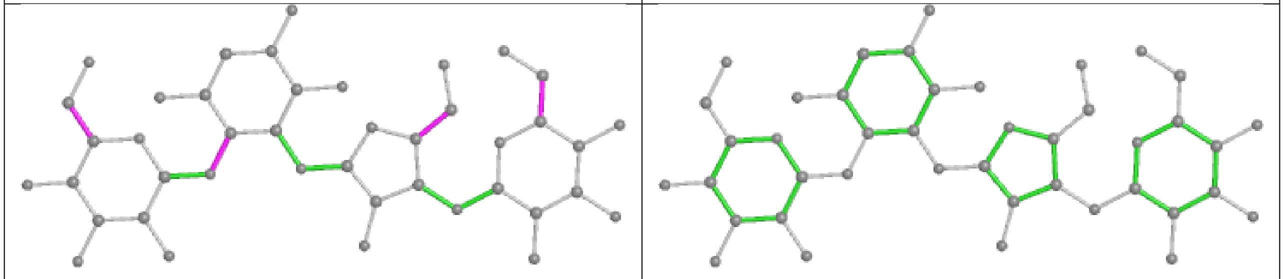
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1681	PAR	4	0
58	XA	1710	PAR	2	0

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 QA 1681

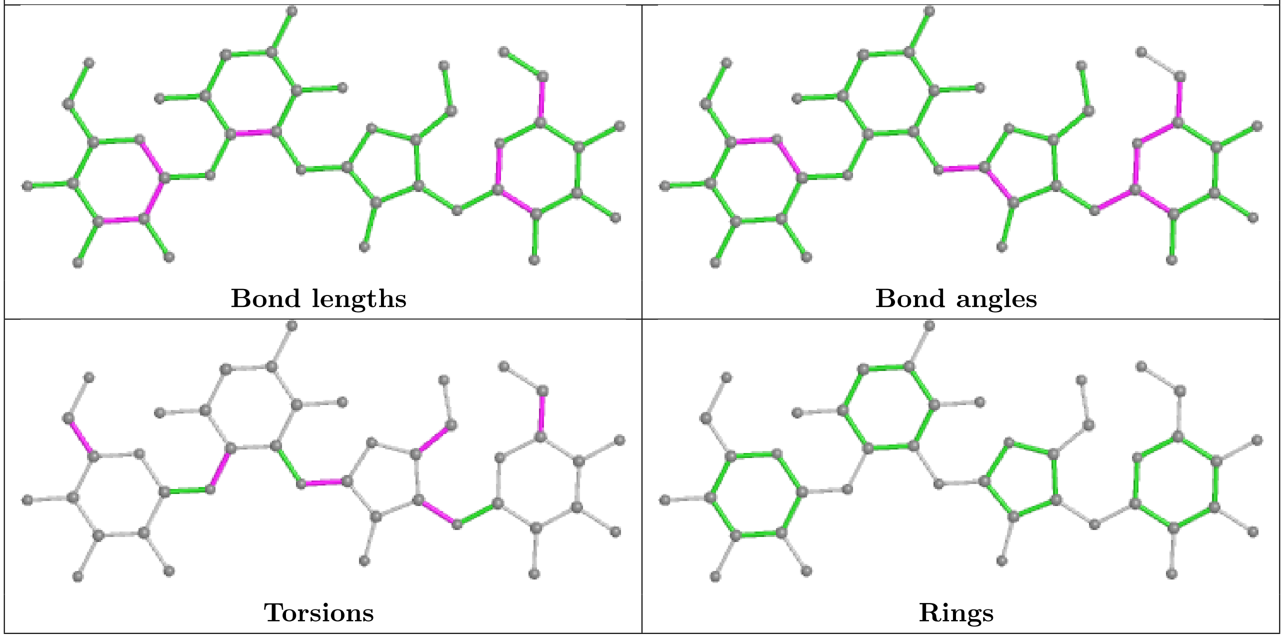


Bond lengths **Bond angles**



Torsions **Rings**

Ligand PAR XA 1710



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	QA	1500/1522 (98%)	0.05	16 (1%) 80 68	40, 98, 191, 460	0
1	XA	1500/1522 (98%)	0.05	10 (0%) 87 78	37, 88, 192, 384	0
2	QB	237/256 (92%)	0.70	26 (10%) 5 3	91, 151, 229, 303	0
2	XB	237/256 (92%)	0.37	7 (2%) 50 34	71, 131, 209, 300	0
3	QC	205/239 (85%)	0.32	1 (0%) 91 83	79, 138, 213, 261	0
3	XC	205/239 (85%)	-0.02	0 100 100	53, 95, 150, 275	0
4	QD	208/209 (99%)	0.12	1 (0%) 91 83	59, 105, 170, 323	0
4	XD	208/209 (99%)	-0.12	0 100 100	43, 92, 156, 208	0
5	QE	151/162 (93%)	0.12	1 (0%) 87 78	66, 112, 178, 228	0
5	XE	151/162 (93%)	-0.16	0 100 100	44, 86, 140, 204	0
6	QF	101/101 (100%)	-0.14	0 100 100	48, 92, 135, 211	0
6	XF	101/101 (100%)	-0.06	0 100 100	47, 96, 150, 271	0
7	QG	155/156 (99%)	0.58	14 (9%) 9 5	86, 136, 192, 401	0
7	XG	155/156 (99%)	0.35	8 (5%) 27 17	63, 118, 165, 229	0
8	QH	138/138 (100%)	0.16	1 (0%) 87 78	66, 110, 155, 278	0
8	XH	138/138 (100%)	-0.00	1 (0%) 87 78	62, 104, 145, 170	0
9	QI	127/128 (99%)	0.84	16 (12%) 3 2	82, 153, 208, 251	0
9	XI	127/128 (99%)	0.25	0 100 100	56, 131, 179, 246	0
10	QJ	99/105 (94%)	0.81	10 (10%) 7 4	101, 158, 246, 398	0
10	XJ	99/105 (94%)	0.61	10 (10%) 7 4	60, 121, 205, 240	0
11	QK	119/129 (92%)	0.89	13 (10%) 5 3	60, 100, 188, 269	0
11	XK	119/129 (92%)	0.51	5 (4%) 36 23	37, 93, 164, 272	0
12	QL	125/132 (94%)	0.31	4 (3%) 47 32	47, 91, 145, 263	0
12	XL	125/132 (94%)	0.17	3 (2%) 59 42	42, 72, 139, 285	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	QM	121/126 (96%)	0.64	12 (9%)	7	4	91, 151, 204, 320	0
13	XM	121/126 (96%)	0.19	3 (2%)	57	41	58, 116, 178, 305	0
14	QN	60/61 (98%)	0.62	1 (1%)	70	55	88, 128, 188, 195	0
14	XN	60/61 (98%)	-0.00	0	100	100	49, 90, 129, 159	0
15	QO	88/89 (98%)	-0.00	0	100	100	41, 92, 137, 169	0
15	XO	88/89 (98%)	0.10	1 (1%)	80	68	56, 97, 143, 170	0
16	QP	84/88 (95%)	0.32	1 (1%)	79	66	62, 95, 137, 206	0
16	XP	84/88 (95%)	0.57	1 (1%)	79	66	74, 110, 158, 267	0
17	QQ	100/105 (95%)	0.26	0	100	100	57, 99, 132, 165	0
17	XQ	100/105 (95%)	0.24	0	100	100	68, 112, 143, 168	0
18	QR	70/88 (79%)	0.19	4 (5%)	23	14	64, 101, 147, 191	0
18	XR	70/88 (79%)	0.20	1 (1%)	75	61	62, 104, 164, 181	0
19	QS	84/93 (90%)	0.71	5 (5%)	21	12	100, 157, 204, 241	0
19	XS	84/93 (90%)	0.56	2 (2%)	59	42	66, 121, 190, 335	0
20	QT	99/106 (93%)	0.39	2 (2%)	65	49	55, 101, 164, 255	0
20	XT	99/106 (93%)	0.73	8 (8%)	12	7	80, 141, 215, 265	0
21	QU	25/27 (92%)	0.69	2 (8%)	12	7	95, 140, 198, 248	0
21	XU	25/27 (92%)	0.28	1 (4%)	38	25	76, 110, 159, 180	0
22	QV	77/77 (100%)	0.14	1 (1%)	77	63	38, 106, 168, 231	0
22	XV	77/77 (100%)	0.20	1 (1%)	77	63	42, 84, 137, 180	0
23	QX	9/25 (36%)	0.42	0	100	100	63, 86, 158, 171	0
23	XX	10/25 (40%)	0.50	1 (10%)	7	4	47, 69, 148, 219	0
24	QY	16/17 (94%)	0.40	1 (6%)	20	11	87, 115, 167, 175	0
24	XY	16/17 (94%)	0.18	0	100	100	68, 95, 153, 191	0
25	RA	2882/2915 (98%)	0.11	118 (4%)	37	24	27, 74, 249, 510	0
25	YA	2882/2915 (98%)	0.13	108 (3%)	41	27	27, 69, 246, 557	0
26	RB	120/122 (98%)	0.04	1 (0%)	86	75	90, 127, 170, 210	0
26	YB	120/122 (98%)	-0.17	0	100	100	61, 90, 124, 152	0
27	RD	272/276 (98%)	-0.14	1 (0%)	92	86	22, 61, 105, 222	0
27	YD	272/276 (98%)	-0.07	1 (0%)	92	86	22, 61, 105, 185	0
28	RE	205/206 (99%)	0.24	5 (2%)	59	42	39, 83, 168, 336	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB($Å^2$)	Q<0.9
28	YE	205/206 (99%)	0.12	3 (1%)	73	60	31, 91, 177, 273	0
29	RF	202/210 (96%)	0.27	4 (1%)	65	49	23, 99, 171, 216	0
29	YF	202/210 (96%)	0.09	4 (1%)	65	49	32, 78, 149, 227	0
30	RG	181/182 (99%)	0.67	11 (6%)	21	12	92, 150, 197, 231	0
30	YG	181/182 (99%)	0.22	4 (2%)	62	45	61, 98, 160, 244	0
31	RH	170/180 (94%)	1.43	41 (24%)	0	0	102, 193, 270, 361	0
31	YH	170/180 (94%)	0.43	4 (2%)	59	42	53, 105, 164, 210	0
32	RI	146/148 (98%)	0.53	10 (6%)	17	10	67, 125, 195, 258	0
32	YI	146/148 (98%)	0.50	8 (5%)	25	15	48, 123, 189, 271	0
33	RN	138/140 (98%)	0.19	3 (2%)	62	45	51, 93, 154, 202	0
33	YN	138/140 (98%)	0.26	2 (1%)	75	61	47, 92, 157, 220	0
34	RO	122/122 (100%)	0.15	0	100	100	48, 80, 114, 148	0
34	YO	122/122 (100%)	0.05	0	100	100	27, 64, 103, 120	0
35	RP	150/150 (100%)	0.50	5 (3%)	46	31	28, 99, 159, 288	0
35	YP	150/150 (100%)	0.20	4 (2%)	54	38	31, 90, 162, 231	0
36	RQ	141/141 (100%)	0.61	8 (5%)	23	14	54, 102, 180, 226	0
36	YQ	141/141 (100%)	0.18	4 (2%)	53	37	35, 73, 140, 222	0
37	RR	118/118 (100%)	-0.14	0	100	100	29, 70, 104, 138	0
37	YR	118/118 (100%)	0.10	1 (0%)	86	75	51, 91, 139, 190	0
38	RS	111/112 (99%)	0.50	4 (3%)	42	28	81, 120, 204, 273	0
38	YS	111/112 (99%)	0.13	2 (1%)	68	53	66, 101, 156, 201	0
39	RT	137/146 (93%)	0.07	2 (1%)	73	60	50, 91, 188, 276	0
39	YT	137/146 (93%)	0.03	0	100	100	51, 89, 212, 242	0
40	RU	117/118 (99%)	0.23	6 (5%)	28	17	35, 81, 155, 298	0
40	YU	117/118 (99%)	-0.04	1 (0%)	84	73	40, 81, 152, 243	0
41	RV	101/101 (100%)	0.73	7 (6%)	16	10	55, 114, 183, 398	0
41	YV	101/101 (100%)	0.39	4 (3%)	38	25	44, 111, 174, 335	0
42	RW	113/113 (100%)	0.10	3 (2%)	54	38	36, 63, 115, 296	0
42	YW	113/113 (100%)	0.14	5 (4%)	34	21	37, 74, 134, 258	0
43	RX	92/96 (95%)	0.34	1 (1%)	80	68	51, 77, 128, 164	0
43	YX	92/96 (95%)	0.32	2 (2%)	62	45	37, 73, 112, 140	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	RY	102/110 (92%)	0.93	15 (14%) 2 1	55, 119, 185, 325	0
44	YY	102/110 (92%)	0.20	4 (3%) 39 25	42, 92, 162, 273	0
45	RZ	183/206 (88%)	0.89	21 (11%) 4 3	104, 153, 230, 292	0
45	YZ	183/206 (88%)	0.49	4 (2%) 62 45	55, 116, 202, 300	0
46	R0	82/85 (96%)	0.44	2 (2%) 59 42	48, 88, 127, 238	0
46	Y0	82/85 (96%)	0.11	0 100 100	44, 71, 99, 142	0
47	R1	97/98 (98%)	0.43	3 (3%) 49 33	37, 80, 161, 290	0
47	Y1	97/98 (98%)	0.38	4 (4%) 37 24	39, 75, 176, 210	0
48	R2	69/72 (95%)	0.67	7 (10%) 7 4	63, 105, 160, 274	0
48	Y2	69/72 (95%)	0.17	3 (4%) 35 22	47, 80, 151, 219	0
49	R3	59/60 (98%)	0.60	3 (5%) 28 17	63, 97, 155, 205	0
49	Y3	59/60 (98%)	0.73	9 (15%) 2 1	55, 89, 162, 293	0
50	R4	71/71 (100%)	1.66	18 (25%) 0 0	150, 244, 350, 423	0
50	Y4	71/71 (100%)	0.85	12 (16%) 1 1	69, 162, 340, 411	0
51	R5	59/60 (98%)	0.24	4 (6%) 17 10	40, 77, 216, 261	0
51	Y5	58/60 (96%)	0.47	7 (12%) 4 3	44, 97, 231, 342	0
52	R6	49/54 (90%)	3.45	36 (73%) 0 0	119, 194, 264, 286	0
52	Y6	49/54 (90%)	3.18	40 (81%) 0 0	115, 171, 260, 295	0
53	R7	49/49 (100%)	-0.21	1 (2%) 65 49	27, 54, 110, 166	0
53	Y7	49/49 (100%)	-0.23	1 (2%) 65 49	32, 51, 111, 180	0
54	R8	64/65 (98%)	0.23	2 (3%) 49 33	42, 82, 134, 223	0
54	Y8	64/65 (98%)	-0.03	0 100 100	35, 68, 120, 229	0
55	R9	37/37 (100%)	5.80	36 (97%) 0 0	134, 200, 317, 510	0
55	Y9	37/37 (100%)	5.50	36 (97%) 0 0	134, 206, 322, 404	0
56	Z5	2/3 (66%)	0.18	0 100 100	50, 50, 50, 60	0
56	Z6	2/3 (66%)	0.04	0 100 100	38, 38, 38, 41	0
All	All	20878/21490 (97%)	0.25	850 (4%) 37 24	22, 92, 205, 557	0

The worst 5 of 850 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	R9	14	CYS	17.4
25	YA	2165	G	14.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	YA	2179	C	13.2
55	Y9	34	GLN	12.6
25	RA	2138	G	11.3

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
56	PPU	Z6	101	37/38	0.94	0.26	36,37,38,38	0
56	PPU	Z5	101	37/38	0.95	0.27	45,47,48,48	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
57	MG	YA	3277	1/1	0.36	0.37	80,80,80,80	0
57	MG	YA	3194	1/1	0.42	0.76	60,60,60,60	0
57	MG	RA	3218	1/1	0.43	0.19	48,48,48,48	0
57	MG	QF	201	1/1	0.48	0.34	57,57,57,57	0
57	MG	QA	1656	1/1	0.50	0.40	63,63,63,63	0
57	MG	XA	1675	1/1	0.51	0.41	59,59,59,59	0
57	MG	RA	3190	1/1	0.52	0.17	69,69,69,69	0
57	MG	XA	1632	1/1	0.53	0.35	58,58,58,58	0
57	MG	YA	3153	1/1	0.54	0.27	52,52,52,52	0
57	MG	YA	3176	1/1	0.56	0.26	89,89,89,89	0
57	MG	QY	101	1/1	0.57	0.27	66,66,66,66	0
57	MG	YA	3333	1/1	0.57	0.58	69,69,69,69	0
57	MG	YA	3308	1/1	0.59	0.33	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1686	1/1	0.59	0.36	72,72,72,72	0
57	MG	QA	1658	1/1	0.60	0.73	62,62,62,62	0
57	MG	RA	3203	1/1	0.60	0.30	70,70,70,70	0
57	MG	XF	201	1/1	0.60	0.25	65,65,65,65	0
57	MG	QA	1627	1/1	0.61	0.31	69,69,69,69	0
57	MG	YA	3211	1/1	0.62	0.33	50,50,50,50	0
57	MG	YA	3174	1/1	0.62	1.17	74,74,74,74	0
57	MG	RA	3138	1/1	0.62	0.28	61,61,61,61	0
57	MG	XA	1648	1/1	0.62	0.35	59,59,59,59	0
57	MG	RA	3202	1/1	0.63	0.27	55,55,55,55	0
57	MG	YA	3295	1/1	0.64	0.53	47,47,47,47	0
57	MG	YA	3260	1/1	0.64	0.29	34,34,34,34	0
57	MG	YA	3315	1/1	0.64	0.39	50,50,50,50	0
57	MG	RA	3189	1/1	0.64	0.20	58,58,58,58	0
57	MG	RA	3059	1/1	0.65	0.20	10,10,10,10	0
57	MG	YA	3196	1/1	0.66	0.20	90,90,90,90	0
57	MG	QA	1640	1/1	0.66	0.85	63,63,63,63	0
57	MG	YA	3339	1/1	0.66	0.77	78,78,78,78	0
57	MG	YA	3355	1/1	0.66	0.63	67,67,67,67	0
57	MG	RA	3308	1/1	0.67	0.52	48,48,48,48	0
57	MG	YA	3338	1/1	0.67	0.38	89,89,89,89	0
57	MG	RA	3298	1/1	0.68	0.31	53,53,53,53	0
57	MG	QA	1629	1/1	0.68	0.31	52,52,52,52	0
57	MG	YA	3117	1/1	0.69	0.63	49,49,49,49	0
57	MG	YA	3337	1/1	0.69	0.84	57,57,57,57	0
57	MG	RA	3325	1/1	0.69	0.21	60,60,60,60	0
57	MG	XA	1705	1/1	0.69	0.30	52,52,52,52	0
57	MG	RA	3271	1/1	0.69	0.42	43,43,43,43	0
57	MG	RA	3062	1/1	0.70	0.19	61,61,61,61	0
57	MG	YA	3216	1/1	0.70	0.40	40,40,40,40	0
57	MG	YA	3302	1/1	0.71	0.66	53,53,53,53	0
57	MG	RA	3215	1/1	0.71	0.20	33,33,33,33	0
57	MG	YA	3208	1/1	0.72	0.68	49,49,49,49	0
57	MG	RA	3177	1/1	0.72	0.23	31,31,31,31	0
57	MG	YA	3283	1/1	0.72	0.56	64,64,64,64	0
57	MG	RR	201	1/1	0.72	0.60	25,25,25,25	0
57	MG	RA	3209	1/1	0.73	0.40	59,59,59,59	0
57	MG	QA	1624	1/1	0.73	0.27	77,77,77,77	0
57	MG	YA	3113	1/1	0.73	1.33	53,53,53,53	0
57	MG	QA	1661	1/1	0.73	0.45	37,37,37,37	0
57	MG	YA	3146	1/1	0.73	0.27	98,98,98,98	0
57	MG	YA	3298	1/1	0.73	0.46	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1633	1/1	0.73	0.34	52,52,52,52	0
57	MG	QA	1668	1/1	0.74	0.55	36,36,36,36	0
57	MG	RA	3176	1/1	0.74	0.32	28,28,28,28	0
57	MG	YA	3193	1/1	0.74	0.32	56,56,56,56	0
57	MG	RA	3251	1/1	0.74	0.45	46,46,46,46	0
57	MG	RA	3311	1/1	0.74	0.12	56,56,56,56	0
57	MG	RA	3264	1/1	0.74	0.47	63,63,63,63	0
57	MG	XA	1694	1/1	0.74	0.22	69,69,69,69	0
57	MG	YQ	201	1/1	0.74	0.21	61,61,61,61	0
57	MG	XA	1636	1/1	0.75	0.18	66,66,66,66	0
57	MG	RA	3213	1/1	0.75	0.80	57,57,57,57	0
57	MG	YA	3292	1/1	0.75	0.67	74,74,74,74	0
57	MG	YA	3191	1/1	0.75	0.51	62,62,62,62	0
57	MG	QA	1673	1/1	0.75	0.60	63,63,63,63	0
57	MG	YA	3227	1/1	0.75	0.66	52,52,52,52	0
57	MG	XA	1677	1/1	0.75	0.12	81,81,81,81	0
59	ZN	QD	301	1/1	0.75	0.34	77,77,77,77	0
57	MG	QA	1603	1/1	0.76	0.62	80,80,80,80	0
57	MG	YA	3181	1/1	0.76	0.12	52,52,52,52	0
57	MG	XA	1706	1/1	0.76	0.80	66,66,66,66	0
57	MG	XA	1649	1/1	0.76	0.49	39,39,39,39	0
57	MG	YP	201	1/1	0.76	0.42	66,66,66,66	0
57	MG	YA	3321	1/1	0.76	0.80	34,34,34,34	0
57	MG	YY	201	1/1	0.76	0.19	45,45,45,45	0
57	MG	XA	1623	1/1	0.76	0.28	48,48,48,48	0
57	MG	XA	1695	1/1	0.77	0.15	78,78,78,78	0
57	MG	RA	3256	1/1	0.77	1.66	78,78,78,78	0
57	MG	XA	1659	1/1	0.77	0.21	105,105,105,105	0
57	MG	XA	1662	1/1	0.77	0.52	38,38,38,38	0
57	MG	YA	3064	1/1	0.77	0.19	25,25,25,25	0
57	MG	RA	3313	1/1	0.77	0.78	68,68,68,68	0
57	MG	RA	3197	1/1	0.77	0.46	44,44,44,44	0
57	MG	XA	1643	1/1	0.77	0.40	59,59,59,59	0
57	MG	RA	3270	1/1	0.77	0.68	41,41,41,41	0
57	MG	YA	3166	1/1	0.77	0.27	51,51,51,51	0
57	MG	XA	1684	1/1	0.78	0.30	56,56,56,56	0
57	MG	YA	3275	1/1	0.78	0.31	46,46,46,46	0
57	MG	YA	3175	1/1	0.78	0.51	63,63,63,63	0
57	MG	RA	3201	1/1	0.78	0.41	65,65,65,65	0
57	MG	YA	3138	1/1	0.78	0.26	40,40,40,40	0
57	MG	RA	3280	1/1	0.79	0.48	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	YA	3226	1/1	0.79	0.48	41,41,41,41	0
57	MG	RA	3226	1/1	0.79	0.35	60,60,60,60	0
57	MG	YA	3353	1/1	0.79	0.36	66,66,66,66	0
57	MG	YA	3257	1/1	0.79	1.11	35,35,35,35	0
57	MG	RA	3303	1/1	0.79	0.65	51,51,51,51	0
57	MG	RA	3113	1/1	0.79	0.21	27,27,27,27	0
57	MG	RA	3055	1/1	0.79	0.25	15,15,15,15	0
57	MG	RA	3274	1/1	0.79	0.49	46,46,46,46	0
57	MG	YA	3297	1/1	0.80	0.53	61,61,61,61	0
57	MG	RA	3011	1/1	0.80	0.33	46,46,46,46	0
57	MG	RA	3179	1/1	0.80	0.49	47,47,47,47	0
57	MG	YA	3199	1/1	0.80	0.29	55,55,55,55	0
57	MG	RA	3134	1/1	0.80	0.16	27,27,27,27	0
57	MG	RA	3315	1/1	0.80	0.14	67,67,67,67	0
57	MG	RA	3214	1/1	0.80	0.25	46,46,46,46	0
57	MG	QA	1638	1/1	0.80	0.17	53,53,53,53	0
57	MG	R0	101	1/1	0.80	0.25	14,14,14,14	0
57	MG	R5	101	1/1	0.80	1.08	162,162,162,162	0
57	MG	RA	3149	1/1	0.80	0.16	41,41,41,41	0
57	MG	XA	1626	1/1	0.80	0.26	31,31,31,31	0
57	MG	RA	3291	1/1	0.80	0.34	45,45,45,45	0
57	MG	YA	3182	1/1	0.80	0.25	62,62,62,62	0
57	MG	RA	3170	1/1	0.80	0.42	35,35,35,35	0
57	MG	RA	3091	1/1	0.80	0.30	39,39,39,39	0
57	MG	RA	3191	1/1	0.81	0.22	49,49,49,49	0
57	MG	YA	3342	1/1	0.81	0.29	56,56,56,56	0
57	MG	RA	3044	1/1	0.81	0.41	65,65,65,65	0
57	MG	RA	3228	1/1	0.81	0.34	23,23,23,23	0
57	MG	RA	3312	1/1	0.81	0.27	55,55,55,55	0
57	MG	RA	3163	1/1	0.81	0.38	27,27,27,27	0
57	MG	YU	201	1/1	0.81	0.34	62,62,62,62	0
57	MG	XA	1646	1/1	0.81	0.17	72,72,72,72	0
57	MG	Y0	102	1/1	0.81	0.63	45,45,45,45	0
57	MG	YA	3205	1/1	0.81	0.35	73,73,73,73	0
57	MG	YA	3310	1/1	0.82	0.56	42,42,42,42	0
57	MG	RA	3233	1/1	0.82	0.40	46,46,46,46	0
57	MG	YA	3316	1/1	0.82	0.34	30,30,30,30	0
57	MG	YE	302	1/1	0.82	0.30	49,49,49,49	0
57	MG	RA	3322	1/1	0.82	0.53	40,40,40,40	0
57	MG	YP	202	1/1	0.82	0.19	52,52,52,52	0
57	MG	YA	3329	1/1	0.82	0.46	56,56,56,56	0
57	MG	RA	3200	1/1	0.82	0.46	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	RA	3220	1/1	0.82	0.45	75,75,75,75	0
57	MG	YA	3230	1/1	0.82	0.35	43,43,43,43	0
57	MG	YA	3288	1/1	0.82	0.53	58,58,58,58	0
57	MG	RA	3167	1/1	0.83	0.67	57,57,57,57	0
57	MG	YA	3336	1/1	0.83	0.23	60,60,60,60	0
57	MG	QA	1666	1/1	0.83	0.22	50,50,50,50	0
57	MG	YA	3201	1/1	0.83	0.20	63,63,63,63	0
57	MG	YA	3158	1/1	0.83	0.44	76,76,76,76	0
57	MG	YA	3207	1/1	0.83	0.28	25,25,25,25	0
57	MG	RA	3174	1/1	0.83	0.25	19,19,19,19	0
57	MG	YA	3055	1/1	0.83	0.54	52,52,52,52	0
57	MG	RA	3260	1/1	0.83	0.23	45,45,45,45	0
57	MG	YA	3303	1/1	0.83	1.31	63,63,63,63	0
57	MG	RA	3281	1/1	0.83	0.45	53,53,53,53	0
57	MG	RA	3289	1/1	0.83	0.37	26,26,26,26	0
57	MG	YA	3135	1/1	0.83	0.20	43,43,43,43	0
57	MG	YA	3136	1/1	0.83	0.55	30,30,30,30	0
57	MG	YA	3137	1/1	0.83	0.74	51,51,51,51	0
57	MG	RA	3185	1/1	0.83	0.45	60,60,60,60	0
57	MG	YA	3284	1/1	0.84	0.35	59,59,59,59	0
57	MG	YA	3080	1/1	0.84	0.23	17,17,17,17	0
57	MG	YA	3291	1/1	0.84	0.42	71,71,71,71	0
57	MG	RB	202	1/1	0.84	0.16	69,69,69,69	0
57	MG	YA	3294	1/1	0.84	0.14	62,62,62,62	0
57	MG	QA	1663	1/1	0.84	0.36	55,55,55,55	0
57	MG	YA	3349	1/1	0.84	0.41	46,46,46,46	0
57	MG	YA	3352	1/1	0.84	0.43	47,47,47,47	0
57	MG	YA	3133	1/1	0.84	0.24	71,71,71,71	0
57	MG	YA	3354	1/1	0.84	0.49	50,50,50,50	0
57	MG	RA	3262	1/1	0.84	0.29	99,99,99,99	0
57	MG	RA	3285	1/1	0.84	0.32	58,58,58,58	0
57	MG	RA	3124	1/1	0.84	0.40	33,33,33,33	0
57	MG	RA	3068	1/1	0.84	0.20	47,47,47,47	0
57	MG	XA	1664	1/1	0.84	0.51	38,38,38,38	0
57	MG	YA	3262	1/1	0.84	0.35	40,40,40,40	0
57	MG	QA	1677	1/1	0.84	0.32	29,29,29,29	0
57	MG	RA	3182	1/1	0.84	0.27	48,48,48,48	0
57	MG	YA	3072	1/1	0.84	0.18	27,27,27,27	0
57	MG	YA	3332	1/1	0.85	0.58	57,57,57,57	0
57	MG	XA	1704	1/1	0.85	0.30	44,44,44,44	0
57	MG	RA	3009	1/1	0.85	0.54	52,52,52,52	0
57	MG	RA	3267	1/1	0.85	0.23	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3140	1/1	0.85	0.29	25,25,25,25	0
57	MG	XA	1627	1/1	0.85	0.19	98,98,98,98	0
57	MG	YA	3203	1/1	0.85	0.66	51,51,51,51	0
57	MG	QA	1622	1/1	0.85	0.30	70,70,70,70	0
57	MG	YA	3162	1/1	0.85	0.14	70,70,70,70	0
57	MG	YA	3165	1/1	0.85	0.09	59,59,59,59	0
57	MG	XA	1635	1/1	0.85	0.45	58,58,58,58	0
57	MG	YA	3215	1/1	0.85	0.32	47,47,47,47	0
57	MG	YA	3073	1/1	0.85	0.60	38,38,38,38	0
57	MG	XA	1680	1/1	0.85	0.29	65,65,65,65	0
57	MG	RA	3299	1/1	0.85	0.36	53,53,53,53	0
57	MG	YA	3179	1/1	0.85	0.32	50,50,50,50	0
57	MG	YA	3234	1/1	0.85	0.56	25,25,25,25	0
57	MG	RA	3026	1/1	0.85	0.28	11,11,11,11	0
57	MG	QA	1643	1/1	0.85	0.27	23,23,23,23	0
57	MG	Y0	103	1/1	0.85	0.44	46,46,46,46	0
57	MG	RA	3192	1/1	0.85	0.27	31,31,31,31	0
57	MG	RA	3155	1/1	0.86	0.54	43,43,43,43	0
57	MG	RA	3301	1/1	0.86	0.31	48,48,48,48	0
57	MG	YA	3210	1/1	0.86	0.41	40,40,40,40	0
57	MG	RA	3100	1/1	0.86	0.29	28,28,28,28	0
57	MG	XA	1629	1/1	0.86	0.18	63,63,63,63	0
57	MG	YA	3149	1/1	0.86	0.22	27,27,27,27	0
57	MG	QA	1641	1/1	0.86	0.25	59,59,59,59	0
57	MG	RA	3114	1/1	0.86	0.39	21,21,21,21	0
57	MG	QA	1625	1/1	0.86	0.14	22,22,22,22	0
57	MG	QA	1679	1/1	0.86	0.33	52,52,52,52	0
57	MG	YA	3245	1/1	0.86	0.34	36,36,36,36	0
57	MG	YA	3031	1/1	0.86	0.51	36,36,36,36	0
57	MG	RA	3314	1/1	0.86	0.34	59,59,59,59	0
57	MG	RA	3277	1/1	0.86	0.59	59,59,59,59	0
57	MG	YA	3274	1/1	0.86	0.35	60,60,60,60	0
57	MG	QA	1670	1/1	0.86	0.35	37,37,37,37	0
57	MG	RA	3075	1/1	0.86	0.15	58,58,58,58	0
57	MG	RA	3250	1/1	0.86	0.32	57,57,57,57	0
57	MG	YA	3109	1/1	0.86	0.17	42,42,42,42	0
57	MG	RB	205	1/1	0.86	0.30	61,61,61,61	0
57	MG	RA	3142	1/1	0.86	0.34	48,48,48,48	0
57	MG	YA	3122	1/1	0.86	0.15	26,26,26,26	0
57	MG	YA	3293	1/1	0.86	0.77	60,60,60,60	0
57	MG	YA	3127	1/1	0.86	0.12	54,54,54,54	0
57	MG	YA	3128	1/1	0.86	0.11	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3131	1/1	0.86	0.21	39,39,39,39	0
57	MG	RA	3207	1/1	0.86	0.19	45,45,45,45	0
57	MG	QM	201	1/1	0.86	0.19	104,104,104,104	0
57	MG	YA	3114	1/1	0.87	0.23	39,39,39,39	0
57	MG	YA	3313	1/1	0.87	0.30	24,24,24,24	0
57	MG	QA	1634	1/1	0.87	0.28	58,58,58,58	0
57	MG	RA	3069	1/1	0.87	0.13	39,39,39,39	0
57	MG	RA	3219	1/1	0.87	0.27	58,58,58,58	0
57	MG	RA	3158	1/1	0.87	0.25	26,26,26,26	0
57	MG	YA	3129	1/1	0.87	0.27	50,50,50,50	0
57	MG	YA	3190	1/1	0.87	0.28	27,27,27,27	0
57	MG	YA	3268	1/1	0.87	0.28	52,52,52,52	0
57	MG	YA	3273	1/1	0.87	0.88	32,32,32,32	0
57	MG	RA	3159	1/1	0.87	0.35	30,30,30,30	0
57	MG	RA	3266	1/1	0.87	1.44	53,53,53,53	0
57	MG	RA	3294	1/1	0.87	0.22	39,39,39,39	0
57	MG	YA	3279	1/1	0.87	0.53	57,57,57,57	0
57	MG	RA	3178	1/1	0.87	0.36	33,33,33,33	0
57	MG	RA	3326	1/1	0.87	0.99	57,57,57,57	0
57	MG	RA	3229	1/1	0.87	0.35	37,37,37,37	0
57	MG	YA	3202	1/1	0.87	0.20	32,32,32,32	0
57	MG	YA	3356	1/1	0.87	0.54	61,61,61,61	0
57	MG	RA	3300	1/1	0.87	0.25	47,47,47,47	0
57	MG	YA	3147	1/1	0.87	0.50	34,34,34,34	0
57	MG	YA	3148	1/1	0.87	0.44	39,39,39,39	0
57	MG	QA	1680	1/1	0.87	0.58	53,53,53,53	0
57	MG	RA	3302	1/1	0.87	0.46	37,37,37,37	0
57	MG	RA	3010	1/1	0.87	0.31	39,39,39,39	0
57	MG	YA	3100	1/1	0.87	0.10	59,59,59,59	0
57	MG	XA	1618	1/1	0.87	0.22	37,37,37,37	0
57	MG	RA	3305	1/1	0.87	0.40	48,48,48,48	0
57	MG	YA	3059	1/1	0.88	0.20	12,12,12,12	0
57	MG	YA	3183	1/1	0.88	0.17	47,47,47,47	0
57	MG	RA	3273	1/1	0.88	0.58	30,30,30,30	0
57	MG	RA	3321	1/1	0.88	0.48	32,32,32,32	0
57	MG	YA	3192	1/1	0.88	0.23	48,48,48,48	0
57	MG	YA	3322	1/1	0.88	0.21	39,39,39,39	0
57	MG	YA	3326	1/1	0.88	0.40	34,34,34,34	0
57	MG	YA	3327	1/1	0.88	0.52	51,51,51,51	0
57	MG	XA	1628	1/1	0.88	0.48	36,36,36,36	0
57	MG	YA	3140	1/1	0.88	0.42	50,50,50,50	0
57	MG	YA	3270	1/1	0.88	0.51	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3335	1/1	0.88	0.36	59,59,59,59	0
57	MG	QA	1662	1/1	0.88	0.19	48,48,48,48	0
57	MG	RA	3204	1/1	0.88	0.16	47,47,47,47	0
57	MG	YA	3102	1/1	0.88	0.16	20,20,20,20	0
57	MG	RA	3181	1/1	0.88	0.33	29,29,29,29	0
57	MG	QA	1630	1/1	0.88	0.16	24,24,24,24	0
57	MG	YA	3347	1/1	0.88	0.20	57,57,57,57	0
57	MG	YA	3282	1/1	0.88	0.23	43,43,43,43	0
57	MG	XA	1638	1/1	0.88	0.32	39,39,39,39	0
57	MG	QA	1617	1/1	0.88	0.28	38,38,38,38	0
57	MG	QA	1639	1/1	0.88	0.23	67,67,67,67	0
57	MG	YA	3126	1/1	0.88	0.17	17,17,17,17	0
57	MG	RA	3290	1/1	0.88	0.35	44,44,44,44	0
57	MG	YA	3214	1/1	0.88	0.28	89,89,89,89	0
57	MG	RA	3232	1/1	0.88	0.43	36,36,36,36	0
57	MG	RA	3130	1/1	0.88	0.96	59,59,59,59	0
57	MG	YA	3219	1/1	0.88	0.52	83,83,83,83	0
57	MG	YA	3222	1/1	0.88	0.20	60,60,60,60	0
57	MG	YA	3301	1/1	0.88	0.64	48,48,48,48	0
57	MG	YA	3225	1/1	0.88	0.45	56,56,56,56	0
57	MG	YA	3045	1/1	0.88	0.30	9,9,9,9	0
57	MG	RA	3217	1/1	0.88	0.23	46,46,46,46	0
57	MG	YA	3198	1/1	0.89	0.49	62,62,62,62	0
57	MG	RA	3269	1/1	0.89	0.27	67,67,67,67	0
57	MG	XA	1676	1/1	0.89	0.22	41,41,41,41	0
57	MG	RA	3151	1/1	0.89	0.36	37,37,37,37	0
57	MG	YA	3082	1/1	0.89	0.37	51,51,51,51	0
57	MG	YA	3151	1/1	0.89	0.58	69,69,69,69	0
57	MG	QA	1660	1/1	0.89	0.41	31,31,31,31	0
57	MG	XA	1681	1/1	0.89	0.45	21,21,21,21	0
57	MG	YA	3161	1/1	0.89	0.50	51,51,51,51	0
57	MG	RA	3254	1/1	0.89	0.19	27,27,27,27	0
57	MG	QA	1604	1/1	0.89	0.60	47,47,47,47	0
57	MG	QA	1648	1/1	0.89	0.23	71,71,71,71	0
57	MG	RA	3278	1/1	0.89	0.23	34,34,34,34	0
57	MG	XA	1698	1/1	0.89	0.79	76,76,76,76	0
57	MG	RA	3160	1/1	0.89	0.23	82,82,82,82	0
57	MG	RA	3118	1/1	0.89	0.27	62,62,62,62	0
57	MG	RA	3265	1/1	0.89	0.45	58,58,58,58	0
57	MG	XA	1707	1/1	0.89	0.80	50,50,50,50	0
57	MG	XA	1612	1/1	0.89	0.15	68,68,68,68	0
57	MG	YA	3188	1/1	0.89	0.46	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	XX	101	1/1	0.89	0.47	57,57,57,57	0
57	MG	XA	1656	1/1	0.89	0.25	56,56,56,56	0
57	MG	QA	1669	1/1	0.89	0.34	59,59,59,59	0
57	MG	RA	3129	1/1	0.89	0.25	42,42,42,42	0
57	MG	YA	3319	1/1	0.89	0.38	45,45,45,45	0
57	MG	RA	3268	1/1	0.89	0.39	45,45,45,45	0
57	MG	Y7	101	1/1	0.89	0.24	33,33,33,33	0
57	MG	XA	1671	1/1	0.89	0.53	39,39,39,39	0
57	MG	RA	3297	1/1	0.90	0.57	48,48,48,48	0
57	MG	YA	3139	1/1	0.90	0.20	76,76,76,76	0
57	MG	YA	3070	1/1	0.90	0.25	29,29,29,29	0
57	MG	RA	3109	1/1	0.90	0.44	34,34,34,34	0
57	MG	RA	3320	1/1	0.90	0.43	62,62,62,62	0
57	MG	YA	3328	1/1	0.90	0.36	49,49,49,49	0
57	MG	QA	1611	1/1	0.90	0.46	21,21,21,21	0
57	MG	RA	3240	1/1	0.90	0.64	17,17,17,17	0
57	MG	RA	3164	1/1	0.90	0.25	45,45,45,45	0
57	MG	RA	3198	1/1	0.90	0.64	49,49,49,49	0
57	MG	RA	3252	1/1	0.90	0.28	47,47,47,47	0
57	MG	YA	3280	1/1	0.90	0.42	25,25,25,25	0
57	MG	RB	204	1/1	0.90	0.28	51,51,51,51	0
57	MG	XA	1700	1/1	0.90	0.57	50,50,50,50	0
57	MG	RA	3304	1/1	0.90	0.20	44,44,44,44	0
57	MG	RA	3288	1/1	0.90	0.28	49,49,49,49	0
57	MG	RA	3307	1/1	0.90	0.38	38,38,38,38	0
57	MG	RA	3186	1/1	0.90	0.25	28,28,28,28	0
57	MG	XA	1604	1/1	0.90	0.43	44,44,44,44	0
57	MG	QA	1647	1/1	0.90	0.34	35,35,35,35	0
57	MG	YA	3180	1/1	0.90	0.21	52,52,52,52	0
57	MG	YA	3224	1/1	0.90	0.34	41,41,41,41	0
57	MG	YA	3006	1/1	0.90	0.28	22,22,22,22	0
57	MG	YA	3132	1/1	0.90	0.26	37,37,37,37	0
57	MG	QA	1618	1/1	0.90	0.29	58,58,58,58	0
57	MG	YA	3228	1/1	0.90	0.91	57,57,57,57	0
57	MG	XA	1665	1/1	0.90	0.57	35,35,35,35	0
57	MG	XA	1619	1/1	0.90	0.60	40,40,40,40	0
57	MG	YA	3312	1/1	0.90	0.16	26,26,26,26	0
57	MG	YA	3238	1/1	0.90	0.40	28,28,28,28	0
57	MG	YA	3240	1/1	0.90	0.67	43,43,43,43	0
57	MG	RA	3261	1/1	0.90	0.30	56,56,56,56	0
57	MG	XA	1701	1/1	0.91	0.23	47,47,47,47	0
57	MG	RA	3084	1/1	0.91	0.41	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3152	1/1	0.91	0.12	54,54,54,54	0
57	MG	RA	3154	1/1	0.91	0.11	26,26,26,26	0
57	MG	RA	3002	1/1	0.91	0.26	47,47,47,47	0
57	MG	XA	1708	1/1	0.91	0.28	33,33,33,33	0
57	MG	RA	3003	1/1	0.91	0.56	42,42,42,42	0
57	MG	XV	101	1/1	0.91	0.25	34,34,34,34	0
57	MG	XA	1644	1/1	0.91	0.41	42,42,42,42	0
57	MG	YA	3141	1/1	0.91	0.39	48,48,48,48	0
57	MG	YA	3143	1/1	0.91	0.23	9,9,9,9	0
57	MG	RA	3102	1/1	0.91	0.14	38,38,38,38	0
57	MG	YA	3019	1/1	0.91	0.49	29,29,29,29	0
57	MG	YA	3317	1/1	0.91	0.50	38,38,38,38	0
57	MG	YA	3021	1/1	0.91	0.53	24,24,24,24	0
57	MG	RA	3132	1/1	0.91	0.13	52,52,52,52	0
57	MG	RA	3216	1/1	0.91	0.27	51,51,51,51	0
57	MG	RA	3103	1/1	0.91	0.15	25,25,25,25	0
57	MG	YA	3156	1/1	0.91	0.30	67,67,67,67	0
57	MG	YA	3229	1/1	0.91	0.40	19,19,19,19	0
57	MG	RA	3135	1/1	0.91	0.19	64,64,64,64	0
57	MG	YA	3330	1/1	0.91	0.36	45,45,45,45	0
57	MG	XA	1660	1/1	0.91	0.93	53,53,53,53	0
57	MG	RA	3042	1/1	0.91	0.33	9,9,9,9	0
57	MG	YA	3163	1/1	0.91	0.40	39,39,39,39	0
57	MG	YA	3244	1/1	0.91	0.34	33,33,33,33	0
57	MG	RA	3194	1/1	0.91	0.16	43,43,43,43	0
57	MG	RA	3225	1/1	0.91	0.55	46,46,46,46	0
57	MG	XA	1667	1/1	0.91	0.50	23,23,23,23	0
57	MG	YA	3340	1/1	0.91	0.63	55,55,55,55	0
57	MG	YA	3261	1/1	0.91	0.23	43,43,43,43	0
57	MG	QA	1659	1/1	0.91	0.51	40,40,40,40	0
57	MG	YA	3265	1/1	0.91	0.60	65,65,65,65	0
57	MG	YA	3086	1/1	0.91	0.30	51,51,51,51	0
57	MG	YA	3096	1/1	0.91	0.51	26,26,26,26	0
57	MG	XA	1606	1/1	0.91	0.40	40,40,40,40	0
57	MG	RA	3172	1/1	0.91	0.29	34,34,34,34	0
57	MG	RA	3199	1/1	0.91	0.92	44,44,44,44	0
57	MG	YB	203	1/1	0.91	0.30	37,37,37,37	0
57	MG	RA	3306	1/1	0.91	0.33	47,47,47,47	0
57	MG	QA	1626	1/1	0.91	0.20	65,65,65,65	0
57	MG	XA	1625	1/1	0.91	0.12	32,32,32,32	0
57	MG	YA	3119	1/1	0.91	0.24	42,42,42,42	0
57	MG	YA	3121	1/1	0.91	0.24	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3143	1/1	0.91	0.45	19,19,19,19	0
57	MG	RA	3234	1/1	0.91	0.48	16,16,16,16	0
57	MG	RA	3116	1/1	0.91	0.23	50,50,50,50	0
57	MG	RA	3244	1/1	0.91	0.17	47,47,47,47	0
58	PAR	QA	1681	42/42	0.91	0.27	71,71,72,72	0
57	MG	XA	1631	1/1	0.91	0.25	63,63,63,63	0
57	MG	XA	1696	1/1	0.92	0.78	65,65,65,65	0
57	MG	RA	3127	1/1	0.92	0.15	24,24,24,24	0
57	MG	RA	3153	1/1	0.92	0.25	34,34,34,34	0
57	MG	XA	1634	1/1	0.92	0.41	38,38,38,38	0
57	MG	RA	3205	1/1	0.92	0.29	59,59,59,59	0
57	MG	RA	3093	1/1	0.92	0.38	18,18,18,18	0
57	MG	YA	3300	1/1	0.92	0.17	45,45,45,45	0
57	MG	QA	1635	1/1	0.92	0.32	58,58,58,58	0
57	MG	RA	3323	1/1	0.92	0.67	39,39,39,39	0
57	MG	RA	3324	1/1	0.92	0.40	38,38,38,38	0
57	MG	YA	3305	1/1	0.92	0.49	53,53,53,53	0
57	MG	RA	3210	1/1	0.92	0.15	68,68,68,68	0
57	MG	XA	1647	1/1	0.92	0.21	82,82,82,82	0
57	MG	YA	3311	1/1	0.92	0.58	69,69,69,69	0
57	MG	RA	3183	1/1	0.92	0.13	37,37,37,37	0
57	MG	YA	3002	1/1	0.92	0.20	22,22,22,22	0
57	MG	RA	3001	1/1	0.92	0.23	27,27,27,27	0
57	MG	XA	1653	1/1	0.92	0.19	42,42,42,42	0
57	MG	YA	3020	1/1	0.92	0.43	16,16,16,16	0
57	MG	YA	3217	1/1	0.92	0.15	45,45,45,45	0
57	MG	YA	3142	1/1	0.92	0.60	58,58,58,58	0
57	MG	RB	203	1/1	0.92	0.25	47,47,47,47	0
57	MG	YA	3324	1/1	0.92	0.37	40,40,40,40	0
57	MG	YA	3025	1/1	0.92	0.41	23,23,23,23	0
57	MG	YA	3029	1/1	0.92	0.28	17,17,17,17	0
57	MG	RA	3296	1/1	0.92	0.30	45,45,45,45	0
57	MG	RA	3012	1/1	0.92	0.60	27,27,27,27	0
57	MG	YA	3049	1/1	0.92	0.32	15,15,15,15	0
57	MG	YA	3054	1/1	0.92	0.45	23,23,23,23	0
57	MG	YA	3155	1/1	0.92	0.27	37,37,37,37	0
57	MG	RA	3187	1/1	0.92	0.22	68,68,68,68	0
57	MG	RA	3263	1/1	0.92	0.47	33,33,33,33	0
57	MG	RA	3015	1/1	0.92	0.12	16,16,16,16	0
57	MG	RA	3136	1/1	0.92	0.39	15,15,15,15	0
57	MG	QE	201	1/1	0.92	0.71	59,59,59,59	0
57	MG	YA	3164	1/1	0.92	0.23	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3258	1/1	0.92	0.54	52,52,52,52	0
57	MG	YA	3343	1/1	0.92	0.27	46,46,46,46	0
57	MG	YA	3344	1/1	0.92	0.28	55,55,55,55	0
57	MG	XA	1672	1/1	0.92	0.35	36,36,36,36	0
57	MG	RA	3166	1/1	0.92	0.36	36,36,36,36	0
57	MG	YA	3170	1/1	0.92	0.24	54,54,54,54	0
57	MG	YA	3172	1/1	0.92	0.44	52,52,52,52	0
57	MG	YA	3267	1/1	0.92	0.28	42,42,42,42	0
57	MG	YA	3173	1/1	0.92	0.61	43,43,43,43	0
57	MG	RA	3139	1/1	0.92	0.30	26,26,26,26	0
57	MG	RA	3168	1/1	0.92	0.20	26,26,26,26	0
57	MG	QA	1665	1/1	0.92	0.26	55,55,55,55	0
57	MG	YA	3099	1/1	0.92	0.43	19,19,19,19	0
57	MG	RA	3078	1/1	0.92	0.25	7,7,7,7	0
57	MG	QA	1619	1/1	0.92	0.21	40,40,40,40	0
57	MG	YA	3103	1/1	0.92	0.39	36,36,36,36	0
57	MG	RA	3050	1/1	0.92	0.41	14,14,14,14	0
57	MG	XA	1690	1/1	0.92	0.61	50,50,50,50	0
57	MG	XA	1692	1/1	0.92	0.29	58,58,58,58	0
57	MG	YA	3287	1/1	0.92	0.29	44,44,44,44	0
57	MG	RA	3125	1/1	0.92	0.29	54,54,54,54	0
57	MG	RA	3239	1/1	0.92	0.30	7,7,7,7	0
57	MG	YA	3125	1/1	0.93	0.20	54,54,54,54	0
57	MG	YA	3296	1/1	0.93	0.54	48,48,48,48	0
57	MG	RA	3072	1/1	0.93	0.51	52,52,52,52	0
57	MG	RA	3258	1/1	0.93	0.40	48,48,48,48	0
57	MG	RA	3184	1/1	0.93	0.13	49,49,49,49	0
57	MG	RA	3157	1/1	0.93	0.38	42,42,42,42	0
57	MG	YA	3130	1/1	0.93	0.39	42,42,42,42	0
57	MG	XA	1652	1/1	0.93	0.34	72,72,72,72	0
57	MG	QA	1672	1/1	0.93	0.35	41,41,41,41	0
57	MG	YA	3306	1/1	0.93	0.44	50,50,50,50	0
57	MG	XA	1655	1/1	0.93	0.50	53,53,53,53	0
57	MG	RA	3027	1/1	0.93	0.41	27,27,27,27	0
57	MG	YA	3005	1/1	0.93	0.21	23,23,23,23	0
57	MG	QA	1644	1/1	0.93	0.55	54,54,54,54	0
57	MG	YA	3008	1/1	0.93	0.45	33,33,33,33	0
57	MG	YA	3016	1/1	0.93	0.30	6,6,6,6	0
57	MG	RA	3005	1/1	0.93	0.27	26,26,26,26	0
57	MG	RA	3045	1/1	0.93	0.28	5,5,5,5	0
57	MG	XA	1605	1/1	0.93	0.60	34,34,34,34	0
57	MG	YA	3223	1/1	0.93	0.22	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3165	1/1	0.93	0.06	36,36,36,36	0
57	MG	RA	3193	1/1	0.93	0.23	46,46,46,46	0
57	MG	XA	1670	1/1	0.93	0.47	37,37,37,37	0
57	MG	YA	3035	1/1	0.93	0.55	27,27,27,27	0
57	MG	RA	3008	1/1	0.93	0.55	12,12,12,12	0
57	MG	RA	3196	1/1	0.93	0.36	56,56,56,56	0
57	MG	XA	1622	1/1	0.93	0.59	33,33,33,33	0
57	MG	QA	1645	1/1	0.93	0.19	73,73,73,73	0
57	MG	RA	3309	1/1	0.93	0.51	54,54,54,54	0
57	MG	RA	3310	1/1	0.93	0.17	39,39,39,39	0
57	MG	RA	3057	1/1	0.93	0.29	48,48,48,48	0
57	MG	XA	1683	1/1	0.93	0.11	48,48,48,48	0
57	MG	RA	3108	1/1	0.93	0.17	32,32,32,32	0
57	MG	YA	3077	1/1	0.93	0.34	21,21,21,21	0
57	MG	QV	101	1/1	0.93	0.35	50,50,50,50	0
57	MG	XA	1689	1/1	0.93	0.63	51,51,51,51	0
57	MG	YA	3168	1/1	0.93	0.45	25,25,25,25	0
57	MG	QX	101	1/1	0.93	0.11	66,66,66,66	0
57	MG	YA	3171	1/1	0.93	0.66	85,85,85,85	0
57	MG	YA	3087	1/1	0.93	0.38	31,31,31,31	0
57	MG	YA	3095	1/1	0.93	0.24	42,42,42,42	0
57	MG	XA	1691	1/1	0.93	0.11	105,105,105,105	0
57	MG	QA	1642	1/1	0.93	0.21	62,62,62,62	0
57	MG	XA	1693	1/1	0.93	0.43	40,40,40,40	0
57	MG	XA	1633	1/1	0.93	0.77	47,47,47,47	0
57	MG	QA	1601	1/1	0.93	0.15	31,31,31,31	0
57	MG	RA	3070	1/1	0.93	0.35	9,9,9,9	0
57	MG	YA	3111	1/1	0.93	0.19	26,26,26,26	0
57	MG	XA	1697	1/1	0.93	0.41	47,47,47,47	0
57	MG	YP	203	1/1	0.93	0.33	32,32,32,32	0
57	MG	YA	3187	1/1	0.93	0.14	87,87,87,87	0
57	MG	YA	3286	1/1	0.93	1.02	67,67,67,67	0
57	MG	RA	3120	1/1	0.93	0.54	50,50,50,50	0
57	MG	YA	3116	1/1	0.93	0.39	40,40,40,40	0
57	MG	XA	1699	1/1	0.93	0.44	35,35,35,35	0
57	MG	RA	3122	1/1	0.93	0.16	24,24,24,24	0
57	MG	RA	3253	1/1	0.93	0.34	29,29,29,29	0
57	MG	RA	3071	1/1	0.93	0.26	32,32,32,32	0
57	MG	XA	1607	1/1	0.94	0.43	29,29,29,29	0
57	MG	YA	3017	1/1	0.94	0.09	6,6,6,6	0
57	MG	YA	3289	1/1	0.94	0.95	69,69,69,69	0
57	MG	XA	1609	1/1	0.94	0.32	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	RA	3101	1/1	0.94	0.20	32,32,32,32	0
57	MG	RA	3236	1/1	0.94	0.63	71,71,71,71	0
57	MG	RA	3206	1/1	0.94	0.15	51,51,51,51	0
57	MG	RA	3272	1/1	0.94	0.61	44,44,44,44	0
57	MG	RA	3123	1/1	0.94	0.20	74,74,74,74	0
57	MG	YA	3204	1/1	0.94	0.20	75,75,75,75	0
57	MG	QA	1646	1/1	0.94	0.32	61,61,61,61	0
57	MG	YA	3206	1/1	0.94	0.41	70,70,70,70	0
57	MG	YA	3040	1/1	0.94	0.18	8,8,8,8	0
57	MG	RA	3276	1/1	0.94	0.34	44,44,44,44	0
57	MG	YA	3209	1/1	0.94	0.63	28,28,28,28	0
57	MG	RA	3247	1/1	0.94	0.18	55,55,55,55	0
57	MG	XA	1682	1/1	0.94	0.35	60,60,60,60	0
57	MG	YA	3212	1/1	0.94	0.20	32,32,32,32	0
57	MG	RA	3249	1/1	0.94	0.41	41,41,41,41	0
57	MG	YA	3056	1/1	0.94	0.27	11,11,11,11	0
57	MG	QX	102	1/1	0.94	0.20	43,43,43,43	0
57	MG	QA	1657	1/1	0.94	0.27	29,29,29,29	0
57	MG	YA	3314	1/1	0.94	0.44	37,37,37,37	0
57	MG	YA	3218	1/1	0.94	0.28	25,25,25,25	0
57	MG	RA	3282	1/1	0.94	0.33	39,39,39,39	0
57	MG	RA	3319	1/1	0.94	0.28	32,32,32,32	0
57	MG	YA	3318	1/1	0.94	0.31	34,34,34,34	0
57	MG	RA	3283	1/1	0.94	0.46	65,65,65,65	0
57	MG	RA	3284	1/1	0.94	0.53	32,32,32,32	0
57	MG	YA	3078	1/1	0.94	0.53	15,15,15,15	0
57	MG	YA	3157	1/1	0.94	0.47	51,51,51,51	0
57	MG	YA	3325	1/1	0.94	0.50	42,42,42,42	0
57	MG	RA	3171	1/1	0.94	0.23	57,57,57,57	0
57	MG	YA	3159	1/1	0.94	0.15	44,44,44,44	0
57	MG	YA	3160	1/1	0.94	0.17	18,18,18,18	0
57	MG	XA	1637	1/1	0.94	0.13	74,74,74,74	0
57	MG	RA	3286	1/1	0.94	0.62	57,57,57,57	0
57	MG	YA	3237	1/1	0.94	0.24	26,26,26,26	0
57	MG	RA	3128	1/1	0.94	0.25	60,60,60,60	0
57	MG	QA	1628	1/1	0.94	0.20	64,64,64,64	0
57	MG	XA	1645	1/1	0.94	0.31	31,31,31,31	0
57	MG	RA	3195	1/1	0.94	0.25	15,15,15,15	0
57	MG	YA	3250	1/1	0.94	0.18	27,27,27,27	0
57	MG	YA	3252	1/1	0.94	0.49	27,27,27,27	0
57	MG	RA	3110	1/1	0.94	0.48	54,54,54,54	0
57	MG	RA	3131	1/1	0.94	0.39	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1671	1/1	0.94	0.34	23,23,23,23	0
57	MG	XA	1650	1/1	0.94	0.28	54,54,54,54	0
57	MG	RA	3224	1/1	0.94	0.19	28,28,28,28	0
57	MG	RE	302	1/1	0.94	0.32	20,20,20,20	0
57	MG	YA	3266	1/1	0.94	0.53	65,65,65,65	0
57	MG	QA	1623	1/1	0.94	0.31	54,54,54,54	0
57	MG	YA	3115	1/1	0.94	0.45	23,23,23,23	0
57	MG	XB	301	1/1	0.94	0.18	51,51,51,51	0
57	MG	YA	3272	1/1	0.94	0.41	32,32,32,32	0
57	MG	RA	3115	1/1	0.94	0.20	12,12,12,12	0
57	MG	XA	1657	1/1	0.94	0.63	49,49,49,49	0
57	MG	QA	1650	1/1	0.94	0.37	41,41,41,41	0
57	MG	YA	3276	1/1	0.94	0.68	43,43,43,43	0
57	MG	RA	3161	1/1	0.94	0.42	55,55,55,55	0
57	MG	YA	3278	1/1	0.94	0.44	50,50,50,50	0
57	MG	YA	3185	1/1	0.94	0.48	37,37,37,37	0
57	MG	YA	3123	1/1	0.94	0.70	46,46,46,46	0
57	MG	YA	3281	1/1	0.94	0.31	33,33,33,33	0
57	MG	XA	1661	1/1	0.94	0.39	44,44,44,44	0
57	MG	Y3	101	1/1	0.94	0.30	28,28,28,28	0
57	MG	RA	3029	1/1	0.94	0.30	18,18,18,18	0
57	MG	QA	1676	1/1	0.94	0.39	63,63,63,63	0
57	MG	YA	3011	1/1	0.94	0.46	30,30,30,30	0
59	ZN	QN	101	1/1	0.94	0.14	135,135,135,135	0
57	MG	QA	1620	1/1	0.95	0.20	66,66,66,66	0
57	MG	QA	1652	1/1	0.95	0.49	34,34,34,34	0
57	MG	RA	3180	1/1	0.95	0.14	28,28,28,28	0
57	MG	YA	3154	1/1	0.95	0.23	18,18,18,18	0
57	MG	XA	1702	1/1	0.95	0.31	43,43,43,43	0
57	MG	YA	3079	1/1	0.95	0.50	21,21,21,21	0
57	MG	RA	3049	1/1	0.95	0.17	7,7,7,7	0
57	MG	YA	3221	1/1	0.95	0.27	37,37,37,37	0
57	MG	YA	3304	1/1	0.95	0.54	42,42,42,42	0
57	MG	RA	3275	1/1	0.95	0.65	59,59,59,59	0
57	MG	RA	3243	1/1	0.95	0.19	84,84,84,84	0
57	MG	YA	3307	1/1	0.95	0.23	12,12,12,12	0
57	MG	RA	3077	1/1	0.95	0.27	5,5,5,5	0
57	MG	YA	3309	1/1	0.95	0.37	37,37,37,37	0
57	MG	YA	3088	1/1	0.95	0.42	56,56,56,56	0
57	MG	YA	3092	1/1	0.95	0.28	45,45,45,45	0
57	MG	XA	1663	1/1	0.95	0.28	26,26,26,26	0
57	MG	RA	3014	1/1	0.95	0.38	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	YA	3097	1/1	0.95	0.38	30,30,30,30	0
57	MG	XD	302	1/1	0.95	0.26	82,82,82,82	0
57	MG	YA	3167	1/1	0.95	0.38	43,43,43,43	0
57	MG	YA	3235	1/1	0.95	0.46	16,16,16,16	0
57	MG	RA	3279	1/1	0.95	0.90	40,40,40,40	0
57	MG	YA	3169	1/1	0.95	0.12	49,49,49,49	0
57	MG	YA	3239	1/1	0.95	0.51	31,31,31,31	0
57	MG	RA	3133	1/1	0.95	0.34	45,45,45,45	0
57	MG	YA	3241	1/1	0.95	0.20	19,19,19,19	0
57	MG	XA	1668	1/1	0.95	0.53	48,48,48,48	0
57	MG	QA	1631	1/1	0.95	0.12	69,69,69,69	0
57	MG	YA	3246	1/1	0.95	0.60	38,38,38,38	0
57	MG	YA	3247	1/1	0.95	0.34	45,45,45,45	0
57	MG	YA	3004	1/1	0.95	0.30	14,14,14,14	0
57	MG	RA	3090	1/1	0.95	0.62	31,31,31,31	0
57	MG	YA	3331	1/1	0.95	0.27	51,51,51,51	0
57	MG	RA	3316	1/1	0.95	0.74	42,42,42,42	0
57	MG	YA	3007	1/1	0.95	0.16	16,16,16,16	0
57	MG	YA	3178	1/1	0.95	0.17	56,56,56,56	0
57	MG	RA	3317	1/1	0.95	0.76	51,51,51,51	0
57	MG	RA	3117	1/1	0.95	0.13	65,65,65,65	0
57	MG	YA	3263	1/1	0.95	0.34	22,22,22,22	0
57	MG	YA	3264	1/1	0.95	0.39	30,30,30,30	0
57	MG	YA	3012	1/1	0.95	0.22	6,6,6,6	0
57	MG	RA	3137	1/1	0.95	0.47	24,24,24,24	0
57	MG	XA	1678	1/1	0.95	0.22	45,45,45,45	0
57	MG	RA	3019	1/1	0.95	0.28	18,18,18,18	0
57	MG	QA	1613	1/1	0.95	0.48	40,40,40,40	0
57	MG	RA	3097	1/1	0.95	0.46	31,31,31,31	0
57	MG	YA	3350	1/1	0.95	0.24	40,40,40,40	0
57	MG	YA	3351	1/1	0.95	0.40	39,39,39,39	0
57	MG	RA	3259	1/1	0.95	0.41	50,50,50,50	0
57	MG	QA	1678	1/1	0.95	0.45	43,43,43,43	0
57	MG	QA	1612	1/1	0.95	0.45	39,39,39,39	0
57	MG	YA	3033	1/1	0.95	0.29	11,11,11,11	0
57	MG	RA	3222	1/1	0.95	0.41	4,4,4,4	0
57	MG	YB	201	1/1	0.95	0.20	46,46,46,46	0
57	MG	RA	3169	1/1	0.95	0.28	26,26,26,26	0
57	MG	YD	301	1/1	0.95	0.32	19,19,19,19	0
57	MG	YE	301	1/1	0.95	0.25	28,28,28,28	0
57	MG	RA	3144	1/1	0.95	0.34	60,60,60,60	0
57	MG	YA	3046	1/1	0.95	0.34	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	YA	3200	1/1	0.95	0.25	45,45,45,45	0
57	MG	YA	3048	1/1	0.95	0.39	18,18,18,18	0
57	MG	RA	3145	1/1	0.95	0.41	40,40,40,40	0
57	MG	YA	3050	1/1	0.95	0.43	21,21,21,21	0
57	MG	YA	3052	1/1	0.95	0.43	22,22,22,22	0
57	MG	RA	3227	1/1	0.95	0.39	27,27,27,27	0
57	MG	RF	301	1/1	0.95	0.07	62,62,62,62	0
57	MG	RA	3146	1/1	0.95	0.17	41,41,41,41	0
57	MG	Y5	101	1/1	0.95	0.21	17,17,17,17	0
57	MG	YA	3057	1/1	0.95	0.17	13,13,13,13	0
57	MG	RA	3147	1/1	0.95	0.25	27,27,27,27	0
58	PAR	XA	1710	42/42	0.95	0.24	56,56,57,57	0
57	MG	RA	3035	1/1	0.95	0.72	49,49,49,49	0
57	MG	QA	1664	1/1	0.95	0.24	30,30,30,30	0
59	ZN	XN	101	1/1	0.95	0.16	81,81,81,81	0
57	MG	YA	3285	1/1	0.96	0.16	46,46,46,46	0
57	MG	YA	3186	1/1	0.96	0.19	22,22,22,22	0
57	MG	QA	1614	1/1	0.96	0.27	30,30,30,30	0
57	MG	RA	3092	1/1	0.96	0.30	29,29,29,29	0
57	MG	RA	3175	1/1	0.96	0.25	31,31,31,31	0
57	MG	XA	1640	1/1	0.96	0.48	41,41,41,41	0
57	MG	YA	3107	1/1	0.96	0.25	45,45,45,45	0
57	MG	YA	3108	1/1	0.96	0.16	32,32,32,32	0
57	MG	QA	1653	1/1	0.96	0.41	30,30,30,30	0
57	MG	YA	3195	1/1	0.96	0.22	39,39,39,39	0
57	MG	RA	3096	1/1	0.96	0.38	5,5,5,5	0
57	MG	YA	3197	1/1	0.96	0.08	53,53,53,53	0
57	MG	QA	1654	1/1	0.96	0.34	68,68,68,68	0
57	MG	QA	1615	1/1	0.96	0.13	57,57,57,57	0
57	MG	RA	3051	1/1	0.96	0.19	22,22,22,22	0
57	MG	RA	3318	1/1	0.96	0.35	40,40,40,40	0
57	MG	RA	3052	1/1	0.96	0.33	4,4,4,4	0
57	MG	YA	3118	1/1	0.96	0.41	58,58,58,58	0
57	MG	QV	102	1/1	0.96	0.19	27,27,27,27	0
57	MG	YA	3120	1/1	0.96	0.32	14,14,14,14	0
57	MG	RA	3104	1/1	0.96	0.20	33,33,33,33	0
57	MG	RA	3013	1/1	0.96	0.27	16,16,16,16	0
57	MG	XA	1654	1/1	0.96	0.08	78,78,78,78	0
57	MG	YA	3124	1/1	0.96	0.27	38,38,38,38	0
57	MG	RA	3058	1/1	0.96	0.43	19,19,19,19	0
57	MG	QA	1674	1/1	0.96	0.09	56,56,56,56	0
57	MG	YA	3009	1/1	0.96	0.36	10,10,10,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3111	1/1	0.96	0.15	33,33,33,33	0
57	MG	XA	1658	1/1	0.96	0.33	30,30,30,30	0
57	MG	YA	3015	1/1	0.96	0.51	20,20,20,20	0
57	MG	RA	3230	1/1	0.96	0.36	22,22,22,22	0
57	MG	RA	3150	1/1	0.96	0.17	37,37,37,37	0
57	MG	RA	3112	1/1	0.96	0.12	58,58,58,58	0
57	MG	YA	3134	1/1	0.96	0.31	21,21,21,21	0
57	MG	RA	3060	1/1	0.96	0.37	15,15,15,15	0
57	MG	YA	3323	1/1	0.96	0.27	49,49,49,49	0
57	MG	RA	3235	1/1	0.96	0.28	18,18,18,18	0
57	MG	YA	3024	1/1	0.96	0.41	28,28,28,28	0
57	MG	RA	3061	1/1	0.96	0.33	11,11,11,11	0
57	MG	YA	3026	1/1	0.96	0.28	15,15,15,15	0
57	MG	QA	1675	1/1	0.96	0.21	36,36,36,36	0
57	MG	XA	1666	1/1	0.96	0.28	48,48,48,48	0
57	MG	RA	3287	1/1	0.96	0.36	26,26,26,26	0
57	MG	RA	3064	1/1	0.96	0.51	9,9,9,9	0
57	MG	YA	3145	1/1	0.96	0.28	23,23,23,23	0
57	MG	RA	3156	1/1	0.96	0.47	55,55,55,55	0
57	MG	YA	3334	1/1	0.96	0.23	67,67,67,67	0
57	MG	XA	1602	1/1	0.96	0.56	19,19,19,19	0
57	MG	QA	1637	1/1	0.96	0.22	44,44,44,44	0
57	MG	RA	3021	1/1	0.96	0.31	2,2,2,2	0
57	MG	RA	3292	1/1	0.96	0.23	37,37,37,37	0
57	MG	YA	3152	1/1	0.96	0.17	41,41,41,41	0
57	MG	RA	3293	1/1	0.96	0.16	58,58,58,58	0
57	MG	RA	3024	1/1	0.96	0.16	22,22,22,22	0
57	MG	XA	1679	1/1	0.96	0.57	27,27,27,27	0
57	MG	XA	1611	1/1	0.96	0.10	20,20,20,20	0
57	MG	YA	3345	1/1	0.96	0.48	67,67,67,67	0
57	MG	YA	3346	1/1	0.96	0.20	28,28,28,28	0
57	MG	RA	3295	1/1	0.96	0.42	29,29,29,29	0
57	MG	YA	3348	1/1	0.96	0.16	49,49,49,49	0
57	MG	YA	3251	1/1	0.96	0.36	44,44,44,44	0
57	MG	XA	1615	1/1	0.96	0.26	25,25,25,25	0
57	MG	YA	3255	1/1	0.96	0.28	32,32,32,32	0
57	MG	QA	1632	1/1	0.96	0.16	28,28,28,28	0
57	MG	QA	1667	1/1	0.96	0.39	38,38,38,38	0
57	MG	YA	3259	1/1	0.96	0.20	54,54,54,54	0
57	MG	YA	3066	1/1	0.96	0.13	9,9,9,9	0
57	MG	YA	3067	1/1	0.96	0.43	22,22,22,22	0
57	MG	YA	3068	1/1	0.96	0.21	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1620	1/1	0.96	0.16	52,52,52,52	0
57	MG	YB	204	1/1	0.96	0.36	27,27,27,27	0
57	MG	XA	1688	1/1	0.96	0.61	60,60,60,60	0
57	MG	QA	1649	1/1	0.96	0.07	81,81,81,81	0
57	MG	YA	3076	1/1	0.96	0.21	22,22,22,22	0
57	MG	RA	3030	1/1	0.96	0.44	15,15,15,15	0
57	MG	RA	3033	1/1	0.96	0.38	19,19,19,19	0
57	MG	RA	3255	1/1	0.96	0.35	35,35,35,35	0
57	MG	RA	3081	1/1	0.96	0.17	24,24,24,24	0
57	MG	RA	3082	1/1	0.96	0.24	39,39,39,39	0
57	MG	YA	3084	1/1	0.96	0.34	12,12,12,12	0
57	MG	Y0	101	1/1	0.96	0.24	10,10,10,10	0
57	MG	YA	3085	1/1	0.96	0.36	7,7,7,7	0
57	MG	QA	1616	1/1	0.96	0.34	35,35,35,35	0
57	MG	XA	1630	1/1	0.96	0.45	47,47,47,47	0
57	MG	RA	3085	1/1	0.96	0.29	21,21,21,21	0
57	MG	YA	3091	1/1	0.96	0.48	17,17,17,17	0
57	MG	RA	3089	1/1	0.96	0.31	18,18,18,18	0
57	MG	YA	3093	1/1	0.96	0.24	32,32,32,32	0
57	MG	RA	3006	1/1	0.96	0.55	10,10,10,10	0
57	MG	RA	3211	1/1	0.96	0.12	62,62,62,62	0
57	MG	RA	3212	1/1	0.96	0.63	46,46,46,46	0
57	MG	RA	3076	1/1	0.97	0.22	4,4,4,4	0
57	MG	YA	3042	1/1	0.97	0.45	11,11,11,11	0
57	MG	YA	3044	1/1	0.97	0.43	15,15,15,15	0
57	MG	RA	3105	1/1	0.97	0.18	19,19,19,19	0
57	MG	RA	3242	1/1	0.97	0.24	20,20,20,20	0
57	MG	YA	3047	1/1	0.97	0.32	14,14,14,14	0
57	MG	RA	3107	1/1	0.97	0.26	21,21,21,21	0
57	MG	RA	3056	1/1	0.97	0.40	14,14,14,14	0
57	MG	YA	3213	1/1	0.97	0.22	31,31,31,31	0
57	MG	XA	1639	1/1	0.97	0.44	43,43,43,43	0
57	MG	QA	1606	1/1	0.97	0.41	20,20,20,20	0
57	MG	XA	1641	1/1	0.97	0.27	21,21,21,21	0
57	MG	RA	3248	1/1	0.97	0.43	46,46,46,46	0
57	MG	RB	201	1/1	0.97	0.13	99,99,99,99	0
57	MG	RA	3141	1/1	0.97	0.09	36,36,36,36	0
57	MG	RA	3079	1/1	0.97	0.39	53,53,53,53	0
57	MG	YA	3060	1/1	0.97	0.18	33,33,33,33	0
57	MG	YA	3144	1/1	0.97	0.29	33,33,33,33	0
57	MG	YA	3062	1/1	0.97	0.24	17,17,17,17	0
57	MG	RA	3208	1/1	0.97	0.28	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3065	1/1	0.97	0.20	55,55,55,55	0
57	MG	RA	3080	1/1	0.97	0.40	36,36,36,36	0
57	MG	RE	301	1/1	0.97	0.34	24,24,24,24	0
57	MG	RA	3023	1/1	0.97	0.34	14,14,14,14	0
57	MG	YA	3320	1/1	0.97	0.11	63,63,63,63	0
57	MG	XA	1703	1/1	0.97	0.35	46,46,46,46	0
57	MG	YA	3231	1/1	0.97	0.45	24,24,24,24	0
57	MG	YA	3071	1/1	0.97	0.34	8,8,8,8	0
57	MG	XA	1651	1/1	0.97	0.49	62,62,62,62	0
57	MG	QA	1607	1/1	0.97	0.16	35,35,35,35	0
57	MG	YA	3074	1/1	0.97	0.53	19,19,19,19	0
57	MG	YA	3075	1/1	0.97	0.28	10,10,10,10	0
57	MG	RA	3083	1/1	0.97	0.21	18,18,18,18	0
57	MG	QA	1602	1/1	0.97	0.52	22,22,22,22	0
57	MG	RA	3257	1/1	0.97	1.02	52,52,52,52	0
57	MG	XA	1709	1/1	0.97	0.23	38,38,38,38	0
57	MG	RA	3148	1/1	0.97	0.22	38,38,38,38	0
57	MG	XA	1603	1/1	0.97	0.32	16,16,16,16	0
57	MG	YA	3248	1/1	0.97	0.31	34,34,34,34	0
57	MG	YA	3083	1/1	0.97	0.38	23,23,23,23	0
57	MG	RA	3047	1/1	0.97	0.43	27,27,27,27	0
57	MG	RA	3086	1/1	0.97	0.33	9,9,9,9	0
57	MG	YA	3253	1/1	0.97	0.36	37,37,37,37	0
57	MG	YA	3254	1/1	0.97	0.21	11,11,11,11	0
57	MG	RA	3088	1/1	0.97	0.44	23,23,23,23	0
57	MG	YA	3341	1/1	0.97	0.20	39,39,39,39	0
57	MG	YA	3256	1/1	0.97	0.20	33,33,33,33	0
57	MG	YA	3001	1/1	0.97	0.24	39,39,39,39	0
57	MG	RA	3119	1/1	0.97	0.46	40,40,40,40	0
57	MG	YA	3089	1/1	0.97	0.26	51,51,51,51	0
57	MG	YA	3003	1/1	0.97	0.45	24,24,24,24	0
57	MG	XA	1608	1/1	0.97	0.13	21,21,21,21	0
57	MG	RA	3048	1/1	0.97	0.43	12,12,12,12	0
57	MG	RA	3063	1/1	0.97	0.46	3,3,3,3	0
57	MG	RA	3188	1/1	0.97	0.25	53,53,53,53	0
57	MG	RA	3223	1/1	0.97	0.33	6,6,6,6	0
57	MG	YA	3177	1/1	0.97	0.31	19,19,19,19	0
57	MG	QA	1651	1/1	0.97	0.29	29,29,29,29	0
57	MG	YA	3010	1/1	0.97	0.22	11,11,11,11	0
57	MG	YA	3269	1/1	0.97	0.37	59,59,59,59	0
57	MG	RA	3066	1/1	0.97	0.24	3,3,3,3	0
57	MG	YA	3271	1/1	0.97	0.28	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1669	1/1	0.97	0.25	21,21,21,21	0
57	MG	YA	3105	1/1	0.97	0.32	11,11,11,11	0
57	MG	YA	3014	1/1	0.97	0.45	8,8,8,8	0
57	MG	RA	3067	1/1	0.97	0.28	13,13,13,13	0
57	MG	RA	3094	1/1	0.97	0.32	45,45,45,45	0
57	MG	YA	3110	1/1	0.97	0.27	7,7,7,7	0
57	MG	QA	1605	1/1	0.97	0.47	30,30,30,30	0
57	MG	YA	3018	1/1	0.97	0.27	28,28,28,28	0
57	MG	XA	1624	1/1	0.97	0.44	41,41,41,41	0
57	MG	RA	3016	1/1	0.97	0.23	15,15,15,15	0
57	MG	RA	3098	1/1	0.97	0.35	5,5,5,5	0
57	MG	YA	3023	1/1	0.97	0.32	17,17,17,17	0
57	MG	RA	3099	1/1	0.97	0.41	14,14,14,14	0
57	MG	RA	3031	1/1	0.97	0.31	30,30,30,30	0
57	MG	Y1	101	1/1	0.97	0.10	35,35,35,35	0
57	MG	RA	3053	1/1	0.97	0.34	5,5,5,5	0
57	MG	RA	3054	1/1	0.97	0.35	10,10,10,10	0
57	MG	YA	3030	1/1	0.97	0.31	17,17,17,17	0
57	MG	QA	1621	1/1	0.97	0.52	61,61,61,61	0
57	MG	RA	3237	1/1	0.97	0.28	21,21,21,21	0
57	MG	RA	3238	1/1	0.97	0.09	57,57,57,57	0
57	MG	YA	3037	1/1	0.97	0.16	23,23,23,23	0
57	MG	YA	3039	1/1	0.97	0.26	12,12,12,12	0
57	MG	YA	3053	1/1	0.98	0.34	22,22,22,22	0
57	MG	YA	3243	1/1	0.98	0.21	45,45,45,45	0
57	MG	XA	1674	1/1	0.98	0.24	4,4,4,4	0
57	MG	RA	3106	1/1	0.98	0.17	12,12,12,12	0
57	MG	QA	1610	1/1	0.98	0.31	20,20,20,20	0
57	MG	RA	3022	1/1	0.98	0.27	4,4,4,4	0
57	MG	RA	3032	1/1	0.98	0.36	40,40,40,40	0
57	MG	YA	3249	1/1	0.98	0.41	70,70,70,70	0
57	MG	QA	1609	1/1	0.98	0.16	42,42,42,42	0
57	MG	YA	3061	1/1	0.98	0.21	2,2,2,2	0
57	MG	XA	1642	1/1	0.98	0.38	27,27,27,27	0
57	MG	YA	3184	1/1	0.98	0.18	41,41,41,41	0
57	MG	YA	3063	1/1	0.98	0.26	12,12,12,12	0
57	MG	RA	3034	1/1	0.98	0.46	16,16,16,16	0
57	MG	QA	1636	1/1	0.98	0.14	12,12,12,12	0
57	MG	RA	3036	1/1	0.98	0.12	10,10,10,10	0
57	MG	YA	3189	1/1	0.98	0.51	51,51,51,51	0
57	MG	XA	1610	1/1	0.98	0.15	21,21,21,21	0
57	MG	XA	1685	1/1	0.98	0.28	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3069	1/1	0.98	0.22	10,10,10,10	0
57	MG	RA	3073	1/1	0.98	0.30	26,26,26,26	0
57	MG	YA	3013	1/1	0.98	0.31	13,13,13,13	0
57	MG	XA	1687	1/1	0.98	0.57	33,33,33,33	0
57	MG	RA	3074	1/1	0.98	0.23	8,8,8,8	0
57	MG	XA	1613	1/1	0.98	0.36	17,17,17,17	0
57	MG	XA	1614	1/1	0.98	0.35	13,13,13,13	0
57	MG	RA	3162	1/1	0.98	0.19	18,18,18,18	0
57	MG	XA	1616	1/1	0.98	0.37	29,29,29,29	0
57	MG	XA	1617	1/1	0.98	0.22	41,41,41,41	0
57	MG	RA	3095	1/1	0.98	0.35	18,18,18,18	0
57	MG	RA	3241	1/1	0.98	0.28	35,35,35,35	0
57	MG	RA	3038	1/1	0.98	0.24	15,15,15,15	0
57	MG	XA	1621	1/1	0.98	0.29	25,25,25,25	0
57	MG	RA	3040	1/1	0.98	0.32	12,12,12,12	0
57	MG	YA	3027	1/1	0.98	0.58	39,39,39,39	0
57	MG	YA	3028	1/1	0.98	0.23	6,6,6,6	0
57	MG	RA	3025	1/1	0.98	0.23	6,6,6,6	0
57	MG	RA	3245	1/1	0.98	0.43	39,39,39,39	0
57	MG	RA	3043	1/1	0.98	0.20	12,12,12,12	0
57	MG	YA	3150	1/1	0.98	0.29	34,34,34,34	0
57	MG	RA	3121	1/1	0.98	0.18	40,40,40,40	0
57	MG	YA	3034	1/1	0.98	0.32	16,16,16,16	0
57	MG	RA	3017	1/1	0.98	0.33	15,15,15,15	0
57	MG	YA	3094	1/1	0.98	0.23	23,23,23,23	0
57	MG	YA	3036	1/1	0.98	0.27	19,19,19,19	0
57	MG	RA	3018	1/1	0.98	0.17	24,24,24,24	0
57	MG	YB	202	1/1	0.98	0.17	51,51,51,51	0
57	MG	RA	3046	1/1	0.98	0.27	13,13,13,13	0
57	MG	YA	3220	1/1	0.98	0.15	55,55,55,55	0
57	MG	YA	3098	1/1	0.98	0.44	21,21,21,21	0
57	MG	RA	3028	1/1	0.98	0.34	24,24,24,24	0
57	MG	YA	3041	1/1	0.98	0.42	12,12,12,12	0
57	MG	YA	3101	1/1	0.98	0.26	5,5,5,5	0
57	MG	RA	3173	1/1	0.98	0.33	42,42,42,42	0
57	MG	YA	3043	1/1	0.98	0.38	31,31,31,31	0
57	MG	YA	3104	1/1	0.98	0.36	16,16,16,16	0
57	MG	RP	201	1/1	0.98	0.38	31,31,31,31	0
57	MG	YA	3299	1/1	0.98	0.34	32,32,32,32	0
57	MG	YA	3106	1/1	0.98	0.15	27,27,27,27	0
57	MG	RA	3126	1/1	0.98	0.25	51,51,51,51	0
57	MG	XA	1711	1/1	0.98	0.12	27,27,27,27	0

Continued on next page...

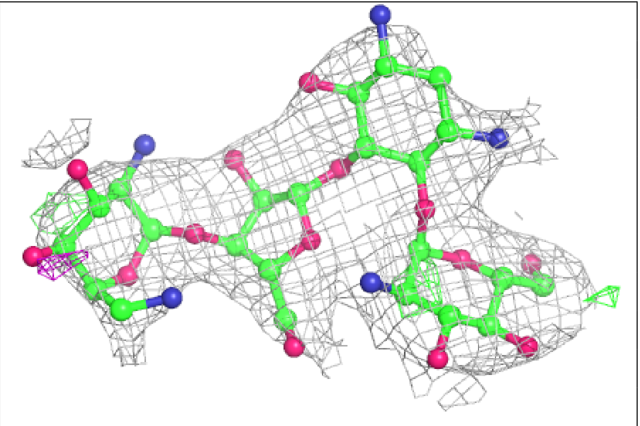
Continued from previous page...

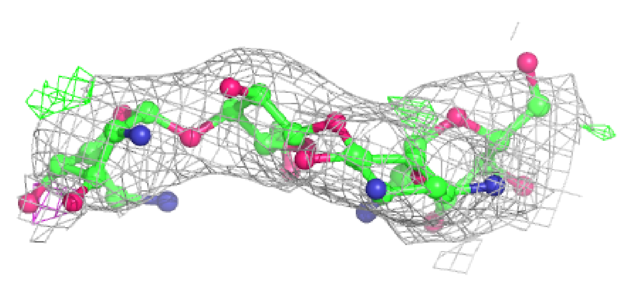
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	YA	3232	1/1	0.98	0.56	20,20,20,20	0
57	MG	YA	3233	1/1	0.98	0.38	24,24,24,24	0
57	MG	QA	1655	1/1	0.98	0.69	19,19,19,19	0
57	MG	RA	3065	1/1	0.98	0.19	13,13,13,13	0
57	MG	YA	3236	1/1	0.98	0.45	10,10,10,10	0
57	MG	XA	1601	1/1	0.98	0.89	35,35,35,35	0
57	MG	YA	3112	1/1	0.98	0.32	44,44,44,44	0
57	MG	XA	1673	1/1	0.98	0.51	21,21,21,21	0
59	ZN	XD	301	1/1	0.98	0.31	49,49,49,49	0
57	MG	XV	102	1/1	0.98	0.18	14,14,14,14	0
57	MG	YA	3022	1/1	0.99	0.39	16,16,16,16	0
57	MG	QA	1608	1/1	0.99	0.08	18,18,18,18	0
57	MG	YA	3051	1/1	0.99	0.29	8,8,8,8	0
57	MG	RA	3246	1/1	0.99	0.11	68,68,68,68	0
57	MG	YA	3038	1/1	0.99	0.25	10,10,10,10	0
57	MG	RA	3039	1/1	0.99	0.28	13,13,13,13	0
57	MG	RA	3004	1/1	0.99	0.44	11,11,11,11	0
57	MG	YA	3290	1/1	0.99	0.22	28,28,28,28	0
57	MG	RA	3041	1/1	0.99	0.31	24,24,24,24	0
57	MG	YA	3090	1/1	0.99	0.30	13,13,13,13	0
57	MG	RA	3007	1/1	0.99	0.38	7,7,7,7	0
57	MG	YA	3058	1/1	0.99	0.34	21,21,21,21	0
57	MG	RA	3221	1/1	0.99	0.34	23,23,23,23	0
57	MG	RA	3231	1/1	0.99	0.37	22,22,22,22	0
57	MG	RA	3020	1/1	0.99	0.18	9,9,9,9	0
57	MG	YA	3032	1/1	0.99	0.52	9,9,9,9	0
57	MG	RA	3037	1/1	0.99	0.24	12,12,12,12	0
57	MG	YA	3242	1/1	0.99	0.44	21,21,21,21	0
57	MG	RA	3087	1/1	0.99	0.21	30,30,30,30	0
57	MG	YA	3081	1/1	0.99	0.35	45,45,45,45	0

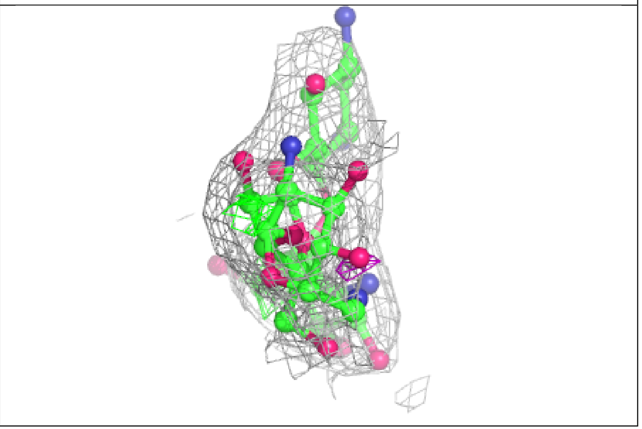
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR QA 1681:

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

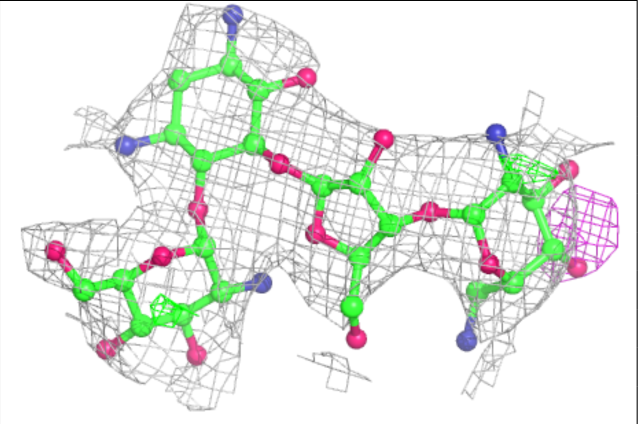


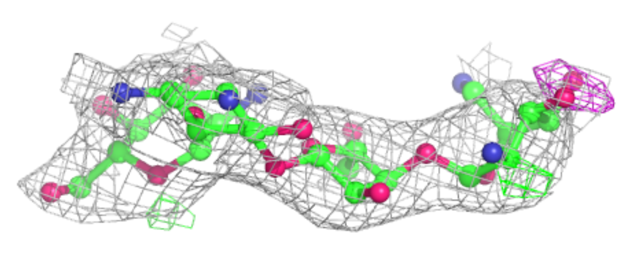


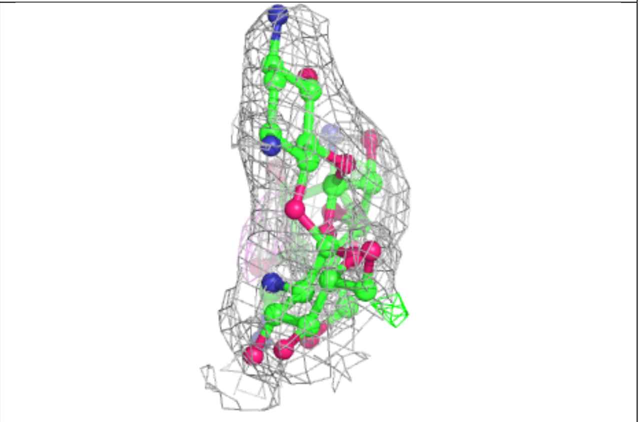


Electron density around PAR XA 1710:

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.