



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:32 AM UTC

PDB ID : 4TUC / pdb_00004tuc
Title : Crystal structure of ASL-SufJ bound to Codon ACC-A on the Ribosome
Authors : Fagan, C.E.; Dunham, C.M.
Deposited on : 2014-06-24
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

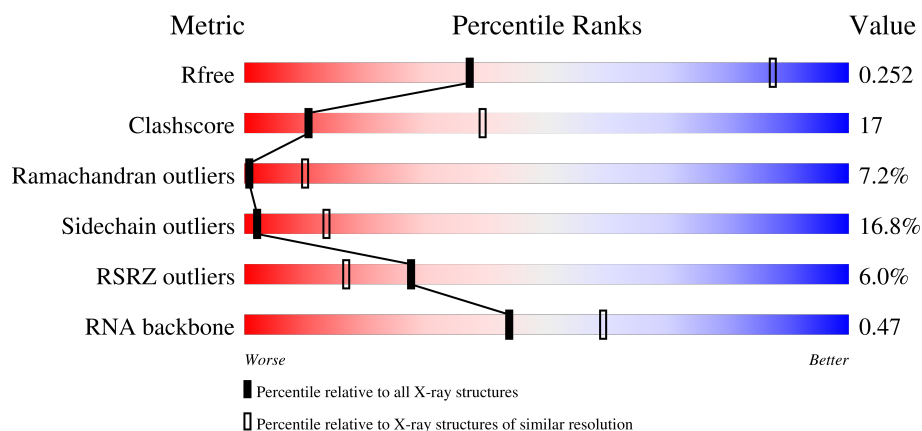
1 Overall quality at a glance

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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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 $\leq 5\%$. 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	6% 54% 37% 8%
1	XA	1522	3% 52% 37% 9%
2	QB	256	6% 46% 38% 8% 7%
2	XB	256	5% 45% 38% 9% 7%

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	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	18	
24	XY	18	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

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	

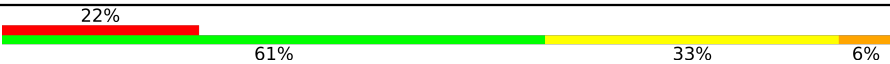
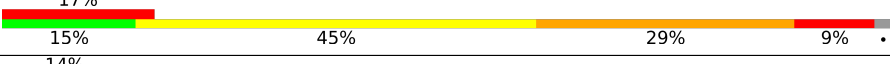
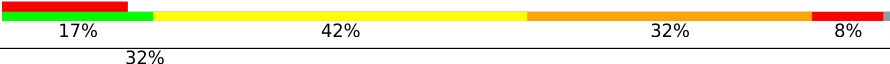
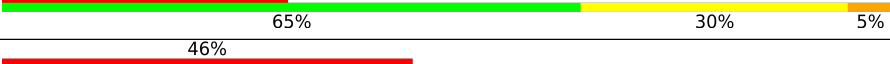
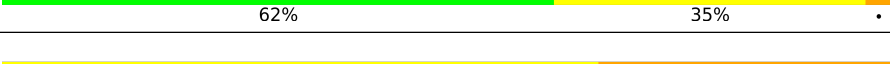
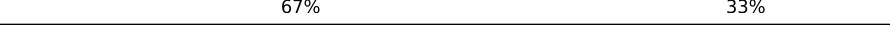
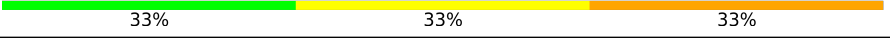
Continued on next page...

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	1602	-	-	-	X
57	MG	QA	1610	-	-	-	X
57	MG	QA	1642	-	-	-	X
57	MG	QA	1664	-	-	-	X
57	MG	QN	102	-	-	-	X
57	MG	RA	3014	-	-	-	X
57	MG	RA	3027	-	-	-	X
57	MG	RA	3032	-	-	-	X
57	MG	RA	3047	-	-	-	X
57	MG	RA	3063	-	-	-	X
57	MG	RA	3064	-	-	-	X
57	MG	RA	3066	-	-	-	X
57	MG	RA	3085	-	-	-	X
57	MG	RA	3120	-	-	-	X
57	MG	RA	3141	-	-	-	X
57	MG	RB	202	-	-	-	X
57	MG	XA	1616	-	-	-	X
57	MG	XA	1633	-	-	-	X
57	MG	XA	1635	-	-	-	X
57	MG	XA	1677	-	-	-	X
57	MG	XA	1681	-	-	-	X
57	MG	YA	3007	-	-	-	X
57	MG	YA	3016	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3019	-	-	-	X
57	MG	YA	3032	-	-	-	X
57	MG	YA	3038	-	-	-	X
57	MG	YA	3041	-	-	-	X
57	MG	YA	3042	-	-	-	X
57	MG	YA	3046	-	-	-	X
57	MG	YA	3061	-	-	-	X
57	MG	YA	3115	-	-	-	X
57	MG	YA	3119	-	-	-	X
57	MG	YA	3139	-	-	-	X
57	MG	YA	3240	-	-	-	X
57	MG	YA	3262	-	-	-	X
57	MG	YB	202	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 292042 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
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

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

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

- 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	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- 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	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- 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	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- 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	0	0	0
			1116	705	215	193	3			
8	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

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

- 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	0	0	0
			801	504	157	139	1			

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

- 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
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

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

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

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	11	Total	C	N	O	P	0	0	0
			220	98	43	68	11			
23	XX	10	Total	C	N	O	P	0	0	0
			214	97	43	65	9			

- Molecule 24 is a RNA chain called A-site ASL-SufJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	15	Total	C	N	O	P	0	0	0
			319	142	55	107	15			
24	XY	15	Total	C	N	O	P	0	0	0
			319	142	55	107	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2882	Total	C	N	O	P	0	0	0
			62069	27627	11609	19952	2881			
25	YA	2882	Total	C	N	O	P	0	0	0
			62070	27627	11611	19951	2881			

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

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

Continued on next page...

Continued from previous page...

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

- 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	0	0	0
			2115	1335	420	357	3			
27	YD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- 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	0	0	0
			1568	991	300	271	6			
28	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- 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	0	0	0
			1585	1011	297	275	2			
29	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- 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	0	0	0
			1474	942	268	260	4			
30	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- 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	0	0	0
			1307	829	245	232	1			
31	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- 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
			1143	711	231	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	C	N	O	S	0	0	0
			968	604	203	160	1			
37	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

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

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

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

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

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

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

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

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

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

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

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
			648	401	138	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	0	0	0
			581	358	118	104	1			
48	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

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

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

- 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	0	0	0
			581	364	108	104	5			
50	Y4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- 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	0	0	0
			459	288	90	76	5			
51	Y5	58	Total	C	N	O	S	0	0	0
			454	285	89	75	5			

- 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	0	0	0
			424	264	87	69	4			
52	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- 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	0	0	0
			430	263	108	57	2			
53	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- 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	0	0	0
			517	331	102	82	2			
54	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- 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	0	0	0
			307	188	68	47	4			
55	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	86	Total	Mg	0	0
			86	86		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QM	2	Total	Mg	0	0
			2	2		
57	QN	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QV	2	Total 2	Mg 2	0	0
57	QX	2	Total 2	Mg 2	0	0
57	RA	247	Total 247	Mg 247	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	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	R3	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	XA	101	Total 101	Mg 101	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	XY	1	Total 1	Mg 1	0	0
57	YA	277	Total 277	Mg 277	0	0
57	YB	4	Total 4	Mg 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YE	2	Total 2	Mg 2	0	0
57	YP	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0

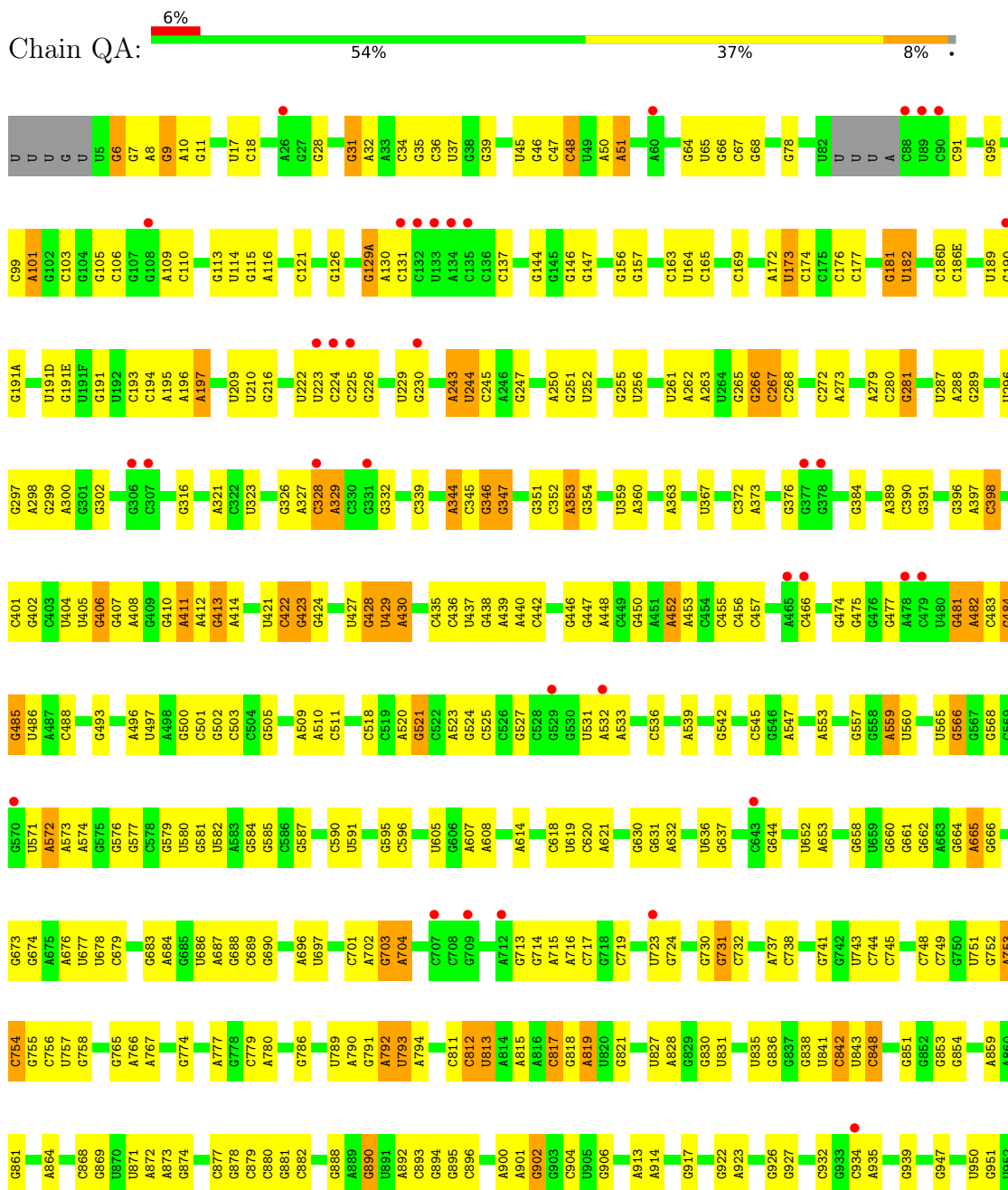
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

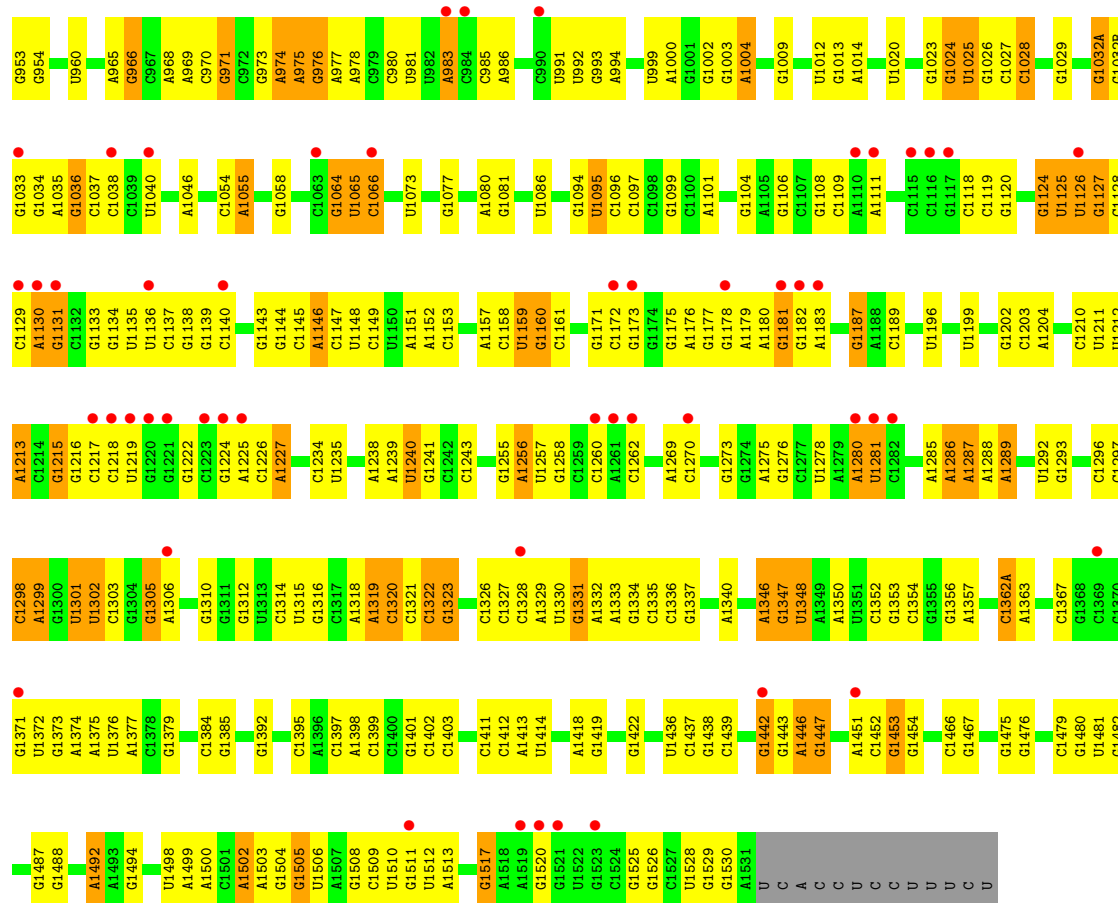
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	QD	1	Total 1	Zn 1	0	0
58	QN	1	Total 1	Zn 1	0	0
58	XD	1	Total 1	Zn 1	0	0
58	XN	1	Total 1	Zn 1	0	0

3 Residue-property plots [i](#)

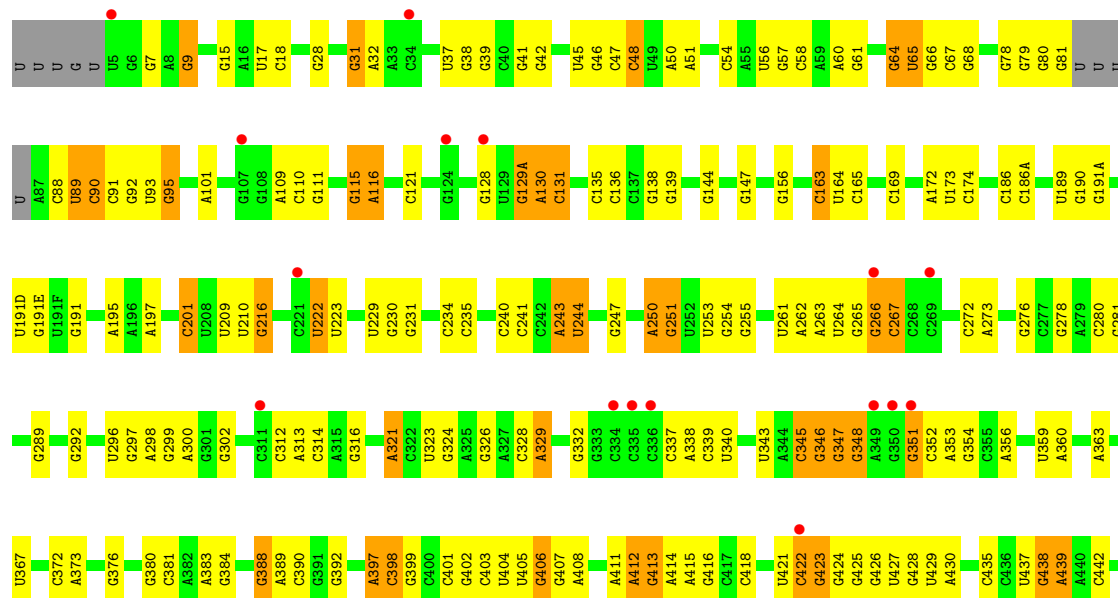
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

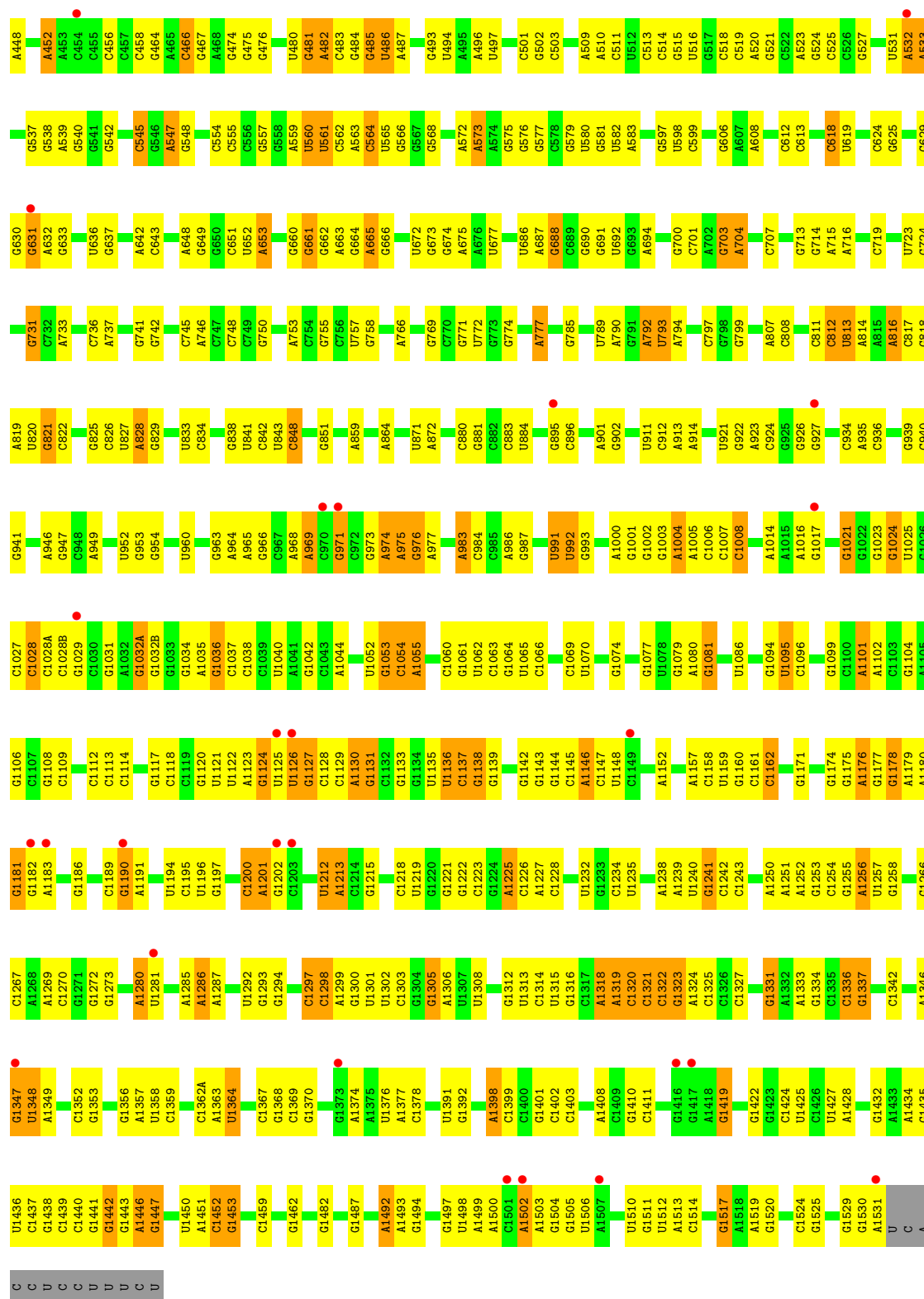
• Molecule 1: 16S rRNA





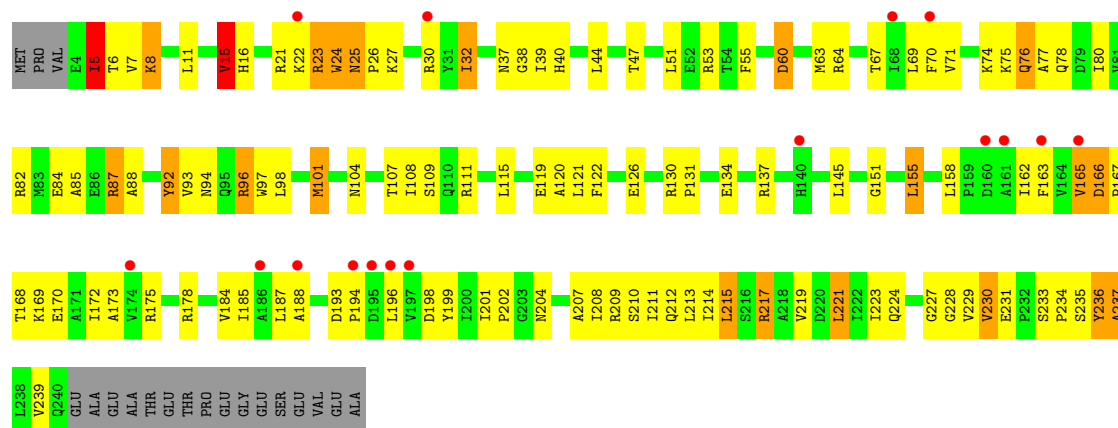
• Molecule 1: 16S rRNA



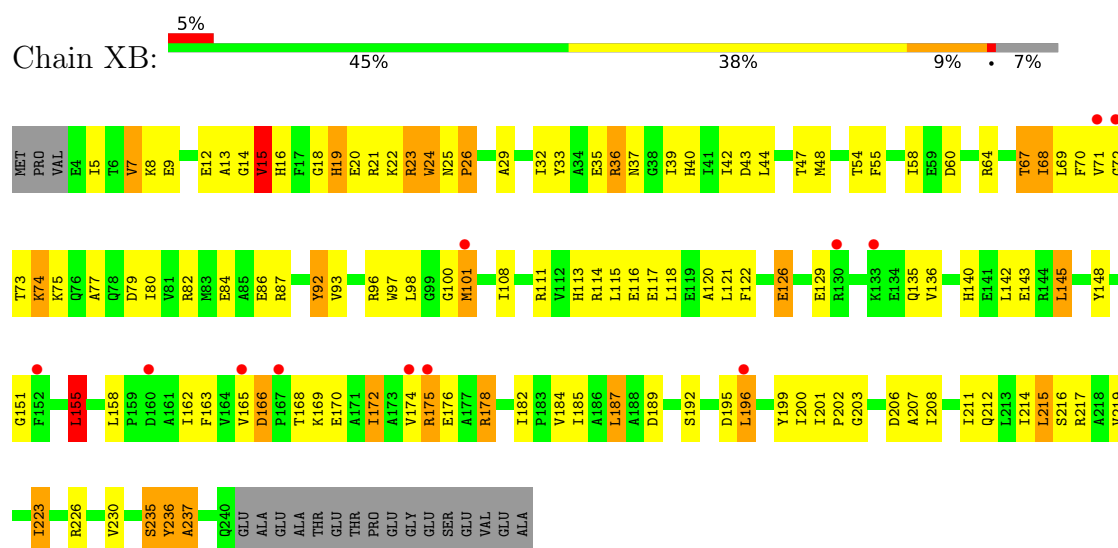


• Molecule 2: 30S ribosomal protein S2

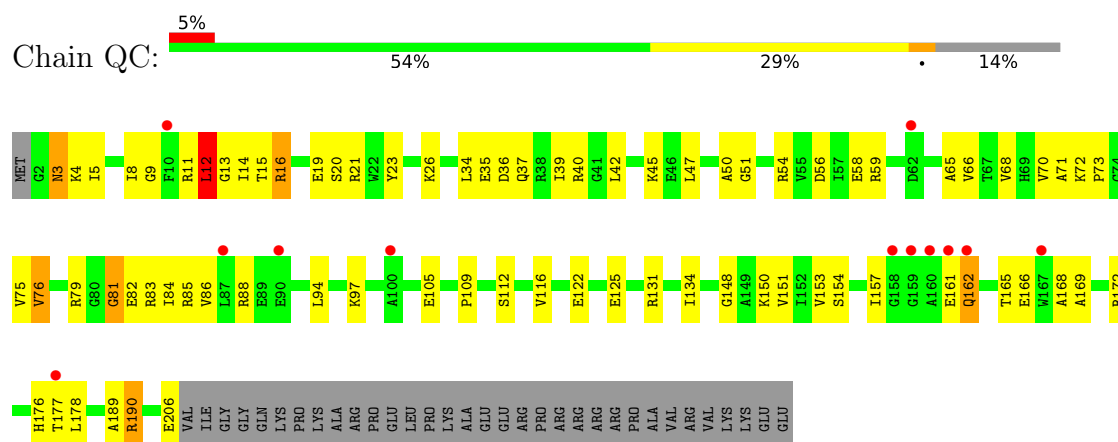




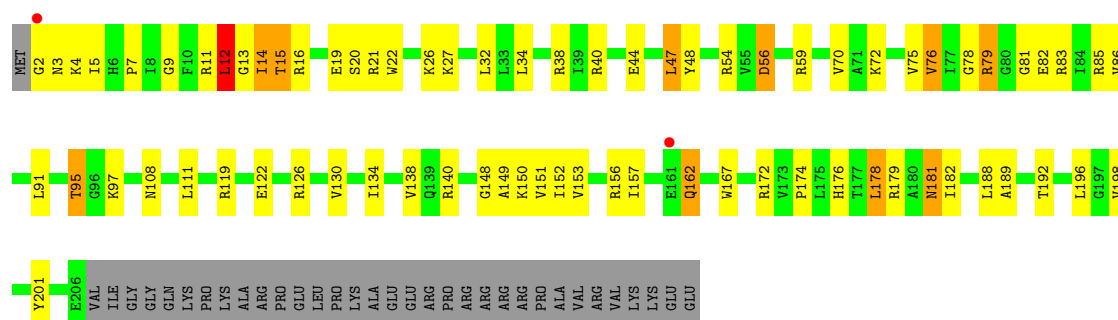
• Molecule 2: 30S ribosomal protein S2



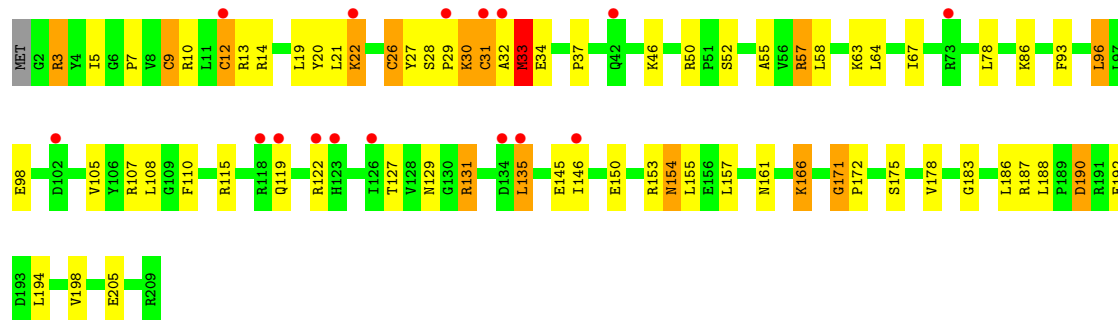
• Molecule 3: 30S ribosomal protein S3



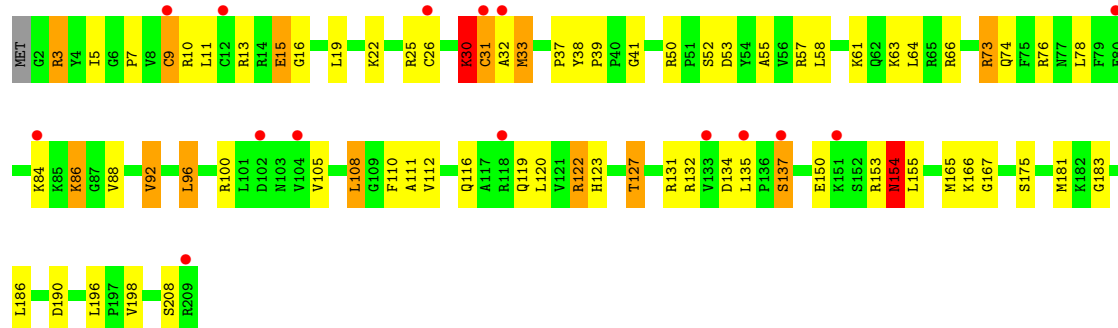
• Molecule 3: 30S ribosomal protein S3



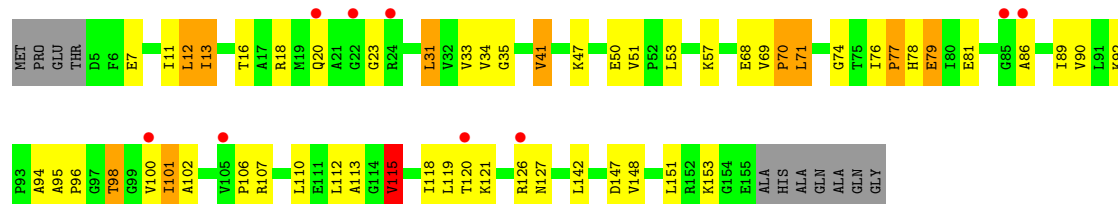
• Molecule 4: 30S ribosomal protein S4



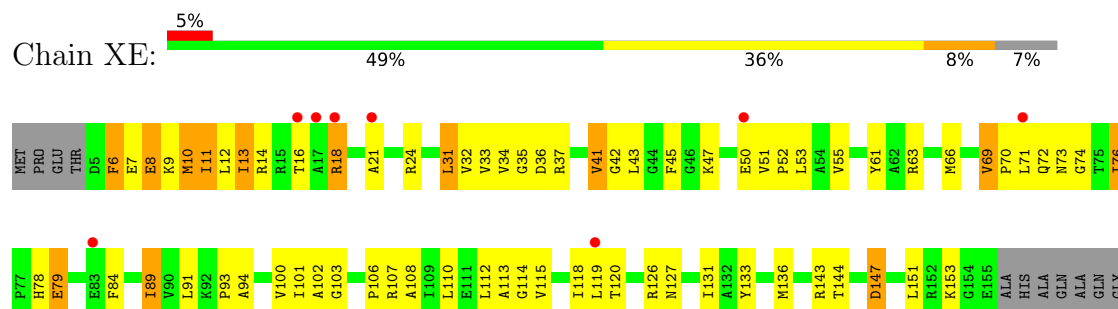
• Molecule 4: 30S ribosomal protein S4



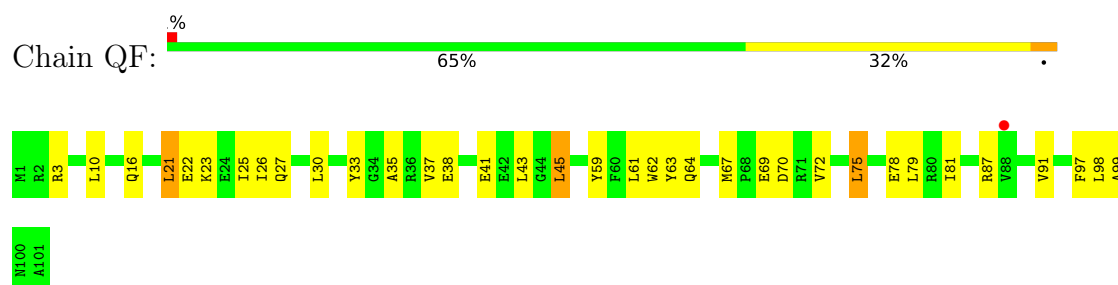
• Molecule 5: 30S ribosomal protein S5



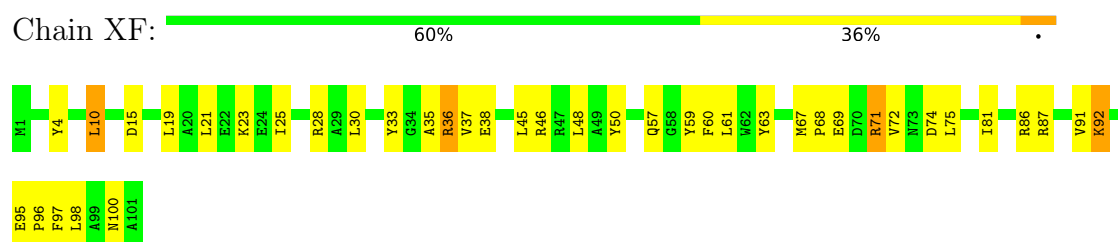
- Molecule 5: 30S ribosomal protein S5



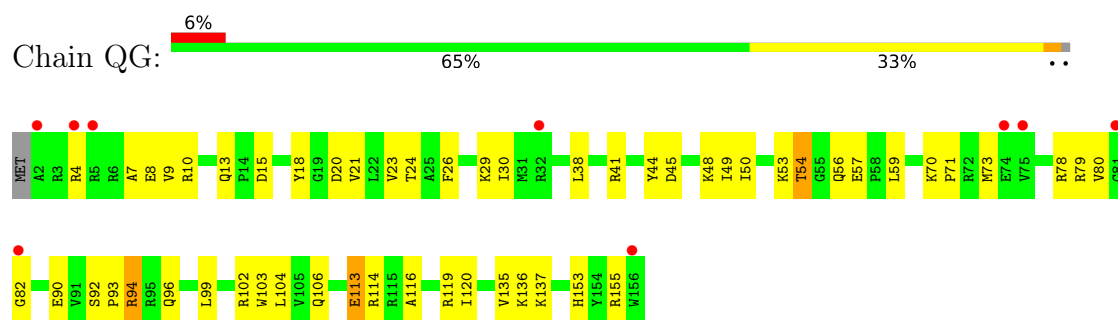
- Molecule 6: 30S ribosomal protein S6



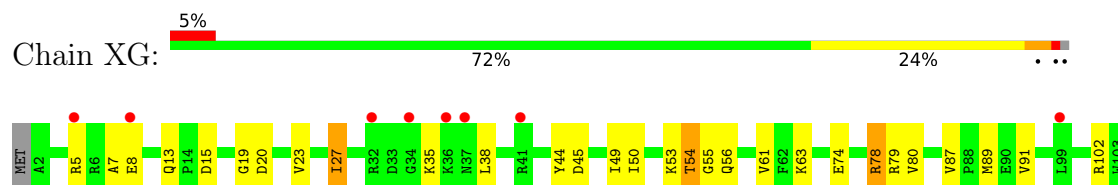
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7

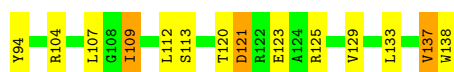




- Molecule 8: 30S ribosomal protein S8



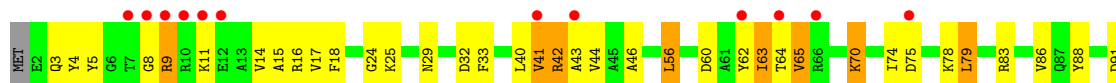
- Molecule 8: 30S ribosomal protein S8



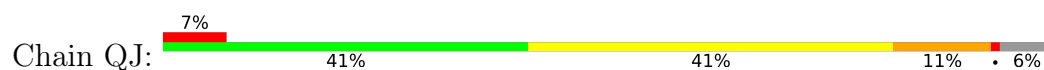
- Molecule 9: 30S ribosomal protein S9

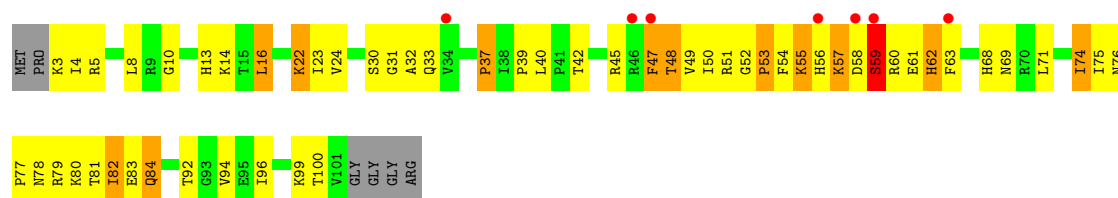


- Molecule 9: 30S ribosomal protein S9

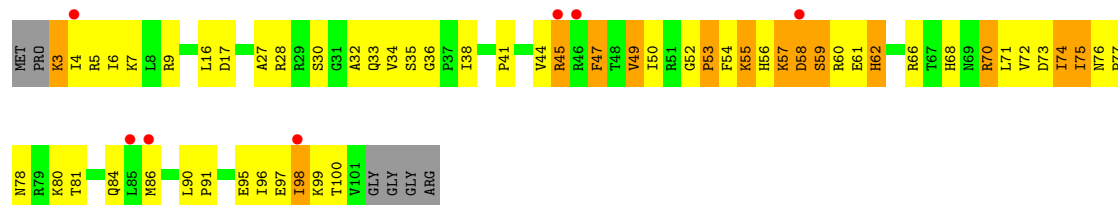
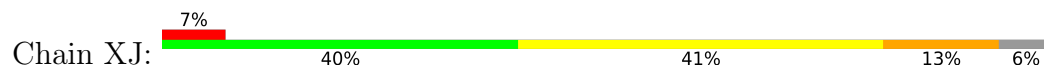


- Molecule 10: 30S ribosomal protein S10

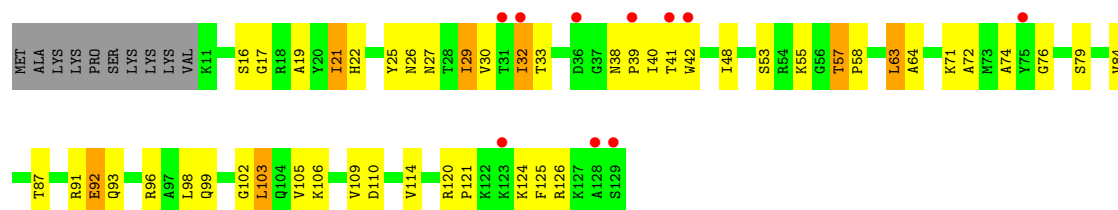




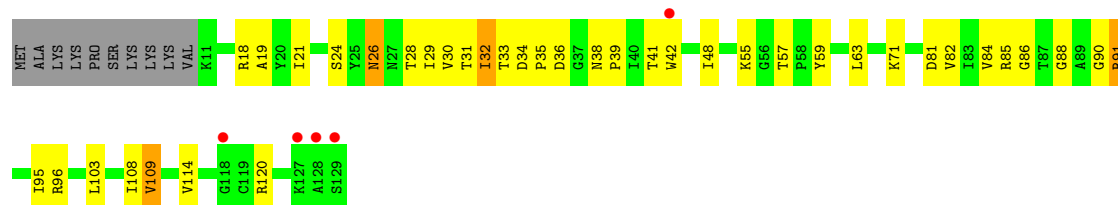
• Molecule 10: 30S ribosomal protein S10



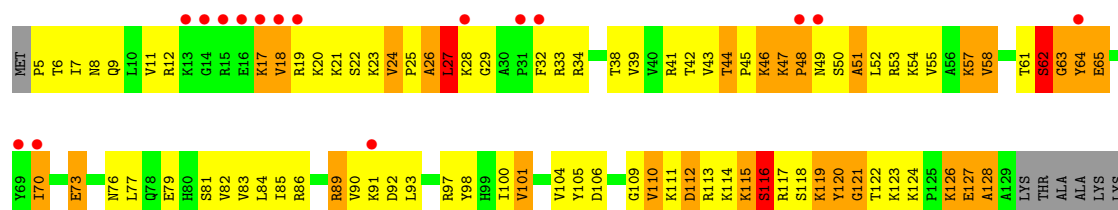
• Molecule 11: 30S ribosomal protein S11



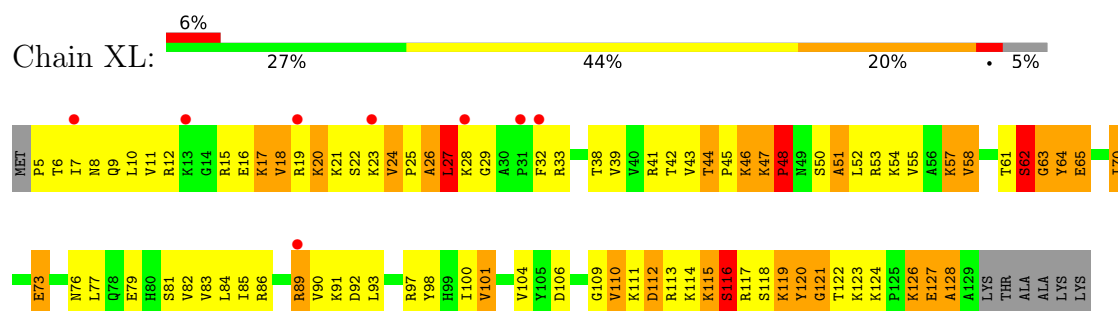
• Molecule 11: 30S ribosomal protein S11



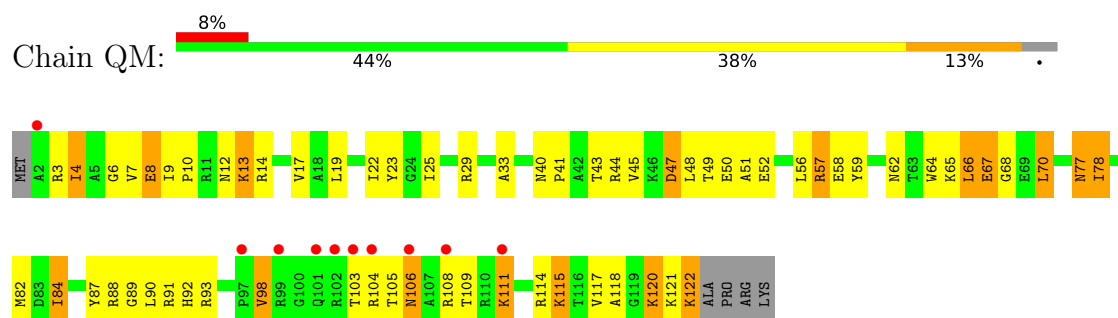
• Molecule 12: 30S ribosomal protein S12



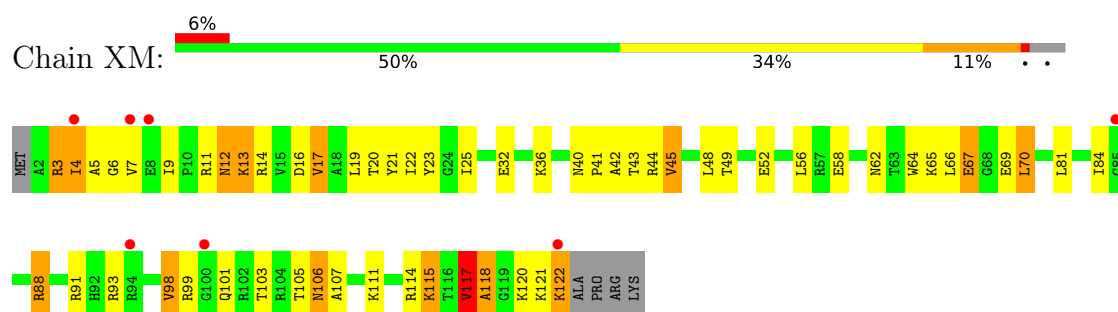
- Molecule 12: 30S ribosomal protein S12



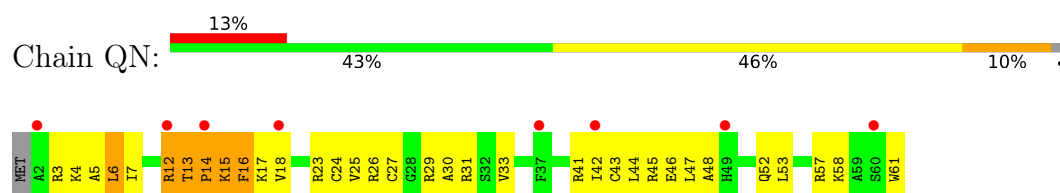
- Molecule 13: 30S ribosomal protein S13



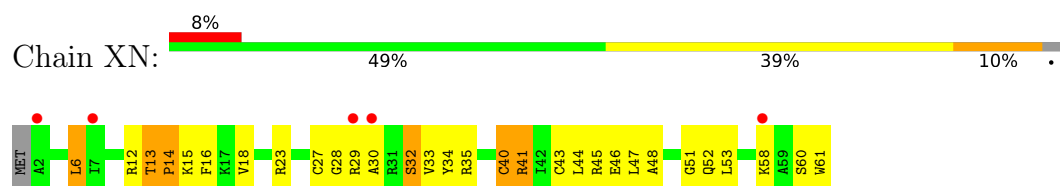
- Molecule 13: 30S ribosomal protein S13



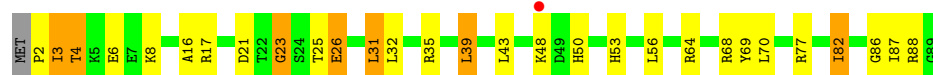
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15



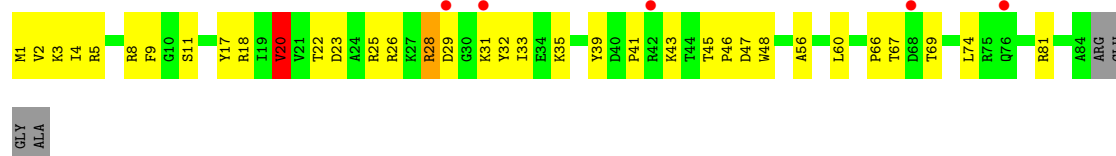
- Molecule 15: 30S ribosomal protein S15



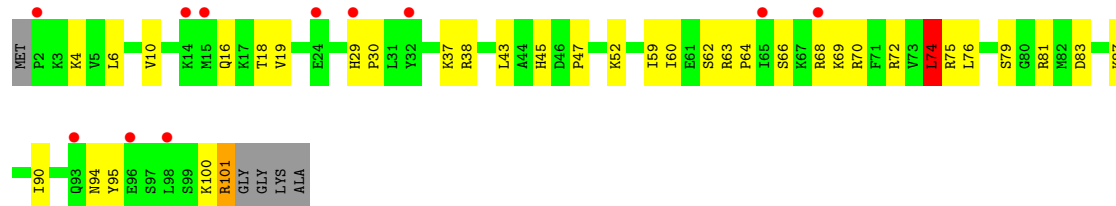
- Molecule 16: 30S ribosomal protein S16



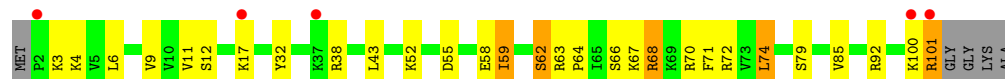
- Molecule 16: 30S ribosomal protein S16



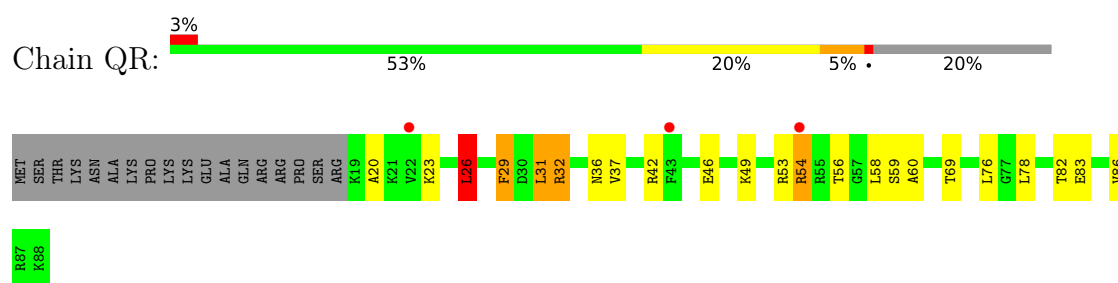
- Molecule 17: 30S ribosomal protein S17



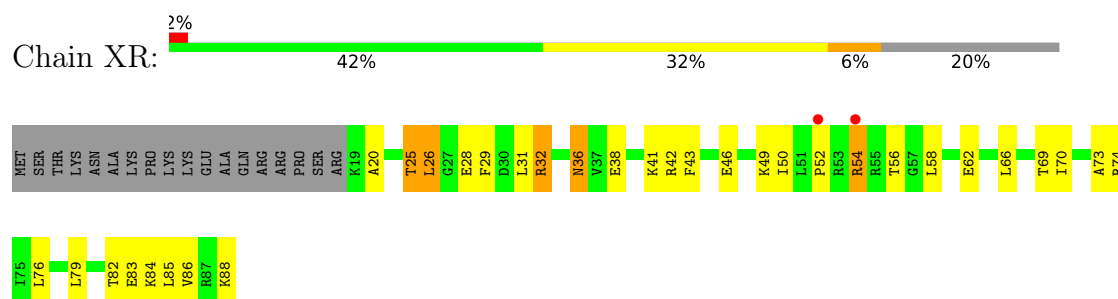
- Molecule 17: 30S ribosomal protein S17



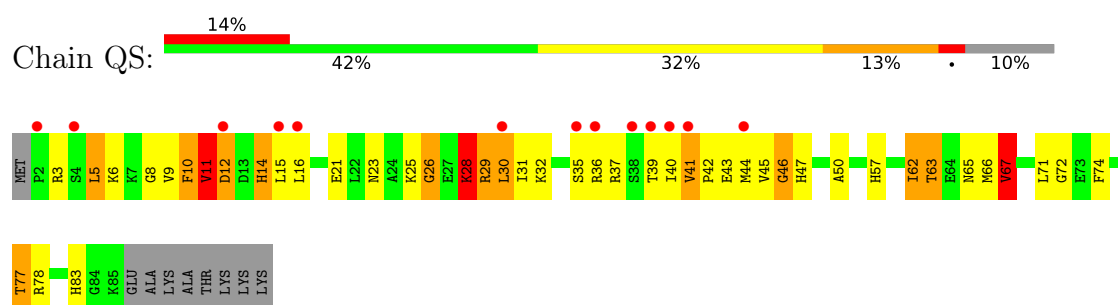
- Molecule 18: 30S ribosomal protein S18



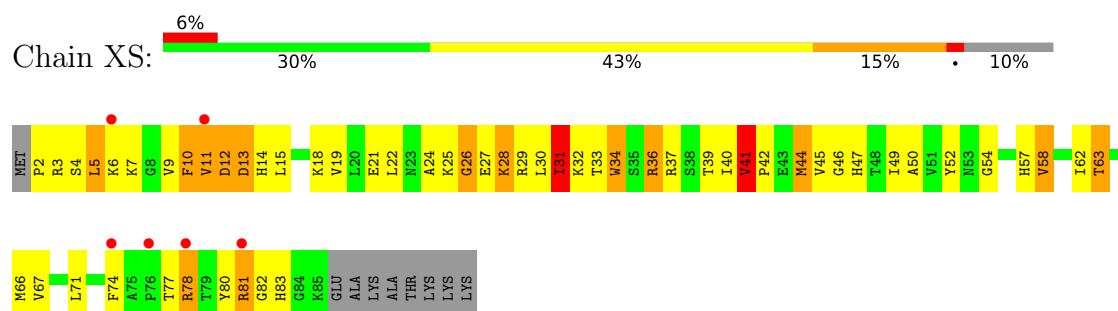
- Molecule 18: 30S ribosomal protein S18



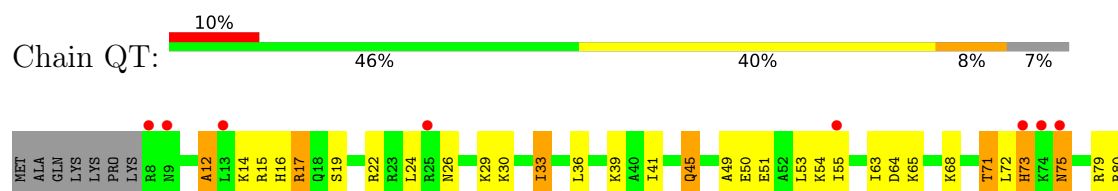
- Molecule 19: 30S ribosomal protein S19

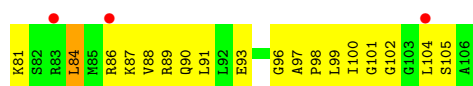


- Molecule 19: 30S ribosomal protein S19

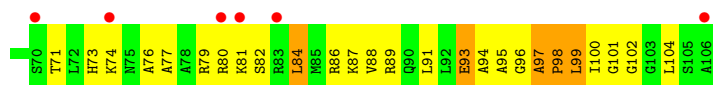
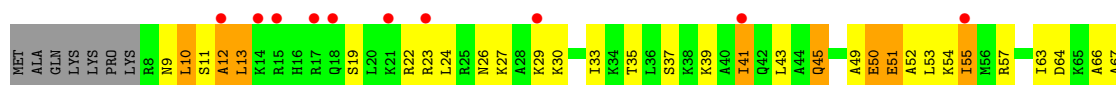


- Molecule 20: 30S ribosomal protein S20

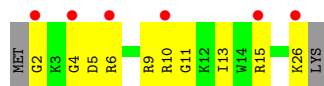




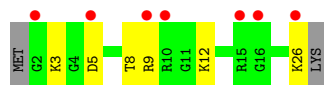
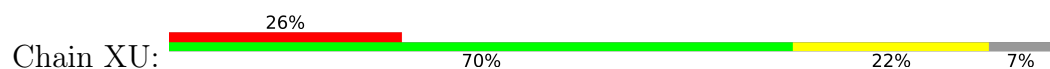
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



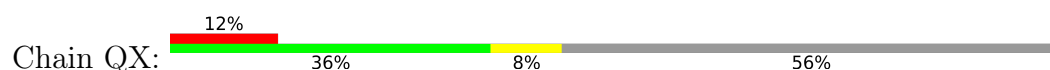
- Molecule 22: P-site tRNA fMet



- Molecule 22: P-site tRNA fMet



- Molecule 23: messenger RNA

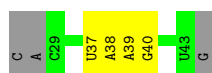




- Molecule 23: messenger RNA



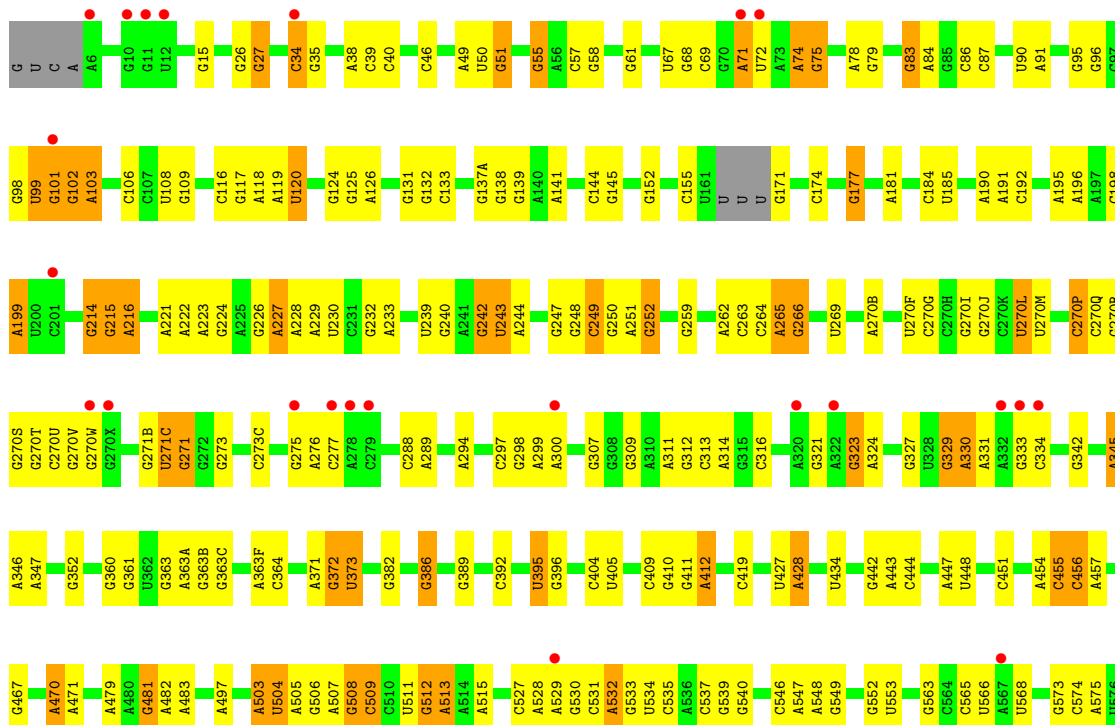
- Molecule 24: A-site ASL-SufJ

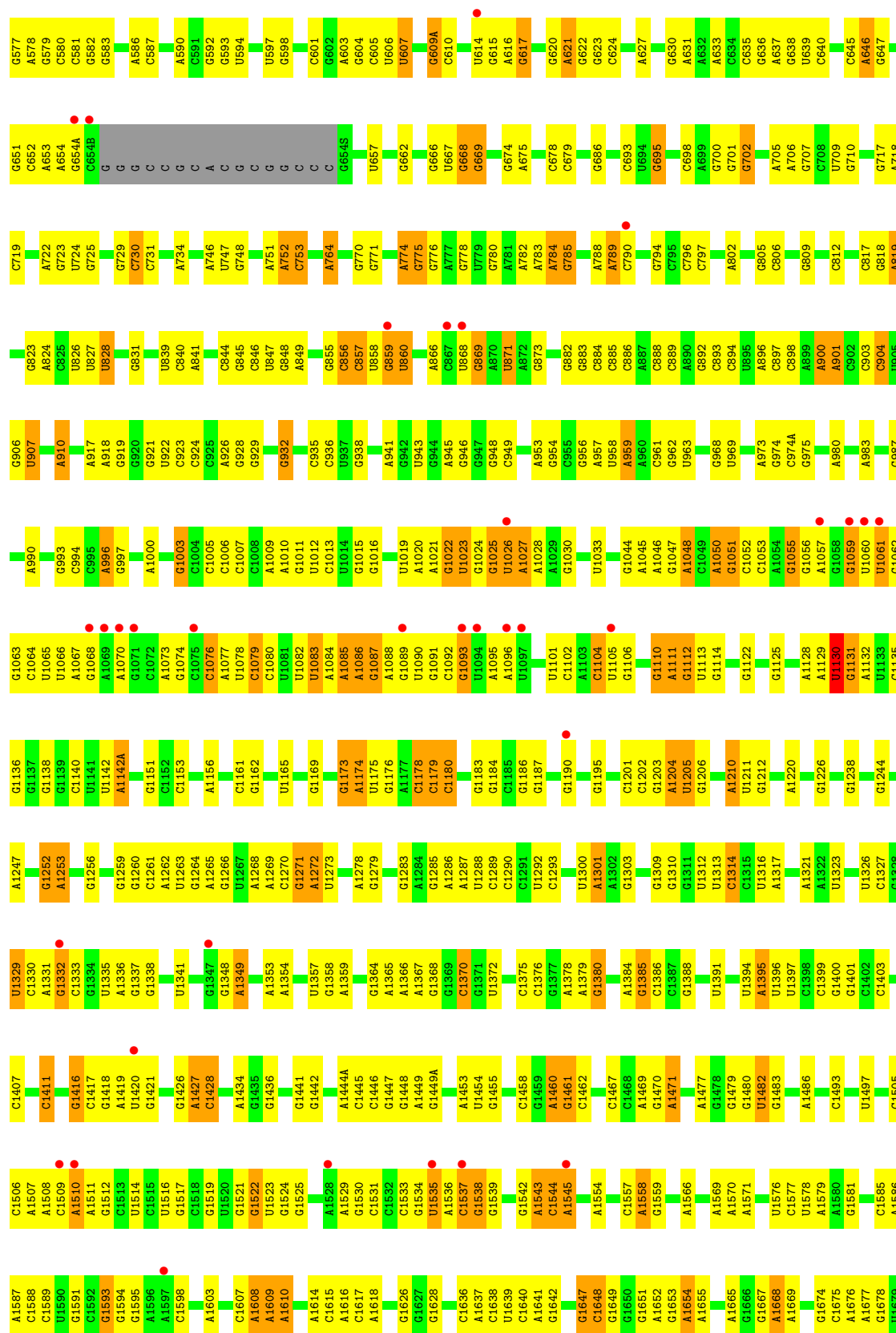


- Molecule 24: A-site ASL-SufJ



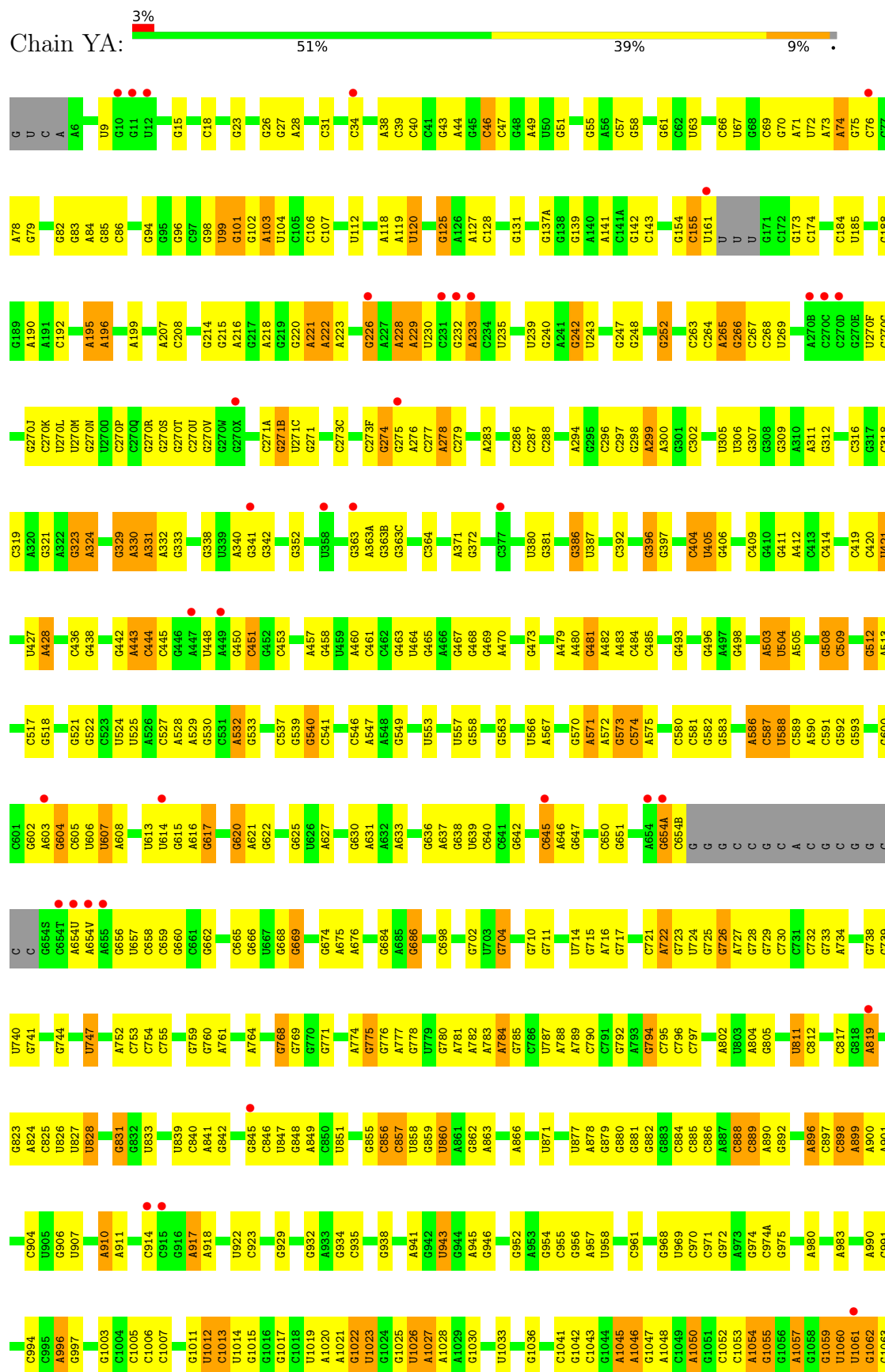
- Molecule 25: 23S rRNA



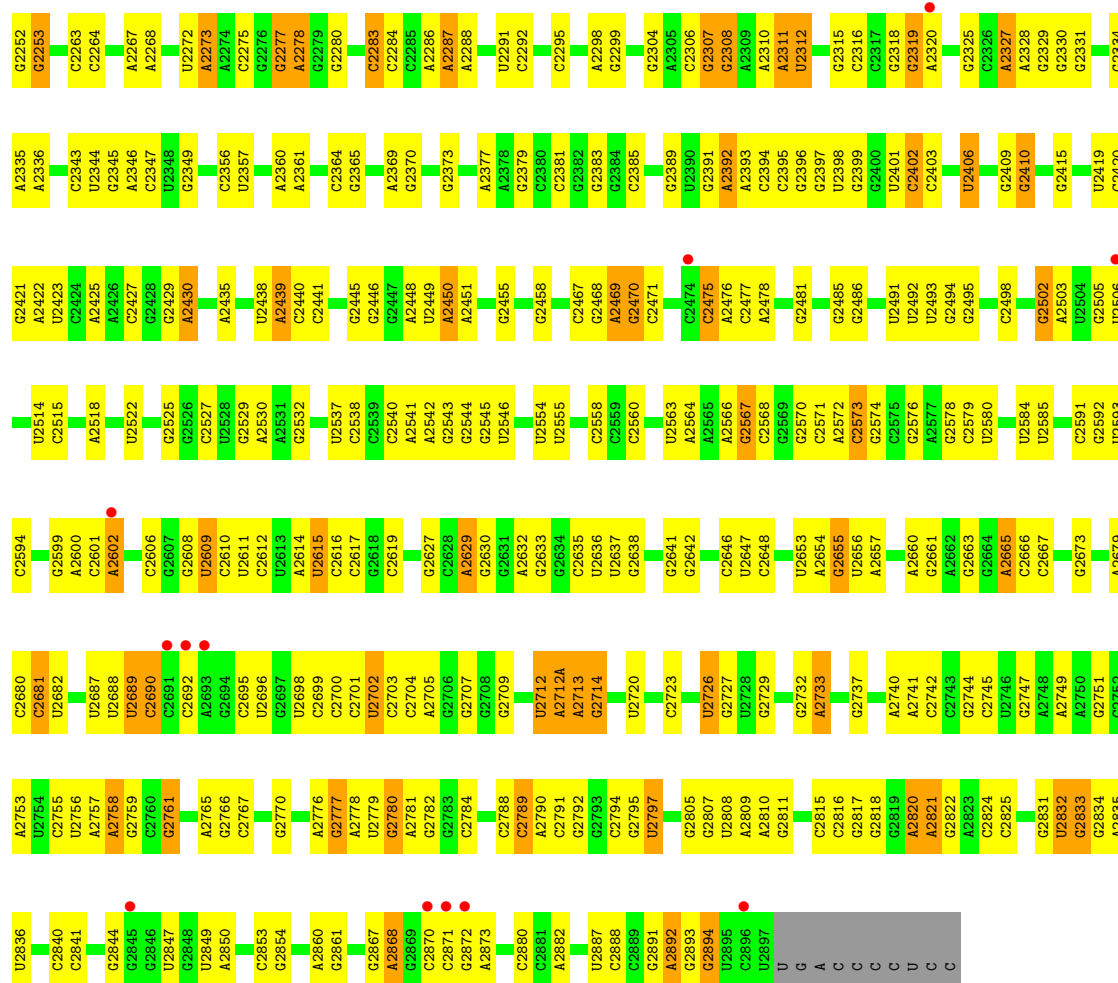




● Molecule 25: 23S rRNA



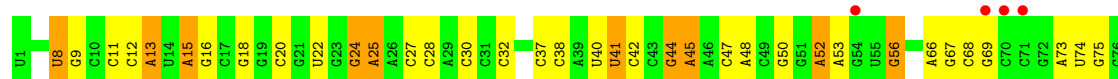
G2165	U2099	C1996	C1902	C1800	G1594	G1512	G1424	A1331	G1236	U1142	G1084
G2166	G2100	C1999	G1903	G1801	G1595	C1513	G1425	G1332	A1237	A1142A	U1065
U2167	U2101	C2008	G1906	A1802	A1596	U1514	G1426	G1338	G1238	A1143	U1066
A2169	C2103	G2009	G1913	A1804	C1598	C1515	A1427	G1339	A1238	G1149	A1067
A2170	G2104	G2010	A1914	C1805	C1605	G1519	G1428	U1340	A1247	C1150	A1068
A2171	C2105	U2011	G1915	U1812	G1606	U1520	G1429	U1341	G1248	G1151	A1070
U2172	G2106	U2012	U1916	G1813	C1607	G1521	A1434	A1342	U1249	C1152	G1071
C2174	C2111	G2013	A1917	A1814	A1608	G1522	G1434	G1343	C1250	G1153	C1076
C2175	G2112	A2014	A1815	G1726	A1609	U1523	G1442	G1344	C1251	G1154	A1077
A2176	U2113	A2015	G1816	A1610	A1610	G1524	G1443	C1345	A1252	A1155	U1078
C2177	A2114	U2016	G1817	C1817	G1728	C1532	G1444	G1348	A1253	A1156	C1079
C2178	G2115	C1920	U1818	U1818	A1729	C1533	A1444A	A1349	G1256	C1161	C1080
C2179	G2116	A2020	A1819	A1819	A1730	G1534	G1445	C1257	C1257	G1162	U1081
G2180	A2117	G1929	G1930	U1820	G1731	U1535	G1448	U1352	C1258	U1082	U1082
G2181	U2118	U2022	U1931	A1834	A1618	C1537	G1449	A1353	U1165	U1083	A1084
A2188	A2120	G2023	G1826	G1826	G1733	G1538	G1450	A1354	U1167	A1085	A1085
U2189	G2121	G2029	A1829	A1829	G1742	G1539	U1454	U1357	G1168	A1086	A1086
G2190	U2122	A2030	C1934	C1934	G1743	G1540	G1455	A1360	G1169	U1087	U1087
G2191	G2123	G2031	U1833	U1833	A1749	A1543	G1456	G1364	G1173	A1088	A1088
G2192	G2124	G2032	U1834	G1835	A1755	A1544	G1459	A1365	U1175	A1089	A1089
G2193	G2125	A2033	G1835	G1835	G1754	A1545	A1460	G1368	A1177	U1090	U1090
G2194	A2126	G2037	C1838	C1838	A1755	C1548	G1461	G1368	G1176	G1093	G1093
A2198	G2127	G2037	C1838	C1838	A1755	C1548	G1461	G1368	G1176	U1094	U1094
C2207	G2128	A2042	G1843	C1843	G1756	C1549	G1467	A1379	C1180	A1095	A1095
U2208	G2131	C2043	C1844	C1844	U1757	C1549	C1467	A1379	C1180	U1096	U1096
C2209	U2132	G2051	G1845	G1845	G1759	A1553	A1468	A1384	G1184	U1103	U1103
G2210	G2133	A2051	G1846	G1846	A1760	A1554	A1469	G1385	C1185	U1104	U1104
G2211	C2136	G2052	A1853	A1853	C1761	G1555	A1471	G1389	G1186	G1106	G1106
A2212	U2137	C2053	A1853	A1853	A1762	A1558	A1471	G1389	G1187	G1107	G1107
U2213	C2138	A2054	G1856	G1856	G1763	G1559	C1474	U1392	U1188	U1108	U1108
G2215	C2139	G2056	G1859	G1859	G1764	G1560	C1474	U1392	U1188	C1109	C1109
C2140	C2140	C2056	A1859	A1859	G1771	G1566	C1474	U1394	G1195	A1111	A1111
G2141	G2141	A2059	U1864	U1864	G1772	A1566	G1478	A1393	G1296	G1112	G1112
C2142	C2142	A2060	G1869	G1869	A1773	A1567	G1479	U1394	G1296	U1113	U1113
U2144	U2144	G2061	G1869	G1869	C1778	G1567	G1480	A1395	G1301	G1114	G1114
C2226	C2226	A2062	C1870	C1870	U1778	A1569	U1482	A1395	G1301	C1201	C1201
A2227	G2145	C2063	A1871	A1871	U1779	A1569	G1483	A1395	G1301	G1122	G1122
C2146	G2146	G2064	A1872	A1872	U1780	A1570	G1484	C1398	A1301	G1125	G1125
G2147	C2147	C2065	A1884	A1884	G1781	A1570	G1485	C1398	A1301	A1128	A1128
G2148	G2148	G2066	A1885	A1885	C1782	G1581	A1495	C1403	G1309	U1130	U1130
U2149	U2149	G2067	A1886	A1886	C1783	U1576	A1496	C1403	G1309	G1131	G1131
U2150	U2150	U2068	C1887	C1887	A1784	U1577	A1496	C1403	G1309	C1135	C1135
G2151	G2151	G2069	G1888	G1888	A1785	U1578	A1496	C1403	G1309	G1137	G1137
G2152	G2152	C2073	A1889	A1889	U1679	A1579	A1496	C1403	G1309	G1138	G1138
G2153	G2153	C2073	A1890	A1890	U1680	A1580	A1496	C1403	G1309	G1139	G1139
G2154	G2154	C2078	A1891	A1891	C1683	G1581	A1496	C1403	G1309	C1140	C1140
G2155	G2155	U2079	C1887	C1887	C1684	U1585	A1496	C1403	G1309	U1141	U1141
G2156	G2156	U2079	G1888	G1888	C1684	A1586	A1496	C1403	G1309	G1216	G1216
U2243	U2243	U2086	A1892	A1892	C1685	A1587	A1496	C1403	G1309	C1217	C1217
U2244	U2244	G2087	A1893	A1893	C1686	A1587	A1496	C1403	G1309	G1218	G1218
U2245	U2245	G2088	A1894	A1894	C1687	U1590	A1496	C1403	G1309	G1219	G1219
G2246	G2246	C2097	C1894	C1894	A1690	C1591	A1496	C1403	G1309	C1220	C1220
G2250	G2250	U2098	C1895	C1895	U1797	U1592	A1496	C1403	G1309	U1141	U1141
G2251	G2251	U2098	G1899	G1899	U1799	G1593	A1496	C1403	G1309	U1141	U1141



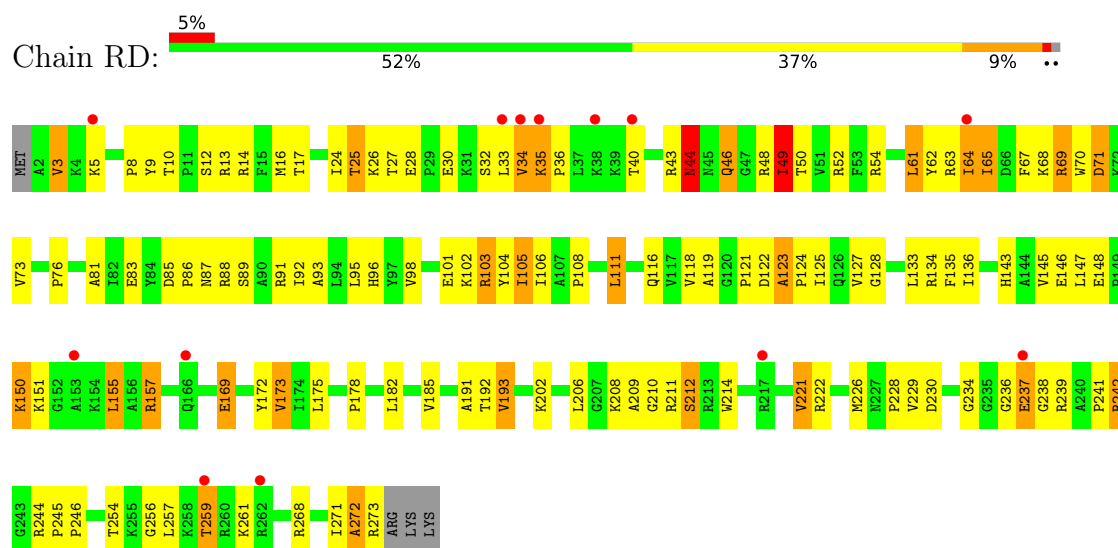
• Molecule 26: 5S rRNA

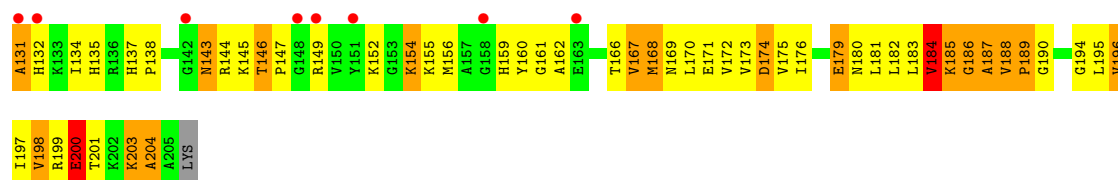


• Molecule 26: 5S rRNA

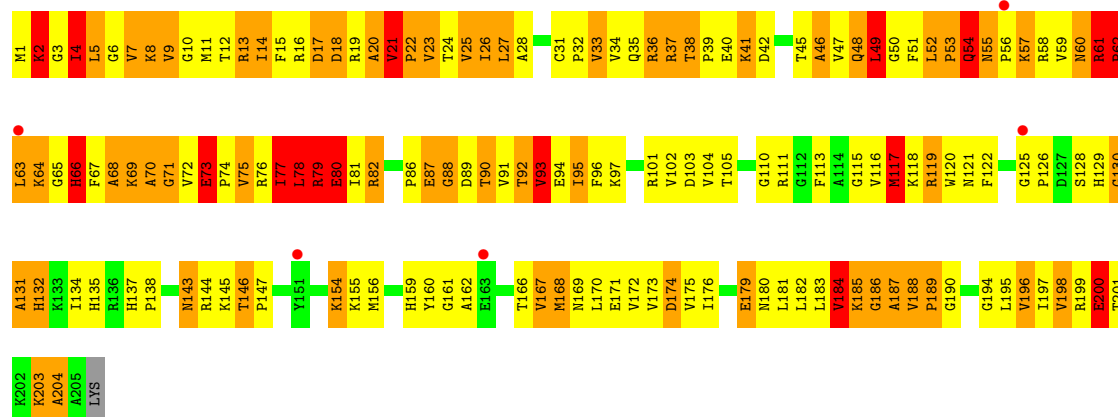
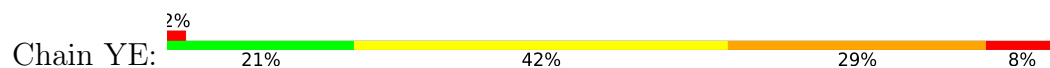


- Molecule 27: 50S ribosomal protein L2

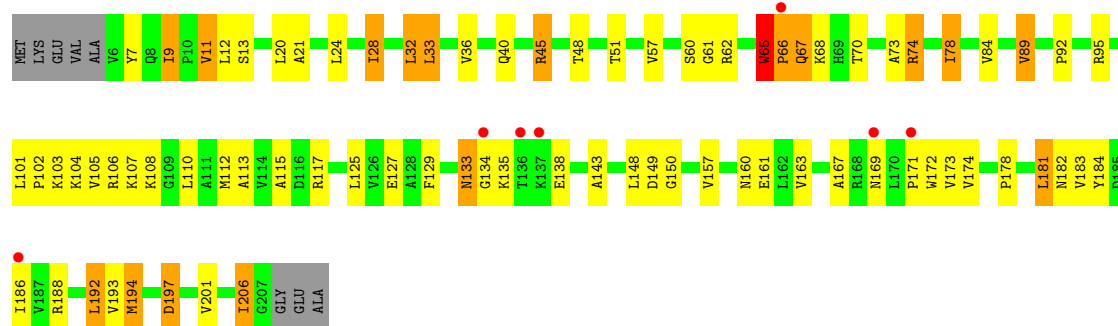




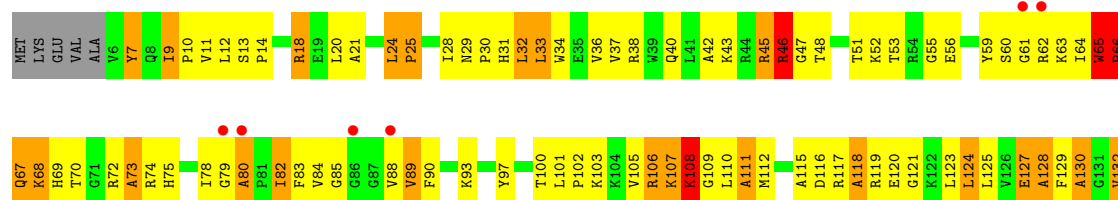
• Molecule 28: 50S ribosomal protein L3

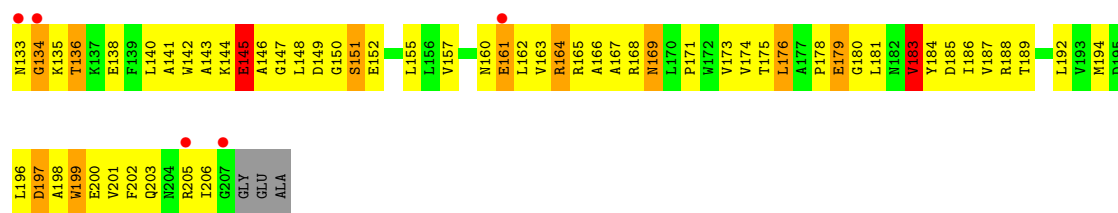


• Molecule 29: 50S ribosomal protein L4

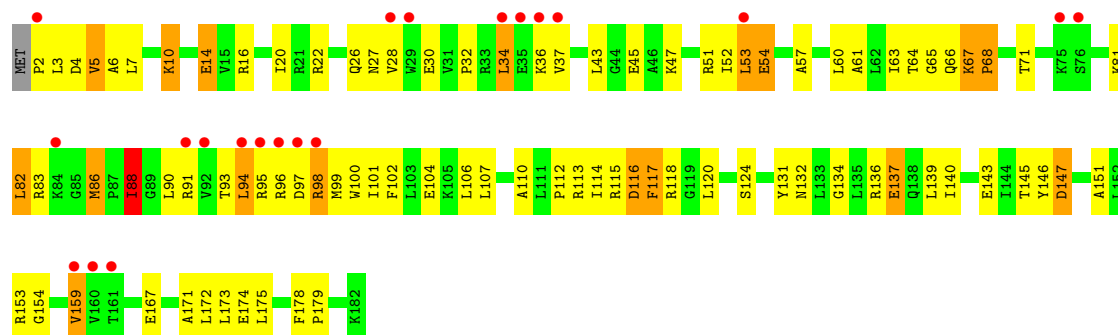


• Molecule 29: 50S ribosomal protein L4

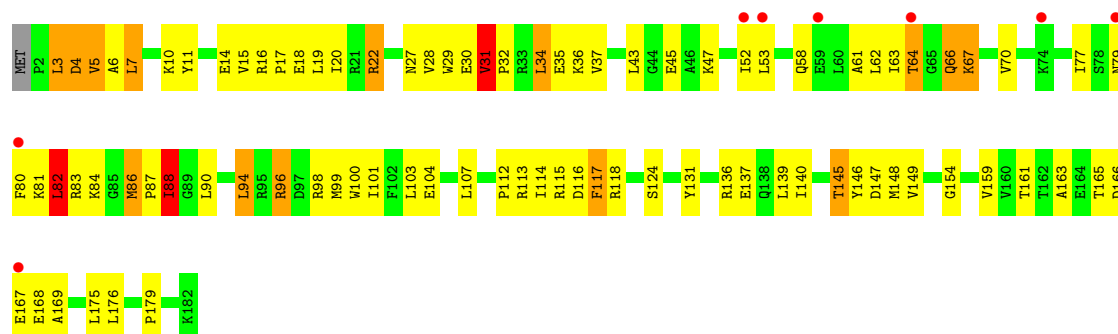




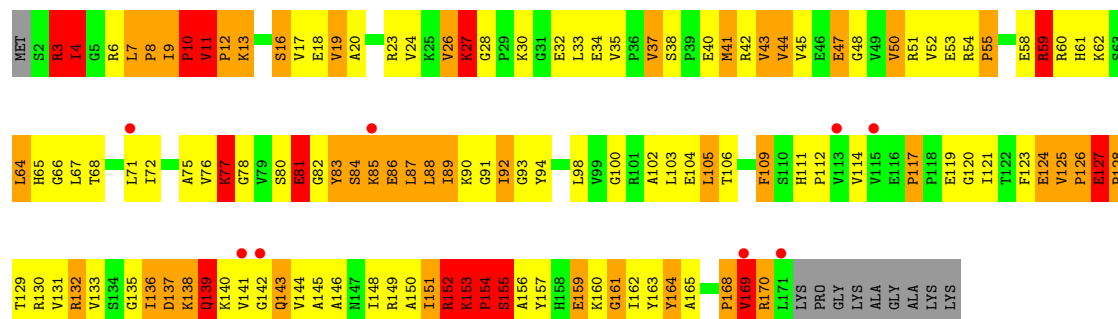
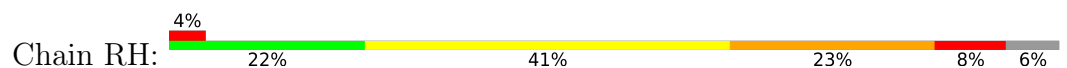
● Molecule 30: 50S ribosomal protein L5



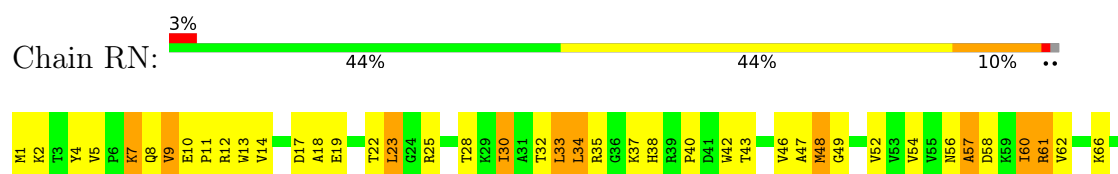
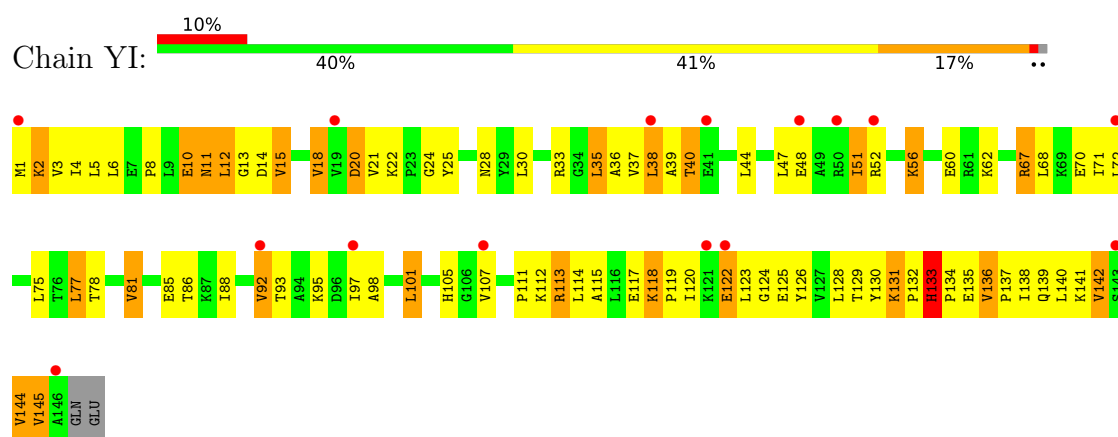
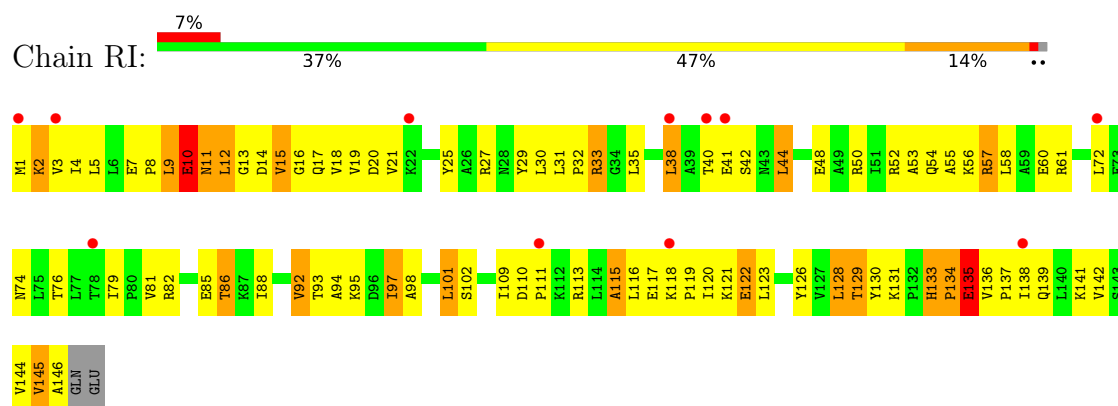
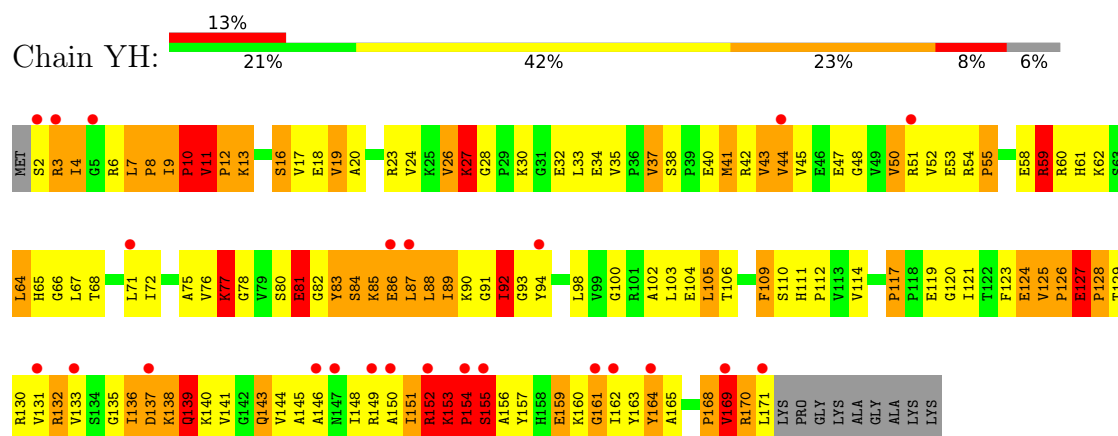
● Molecule 30: 50S ribosomal protein L5



● Molecule 31: 50S ribosomal protein L6

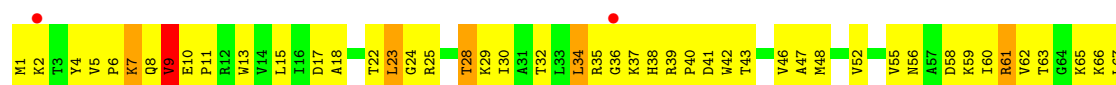


- Molecule 31: 50S ribosomal protein L6

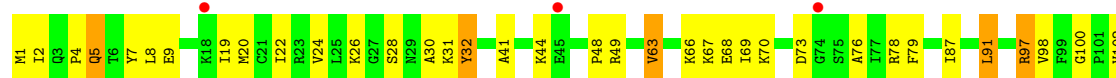




• Molecule 33: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L14



• Molecule 34: 50S ribosomal protein L14

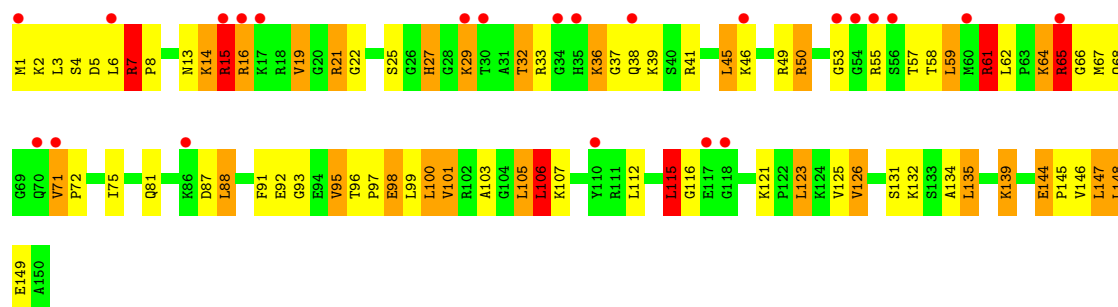


• Molecule 35: 50S ribosomal protein L15

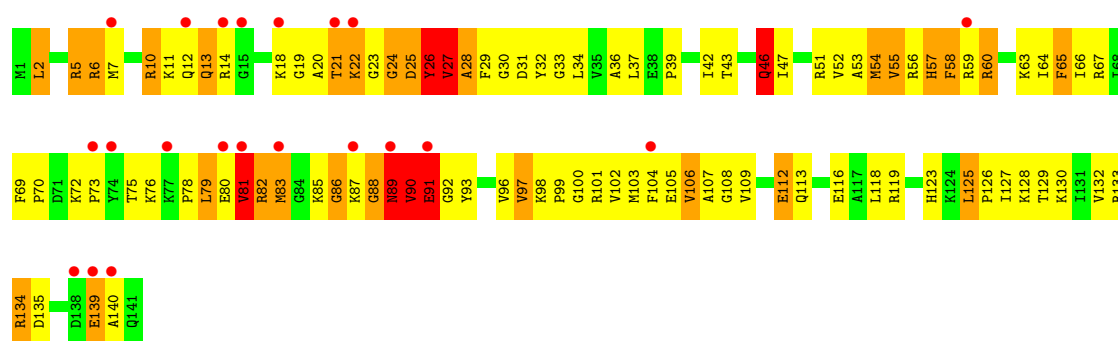


• Molecule 35: 50S ribosomal protein L15

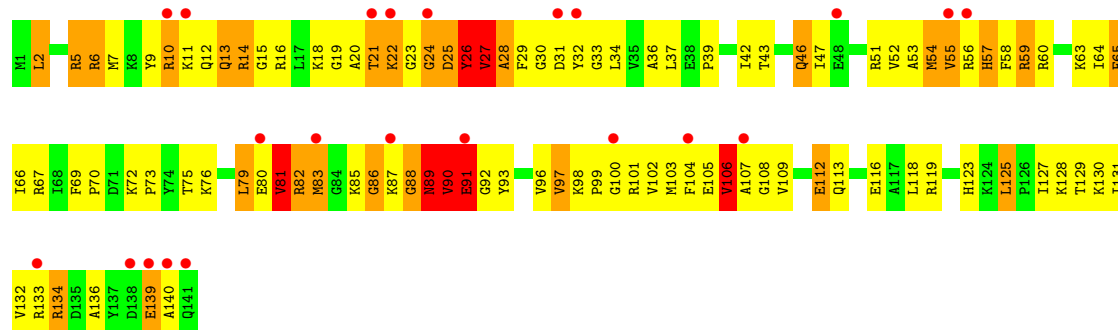




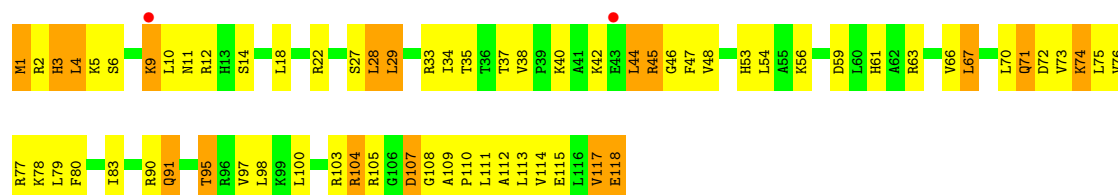
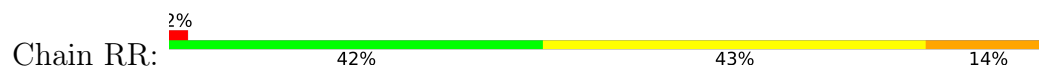
- Molecule 36: 50S ribosomal protein L16



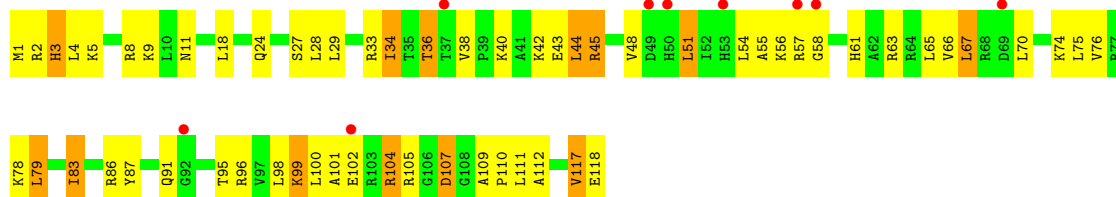
- Molecule 36: 50S ribosomal protein L16



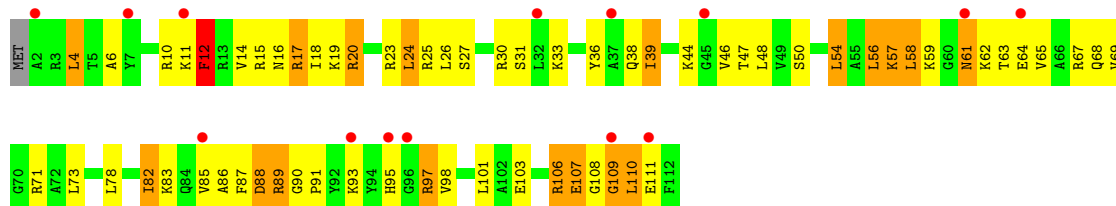
- Molecule 37: 50S ribosomal protein L17



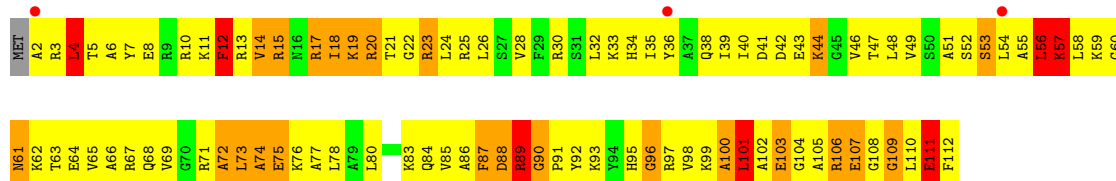
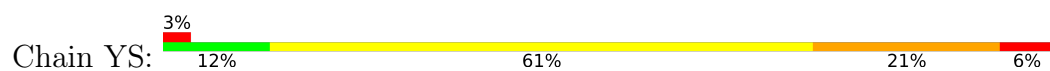
- Molecule 37: 50S ribosomal protein L17



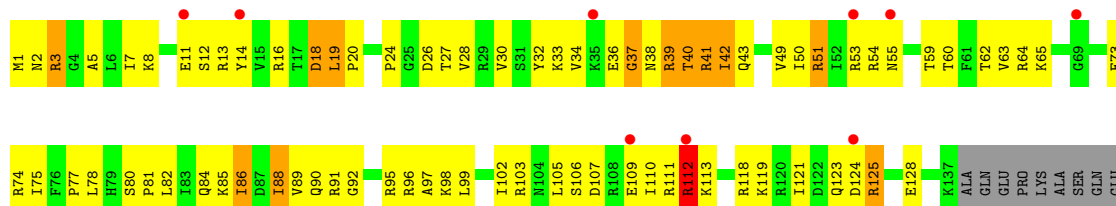
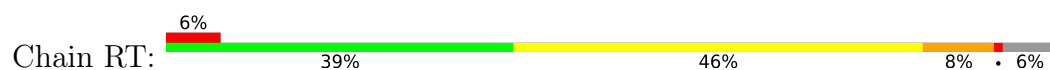
• Molecule 38: 50S ribosomal protein L18



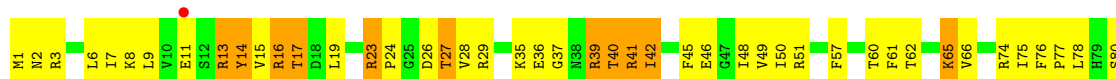
• Molecule 38: 50S ribosomal protein L18



• Molecule 39: 50S ribosomal protein L19

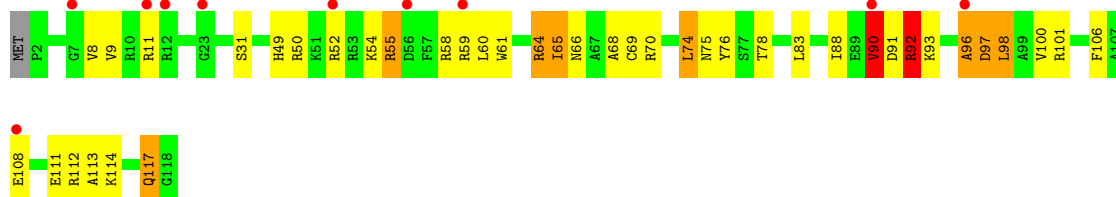


• Molecule 39: 50S ribosomal protein L19

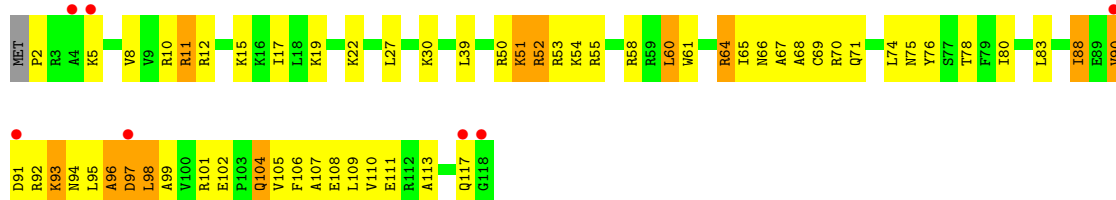




- Molecule 40: 50S ribosomal protein L20



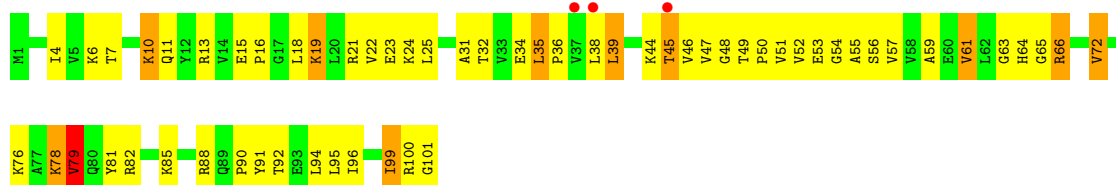
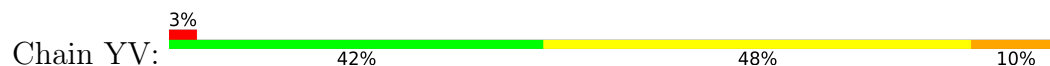
- Molecule 40: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L21

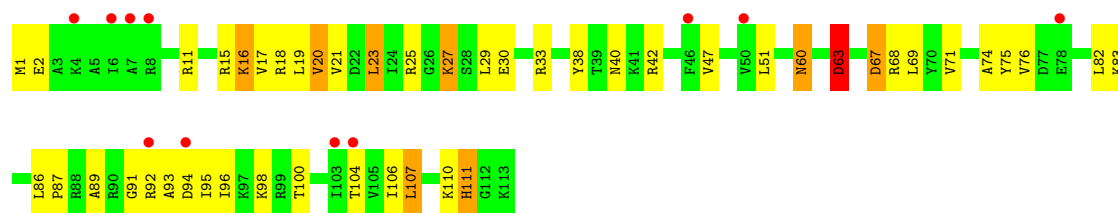


- Molecule 41: 50S ribosomal protein L21

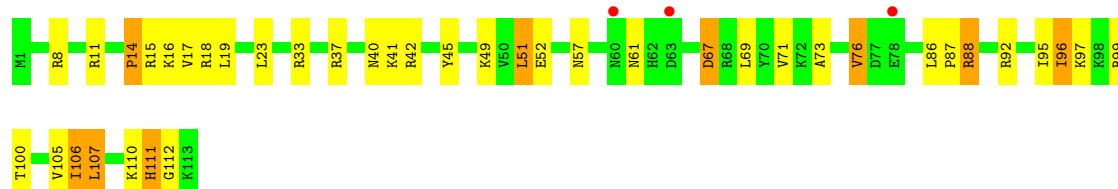


- Molecule 42: 50S ribosomal protein L22

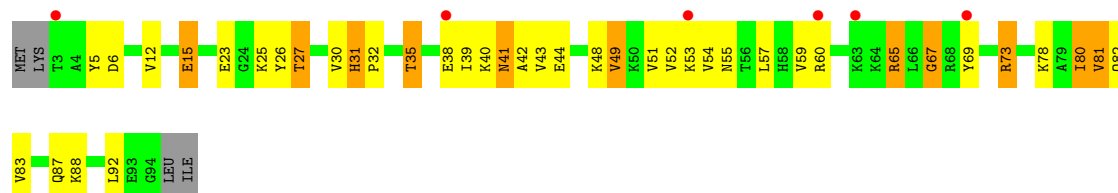




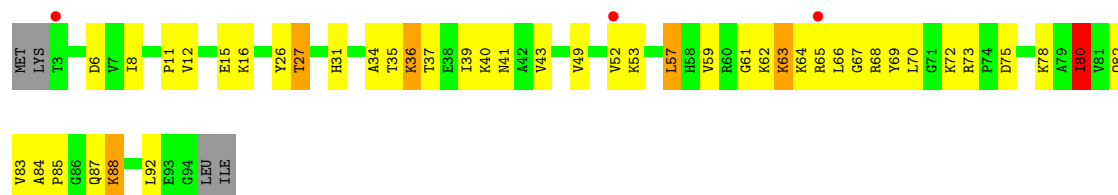
• Molecule 42: 50S ribosomal protein L22



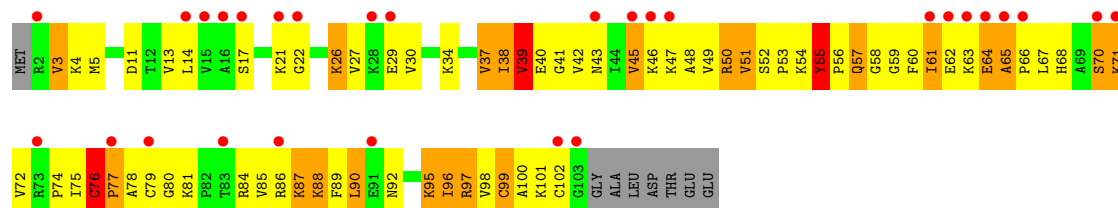
• Molecule 43: 50S ribosomal protein L23



• Molecule 43: 50S ribosomal protein L23

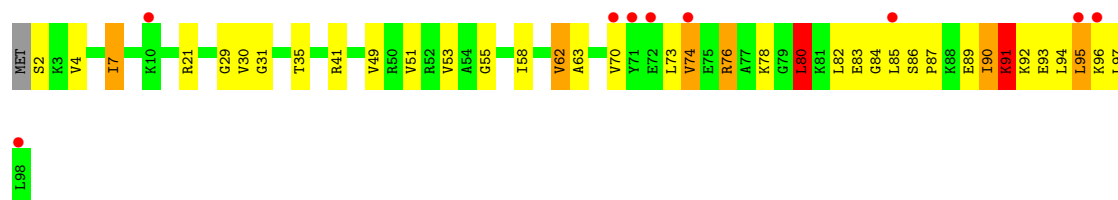


• Molecule 44: 50S ribosomal protein L24

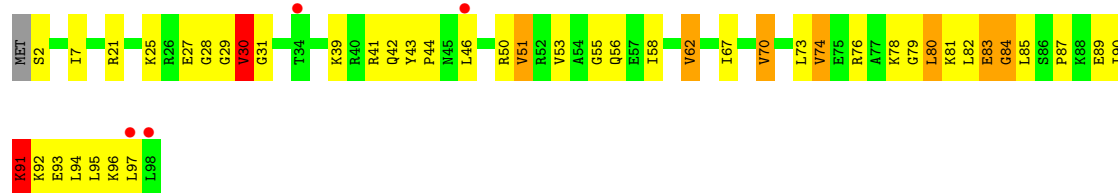




• Molecule 47: 50S ribosomal protein L28



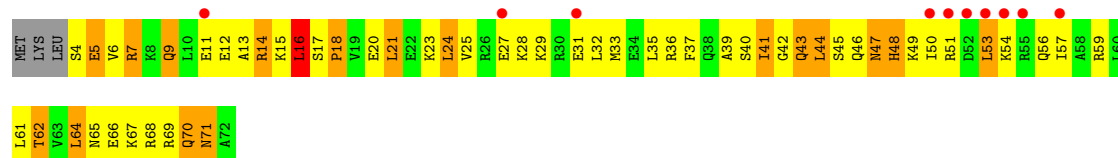
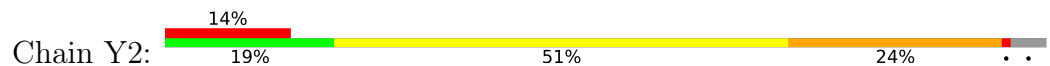
• Molecule 47: 50S ribosomal protein L28



• Molecule 48: 50S ribosomal protein L29

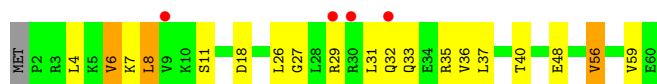


• Molecule 48: 50S ribosomal protein L29

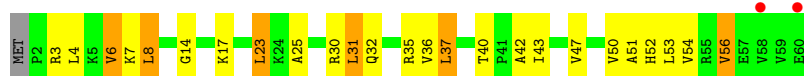


• Molecule 49: 50S ribosomal protein L30





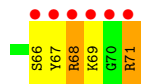
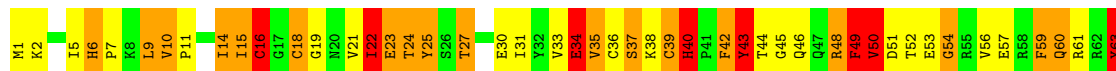
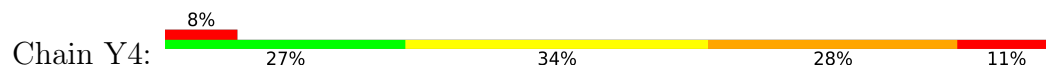
- Molecule 49: 50S ribosomal protein L30



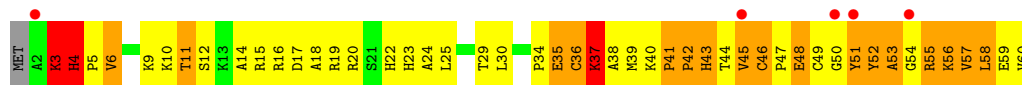
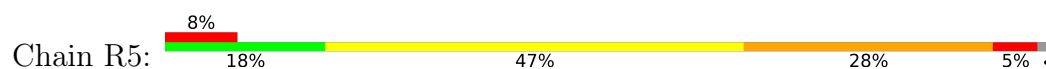
- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31



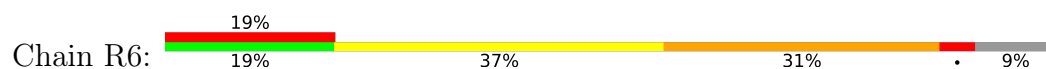
- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32

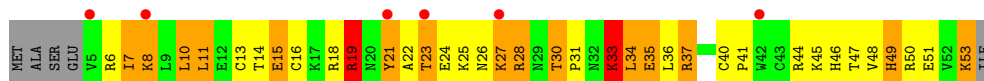
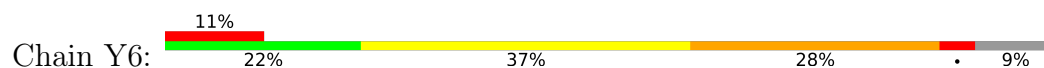


- Molecule 52: 50S ribosomal protein L33





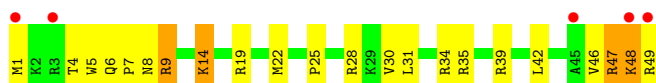
- Molecule 52: 50S ribosomal protein L33



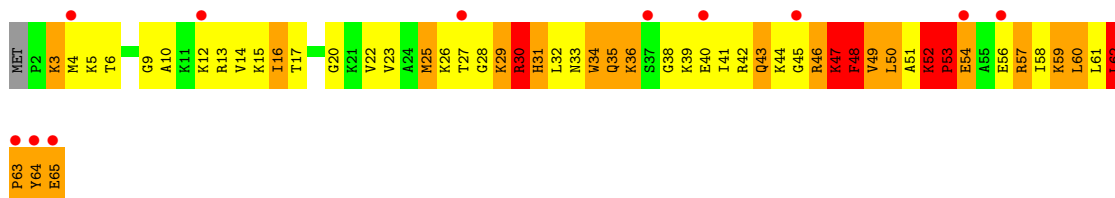
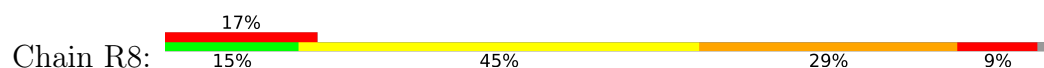
- Molecule 53: 50S ribosomal protein L34



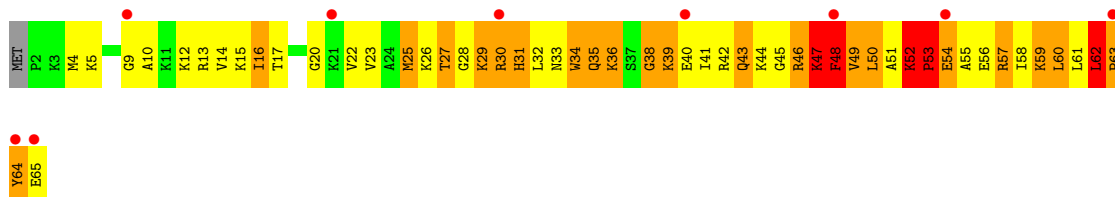
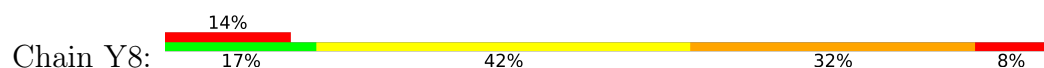
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35

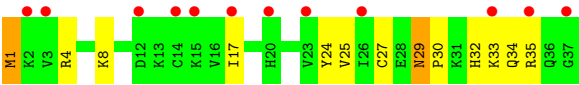


- Molecule 54: 50S ribosomal protein L35

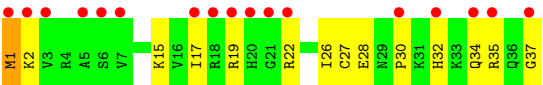


- Molecule 55: 50S ribosomal protein L36





● 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	209.35Å 450.71Å 622.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 3.60 49.51 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.51-3.60) 99.2 (49.51-3.60)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.214 , 0.253 0.215 , 0.252	Depositor DCC
R_{free} test set	35437 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	96.4	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 99.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	292042	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.16	0/36098	0.34	0/56341
1	XA	0.17	0/36101	0.36	0/56346
2	QB	0.40	0/1959	0.87	4/2642 (0.2%)
2	XB	0.40	0/1959	0.89	4/2642 (0.2%)
3	QC	0.44	0/1629	0.87	0/2195
3	XC	0.48	0/1629	0.86	0/2195
4	QD	0.34	0/1733	0.81	4/2318 (0.2%)
4	XD	0.51	0/1733	0.96	5/2318 (0.2%)
5	QE	0.50	1/1171 (0.1%)	0.97	5/1576 (0.3%)
5	XE	0.54	0/1171	1.13	5/1576 (0.3%)
6	QF	0.46	0/856	0.80	0/1154
6	XF	0.51	0/856	0.87	0/1154
7	QG	0.43	0/1276	0.84	0/1709
7	XG	0.46	0/1276	0.88	2/1709 (0.1%)
8	QH	0.44	0/1136	0.93	4/1527 (0.3%)
8	XH	0.47	0/1136	0.92	4/1527 (0.3%)
9	QI	0.41	0/1029	0.90	1/1379 (0.1%)
9	XI	0.43	0/1029	0.89	2/1379 (0.1%)
10	QJ	0.56	1/814 (0.1%)	1.01	6/1095 (0.5%)
10	XJ	0.52	2/814 (0.2%)	1.03	6/1095 (0.5%)
11	QK	0.50	0/900	0.94	3/1213 (0.2%)
11	XK	0.52	0/900	0.94	0/1213
12	QL	0.59	1/991 (0.1%)	1.23	10/1327 (0.8%)
12	XL	0.59	0/991	1.26	12/1327 (0.9%)
13	QM	0.42	0/974	0.97	0/1303
13	XM	0.47	0/974	0.97	1/1303 (0.1%)
14	QN	0.49	0/501	0.95	1/664 (0.2%)
14	XN	0.57	0/501	1.04	3/664 (0.5%)
15	QO	0.45	0/745	0.80	0/992
15	XO	0.50	0/745	0.89	0/992
16	QP	0.48	0/721	0.94	2/970 (0.2%)
16	XP	0.47	0/721	0.88	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.42	0/847	0.85	0/1131
17	XQ	0.43	0/847	0.83	0/1131
18	QR	0.44	0/579	0.89	0/768
18	XR	0.47	0/579	0.85	1/768 (0.1%)
19	QS	0.45	0/689	0.99	3/926 (0.3%)
19	XS	0.48	0/689	1.01	6/926 (0.6%)
20	QT	0.46	0/765	0.95	2/1007 (0.2%)
20	XT	0.45	0/765	0.98	2/1007 (0.2%)
21	QU	0.38	0/221	0.79	0/288
21	XU	0.37	0/221	0.82	0/288
22	QV	0.16	0/1836	0.32	0/2859
22	XV	0.19	0/1836	0.36	0/2859
23	QX	0.22	0/246	0.32	0/381
23	XX	0.33	0/238	0.58	0/369
24	QY	0.26	0/355	0.33	0/551
24	XY	0.25	0/355	0.44	0/551
25	RA	0.20	0/69518	0.38	2/108523 (0.0%)
25	YA	0.23	0/69520	0.43	10/108527 (0.0%)
26	RB	0.18	0/2878	0.36	0/4490
26	YB	0.21	0/2878	0.40	0/4490
27	RD	0.64	0/2165	1.07	8/2919 (0.3%)
27	YD	0.72	0/2165	1.29	33/2919 (1.1%)
28	RE	0.62	0/1601	1.35	29/2160 (1.3%)
28	YE	0.62	0/1601	1.35	29/2160 (1.3%)
29	RF	0.38	0/1620	0.84	2/2194 (0.1%)
29	YF	0.62	0/1620	1.20	19/2194 (0.9%)
30	RG	0.41	0/1499	0.91	0/2016
30	YG	0.51	0/1499	0.91	2/2016 (0.1%)
31	RH	0.57	0/1332	1.22	14/1802 (0.8%)
31	YH	0.57	0/1332	1.21	14/1802 (0.8%)
32	RI	0.40	0/1151	0.91	2/1558 (0.1%)
32	YI	0.41	0/1151	0.88	3/1558 (0.2%)
33	RN	0.52	0/1131	1.01	2/1525 (0.1%)
33	YN	0.55	0/1131	0.95	1/1525 (0.1%)
34	RO	0.55	0/943	0.98	3/1269 (0.2%)
34	YO	0.60	0/943	0.97	0/1269
35	RP	0.40	0/1162	0.90	2/1544 (0.1%)
35	YP	0.44	0/1158	0.96	2/1535 (0.1%)
36	RQ	0.71	0/1143	1.36	19/1527 (1.2%)
36	YQ	0.71	0/1143	1.35	19/1527 (1.2%)
37	RR	0.55	0/982	0.99	1/1312 (0.1%)
37	YR	0.57	0/982	1.04	3/1312 (0.2%)
38	RS	0.43	0/892	0.88	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.53	0/892	1.14	7/1187 (0.6%)
39	RT	0.53	0/1155	0.98	3/1542 (0.2%)
39	YT	0.56	0/1155	1.05	7/1542 (0.5%)
40	RU	0.54	0/982	1.04	6/1306 (0.5%)
40	YU	0.65	0/982	1.07	2/1306 (0.2%)
41	RV	0.47	0/790	0.97	4/1057 (0.4%)
41	YV	0.58	0/790	1.01	2/1057 (0.2%)
42	RW	0.65	0/911	0.98	1/1220 (0.1%)
42	YW	0.60	0/911	1.00	0/1220
43	RX	0.59	0/739	0.96	4/993 (0.4%)
43	YX	0.60	0/739	1.00	1/993 (0.1%)
44	RY	0.54	0/798	1.07	6/1064 (0.6%)
44	YY	0.59	0/798	1.09	5/1064 (0.5%)
45	RZ	0.37	0/1493	0.88	7/2026 (0.3%)
45	YZ	0.38	0/1493	0.93	4/2026 (0.2%)
46	R0	0.56	0/657	1.04	5/874 (0.6%)
46	Y0	0.60	0/657	0.98	1/874 (0.1%)
47	R1	0.56	0/770	0.97	0/1022
47	Y1	0.59	0/770	0.96	1/1022 (0.1%)
48	R2	0.47	0/583	1.00	2/771 (0.3%)
48	Y2	0.60	0/583	1.32	8/771 (1.0%)
49	R3	0.47	0/474	0.91	2/635 (0.3%)
49	Y3	0.53	0/474	0.86	0/635
50	R4	0.47	0/594	1.24	10/795 (1.3%)
50	Y4	0.48	0/594	1.16	6/795 (0.8%)
51	R5	0.64	0/473	1.24	5/639 (0.8%)
51	Y5	0.68	0/468	1.15	4/632 (0.6%)
52	R6	0.53	0/431	1.01	2/575 (0.3%)
52	Y6	0.56	0/431	1.00	2/575 (0.3%)
53	R7	0.62	0/438	1.05	2/575 (0.3%)
53	Y7	0.69	0/438	1.02	3/575 (0.5%)
54	R8	0.79	0/525	1.40	9/691 (1.3%)
54	Y8	0.79	0/525	1.40	9/691 (1.3%)
55	R9	0.35	0/310	0.81	0/407
55	Y9	0.46	0/310	0.80	0/407
56	Z5	0.45	0/40	0.62	0/60
56	Z6	0.45	0/40	0.62	0/60
All	All	0.33	5/316490 (0.0%)	0.62	448/473169 (0.1%)

All (5) bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	QJ	59	SER	C-N	-8.53	1.26	1.33
12	QL	48	PRO	N-CD	5.49	1.55	1.47
5	QE	70	PRO	N-CD	5.41	1.55	1.47
10	XJ	53	PRO	N-CD	5.36	1.55	1.47
10	XJ	52	GLY	C-N	5.05	1.40	1.34

The worst 5 of 448 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	1884	A	P-O3'-C3'	17.39	146.28	120.20
5	XE	69	VAL	O-C-N	17.36	140.88	121.10
50	R4	39	CYS	N-CA-C	-13.59	95.96	112.54
5	XE	69	VAL	CA-C-N	-12.70	103.97	119.84
5	XE	69	VAL	C-N-CA	-12.70	103.97	119.84

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	461	0
1	XA	32249	0	16278	468	0
2	QB	1924	0	1975	65	0
2	XB	1924	0	1975	89	0
3	QC	1605	0	1668	51	0
3	XC	1605	0	1668	61	0
4	QD	1703	0	1764	61	0
4	XD	1703	0	1764	54	0
5	QE	1155	0	1213	69	0
5	XE	1155	0	1213	79	0
6	QF	843	0	857	21	0
6	XF	843	0	857	22	0
7	QG	1257	0	1296	36	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	20	0
8	QH	1116	0	1175	36	0
8	XH	1116	0	1177	29	0
9	QI	1010	0	1037	36	0
9	XI	1010	0	1037	50	0
10	QJ	801	0	849	67	0
10	XJ	801	0	849	60	0
11	QK	885	0	904	28	0
11	XK	885	0	904	27	0
12	QL	975	0	1062	102	0
12	XL	975	0	1062	106	0
13	QM	964	0	1034	71	0
13	XM	964	0	1034	47	0
14	QN	492	0	529	23	0
14	XN	492	0	529	18	0
15	QO	734	0	771	21	0
15	XO	734	0	771	17	0
16	QP	705	0	725	15	0
16	XP	705	0	725	23	0
17	QQ	834	0	904	19	0
17	XQ	834	0	904	19	0
18	QR	574	0	644	11	0
18	XR	574	0	644	21	0
19	QS	674	0	699	55	0
19	XS	674	0	699	43	0
20	QT	763	0	860	40	0
20	XT	763	0	861	65	0
21	QU	217	0	234	9	0
21	XU	217	0	234	4	0
22	QV	1644	0	836	20	0
22	XV	1644	0	836	15	0
23	QX	220	0	109	1	0
23	XX	214	0	111	2	0
24	QY	319	0	162	2	0
24	XY	319	0	162	5	0
25	RA	62069	0	31285	901	0
25	YA	62070	0	31285	985	0
26	RB	2573	0	1306	41	0
26	YB	2573	0	1306	49	0
27	RD	2115	0	2195	99	0
27	YD	2115	0	2195	345	0
28	RE	1568	0	1634	309	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	306	0
29	RF	1585	0	1632	57	0
29	YF	1585	0	1632	199	0
30	RG	1474	0	1535	106	0
30	YG	1474	0	1535	62	0
31	RH	1307	0	1382	237	0
31	YH	1307	0	1382	245	0
32	RI	1136	0	1223	71	0
32	YI	1136	0	1223	52	0
33	RN	1104	0	1180	51	0
33	YN	1104	0	1180	57	0
34	RO	933	0	996	27	0
34	YO	933	0	996	29	0
35	RP	1145	0	1227	72	0
35	YP	1143	0	1224	85	0
36	RQ	1122	0	1179	173	0
36	YQ	1122	0	1179	187	0
37	RR	968	0	1033	52	0
37	YR	968	0	1033	37	0
38	RS	882	0	943	54	0
38	YS	882	0	943	172	0
39	RT	1141	0	1202	77	0
39	YT	1141	0	1202	56	0
40	RU	964	0	1022	28	0
40	YU	964	0	1022	62	0
41	RV	779	0	852	21	0
41	YV	779	0	852	47	0
42	RW	900	0	964	27	0
42	YW	900	0	964	25	0
43	RX	725	0	778	29	0
43	YX	725	0	778	23	0
44	RY	785	0	878	52	0
44	YY	785	0	878	47	0
45	RZ	1461	0	1493	48	0
45	YZ	1461	0	1493	65	0
46	R0	648	0	672	30	0
46	Y0	648	0	672	39	0
47	R1	763	0	848	27	0
47	Y1	763	0	848	36	0
48	R2	581	0	629	18	0
48	Y2	581	0	629	79	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	18	0
50	R4	581	0	575	194	0
50	Y4	581	0	577	56	0
51	R5	459	0	480	76	0
51	Y5	454	0	475	39	0
52	R6	424	0	450	28	0
52	Y6	424	0	450	33	0
53	R7	430	0	480	22	0
53	Y7	430	0	480	21	0
54	R8	517	0	582	119	0
54	Y8	517	0	582	122	0
55	R9	307	0	338	10	0
55	Y9	307	0	338	12	0
56	Z5	74	0	51	12	0
56	Z6	74	0	51	10	0
57	QA	86	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	2	0	0	0	0
57	QN	1	0	0	0	0
57	QV	2	0	0	0	0
57	QX	2	0	0	0	0
57	R0	1	0	0	0	0
57	R3	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	247	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	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	101	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	XY	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y5	1	0	0	0	0
57	YA	277	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	YE	2	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	1	0	0	0	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
All	All	292042	0	198293	8021	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 8021 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
30:RG:67:LYS:HE2	50:R4:6:HIS:CE1	1.69	1.26
51:Y5:49:CYS:SG	51:Y5:60:VAL:HG12	1.75	1.26
19:QS:5:LEU:CD2	50:R4:67:TYR:CZ	2.18	1.26

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	10
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1	12
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	3	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	XC	203/239 (85%)	172 (85%)	28 (14%)	3 (2%)	8	37
4	QD	206/209 (99%)	186 (90%)	17 (8%)	3 (2%)	8	37
4	XD	206/209 (99%)	176 (85%)	25 (12%)	5 (2%)	4	29
5	QE	149/162 (92%)	137 (92%)	8 (5%)	4 (3%)	4	27
5	XE	149/162 (92%)	134 (90%)	13 (9%)	2 (1%)	9	39
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%)	9	39
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	9	39
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	18	51
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	3	26
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	2	20
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	3	24
10	QJ	97/105 (92%)	77 (79%)	16 (16%)	4 (4%)	2	19
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	1	15
11	QK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	7	35
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	7	35
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	4
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	4
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	9
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	9
14	QN	58/61 (95%)	50 (86%)	4 (7%)	4 (7%)	1	11
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	5
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	41
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	30
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	10	41
16	XP	82/88 (93%)	72 (88%)	9 (11%)	1 (1%)	10	41
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	6	32
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	18
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	8	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	3
19	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	3
20	QT	97/106 (92%)	77 (79%)	14 (14%)	6 (6%)	1	12
20	XT	97/106 (92%)	77 (79%)	16 (16%)	4 (4%)	2	19
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	18
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	18
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	18
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	10
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%)	181 (90%)	13 (6%)	6 (3%)	3	25
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	5
30	RG	179/182 (98%)	139 (78%)	25 (14%)	15 (8%)	0	7
30	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	11
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	0
31	YH	168/180 (93%)	94 (56%)	37 (22%)	37 (22%)	0	0
32	RI	144/148 (97%)	109 (76%)	24 (17%)	11 (8%)	1	9
32	YI	144/148 (97%)	107 (74%)	23 (16%)	14 (10%)	0	6
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	0	7
33	YN	136/140 (97%)	107 (79%)	16 (12%)	13 (10%)	0	6
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	7	35
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	7	35
35	RP	148/150 (99%)	109 (74%)	26 (18%)	13 (9%)	0	7
35	YP	146/150 (97%)	100 (68%)	35 (24%)	11 (8%)	1	9
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	5
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	5
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	18
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	1	15
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	5
38	YS	109/112 (97%)	62 (57%)	29 (27%)	18 (16%)	0	2
39	RT	135/146 (92%)	107 (79%)	16 (12%)	12 (9%)	0	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	9
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	23
40	YU	115/118 (98%)	101 (88%)	12 (10%)	2 (2%)	7	35
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	13
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	8
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	2	22
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	6	34
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	5	30
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	5	30
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	2
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	4
45	RZ	181/206 (88%)	127 (70%)	34 (19%)	20 (11%)	0	5
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	0	6
46	R0	80/85 (94%)	66 (82%)	13 (16%)	1 (1%)	9	39
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	6
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	12
48	R2	67/72 (93%)	54 (81%)	9 (13%)	4 (6%)	1	13
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	3
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	23
49	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	6	34
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%)	10 (18%)	14 (25%)	0	0
51	Y5	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	2	22
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%)	5	31
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	5	31
54	R8	62/65 (95%)	36 (58%)	14 (23%)	12 (19%)	0	1
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	11467/12128 (94%)	9027 (79%)	1609 (14%)	831 (7%)	1	10

5 of 831 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	33	MET
12	QL	18	VAL

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%)	170 (83%)	35 (17%)	2	13
2	XB	205/220 (93%)	180 (88%)	25 (12%)	5	23
3	QC	159/188 (85%)	146 (92%)	13 (8%)	10	36
3	XC	159/188 (85%)	145 (91%)	14 (9%)	9	33
4	QD	180/181 (99%)	161 (89%)	19 (11%)	6	28
4	XD	180/181 (99%)	155 (86%)	25 (14%)	3	19
5	QE	116/123 (94%)	101 (87%)	15 (13%)	4	22
5	XE	116/123 (94%)	100 (86%)	16 (14%)	3	20
6	QF	90/90 (100%)	79 (88%)	11 (12%)	5	23
6	XF	90/90 (100%)	78 (87%)	12 (13%)	4	21
7	QG	126/127 (99%)	115 (91%)	11 (9%)	9	34
7	XG	126/127 (99%)	112 (89%)	14 (11%)	6	27
8	QH	119/119 (100%)	105 (88%)	14 (12%)	5	24
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	QI	98/99 (99%)	80 (82%)	18 (18%)	1	10
9	XI	98/99 (99%)	77 (79%)	21 (21%)	1	7
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4	21
10	XJ	89/92 (97%)	74 (83%)	15 (17%)	2	13
11	QK	90/99 (91%)	79 (88%)	11 (12%)	5	23
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	30
12	QL	104/109 (95%)	87 (84%)	17 (16%)	2	15
12	XL	104/109 (95%)	86 (83%)	18 (17%)	2	12
13	QM	97/101 (96%)	73 (75%)	24 (25%)	1	4
13	XM	97/101 (96%)	79 (81%)	18 (19%)	1	10
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	10
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	19
15	QO	79/80 (99%)	72 (91%)	7 (9%)	9	33
15	XO	79/80 (99%)	68 (86%)	11 (14%)	3	19
16	QP	72/74 (97%)	62 (86%)	10 (14%)	3	19
16	XP	72/74 (97%)	66 (92%)	6 (8%)	10	35
17	QQ	95/97 (98%)	86 (90%)	9 (10%)	8	32
17	XQ	95/97 (98%)	88 (93%)	7 (7%)	13	39
18	QR	61/77 (79%)	50 (82%)	11 (18%)	2	11
18	XR	61/77 (79%)	50 (82%)	11 (18%)	2	11
19	QS	73/80 (91%)	58 (80%)	15 (20%)	1	8
19	XS	73/80 (91%)	56 (77%)	17 (23%)	1	5
20	QT	76/82 (93%)	66 (87%)	10 (13%)	4	21
20	XT	76/82 (93%)	65 (86%)	11 (14%)	3	18
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
27	RD	214/218 (98%)	170 (79%)	44 (21%)	1	8
27	YD	214/218 (98%)	173 (81%)	41 (19%)	1	9
28	RE	165/166 (99%)	125 (76%)	40 (24%)	1	5
28	YE	165/166 (99%)	125 (76%)	40 (24%)	1	5
29	RF	161/166 (97%)	138 (86%)	23 (14%)	3	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	YF	161/166 (97%)	138 (86%)	23 (14%)	3	19
30	RG	155/156 (99%)	135 (87%)	20 (13%)	4	22
30	YG	155/156 (99%)	131 (84%)	24 (16%)	2	16
31	RH	142/148 (96%)	111 (78%)	31 (22%)	1	7
31	YH	142/148 (96%)	112 (79%)	30 (21%)	1	7
32	RI	122/124 (98%)	101 (83%)	21 (17%)	2	12
32	YI	122/124 (98%)	93 (76%)	29 (24%)	1	5
33	RN	117/119 (98%)	94 (80%)	23 (20%)	1	8
33	YN	117/119 (98%)	94 (80%)	23 (20%)	1	8
34	RO	100/100 (100%)	91 (91%)	9 (9%)	9	33
34	YO	100/100 (100%)	85 (85%)	15 (15%)	3	17
35	RP	116/116 (100%)	85 (73%)	31 (27%)	0	3
35	YP	115/116 (99%)	78 (68%)	37 (32%)	0	2
36	RQ	111/111 (100%)	95 (86%)	16 (14%)	3	18
36	YQ	111/111 (100%)	95 (86%)	16 (14%)	3	18
37	RR	101/101 (100%)	81 (80%)	20 (20%)	1	8
37	YR	101/101 (100%)	80 (79%)	21 (21%)	1	7
38	RS	87/88 (99%)	67 (77%)	20 (23%)	1	6
38	YS	87/88 (99%)	73 (84%)	14 (16%)	2	15
39	RT	120/127 (94%)	101 (84%)	19 (16%)	2	15
39	YT	120/127 (94%)	94 (78%)	26 (22%)	1	7
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3	17
40	YU	93/94 (99%)	79 (85%)	14 (15%)	3	17
41	RV	82/82 (100%)	63 (77%)	19 (23%)	1	5
41	YV	82/82 (100%)	66 (80%)	16 (20%)	1	9
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%)	61 (82%)	13 (18%)	2	12
43	YX	74/78 (95%)	59 (80%)	15 (20%)	1	8
44	RY	85/91 (93%)	56 (66%)	29 (34%)	0	1
44	YY	85/91 (93%)	62 (73%)	23 (27%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	RZ	162/179 (90%)	140 (86%)	22 (14%)	3	20
45	YZ	162/179 (90%)	141 (87%)	21 (13%)	4	21
46	R0	65/67 (97%)	58 (89%)	7 (11%)	6	28
46	Y0	65/67 (97%)	57 (88%)	8 (12%)	4	23
47	R1	82/83 (99%)	74 (90%)	8 (10%)	7	31
47	Y1	82/83 (99%)	69 (84%)	13 (16%)	2	15
48	R2	64/67 (96%)	48 (75%)	16 (25%)	0	4
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	27
49	R3	51/52 (98%)	43 (84%)	8 (16%)	2	15
49	Y3	51/52 (98%)	44 (86%)	7 (14%)	3	20
50	R4	63/63 (100%)	48 (76%)	15 (24%)	1	5
50	Y4	63/63 (100%)	43 (68%)	20 (32%)	0	2
51	R5	51/52 (98%)	40 (78%)	11 (22%)	1	7
51	Y5	51/52 (98%)	37 (72%)	14 (28%)	0	3
52	R6	48/52 (92%)	32 (67%)	16 (33%)	0	2
52	Y6	48/52 (92%)	34 (71%)	14 (29%)	0	2
53	R7	42/42 (100%)	35 (83%)	7 (17%)	2	14
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%)	39 (72%)	15 (28%)	0	3
55	R9	34/34 (100%)	30 (88%)	4 (12%)	5	24
55	Y9	34/34 (100%)	31 (91%)	3 (9%)	9	33
All	All	9701/10066 (96%)	8068 (83%)	1633 (17%)	2	13

5 of 1633 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	XH	109	ILE
28	YE	77	ILE
52	Y6	19	ARG
10	XJ	45	ARG
8	XH	80	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
6	XF	73	ASN
28	YE	55	ASN
9	XI	3	GLN
27	YD	44	ASN
31	YH	158	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	264 (17%)	39 (2%)
1	XA	1498/1522 (98%)	283 (18%)	36 (2%)
22	QV	76/77 (98%)	16 (21%)	1 (1%)
22	XV	76/77 (98%)	14 (18%)	1 (1%)
23	QX	9/25 (36%)	1 (11%)	0
23	XX	9/25 (36%)	3 (33%)	0
24	QY	14/18 (77%)	1 (7%)	0
24	XY	14/18 (77%)	3 (21%)	0
25	RA	2879/2915 (98%)	590 (20%)	51 (1%)
25	YA	2879/2915 (98%)	606 (21%)	53 (1%)
26	RB	119/122 (97%)	15 (12%)	2 (1%)
26	YB	119/122 (97%)	22 (18%)	2 (1%)
56	Z5	1/3 (33%)	0	0
56	Z6	1/3 (33%)	0	0
All	All	9192/9364 (98%)	1818 (19%)	185 (2%)

5 of 1818 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 185 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	703	G
25	YA	587	C
1	XA	992	U
25	YA	71	A
25	YA	974(A)	C

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	Z6	101	25,56	37,40,41	2.58	8 (21%)	47,57,60	2.56	15 (31%)
56	PPU	Z5	101	25,56	37,40,41	2.58	8 (21%)	47,57,60	2.55	15 (31%)

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

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	101	PPU	O-C	9.60	1.41	1.23
56	Z5	101	PPU	O-C	9.59	1.41	1.23
56	Z6	101	PPU	C9-N6	-6.26	1.31	1.45
56	Z5	101	PPU	C9-N6	-6.21	1.32	1.45
56	Z5	101	PPU	C10-N6	-5.89	1.32	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	101	PPU	C3'-N3'-C	-8.53	110.22	123.20
56	Z5	101	PPU	C3'-N3'-C	-8.49	110.29	123.20
56	Z6	101	PPU	C2'-C1'-N9	-5.95	98.52	113.30
56	Z5	101	PPU	C2'-C1'-N9	-5.95	98.52	113.30
56	Z6	101	PPU	C5-C4-N3	-5.02	119.81	126.72

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 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z6	101	PPU	9	0
56	Z5	101	PPU	9	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 752 ligands modelled in this entry, 752 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.36	86 (5%) 29 17	68, 119, 216, 326	0
1	XA	1500/1522 (98%)	0.16	42 (2%) 55 31	51, 103, 202, 332	0
2	QB	237/256 (92%)	0.47	16 (6%) 23 15	120, 181, 240, 264	0
2	XB	237/256 (92%)	0.32	12 (5%) 33 19	99, 157, 210, 239	0
3	QC	205/239 (85%)	0.46	12 (5%) 28 17	121, 172, 216, 250	0
3	XC	205/239 (85%)	0.15	2 (0%) 79 54	79, 131, 185, 239	0
4	QD	208/209 (99%)	0.59	16 (7%) 19 13	92, 126, 170, 212	0
4	XD	208/209 (99%)	0.61	15 (7%) 21 14	83, 130, 180, 211	0
5	QE	151/162 (93%)	0.49	9 (5%) 27 17	93, 140, 182, 216	0
5	XE	151/162 (93%)	0.73	8 (5%) 32 19	77, 121, 174, 245	0
6	QF	101/101 (100%)	0.04	1 (0%) 79 54	76, 116, 161, 205	0
6	XF	101/101 (100%)	0.17	0 100 100	77, 120, 162, 198	0
7	QG	155/156 (99%)	0.51	9 (5%) 29 17	92, 148, 197, 212	0
7	XG	155/156 (99%)	0.44	8 (5%) 33 19	82, 123, 165, 203	0
8	QH	138/138 (100%)	0.49	9 (6%) 25 16	86, 140, 178, 207	0
8	XH	138/138 (100%)	0.24	4 (2%) 53 30	84, 119, 161, 178	0
9	QI	127/128 (99%)	1.13	24 (18%) 3 3	122, 188, 231, 267	0
9	XI	127/128 (99%)	0.83	22 (17%) 4 4	76, 150, 201, 226	0
10	QJ	99/105 (94%)	0.70	7 (7%) 22 14	122, 205, 256, 279	0
10	XJ	99/105 (94%)	0.81	7 (7%) 22 14	82, 158, 223, 244	0
11	QK	119/129 (92%)	0.54	10 (8%) 17 12	80, 122, 188, 209	0
11	XK	119/129 (92%)	0.31	5 (4%) 40 22	64, 104, 171, 198	0
12	QL	125/132 (94%)	0.90	16 (12%) 7 7	67, 114, 162, 222	0
12	XL	125/132 (94%)	0.63	8 (6%) 25 16	50, 90, 150, 212	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%)	0.52	10 (8%) 17 12	106, 172, 212, 249	0
13	XM	121/126 (96%)	0.42	7 (5%) 29 17	67, 128, 184, 225	0
14	QN	60/61 (98%)	1.08	8 (13%) 7 6	135, 164, 205, 221	0
14	XN	60/61 (98%)	0.68	5 (8%) 17 12	88, 114, 157, 184	0
15	QO	88/89 (98%)	0.35	1 (1%) 78 52	78, 118, 156, 167	0
15	XO	88/89 (98%)	0.51	4 (4%) 38 21	62, 104, 151, 183	0
16	QP	84/88 (95%)	0.51	4 (4%) 35 20	70, 109, 154, 202	0
16	XP	84/88 (95%)	0.58	5 (5%) 27 17	92, 122, 166, 208	0
17	QQ	100/105 (95%)	0.82	11 (11%) 10 9	74, 116, 157, 175	0
17	XQ	100/105 (95%)	0.53	5 (5%) 34 19	70, 114, 154, 184	0
18	QR	70/88 (79%)	0.34	3 (4%) 40 22	83, 124, 172, 203	0
18	XR	70/88 (79%)	0.21	2 (2%) 53 30	72, 116, 171, 191	0
19	QS	84/93 (90%)	0.98	13 (15%) 5 5	118, 184, 216, 227	0
19	XS	84/93 (90%)	0.64	6 (7%) 22 14	74, 141, 182, 215	0
20	QT	99/106 (93%)	0.66	11 (11%) 10 8	72, 121, 165, 219	0
20	XT	99/106 (93%)	1.10	16 (16%) 4 5	85, 134, 187, 220	0
21	QU	25/27 (92%)	1.13	6 (24%) 2 2	132, 164, 200, 248	0
21	XU	25/27 (92%)	1.66	7 (28%) 1 1	98, 126, 181, 218	0
22	QV	77/77 (100%)	0.13	0 100 100	66, 116, 162, 216	0
22	XV	77/77 (100%)	0.06	1 (1%) 75 48	62, 90, 128, 178	0
23	QX	11/25 (44%)	1.62	3 (27%) 1 2	93, 112, 226, 253	0
23	XX	10/25 (40%)	1.31	3 (30%) 1 1	70, 95, 186, 197	0
24	QY	15/18 (83%)	0.48	0 100 100	107, 141, 236, 256	0
24	XY	15/18 (83%)	0.04	0 100 100	89, 117, 219, 223	0
25	RA	2882/2915 (98%)	0.15	90 (3%) 51 29	43, 86, 233, 352	0
25	YA	2882/2915 (98%)	0.08	84 (2%) 53 30	31, 70, 224, 366	0
26	RB	120/122 (98%)	0.67	11 (9%) 14 11	103, 157, 198, 227	0
26	YB	120/122 (98%)	0.33	4 (3%) 49 28	68, 118, 143, 176	0
27	RD	272/276 (98%)	0.39	13 (4%) 35 20	43, 78, 129, 207	0
27	YD	272/276 (98%)	0.67	29 (10%) 11 9	33, 69, 112, 205	0
28	RE	205/206 (99%)	0.80	19 (9%) 14 10	50, 100, 166, 224	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%)	0.39	5 (2%) 59 34	37, 93, 167, 230	0
29	RF	202/210 (96%)	0.43	7 (3%) 47 27	38, 104, 162, 221	0
29	YF	202/210 (96%)	0.47	11 (5%) 31 18	32, 84, 147, 201	0
30	RG	181/182 (99%)	0.80	21 (11%) 9 8	125, 179, 223, 250	0
30	YG	181/182 (99%)	0.51	8 (4%) 39 22	81, 135, 183, 245	0
31	RH	170/180 (94%)	0.54	8 (4%) 36 20	108, 184, 228, 277	0
31	YH	170/180 (94%)	0.87	24 (14%) 6 6	83, 119, 170, 234	0
32	RI	146/148 (98%)	0.70	11 (7%) 20 14	67, 164, 206, 249	0
32	YI	146/148 (98%)	0.75	15 (10%) 12 10	63, 158, 202, 226	0
33	RN	138/140 (98%)	0.47	4 (2%) 53 30	60, 111, 165, 197	0
33	YN	138/140 (98%)	0.63	14 (10%) 12 10	49, 91, 148, 194	0
34	RO	122/122 (100%)	0.25	4 (3%) 49 28	56, 85, 126, 144	0
34	YO	122/122 (100%)	0.06	0 100 100	47, 77, 118, 145	0
35	RP	150/150 (100%)	0.68	20 (13%) 7 6	45, 109, 175, 219	0
35	YP	150/150 (100%)	0.82	23 (15%) 5 5	33, 86, 155, 210	0
36	RQ	141/141 (100%)	0.86	21 (14%) 5 5	76, 118, 174, 231	0
36	YQ	141/141 (100%)	0.91	22 (15%) 5 5	46, 85, 138, 230	0
37	RR	118/118 (100%)	0.45	2 (1%) 69 41	52, 84, 121, 150	0
37	YR	118/118 (100%)	0.66	9 (7%) 20 13	48, 83, 127, 171	0
38	RS	111/112 (99%)	0.96	14 (12%) 8 7	126, 160, 218, 229	0
38	YS	111/112 (99%)	0.55	3 (2%) 56 32	93, 124, 171, 199	0
39	RT	137/146 (93%)	0.58	9 (6%) 24 15	60, 95, 190, 262	0
39	YT	137/146 (93%)	0.27	1 (0%) 84 61	59, 92, 179, 223	0
40	RU	117/118 (99%)	0.58	10 (8%) 16 12	52, 104, 157, 243	0
40	YU	117/118 (99%)	0.58	7 (5%) 27 17	46, 83, 151, 203	0
41	RV	101/101 (100%)	0.43	5 (4%) 34 19	62, 125, 186, 258	0
41	YV	101/101 (100%)	0.40	3 (2%) 52 30	42, 106, 174, 235	0
42	RW	113/113 (100%)	0.67	11 (9%) 13 10	48, 81, 135, 217	0
42	YW	113/113 (100%)	0.21	3 (2%) 56 32	40, 74, 140, 199	0
43	RX	92/96 (95%)	0.62	6 (6%) 25 16	61, 93, 139, 182	0
43	YX	92/96 (95%)	0.53	3 (3%) 49 28	49, 74, 115, 162	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%)	1.31	29 (28%) 1 1	84, 131, 189, 225	0
44	YY	102/110 (92%)	0.90	13 (12%) 8 7	69, 107, 159, 251	0
45	RZ	183/206 (88%)	0.63	8 (4%) 39 22	99, 165, 224, 280	0
45	YZ	183/206 (88%)	0.72	13 (7%) 22 14	82, 124, 202, 240	0
46	R0	82/85 (96%)	0.73	10 (12%) 8 7	64, 104, 143, 168	0
46	Y0	82/85 (96%)	0.48	4 (4%) 35 20	46, 79, 114, 140	0
47	R1	97/98 (98%)	0.79	9 (9%) 14 10	55, 89, 182, 204	0
47	Y1	97/98 (98%)	0.46	4 (4%) 41 23	36, 73, 178, 200	0
48	R2	69/72 (95%)	0.58	4 (5%) 29 17	83, 120, 172, 193	0
48	Y2	69/72 (95%)	0.85	10 (14%) 6 6	65, 84, 157, 226	0
49	R3	59/60 (98%)	0.46	4 (6%) 23 15	79, 111, 172, 193	0
49	Y3	59/60 (98%)	0.33	2 (3%) 48 27	57, 89, 148, 197	0
50	R4	71/71 (100%)	0.81	7 (9%) 13 10	158, 229, 303, 319	0
50	Y4	71/71 (100%)	0.72	6 (8%) 16 12	127, 173, 251, 269	0
51	R5	59/60 (98%)	0.62	5 (8%) 16 12	48, 92, 214, 226	0
51	Y5	58/60 (96%)	0.53	2 (3%) 48 27	41, 85, 195, 229	0
52	R6	49/54 (90%)	1.22	10 (20%) 3 3	142, 185, 226, 245	0
52	Y6	49/54 (90%)	0.91	6 (12%) 8 7	115, 172, 221, 241	0
53	R7	49/49 (100%)	1.02	11 (22%) 2 2	41, 66, 126, 203	0
53	Y7	49/49 (100%)	0.72	5 (10%) 12 10	31, 53, 115, 183	0
54	R8	64/65 (98%)	1.12	11 (17%) 4 4	56, 99, 146, 240	0
54	Y8	64/65 (98%)	1.12	9 (14%) 6 6	43, 78, 132, 225	0
55	R9	37/37 (100%)	1.71	12 (32%) 1 1	128, 172, 212, 231	0
55	Y9	37/37 (100%)	1.93	17 (45%) 0 1	103, 149, 207, 229	0
56	Z5	2/3 (66%)	0.36	0 100 100	77, 77, 77, 85	0
56	Z6	2/3 (66%)	0.28	0 100 100	51, 51, 51, 59	0
All	All	20878/21492 (97%)	0.41	1244 (5%) 27 17	31, 107, 207, 366	0

The worst 5 of 1244 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	R0	71	ASP	7.8
9	XI	106	ALA	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
53	R7	49	ARG	7.1
30	RG	34	LEU	6.8
36	YQ	80	GLU	6.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PPU	Z5	101	37/38	0.92	0.16	74,76,77,78	0
56	PPU	Z6	101	37/38	0.95	0.11	52,54,54,55	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	RB	202	1/1	-0.23	0.47	118,118,118,118	0
57	MG	QN	102	1/1	-0.17	0.44	143,143,143,143	0
57	MG	RA	3153	1/1	0.21	0.19	80,80,80,80	0
57	MG	RA	3137	1/1	0.29	0.27	81,81,81,81	0
57	MG	QV	101	1/1	0.31	0.23	119,119,119,119	0
57	MG	QA	1642	1/1	0.34	0.49	137,137,137,137	0
57	MG	RA	3209	1/1	0.35	0.32	79,79,79,79	0
57	MG	QA	1674	1/1	0.37	0.31	97,97,97,97	0
57	MG	Y0	101	1/1	0.40	0.24	49,49,49,49	0
57	MG	YB	202	1/1	0.41	0.54	79,79,79,79	0
57	MG	QA	1652	1/1	0.44	0.21	115,115,115,115	0
57	MG	XA	1650	1/1	0.44	0.30	80,80,80,80	0
57	MG	RA	3213	1/1	0.45	0.16	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3069	1/1	0.47	0.37	52,52,52,52	0
57	MG	QA	1657	1/1	0.47	0.39	89,89,89,89	0
57	MG	XA	1681	1/1	0.47	0.41	98,98,98,98	0
57	MG	RA	3133	1/1	0.48	0.22	79,79,79,79	0
57	MG	RA	3175	1/1	0.48	0.25	56,56,56,56	0
57	MG	RA	3217	1/1	0.48	0.27	88,88,88,88	0
57	MG	RA	3171	1/1	0.50	0.26	100,100,100,100	0
57	MG	RA	3189	1/1	0.52	0.17	97,97,97,97	0
57	MG	QA	1680	1/1	0.53	0.24	123,123,123,123	0
57	MG	R0	101	1/1	0.55	0.19	68,68,68,68	0
57	MG	YA	3061	1/1	0.55	0.47	65,65,65,65	0
57	MG	RA	3206	1/1	0.55	0.17	76,76,76,76	0
57	MG	YA	3072	1/1	0.55	0.17	46,46,46,46	0
57	MG	XA	1660	1/1	0.55	0.17	118,118,118,118	0
57	MG	XA	1663	1/1	0.55	0.14	127,127,127,127	0
57	MG	YA	3139	1/1	0.56	0.46	66,66,66,66	0
57	MG	RA	3066	1/1	0.56	0.61	74,74,74,74	0
57	MG	YB	203	1/1	0.56	0.33	125,125,125,125	0
57	MG	YA	3064	1/1	0.56	0.30	75,75,75,75	0
57	MG	YA	3262	1/1	0.57	0.46	86,86,86,86	0
57	MG	YA	3046	1/1	0.57	0.41	69,69,69,69	0
57	MG	RA	3163	1/1	0.57	0.21	82,82,82,82	0
57	MG	RA	3120	1/1	0.57	0.41	76,76,76,76	0
57	MG	XA	1687	1/1	0.58	0.11	104,104,104,104	0
57	MG	XA	1698	1/1	0.58	0.27	64,64,64,64	0
57	MG	QA	1643	1/1	0.58	0.15	89,89,89,89	0
57	MG	QA	1655	1/1	0.59	0.37	93,93,93,93	0
57	MG	QA	1618	1/1	0.59	0.30	119,119,119,119	0
57	MG	RA	3004	1/1	0.59	0.35	96,96,96,96	0
57	MG	YA	3181	1/1	0.59	0.26	109,109,109,109	0
57	MG	XA	1694	1/1	0.60	0.33	74,74,74,74	0
57	MG	QA	1617	1/1	0.60	0.27	96,96,96,96	0
57	MG	RA	3245	1/1	0.60	0.14	64,64,64,64	0
57	MG	YA	3115	1/1	0.60	0.50	75,75,75,75	0
57	MG	RA	3027	1/1	0.60	0.69	74,74,74,74	0
57	MG	RA	3159	1/1	0.61	0.24	68,68,68,68	0
57	MG	QA	1667	1/1	0.61	0.18	102,102,102,102	0
57	MG	RA	3014	1/1	0.61	0.60	73,73,73,73	0
57	MG	YA	3216	1/1	0.61	0.24	50,50,50,50	0
57	MG	QH	201	1/1	0.62	0.13	94,94,94,94	0
57	MG	YA	3229	1/1	0.62	0.14	74,74,74,74	0
57	MG	XA	1633	1/1	0.63	0.57	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3240	1/1	0.63	0.60	93,93,93,93	0
57	MG	XA	1622	1/1	0.64	0.35	79,79,79,79	0
57	MG	RA	3197	1/1	0.64	0.14	57,57,57,57	0
57	MG	XA	1658	1/1	0.65	0.23	123,123,123,123	0
57	MG	YA	3130	1/1	0.65	0.19	33,33,33,33	0
57	MG	RA	3201	1/1	0.65	0.19	70,70,70,70	0
57	MG	RA	3216	1/1	0.65	0.36	76,76,76,76	0
57	MG	YA	3200	1/1	0.65	0.35	61,61,61,61	0
57	MG	R8	101	1/1	0.65	0.19	50,50,50,50	0
57	MG	YA	3121	1/1	0.66	0.24	46,46,46,46	0
57	MG	XA	1662	1/1	0.66	0.35	80,80,80,80	0
57	MG	QA	1653	1/1	0.66	0.16	115,115,115,115	0
57	MG	XA	1677	1/1	0.66	0.51	103,103,103,103	0
57	MG	YA	3038	1/1	0.66	0.46	60,60,60,60	0
57	MG	QA	1668	1/1	0.66	0.18	67,67,67,67	0
57	MG	QA	1635	1/1	0.67	0.28	69,69,69,69	0
57	MG	QA	1602	1/1	0.67	0.59	75,75,75,75	0
57	MG	XA	1635	1/1	0.67	0.42	91,91,91,91	0
57	MG	YA	3187	1/1	0.67	0.11	74,74,74,74	0
57	MG	YA	3154	1/1	0.68	0.31	80,80,80,80	0
57	MG	YA	3169	1/1	0.68	0.18	65,65,65,65	0
57	MG	QA	1625	1/1	0.68	0.27	90,90,90,90	0
57	MG	RA	3073	1/1	0.68	0.26	58,58,58,58	0
57	MG	QA	1684	1/1	0.68	0.29	83,83,83,83	0
57	MG	R3	101	1/1	0.68	0.33	69,69,69,69	0
57	MG	QA	1664	1/1	0.69	0.43	88,88,88,88	0
57	MG	YA	3162	1/1	0.69	0.23	68,68,68,68	0
57	MG	RA	3168	1/1	0.69	0.33	77,77,77,77	0
57	MG	QA	1605	1/1	0.69	0.37	69,69,69,69	0
57	MG	RA	3110	1/1	0.69	0.32	89,89,89,89	0
57	MG	YA	3188	1/1	0.69	0.25	84,84,84,84	0
57	MG	RA	3047	1/1	0.69	0.42	53,53,53,53	0
57	MG	RA	3234	1/1	0.70	0.27	60,60,60,60	0
57	MG	XA	1689	1/1	0.70	0.20	89,89,89,89	0
57	MG	XA	1692	1/1	0.70	0.18	66,66,66,66	0
57	MG	RA	3222	1/1	0.70	0.18	62,62,62,62	0
57	MG	YA	3235	1/1	0.70	0.20	45,45,45,45	0
57	MG	RA	3063	1/1	0.71	0.87	72,72,72,72	0
57	MG	YA	3007	1/1	0.71	0.61	62,62,62,62	0
57	MG	YA	3140	1/1	0.71	0.30	51,51,51,51	0
57	MG	YA	3108	1/1	0.71	0.37	65,65,65,65	0
57	MG	YA	3019	1/1	0.71	0.42	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3030	1/1	0.71	0.36	32,32,32,32	0
57	MG	YA	3127	1/1	0.72	0.36	68,68,68,68	0
57	MG	QX	102	1/1	0.72	0.13	93,93,93,93	0
57	MG	YA	3137	1/1	0.72	0.24	60,60,60,60	0
57	MG	XA	1664	1/1	0.72	0.32	100,100,100,100	0
57	MG	QA	1675	1/1	0.72	0.27	72,72,72,72	0
57	MG	YA	3153	1/1	0.72	0.28	68,68,68,68	0
57	MG	RA	3081	1/1	0.72	0.23	85,85,85,85	0
57	MG	RA	3100	1/1	0.72	0.25	67,67,67,67	0
57	MG	YA	3269	1/1	0.72	0.21	74,74,74,74	0
57	MG	XA	1616	1/1	0.72	0.41	67,67,67,67	0
57	MG	YA	3175	1/1	0.72	0.28	70,70,70,70	0
57	MG	QA	1633	1/1	0.72	0.21	128,128,128,128	0
57	MG	QA	1610	1/1	0.73	0.42	66,66,66,66	0
57	MG	XY	101	1/1	0.73	0.10	53,53,53,53	0
57	MG	YA	3063	1/1	0.73	0.38	72,72,72,72	0
57	MG	QA	1661	1/1	0.73	0.30	72,72,72,72	0
57	MG	RA	3152	1/1	0.73	0.22	62,62,62,62	0
57	MG	XA	1601	1/1	0.73	0.35	74,74,74,74	0
57	MG	YA	3032	1/1	0.73	0.48	63,63,63,63	0
57	MG	RA	3182	1/1	0.73	0.15	88,88,88,88	0
57	MG	YA	3119	1/1	0.74	0.45	50,50,50,50	0
57	MG	QA	1676	1/1	0.74	0.27	111,111,111,111	0
57	MG	RA	3076	1/1	0.74	0.37	52,52,52,52	0
57	MG	RA	3125	1/1	0.74	0.24	87,87,87,87	0
57	MG	YA	3016	1/1	0.74	0.56	63,63,63,63	0
57	MG	XA	1642	1/1	0.75	0.39	90,90,90,90	0
57	MG	XA	1647	1/1	0.75	0.25	94,94,94,94	0
57	MG	XA	1649	1/1	0.75	0.17	82,82,82,82	0
57	MG	XA	1610	1/1	0.75	0.26	72,72,72,72	0
57	MG	YA	3225	1/1	0.75	0.29	71,71,71,71	0
57	MG	RA	3085	1/1	0.75	0.58	59,59,59,59	0
57	MG	YA	3073	1/1	0.75	0.17	64,64,64,64	0
57	MG	YA	3095	1/1	0.75	0.32	71,71,71,71	0
57	MG	YA	3249	1/1	0.75	0.35	49,49,49,49	0
57	MG	YA	3159	1/1	0.75	0.30	105,105,105,105	0
57	MG	RA	3023	1/1	0.75	0.34	40,40,40,40	0
57	MG	RB	201	1/1	0.75	0.10	166,166,166,166	0
57	MG	YA	3042	1/1	0.75	0.43	62,62,62,62	0
57	MG	QA	1634	1/1	0.75	0.13	62,62,62,62	0
57	MG	RA	3139	1/1	0.76	0.34	78,78,78,78	0
57	MG	RA	3164	1/1	0.76	0.30	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1648	1/1	0.76	0.13	94,94,94,94	0
57	MG	RA	3069	1/1	0.76	0.17	58,58,58,58	0
57	MG	YA	3015	1/1	0.76	0.33	34,34,34,34	0
57	MG	QA	1640	1/1	0.76	0.14	91,91,91,91	0
57	MG	XA	1648	1/1	0.76	0.22	59,59,59,59	0
57	MG	RA	3212	1/1	0.77	0.15	68,68,68,68	0
57	MG	YA	3026	1/1	0.77	0.27	40,40,40,40	0
57	MG	QA	1670	1/1	0.77	0.21	65,65,65,65	0
57	MG	XA	1651	1/1	0.77	0.30	78,78,78,78	0
57	MG	YA	3250	1/1	0.77	0.23	32,32,32,32	0
57	MG	YA	3035	1/1	0.77	0.40	64,64,64,64	0
57	MG	QA	1622	1/1	0.77	0.21	104,104,104,104	0
57	MG	XA	1682	1/1	0.77	0.29	114,114,114,114	0
57	MG	RA	3064	1/1	0.77	0.94	82,82,82,82	0
57	MG	XA	1630	1/1	0.77	0.25	57,57,57,57	0
57	MG	RA	3141	1/1	0.78	0.42	83,83,83,83	0
57	MG	QA	1630	1/1	0.78	0.25	111,111,111,111	0
57	MG	RA	3235	1/1	0.78	0.20	71,71,71,71	0
57	MG	RA	3097	1/1	0.78	0.36	44,44,44,44	0
57	MG	XA	1684	1/1	0.78	0.38	91,91,91,91	0
57	MG	RA	3179	1/1	0.78	0.23	66,66,66,66	0
57	MG	QA	1628	1/1	0.78	0.14	84,84,84,84	0
57	MG	YA	3104	1/1	0.78	0.26	34,34,34,34	0
57	MG	RA	3109	1/1	0.78	0.30	70,70,70,70	0
57	MG	XA	1634	1/1	0.78	0.38	67,67,67,67	0
57	MG	YA	3041	1/1	0.78	0.51	63,63,63,63	0
57	MG	QA	1651	1/1	0.78	0.26	102,102,102,102	0
57	MG	XA	1637	1/1	0.78	0.16	105,105,105,105	0
57	MG	RA	3046	1/1	0.79	0.32	47,47,47,47	0
57	MG	QM	202	1/1	0.79	0.22	113,113,113,113	0
57	MG	YA	3020	1/1	0.79	0.25	35,35,35,35	0
57	MG	YA	3076	1/1	0.79	0.25	41,41,41,41	0
57	MG	YA	3085	1/1	0.79	0.24	63,63,63,63	0
57	MG	QA	1614	1/1	0.79	0.25	60,60,60,60	0
57	MG	RA	3186	1/1	0.79	0.38	84,84,84,84	0
57	MG	RA	3032	1/1	0.79	0.41	59,59,59,59	0
57	MG	RA	3102	1/1	0.79	0.12	61,61,61,61	0
57	MG	YA	3158	1/1	0.79	0.10	67,67,67,67	0
57	MG	XA	1618	1/1	0.80	0.20	69,69,69,69	0
57	MG	RA	3224	1/1	0.80	0.36	60,60,60,60	0
57	MG	RA	3043	1/1	0.80	0.23	46,46,46,46	0
57	MG	YA	3025	1/1	0.80	0.68	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1631	1/1	0.80	0.12	63,63,63,63	0
57	MG	RA	3143	1/1	0.80	0.24	62,62,62,62	0
57	MG	YA	3047	1/1	0.81	0.42	59,59,59,59	0
57	MG	YA	3048	1/1	0.81	0.47	76,76,76,76	0
57	MG	RA	3055	1/1	0.81	0.21	45,45,45,45	0
57	MG	QA	1632	1/1	0.81	0.36	62,62,62,62	0
57	MG	YA	3208	1/1	0.81	0.23	88,88,88,88	0
57	MG	YA	3265	1/1	0.81	0.47	81,81,81,81	0
57	MG	YA	3209	1/1	0.81	0.10	80,80,80,80	0
57	MG	XA	1671	1/1	0.81	0.23	89,89,89,89	0
57	MG	XA	1605	1/1	0.81	0.52	60,60,60,60	0
57	MG	XF	201	1/1	0.81	0.12	104,104,104,104	0
57	MG	YA	3194	1/1	0.82	0.34	47,47,47,47	0
57	MG	YA	3195	1/1	0.82	0.13	45,45,45,45	0
57	MG	YA	3198	1/1	0.82	0.13	89,89,89,89	0
57	MG	QA	1604	1/1	0.82	0.23	74,74,74,74	0
57	MG	QX	101	1/1	0.82	0.16	96,96,96,96	0
57	MG	QA	1636	1/1	0.82	0.25	73,73,73,73	0
57	MG	XA	1690	1/1	0.82	0.18	98,98,98,98	0
57	MG	RR	201	1/1	0.82	0.33	52,52,52,52	0
57	MG	YA	3150	1/1	0.82	0.18	84,84,84,84	0
57	MG	RA	3118	1/1	0.82	0.19	41,41,41,41	0
57	MG	XA	1669	1/1	0.82	0.39	66,66,66,66	0
57	MG	YA	3246	1/1	0.82	0.17	35,35,35,35	0
57	MG	RA	3091	1/1	0.82	0.22	53,53,53,53	0
57	MG	XA	1676	1/1	0.82	0.30	73,73,73,73	0
57	MG	YA	3103	1/1	0.82	0.17	79,79,79,79	0
57	MG	RA	3052	1/1	0.82	0.30	39,39,39,39	0
57	MG	YA	3013	1/1	0.82	0.41	63,63,63,63	0
57	MG	YA	3270	1/1	0.82	0.17	59,59,59,59	0
57	MG	QA	1649	1/1	0.82	0.20	76,76,76,76	0
57	MG	XA	1652	1/1	0.82	0.20	104,104,104,104	0
57	MG	YA	3049	1/1	0.82	0.37	69,69,69,69	0
57	MG	RA	3124	1/1	0.83	0.33	56,56,56,56	0
57	MG	YA	3117	1/1	0.83	0.32	70,70,70,70	0
57	MG	RA	3002	1/1	0.83	0.27	48,48,48,48	0
57	MG	RA	3241	1/1	0.83	0.24	56,56,56,56	0
57	MG	RA	3144	1/1	0.83	0.27	54,54,54,54	0
57	MG	YA	3062	1/1	0.83	0.30	39,39,39,39	0
57	MG	XA	1619	1/1	0.83	0.44	63,63,63,63	0
57	MG	YA	3022	1/1	0.83	0.33	66,66,66,66	0
57	MG	YA	3066	1/1	0.83	0.34	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3226	1/1	0.83	0.33	67,67,67,67	0
57	MG	YA	3146	1/1	0.83	0.27	49,49,49,49	0
57	MG	RA	3174	1/1	0.83	0.20	77,77,77,77	0
57	MG	XA	1653	1/1	0.83	0.25	56,56,56,56	0
57	MG	RA	3150	1/1	0.83	0.15	58,58,58,58	0
57	MG	XA	1631	1/1	0.83	0.28	67,67,67,67	0
57	MG	QA	1672	1/1	0.83	0.17	56,56,56,56	0
57	MG	YA	3160	1/1	0.83	0.11	37,37,37,37	0
57	MG	RA	3013	1/1	0.83	0.39	43,43,43,43	0
57	MG	YA	3100	1/1	0.83	0.45	44,44,44,44	0
57	MG	RA	3185	1/1	0.83	0.13	66,66,66,66	0
57	MG	QA	1616	1/1	0.83	0.23	93,93,93,93	0
57	MG	YA	3186	1/1	0.83	0.28	88,88,88,88	0
57	MG	YE	302	1/1	0.83	0.21	35,35,35,35	0
57	MG	RA	3140	1/1	0.83	0.09	74,74,74,74	0
57	MG	YA	3212	1/1	0.84	0.12	50,50,50,50	0
57	MG	RA	3079	1/1	0.84	0.34	48,48,48,48	0
57	MG	RA	3034	1/1	0.84	0.41	44,44,44,44	0
57	MG	RE	301	1/1	0.84	0.21	39,39,39,39	0
57	MG	XA	1678	1/1	0.84	0.56	79,79,79,79	0
57	MG	YA	3111	1/1	0.84	0.21	61,61,61,61	0
57	MG	YA	3237	1/1	0.84	0.20	54,54,54,54	0
57	MG	RA	3026	1/1	0.84	0.12	39,39,39,39	0
57	MG	XA	1629	1/1	0.84	0.10	67,67,67,67	0
57	MG	RA	3090	1/1	0.84	0.18	61,61,61,61	0
57	MG	QA	1629	1/1	0.84	0.22	60,60,60,60	0
57	MG	RA	3094	1/1	0.84	0.33	41,41,41,41	0
57	MG	RA	3149	1/1	0.84	0.13	108,108,108,108	0
57	MG	QA	1623	1/1	0.84	0.16	79,79,79,79	0
57	MG	YA	3031	1/1	0.84	0.43	70,70,70,70	0
57	MG	RA	3078	1/1	0.84	0.21	67,67,67,67	0
57	MG	XA	1639	1/1	0.84	0.27	49,49,49,49	0
57	MG	XA	1615	1/1	0.84	0.27	58,58,58,58	0
57	MG	XV	101	1/1	0.84	0.23	49,49,49,49	0
57	MG	XA	1659	1/1	0.85	0.24	84,84,84,84	0
57	MG	YA	3171	1/1	0.85	0.17	51,51,51,51	0
57	MG	RA	3059	1/1	0.85	0.26	38,38,38,38	0
57	MG	YA	3075	1/1	0.85	0.17	45,45,45,45	0
57	MG	QA	1662	1/1	0.85	0.26	62,62,62,62	0
57	MG	QA	1678	1/1	0.85	0.07	109,109,109,109	0
57	MG	QA	1679	1/1	0.85	0.37	106,106,106,106	0
57	MG	YA	3190	1/1	0.85	0.40	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1671	1/1	0.85	0.12	134,134,134,134	0
57	MG	RA	3219	1/1	0.85	0.30	47,47,47,47	0
57	MG	XA	1675	1/1	0.85	0.38	57,57,57,57	0
57	MG	RA	3112	1/1	0.85	0.21	75,75,75,75	0
57	MG	YA	3202	1/1	0.85	0.27	66,66,66,66	0
57	MG	RA	3117	1/1	0.85	0.16	91,91,91,91	0
57	MG	RA	3071	1/1	0.85	0.29	67,67,67,67	0
57	MG	RA	3033	1/1	0.85	0.62	77,77,77,77	0
57	MG	QA	1683	1/1	0.85	0.26	80,80,80,80	0
57	MG	RA	3038	1/1	0.85	0.26	56,56,56,56	0
57	MG	QA	1646	1/1	0.85	0.17	91,91,91,91	0
57	MG	RA	3008	1/1	0.85	0.22	62,62,62,62	0
57	MG	YA	3131	1/1	0.85	0.20	78,78,78,78	0
57	MG	RA	3012	1/1	0.85	0.12	39,39,39,39	0
57	MG	RA	3088	1/1	0.85	0.32	59,59,59,59	0
57	MG	QA	1621	1/1	0.85	0.20	102,102,102,102	0
57	MG	YA	3145	1/1	0.85	0.20	49,49,49,49	0
57	MG	YA	3055	1/1	0.85	0.17	46,46,46,46	0
57	MG	YA	3058	1/1	0.85	0.46	69,69,69,69	0
57	MG	RA	3142	1/1	0.85	0.39	46,46,46,46	0
57	MG	RA	3198	1/1	0.85	0.35	81,81,81,81	0
57	MG	RA	3199	1/1	0.85	0.31	47,47,47,47	0
57	MG	YA	3274	1/1	0.85	0.10	68,68,68,68	0
57	MG	QA	1611	1/1	0.85	0.30	60,60,60,60	0
57	MG	RA	3057	1/1	0.85	0.22	44,44,44,44	0
57	MG	YE	301	1/1	0.85	0.17	32,32,32,32	0
57	MG	YA	3012	1/1	0.85	0.21	26,26,26,26	0
57	MG	YA	3168	1/1	0.85	0.10	69,69,69,69	0
57	MG	RA	3025	1/1	0.86	0.20	44,44,44,44	0
57	MG	XA	1667	1/1	0.86	0.24	54,54,54,54	0
57	MG	YA	3211	1/1	0.86	0.20	81,81,81,81	0
57	MG	XA	1604	1/1	0.86	0.54	83,83,83,83	0
57	MG	YA	3215	1/1	0.86	0.13	73,73,73,73	0
57	MG	QA	1677	1/1	0.86	0.16	69,69,69,69	0
57	MG	YA	3222	1/1	0.86	0.21	90,90,90,90	0
57	MG	XA	1606	1/1	0.86	0.23	85,85,85,85	0
57	MG	YA	3051	1/1	0.86	0.54	58,58,58,58	0
57	MG	XA	1608	1/1	0.86	0.23	46,46,46,46	0
57	MG	RA	3122	1/1	0.86	0.13	85,85,85,85	0
57	MG	YA	3118	1/1	0.86	0.20	32,32,32,32	0
57	MG	YA	3174	1/1	0.86	0.09	40,40,40,40	0
57	MG	YA	3243	1/1	0.86	0.21	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1638	1/1	0.86	0.21	71,71,71,71	0
57	MG	YA	3180	1/1	0.86	0.30	66,66,66,66	0
57	MG	RA	3007	1/1	0.86	0.33	41,41,41,41	0
57	MG	RA	3190	1/1	0.86	0.10	45,45,45,45	0
57	MG	RD	301	1/1	0.86	0.23	73,73,73,73	0
57	MG	QA	1656	1/1	0.86	0.09	78,78,78,78	0
57	MG	XA	1656	1/1	0.86	0.11	92,92,92,92	0
57	MG	YA	3191	1/1	0.86	0.22	60,60,60,60	0
57	MG	RF	301	1/1	0.86	0.10	88,88,88,88	0
57	MG	RA	3077	1/1	0.86	0.23	38,38,38,38	0
57	MG	YB	204	1/1	0.86	0.53	82,82,82,82	0
57	MG	RA	3048	1/1	0.86	0.30	42,42,42,42	0
57	MG	RA	3200	1/1	0.86	0.32	93,93,93,93	0
57	MG	RA	3231	1/1	0.86	0.27	52,52,52,52	0
57	MG	XA	1695	1/1	0.87	0.22	57,57,57,57	0
57	MG	XA	1626	1/1	0.87	0.13	49,49,49,49	0
57	MG	YA	3206	1/1	0.87	0.17	58,58,58,58	0
57	MG	XA	1700	1/1	0.87	0.18	90,90,90,90	0
57	MG	XD	1701	1/1	0.87	0.12	151,151,151,151	0
57	MG	RA	3166	1/1	0.87	0.15	42,42,42,42	0
57	MG	RA	3050	1/1	0.87	0.21	51,51,51,51	0
57	MG	QA	1669	1/1	0.87	0.25	94,94,94,94	0
57	MG	RA	3220	1/1	0.87	0.50	78,78,78,78	0
57	MG	XA	1665	1/1	0.87	0.12	64,64,64,64	0
57	MG	YA	3223	1/1	0.87	0.30	69,69,69,69	0
57	MG	XA	1666	1/1	0.87	0.09	62,62,62,62	0
57	MG	R5	101	1/1	0.87	0.17	38,38,38,38	0
57	MG	RA	3173	1/1	0.87	0.13	66,66,66,66	0
57	MG	RA	3130	1/1	0.87	0.24	42,42,42,42	0
57	MG	XA	1673	1/1	0.87	0.29	58,58,58,58	0
57	MG	RA	3155	1/1	0.87	0.39	80,80,80,80	0
57	MG	YA	3094	1/1	0.87	0.27	32,32,32,32	0
57	MG	XA	1641	1/1	0.87	0.11	71,71,71,71	0
57	MG	RA	3157	1/1	0.87	0.08	49,49,49,49	0
57	MG	YA	3102	1/1	0.87	0.36	58,58,58,58	0
57	MG	YA	3178	1/1	0.87	0.23	48,48,48,48	0
57	MG	RA	3086	1/1	0.87	0.19	64,64,64,64	0
57	MG	RA	3236	1/1	0.87	0.21	80,80,80,80	0
57	MG	RA	3207	1/1	0.87	0.26	68,68,68,68	0
57	MG	RA	3208	1/1	0.87	0.14	52,52,52,52	0
57	MG	QA	1637	1/1	0.87	0.11	79,79,79,79	0
57	MG	XA	1688	1/1	0.87	0.30	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1617	1/1	0.87	0.21	50,50,50,50	0
57	MG	RA	3210	1/1	0.87	0.10	53,53,53,53	0
57	MG	RA	3111	1/1	0.87	0.21	67,67,67,67	0
57	MG	YP	201	1/1	0.87	0.18	39,39,39,39	0
57	MG	RA	3188	1/1	0.87	0.10	94,94,94,94	0
57	MG	YA	3133	1/1	0.88	0.23	60,60,60,60	0
57	MG	QA	1666	1/1	0.88	0.18	97,97,97,97	0
57	MG	YA	3034	1/1	0.88	0.34	35,35,35,35	0
57	MG	RA	3040	1/1	0.88	0.28	36,36,36,36	0
57	MG	XA	1670	1/1	0.88	0.25	67,67,67,67	0
57	MG	RA	3193	1/1	0.88	0.13	73,73,73,73	0
57	MG	YA	3149	1/1	0.88	0.18	51,51,51,51	0
57	MG	QA	1620	1/1	0.88	0.10	75,75,75,75	0
57	MG	YA	3045	1/1	0.88	0.34	32,32,32,32	0
57	MG	YA	3254	1/1	0.88	0.29	58,58,58,58	0
57	MG	RA	3054	1/1	0.88	0.20	49,49,49,49	0
57	MG	YA	3113	1/1	0.88	0.23	50,50,50,50	0
57	MG	YA	3070	1/1	0.88	0.30	53,53,53,53	0
57	MG	XX	101	1/1	0.88	0.16	74,74,74,74	0
57	MG	RA	3243	1/1	0.88	0.25	57,57,57,57	0
57	MG	YB	201	1/1	0.88	0.07	100,100,100,100	0
57	MG	QA	1615	1/1	0.88	0.17	100,100,100,100	0
57	MG	YA	3050	1/1	0.88	0.42	42,42,42,42	0
57	MG	YA	3122	1/1	0.88	0.20	61,61,61,61	0
57	MG	YA	3082	1/1	0.88	0.33	37,37,37,37	0
57	MG	YA	3128	1/1	0.88	0.27	73,73,73,73	0
57	MG	QA	1639	1/1	0.88	0.19	59,59,59,59	0
57	MG	YA	3092	1/1	0.88	0.21	76,76,76,76	0
57	MG	YA	3207	1/1	0.89	0.08	53,53,53,53	0
57	MG	RA	3119	1/1	0.89	0.19	59,59,59,59	0
57	MG	RA	3099	1/1	0.89	0.17	55,55,55,55	0
57	MG	YA	3079	1/1	0.89	0.26	30,30,30,30	0
57	MG	XA	1691	1/1	0.89	0.06	145,145,145,145	0
57	MG	YA	3033	1/1	0.89	0.39	47,47,47,47	0
57	MG	YA	3089	1/1	0.89	0.20	41,41,41,41	0
57	MG	RA	3010	1/1	0.89	0.24	79,79,79,79	0
57	MG	RA	3227	1/1	0.89	0.16	48,48,48,48	0
57	MG	RA	3228	1/1	0.89	0.37	50,50,50,50	0
57	MG	YA	3096	1/1	0.89	0.26	32,32,32,32	0
57	MG	XA	1697	1/1	0.89	0.25	61,61,61,61	0
57	MG	RA	3123	1/1	0.89	0.17	92,92,92,92	0
57	MG	QA	1654	1/1	0.89	0.08	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1668	1/1	0.89	0.13	70,70,70,70	0
57	MG	RA	3176	1/1	0.89	0.17	42,42,42,42	0
57	MG	YA	3244	1/1	0.89	0.44	69,69,69,69	0
57	MG	YA	3245	1/1	0.89	0.54	64,64,64,64	0
57	MG	RA	3005	1/1	0.89	0.34	42,42,42,42	0
57	MG	XA	1644	1/1	0.89	0.17	84,84,84,84	0
57	MG	XA	1672	1/1	0.89	0.39	69,69,69,69	0
57	MG	YA	3004	1/1	0.89	0.17	30,30,30,30	0
57	MG	YA	3182	1/1	0.89	0.22	44,44,44,44	0
57	MG	YA	3264	1/1	0.89	0.21	62,62,62,62	0
57	MG	RA	3030	1/1	0.89	0.27	42,42,42,42	0
57	MG	XA	1613	1/1	0.89	0.47	52,52,52,52	0
57	MG	QA	1647	1/1	0.89	0.12	118,118,118,118	0
57	MG	YA	3271	1/1	0.89	0.24	58,58,58,58	0
57	MG	YA	3189	1/1	0.89	0.08	61,61,61,61	0
57	MG	YA	3275	1/1	0.89	0.34	75,75,75,75	0
57	MG	RA	3135	1/1	0.89	0.22	42,42,42,42	0
57	MG	RA	3211	1/1	0.89	0.07	65,65,65,65	0
57	MG	RA	3060	1/1	0.89	0.32	38,38,38,38	0
57	MG	RA	3113	1/1	0.89	0.11	37,37,37,37	0
57	MG	RA	3016	1/1	0.89	0.25	38,38,38,38	0
57	MG	YA	3023	1/1	0.89	0.32	29,29,29,29	0
57	MG	QA	1613	1/1	0.89	0.15	75,75,75,75	0
57	MG	RA	3196	1/1	0.89	0.25	52,52,52,52	0
57	MG	RA	3162	1/1	0.90	0.22	38,38,38,38	0
57	MG	YA	3135	1/1	0.90	0.12	63,63,63,63	0
57	MG	RA	3225	1/1	0.90	0.32	64,64,64,64	0
57	MG	XA	1645	1/1	0.90	0.20	51,51,51,51	0
57	MG	QA	1659	1/1	0.90	0.15	66,66,66,66	0
57	MG	YA	3210	1/1	0.90	0.17	48,48,48,48	0
57	MG	RA	3024	1/1	0.90	0.14	55,55,55,55	0
57	MG	RA	3096	1/1	0.90	0.20	44,44,44,44	0
57	MG	YA	3147	1/1	0.90	0.14	43,43,43,43	0
57	MG	XA	1686	1/1	0.90	0.14	61,61,61,61	0
57	MG	QA	1645	1/1	0.90	0.22	58,58,58,58	0
57	MG	XA	1614	1/1	0.90	0.37	50,50,50,50	0
57	MG	QA	1601	1/1	0.90	0.28	67,67,67,67	0
57	MG	RA	3015	1/1	0.90	0.20	44,44,44,44	0
57	MG	YA	3227	1/1	0.90	0.29	57,57,57,57	0
57	MG	RA	3205	1/1	0.90	0.26	46,46,46,46	0
57	MG	RA	3080	1/1	0.90	0.15	62,62,62,62	0
57	MG	YA	3039	1/1	0.90	0.16	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3165	1/1	0.90	0.34	76,76,76,76	0
57	MG	YA	3098	1/1	0.90	0.24	68,68,68,68	0
57	MG	RA	3053	1/1	0.90	0.33	41,41,41,41	0
57	MG	XA	1620	1/1	0.90	0.17	55,55,55,55	0
57	MG	YA	3172	1/1	0.90	0.28	46,46,46,46	0
57	MG	YA	3173	1/1	0.90	0.08	65,65,65,65	0
57	MG	RA	3067	1/1	0.90	0.30	46,46,46,46	0
57	MG	RA	3177	1/1	0.90	0.24	52,52,52,52	0
57	MG	YA	3257	1/1	0.90	0.20	62,62,62,62	0
57	MG	YA	3176	1/1	0.90	0.30	67,67,67,67	0
57	MG	RA	3178	1/1	0.90	0.15	62,62,62,62	0
57	MG	RA	3132	1/1	0.90	0.14	65,65,65,65	0
57	MG	RA	3154	1/1	0.90	0.16	48,48,48,48	0
57	MG	YA	3114	1/1	0.90	0.20	35,35,35,35	0
57	MG	YA	3184	1/1	0.90	0.09	82,82,82,82	0
57	MG	XA	1632	1/1	0.90	0.09	51,51,51,51	0
57	MG	RA	3183	1/1	0.90	0.21	62,62,62,62	0
57	MG	RA	3068	1/1	0.90	0.16	61,61,61,61	0
57	MG	QA	1606	1/1	0.90	0.38	62,62,62,62	0
57	MG	XA	1636	1/1	0.90	0.08	73,73,73,73	0
57	MG	RA	3158	1/1	0.90	0.09	48,48,48,48	0
57	MG	RA	3044	1/1	0.90	0.20	62,62,62,62	0
57	MG	XA	1674	1/1	0.90	0.14	64,64,64,64	0
57	MG	YA	3065	1/1	0.90	0.20	56,56,56,56	0
57	MG	RA	3160	1/1	0.90	0.08	56,56,56,56	0
57	MG	XA	1643	1/1	0.91	0.28	79,79,79,79	0
57	MG	YA	3005	1/1	0.91	0.07	37,37,37,37	0
57	MG	YA	3056	1/1	0.91	0.25	43,43,43,43	0
57	MG	YA	3057	1/1	0.91	0.19	37,37,37,37	0
57	MG	RA	3115	1/1	0.91	0.20	39,39,39,39	0
57	MG	YA	3203	1/1	0.91	0.13	64,64,64,64	0
57	MG	YA	3008	1/1	0.91	0.21	38,38,38,38	0
57	MG	YA	3010	1/1	0.91	0.37	33,33,33,33	0
57	MG	YA	3134	1/1	0.91	0.18	49,49,49,49	0
57	MG	YA	3011	1/1	0.91	0.25	37,37,37,37	0
57	MG	QA	1686	1/1	0.91	0.12	129,129,129,129	0
57	MG	QA	1612	1/1	0.91	0.29	61,61,61,61	0
57	MG	RA	3244	1/1	0.91	0.23	88,88,88,88	0
57	MG	YA	3213	1/1	0.91	0.14	59,59,59,59	0
57	MG	YA	3214	1/1	0.91	0.28	72,72,72,72	0
57	MG	RA	3098	1/1	0.91	0.31	50,50,50,50	0
57	MG	YA	3017	1/1	0.91	0.11	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3217	1/1	0.91	0.21	33,33,33,33	0
57	MG	YA	3220	1/1	0.91	0.21	57,57,57,57	0
57	MG	YA	3018	1/1	0.91	0.22	28,28,28,28	0
57	MG	XA	1679	1/1	0.91	0.32	47,47,47,47	0
57	MG	RA	3035	1/1	0.91	0.24	49,49,49,49	0
57	MG	RA	3121	1/1	0.91	0.19	57,57,57,57	0
57	MG	YA	3078	1/1	0.91	0.28	35,35,35,35	0
57	MG	RA	3083	1/1	0.91	0.12	62,62,62,62	0
57	MG	YA	3234	1/1	0.91	0.29	46,46,46,46	0
57	MG	XA	1621	1/1	0.91	0.13	63,63,63,63	0
57	MG	YA	3084	1/1	0.91	0.21	51,51,51,51	0
57	MG	YA	3161	1/1	0.91	0.18	47,47,47,47	0
57	MG	YA	3242	1/1	0.91	0.21	38,38,38,38	0
57	MG	XA	1654	1/1	0.91	0.16	58,58,58,58	0
57	MG	YA	3027	1/1	0.91	0.41	37,37,37,37	0
57	MG	YA	3090	1/1	0.91	0.23	39,39,39,39	0
57	MG	YA	3028	1/1	0.91	0.12	30,30,30,30	0
57	MG	RA	3195	1/1	0.91	0.26	59,59,59,59	0
57	MG	XA	1625	1/1	0.91	0.06	53,53,53,53	0
57	MG	RA	3018	1/1	0.91	0.19	47,47,47,47	0
57	MG	RA	3108	1/1	0.91	0.07	51,51,51,51	0
57	MG	YA	3099	1/1	0.91	0.21	31,31,31,31	0
57	MG	QA	1660	1/1	0.91	0.34	56,56,56,56	0
57	MG	YA	3177	1/1	0.91	0.35	47,47,47,47	0
57	MG	RA	3075	1/1	0.91	0.19	40,40,40,40	0
57	MG	RA	3051	1/1	0.91	0.24	60,60,60,60	0
57	MG	RA	3226	1/1	0.91	0.17	44,44,44,44	0
57	MG	RA	3042	1/1	0.91	0.18	44,44,44,44	0
57	MG	YA	3183	1/1	0.91	0.09	79,79,79,79	0
57	MG	XA	1602	1/1	0.91	0.41	47,47,47,47	0
57	MG	RA	3202	1/1	0.91	0.21	55,55,55,55	0
57	MG	RA	3156	1/1	0.91	0.27	63,63,63,63	0
57	MG	RA	3232	1/1	0.91	0.33	45,45,45,45	0
57	MG	QA	1673	1/1	0.91	0.18	65,65,65,65	0
57	MG	RA	3136	1/1	0.91	0.21	44,44,44,44	0
57	MG	YA	3001	1/1	0.91	0.16	30,30,30,30	0
57	MG	YA	3192	1/1	0.91	0.18	69,69,69,69	0
57	MG	YA	3037	1/1	0.92	0.21	29,29,29,29	0
57	MG	RA	3180	1/1	0.92	0.19	69,69,69,69	0
57	MG	XA	1628	1/1	0.92	0.25	67,67,67,67	0
57	MG	RA	3129	1/1	0.92	0.19	68,68,68,68	0
57	MG	YA	3155	1/1	0.92	0.20	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3156	1/1	0.92	0.15	46,46,46,46	0
57	MG	RA	3084	1/1	0.92	0.21	46,46,46,46	0
57	MG	RA	3028	1/1	0.92	0.18	46,46,46,46	0
57	MG	YA	3097	1/1	0.92	0.15	29,29,29,29	0
57	MG	YA	3218	1/1	0.92	0.25	48,48,48,48	0
57	MG	RA	3070	1/1	0.92	0.34	49,49,49,49	0
57	MG	YA	3221	1/1	0.92	0.17	37,37,37,37	0
57	MG	RA	3187	1/1	0.92	0.06	60,60,60,60	0
57	MG	RA	3218	1/1	0.92	0.28	58,58,58,58	0
57	MG	YA	3166	1/1	0.92	0.10	72,72,72,72	0
57	MG	QA	1607	1/1	0.92	0.11	71,71,71,71	0
57	MG	RA	3019	1/1	0.92	0.15	39,39,39,39	0
57	MG	RA	3045	1/1	0.92	0.23	42,42,42,42	0
57	MG	YA	3107	1/1	0.92	0.12	52,52,52,52	0
57	MG	RA	3191	1/1	0.92	0.12	81,81,81,81	0
57	MG	XA	1603	1/1	0.92	0.57	61,61,61,61	0
57	MG	QF	201	1/1	0.92	0.12	77,77,77,77	0
57	MG	RA	3006	1/1	0.92	0.59	81,81,81,81	0
57	MG	QA	1682	1/1	0.92	0.37	77,77,77,77	0
57	MG	RA	3049	1/1	0.92	0.13	40,40,40,40	0
57	MG	RA	3036	1/1	0.92	0.22	42,42,42,42	0
57	MG	RA	3169	1/1	0.92	0.08	60,60,60,60	0
57	MG	RA	3003	1/1	0.92	0.32	53,53,53,53	0
57	MG	RA	3146	1/1	0.92	0.17	58,58,58,58	0
57	MG	RA	3148	1/1	0.92	0.07	96,96,96,96	0
57	MG	RA	3240	1/1	0.92	0.10	52,52,52,52	0
57	MG	RA	3082	1/1	0.92	0.20	38,38,38,38	0
57	MG	RA	3242	1/1	0.92	0.33	71,71,71,71	0
57	MG	YA	3132	1/1	0.92	0.09	62,62,62,62	0
57	MG	YA	3268	1/1	0.92	0.22	71,71,71,71	0
57	MG	RA	3104	1/1	0.92	0.12	54,54,54,54	0
57	MG	XA	1657	1/1	0.92	0.25	52,52,52,52	0
57	MG	RA	3151	1/1	0.92	0.15	74,74,74,74	0
57	MG	YA	3193	1/1	0.92	0.45	31,31,31,31	0
57	MG	YA	3136	1/1	0.92	0.14	46,46,46,46	0
57	MG	YA	3277	1/1	0.92	0.14	58,58,58,58	0
57	MG	RA	3009	1/1	0.92	0.14	43,43,43,43	0
57	MG	YA	3081	1/1	0.92	0.41	29,29,29,29	0
57	MG	XA	1623	1/1	0.92	0.12	73,73,73,73	0
57	MG	YA	3141	1/1	0.92	0.17	58,58,58,58	0
57	MG	YA	3142	1/1	0.92	0.14	38,38,38,38	0
57	MG	YA	3083	1/1	0.92	0.15	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1661	1/1	0.92	0.39	54,54,54,54	0
57	MG	YQ	201	1/1	0.92	0.23	170,170,170,170	0
57	MG	RA	3127	1/1	0.92	0.13	51,51,51,51	0
57	MG	RA	3029	1/1	0.93	0.18	46,46,46,46	0
57	MG	XA	1683	1/1	0.93	0.20	57,57,57,57	0
57	MG	QA	1685	1/1	0.93	0.12	127,127,127,127	0
57	MG	YA	3233	1/1	0.93	0.19	48,48,48,48	0
57	MG	XA	1685	1/1	0.93	0.11	92,92,92,92	0
57	MG	YA	3101	1/1	0.93	0.23	31,31,31,31	0
57	MG	RA	3223	1/1	0.93	0.16	50,50,50,50	0
57	MG	RA	3041	1/1	0.93	0.21	42,42,42,42	0
57	MG	RA	3031	1/1	0.93	0.20	47,47,47,47	0
57	MG	YA	3036	1/1	0.93	0.26	32,32,32,32	0
57	MG	RA	3114	1/1	0.93	0.29	48,48,48,48	0
57	MG	QA	1681	1/1	0.93	0.29	64,64,64,64	0
57	MG	QA	1603	1/1	0.93	0.23	69,69,69,69	0
57	MG	YA	3199	1/1	0.93	0.16	40,40,40,40	0
57	MG	YA	3040	1/1	0.93	0.10	26,26,26,26	0
57	MG	YA	3014	1/1	0.93	0.35	34,34,34,34	0
57	MG	YA	3116	1/1	0.93	0.10	37,37,37,37	0
57	MG	YA	3077	1/1	0.93	0.25	28,28,28,28	0
57	MG	YA	3263	1/1	0.93	0.18	30,30,30,30	0
57	MG	QA	1619	1/1	0.93	0.13	74,74,74,74	0
57	MG	RE	302	1/1	0.93	0.23	41,41,41,41	0
57	MG	YA	3080	1/1	0.93	0.11	53,53,53,53	0
57	MG	XA	1655	1/1	0.93	0.13	63,63,63,63	0
57	MG	YA	3123	1/1	0.93	0.19	42,42,42,42	0
57	MG	YA	3124	1/1	0.93	0.29	31,31,31,31	0
57	MG	YA	3272	1/1	0.93	0.31	54,54,54,54	0
57	MG	YA	3273	1/1	0.93	0.19	51,51,51,51	0
57	MG	RA	3214	1/1	0.93	0.15	55,55,55,55	0
57	MG	RA	3106	1/1	0.93	0.22	46,46,46,46	0
57	MG	QA	1624	1/1	0.93	0.10	83,83,83,83	0
57	MG	XA	1701	1/1	0.93	0.12	56,56,56,56	0
57	MG	YA	3088	1/1	0.93	0.34	43,43,43,43	0
57	MG	RA	3204	1/1	0.93	0.12	52,52,52,52	0
57	MG	YA	3052	1/1	0.93	0.17	32,32,32,32	0
57	MG	YA	3053	1/1	0.93	0.14	44,44,44,44	0
57	MG	RA	3237	1/1	0.93	0.25	39,39,39,39	0
57	MG	RA	3239	1/1	0.93	0.10	55,55,55,55	0
57	MG	YA	3224	1/1	0.93	0.21	57,57,57,57	0
57	MG	RA	3020	1/1	0.93	0.17	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3231	1/1	0.94	0.18	43,43,43,43	0
57	MG	YA	3148	1/1	0.94	0.08	64,64,64,64	0
57	MG	YA	3109	1/1	0.94	0.30	32,32,32,32	0
57	MG	RA	3138	1/1	0.94	0.19	53,53,53,53	0
57	MG	YA	3236	1/1	0.94	0.17	31,31,31,31	0
57	MG	RA	3172	1/1	0.94	0.08	51,51,51,51	0
57	MG	YA	3239	1/1	0.94	0.22	47,47,47,47	0
57	MG	RA	3065	1/1	0.94	0.16	42,42,42,42	0
57	MG	RA	3192	1/1	0.94	0.14	54,54,54,54	0
57	MG	QA	1641	1/1	0.94	0.13	57,57,57,57	0
57	MG	QA	1665	1/1	0.94	0.36	84,84,84,84	0
57	MG	RA	3022	1/1	0.94	0.21	39,39,39,39	0
57	MG	QA	1658	1/1	0.94	0.26	80,80,80,80	0
57	MG	XA	1624	1/1	0.94	0.23	66,66,66,66	0
57	MG	YA	3087	1/1	0.94	0.35	43,43,43,43	0
57	MG	YA	3204	1/1	0.94	0.17	43,43,43,43	0
57	MG	YA	3256	1/1	0.94	0.15	57,57,57,57	0
57	MG	YA	3205	1/1	0.94	0.09	51,51,51,51	0
57	MG	RA	3238	1/1	0.94	0.08	43,43,43,43	0
57	MG	RA	3101	1/1	0.94	0.19	41,41,41,41	0
57	MG	YA	3167	1/1	0.94	0.33	41,41,41,41	0
57	MG	YA	3126	1/1	0.94	0.10	32,32,32,32	0
57	MG	RA	3116	1/1	0.94	0.12	56,56,56,56	0
57	MG	YA	3170	1/1	0.94	0.13	44,44,44,44	0
57	MG	RA	3161	1/1	0.94	0.12	62,62,62,62	0
57	MG	XV	102	1/1	0.94	0.19	32,32,32,32	0
57	MG	RA	3147	1/1	0.94	0.22	71,71,71,71	0
57	MG	RA	3221	1/1	0.94	0.29	36,36,36,36	0
57	MG	XA	1607	1/1	0.94	0.09	93,93,93,93	0
57	MG	YA	3002	1/1	0.94	0.28	31,31,31,31	0
57	MG	YA	3003	1/1	0.94	0.33	32,32,32,32	0
57	MG	RA	3089	1/1	0.94	0.17	51,51,51,51	0
57	MG	XA	1609	1/1	0.94	0.14	46,46,46,46	0
57	MG	RA	3011	1/1	0.94	0.34	43,43,43,43	0
57	MG	QA	1626	1/1	0.94	0.06	79,79,79,79	0
57	MG	RA	3039	1/1	0.94	0.16	39,39,39,39	0
57	MG	YA	3105	1/1	0.94	0.12	41,41,41,41	0
57	MG	YA	3106	1/1	0.94	0.21	60,60,60,60	0
57	MG	XA	1638	1/1	0.94	0.36	48,48,48,48	0
57	MG	RA	3095	1/1	0.94	0.19	39,39,39,39	0
57	MG	YA	3247	1/1	0.95	0.27	44,44,44,44	0
57	MG	RA	3072	1/1	0.95	0.16	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3059	1/1	0.95	0.16	32,32,32,32	0
57	MG	RA	3229	1/1	0.95	0.17	50,50,50,50	0
57	MG	RA	3230	1/1	0.95	0.07	60,60,60,60	0
57	MG	YA	3086	1/1	0.95	0.20	37,37,37,37	0
57	MG	YA	3260	1/1	0.95	0.15	39,39,39,39	0
57	MG	QV	102	1/1	0.95	0.20	45,45,45,45	0
57	MG	YA	3043	1/1	0.95	0.12	39,39,39,39	0
57	MG	XA	1696	1/1	0.95	0.10	65,65,65,65	0
57	MG	XA	1680	1/1	0.95	0.07	47,47,47,47	0
57	MG	YA	3267	1/1	0.95	0.32	67,67,67,67	0
57	MG	RA	3181	1/1	0.95	0.08	82,82,82,82	0
57	MG	YA	3093	1/1	0.95	0.16	46,46,46,46	0
57	MG	RA	3061	1/1	0.95	0.18	38,38,38,38	0
57	MG	YA	3201	1/1	0.95	0.40	63,63,63,63	0
57	MG	YA	3071	1/1	0.95	0.08	30,30,30,30	0
57	MG	RA	3194	1/1	0.95	0.06	75,75,75,75	0
57	MG	RA	3062	1/1	0.95	0.06	70,70,70,70	0
57	MG	RA	3184	1/1	0.95	0.09	40,40,40,40	0
57	MG	YA	3151	1/1	0.95	0.37	30,30,30,30	0
57	MG	YA	3179	1/1	0.95	0.41	48,48,48,48	0
57	MG	YA	3238	1/1	0.95	0.20	41,41,41,41	0
57	MG	QA	1650	1/1	0.95	0.05	65,65,65,65	0
57	MG	RA	3145	1/1	0.95	0.14	52,52,52,52	0
57	MG	YA	3054	1/1	0.95	0.30	28,28,28,28	0
57	MG	QA	1608	1/1	0.95	0.09	71,71,71,71	0
57	MG	RA	3128	1/1	0.95	0.08	44,44,44,44	0
57	MG	YA	3185	1/1	0.95	0.05	57,57,57,57	0
57	MG	QM	201	1/1	0.95	0.10	154,154,154,154	0
58	ZN	QD	301	1/1	0.95	0.24	115,115,115,115	0
58	ZN	XD	1702	1/1	0.95	0.22	103,103,103,103	0
57	MG	RA	3170	1/1	0.96	0.04	38,38,38,38	0
57	MG	RA	3001	1/1	0.96	0.08	42,42,42,42	0
57	MG	QA	1644	1/1	0.96	0.08	62,62,62,62	0
57	MG	YA	3259	1/1	0.96	0.14	33,33,33,33	0
57	MG	RA	3134	1/1	0.96	0.12	46,46,46,46	0
57	MG	YA	3261	1/1	0.96	0.18	34,34,34,34	0
57	MG	YA	3144	1/1	0.96	0.09	66,66,66,66	0
57	MG	RA	3037	1/1	0.96	0.14	41,41,41,41	0
57	MG	YA	3120	1/1	0.96	0.30	53,53,53,53	0
57	MG	RA	3247	1/1	0.96	0.06	58,58,58,58	0
57	MG	RA	3103	1/1	0.96	0.08	50,50,50,50	0
57	MG	YA	3060	1/1	0.96	0.12	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3024	1/1	0.96	0.12	37,37,37,37	0
57	MG	YA	3006	1/1	0.96	0.11	38,38,38,38	0
57	MG	RA	3056	1/1	0.96	0.23	40,40,40,40	0
57	MG	RA	3165	1/1	0.96	0.09	60,60,60,60	0
57	MG	YA	3129	1/1	0.96	0.17	73,73,73,73	0
57	MG	RA	3092	1/1	0.96	0.40	54,54,54,54	0
57	MG	YA	3157	1/1	0.96	0.05	37,37,37,37	0
57	MG	RA	3093	1/1	0.96	0.26	38,38,38,38	0
57	MG	YA	3067	1/1	0.96	0.24	45,45,45,45	0
57	MG	RA	3131	1/1	0.96	0.03	64,64,64,64	0
57	MG	XA	1640	1/1	0.96	0.20	73,73,73,73	0
57	MG	YA	3112	1/1	0.96	0.05	33,33,33,33	0
57	MG	YA	3163	1/1	0.96	0.07	67,67,67,67	0
57	MG	RP	201	1/1	0.96	0.14	132,132,132,132	0
57	MG	RA	3215	1/1	0.96	0.18	65,65,65,65	0
57	MG	YA	3219	1/1	0.96	0.05	60,60,60,60	0
57	MG	YA	3251	1/1	0.96	0.26	32,32,32,32	0
57	MG	YA	3252	1/1	0.96	0.20	43,43,43,43	0
57	MG	YA	3253	1/1	0.96	0.39	29,29,29,29	0
57	MG	QA	1663	1/1	0.97	0.10	73,73,73,73	0
57	MG	RA	3246	1/1	0.97	0.04	69,69,69,69	0
57	MG	RA	3017	1/1	0.97	0.11	43,43,43,43	0
57	MG	YA	3232	1/1	0.97	0.19	43,43,43,43	0
57	MG	YA	3164	1/1	0.97	0.06	67,67,67,67	0
57	MG	YA	3074	1/1	0.97	0.26	38,38,38,38	0
57	MG	XA	1699	1/1	0.97	0.10	87,87,87,87	0
57	MG	YA	3276	1/1	0.97	0.26	162,162,162,162	0
57	MG	RA	3021	1/1	0.97	0.16	38,38,38,38	0
57	MG	XA	1611	1/1	0.97	0.08	51,51,51,51	0
57	MG	YA	3091	1/1	0.97	0.15	42,42,42,42	0
57	MG	XA	1646	1/1	0.97	0.07	97,97,97,97	0
57	MG	RA	3105	1/1	0.97	0.08	42,42,42,42	0
57	MG	YA	3241	1/1	0.97	0.33	31,31,31,31	0
57	MG	RA	3058	1/1	0.97	0.27	47,47,47,47	0
57	MG	QA	1609	1/1	0.97	0.07	61,61,61,61	0
57	MG	YA	3125	1/1	0.97	0.09	39,39,39,39	0
57	MG	YA	3266	1/1	0.97	0.17	33,33,33,33	0
57	MG	YA	3044	1/1	0.97	0.28	33,33,33,33	0
57	MG	YA	3009	1/1	0.97	0.15	39,39,39,39	0
57	MG	RA	3087	1/1	0.98	0.29	37,37,37,37	0
57	MG	QA	1627	1/1	0.98	0.09	62,62,62,62	0
57	MG	XA	1627	1/1	0.98	0.03	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3107	1/1	0.98	0.11	41,41,41,41	0
57	MG	YA	3255	1/1	0.98	0.32	34,34,34,34	0
57	MG	RA	3074	1/1	0.98	0.05	49,49,49,49	0
57	MG	XA	1693	1/1	0.98	0.11	51,51,51,51	0
57	MG	YA	3258	1/1	0.98	0.10	48,48,48,48	0
57	MG	YA	3196	1/1	0.98	0.08	51,51,51,51	0
57	MG	YA	3197	1/1	0.98	0.05	46,46,46,46	0
57	MG	YA	3068	1/1	0.98	0.05	43,43,43,43	0
57	MG	RA	3233	1/1	0.98	0.14	50,50,50,50	0
57	MG	YA	3228	1/1	0.98	0.13	98,98,98,98	0
57	MG	YA	3029	1/1	0.98	0.12	31,31,31,31	0
57	MG	YA	3230	1/1	0.98	0.11	57,57,57,57	0
57	MG	RA	3203	1/1	0.98	0.04	56,56,56,56	0
57	MG	YA	3248	1/1	0.98	0.17	31,31,31,31	0
57	MG	YA	3152	1/1	0.98	0.07	32,32,32,32	0
57	MG	YA	3021	1/1	0.98	0.35	42,42,42,42	0
57	MG	YA	3110	1/1	0.99	0.02	36,36,36,36	0
57	MG	RA	3167	1/1	0.99	0.02	60,60,60,60	0
57	MG	RA	3126	1/1	0.99	0.05	52,52,52,52	0
57	MG	XA	1612	1/1	0.99	0.06	50,50,50,50	0
57	MG	Y5	101	1/1	0.99	0.07	31,31,31,31	0
57	MG	YA	3143	1/1	0.99	0.07	42,42,42,42	0
58	ZN	QN	101	1/1	0.99	0.03	149,149,149,149	0
57	MG	YA	3138	1/1	0.99	0.05	33,33,33,33	0
58	ZN	XN	101	1/1	1.00	0.03	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.