



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 1, 2020 – 08:46 PM BST

PDB ID : 4LFZ  
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-U in the Absence of Paromomycin  
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.  
Deposited on : 2013-06-27  
Resolution : 3.92 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.2

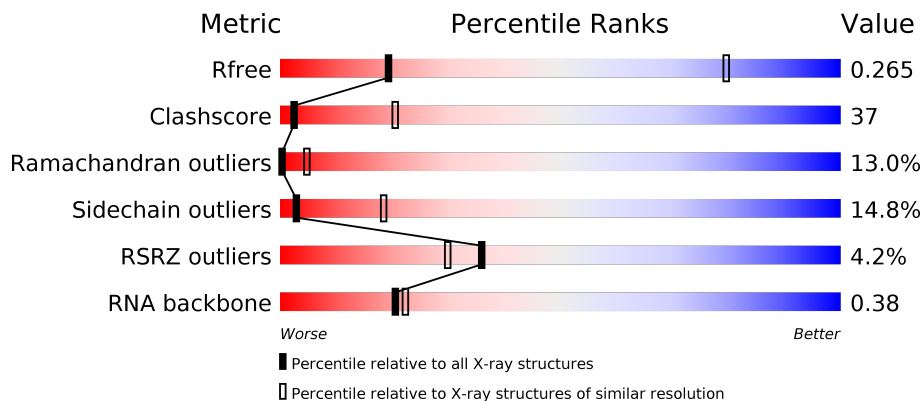
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

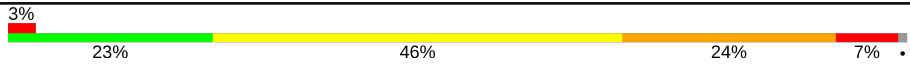
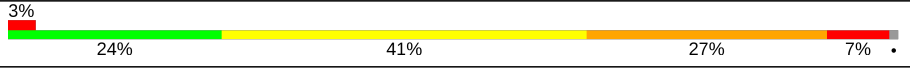
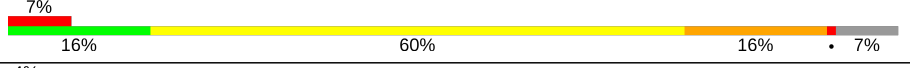
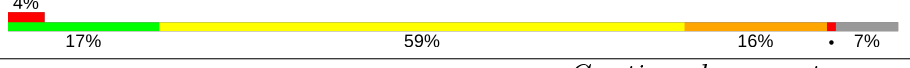
The reported resolution of this entry is 3.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)
RNA backbone	3102	1041 (4.84-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	XA	1522	
2	QB	256	
2	XB	256	

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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	

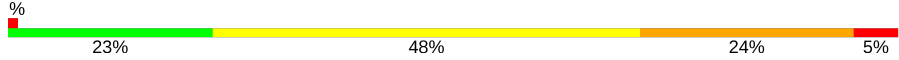
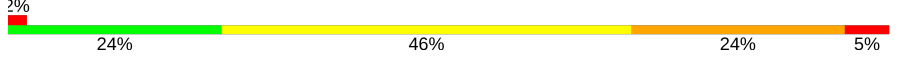

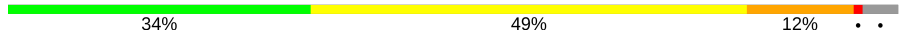
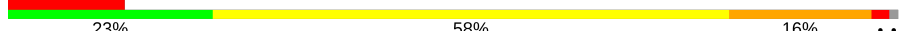
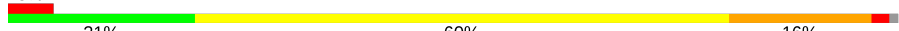
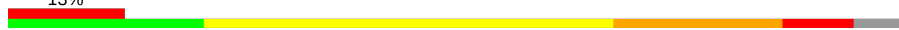



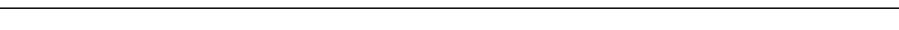

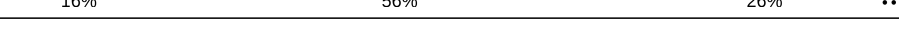




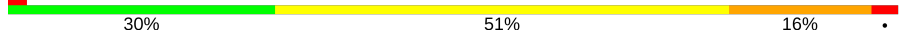

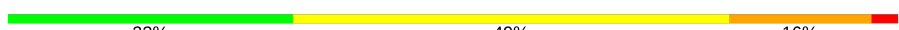
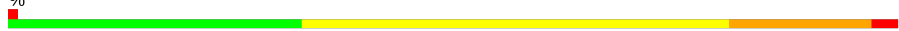


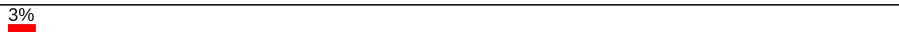
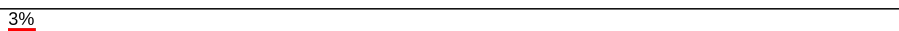
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Mol	Chain	Length	Quality of chain
15	XO	89	4% 31% 56% 11% .
16	QP	88	% 16% 61% 16% . 5%
16	XP	88	2% 17% 61% 15% . 5%
17	QQ	105	3% 36% 48% 11% 5%
17	XQ	105	3% 33% 50% 11% 5%
18	QR	88	% 24% 43% 11% . 20%
18	XR	88	% 24% 43% 11% . 20%
19	QS	93	25% 24% 40% 24% . 10%
19	XS	93	% 22% 42% 23% . 10%
20	QT	106	2% 25% 49% 19% . 7%
20	XT	106	5% 24% 50% 19% . 7%
21	QU	27	37% 19% 56% 19% 7%
21	XU	27	7% 22% 52% 19% 7%
22	QV	77	3% 27% 55% 17% .
22	XV	77	4% 32% 51% 16% .
23	QX	25	4% . . 24% 68%
23	XX	25	. 12% 12% 72%
24	QY	18	22% 28% 28% 22% 22%
24	XY	18	22% 22% 33% 22% 22%
25	RA	2916	5% 20% 40% 30% 9% .
25	YA	2916	4% 16% 38% 35% 10% .
26	RB	122	2% 15% 44% 32% 7% .
26	YB	122	2% 19% 38% 30% 12% .
27	RD	276	% 29% 52% 15% ..
27	YD	276	31% 51% 15% ..

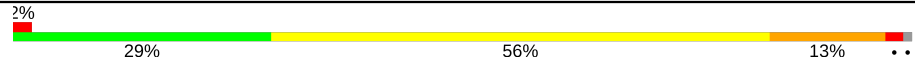
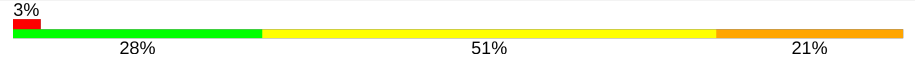
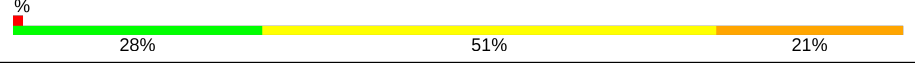
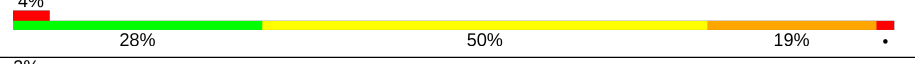
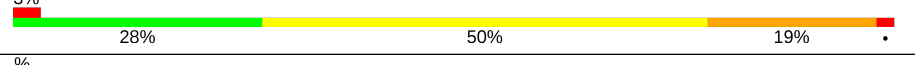
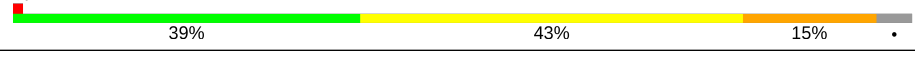
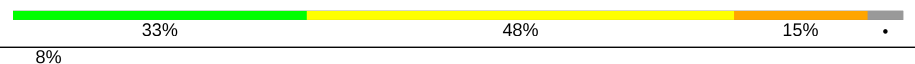

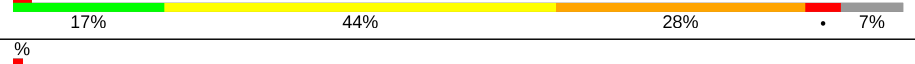
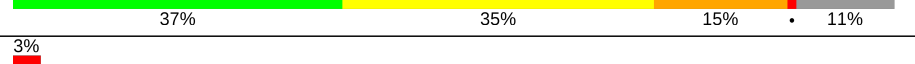
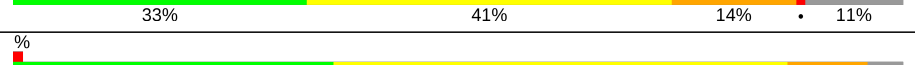

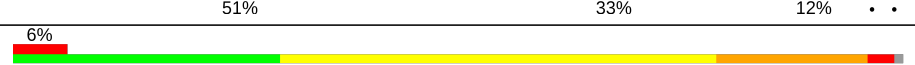
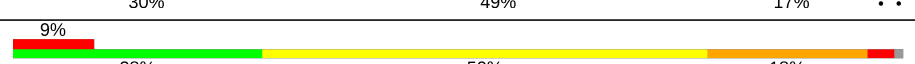
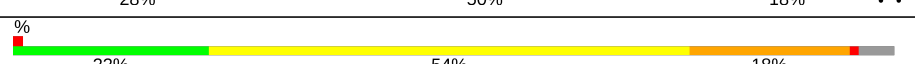
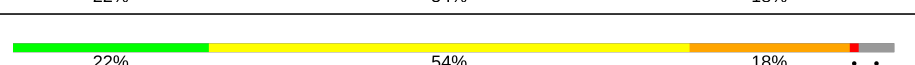
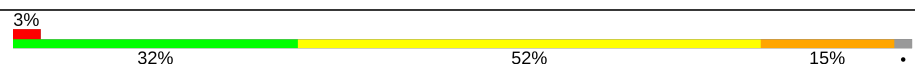
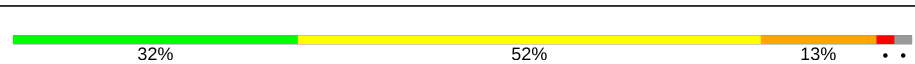


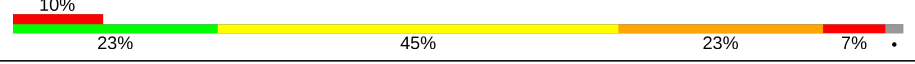
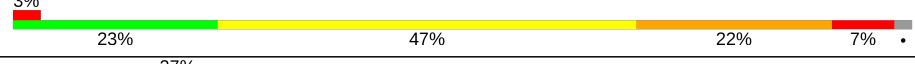



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Mol	Chain	Length	Quality of chain
28	RE	206	 % 23% 48% 24% 5%
28	YE	206	 2% 24% 46% 24% 5%
29	RF	210	 35% 47% 13% ..
29	YF	210	 34% 49% 12% ..
30	RG	182	 13% 23% 58% 16% ..
30	YG	182	 5% 21% 60% 16% ..
31	RH	180	 13% 22% 46% 19% 8% 6%
31	YH	180	 2% 22% 45% 19% 8% 6%
32	RI	148	 3% 28% 56% 12% ..
32	YI	148	 2% 36% 37% 24% ..
33	RN	140	 18% 54% 26% ..
33	YN	140	 16% 56% 26% ..
34	RO	122	 34% 55% 9% .
34	YO	122	 34% 55% 9% .
35	RP	150	 4% 19% 51% 23% 8%
35	YP	150	 2% 19% 51% 23% 7%
36	RQ	141	 2% 30% 51% 16% .
36	YQ	141	 % 30% 50% 16% .
37	RR	118	 32% 49% 16% .
37	YR	118	 % 33% 48% 16% .
38	RS	112	 2% 13% 63% 19% 5% .
38	YS	112	 % 13% 63% 20% ..
39	RT	146	 3% 21% 51% 19% . 6%
39	YT	146	 3% 23% 49% 20% . 6%
40	RU	118	 2% 33% 53% 12% ..

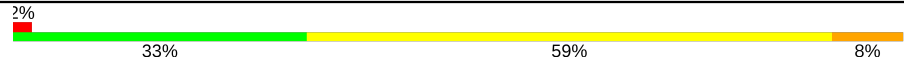

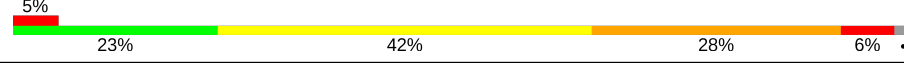
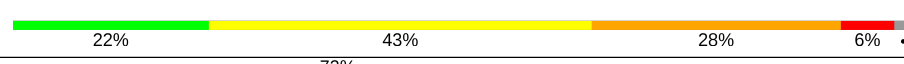
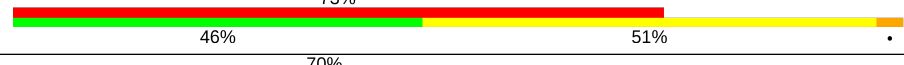
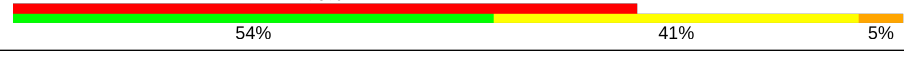

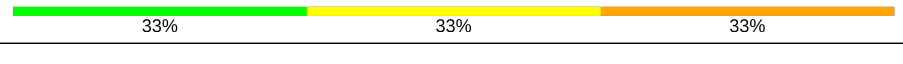
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Mol	Chain	Length	Quality of chain
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4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

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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	Z6	3	
56	Z8	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	1629	-	-	-	X
57	MG	QA	1631	-	-	-	X
57	MG	QF	201	-	-	-	X
57	MG	QX	101	-	-	-	X
57	MG	RA	3003	-	-	-	X
57	MG	RA	3007	-	-	-	X
57	MG	RA	3049	-	-	-	X
57	MG	RA	3062	-	-	-	X
57	MG	RA	3138	-	-	-	X
57	MG	RA	3157	-	-	-	X
57	MG	RA	3173	-	-	-	X
57	MG	RA	3199	-	-	-	X
57	MG	RA	3213	-	-	-	X
57	MG	RA	3219	-	-	-	X
57	MG	RA	3227	-	-	-	X
57	MG	RA	3239	-	-	-	X
57	MG	RP	201	-	-	-	X
57	MG	XA	1642	-	-	-	X
57	MG	YA	3030	-	-	-	X
57	MG	YA	3076	-	-	-	X
57	MG	YA	3100	-	-	-	X
57	MG	YA	3121	-	-	-	X
57	MG	YA	3131	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
57	MG	YA	3152	-	-	-	X
57	MG	YA	3172	-	-	-	X
57	MG	YA	3176	-	-	-	X
57	MG	YA	3183	-	-	-	X
57	MG	YA	3196	-	-	-	X
57	MG	YA	3207	-	-	-	X
57	MG	YA	3242	-	-	-	X
57	MG	YA	3250	-	-	-	X
57	MG	YA	3254	-	-	-	X



## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 291868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			
23	XX	7	Total	C	N	O	P	0	0	0
			145	65	23	50	7			

- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			
24	XY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			

- 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
			62071	27627	11611	19952	2881			
25	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- 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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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			

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

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

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

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

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

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

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

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

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

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

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

- 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	59	Total	C	N	O	S	0	0	0
			459	288	90	76	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 tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
56	Z6	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	Z8	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	64	Total	Mg	0	0
			64	64		
57	RP	1	Total	Mg	0	0
			1	1		
57	QX	1	Total	Mg	0	0
			1	1		
57	YA	269	Total	Mg	0	0
			269	269		
57	QM	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	XX	1	Total Mg 1 1	0	0
57	QV	1	Total Mg 1 1	0	0
57	XA	72	Total Mg 72 72	0	0
57	R0	1	Total Mg 1 1	0	0
57	QH	1	Total Mg 1 1	0	0
57	YQ	1	Total Mg 1 1	0	0
57	R8	1	Total Mg 1 1	0	0
57	RR	2	Total Mg 2 2	0	0
57	RD	1	Total Mg 1 1	0	0
57	Y7	1	Total Mg 1 1	0	0
57	XB	1	Total Mg 1 1	0	0
57	QF	1	Total Mg 1 1	0	0
57	R5	1	Total Mg 1 1	0	0
57	RA	239	Total Mg 239 239	0	0
57	YP	1	Total Mg 1 1	0	0
57	Y5	1	Total Mg 1 1	0	0
57	RE	2	Total Mg 2 2	0	0
57	YB	3	Total Mg 3 3	0	0
57	XV	2	Total Mg 2 2	0	0
57	RB	2	Total Mg 2 2	0	0
57	RF	1	Total Mg 1 1	0	0

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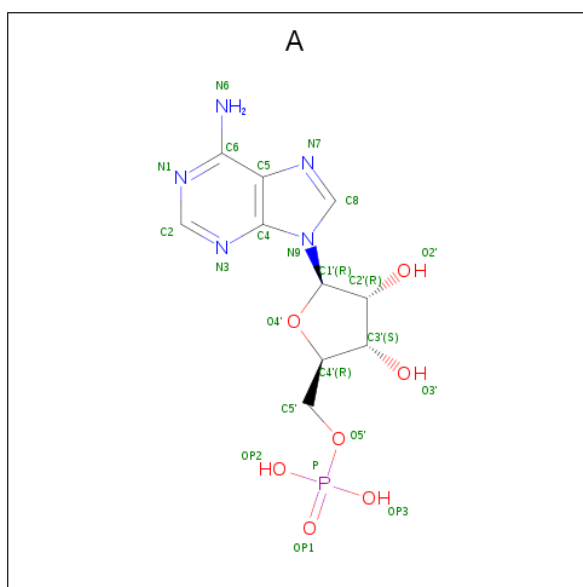
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	XM	1	Total Mg 1 1	0	0
57	YE	1	Total Mg 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	Y9	1	Total Zn 1 1	0	0
58	QN	1	Total Zn 1 1	0	0
58	XN	1	Total Zn 1 1	0	0
58	QD	1	Total Zn 1 1	0	0
58	XD	1	Total Zn 1 1	0	0
58	R9	1	Total Zn 1 1	0	0

- Molecule 59 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).

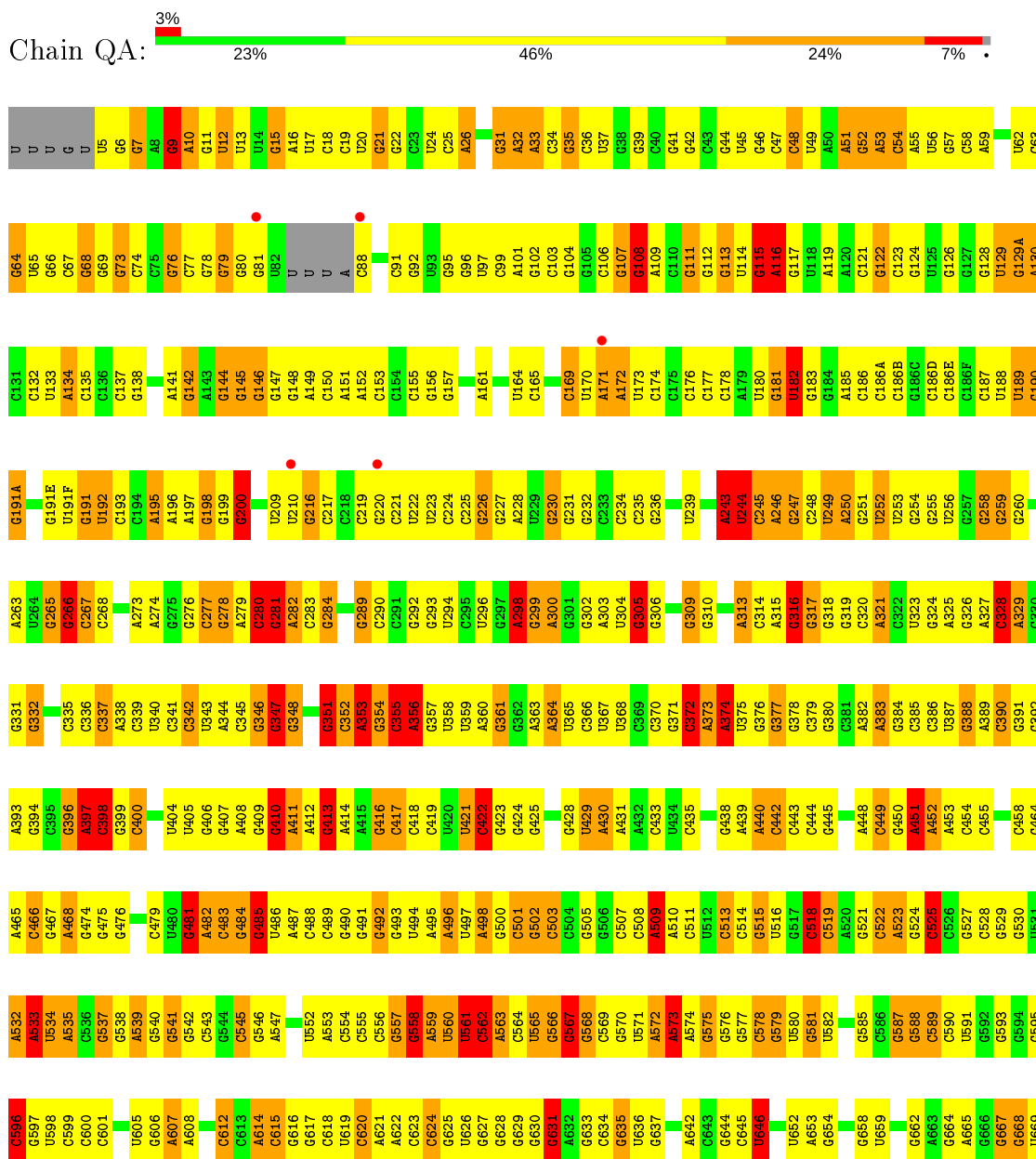


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	XX	1	Total C N O P 22 10 5 6 1	0	0

### 3 Residue-property plots

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

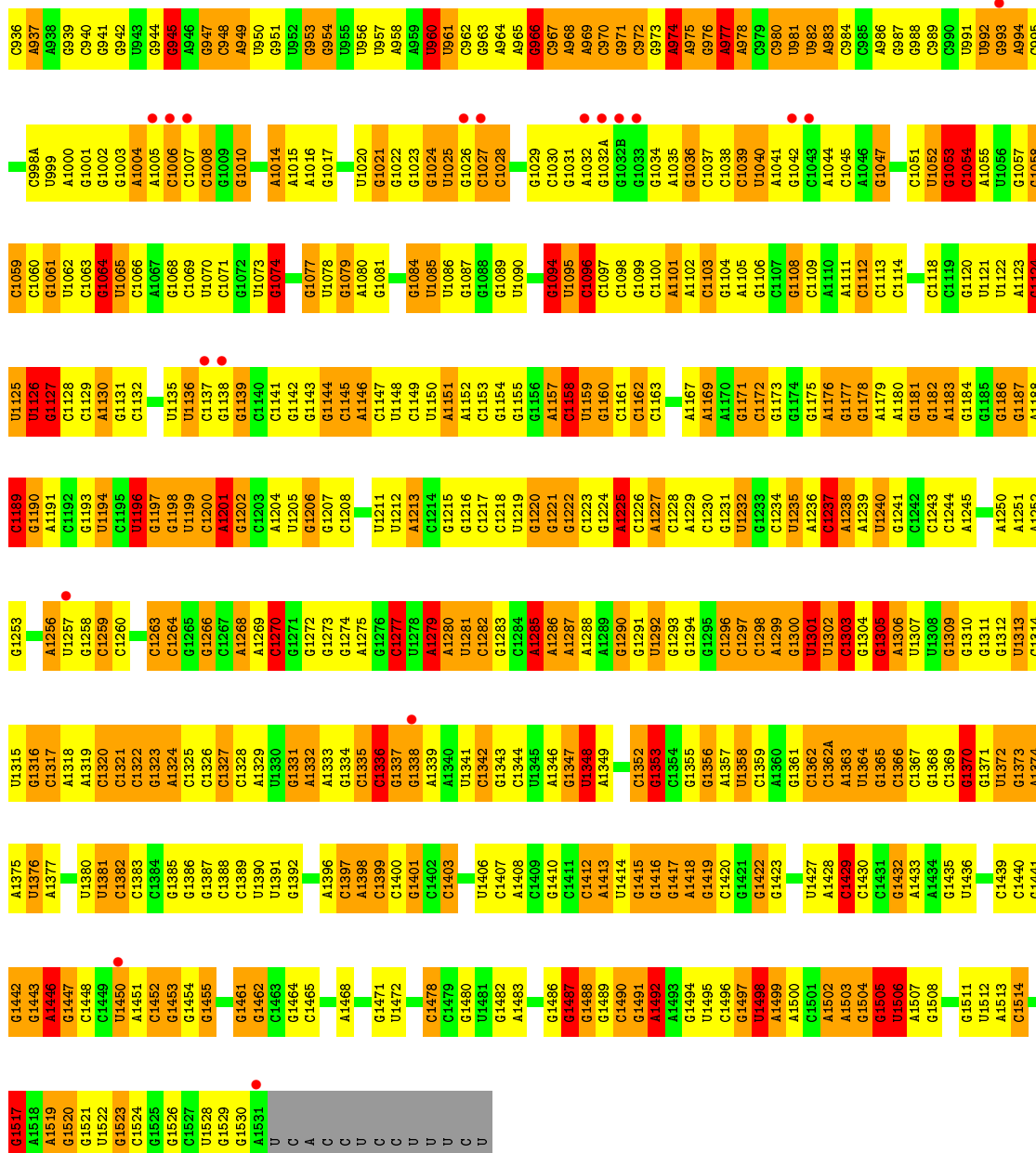
- Molecule 1: 16S rRNA



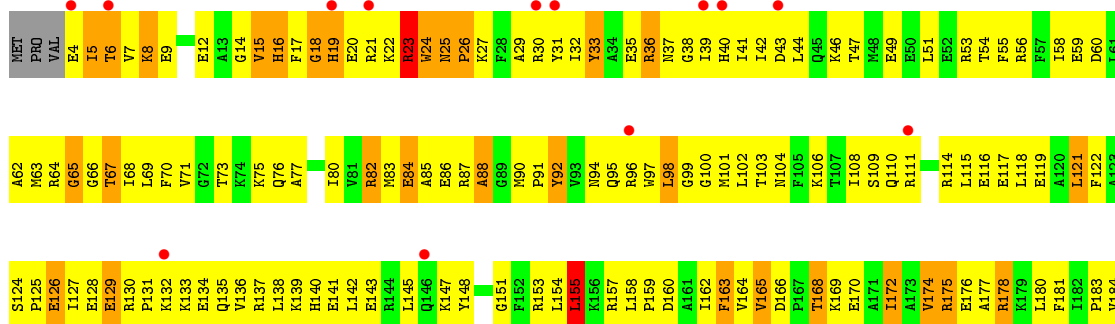
A1513	G1435	G1371	G1312	G1184	G1058	A994	C9824	6869	G799	C736	6670
C1514	U1436	U1372	U1313	G1185	C1059	C995	A935	U870	G800	A737	6671
G1516	C1437	G1373	C1314	G1186	C1060	U999	C936	U871	G803	C738	U672
G1517	G1438	A1374	U1315	G1187	G1061	A1000	A937	A872	U804	C739	G673
A1518	G1439	A1375	G1316	A1188	U1062	G1001	A938	A873	U805	U740	G674
A1519	C1440	U1376	A1317	C1189	C1063	G1002	G939	G874	C805	A675	A675
G1520	G1441	A1377	A1318	G1190	G1064	G1003	C940	C875	G806	C742	A676
G1442	G1442	C1378	A1319	A1191	U1065	A1004	G941	G876	A807	C745	U677
G1443	G1443	G1379	C1320	C1192	C1066	G1005	G942	C877	C808	U746	U678
A1446	A1446	U1380	C1321	G1193	A1067	A1006	U943	C878	C811	A747	C679
G1447	G1447	C1381	C1322	U1194	G1068	G1007	G944	C879	C812	A748	G682
U1450	U1450	G1382	A1323	C1195	C1069	C1008	G945	C880	U813	C749	G683
A1451	A1451	C1383	A1324	U1196	U1070	G1009	A946	C881	A814	G750	A684
G1452	G1452	C1384	C1325	G1197	C1071	A1014	C948	C882	A815	U751	G685
G1453	G1453	G1385	C1326	U1198	G1072	A1015	C949	U883	A816	G752	U686
G1454	G1454	C1386	C1327	U1199	U1073	A1016	U950	U884	A817	A753	A687
G1455	G1455	G1387	A1328	G1200	G1074	A1017	U951	C885	C818	C754	G688
C1459	C1459	C1263	A1201	A1201	C1075	A1018	U952	C886	G951	G755	C689
A1460	A1460	G1266	G1202	G1202	G1076	G1017	U953	C889	U820	C756	C690
G1461	G1461	C1267	C1203	C1203	G1077	C1019	G953	U890	G821	U757	G691
G1469	G1469	A1268	A1204	A1204	U1078	C1018	G954	C891	C822	U758	U692
G1470	G1470	A1269	C1205	G1205	G1079	U1020	U955	U891	C823	A759	G693
G1471	G1471	C1270	G1206	G1206	A1080	G1021	U956	C892	C824	G760	A694
G1472	G1472	G1271	G1207	G1207	U1081	G1022	U957	C893	C825	A761	G695
A1473	A1473	G1272	C1208	C1208	G1082	G1023	A958	C894	G826	C762	A696
G1474	G1474	G1273	C1209	G1209	U1083	G1024	A959	C895	C827	G763	C701
G1475	G1475	G1274	C1210	C1210	G1084	U1025	U960	C896	U828	G764	A702
G1476	G1476	G1275	U1211	U1211	U1085	G1026	U961	C897	A829	C765	G703
G1477	G1477	G1276	A1146	A1146	U1086	C1027	C962	C900	G830	A766	A704
C1478	C1478	C1277	G1147	G1147	G1087	C1028	G963	C901	A827	A767	U705
C1479	C1479	U1278	U1148	U1148	G1088	G1029	A964	A902	U833	A768	U706
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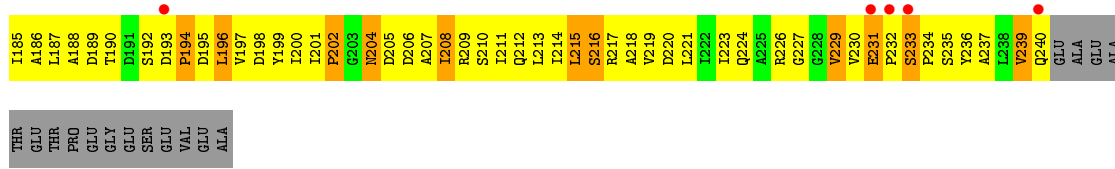




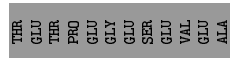
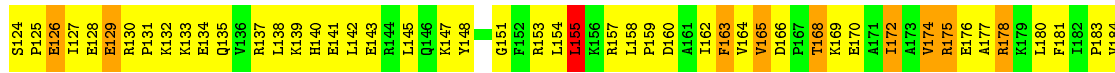
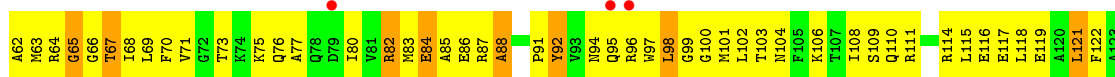
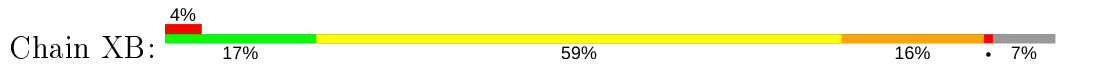


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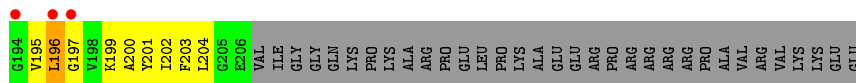
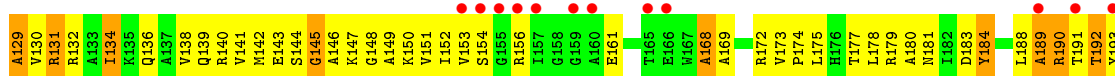
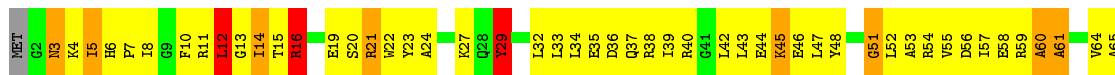
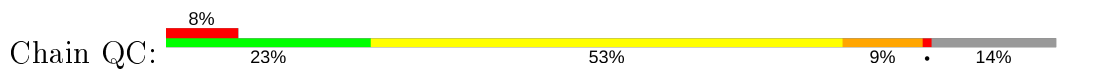




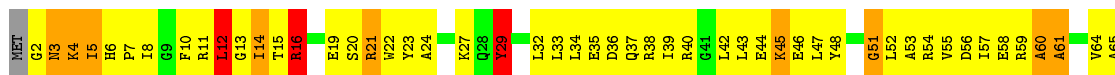
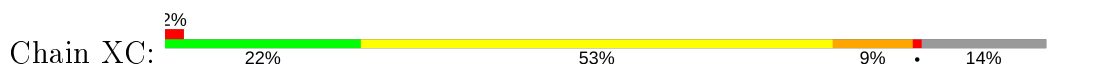
• Molecule 2: 30S ribosomal protein S2

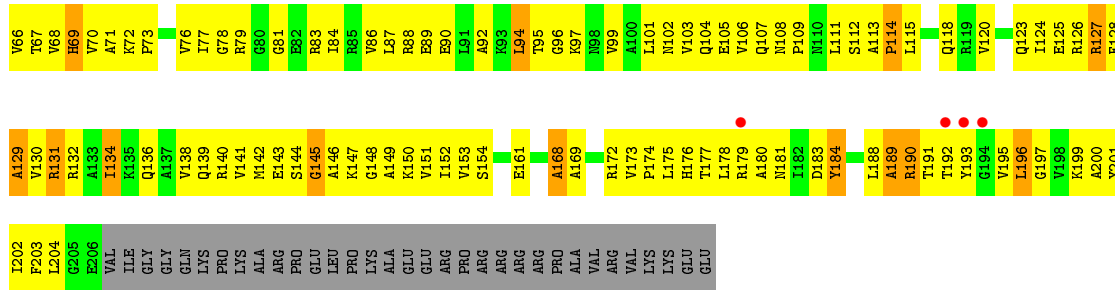


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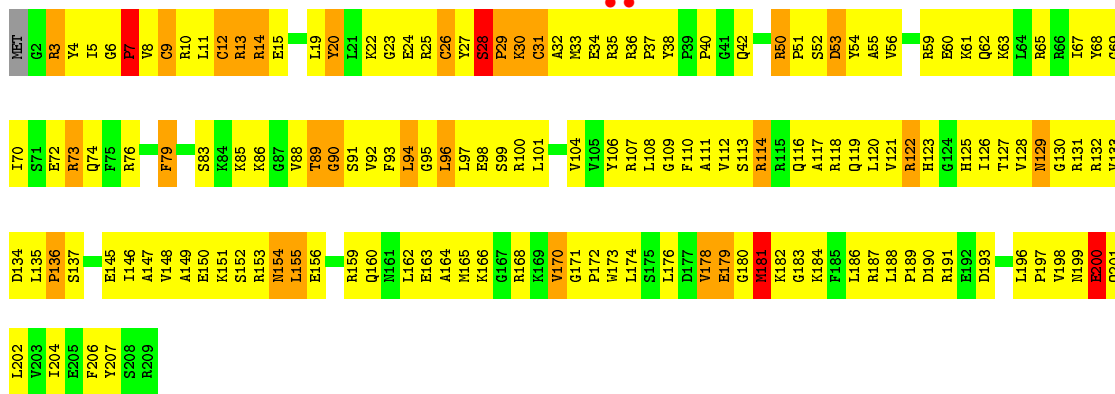


• Molecule 3: 30S ribosomal protein S3

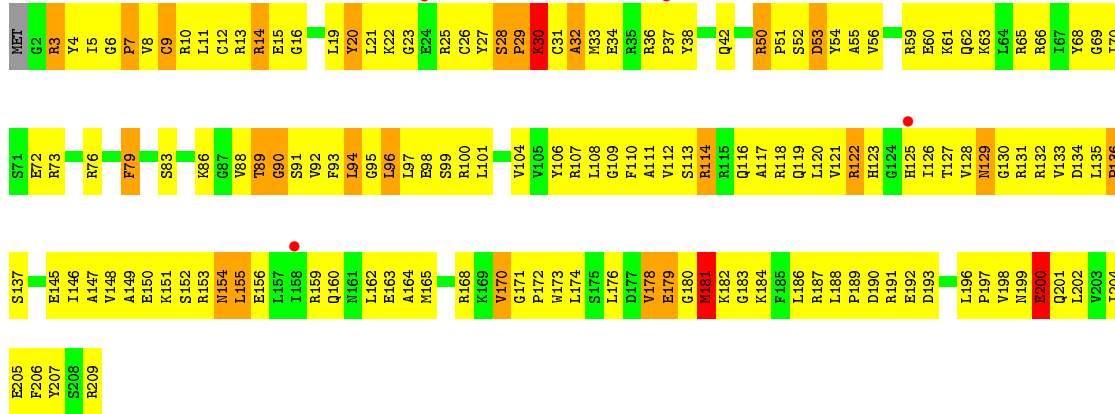




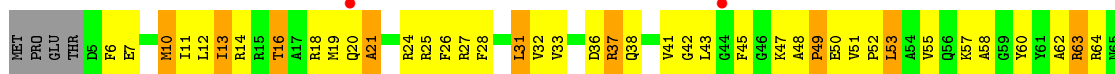
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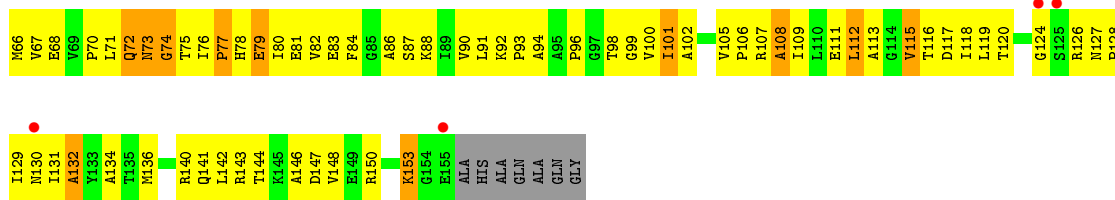


• Molecule 4: 30S ribosomal protein S4

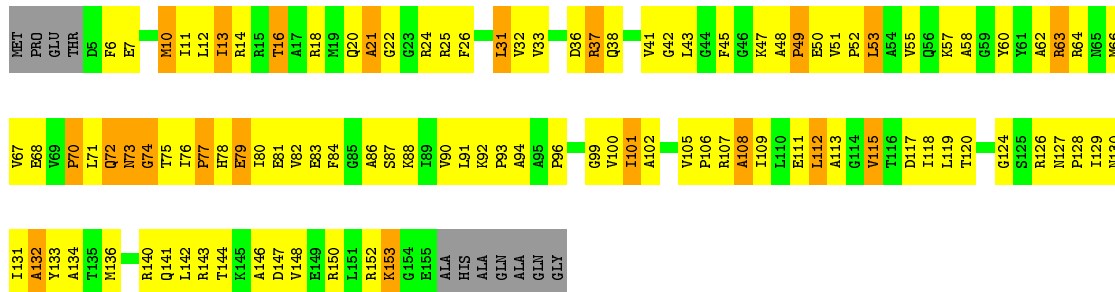
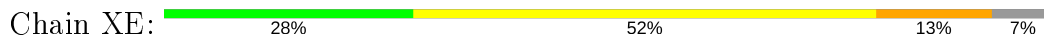


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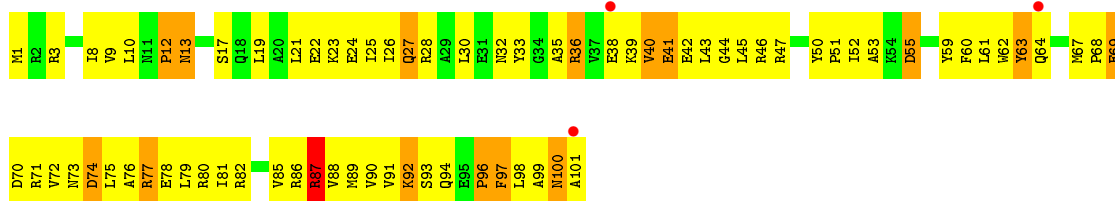




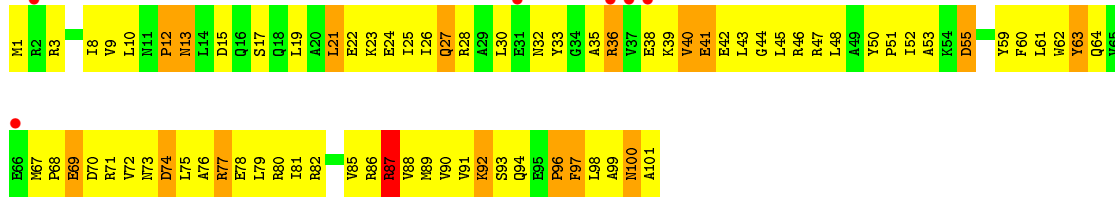
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

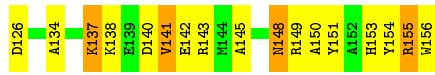
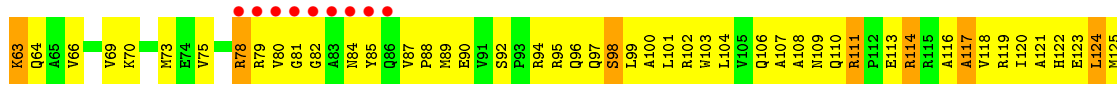


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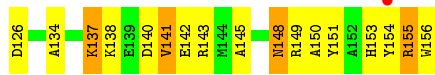


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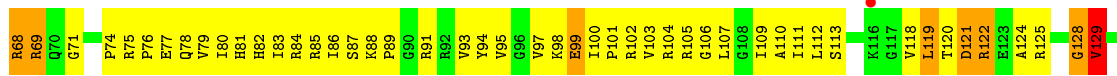
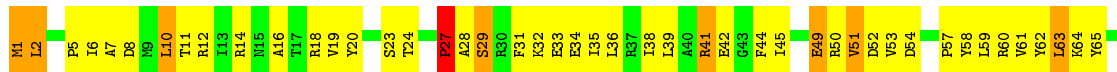




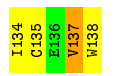
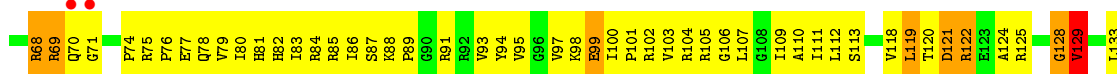
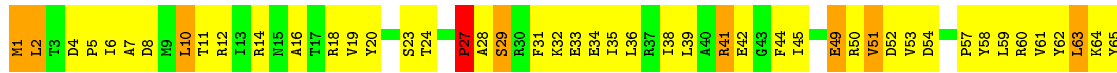
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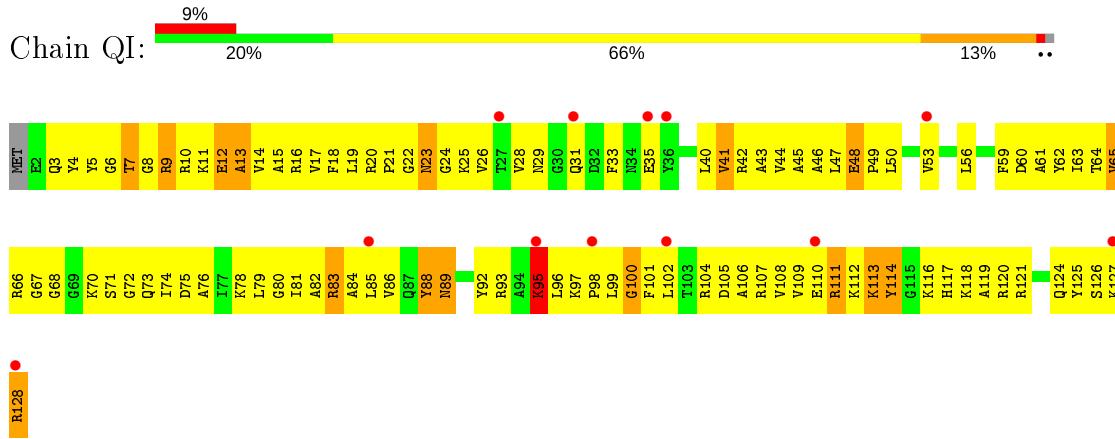
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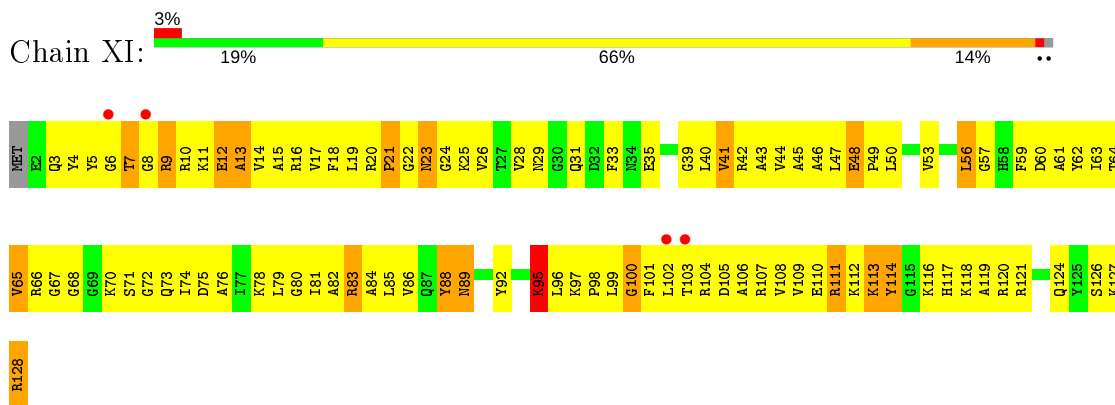
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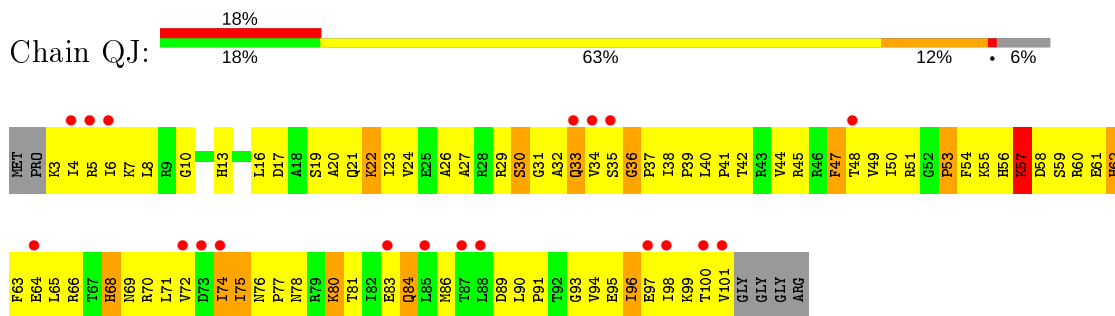
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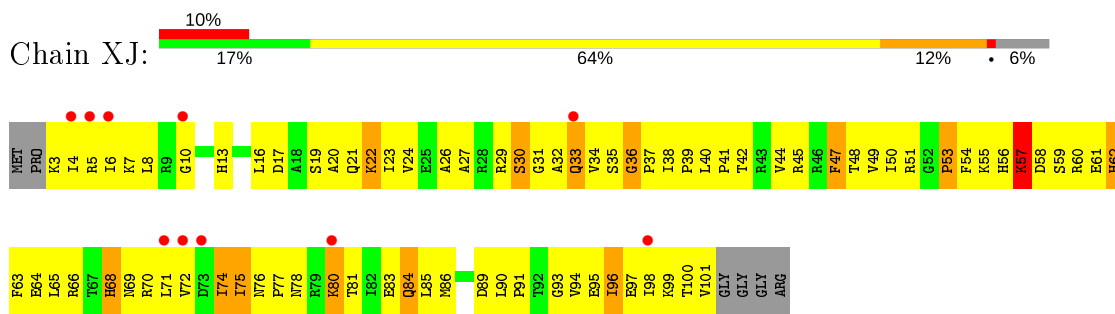
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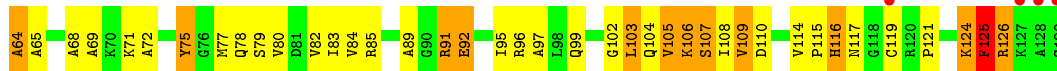
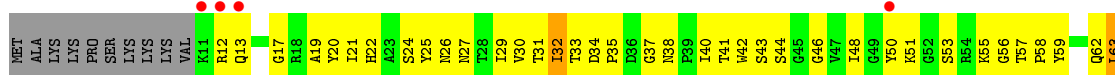
• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10



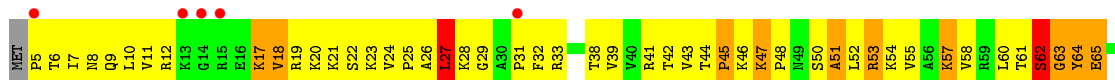
• Molecule 11: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12



• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13

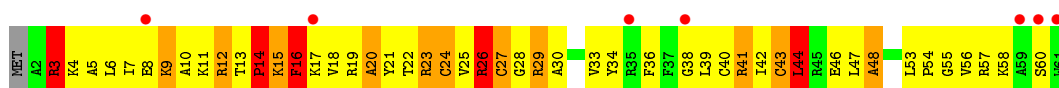
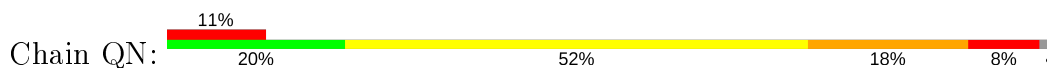




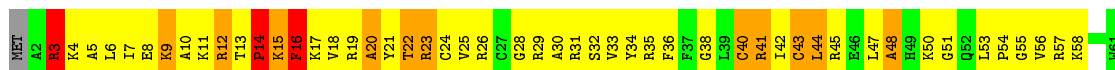
- Molecule 13: 30S ribosomal protein S13



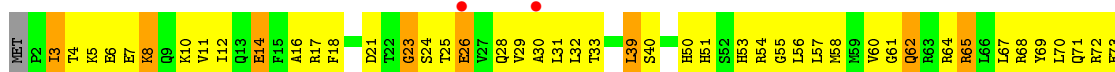
- Molecule 14: 30S ribosomal protein S14



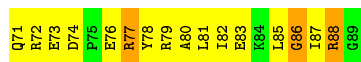
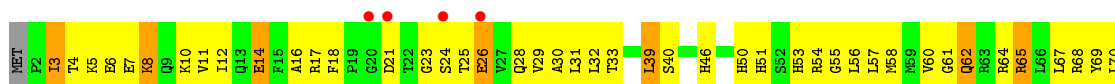
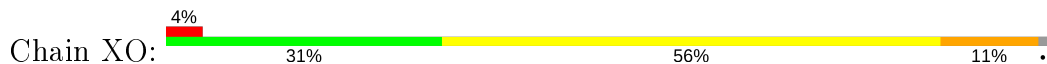
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

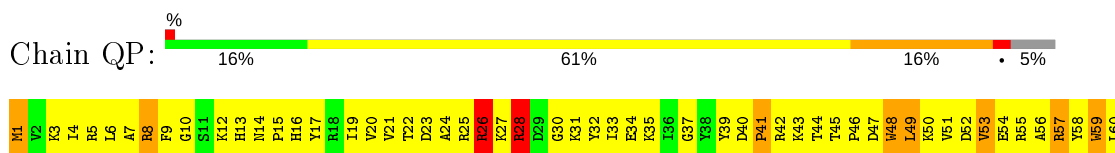


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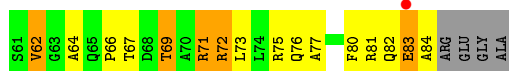
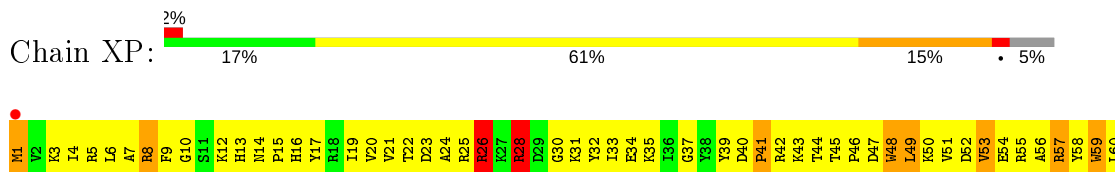


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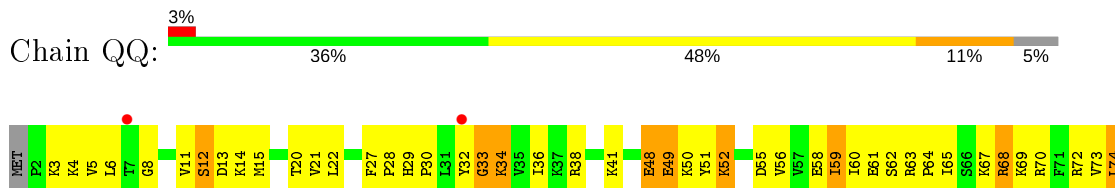




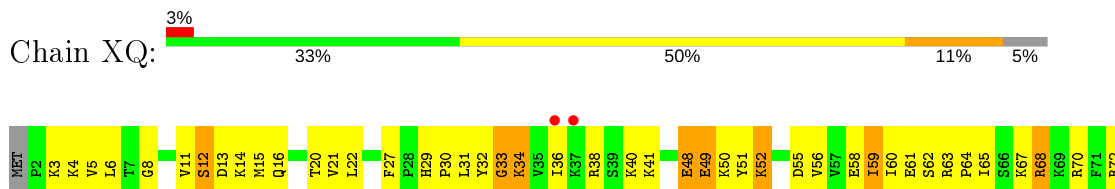
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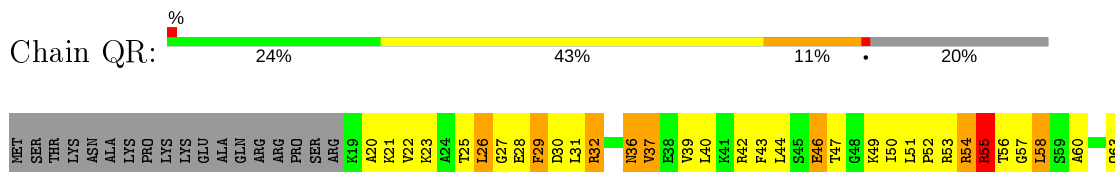
• Molecule 17: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S17

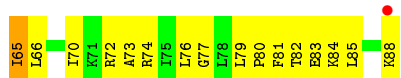


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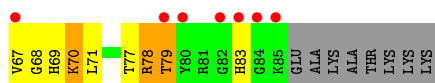
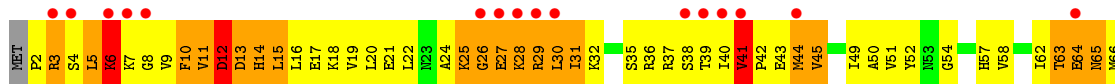
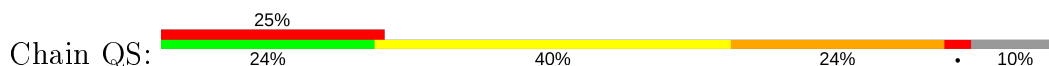




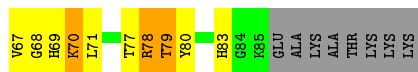
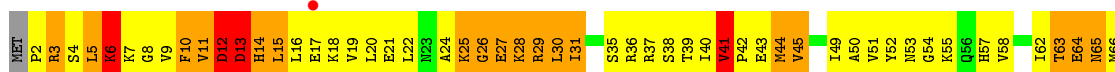
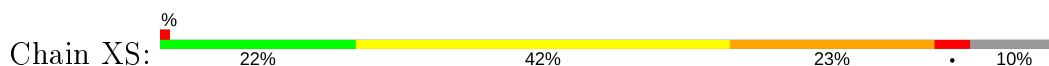
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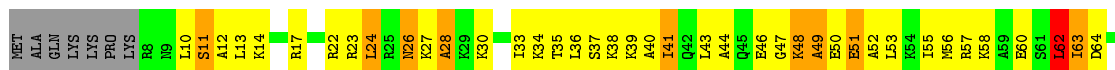
• Molecule 19: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S20

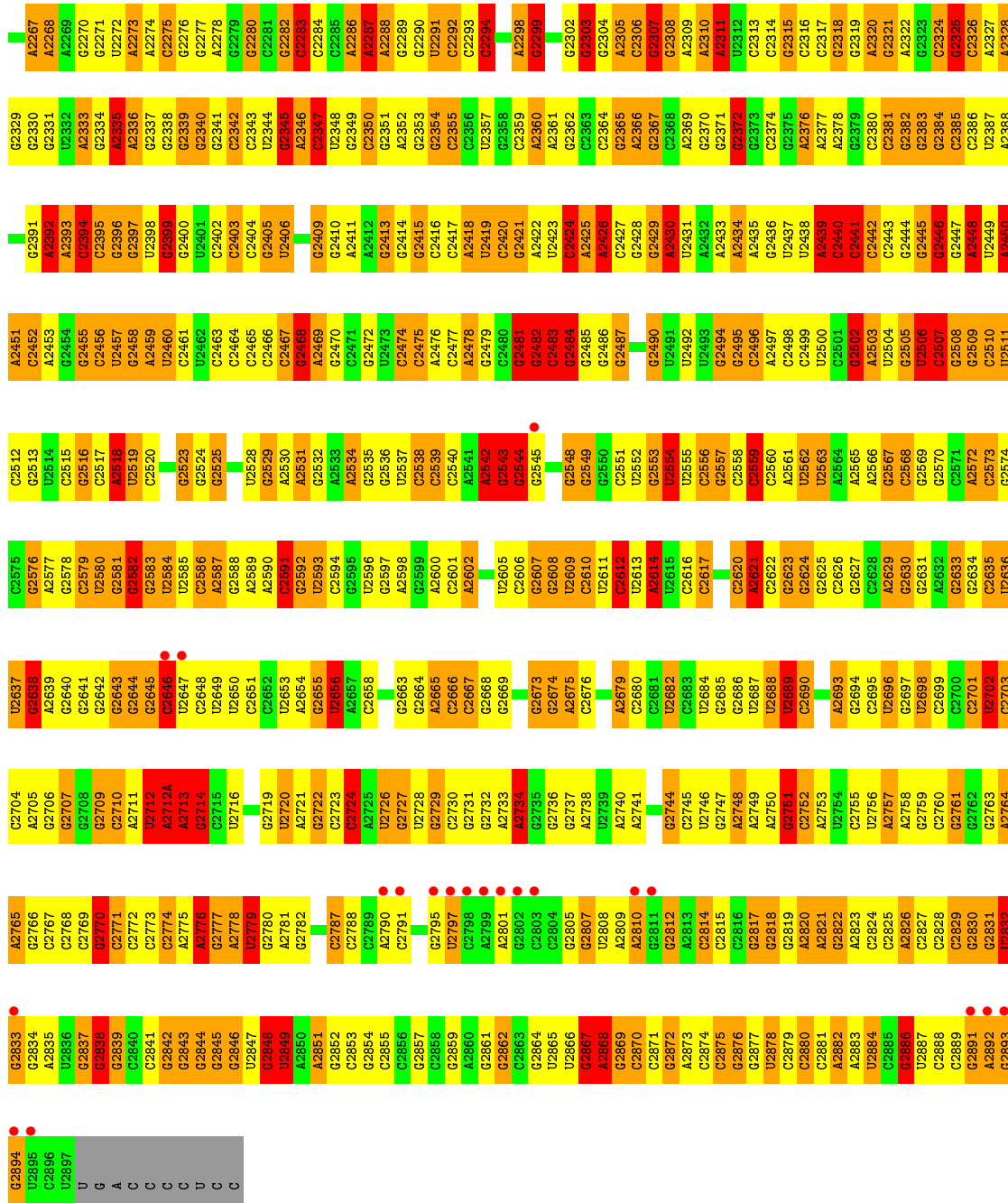




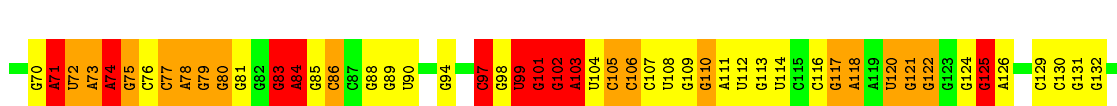
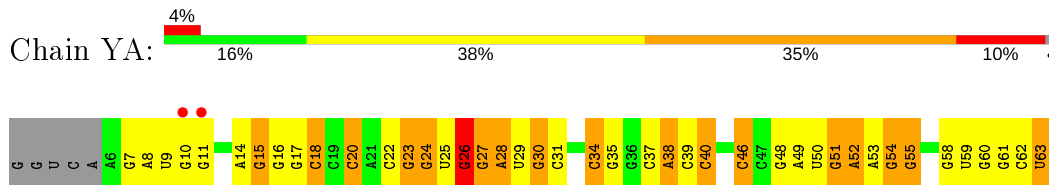


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U1255	C1192	C1063	A1000	A1000	A941	C877	C816	A752	G651	G591	A526
G1256	G1193	U1064	A1001	A1001	G942	U878	C917	A753	C652	C591	C527
C1257	A1194	U1065	G1002	G1002	U943	G879	G818	C754	A653	G593	A528
C1258	G1195	U1066	C1003	C1003	G944	A880	A819	G755	A654	G594	A529
G1259	C1196	A1067	C1004	C1004	A945	G881	A820	C756	G654A	U594	G530
A1260	G1197	G1068	C1005	C1005	G946	G882	A821	U757	C654B	C595	C531
A1261	U1198	A1069	C1006	C1006	G947	G883	G823	U758	G656	G596	A532
C1262	U1199	C1136	C1007	C1007	G948	C884	A824	G759	G	G597	G533
U1263	C1200	G1137	A1070	A1070	G948	C885	A824	G760	G	G598	U534
G1264	C1201	G1138	G1071	C1008	C949	C886	C825	G761	C	G600	C535
A1265	C1202	G1139	U1072	A1009	G950	C887	U826	U762	C	G601	C537
G1266	G1203	C1140	A1073	A1010	G951	A887	U827	U762	C	G602	G539
U1267	A1204	U1141	G1074	G1011	G952	C888	U828	G765	C	A603	G540
A1268	U1205	U142	G1075	G1012	G953	C889	A829	G766	C	G604	C541
A1269	C1206	A142A	A1076	C1013	G954	C890	G830	U767	A	C605	C544
C1270	G1207	G1143	U1078	U1014	C955	G892	G831	G768	C	U606	C544
C1208	C1208	G1144	U1079	G1015	G956	C893	G832	G769	C	U607	G545
G1209	G1209	C1145	C1080	C994	A957	C894	U833	G770	C	A608	C546
A1272	A1210	C1146	U1081	U995	U958	U895	C834	G773	C	A609	A547
U1273	U1211	G1149	U1082	A999	A959	A896	A835	U773	C	G609A	A548
A1274	G1212	G1150	U1083	U1019	A960	C897	G836	A774	C	C610	G549
A1275	A1213	C1150	A1084	A1020	G961	C898	C837	G775	C	C611	G550
G1277	A1214	G1151	A1085	G1022	G962	A899	C838	G776	C	G612	G553
A1278	G1215	C1152	A1086	U1023	U963	A900	U839	A777	C	U613	U554
G1279	G1216	C1153	A1087	G1024	C964	A901	C840	G778	C	U614	U554
G1280	G1217	G1154	U1088	G1025	C965	C902	G841	U779	C	G615	G556
U1281	A1218	G1155	A1088	U1026	G966	C903	G842	G780	C	A616	U557
U1282	C1221	A1156	U1090	A1027	C967	C904	G843	G781	C	G617	G558
G1283	C1222	G1157	G1091	U1028	G968	U969	C844	A782	C	U618	G559
A1284	C1223	C1158	G1092	A1029	U969	U969	G845	A783	C	C618A	C560
G1285	G1224	C1161	U1093	A1029	C970	U970	C846	A784	C	G619	G561
A1286	G1225	G1162	U1094	G1030	G971	G971	U987	A785	C	U620	U562
A1287	G1226	A1095	A1095	A1032	A973	A973	G948	G786	C	A621	G563

G2193	G2194	C2195	C2196	U2197	A2198	G2199	C2200	C2201	A2202	C2203	C2204	C2205	C2206	A2207	C2208	C2209	C2210	C2211	C2212	C2213	C2214	C2215	C2216	C2217	C2218	C2219	C2220	C2221	C2222	C2223	C2224	C2225	C2226	C2227	C2228	C2229	C2230	C2231	C2232	C2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	C2241	C2242	U2243	U2244	C2245	C2246	C2247	C2248	U2249	C2250	C2251	C2252	C2253	C2254	C2255	C2256	C2257	C2258	C2259	C2260	C2261	C2262	C2263	C2264	C2126	G2127	C2128	C2129	C2130	G2131	U2132	C2133	A2134	C2135	C2136	C2137	C2138	C2139	C2140	C2141	C2142	C2143	C2144	C2145	C2146	C2147	C2148	C2149	C2150	C2151	C2152	C2153	C2154	C2155	C2156	C2157	C2158	C2159	C2160	C2161	C2162	C2163	C2164	C2165	C2166	C2167	C2168	C2169	C2170	C2171	C2172	C2173	C2174	C2175	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2183	C2184	C2185	C2186	C2187	C2188	C2189	C2190	C2191	C2192	A2005	C2006	C2007	C2008	C2009	G2010	U2011	G2012	A2013	A2014	C2015	C2016	U2017	C2018	C2019	A2020	C2021	C2022	G2023	G2024	C2025	C2026	C2027	U2028	C2029	A2030	A2031	C2032	A2033	U2034	C2035	C2036	C2037	C2038	C2039	C2040	U2041	A2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	A2051	C2052	C2053	A2054	C2055	C2056	A2057	C2058	C2059	C2060	G2061	A2062	C2063	G2064	C1878	G1879	U1880	C1881	C1882	U1883	A1884	C1885	A1886	C1887	G1888	C1889	A1890	C1891	C1892	C1893	A1894	C1895	U1896	C1897	A1898	C1899	C1900	C1901	C1902	G1903	C1904	C1905	C1906	C1907	C1908	C1909	G1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	C1943	U1944	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	C1802	C1803	C1804	U1805	C1806	U1807	C1808	A1809	C1810	C1811	A1812	C1813	C1814	A1815	C1816	C1817	U1818	A1819	C1820	A1821	C1822	C1823	A1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	U1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	C1943	C1944	C1945	C1946	C1947	C1948	C1949	C1950	C1951	C1952	C1953	C1954	C1955	C1956	C1957	C1958	C1959	C1960	C1961	C1962	C1963	C1964	C1965	C1966	C1967	C1968	C1969	C1970	C1971	C1972	C1973	C1974	C1975	C1976	C1977	C1978	C1979	C1980	C1981	C1982	C1983	C1984	C1985	C1986	C1987	C1988	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	C1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	C2010	C2011	C2012	C2013	C2014	C2015	C2016	C2017	C2018	C2019	C2020	C2021	C2022	C2023	C2024	C2025	C2026	C2027	C2028	C2029	C2030	C2031	C2032	C2033	C2034	C2035	C2036	C2037	C2038	C2039	C2040	C2041	C2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055	C2056	C2057	C2058	C2059	C2060	C2061	C2062	C2063	C2064	C1661	C1662	C1663	A1664	C1665	C1666	C1667	A1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	U1585	A1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	U1601	C1602	A1603	C1604	C1605	C1606	C1607	A1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1473	C1474	G1475	C1476	C1477	C1478	C1479	C1480	C1481	C1482	C1483	C1484	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505	C1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	U1535	A1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1441	A1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1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● Molecule 25: 23S rRNA

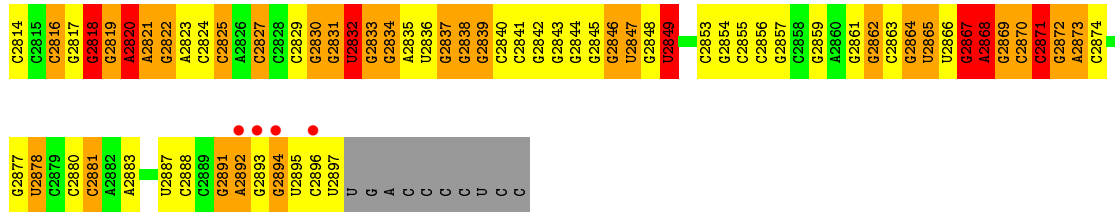




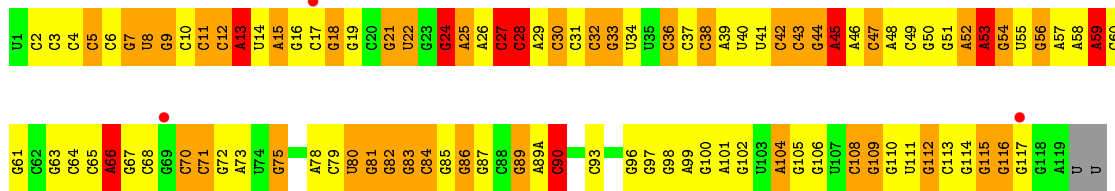
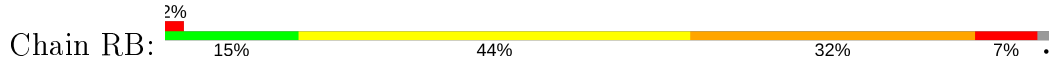


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A1021	A1086	G1150	A1213	A1275	G1337	A1396	U1455	G1520	G1582	C1647	A1791	A1853
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U1023	A1088	G1152	G1215	G1277	G1339	C1398	A1457	U1523	A1586	G1649	G1718	G1857
G1024	G1089	G1153	G1216	A1278	G1340	C1399	C1458	G1524	A1587	G1650	G1719	G1858
G1025	U1090	G1154	C1217	G1279	U1340	G1400	U1459	G1525	C1588	G1651	G1725	A1859
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G1031	U1097	G1160	G1223	G1285	G1346	U1406	C1464	G1530	G1594	G1656	G1731	U1801
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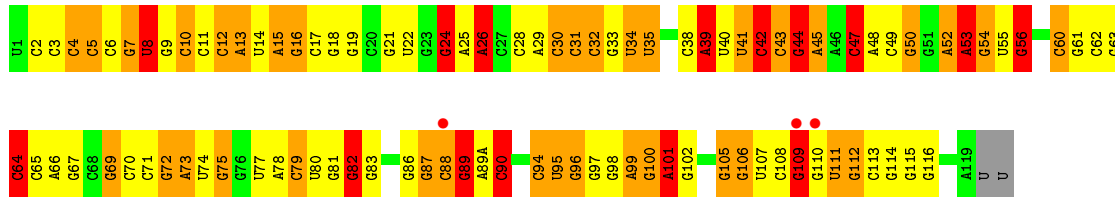
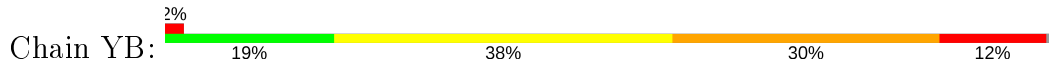
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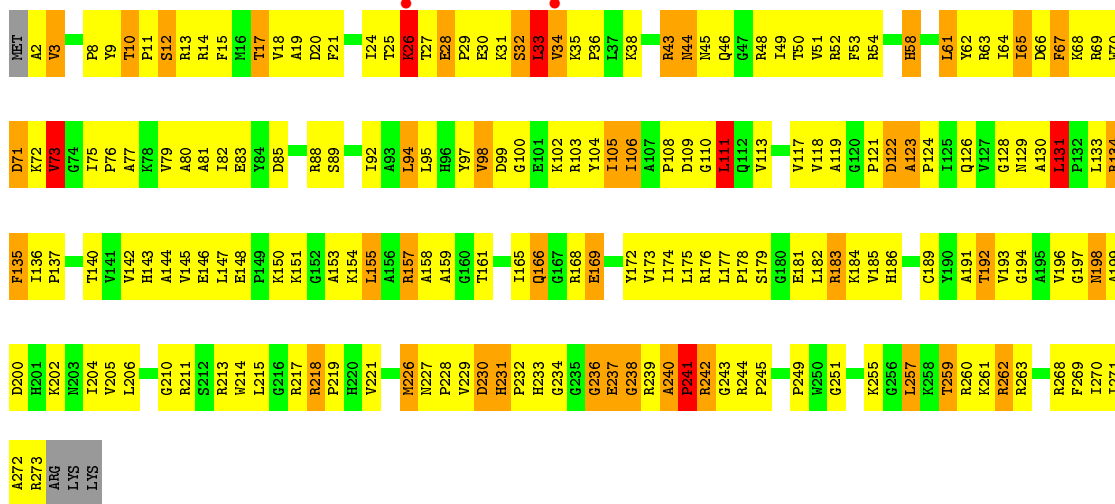
• Molecule 26: 5S rRNA



• Molecule 26: 5S rRNA

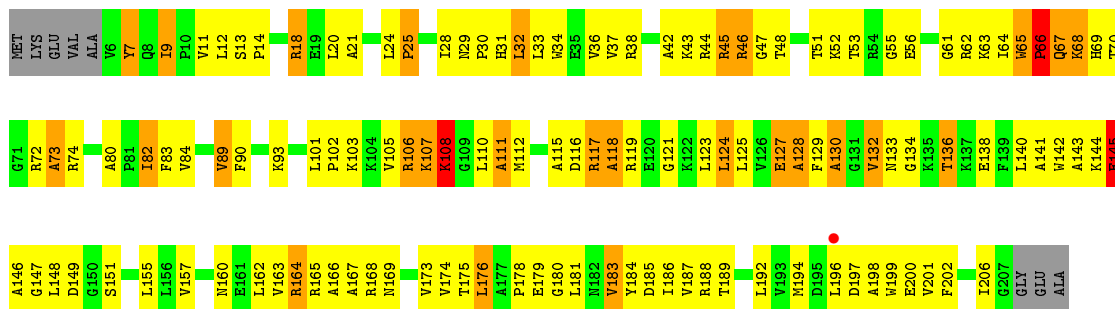


• Molecule 27: 50S ribosomal protein L2

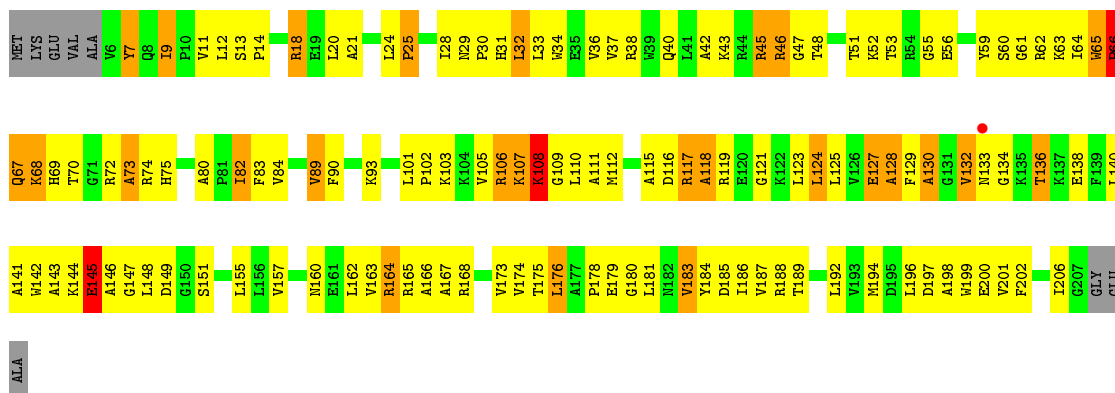


• Molecule 27: 50S ribosomal protein L2

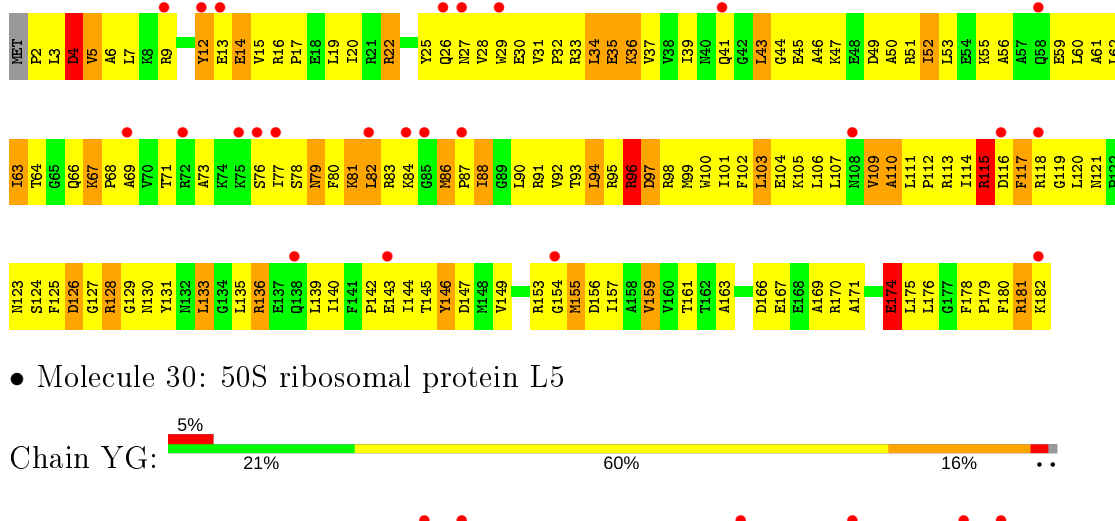
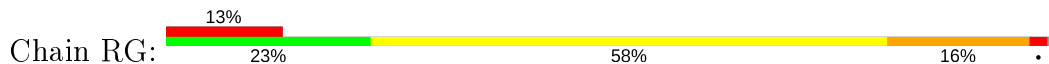




• Molecule 29: 50S ribosomal protein L4

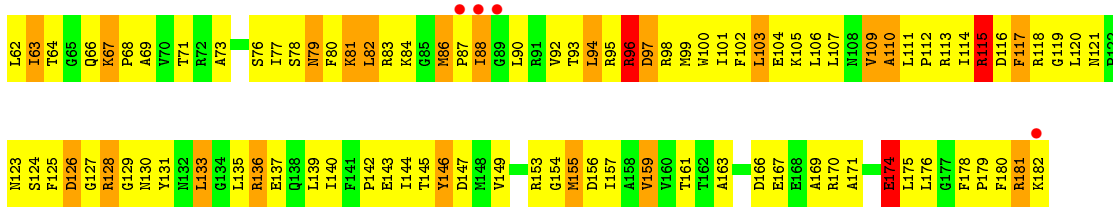


• Molecule 30: 50S ribosomal protein L5

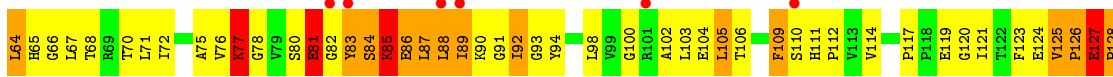
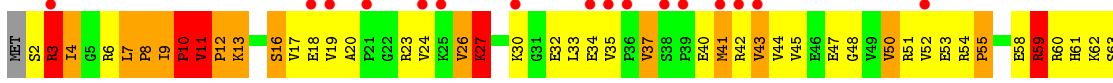
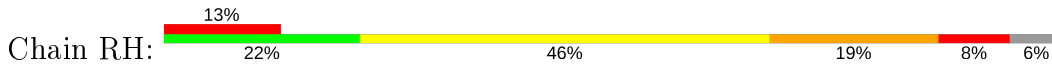


• Molecule 30: 50S ribosomal protein L5

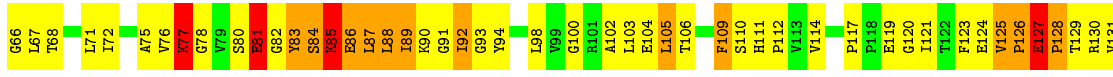
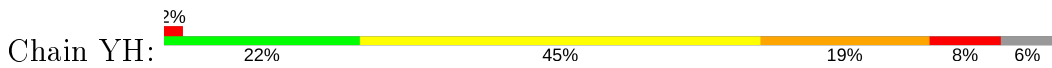




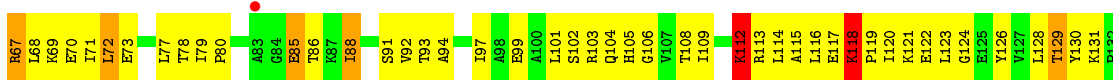
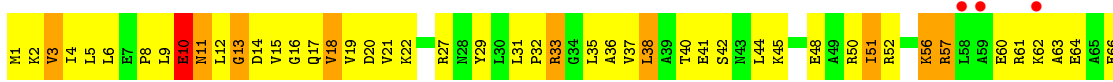
● Molecule 31: 50S ribosomal protein L6



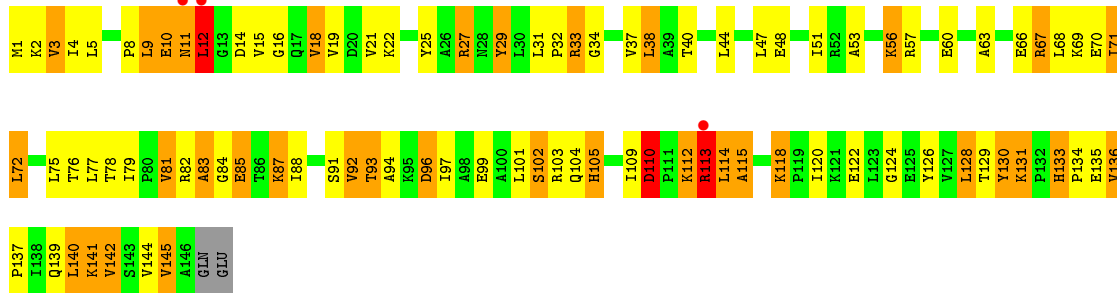
● Molecule 31: 50S ribosomal protein L6



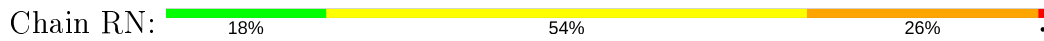
● Molecule 32: 50S ribosomal protein L9



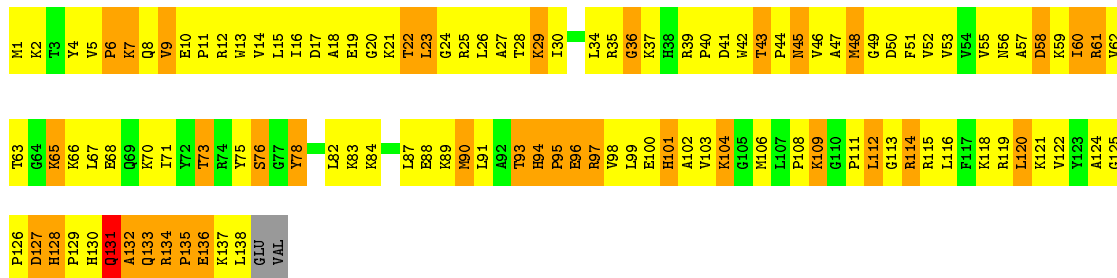
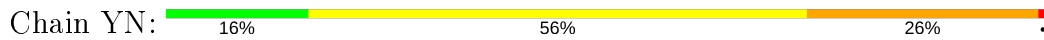
● Molecule 32: 50S ribosomal protein L9



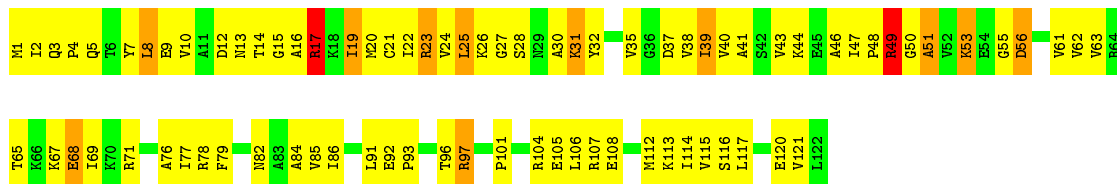
• Molecule 33: 50S ribosomal protein L13



• Molecule 33: 50S ribosomal protein L13

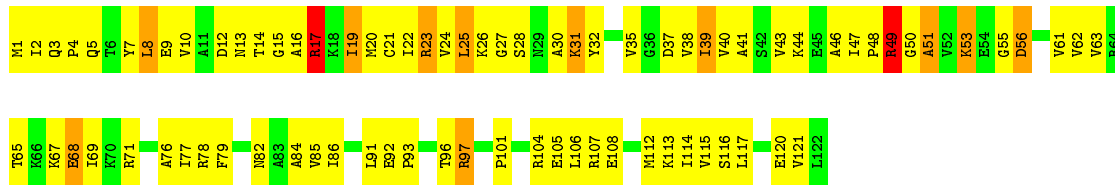


• Molecule 34: 50S ribosomal protein L14



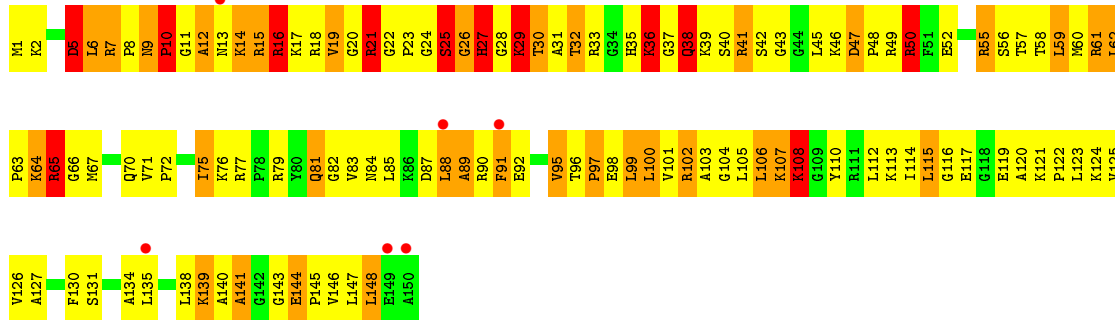
• Molecule 34: 50S ribosomal protein L14

Chain YO: 34% 55% 9%



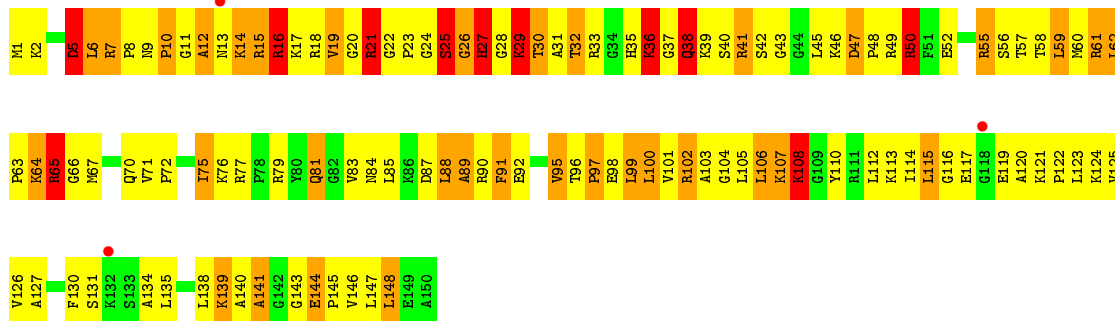
• Molecule 35: 50S ribosomal protein L15

Chain RP: 4% 19% 51% 23% 8%



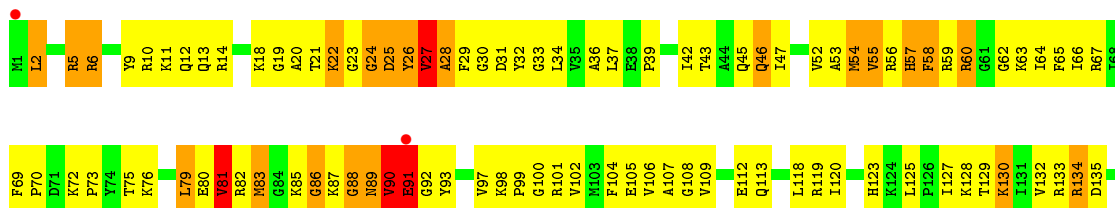
• Molecule 35: 50S ribosomal protein L15

Chain YP: 2% 19% 51% 23% 7%



• Molecule 36: 50S ribosomal protein L16

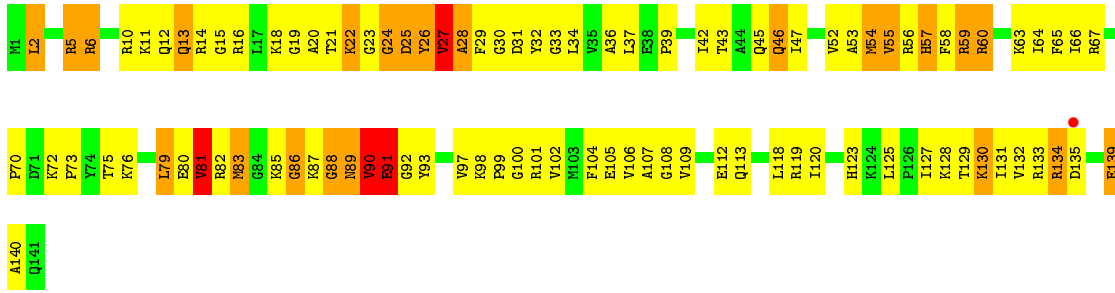
Chain RQ: 2% 30% 51% 16%



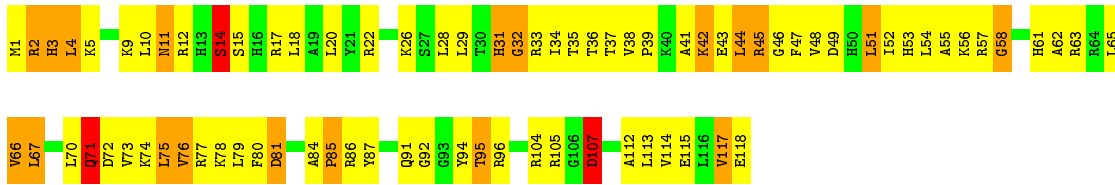
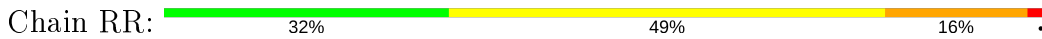




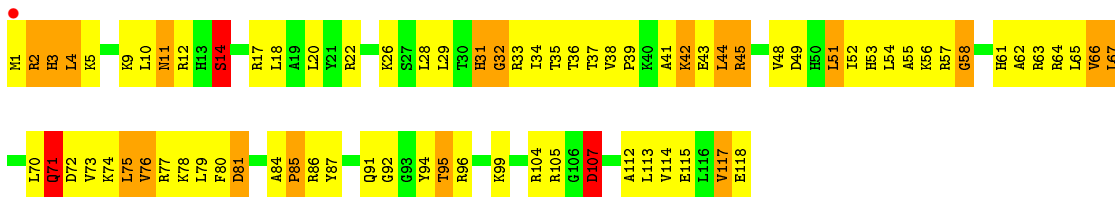
• Molecule 36: 50S ribosomal protein L16



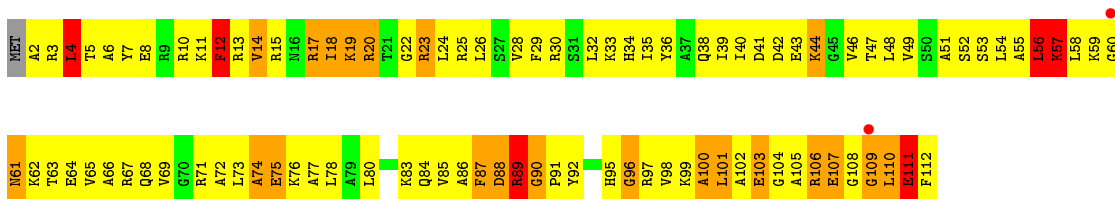
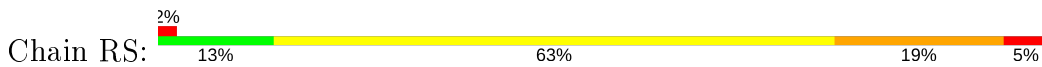
• Molecule 37: 50S ribosomal protein L17



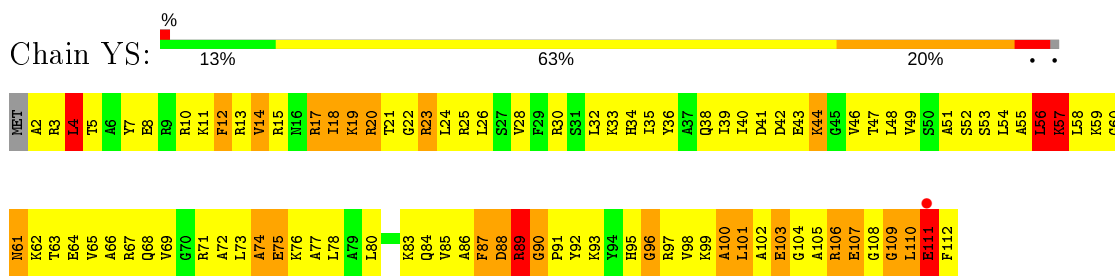
• Molecule 37: 50S ribosomal protein L17



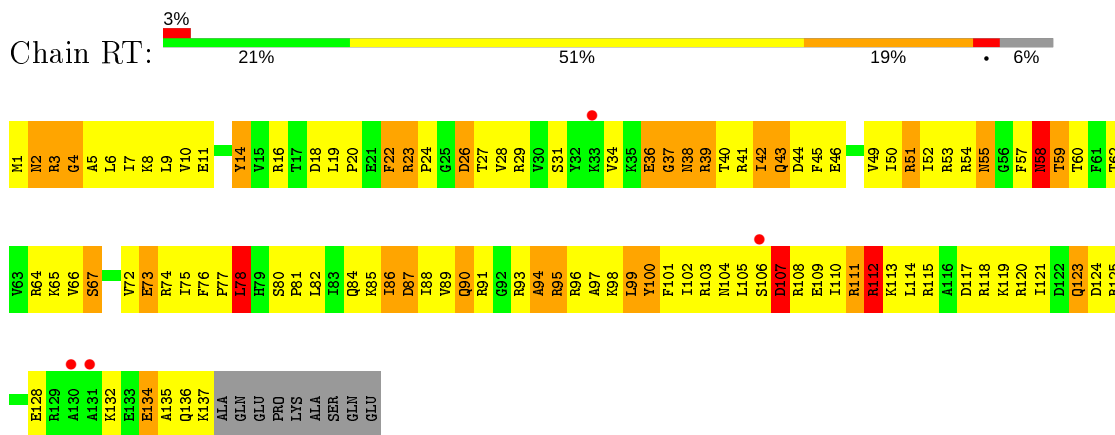
• Molecule 38: 50S ribosomal protein L18



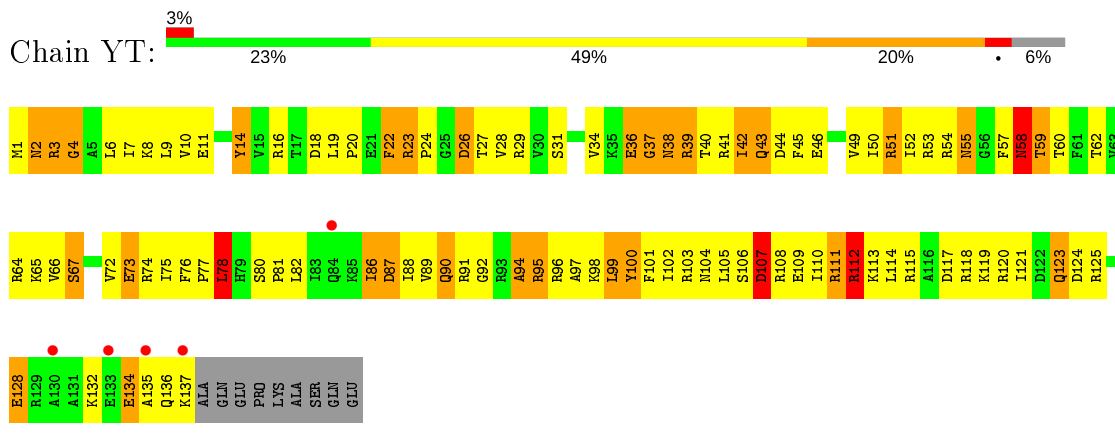
• Molecule 38: 50S ribosomal protein L18



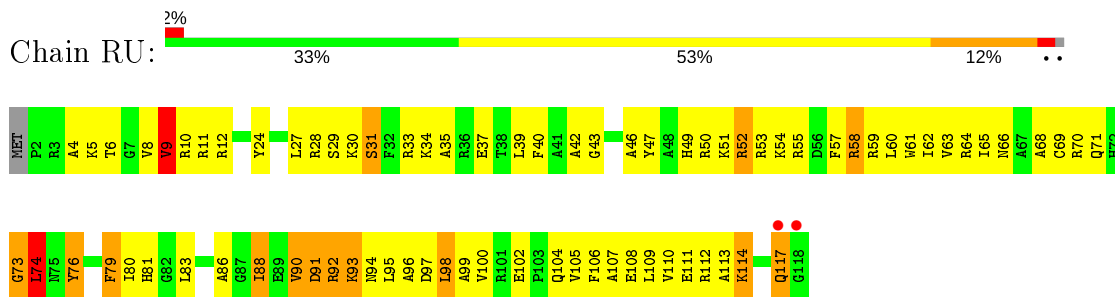
• Molecule 39: 50S ribosomal protein L19



• Molecule 39: 50S ribosomal protein L19

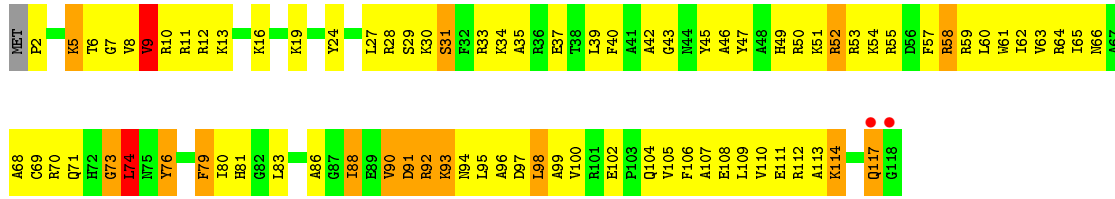


• Molecule 40: 50S ribosomal protein L20

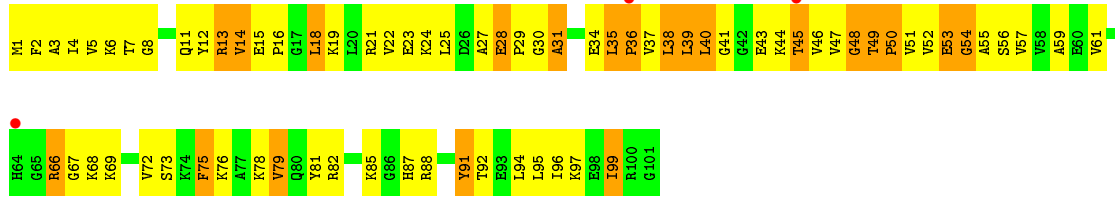


• Molecule 40: 50S ribosomal protein L20

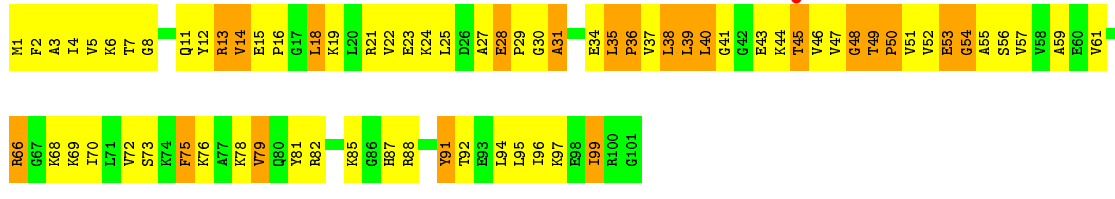




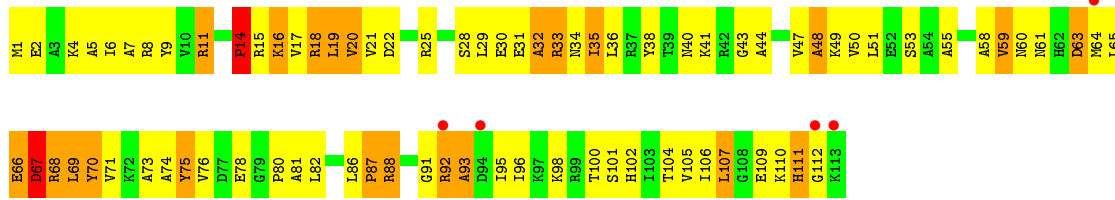
• Molecule 41: 50S ribosomal protein L21



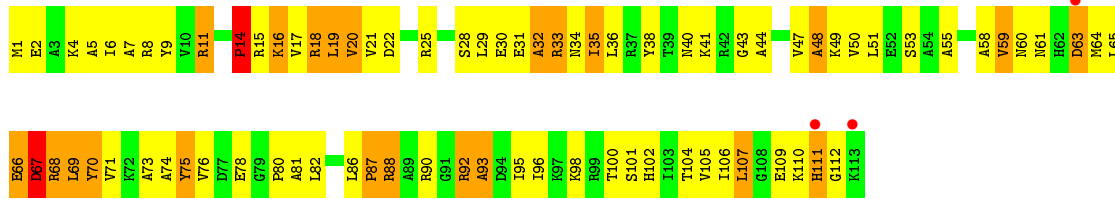
• Molecule 41: 50S ribosomal protein L21



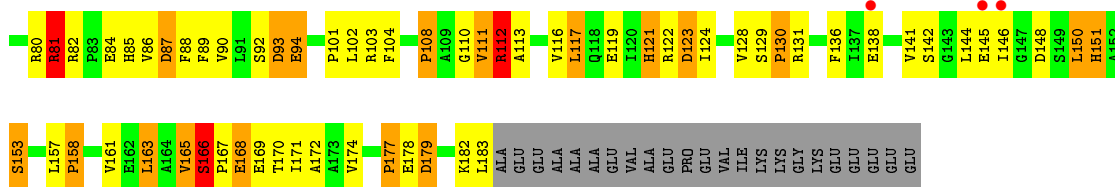
• Molecule 42: 50S ribosomal protein L22



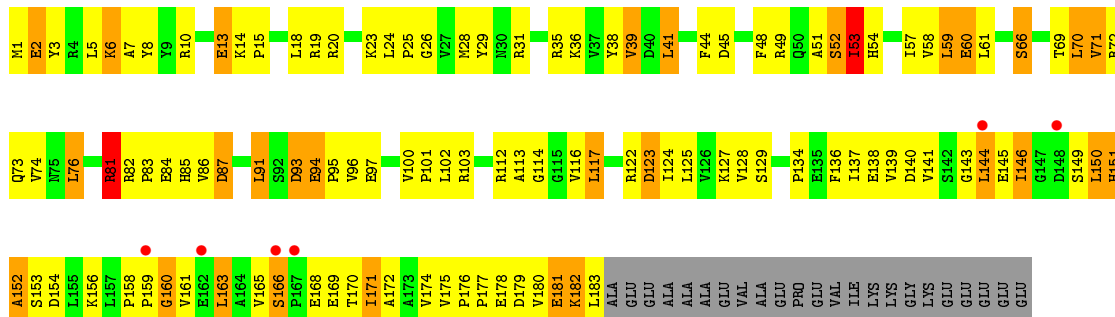
• Molecule 42: 50S ribosomal protein L22



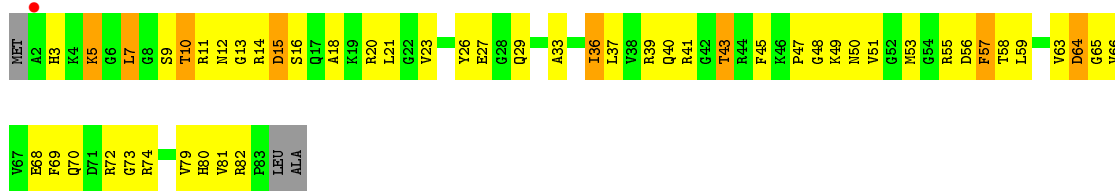
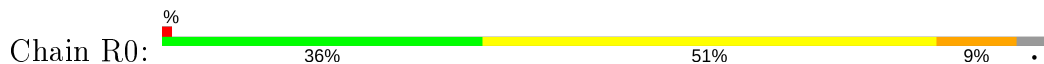




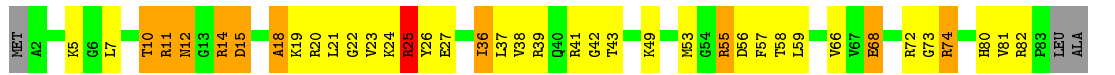
• Molecule 45: 50S ribosomal protein L25



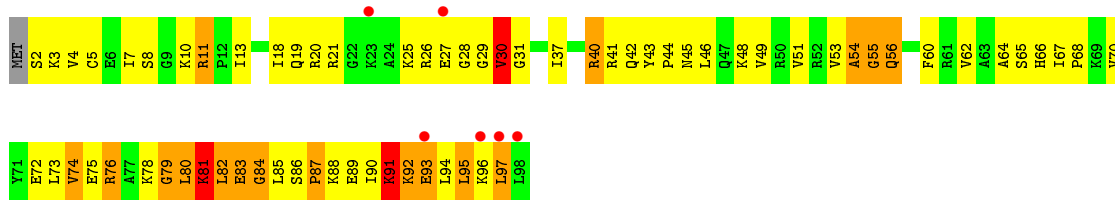
• Molecule 46: 50S ribosomal protein L27



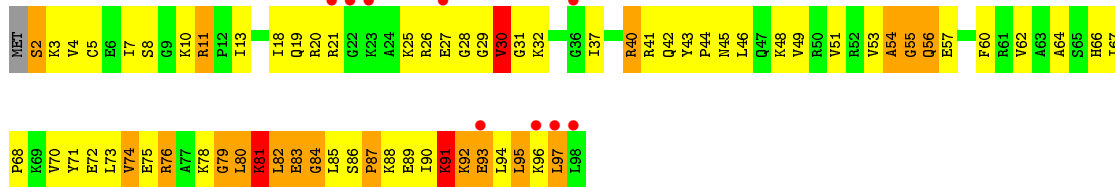
• Molecule 46: 50S ribosomal protein L27



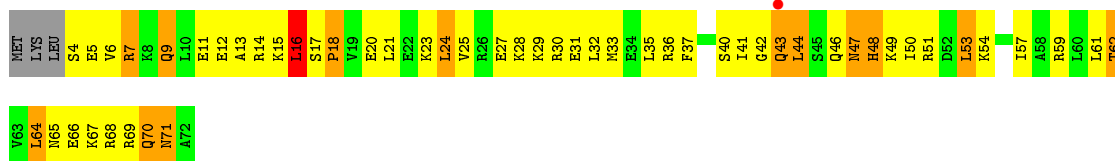
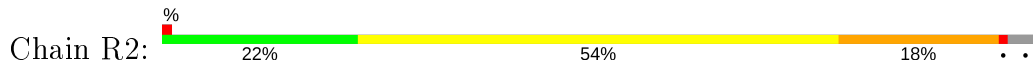
• Molecule 47: 50S ribosomal protein L28



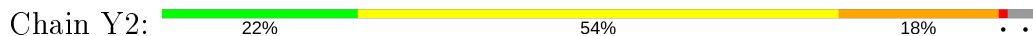
• Molecule 47: 50S ribosomal protein L28



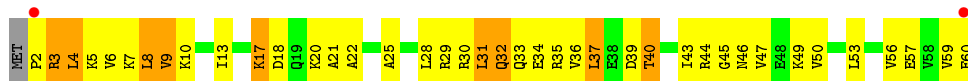
• Molecule 48: 50S ribosomal protein L29



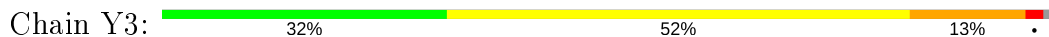
• Molecule 48: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L30

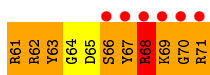


• Molecule 49: 50S ribosomal protein L30

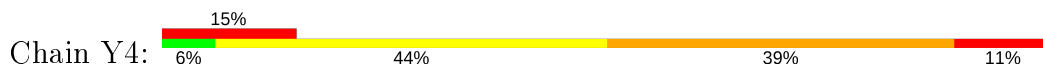


• Molecule 50: 50S ribosomal protein L31

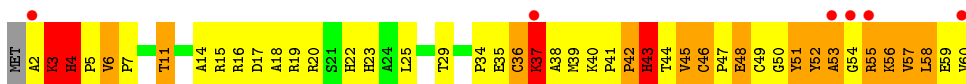
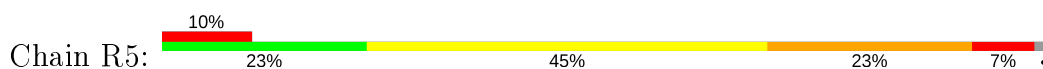




- Molecule 50: 50S ribosomal protein L31



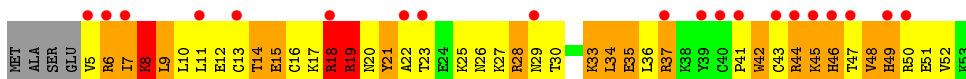
- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32



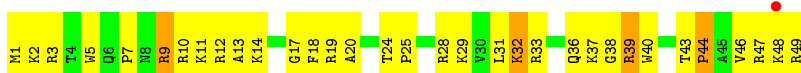
- Molecule 52: 50S ribosomal protein L33



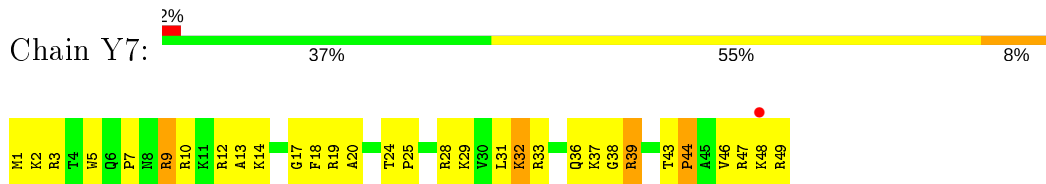
- Molecule 52: 50S ribosomal protein L33



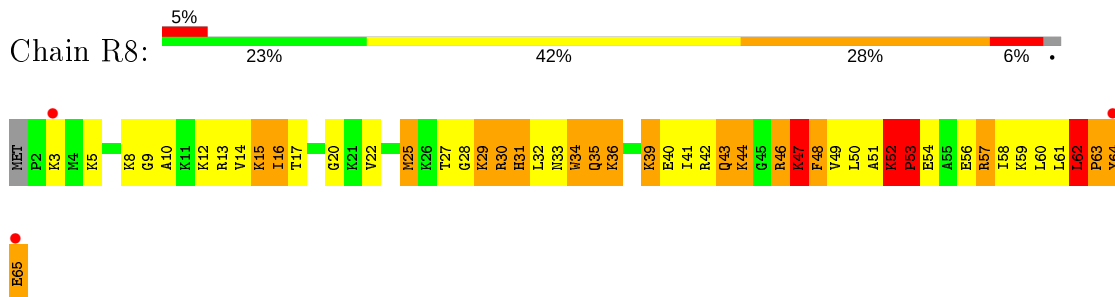
- Molecule 53: 50S ribosomal protein L34



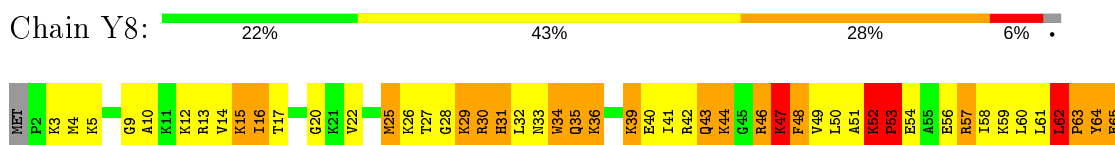
- Molecule 53: 50S ribosomal protein L34



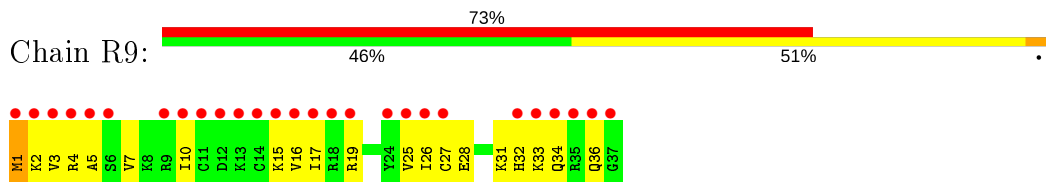
- Molecule 54: 50S ribosomal protein L35



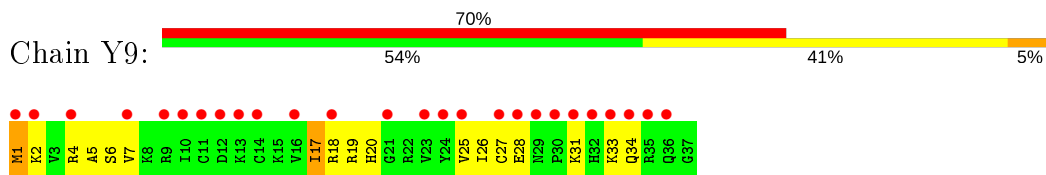
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic



- Molecule 56: tRNA acceptor end mimic







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.38Å 451.02Å 621.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.77 – 3.92 34.83 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.77-3.92) 99.8 (34.83-3.80)	Depositor EDS
$R_{merge}$	0.34	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 3.76Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.208 , 0.265 0.208 , 0.265	Depositor DCC
$R_{free}$ test set	25594 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.6	Xtrriage
Anisotropy	0.150	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	291868	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, MG, 1MG, PPU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	QA	0.84	19/36098 (0.1%)	1.59	747/56341 (1.3%)
1	XA	0.89	21/36101 (0.1%)	1.65	830/56346 (1.5%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.36	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.36	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.60	0/1709
7	XG	0.37	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.47	0/991	0.79	2/1327 (0.2%)
12	XL	0.52	1/991 (0.1%)	0.83	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.40	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.38	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.70	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	QV	0.51	0/1836	1.00	6/2859 (0.2%)
22	XV	0.52	0/1836	0.99	6/2859 (0.2%)
23	QX	0.39	0/185	0.71	0/285
23	XX	0.51	0/160	0.76	0/246
24	QY	0.52	0/311	0.87	0/483
24	XY	0.52	0/311	0.89	0/483
25	RA	1.03	104/69521 (0.1%)	1.85	2693/108529 (2.5%)
25	YA	1.19	254/69543 (0.4%)	1.98	3497/108563 (3.2%)
26	RB	0.82	1/2878 (0.0%)	1.59	60/4490 (1.3%)
26	YB	0.86	1/2878 (0.0%)	1.72	76/4490 (1.7%)
27	RD	0.60	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	1/2165 (0.0%)	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.44	0/1151	0.77	1/1558 (0.1%)
32	YI	0.44	0/1151	0.76	0/1558
33	RN	0.46	0/1131	0.78	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.54	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.95	3/1544 (0.2%)
35	YP	0.49	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.90	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YS	0.45	0/892	0.82	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.47	0/1155	0.73	2/1542 (0.1%)
40	RU	0.48	0/982	0.78	0/1306
40	YU	0.48	0/982	0.78	0/1306
41	RV	0.47	0/790	0.82	0/1057
41	YV	0.47	0/790	0.82	0/1057
42	RW	0.45	0/911	0.75	0/1220
42	YW	0.45	0/911	0.75	0/1220
43	RX	0.56	0/739	0.77	0/993
43	YX	0.56	0/739	0.77	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.44	0/1493	0.70	0/2026
45	YZ	0.43	0/1493	0.70	0/2026
46	R0	0.52	0/657	0.73	0/874
46	Y0	0.55	0/657	0.80	1/874 (0.1%)
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.51	0/583	0.84	1/771 (0.1%)
48	Y2	0.51	0/583	0.83	1/771 (0.1%)
49	R3	0.47	0/474	0.71	0/635
49	Y3	0.43	0/474	0.71	0/635
50	R4	0.38	0/594	0.78	1/795 (0.1%)
50	Y4	0.38	0/594	0.78	1/795 (0.1%)
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.51	0/473	0.74	0/639
52	R6	0.42	0/431	0.76	0/575
52	Y6	0.42	0/431	0.76	0/575
53	R7	0.56	0/438	0.76	0/575
53	Y7	0.56	0/438	0.76	0/575
54	R8	0.62	0/525	0.93	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.35	0/310	0.59	0/407
55	Y9	0.37	0/310	0.61	0/407
56	Z6	0.78	0/40	1.78	1/60 (1.7%)
56	Z8	0.79	0/40	1.81	1/60 (1.7%)
All	All	0.89	404/316298 (0.1%)	1.59	7980/472872 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
45	YZ	0	1

The worst 5 of 404 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	1201	A	C3'-C2'	12.06	1.66	1.52
1	XA	1054	C	C4'-C3'	11.40	1.65	1.53
25	YA	783	A	N7-C5	-11.18	1.32	1.39
25	YA	793	A	N7-C5	-10.74	1.32	1.39
25	YA	783	A	C5-C6	-10.48	1.31	1.41

The worst 5 of 7980 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	761	A	N1-C6-N6	19.13	130.07	118.60
25	RA	2490	G	C6-C5-N7	-18.87	119.08	130.40
25	RA	783	A	C6-C5-N7	-17.19	120.27	132.30
25	RA	783	A	N1-C6-N6	16.89	128.74	118.60
25	YA	783	A	N1-C6-N6	16.68	128.61	118.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
45	YZ	181	GLU	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	1130	0
1	XA	32249	0	16279	1064	1
2	QB	1924	0	1975	289	0
2	XB	1924	0	1975	290	0
3	QC	1605	0	1668	205	0
3	XC	1605	0	1668	211	0
4	QD	1703	0	1764	253	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	XD	1703	0	1765	214	0
5	QE	1155	0	1213	182	0
5	XE	1155	0	1213	147	0
6	QF	843	0	857	94	0
6	XF	843	0	857	99	0
7	QG	1257	0	1296	151	0
7	XG	1257	0	1294	142	0
8	QH	1116	0	1175	167	0
8	XH	1116	0	1177	150	0
9	QI	1010	0	1037	144	0
9	XI	1010	0	1037	152	0
10	QJ	801	0	849	150	0
10	XJ	801	0	849	132	0
11	QK	885	0	904	103	0
11	XK	885	0	904	107	0
12	QL	975	0	1062	100	0
12	XL	975	0	1062	111	0
13	QM	964	0	1034	169	0
13	XM	964	0	1034	163	0
14	QN	492	0	530	102	0
14	XN	492	0	530	99	0
15	QO	734	0	771	76	0
15	XO	734	0	771	78	0
16	QP	705	0	725	120	0
16	XP	705	0	725	113	0
17	QQ	834	0	904	84	0
17	XQ	834	0	904	81	0
18	QR	574	0	644	66	0
18	XR	574	0	644	66	0
19	QS	674	0	699	109	0
19	XS	674	0	699	132	0
20	QT	763	0	860	108	0
20	XT	763	0	861	108	0
21	QU	217	0	234	30	0
21	XU	217	0	234	26	0
22	QV	1644	0	836	44	0
22	XV	1644	0	836	29	0
23	QX	167	0	87	13	0
23	XX	145	0	75	9	0
24	QY	303	0	154	11	0
24	XY	303	0	154	11	0
25	RA	62071	0	31285	1926	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	YA	62091	0	31293	1989	0
26	RB	2573	0	1306	121	0
26	YB	2573	0	1306	103	0
27	RD	2115	0	2195	324	0
27	YD	2115	0	2195	332	0
28	RE	1568	0	1634	270	0
28	YE	1568	0	1634	263	0
29	RF	1585	0	1632	178	0
29	YF	1585	0	1632	178	0
30	RG	1474	0	1535	201	0
30	YG	1474	0	1535	194	0
31	RH	1307	0	1382	226	0
31	YH	1307	0	1382	228	0
32	RI	1136	0	1223	79	1
32	YI	1136	0	1223	72	0
33	RN	1104	0	1180	200	0
33	YN	1104	0	1180	189	0
34	RO	933	0	996	126	0
34	YO	933	0	996	125	0
35	RP	1145	0	1228	256	0
35	YP	1145	0	1228	244	0
36	RQ	1122	0	1179	157	0
36	YQ	1122	0	1178	165	0
37	RR	968	0	1033	115	0
37	YR	968	0	1033	117	0
38	RS	882	0	943	166	0
38	YS	882	0	943	159	0
39	RT	1141	0	1202	151	0
39	YT	1141	0	1202	155	0
40	RU	964	0	1022	130	0
40	YU	964	0	1022	142	0
41	RV	779	0	852	130	0
41	YV	779	0	852	131	0
42	RW	900	0	964	100	0
42	YW	900	0	964	108	0
43	RX	725	0	778	70	0
43	YX	725	0	778	74	0
44	RY	785	0	878	167	0
44	YY	785	0	878	160	0
45	RZ	1461	0	1493	81	0
45	YZ	1461	0	1493	86	0
46	R0	648	0	671	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Y0	648	0	672	51	0
47	R1	763	0	848	142	0
47	Y1	763	0	848	142	0
48	R2	581	0	629	83	0
48	Y2	581	0	629	78	0
49	R3	469	0	518	41	0
49	Y3	469	0	518	46	0
50	R4	581	0	574	159	0
50	Y4	581	0	574	167	0
51	R5	459	0	480	73	0
51	Y5	459	0	480	76	0
52	R6	424	0	450	90	0
52	Y6	424	0	450	97	0
53	R7	430	0	480	42	0
53	Y7	430	0	480	40	0
54	R8	517	0	582	104	0
54	Y8	517	0	582	105	0
55	R9	307	0	335	23	0
55	Y9	307	0	336	24	0
56	Z6	74	0	51	10	0
56	Z8	74	0	51	10	0
57	QA	64	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	239	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	2	0	0	0	0
57	XA	72	0	0	1	0
57	XB	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	2	0	0	0	0
57	XX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	269	0	0	1	0
57	YB	3	0	0	0	0
57	YE	1	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	R9	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y9	1	0	0	0	0
59	XX	22	0	12	1	0
All	All	291868	0	198240	17856	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

The worst 5 of 17856 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)
14:YN:32:SER:CB	14:YN:41:ARG:HB3	1.23	1.54
14:YN:32:SER:HB3	14:YN:41:ARG:CB	1.28	1.54
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
4:XD:22:LYS:CG	4:XD:26:CYS:SG	2.01	1.49

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.02	0.18

## 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%)	153 (65%)	52 (22%)	30 (13%)	0	5
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	5
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	12
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	12
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	0	11
4	XD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	0	8
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	10
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	8
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	12
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	12
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	10
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	12
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0	12
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	9
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	15
11	XK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	18
12	QL	123/132 (93%)	84 (68%)	24 (20%)	15 (12%)	0	6
12	XL	123/132 (93%)	83 (68%)	24 (20%)	16 (13%)	0	5
13	QM	119/126 (94%)	71 (60%)	29 (24%)	19 (16%)	0	3
13	XM	119/126 (94%)	72 (60%)	25 (21%)	22 (18%)	0	2
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	2
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	17
15	XO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	17
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	14
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	14
18	QR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	6
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	6
19	QS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	2
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	2
21	QU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	3
21	XU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	3
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	17
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	17
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	10
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	10
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	6
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	6
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	99 (69%)	32 (22%)	13 (9%)	1	13
32	YI	144/148 (97%)	93 (65%)	30 (21%)	21 (15%)	0	4
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	3
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	3
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	16
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	10
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	10
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3
38	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	15
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	15
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	10
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	10
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	21
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	21
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	1
44	YY	100/110 (91%)	57 (57%)	16 (16%)	27 (27%)	0	1
45	RZ	181/206 (88%)	113 (62%)	46 (25%)	22 (12%)	0	6
45	YZ	181/206 (88%)	128 (71%)	36 (20%)	17 (9%)	0	12
46	R0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	2	23
46	Y0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	2	23
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	6
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	6
48	R2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	4
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	4
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	22
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	22
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	19
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	19
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	2
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	2
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	7621 (66%)	2356 (20%)	1493 (13%)	0	5

5 of 1493 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	6	THR
2	QB	15	VAL
2	QB	26	PRO
2	QB	84	GLU
2	QB	88	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	181 (88%)	24 (12%)	5	25
2	XB	205/220 (93%)	181 (88%)	24 (12%)	5	25
3	QC	159/188 (85%)	143 (90%)	16 (10%)	7	30
3	XC	159/188 (85%)	143 (90%)	16 (10%)	7	30
4	QD	180/181 (99%)	160 (89%)	20 (11%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	180/181 (99%)	165 (92%)	15 (8%)	11	39
5	QE	116/123 (94%)	107 (92%)	9 (8%)	12	41
5	XE	116/123 (94%)	107 (92%)	9 (8%)	12	41
6	QF	90/90 (100%)	76 (84%)	14 (16%)	2	17
6	XF	90/90 (100%)	76 (84%)	14 (16%)	2	17
7	QG	126/127 (99%)	115 (91%)	11 (9%)	10	37
7	XG	126/127 (99%)	115 (91%)	11 (9%)	10	37
8	QH	119/119 (100%)	106 (89%)	13 (11%)	6	28
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	28
9	QI	98/99 (99%)	87 (89%)	11 (11%)	6	27
9	XI	98/99 (99%)	87 (89%)	11 (11%)	6	27
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	9	35
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	9	35
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	30
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	30
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	22
12	XL	104/109 (95%)	89 (86%)	15 (14%)	3	19
13	QM	97/101 (96%)	81 (84%)	16 (16%)	2	15
13	XM	97/101 (96%)	81 (84%)	16 (16%)	2	15
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	11
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7	30
15	QO	79/80 (99%)	73 (92%)	6 (8%)	13	42
15	XO	79/80 (99%)	73 (92%)	6 (8%)	13	42
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	23
16	XP	72/74 (97%)	63 (88%)	9 (12%)	4	23
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	18	47
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	47
18	QR	61/77 (79%)	54 (88%)	7 (12%)	5	26
18	XR	61/77 (79%)	54 (88%)	7 (12%)	5	26
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	18
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	QT	76/82 (93%)	68 (90%)	8 (10%)	7	29
20	XT	76/82 (93%)	68 (90%)	8 (10%)	7	29
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	53
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	53
27	RD	214/218 (98%)	177 (83%)	37 (17%)	2	13
27	YD	214/218 (98%)	178 (83%)	36 (17%)	2	15
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	6
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	6
29	RF	161/166 (97%)	140 (87%)	21 (13%)	4	22
29	YF	161/166 (97%)	140 (87%)	21 (13%)	4	22
30	RG	155/156 (99%)	130 (84%)	25 (16%)	2	16
30	YG	155/156 (99%)	130 (84%)	25 (16%)	2	16
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	9
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	9
32	RI	122/124 (98%)	94 (77%)	28 (23%)	1	6
32	YI	122/124 (98%)	92 (75%)	30 (25%)	0	5
33	RN	117/119 (98%)	98 (84%)	19 (16%)	2	16
33	YN	117/119 (98%)	98 (84%)	19 (16%)	2	16
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7	30
34	YO	100/100 (100%)	90 (90%)	10 (10%)	7	30
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	5
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	5
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	16
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	2	16
37	RR	101/101 (100%)	84 (83%)	17 (17%)	2	15
37	YR	101/101 (100%)	84 (83%)	17 (17%)	2	15
38	RS	87/88 (99%)	74 (85%)	13 (15%)	3	18
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	18
39	RT	120/127 (94%)	97 (81%)	23 (19%)	1	10
39	YT	120/127 (94%)	97 (81%)	23 (19%)	1	10
40	RU	93/94 (99%)	80 (86%)	13 (14%)	3	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	YU	93/94 (99%)	80 (86%)	13 (14%)	3	21
41	RV	82/82 (100%)	71 (87%)	11 (13%)	4	22
41	YV	82/82 (100%)	71 (87%)	11 (13%)	4	22
42	RW	92/92 (100%)	77 (84%)	15 (16%)	2	16
42	YW	92/92 (100%)	77 (84%)	15 (16%)	2	16
43	RX	74/78 (95%)	63 (85%)	11 (15%)	3	18
43	YX	74/78 (95%)	63 (85%)	11 (15%)	3	18
44	RY	85/91 (93%)	70 (82%)	15 (18%)	2	13
44	YY	85/91 (93%)	70 (82%)	15 (18%)	2	13
45	RZ	162/179 (90%)	133 (82%)	29 (18%)	2	12
45	YZ	162/179 (90%)	131 (81%)	31 (19%)	1	10
46	R0	65/67 (97%)	58 (89%)	7 (11%)	6	28
46	Y0	65/67 (97%)	58 (89%)	7 (11%)	6	28
47	R1	82/83 (99%)	67 (82%)	15 (18%)	1	11
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	1	11
48	R2	64/67 (96%)	57 (89%)	7 (11%)	6	28
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	28
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	6
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	6
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	2
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	5
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	5
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	7
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	7
53	R7	42/42 (100%)	39 (93%)	3 (7%)	14	44
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	14	44
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%)	32 (94%)	2 (6%)	19	49
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9702/10066 (96%)	8266 (85%)	1436 (15%)	3 18

5 of 1436 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	8	LEU
7	XG	111	ARG
45	YZ	141	VAL
50	R4	50	VAL
2	XB	73	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
43	RX	55	ASN
2	XB	135	GLN
43	YX	55	ASN
43	RX	87	GLN
48	R2	47	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	385 (25%)	49 (3%)
1	XA	1498/1522 (98%)	378 (25%)	60 (4%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	5 (71%)	1 (14%)
23	XX	6/25 (24%)	3 (50%)	0
24	QY	13/18 (72%)	5 (38%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2879/2916 (98%)	835 (29%)	82 (2%)
25	YA	2880/2916 (98%)	865 (30%)	93 (3%)
26	RB	119/122 (97%)	32 (26%)	3 (2%)
26	YB	119/122 (97%)	42 (35%)	2 (1%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9186/9366 (98%)	2615 (28%)	294 (3%)

5 of 2615 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	7	G
1	QA	9	G
1	QA	10	A
1	QA	22	G
1	QA	32	A

5 of 294 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2848	G
1	XA	595	G
25	YA	2238	G
26	RB	108	C
1	XA	328	C

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

4 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	$\# Z  > 2$
24	1MG	QY	37	24	18,26,27	2.79	3 (16%)	19,39,42	1.47	4 (21%)
24	1MG	XY	37	24	18,26,27	2.81	3 (16%)	19,39,42	1.49	4 (21%)
56	PPU	Z8	76	25,56	32,40,41	2.54	6 (18%)	33,57,60	2.15	5 (15%)
56	PPU	Z6	76	25,56	32,40,41	2.55	5 (15%)	33,57,60	2.16	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	1MG	QY	37	24	-	0/3/25/26	0/3/3/3
24	1MG	XY	37	24	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	Z8	76	25,56	-	2/21/43/44	0/4/4/4
56	PPU	Z6	76	25,56	-	2/21/43/44	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.25	1.41	1.23
56	Z8	76	PPU	O-C	9.21	1.41	1.23
24	XY	37	1MG	C4-N3	8.71	1.49	1.35
24	QY	37	1MG	C4-N3	8.68	1.49	1.35
24	XY	37	1MG	C2-N2	7.15	1.48	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-8.65	110.17	123.21
56	Z8	76	PPU	C3'-N3'-C	-8.63	110.20	123.21
56	Z8	76	PPU	N3-C2-N1	-4.67	121.38	128.68
56	Z6	76	PPU	N3-C2-N1	-4.66	121.39	128.68
24	QY	37	1MG	N2-C2-N1	4.18	123.73	118.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Z8	76	PPU	O-C-CA-N
56	Z6	76	PPU	O-C-CA-N
56	Z8	76	PPU	N3'-C-CA-N
56	Z6	76	PPU	N3'-C-CA-N

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	QY	37	1MG	1	0
24	XY	37	1MG	1	0
56	Z8	76	PPU	10	0
56	Z6	76	PPU	7	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 681 ligands modelled in this entry, 680 are monoatomic - leaving 1 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 i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	QA	1500/1522 (98%)	0.06	50 (3%) 46 37	3, 59, 153, 236	0
1	XA	1500/1522 (98%)	0.01	41 (2%) 54 44	1, 53, 148, 240	0
2	QB	237/256 (92%)	0.31	18 (7%) 13 11	41, 113, 151, 177	0
2	XB	237/256 (92%)	0.11	9 (3%) 40 32	21, 96, 142, 157	0
3	QC	205/239 (85%)	0.36	20 (9%) 7 7	22, 104, 139, 161	0
3	XC	205/239 (85%)	-0.13	4 (1%) 65 56	22, 79, 122, 161	0
4	QD	208/209 (99%)	-0.14	2 (0%) 82 75	8, 69, 116, 153	0
4	XD	208/209 (99%)	0.01	4 (1%) 66 58	16, 74, 114, 159	0
5	QE	151/162 (93%)	0.35	6 (3%) 38 31	32, 95, 133, 161	0
5	XE	151/162 (93%)	-0.21	0 100 100	20, 63, 108, 140	0
6	QF	101/101 (100%)	-0.10	3 (2%) 50 39	15, 68, 105, 139	0
6	XF	101/101 (100%)	0.17	6 (5%) 22 18	4, 66, 107, 134	0
7	QG	155/156 (99%)	0.16	9 (5%) 23 19	26, 89, 133, 154	0
7	XG	155/156 (99%)	0.10	9 (5%) 23 19	28, 83, 124, 148	0
8	QH	138/138 (100%)	-0.10	1 (0%) 87 82	21, 79, 122, 132	0
8	XH	138/138 (100%)	-0.18	2 (1%) 75 66	14, 68, 108, 133	0
9	QI	127/128 (99%)	0.48	12 (9%) 8 8	49, 102, 138, 161	0
9	XI	127/128 (99%)	0.10	4 (3%) 49 38	13, 91, 134, 162	0
10	QJ	99/105 (94%)	0.87	19 (19%) 1 1	57, 108, 148, 192	0
10	XJ	99/105 (94%)	0.52	10 (10%) 7 7	40, 94, 140, 165	0
11	QK	119/129 (92%)	0.31	8 (6%) 17 14	25, 72, 127, 150	0
11	XK	119/129 (92%)	-0.02	4 (3%) 45 36	4, 59, 109, 129	0
12	QL	125/132 (94%)	0.14	8 (6%) 19 15	15, 64, 124, 159	0
12	XL	125/132 (94%)	-0.10	1 (0%) 86 80	6, 48, 102, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	QM	121/126 (96%)	0.18	6 (4%) 28 25	48, 101, 151, 159	0
13	XM	121/126 (96%)	-0.04	1 (0%) 86 80	38, 85, 119, 158	0
14	QN	60/61 (98%)	0.67	7 (11%) 4 5	52, 108, 148, 159	0
14	XN	60/61 (98%)	-0.09	0 100 100	33, 72, 116, 130	0
15	QO	88/89 (98%)	-0.10	3 (3%) 45 36	17, 71, 119, 151	0
15	XO	88/89 (98%)	0.03	4 (4%) 33 28	7, 59, 102, 127	0
16	QP	84/88 (95%)	-0.13	1 (1%) 79 70	14, 59, 114, 134	0
16	XP	84/88 (95%)	-0.13	2 (2%) 59 49	28, 68, 122, 176	0
17	QQ	100/105 (95%)	0.06	3 (3%) 50 39	30, 70, 116, 148	0
17	XQ	100/105 (95%)	0.03	3 (3%) 50 39	19, 71, 106, 144	0
18	QR	70/88 (79%)	0.03	1 (1%) 75 66	22, 70, 125, 150	0
18	XR	70/88 (79%)	-0.07	1 (1%) 75 66	9, 65, 106, 140	0
19	QS	84/93 (90%)	1.05	23 (27%) 0 0	69, 116, 148, 161	0
19	XS	84/93 (90%)	0.09	1 (1%) 79 70	48, 87, 132, 145	0
20	QT	99/106 (93%)	0.13	2 (2%) 65 56	16, 73, 113, 135	0
20	XT	99/106 (93%)	0.24	5 (5%) 28 24	23, 77, 124, 157	0
21	QU	25/27 (92%)	1.63	10 (40%) 0 0	31, 92, 141, 158	0
21	XU	25/27 (92%)	0.90	2 (8%) 12 11	32, 83, 121, 143	0
22	QV	77/77 (100%)	0.29	2 (2%) 56 46	21, 85, 147, 180	0
22	XV	77/77 (100%)	0.27	3 (3%) 39 31	6, 64, 119, 169	0
23	QX	8/25 (32%)	0.72	1 (12%) 3 5	50, 74, 138, 138	0
23	XX	7/25 (28%)	0.86	0 100 100	18, 51, 81, 90	0
24	QY	13/18 (72%)	1.86	4 (30%) 0 0	106, 175, 223, 238	0
24	XY	13/18 (72%)	2.22	4 (30%) 0 0	55, 149, 189, 217	0
25	RA	2882/2916 (98%)	0.03	137 (4%) 30 26	0, 30, 174, 252	0
25	YA	2883/2916 (98%)	-0.07	108 (3%) 41 33	0, 20, 159, 242	0
26	RB	120/122 (98%)	0.24	3 (2%) 57 48	39, 82, 133, 170	0
26	YB	120/122 (98%)	0.10	3 (2%) 57 48	16, 68, 104, 146	0
27	RD	272/276 (98%)	-0.25	2 (0%) 87 82	0, 34, 82, 147	0
27	YD	272/276 (98%)	-0.37	0 100 100	0, 18, 64, 125	0
28	RE	205/206 (99%)	-0.19	2 (0%) 82 75	1, 49, 112, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	YE	205/206 (99%)	-0.18	4 (1%) 65 56	0, 47, 104, 155	0
29	RF	202/210 (96%)	-0.29	1 (0%) 91 85	0, 55, 108, 143	0
29	YF	202/210 (96%)	-0.33	1 (0%) 91 85	0, 32, 96, 124	0
30	RG	181/182 (99%)	0.82	24 (13%) 3 3	39, 113, 160, 177	0
30	YG	181/182 (99%)	0.24	10 (5%) 25 22	18, 92, 131, 177	0
31	RH	170/180 (94%)	0.89	24 (14%) 2 3	45, 112, 156, 177	0
31	YH	170/180 (94%)	-0.09	3 (1%) 68 60	11, 66, 116, 131	0
32	RI	146/148 (98%)	-0.12	4 (2%) 54 44	3, 77, 124, 177	0
32	YI	146/148 (98%)	-0.21	3 (2%) 63 54	3, 64, 125, 140	0
33	RN	138/140 (98%)	-0.04	0 100 100	6, 61, 118, 144	0
33	YN	138/140 (98%)	-0.33	0 100 100	4, 45, 98, 131	0
34	RO	122/122 (100%)	-0.28	0 100 100	2, 42, 80, 107	0
34	YO	122/122 (100%)	-0.28	0 100 100	2, 41, 82, 126	0
35	RP	150/150 (100%)	-0.02	6 (4%) 38 31	1, 58, 130, 158	0
35	YP	150/150 (100%)	-0.16	3 (2%) 65 56	1, 46, 101, 160	0
36	RQ	141/141 (100%)	-0.08	3 (2%) 63 54	3, 58, 103, 133	0
36	YQ	141/141 (100%)	-0.27	1 (0%) 87 82	0, 47, 97, 115	0
37	RR	118/118 (100%)	-0.38	0 100 100	1, 34, 87, 136	0
37	YR	118/118 (100%)	-0.32	1 (0%) 86 80	2, 38, 98, 136	0
38	RS	111/112 (99%)	-0.03	2 (1%) 68 60	23, 83, 117, 138	0
38	YS	111/112 (99%)	0.04	1 (0%) 84 77	13, 73, 115, 168	0
39	RT	137/146 (93%)	-0.02	4 (2%) 51 41	8, 58, 130, 152	0
39	YT	137/146 (93%)	-0.13	5 (3%) 42 34	9, 56, 122, 170	0
40	RU	117/118 (99%)	-0.14	2 (1%) 70 61	1, 49, 113, 166	0
40	YU	117/118 (99%)	-0.42	2 (1%) 70 61	1, 31, 97, 145	0
41	RV	101/101 (100%)	-0.10	3 (2%) 50 39	1, 68, 120, 193	0
41	YV	101/101 (100%)	-0.19	1 (0%) 82 75	1, 45, 97, 171	0
42	RW	113/113 (100%)	-0.06	5 (4%) 34 29	2, 34, 95, 131	0
42	YW	113/113 (100%)	-0.16	3 (2%) 54 44	1, 24, 84, 155	0
43	RX	92/96 (95%)	-0.19	1 (1%) 80 73	4, 44, 91, 131	0
43	YX	92/96 (95%)	-0.09	0 100 100	1, 25, 64, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	RY	102/110 (92%)	0.40	9 (8%) 10 9	10, 84, 138, 174	0
44	YY	102/110 (92%)	-0.31	2 (1%) 65 56	2, 50, 106, 160	0
45	RZ	183/206 (88%)	0.02	3 (1%) 72 62	20, 88, 136, 160	0
45	YZ	183/206 (88%)	-0.08	6 (3%) 46 37	20, 78, 137, 167	0
46	R0	82/85 (96%)	-0.39	1 (1%) 79 70	6, 44, 83, 137	0
46	Y0	82/85 (96%)	-0.39	0 100 100	2, 32, 70, 88	0
47	R1	97/98 (98%)	0.27	6 (6%) 20 17	2, 47, 126, 202	0
47	Y1	97/98 (98%)	0.13	9 (9%) 8 8	0, 32, 114, 142	0
48	R2	69/72 (95%)	-0.17	1 (1%) 75 66	8, 72, 116, 128	0
48	Y2	69/72 (95%)	-0.31	0 100 100	0, 39, 97, 137	0
49	R3	59/60 (98%)	-0.11	2 (3%) 45 36	7, 60, 126, 152	0
49	Y3	59/60 (98%)	-0.41	0 100 100	3, 40, 87, 128	0
50	R4	71/71 (100%)	1.03	14 (19%) 1 1	78, 145, 193, 235	0
50	Y4	71/71 (100%)	0.52	11 (15%) 2 2	69, 122, 166, 194	0
51	R5	59/60 (98%)	0.16	6 (10%) 6 7	4, 39, 139, 166	0
51	Y5	59/60 (98%)	0.06	2 (3%) 45 36	1, 40, 132, 156	0
52	R6	49/54 (90%)	1.93	20 (40%) 0 0	48, 122, 152, 191	0
52	Y6	49/54 (90%)	0.99	8 (16%) 1 2	47, 108, 148, 175	0
53	R7	49/49 (100%)	-0.20	1 (2%) 65 56	1, 27, 75, 161	0
53	Y7	49/49 (100%)	-0.13	1 (2%) 65 56	1, 15, 84, 140	0
54	R8	64/65 (98%)	0.00	3 (4%) 31 26	4, 41, 94, 153	0
54	Y8	64/65 (98%)	-0.09	0 100 100	2, 34, 85, 138	0
55	R9	37/37 (100%)	3.10	27 (72%) 0 0	53, 103, 154, 162	0
55	Y9	37/37 (100%)	2.81	26 (70%) 0 0	60, 98, 136, 154	0
56	Z6	2/3 (66%)	0.66	0 100 100	17, 17, 17, 30	0
56	Z8	2/3 (66%)	0.70	0 100 100	19, 19, 19, 22	0
All	All	20870/21494 (97%)	0.03	869 (4%) 36 30	0, 55, 139, 252	0

The worst 5 of 869 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	RA	2173	A	14.2
25	RA	1084	A	12.3

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Mol	Chain	Res	Type	RSRZ
25	RA	1094	U	11.8
25	RA	1058	G	11.5
40	RU	118	GLY	11.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	1MG	QY	37	24/25	0.88	0.23	130,130,130,130	0
24	1MG	XY	37	24/25	0.90	0.26	56,56,56,56	0
56	PPU	Z8	76	37/38	0.91	0.39	10,10,10,10	0
56	PPU	Z6	76	37/38	0.95	0.32	14,14,14,14	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
57	MG	RA	3219	1/1	0.43	0.72	40,40,40,40	0
57	MG	QF	201	1/1	0.45	1.08	36,36,36,36	0
57	MG	RA	3166	1/1	0.49	0.29	34,34,34,34	0
57	MG	RA	3213	1/1	0.50	0.50	8,8,8,8	0
57	MG	RA	3062	1/1	0.51	1.84	50,50,50,50	0
57	MG	RA	3138	1/1	0.53	0.76	29,29,29,29	0
57	MG	YA	3207	1/1	0.55	0.97	7,7,7,7	0
57	MG	RA	3226	1/1	0.55	0.37	9,9,9,9	0
57	MG	RA	3227	1/1	0.59	0.56	22,22,22,22	0
57	MG	QA	1620	1/1	0.60	0.32	6,6,6,6	0
57	MG	QA	1661	1/1	0.61	0.33	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3196	1/1	0.61	0.51	1,1,1,1	0
57	MG	YA	3236	1/1	0.61	0.28	5,5,5,5	0
57	MG	QA	1629	1/1	0.64	0.85	0,0,0,0	0
57	MG	RA	3239	1/1	0.65	0.49	14,14,14,14	0
57	MG	YA	3183	1/1	0.66	0.55	16,16,16,16	0
57	MG	YA	3131	1/1	0.66	0.41	3,3,3,3	0
57	MG	YA	3254	1/1	0.67	0.63	2,2,2,2	0
57	MG	YA	3076	1/1	0.69	1.29	50,50,50,50	0
57	MG	QA	1631	1/1	0.69	0.42	26,26,26,26	0
57	MG	YA	3176	1/1	0.70	0.51	6,6,6,6	0
57	MG	RA	3153	1/1	0.70	0.34	15,15,15,15	0
57	MG	RA	3225	1/1	0.71	0.25	10,10,10,10	0
57	MG	YA	3100	1/1	0.72	0.91	6,6,6,6	0
57	MG	YA	3219	1/1	0.72	0.17	7,7,7,7	0
57	MG	R8	101	1/1	0.73	0.37	0,0,0,0	0
57	MG	RA	3003	1/1	0.74	0.93	5,5,5,5	0
57	MG	XA	1667	1/1	0.75	0.27	17,17,17,17	0
57	MG	YA	3184	1/1	0.76	0.32	7,7,7,7	0
57	MG	RA	3049	1/1	0.76	1.01	13,13,13,13	0
57	MG	RA	3203	1/1	0.76	0.38	24,24,24,24	0
57	MG	YA	3250	1/1	0.76	1.17	11,11,11,11	0
57	MG	YA	3242	1/1	0.76	0.79	4,4,4,4	0
57	MG	RA	3206	1/1	0.76	0.37	3,3,3,3	0
57	MG	RA	3157	1/1	0.77	0.55	0,0,0,0	0
57	MG	RA	3007	1/1	0.77	0.41	16,16,16,16	0
57	MG	XA	1642	1/1	0.77	0.72	5,5,5,5	0
57	MG	RA	3199	1/1	0.77	0.73	6,6,6,6	0
57	MG	RA	3191	1/1	0.77	0.31	67,67,67,67	0
59	A	XX	101	22/23	0.77	0.30	91,91,91,91	0
57	MG	YA	3152	1/1	0.77	0.66	5,5,5,5	0
57	MG	YA	3166	1/1	0.77	0.30	4,4,4,4	0
57	MG	YA	3172	1/1	0.77	1.39	1,1,1,1	0
57	MG	RA	3173	1/1	0.78	0.50	48,48,48,48	0
57	MG	YA	3030	1/1	0.78	0.95	5,5,5,5	0
57	MG	RP	201	1/1	0.78	1.36	21,21,21,21	0
57	MG	YA	3121	1/1	0.79	0.42	62,62,62,62	0
57	MG	RA	3224	1/1	0.79	0.39	5,5,5,5	0
57	MG	RA	3179	1/1	0.80	0.38	4,4,4,4	0
57	MG	RA	3197	1/1	0.80	0.65	3,3,3,3	0
57	MG	QA	1650	1/1	0.80	0.61	11,11,11,11	0
57	MG	QX	101	1/1	0.80	0.41	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1656	1/1	0.80	1.10	10,10,10,10	0
57	MG	YA	3210	1/1	0.80	0.51	3,3,3,3	0
57	MG	QA	1623	1/1	0.80	0.42	14,14,14,14	0
57	MG	QA	1632	1/1	0.80	0.14	42,42,42,42	0
57	MG	RA	3046	1/1	0.80	0.87	50,50,50,50	0
57	MG	YA	3080	1/1	0.80	1.46	50,50,50,50	0
57	MG	YA	3063	1/1	0.80	0.29	11,11,11,11	0
57	MG	XA	1627	1/1	0.81	0.27	14,14,14,14	0
57	MG	RA	3063	1/1	0.81	0.81	3,3,3,3	0
57	MG	XA	1655	1/1	0.81	0.29	9,9,9,9	0
57	MG	RA	3172	1/1	0.81	0.48	4,4,4,4	0
57	MG	YA	3167	1/1	0.81	0.52	2,2,2,2	0
57	MG	YB	201	1/1	0.81	0.31	7,7,7,7	0
57	MG	RD	301	1/1	0.81	0.47	1,1,1,1	0
57	MG	RA	3221	1/1	0.81	0.33	22,22,22,22	0
57	MG	XA	1663	1/1	0.81	0.54	15,15,15,15	0
57	MG	RA	3009	1/1	0.82	0.36	10,10,10,10	0
57	MG	XA	1646	1/1	0.82	0.28	7,7,7,7	0
57	MG	RA	3130	1/1	0.82	0.61	2,2,2,2	0
57	MG	RA	3207	1/1	0.82	0.27	11,11,11,11	0
57	MG	YA	3114	1/1	0.82	0.33	13,13,13,13	0
57	MG	YA	3145	1/1	0.82	0.33	9,9,9,9	0
57	MG	YP	201	1/1	0.83	0.15	94,94,94,94	0
57	MG	YA	3012	1/1	0.83	1.55	50,50,50,50	0
57	MG	QA	1601	1/1	0.83	0.35	9,9,9,9	0
57	MG	R0	101	1/1	0.83	0.30	0,0,0,0	0
57	MG	XB	301	1/1	0.83	0.33	2,2,2,2	0
57	MG	YA	3159	1/1	0.83	0.20	6,6,6,6	0
57	MG	RA	3137	1/1	0.83	0.44	10,10,10,10	0
57	MG	QA	1638	1/1	0.83	0.64	34,34,34,34	0
57	MG	RA	3022	1/1	0.83	0.36	4,4,4,4	0
57	MG	RA	3202	1/1	0.83	0.15	16,16,16,16	0
57	MG	XA	1629	1/1	0.83	0.17	8,8,8,8	0
57	MG	RA	3176	1/1	0.84	0.31	3,3,3,3	0
57	MG	QA	1649	1/1	0.84	0.41	6,6,6,6	0
57	MG	XA	1650	1/1	0.84	0.28	18,18,18,18	0
57	MG	QA	1618	1/1	0.84	0.51	3,3,3,3	0
57	MG	YA	3039	1/1	0.84	0.28	6,6,6,6	0
57	MG	YA	3252	1/1	0.84	0.75	8,8,8,8	0
57	MG	QA	1637	1/1	0.84	0.31	0,0,0,0	0
57	MG	YA	3140	1/1	0.84	0.25	12,12,12,12	0
57	MG	RA	3069	1/1	0.84	0.82	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3014	1/1	0.84	1.25	50,50,50,50	0
57	MG	RA	3070	1/1	0.84	0.90	0,0,0,0	0
57	MG	YA	3246	1/1	0.84	0.35	7,7,7,7	0
57	MG	YA	3260	1/1	0.84	0.97	50,50,50,50	0
57	MG	QA	1624	1/1	0.85	0.65	0,0,0,0	0
57	MG	RA	3169	1/1	0.85	0.24	16,16,16,16	0
57	MG	XA	1638	1/1	0.85	0.33	20,20,20,20	0
57	MG	YA	3238	1/1	0.85	0.29	11,11,11,11	0
57	MG	XA	1662	1/1	0.85	0.88	11,11,11,11	0
57	MG	QA	1664	1/1	0.85	0.41	54,54,54,54	0
57	MG	YA	3248	1/1	0.85	0.44	0,0,0,0	0
57	MG	QA	1662	1/1	0.85	0.27	37,37,37,37	0
57	MG	RA	3168	1/1	0.85	0.47	1,1,1,1	0
57	MG	YA	3117	1/1	0.85	0.99	6,6,6,6	0
57	MG	YA	3049	1/1	0.85	0.89	50,50,50,50	0
57	MG	YA	3122	1/1	0.86	0.40	3,3,3,3	0
57	MG	RA	3048	1/1	0.86	0.21	3,3,3,3	0
57	MG	YA	3001	1/1	0.86	1.21	50,50,50,50	0
57	MG	RA	3220	1/1	0.86	0.28	26,26,26,26	0
57	MG	YA	3128	1/1	0.86	0.57	12,12,12,12	0
57	MG	XA	1607	1/1	0.86	0.38	16,16,16,16	0
57	MG	YA	3045	1/1	0.86	0.53	13,13,13,13	0
57	MG	RA	3208	1/1	0.86	0.65	15,15,15,15	0
57	MG	RA	3032	1/1	0.86	1.18	50,50,50,50	0
57	MG	YA	3085	1/1	0.86	0.61	13,13,13,13	0
57	MG	RA	3159	1/1	0.86	0.26	6,6,6,6	0
57	MG	YA	3230	1/1	0.86	0.16	8,8,8,8	0
57	MG	QA	1626	1/1	0.86	0.40	57,57,57,57	0
57	MG	RA	3039	1/1	0.86	0.36	10,10,10,10	0
57	MG	RA	3076	1/1	0.86	0.53	7,7,7,7	0
57	MG	YA	3193	1/1	0.86	0.19	3,3,3,3	0
57	MG	QA	1615	1/1	0.86	0.78	4,4,4,4	0
57	MG	YA	3165	1/1	0.86	0.23	11,11,11,11	0
57	MG	YB	202	1/1	0.86	0.67	24,24,24,24	0
57	MG	RA	3071	1/1	0.86	0.23	1,1,1,1	0
57	MG	RA	3222	1/1	0.86	0.34	14,14,14,14	0
57	MG	YA	3212	1/1	0.86	0.25	8,8,8,8	0
57	MG	YA	3175	1/1	0.86	0.24	9,9,9,9	0
57	MG	QA	1646	1/1	0.86	0.53	10,10,10,10	0
57	MG	YA	3247	1/1	0.86	0.39	14,14,14,14	0
57	MG	RA	3025	1/1	0.86	0.14	3,3,3,3	0
57	MG	RA	3006	1/1	0.86	0.97	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	YA	3237	1/1	0.86	0.32	7,7,7,7	0
57	MG	RA	3229	1/1	0.87	1.51	50,50,50,50	0
57	MG	RA	3132	1/1	0.87	0.16	3,3,3,3	0
57	MG	YA	3243	1/1	0.87	0.42	32,32,32,32	0
57	MG	RA	3192	1/1	0.87	0.27	21,21,21,21	0
57	MG	RA	3121	1/1	0.87	0.77	5,5,5,5	0
58	ZN	QN	101	1/1	0.87	0.13	104,104,104,104	0
57	MG	RA	3141	1/1	0.87	0.24	2,2,2,2	0
57	MG	RA	3142	1/1	0.87	0.49	36,36,36,36	0
57	MG	XA	1665	1/1	0.87	0.49	7,7,7,7	0
57	MG	YA	3188	1/1	0.88	0.51	1,1,1,1	0
57	MG	YA	3155	1/1	0.88	0.33	7,7,7,7	0
57	MG	RA	3195	1/1	0.88	0.26	24,24,24,24	0
57	MG	RA	3085	1/1	0.88	0.81	5,5,5,5	0
57	MG	RA	3193	1/1	0.88	0.33	22,22,22,22	0
57	MG	YA	3151	1/1	0.88	0.17	5,5,5,5	0
57	MG	YA	3218	1/1	0.88	0.36	5,5,5,5	0
57	MG	YA	3245	1/1	0.88	0.30	2,2,2,2	0
57	MG	XA	1671	1/1	0.88	0.22	3,3,3,3	0
57	MG	YA	3119	1/1	0.88	0.78	8,8,8,8	0
57	MG	XA	1648	1/1	0.88	0.57	3,3,3,3	0
57	MG	RA	3209	1/1	0.88	0.33	17,17,17,17	0
57	MG	XA	1664	1/1	0.88	0.29	8,8,8,8	0
57	MG	QA	1655	1/1	0.88	0.67	20,20,20,20	0
57	MG	Y7	101	1/1	0.88	0.73	15,15,15,15	0
57	MG	XA	1647	1/1	0.88	0.37	1,1,1,1	0
57	MG	QA	1603	1/1	0.88	0.93	14,14,14,14	0
57	MG	RA	3234	1/1	0.88	0.34	9,9,9,9	0
57	MG	RA	3177	1/1	0.89	0.79	7,7,7,7	0
57	MG	RA	3125	1/1	0.89	0.52	1,1,1,1	0
57	MG	YA	3269	1/1	0.89	0.78	1,1,1,1	0
57	MG	YA	3084	1/1	0.89	0.27	17,17,17,17	0
57	MG	RA	3155	1/1	0.89	0.39	10,10,10,10	0
57	MG	YA	3075	1/1	0.89	0.26	0,0,0,0	0
57	MG	RA	3114	1/1	0.89	0.33	1,1,1,1	0
57	MG	XA	1630	1/1	0.89	0.64	10,10,10,10	0
57	MG	RA	3185	1/1	0.89	0.18	9,9,9,9	0
57	MG	RA	3182	1/1	0.89	0.21	4,4,4,4	0
57	MG	YA	3209	1/1	0.89	0.28	15,15,15,15	0
57	MG	YA	3224	1/1	0.89	0.38	0,0,0,0	0
57	MG	RA	3033	1/1	0.89	0.58	50,50,50,50	0
57	MG	RA	3052	1/1	0.89	0.87	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3200	1/1	0.89	0.92	4,4,4,4	0
57	MG	YA	3146	1/1	0.89	0.44	0,0,0,0	0
57	MG	YA	3074	1/1	0.89	0.18	11,11,11,11	0
57	MG	RA	3083	1/1	0.89	0.39	6,6,6,6	0
57	MG	XA	1603	1/1	0.89	0.62	8,8,8,8	0
57	MG	YA	3263	1/1	0.89	0.76	4,4,4,4	0
57	MG	RA	3233	1/1	0.89	0.64	2,2,2,2	0
57	MG	R5	101	1/1	0.89	0.52	5,5,5,5	0
57	MG	XA	1657	1/1	0.89	0.42	8,8,8,8	0
57	MG	YA	3066	1/1	0.89	0.59	7,7,7,7	0
57	MG	RA	3088	1/1	0.89	0.61	15,15,15,15	0
57	MG	QA	1636	1/1	0.89	0.12	16,16,16,16	0
57	MG	RA	3178	1/1	0.90	0.25	1,1,1,1	0
57	MG	QH	201	1/1	0.90	0.21	47,47,47,47	0
57	MG	RA	3162	1/1	0.90	0.23	2,2,2,2	0
57	MG	XA	1652	1/1	0.90	0.33	66,66,66,66	0
57	MG	YA	3174	1/1	0.90	0.22	40,40,40,40	0
57	MG	RA	3171	1/1	0.90	0.19	12,12,12,12	0
57	MG	RA	3187	1/1	0.90	0.48	3,3,3,3	0
57	MG	RR	202	1/1	0.90	0.34	0,0,0,0	0
57	MG	YA	3173	1/1	0.90	0.30	35,35,35,35	0
57	MG	YA	3185	1/1	0.90	0.14	2,2,2,2	0
57	MG	RA	3170	1/1	0.90	1.02	5,5,5,5	0
57	MG	YA	3239	1/1	0.90	0.20	5,5,5,5	0
57	MG	YA	3256	1/1	0.90	0.39	7,7,7,7	0
57	MG	YA	3160	1/1	0.90	0.49	1,1,1,1	0
57	MG	YA	3103	1/1	0.90	0.14	5,5,5,5	0
57	MG	YA	3101	1/1	0.90	0.59	2,2,2,2	0
57	MG	RE	302	1/1	0.90	0.25	1,1,1,1	0
57	MG	RA	3005	1/1	0.90	0.62	12,12,12,12	0
57	MG	RA	3117	1/1	0.90	0.15	25,25,25,25	0
57	MG	XA	1636	1/1	0.90	0.38	3,3,3,3	0
57	MG	XA	1605	1/1	0.90	0.57	3,3,3,3	0
57	MG	RA	3140	1/1	0.90	0.73	9,9,9,9	0
57	MG	YA	3071	1/1	0.90	0.19	28,28,28,28	0
57	MG	XA	1631	1/1	0.90	0.20	31,31,31,31	0
57	MG	RA	3188	1/1	0.90	0.34	5,5,5,5	0
57	MG	RA	3175	1/1	0.90	0.12	1,1,1,1	0
57	MG	XV	102	1/1	0.90	0.66	9,9,9,9	0
57	MG	RA	3026	1/1	0.90	0.63	50,50,50,50	0
57	MG	RA	3214	1/1	0.91	0.34	5,5,5,5	0
57	MG	XA	1609	1/1	0.91	0.52	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3198	1/1	0.91	0.18	12,12,12,12	0
57	MG	YA	3099	1/1	0.91	0.76	10,10,10,10	0
57	MG	XA	1653	1/1	0.91	0.35	8,8,8,8	0
57	MG	YA	3203	1/1	0.91	0.15	53,53,53,53	0
57	MG	YA	3265	1/1	0.91	1.06	4,4,4,4	0
57	MG	YA	3169	1/1	0.91	0.16	6,6,6,6	0
57	MG	YA	3156	1/1	0.91	0.58	2,2,2,2	0
57	MG	QA	1657	1/1	0.91	0.14	7,7,7,7	0
58	ZN	Y9	101	1/1	0.91	0.47	138,138,138,138	0
57	MG	RA	3001	1/1	0.91	0.59	3,3,3,3	0
57	MG	YA	3268	1/1	0.91	0.53	6,6,6,6	0
58	ZN	QD	301	1/1	0.91	0.35	50,50,50,50	0
57	MG	YA	3192	1/1	0.91	0.52	11,11,11,11	0
57	MG	RA	3018	1/1	0.91	0.73	6,6,6,6	0
57	MG	RA	3223	1/1	0.91	0.30	47,47,47,47	0
57	MG	XA	1641	1/1	0.91	1.19	21,21,21,21	0
57	MG	YA	3202	1/1	0.91	0.25	1,1,1,1	0
57	MG	XA	1666	1/1	0.91	0.32	50,50,50,50	0
57	MG	XA	1635	1/1	0.91	0.57	4,4,4,4	0
57	MG	QA	1628	1/1	0.91	0.21	8,8,8,8	0
57	MG	RA	3194	1/1	0.91	0.28	6,6,6,6	0
57	MG	YA	3201	1/1	0.91	0.56	9,9,9,9	0
57	MG	RA	3044	1/1	0.91	0.85	10,10,10,10	0
57	MG	YA	3153	1/1	0.91	0.41	20,20,20,20	0
57	MG	QA	1612	1/1	0.92	0.46	7,7,7,7	0
57	MG	YA	3133	1/1	0.92	0.13	1,1,1,1	0
57	MG	YA	3006	1/1	0.92	0.56	3,3,3,3	0
57	MG	RA	3101	1/1	0.92	0.45	11,11,11,11	0
58	ZN	R9	101	1/1	0.92	0.40	145,145,145,145	0
57	MG	RA	3174	1/1	0.92	0.52	4,4,4,4	0
57	MG	YA	3127	1/1	0.92	0.29	2,2,2,2	0
57	MG	RE	301	1/1	0.92	0.27	12,12,12,12	0
57	MG	YA	3050	1/1	0.92	0.45	50,50,50,50	0
57	MG	QA	1614	1/1	0.92	0.51	9,9,9,9	0
57	MG	YA	3171	1/1	0.92	0.40	13,13,13,13	0
57	MG	YA	3222	1/1	0.92	0.19	8,8,8,8	0
57	MG	YA	3016	1/1	0.92	0.22	6,6,6,6	0
57	MG	XA	1606	1/1	0.92	0.56	10,10,10,10	0
57	MG	YA	3024	1/1	0.92	0.54	50,50,50,50	0
57	MG	RA	3235	1/1	0.92	0.62	1,1,1,1	0
57	MG	RA	3216	1/1	0.92	0.52	7,7,7,7	0
57	MG	YA	3194	1/1	0.92	0.17	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	RA	3131	1/1	0.92	0.68	9,9,9,9	0
57	MG	YA	3149	1/1	0.92	0.20	15,15,15,15	0
57	MG	RA	3036	1/1	0.92	0.78	6,6,6,6	0
57	MG	XM	201	1/1	0.92	0.11	85,85,85,85	0
57	MG	YA	3002	1/1	0.92	1.06	50,50,50,50	0
57	MG	QA	1609	1/1	0.92	0.72	4,4,4,4	0
57	MG	YA	3157	1/1	0.92	0.63	0,0,0,0	0
57	MG	QA	1640	1/1	0.92	0.35	9,9,9,9	0
57	MG	YA	3186	1/1	0.92	0.62	11,11,11,11	0
57	MG	YA	3198	1/1	0.92	0.25	51,51,51,51	0
57	MG	RA	3116	1/1	0.92	0.46	9,9,9,9	0
57	MG	QA	1613	1/1	0.92	0.68	15,15,15,15	0
57	MG	XA	1624	1/1	0.92	0.59	3,3,3,3	0
57	MG	QA	1643	1/1	0.92	0.29	33,33,33,33	0
57	MG	QA	1642	1/1	0.92	0.49	16,16,16,16	0
57	MG	YA	3135	1/1	0.92	0.25	6,6,6,6	0
57	MG	YA	3234	1/1	0.92	0.53	17,17,17,17	0
57	MG	RA	3055	1/1	0.92	0.93	5,5,5,5	0
57	MG	RA	3230	1/1	0.92	0.74	5,5,5,5	0
57	MG	XA	1621	1/1	0.92	0.33	3,3,3,3	0
57	MG	RA	3129	1/1	0.92	0.21	31,31,31,31	0
57	MG	YA	3261	1/1	0.92	0.30	4,4,4,4	0
57	MG	YB	203	1/1	0.92	0.23	37,37,37,37	0
57	MG	XA	1649	1/1	0.92	0.20	0,0,0,0	0
57	MG	YA	3154	1/1	0.92	0.23	1,1,1,1	0
57	MG	YA	3141	1/1	0.92	0.53	0,0,0,0	0
57	MG	YA	3179	1/1	0.92	0.24	0,0,0,0	0
57	MG	YA	3181	1/1	0.92	0.34	3,3,3,3	0
57	MG	RA	3110	1/1	0.92	0.48	3,3,3,3	0
57	MG	XA	1608	1/1	0.92	0.13	37,37,37,37	0
57	MG	YA	3225	1/1	0.92	0.24	10,10,10,10	0
57	MG	RA	3028	1/1	0.92	0.46	14,14,14,14	0
57	MG	QA	1622	1/1	0.93	0.33	14,14,14,14	0
57	MG	YA	3088	1/1	0.93	0.58	50,50,50,50	0
57	MG	RA	3041	1/1	0.93	0.44	4,4,4,4	0
57	MG	YA	3115	1/1	0.93	0.32	4,4,4,4	0
57	MG	RA	3089	1/1	0.93	0.57	11,11,11,11	0
57	MG	YA	3054	1/1	0.93	0.31	1,1,1,1	0
57	MG	XA	1625	1/1	0.93	0.17	5,5,5,5	0
57	MG	RA	3067	1/1	0.93	0.25	2,2,2,2	0
57	MG	QA	1656	1/1	0.93	0.14	30,30,30,30	0
57	MG	YA	3142	1/1	0.93	0.66	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3231	1/1	0.93	0.30	14,14,14,14	0
57	MG	QA	1627	1/1	0.93	0.21	10,10,10,10	0
57	MG	RA	3238	1/1	0.93	0.49	16,16,16,16	0
57	MG	QA	1619	1/1	0.93	0.45	4,4,4,4	0
57	MG	YA	3267	1/1	0.93	0.41	4,4,4,4	0
57	MG	RA	3079	1/1	0.93	0.68	5,5,5,5	0
57	MG	XA	1601	1/1	0.93	0.95	1,1,1,1	0
57	MG	YA	3229	1/1	0.93	0.24	3,3,3,3	0
57	MG	QA	1602	1/1	0.93	0.81	12,12,12,12	0
57	MG	YA	3094	1/1	0.93	0.91	11,11,11,11	0
57	MG	RB	201	1/1	0.93	0.13	8,8,8,8	0
57	MG	YA	3028	1/1	0.93	0.37	6,6,6,6	0
57	MG	XA	1654	1/1	0.93	0.29	26,26,26,26	0
57	MG	RA	3218	1/1	0.93	0.32	23,23,23,23	0
57	MG	YA	3259	1/1	0.93	0.72	8,8,8,8	0
57	MG	YA	3069	1/1	0.93	0.51	2,2,2,2	0
57	MG	XA	1661	1/1	0.93	0.16	2,2,2,2	0
57	MG	RA	3045	1/1	0.93	0.12	1,1,1,1	0
57	MG	YA	3132	1/1	0.93	0.10	5,5,5,5	0
57	MG	YA	3053	1/1	0.93	0.53	4,4,4,4	0
57	MG	RA	3152	1/1	0.93	0.14	4,4,4,4	0
57	MG	RA	3050	1/1	0.93	0.56	11,11,11,11	0
57	MG	YA	3189	1/1	0.93	0.55	6,6,6,6	0
57	MG	RA	3232	1/1	0.93	0.39	13,13,13,13	0
57	MG	YA	3168	1/1	0.94	0.29	41,41,41,41	0
57	MG	QA	1644	1/1	0.94	0.26	4,4,4,4	0
57	MG	RA	3236	1/1	0.94	0.44	0,0,0,0	0
57	MG	RB	202	1/1	0.94	0.08	4,4,4,4	0
57	MG	YA	3086	1/1	0.94	0.78	6,6,6,6	0
57	MG	XA	1637	1/1	0.94	0.43	25,25,25,25	0
57	MG	YA	3253	1/1	0.94	0.59	6,6,6,6	0
57	MG	RA	3186	1/1	0.94	0.23	8,8,8,8	0
57	MG	YA	3258	1/1	0.94	0.52	1,1,1,1	0
57	MG	XA	1634	1/1	0.94	0.55	0,0,0,0	0
57	MG	YA	3208	1/1	0.94	0.21	15,15,15,15	0
57	MG	YA	3180	1/1	0.94	0.41	38,38,38,38	0
57	MG	RA	3164	1/1	0.94	0.16	4,4,4,4	0
57	MG	YA	3032	1/1	0.94	0.28	1,1,1,1	0
57	MG	YA	3150	1/1	0.94	0.41	4,4,4,4	0
57	MG	YA	3211	1/1	0.94	0.60	7,7,7,7	0
57	MG	XA	1651	1/1	0.94	0.27	25,25,25,25	0
57	MG	XV	101	1/1	0.94	0.45	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	QA	1651	1/1	0.94	0.22	9,9,9,9	0
57	MG	QA	1607	1/1	0.94	0.11	13,13,13,13	0
57	MG	YA	3124	1/1	0.94	0.21	9,9,9,9	0
57	MG	YA	3043	1/1	0.94	1.15	2,2,2,2	0
57	MG	YA	3164	1/1	0.94	0.46	8,8,8,8	0
57	MG	XA	1670	1/1	0.94	0.17	43,43,43,43	0
57	MG	YA	3144	1/1	0.94	0.13	4,4,4,4	0
57	MG	RA	3183	1/1	0.94	0.33	57,57,57,57	0
57	MG	XA	1668	1/1	0.94	0.23	18,18,18,18	0
57	MG	YA	3106	1/1	0.94	0.34	8,8,8,8	0
57	MG	RA	3112	1/1	0.94	0.17	6,6,6,6	0
57	MG	YA	3015	1/1	0.94	1.11	50,50,50,50	0
57	MG	QA	1639	1/1	0.94	0.19	3,3,3,3	0
57	MG	RA	3010	1/1	0.94	0.51	14,14,14,14	0
57	MG	YA	3251	1/1	0.94	0.17	9,9,9,9	0
57	MG	YA	3266	1/1	0.94	0.27	2,2,2,2	0
57	MG	RA	3237	1/1	0.94	1.23	1,1,1,1	0
57	MG	YA	3205	1/1	0.94	0.14	10,10,10,10	0
57	MG	RA	3145	1/1	0.94	0.47	3,3,3,3	0
57	MG	RA	3215	1/1	0.94	0.17	27,27,27,27	0
57	MG	QA	1633	1/1	0.94	0.58	4,4,4,4	0
57	MG	RA	3004	1/1	0.94	0.96	10,10,10,10	0
57	MG	XA	1658	1/1	0.94	0.43	9,9,9,9	0
57	MG	RA	3143	1/1	0.94	0.30	7,7,7,7	0
57	MG	YA	3240	1/1	0.94	0.17	72,72,72,72	0
57	MG	QA	1648	1/1	0.94	0.32	12,12,12,12	0
57	MG	RA	3013	1/1	0.94	0.53	4,4,4,4	0
57	MG	XA	1620	1/1	0.94	0.16	2,2,2,2	0
57	MG	YE	301	1/1	0.94	0.18	0,0,0,0	0
57	MG	YA	3221	1/1	0.94	0.50	18,18,18,18	0
57	MG	YA	3004	1/1	0.94	0.40	12,12,12,12	0
57	MG	RA	3211	1/1	0.94	0.24	2,2,2,2	0
57	MG	YA	3011	1/1	0.94	0.32	0,0,0,0	0
57	MG	RA	3190	1/1	0.95	0.20	16,16,16,16	0
57	MG	RA	3020	1/1	0.95	0.73	50,50,50,50	0
57	MG	RA	3134	1/1	0.95	0.13	25,25,25,25	0
57	MG	YA	3111	1/1	0.95	0.21	15,15,15,15	0
57	MG	RA	3093	1/1	0.95	0.59	10,10,10,10	0
57	MG	XA	1672	1/1	0.95	0.41	0,0,0,0	0
57	MG	RA	3120	1/1	0.95	0.22	1,1,1,1	0
57	MG	RA	3029	1/1	0.95	0.37	1,1,1,1	0
57	MG	YA	3026	1/1	0.95	1.12	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3161	1/1	0.95	0.20	1,1,1,1	0
57	MG	RA	3135	1/1	0.95	0.17	7,7,7,7	0
57	MG	RA	3181	1/1	0.95	0.20	3,3,3,3	0
57	MG	RA	3111	1/1	0.95	0.46	11,11,11,11	0
57	MG	RA	3016	1/1	0.95	0.39	8,8,8,8	0
57	MG	RA	3068	1/1	0.95	0.12	6,6,6,6	0
57	MG	YA	3072	1/1	0.95	0.21	2,2,2,2	0
57	MG	YA	3264	1/1	0.95	0.17	9,9,9,9	0
57	MG	YA	3052	1/1	0.95	0.70	14,14,14,14	0
57	MG	YA	3215	1/1	0.95	0.18	14,14,14,14	0
57	MG	YA	3118	1/1	0.95	0.28	14,14,14,14	0
57	MG	YA	3019	1/1	0.95	0.47	5,5,5,5	0
57	MG	RA	3094	1/1	0.95	0.47	0,0,0,0	0
57	MG	YA	3136	1/1	0.95	0.12	21,21,21,21	0
57	MG	YA	3007	1/1	0.95	0.17	7,7,7,7	0
57	MG	YA	3033	1/1	0.95	0.45	4,4,4,4	0
57	MG	YA	3078	1/1	0.95	0.36	2,2,2,2	0
57	MG	RA	3015	1/1	0.95	0.69	5,5,5,5	0
57	MG	QA	1641	1/1	0.95	0.23	7,7,7,7	0
57	MG	QA	1625	1/1	0.95	0.30	0,0,0,0	0
57	MG	YA	3163	1/1	0.95	0.21	4,4,4,4	0
57	MG	QA	1605	1/1	0.95	1.07	7,7,7,7	0
57	MG	YA	3125	1/1	0.95	0.41	12,12,12,12	0
57	MG	RA	3058	1/1	0.95	0.74	3,3,3,3	0
57	MG	RA	3092	1/1	0.95	0.53	7,7,7,7	0
57	MG	RA	3014	1/1	0.95	0.28	13,13,13,13	0
57	MG	XA	1660	1/1	0.95	0.14	24,24,24,24	0
57	MG	YA	3120	1/1	0.95	0.60	8,8,8,8	0
57	MG	RA	3047	1/1	0.95	0.62	5,5,5,5	0
57	MG	XA	1611	1/1	0.95	0.31	7,7,7,7	0
57	MG	XA	1628	1/1	0.95	0.54	10,10,10,10	0
57	MG	RA	3102	1/1	0.95	0.27	4,4,4,4	0
57	MG	YA	3190	1/1	0.95	0.24	21,21,21,21	0
57	MG	YA	3123	1/1	0.95	0.19	18,18,18,18	0
57	MG	YA	3255	1/1	0.95	1.32	0,0,0,0	0
57	MG	QA	1611	1/1	0.95	0.31	6,6,6,6	0
57	MG	XA	1622	1/1	0.95	0.13	7,7,7,7	0
57	MG	RA	3204	1/1	0.95	0.27	18,18,18,18	0
57	MG	RA	3043	1/1	0.95	0.21	10,10,10,10	0
57	MG	YA	3227	1/1	0.95	0.28	0,0,0,0	0
57	MG	YA	3096	1/1	0.95	0.52	3,3,3,3	0
57	MG	YA	3134	1/1	0.95	0.78	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	YA	3068	1/1	0.96	0.51	2,2,2,2	0
57	MG	XX	102	1/1	0.96	0.09	50,50,50,50	0
57	MG	RA	3184	1/1	0.96	0.26	8,8,8,8	0
57	MG	RA	3149	1/1	0.96	0.15	20,20,20,20	0
57	MG	RA	3084	1/1	0.96	0.16	4,4,4,4	0
57	MG	RA	3008	1/1	0.96	0.46	0,0,0,0	0
57	MG	RA	3150	1/1	0.96	0.32	37,37,37,37	0
57	MG	RA	3136	1/1	0.96	0.37	0,0,0,0	0
57	MG	YA	3035	1/1	0.96	0.33	9,9,9,9	0
57	MG	RF	301	1/1	0.96	0.39	2,2,2,2	0
57	MG	RA	3064	1/1	0.96	0.18	5,5,5,5	0
57	MG	RA	3024	1/1	0.96	0.23	16,16,16,16	0
57	MG	YA	3143	1/1	0.96	0.15	8,8,8,8	0
57	MG	RA	3151	1/1	0.96	0.41	9,9,9,9	0
57	MG	RA	3205	1/1	0.96	0.31	12,12,12,12	0
57	MG	YA	3139	1/1	0.96	0.40	7,7,7,7	0
57	MG	QA	1604	1/1	0.96	0.27	0,0,0,0	0
57	MG	RA	3053	1/1	0.96	0.16	2,2,2,2	0
57	MG	QA	1621	1/1	0.96	0.11	5,5,5,5	0
57	MG	RA	3095	1/1	0.96	0.80	1,1,1,1	0
57	MG	YA	3178	1/1	0.96	0.13	2,2,2,2	0
57	MG	YA	3070	1/1	0.96	0.40	15,15,15,15	0
57	MG	RA	3031	1/1	0.96	0.74	5,5,5,5	0
57	MG	RA	3154	1/1	0.96	0.18	11,11,11,11	0
57	MG	RA	3077	1/1	0.96	0.55	0,0,0,0	0
57	MG	RA	3091	1/1	0.96	0.44	9,9,9,9	0
57	MG	RA	3217	1/1	0.96	0.21	74,74,74,74	0
57	MG	RA	3139	1/1	0.96	0.24	2,2,2,2	0
57	MG	RA	3017	1/1	0.96	0.39	11,11,11,11	0
57	MG	YA	3034	1/1	0.96	0.54	2,2,2,2	0
57	MG	XA	1643	1/1	0.96	0.37	5,5,5,5	0
57	MG	RA	3126	1/1	0.96	0.44	2,2,2,2	0
57	MG	YA	3195	1/1	0.96	0.39	9,9,9,9	0
57	MG	RA	3035	1/1	0.96	0.41	11,11,11,11	0
57	MG	XA	1659	1/1	0.96	0.32	0,0,0,0	0
57	MG	RA	3160	1/1	0.96	0.33	4,4,4,4	0
57	MG	RA	3019	1/1	0.96	0.38	8,8,8,8	0
57	MG	RA	3051	1/1	0.96	0.47	7,7,7,7	0
57	MG	RA	3122	1/1	0.96	0.56	5,5,5,5	0
57	MG	RA	3119	1/1	0.96	0.39	3,3,3,3	0
57	MG	XA	1618	1/1	0.96	0.50	3,3,3,3	0
57	MG	RA	3167	1/1	0.96	0.23	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	QA	1645	1/1	0.96	0.13	38,38,38,38	0
57	MG	RA	3180	1/1	0.96	0.11	6,6,6,6	0
57	MG	RA	3147	1/1	0.96	0.23	9,9,9,9	0
57	MG	QA	1616	1/1	0.96	0.09	29,29,29,29	0
57	MG	YA	3158	1/1	0.96	0.27	6,6,6,6	0
57	MG	RA	3189	1/1	0.96	0.27	4,4,4,4	0
57	MG	RA	3074	1/1	0.96	0.12	8,8,8,8	0
57	MG	YA	3232	1/1	0.96	0.41	2,2,2,2	0
57	MG	RA	3161	1/1	0.96	0.13	1,1,1,1	0
57	MG	RA	3061	1/1	0.96	0.16	53,53,53,53	0
57	MG	YA	3089	1/1	0.96	0.43	5,5,5,5	0
57	MG	YA	3116	1/1	0.96	0.42	3,3,3,3	0
57	MG	QA	1663	1/1	0.96	0.10	47,47,47,47	0
57	MG	RA	3201	1/1	0.96	0.77	10,10,10,10	0
57	MG	YA	3082	1/1	0.96	0.23	3,3,3,3	0
57	MG	YA	3095	1/1	0.96	0.48	2,2,2,2	0
57	MG	YA	3097	1/1	0.96	0.65	5,5,5,5	0
57	MG	YA	3041	1/1	0.96	0.73	0,0,0,0	0
57	MG	RA	3090	1/1	0.96	0.15	75,75,75,75	0
57	MG	YA	3104	1/1	0.96	0.59	10,10,10,10	0
57	MG	YA	3204	1/1	0.96	0.10	11,11,11,11	0
57	MG	YQ	201	1/1	0.96	0.21	99,99,99,99	0
57	MG	XA	1645	1/1	0.97	0.23	1,1,1,1	0
57	MG	YA	3093	1/1	0.97	0.36	7,7,7,7	0
57	MG	YA	3048	1/1	0.97	0.22	4,4,4,4	0
57	MG	YA	3061	1/1	0.97	0.12	17,17,17,17	0
57	MG	QA	1647	1/1	0.97	0.26	33,33,33,33	0
57	MG	YA	3228	1/1	0.97	0.50	17,17,17,17	0
57	MG	YA	3191	1/1	0.97	0.05	7,7,7,7	0
57	MG	YA	3112	1/1	0.97	0.13	21,21,21,21	0
57	MG	YA	3102	1/1	0.97	0.48	14,14,14,14	0
57	MG	YA	3129	1/1	0.97	0.70	15,15,15,15	0
57	MG	QA	1654	1/1	0.97	0.13	17,17,17,17	0
57	MG	YA	3056	1/1	0.97	0.18	5,5,5,5	0
57	MG	YA	3223	1/1	0.97	0.42	34,34,34,34	0
57	MG	XA	1614	1/1	0.97	0.15	26,26,26,26	0
57	MG	YA	3262	1/1	0.97	0.55	8,8,8,8	0
57	MG	RA	3115	1/1	0.97	0.44	6,6,6,6	0
57	MG	QA	1617	1/1	0.97	0.20	4,4,4,4	0
57	MG	YA	3197	1/1	0.97	0.15	1,1,1,1	0
57	MG	YA	3055	1/1	0.97	0.26	0,0,0,0	0
57	MG	QA	1635	1/1	0.97	0.41	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1632	1/1	0.97	0.81	14,14,14,14	0
57	MG	YA	3064	1/1	0.97	0.35	8,8,8,8	0
57	MG	RA	3012	1/1	0.97	0.50	4,4,4,4	0
57	MG	RA	3163	1/1	0.97	1.01	12,12,12,12	0
57	MG	RA	3002	1/1	0.97	0.89	6,6,6,6	0
57	MG	YA	3098	1/1	0.97	0.29	1,1,1,1	0
57	MG	RA	3118	1/1	0.97	0.22	2,2,2,2	0
57	MG	YA	3137	1/1	0.97	0.21	10,10,10,10	0
57	MG	XA	1669	1/1	0.97	0.19	38,38,38,38	0
57	MG	RA	3144	1/1	0.97	0.26	0,0,0,0	0
57	MG	YA	3081	1/1	0.97	0.50	9,9,9,9	0
57	MG	YA	3059	1/1	0.97	0.32	5,5,5,5	0
57	MG	YA	3047	1/1	0.97	0.60	3,3,3,3	0
57	MG	RA	3054	1/1	0.97	0.28	3,3,3,3	0
57	MG	RA	3021	1/1	0.97	0.22	2,2,2,2	0
57	MG	XA	1644	1/1	0.97	0.14	5,5,5,5	0
57	MG	YA	3130	1/1	0.97	0.21	20,20,20,20	0
57	MG	YA	3005	1/1	0.97	0.25	3,3,3,3	0
57	MG	YA	3217	1/1	0.97	0.17	35,35,35,35	0
57	MG	YA	3170	1/1	0.97	0.20	8,8,8,8	0
57	MG	YA	3040	1/1	0.97	0.55	10,10,10,10	0
57	MG	YA	3138	1/1	0.97	0.12	0,0,0,0	0
57	MG	YA	3126	1/1	0.97	0.35	7,7,7,7	0
57	MG	YA	3087	1/1	0.97	0.68	11,11,11,11	0
57	MG	XA	1626	1/1	0.97	0.16	6,6,6,6	0
57	MG	YA	3162	1/1	0.97	0.18	0,0,0,0	0
57	MG	YA	3199	1/1	0.97	0.11	55,55,55,55	0
57	MG	RA	3108	1/1	0.97	0.09	0,0,0,0	0
57	MG	YA	3083	1/1	0.97	0.50	9,9,9,9	0
57	MG	YA	3003	1/1	0.97	0.17	2,2,2,2	0
57	MG	YA	3233	1/1	0.97	0.22	7,7,7,7	0
57	MG	RA	3065	1/1	0.97	0.37	7,7,7,7	0
57	MG	QA	1659	1/1	0.97	0.23	4,4,4,4	0
57	MG	YA	3077	1/1	0.97	0.30	2,2,2,2	0
57	MG	RA	3086	1/1	0.97	0.24	0,0,0,0	0
57	MG	RA	3097	1/1	0.97	0.47	2,2,2,2	0
57	MG	YA	3021	1/1	0.97	0.43	12,12,12,12	0
57	MG	YA	3046	1/1	0.97	0.40	3,3,3,3	0
57	MG	QA	1652	1/1	0.97	0.16	12,12,12,12	0
57	MG	RA	3106	1/1	0.97	0.36	13,13,13,13	0
57	MG	RA	3103	1/1	0.97	0.48	9,9,9,9	0
57	MG	RA	3124	1/1	0.97	0.34	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3010	1/1	0.97	0.40	5,5,5,5	0
57	MG	RA	3200	1/1	0.97	0.14	1,1,1,1	0
57	MG	XA	1610	1/1	0.97	0.23	3,3,3,3	0
57	MG	RA	3034	1/1	0.97	0.86	9,9,9,9	0
57	MG	RA	3040	1/1	0.97	0.37	14,14,14,14	0
57	MG	YA	3113	1/1	0.97	0.20	1,1,1,1	0
57	MG	RA	3146	1/1	0.97	0.13	5,5,5,5	0
57	MG	RA	3027	1/1	0.97	0.49	13,13,13,13	0
57	MG	YA	3058	1/1	0.97	0.52	15,15,15,15	0
57	MG	RA	3196	1/1	0.98	0.18	0,0,0,0	0
57	MG	RR	201	1/1	0.98	0.24	13,13,13,13	0
57	MG	YA	3105	1/1	0.98	0.18	4,4,4,4	0
57	MG	RA	3080	1/1	0.98	0.34	21,21,21,21	0
57	MG	YA	3220	1/1	0.98	0.66	33,33,33,33	0
57	MG	RA	3075	1/1	0.98	0.19	3,3,3,3	0
57	MG	YA	3009	1/1	0.98	0.73	8,8,8,8	0
57	MG	RA	3060	1/1	0.98	0.30	6,6,6,6	0
57	MG	YA	3107	1/1	0.98	0.46	15,15,15,15	0
57	MG	RA	3100	1/1	0.98	0.14	2,2,2,2	0
57	MG	YA	3213	1/1	0.98	0.13	19,19,19,19	0
57	MG	YA	3147	1/1	0.98	0.57	4,4,4,4	0
57	MG	RA	3133	1/1	0.98	0.16	0,0,0,0	0
57	MG	YA	3060	1/1	0.98	0.59	10,10,10,10	0
57	MG	Y5	101	1/1	0.98	0.36	6,6,6,6	0
57	MG	RA	3113	1/1	0.98	0.11	0,0,0,0	0
57	MG	RA	3087	1/1	0.98	0.93	11,11,11,11	0
57	MG	RA	3011	1/1	0.98	0.18	6,6,6,6	0
57	MG	RA	3098	1/1	0.98	0.63	14,14,14,14	0
57	MG	RA	3109	1/1	0.98	0.23	8,8,8,8	0
57	MG	YA	3092	1/1	0.98	0.25	12,12,12,12	0
57	MG	YA	3091	1/1	0.98	0.39	13,13,13,13	0
57	MG	XA	1615	1/1	0.98	0.28	6,6,6,6	0
57	MG	RA	3059	1/1	0.98	0.44	11,11,11,11	0
57	MG	RA	3081	1/1	0.98	0.71	1,1,1,1	0
57	MG	RA	3099	1/1	0.98	0.24	10,10,10,10	0
57	MG	QV	101	1/1	0.98	0.26	1,1,1,1	0
57	MG	QA	1608	1/1	0.98	0.09	10,10,10,10	0
57	MG	YA	3108	1/1	0.98	0.49	1,1,1,1	0
57	MG	XA	1640	1/1	0.98	0.12	75,75,75,75	0
57	MG	RA	3096	1/1	0.98	0.58	4,4,4,4	0
57	MG	XA	1633	1/1	0.98	0.21	3,3,3,3	0
57	MG	YA	3187	1/1	0.98	0.13	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3025	1/1	0.98	0.19	4,4,4,4	0
57	MG	XA	1612	1/1	0.98	0.17	19,19,19,19	0
57	MG	YA	3017	1/1	0.98	0.17	1,1,1,1	0
57	MG	YA	3249	1/1	0.98	0.31	10,10,10,10	0
57	MG	YA	3008	1/1	0.98	0.32	10,10,10,10	0
57	MG	YA	3042	1/1	0.98	0.57	2,2,2,2	0
57	MG	YA	3109	1/1	0.98	0.31	2,2,2,2	0
57	MG	YA	3051	1/1	0.98	0.44	3,3,3,3	0
57	MG	YA	3235	1/1	0.98	0.37	3,3,3,3	0
57	MG	YA	3044	1/1	0.98	0.31	6,6,6,6	0
57	MG	XA	1616	1/1	0.98	0.31	1,1,1,1	0
57	MG	YA	3231	1/1	0.98	0.11	45,45,45,45	0
57	MG	YA	3013	1/1	0.98	0.54	5,5,5,5	0
57	MG	YA	3031	1/1	0.98	0.60	0,0,0,0	0
57	MG	RA	3156	1/1	0.98	0.13	9,9,9,9	0
57	MG	QA	1606	1/1	0.98	0.13	16,16,16,16	0
57	MG	YA	3148	1/1	0.98	0.14	7,7,7,7	0
57	MG	RA	3228	1/1	0.98	0.51	11,11,11,11	0
57	MG	YA	3038	1/1	0.98	0.16	7,7,7,7	0
57	MG	YA	3241	1/1	0.98	0.18	5,5,5,5	0
57	MG	XA	1604	1/1	0.98	0.96	10,10,10,10	0
57	MG	RA	3056	1/1	0.98	0.36	5,5,5,5	0
57	MG	XA	1623	1/1	0.98	0.16	14,14,14,14	0
57	MG	RA	3037	1/1	0.98	0.51	5,5,5,5	0
57	MG	YA	3073	1/1	0.98	0.25	1,1,1,1	0
57	MG	YA	3029	1/1	0.98	0.81	10,10,10,10	0
57	MG	RA	3212	1/1	0.98	0.51	1,1,1,1	0
58	ZN	XN	101	1/1	0.98	0.20	84,84,84,84	0
57	MG	YA	3036	1/1	0.98	0.32	2,2,2,2	0
57	MG	YA	3079	1/1	0.98	0.23	4,4,4,4	0
57	MG	RA	3030	1/1	0.98	0.36	5,5,5,5	0
57	MG	RA	3042	1/1	0.98	0.18	2,2,2,2	0
57	MG	QA	1634	1/1	0.98	0.18	7,7,7,7	0
57	MG	YA	3057	1/1	0.98	0.88	4,4,4,4	0
57	MG	YA	3090	1/1	0.98	0.43	1,1,1,1	0
57	MG	QA	1630	1/1	0.98	0.15	7,7,7,7	0
57	MG	YA	3216	1/1	0.98	0.16	19,19,19,19	0
57	MG	RA	3123	1/1	0.98	0.12	7,7,7,7	0
57	MG	XA	1617	1/1	0.98	0.22	15,15,15,15	0
57	MG	YA	3226	1/1	0.98	0.38	1,1,1,1	0
57	MG	RA	3105	1/1	0.98	0.47	11,11,11,11	0
57	MG	YA	3027	1/1	0.98	0.10	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3072	1/1	0.98	0.41	3,3,3,3	0
57	MG	RA	3023	1/1	0.98	0.32	16,16,16,16	0
57	MG	YA	3018	1/1	0.98	0.69	3,3,3,3	0
57	MG	YA	3206	1/1	0.98	0.34	26,26,26,26	0
57	MG	XA	1619	1/1	0.98	0.28	5,5,5,5	0
57	MG	YA	3177	1/1	0.99	0.21	3,3,3,3	0
57	MG	YA	3257	1/1	0.99	0.23	3,3,3,3	0
57	MG	RA	3073	1/1	0.99	0.35	2,2,2,2	0
57	MG	RA	3104	1/1	0.99	0.21	3,3,3,3	0
57	MG	YA	3065	1/1	0.99	0.15	5,5,5,5	0
57	MG	YA	3062	1/1	0.99	0.39	6,6,6,6	0
57	MG	RA	3158	1/1	0.99	0.27	15,15,15,15	0
57	MG	QA	1653	1/1	0.99	0.07	67,67,67,67	0
57	MG	XA	1613	1/1	0.99	0.08	0,0,0,0	0
57	MG	RA	3078	1/1	0.99	0.35	3,3,3,3	0
57	MG	QA	1660	1/1	0.99	0.75	2,2,2,2	0
57	MG	YA	3020	1/1	0.99	0.86	0,0,0,0	0
57	MG	XA	1639	1/1	0.99	0.12	5,5,5,5	0
57	MG	RA	3127	1/1	0.99	0.22	0,0,0,0	0
57	MG	YA	3067	1/1	0.99	0.34	5,5,5,5	0
57	MG	RA	3210	1/1	0.99	0.17	45,45,45,45	0
57	MG	YA	3214	1/1	0.99	0.20	2,2,2,2	0
57	MG	RA	3165	1/1	0.99	0.48	13,13,13,13	0
57	MG	RA	3107	1/1	0.99	0.19	10,10,10,10	0
58	ZN	XD	301	1/1	0.99	0.42	50,50,50,50	0
57	MG	YA	3022	1/1	0.99	0.28	1,1,1,1	0
57	MG	YA	3110	1/1	0.99	0.12	2,2,2,2	0
57	MG	RA	3057	1/1	0.99	0.30	2,2,2,2	0
57	MG	RA	3066	1/1	0.99	0.53	6,6,6,6	0
57	MG	RA	3148	1/1	0.99	0.34	5,5,5,5	0
57	MG	RA	3082	1/1	0.99	0.30	0,0,0,0	0
57	MG	YA	3182	1/1	0.99	0.13	8,8,8,8	0
57	MG	QA	1658	1/1	0.99	0.24	16,16,16,16	0
57	MG	YA	3037	1/1	0.99	0.25	13,13,13,13	0
57	MG	RA	3038	1/1	0.99	0.32	8,8,8,8	0
57	MG	RA	3128	1/1	0.99	0.44	7,7,7,7	0
57	MG	XA	1602	1/1	0.99	0.20	7,7,7,7	0
57	MG	QM	201	1/1	0.99	0.14	44,44,44,44	0
57	MG	YA	3023	1/1	0.99	0.32	2,2,2,2	0
57	MG	QA	1610	1/1	0.99	0.23	7,7,7,7	0
57	MG	YA	3244	1/1	1.00	0.10	9,9,9,9	0

## 6.5 Other polymers

There are no such residues in this entry.