



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:55 PM GMT

PDB ID : 4LEL
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCG-G on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-25
Resolution : 3.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

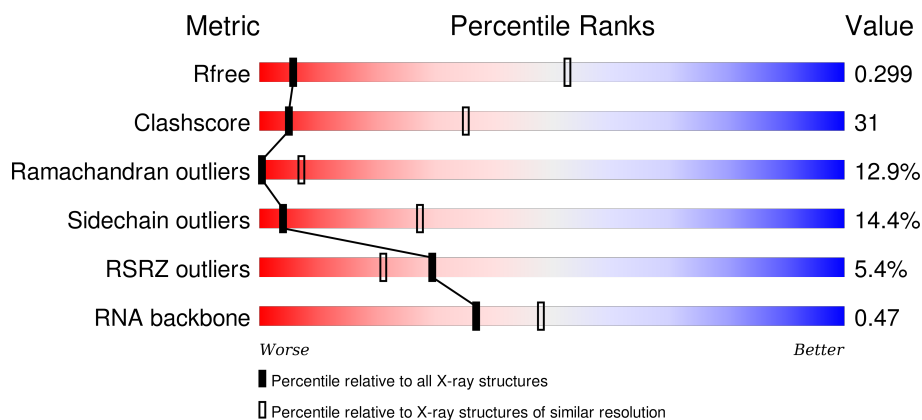
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)
RNA backbone	2183	1078 (5.00-2.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div>44%</div> <div>43%</div> <div>11%</div> <div>..</div> </div>
1	XA	1522	<div> <div>%</div> <div>42%</div> <div>44%</div> <div>12%</div> <div>..</div> </div>
2	QB	256	<div> <div>10%</div> <div>17%</div> <div>58%</div> <div>16%</div> <div>7%</div> </div>
2	XB	256	<div> <div>5%</div> <div>17%</div> <div>59%</div> <div>16%</div> <div>7%</div> </div>

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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	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	18	
24	XY	18	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

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

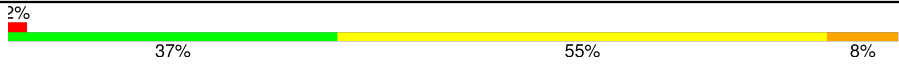
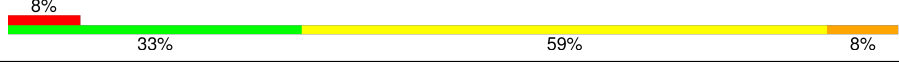
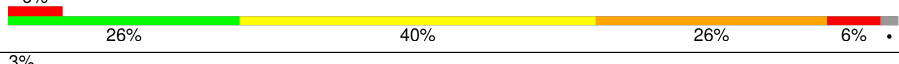
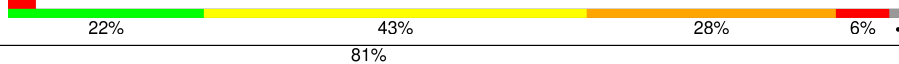
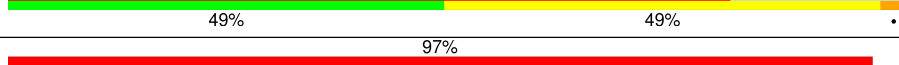

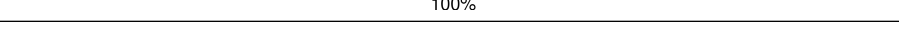
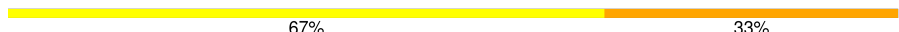
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Mol	Chain	Length	Quality of chain
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	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	1617	-	-	-	X
57	MG	QA	1632	-	-	-	X
57	MG	QA	1647	-	-	-	X
57	MG	QA	1658	-	-	-	X
57	MG	QA	1660	-	-	-	X
57	MG	QV	101	-	-	-	X
57	MG	RA	3002	-	-	-	X
57	MG	RA	3004	-	-	-	X
57	MG	RA	3008	-	-	-	X
57	MG	RA	3009	-	-	-	X
57	MG	RA	3012	-	-	-	X
57	MG	RA	3015	-	-	-	X
57	MG	RA	3019	-	-	-	X
57	MG	RA	3021	-	-	-	X
57	MG	RA	3022	-	-	-	X
57	MG	RA	3024	-	-	-	X
57	MG	RA	3026	-	-	-	X
57	MG	RA	3031	-	-	-	X
57	MG	RA	3033	-	-	-	X
57	MG	RA	3034	-	-	-	X
57	MG	RA	3035	-	-	-	X
57	MG	RA	3036	-	-	-	X
57	MG	RA	3047	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3049	-	-	-	X
57	MG	RA	3052	-	-	-	X
57	MG	RA	3054	-	-	-	X
57	MG	RA	3056	-	-	-	X
57	MG	RA	3058	-	-	-	X
57	MG	RA	3062	-	-	-	X
57	MG	RA	3063	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3077	-	-	-	X
57	MG	RA	3086	-	-	-	X
57	MG	RA	3088	-	-	-	X
57	MG	RA	3089	-	-	-	X
57	MG	RA	3094	-	-	-	X
57	MG	RA	3097	-	-	-	X
57	MG	RA	3098	-	-	-	X
57	MG	RA	3099	-	-	-	X
57	MG	RA	3101	-	-	-	X
57	MG	RA	3120	-	-	-	X
57	MG	RA	3121	-	-	-	X
57	MG	RA	3124	-	-	-	X
57	MG	RA	3156	-	-	-	X
57	MG	RA	3161	-	-	-	X
57	MG	RA	3170	-	-	-	X
57	MG	RA	3174	-	-	-	X
57	MG	RA	3175	-	-	-	X
57	MG	RA	3179	-	-	-	X
57	MG	RA	3184	-	-	-	X
57	MG	RA	3209	-	-	-	X
57	MG	RA	3222	-	-	-	X
57	MG	RA	3224	-	-	-	X
57	MG	RA	3225	-	-	-	X
57	MG	RA	3237	-	-	-	X
57	MG	RD	301	-	-	-	X
57	MG	RP	201	-	-	-	X
57	MG	RP	202	-	-	-	X
57	MG	XA	1603	-	-	-	X
57	MG	XA	1604	-	-	-	X
57	MG	XA	1611	-	-	-	X
57	MG	XA	1620	-	-	-	X
57	MG	XA	1625	-	-	-	X
57	MG	XA	1634	-	-	-	X
57	MG	XA	1635	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	XA	1642	-	-	-	X
57	MG	XA	1643	-	-	-	X
57	MG	XA	1651	-	-	-	X
57	MG	XA	1654	-	-	-	X
57	MG	XA	1662	-	-	-	X
57	MG	XA	1669	-	-	-	X
57	MG	XA	1670	-	-	-	X
57	MG	YA	3002	-	-	-	X
57	MG	YA	3005	-	-	-	X
57	MG	YA	3009	-	-	-	X
57	MG	YA	3011	-	-	-	X
57	MG	YA	3013	-	-	-	X
57	MG	YA	3016	-	-	-	X
57	MG	YA	3023	-	-	-	X
57	MG	YA	3025	-	-	-	X
57	MG	YA	3027	-	-	-	X
57	MG	YA	3031	-	-	-	X
57	MG	YA	3033	-	-	-	X
57	MG	YA	3034	-	-	-	X
57	MG	YA	3035	-	-	-	X
57	MG	YA	3036	-	-	-	X
57	MG	YA	3037	-	-	-	X
57	MG	YA	3041	-	-	-	X
57	MG	YA	3043	-	-	-	X
57	MG	YA	3047	-	-	-	X
57	MG	YA	3049	-	-	-	X
57	MG	YA	3050	-	-	-	X
57	MG	YA	3058	-	-	-	X
57	MG	YA	3060	-	-	-	X
57	MG	YA	3066	-	-	-	X
57	MG	YA	3069	-	-	-	X
57	MG	YA	3073	-	-	-	X
57	MG	YA	3075	-	-	-	X
57	MG	YA	3081	-	-	-	X
57	MG	YA	3088	-	-	-	X
57	MG	YA	3091	-	-	-	X
57	MG	YA	3092	-	-	-	X
57	MG	YA	3095	-	-	-	X
57	MG	YA	3096	-	-	-	X
57	MG	YA	3100	-	-	-	X
57	MG	YA	3101	-	-	-	X
57	MG	YA	3102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3106	-	-	-	X
57	MG	YA	3108	-	-	-	X
57	MG	YA	3109	-	-	-	X
57	MG	YA	3110	-	-	-	X
57	MG	YA	3112	-	-	-	X
57	MG	YA	3116	-	-	-	X
57	MG	YA	3124	-	-	-	X
57	MG	YA	3141	-	-	-	X
57	MG	YA	3145	-	-	-	X
57	MG	YA	3155	-	-	-	X
57	MG	YA	3161	-	-	-	X
57	MG	YA	3170	-	-	-	X
57	MG	YA	3173	-	-	-	X
57	MG	YA	3182	-	-	-	X
57	MG	YA	3206	-	-	-	X
57	MG	YA	3207	-	-	-	X
57	MG	YA	3209	-	-	-	X
57	MG	YA	3218	-	-	-	X
57	MG	YA	3229	-	-	-	X
57	MG	YA	3234	-	-	-	X
57	MG	YA	3235	-	-	-	X
57	MG	YA	3239	-	-	-	X
57	MG	YA	3240	-	-	-	X
57	MG	YA	3248	-	-	-	X
57	MG	YA	3252	-	-	-	X
57	MG	YA	3254	-	-	-	X
57	MG	YA	3257	-	-	-	X
57	MG	YA	3259	-	-	-	X
57	MG	YA	3261	-	-	-	X
57	MG	YA	3263	-	-	-	X
57	MG	YA	3264	-	-	-	X
57	MG	YD	301	-	-	-	X
57	MG	YD	302	-	-	-	X
58	PAR	XA	1671	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291958 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is a protein called 30S ribosomal protein 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
			173	77	33	55	8			
23	XX	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			

- 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
26	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RR	118	Total	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
42	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	Y5	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).

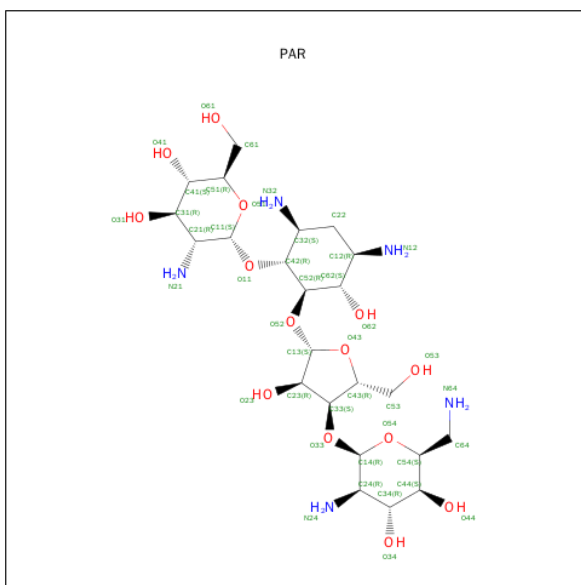
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	65	Total	Mg	0	0
			65	65		
57	RP	2	Total	Mg	0	0
			2	2		
57	YA	267	Total	Mg	0	0
			267	267		
57	QM	1	Total	Mg	0	0
			1	1		
57	YD	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XX	1	Total 1	Mg 1	0	0
57	QV	1	Total 1	Mg 1	0	0
57	XA	70	Total 70	Mg 70	0	0
57	R0	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	RD	1	Total 1	Mg 1	0	0
57	XB	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	RA	242	Total 242	Mg 242	0	0
57	YP	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	YB	3	Total 3	Mg 3	0	0
57	XV	1	Total 1	Mg 1	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	YE	1	Total 1	Mg 1	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

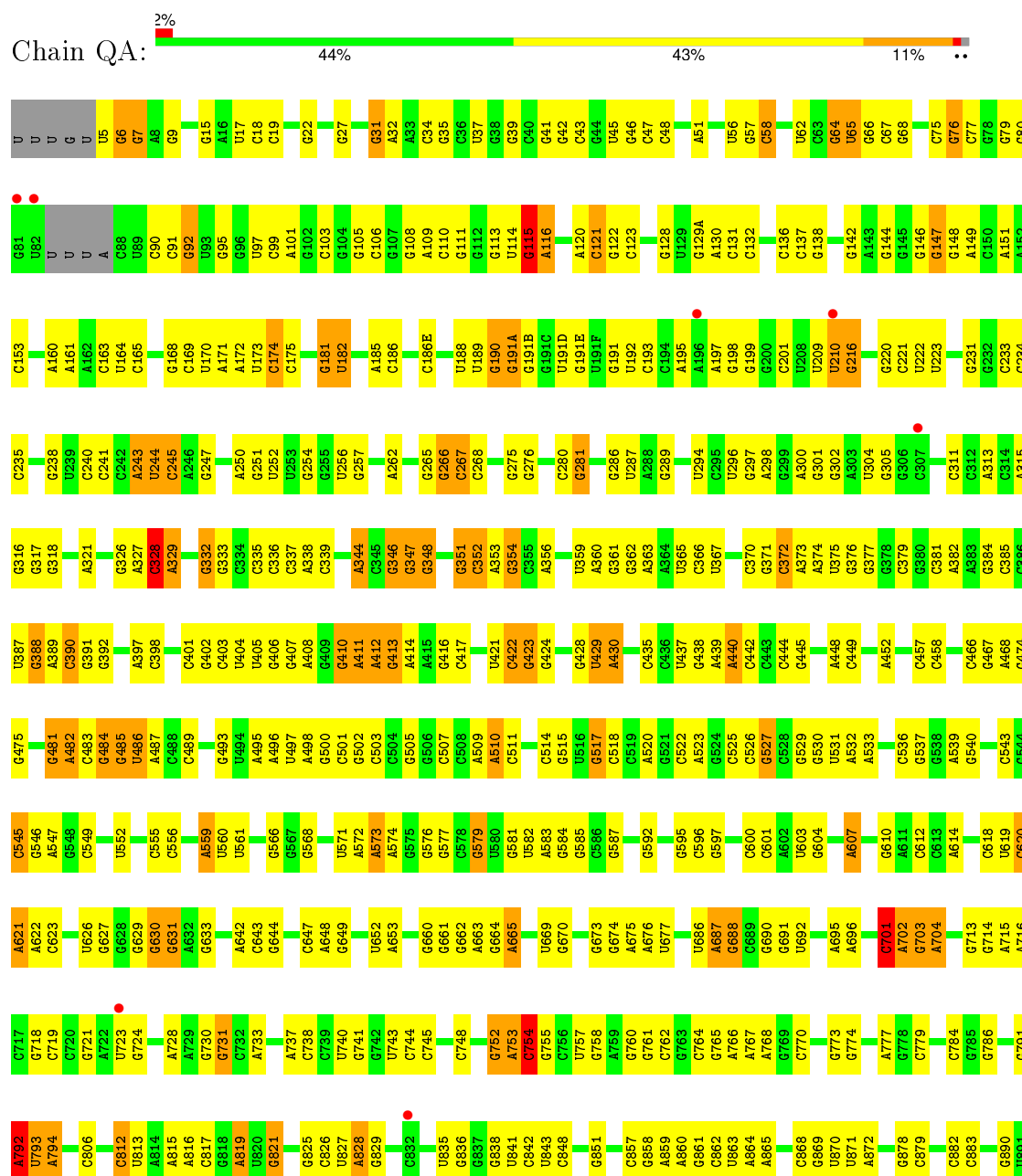
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

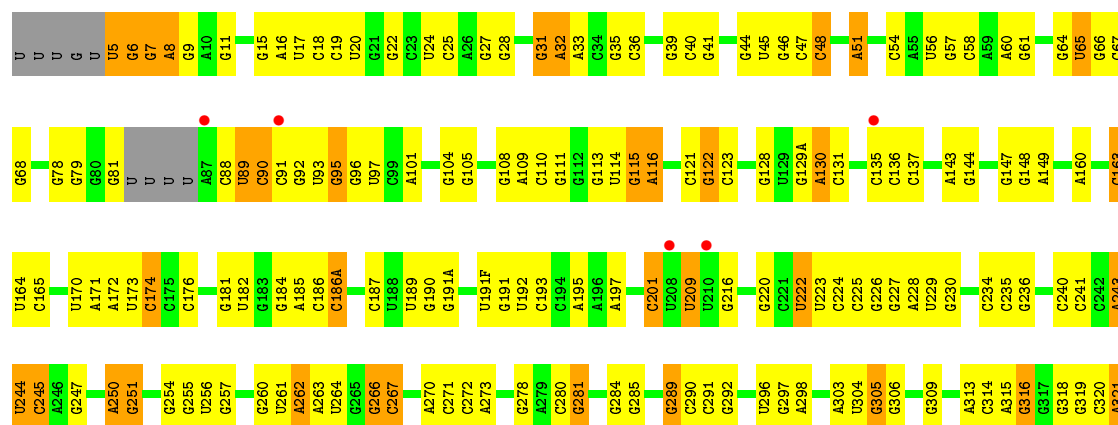
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	XD	1	Total Zn 1 1	0	0
59	QD	1	Total Zn 1 1	0	0
59	QN	1	Total Zn 1 1	0	0
59	XN	1	Total Zn 1 1	0	0

3 Residue-property plots

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

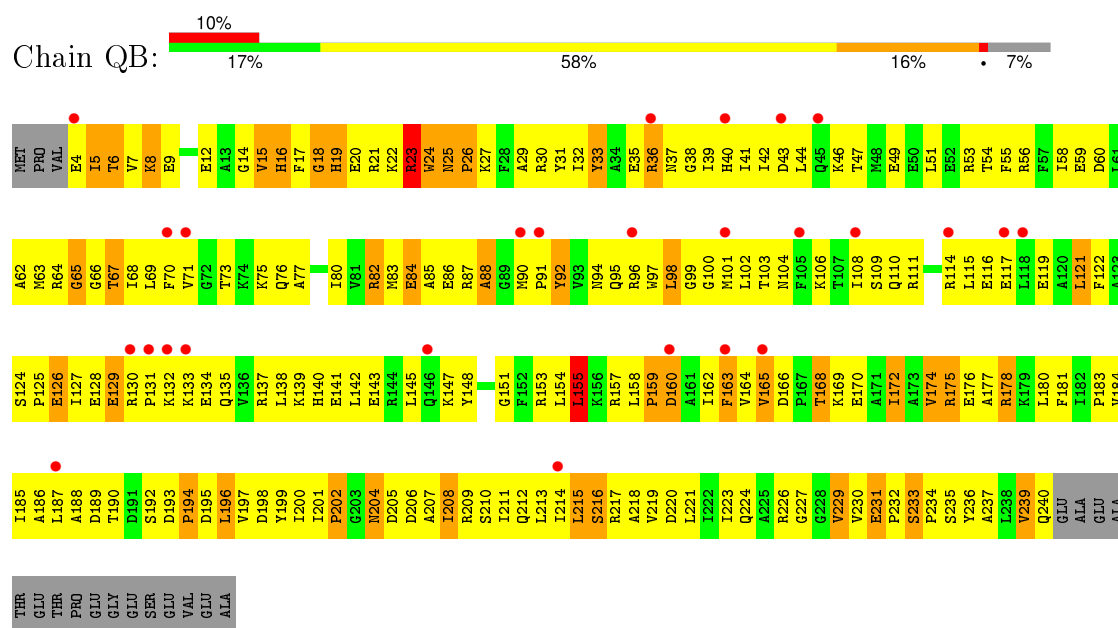
● Molecule 1: 16S rRNA



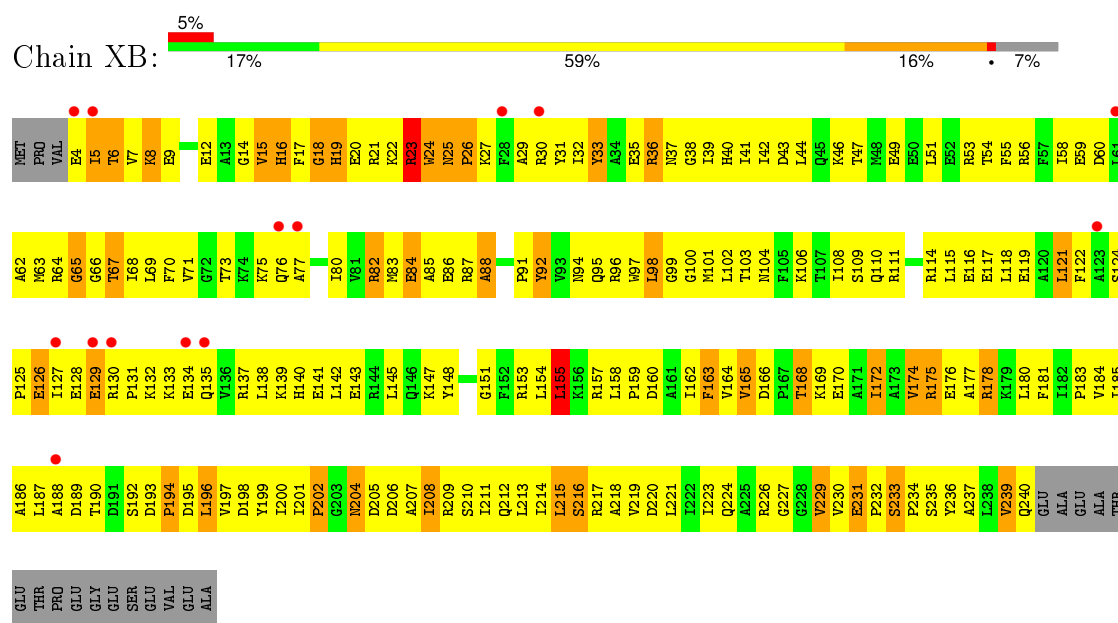




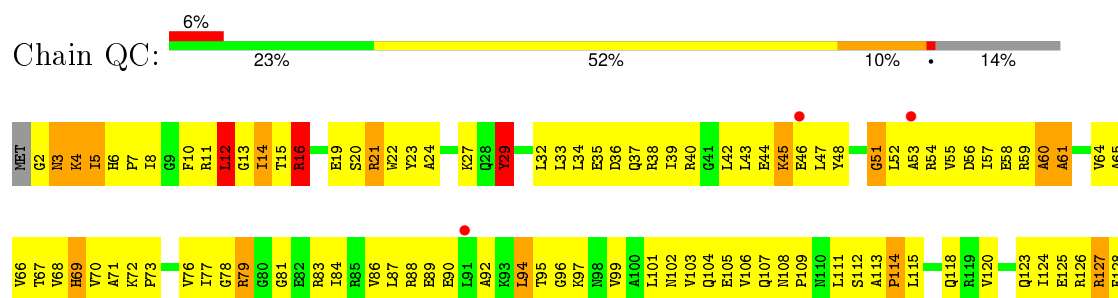
- Molecule 2: 30S ribosomal protein S2

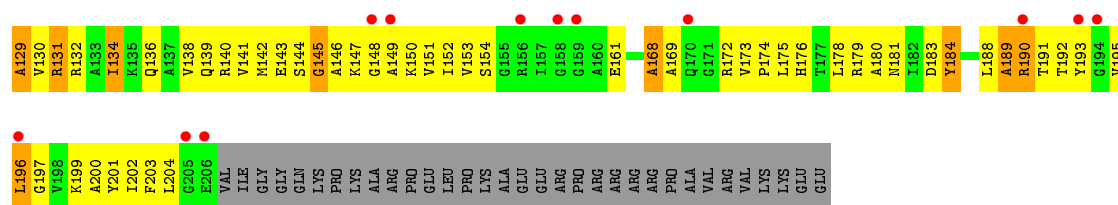


- Molecule 2: 30S ribosomal protein S2

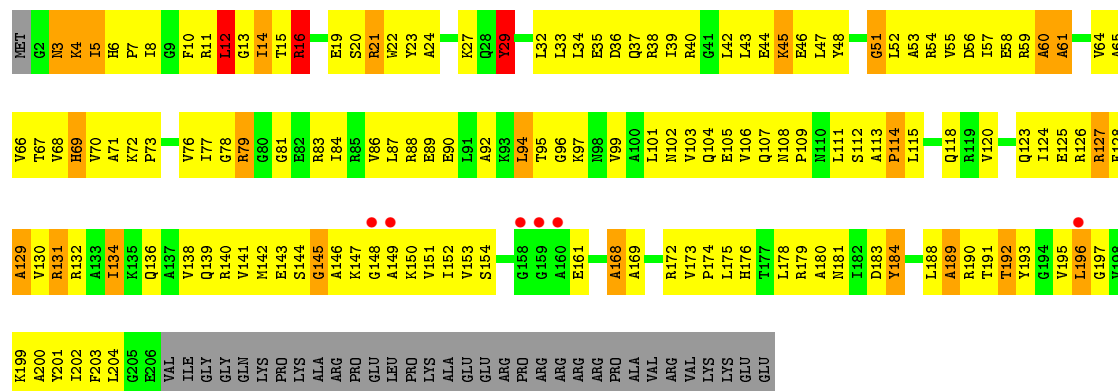


- Molecule 3: 30S ribosomal protein S3

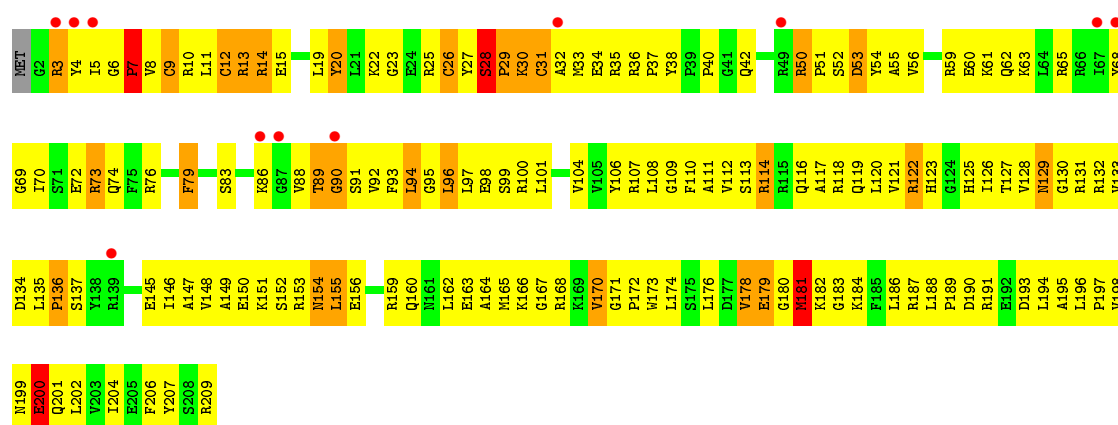




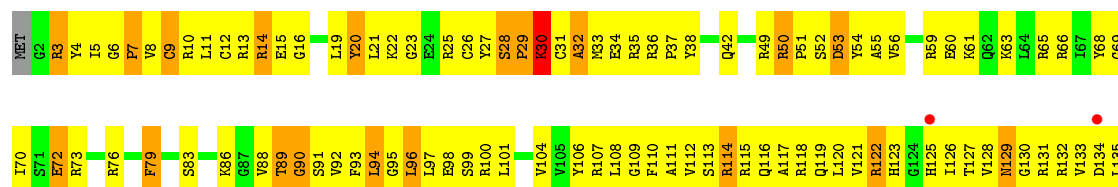
• Molecule 3: 30S ribosomal protein S3

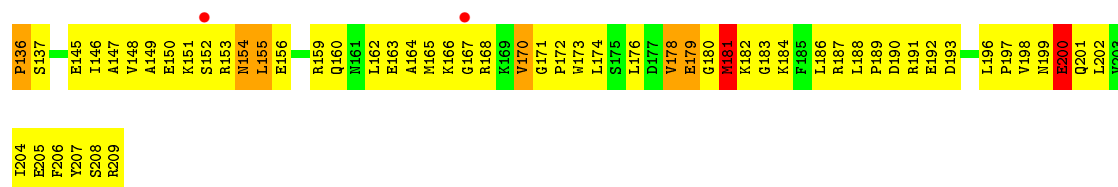


• Molecule 4: 30S ribosomal protein S4

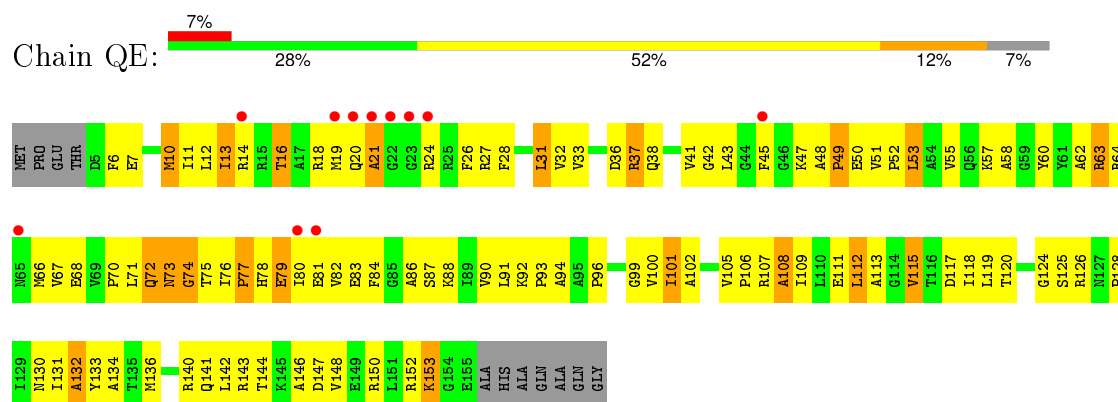


• Molecule 4: 30S ribosomal protein S4

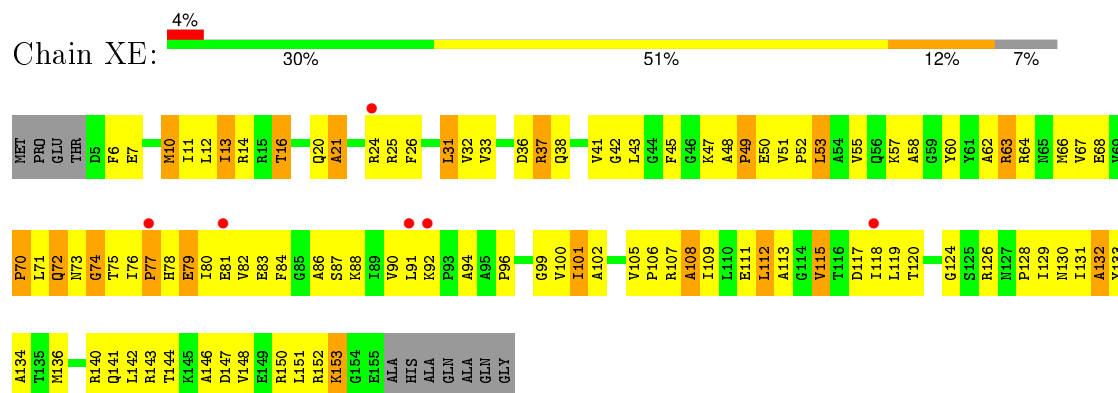




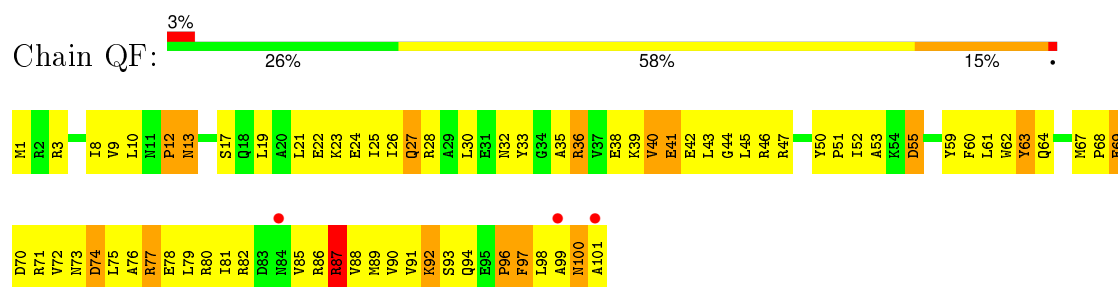
• Molecule 5: 30S ribosomal protein S5



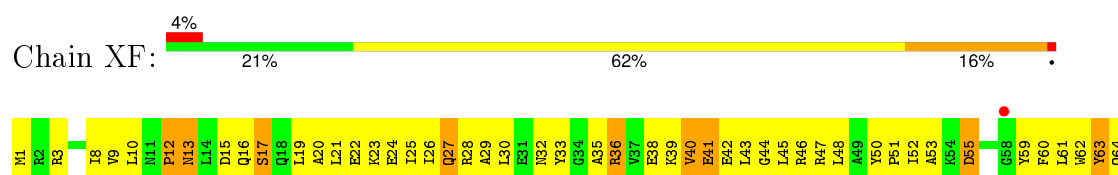
• Molecule 5: 30S ribosomal protein S5

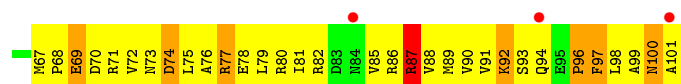


• Molecule 6: 30S ribosomal protein S6

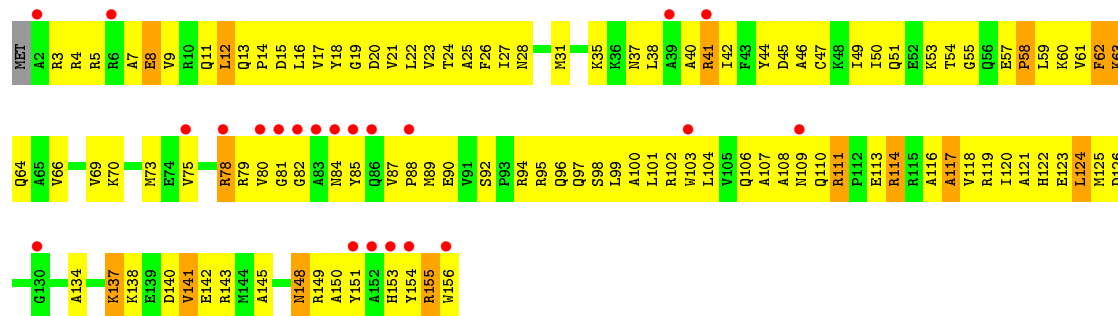


• Molecule 6: 30S ribosomal protein S6

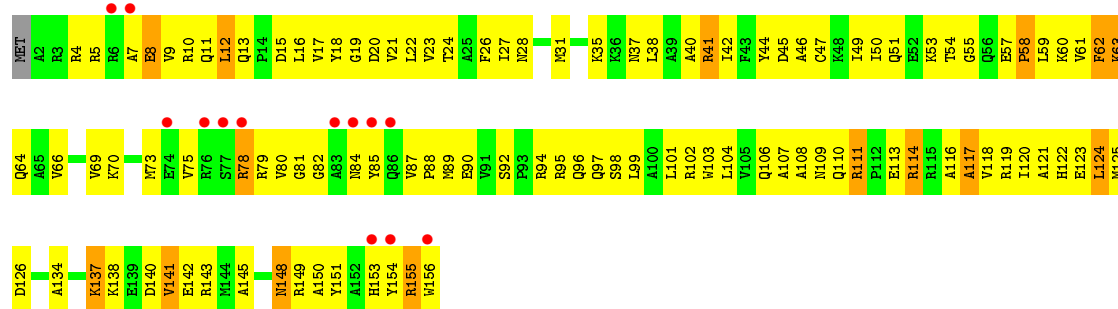




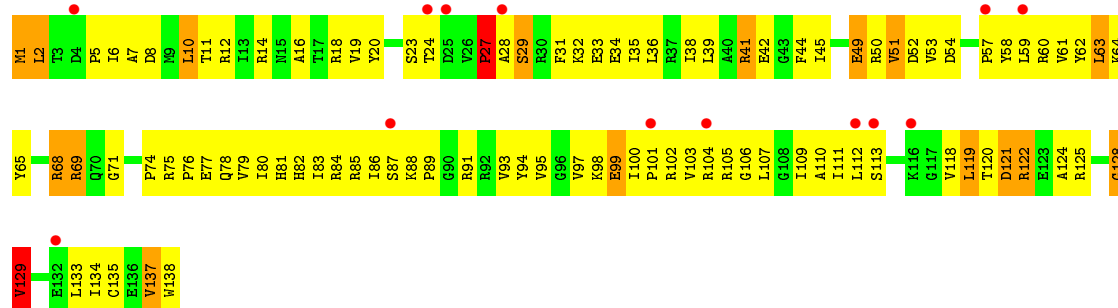
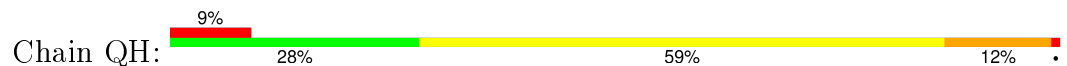
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7

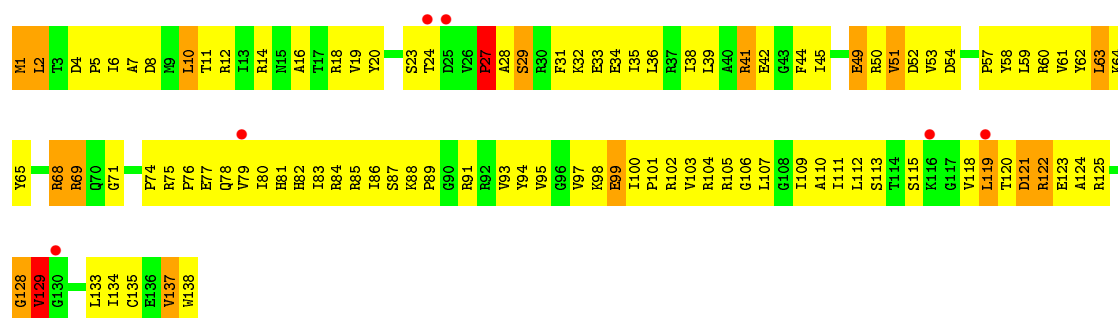


• Molecule 8: 30S ribosomal protein S8

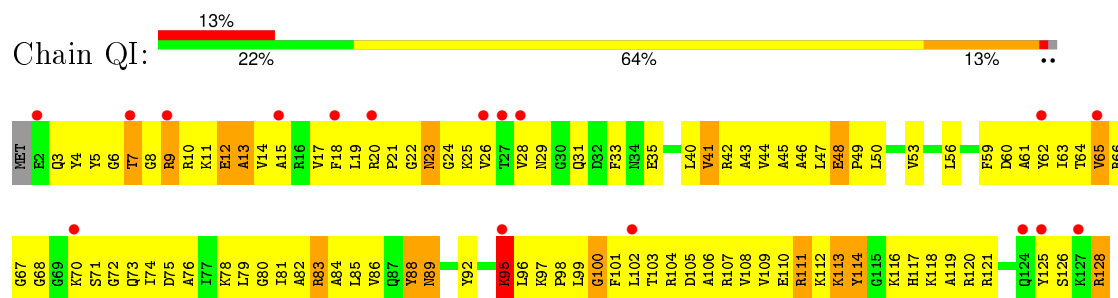


• Molecule 8: 30S ribosomal protein S8

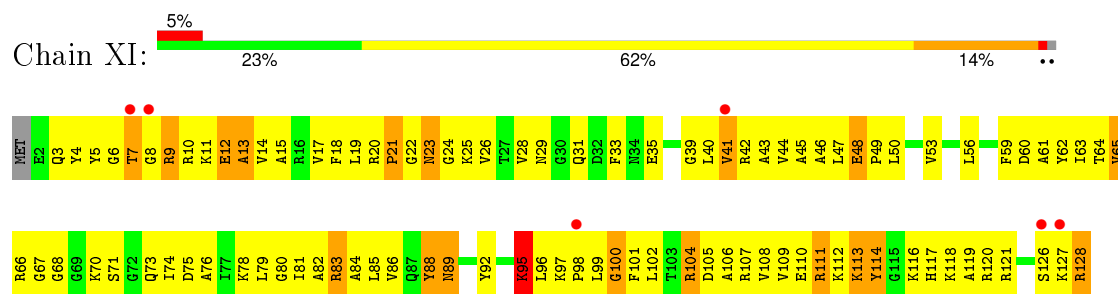




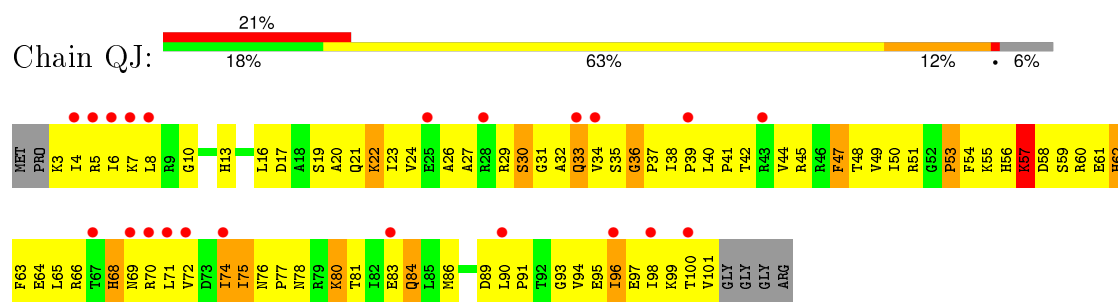
- Molecule 9: 30S ribosomal protein S9



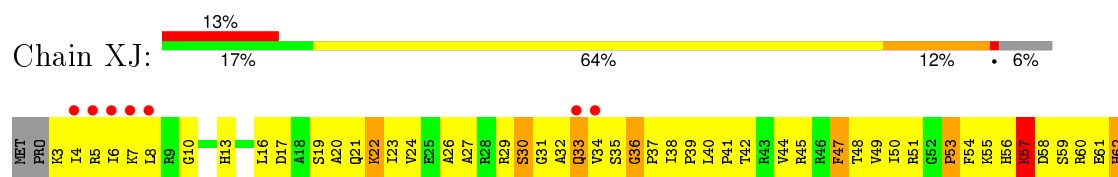
- Molecule 9: 30S ribosomal protein S9

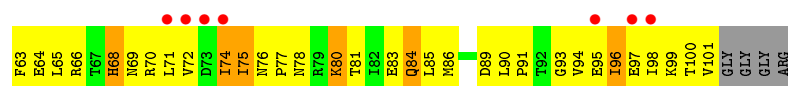


- Molecule 10: 30S ribosomal protein S10

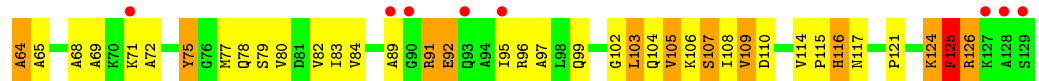


- Molecule 10: 30S ribosomal protein S10

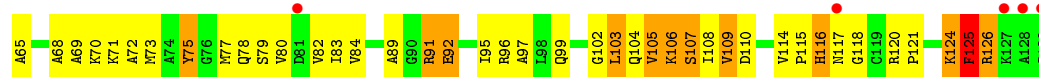




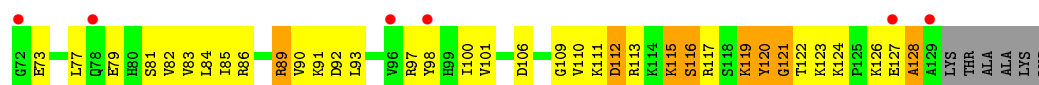
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

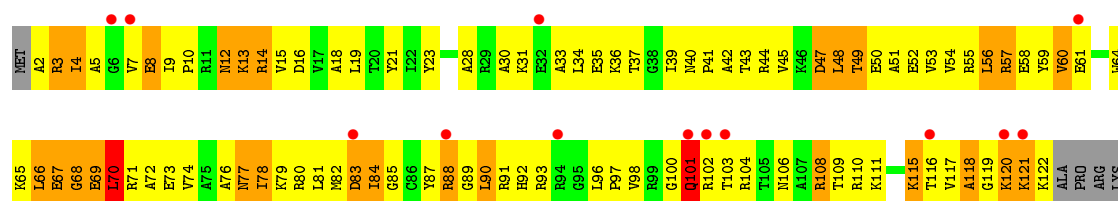


- Molecule 12: 30S ribosomal protein S12

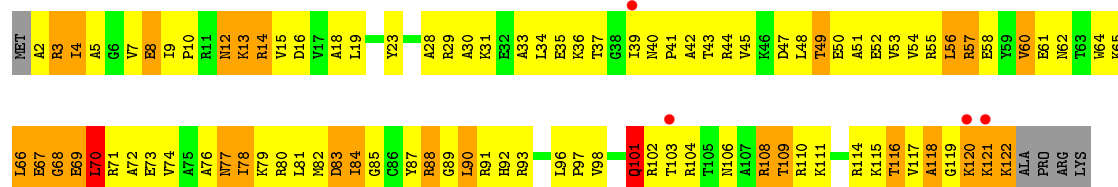


- Molecule 13: 30S ribosomal protein S13

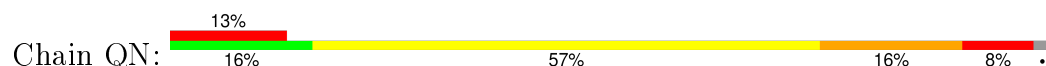




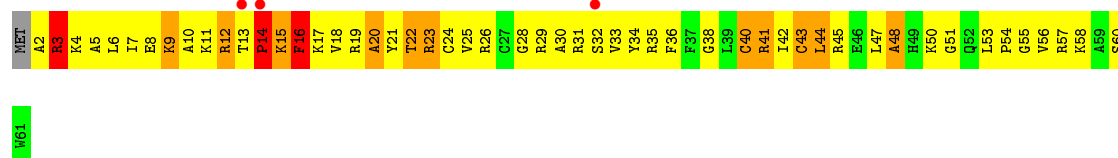
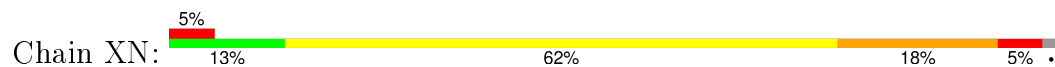
• Molecule 13: 30S ribosomal protein S13



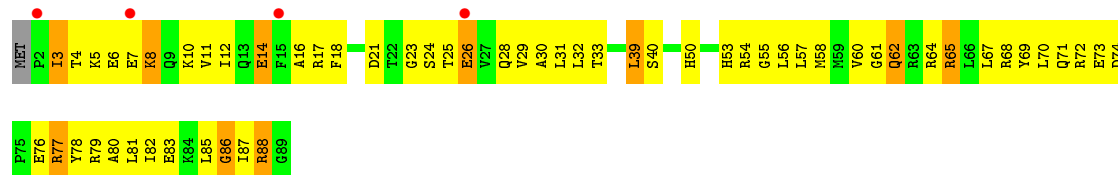
• Molecule 14: 30S ribosomal protein S14



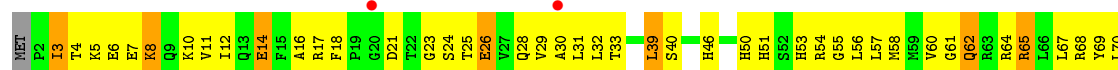
• Molecule 14: 30S ribosomal protein S14

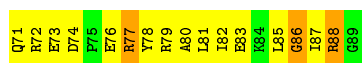


• Molecule 15: 30S ribosomal protein S15

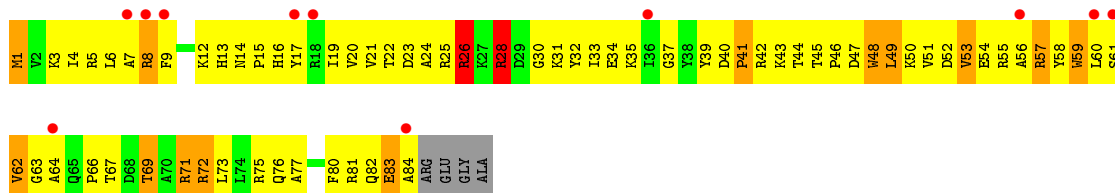


• Molecule 15: 30S ribosomal protein S15

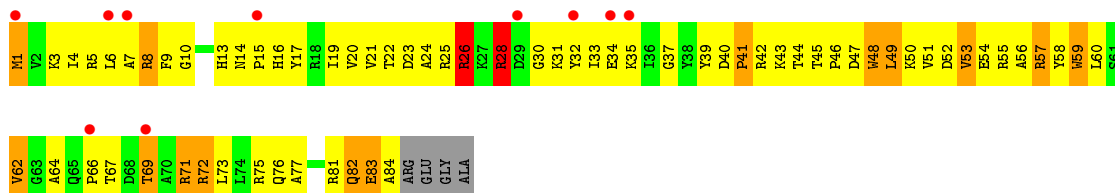




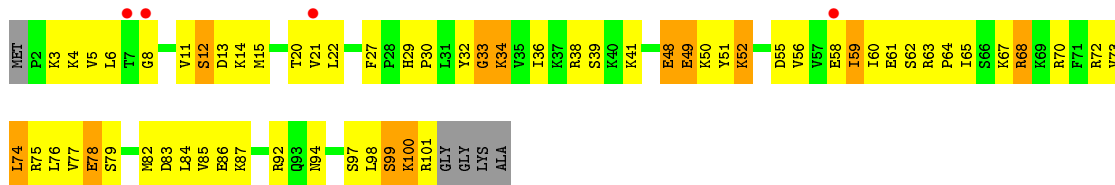
- Molecule 16: 30S ribosomal protein S16



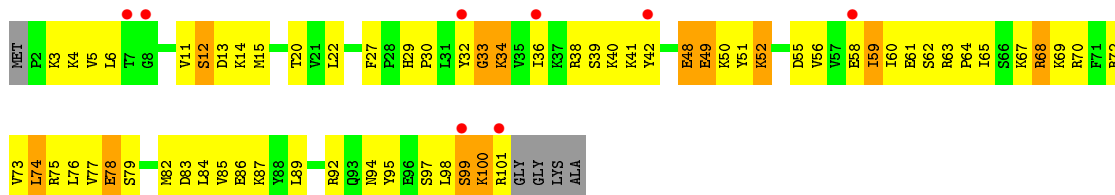
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

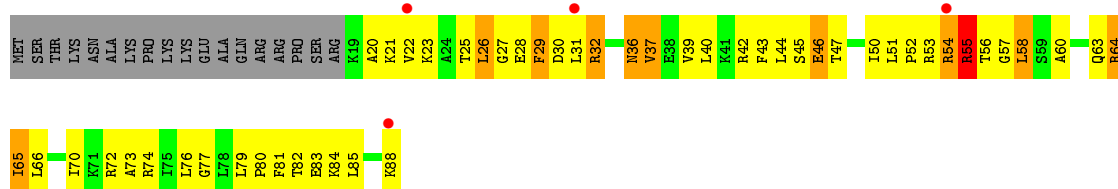
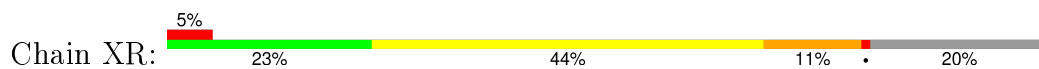


- Molecule 18: 30S ribosomal protein S18

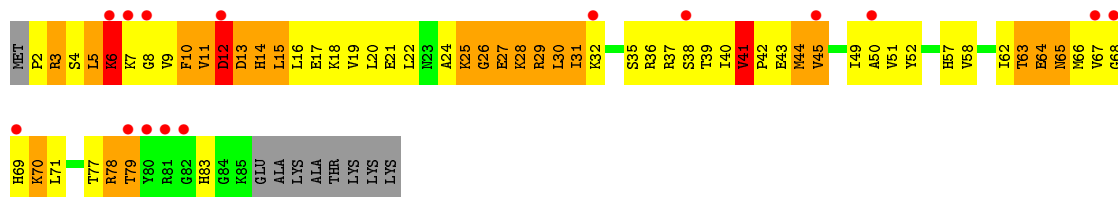
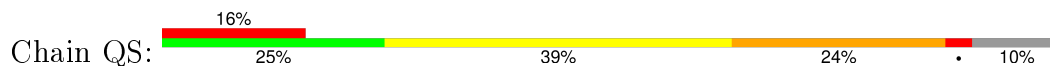




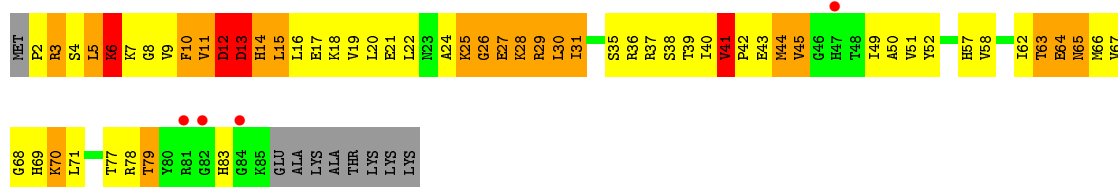
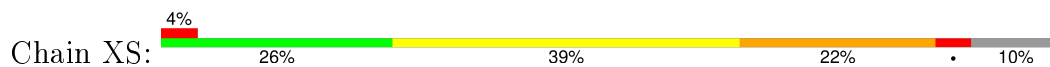
- Molecule 18: 30S ribosomal protein S18



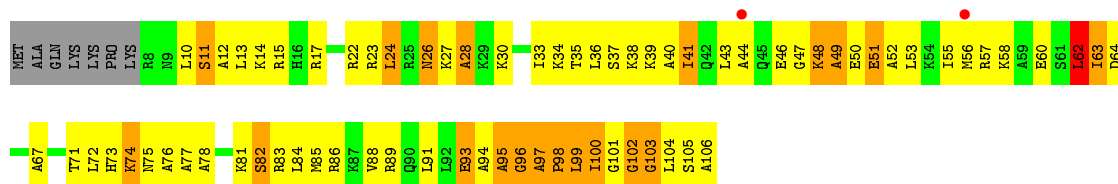
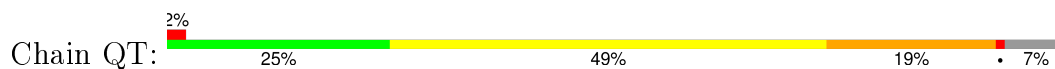
- Molecule 19: 30S ribosomal protein S19



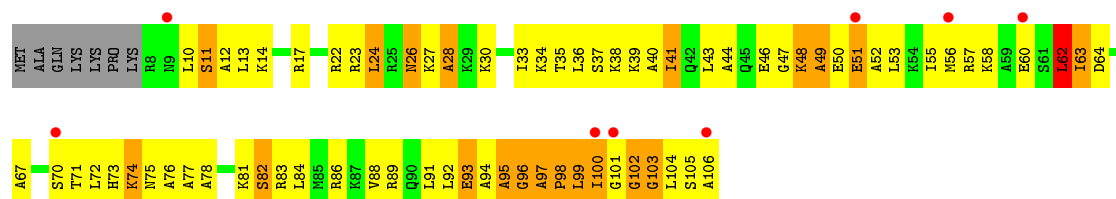
- Molecule 19: 30S ribosomal protein S19



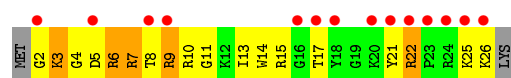
- Molecule 20: 30S ribosomal protein S20



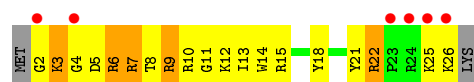
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21



- Molecule 22: P-site tRNA fMet



- Molecule 22: P-site tRNA fMet



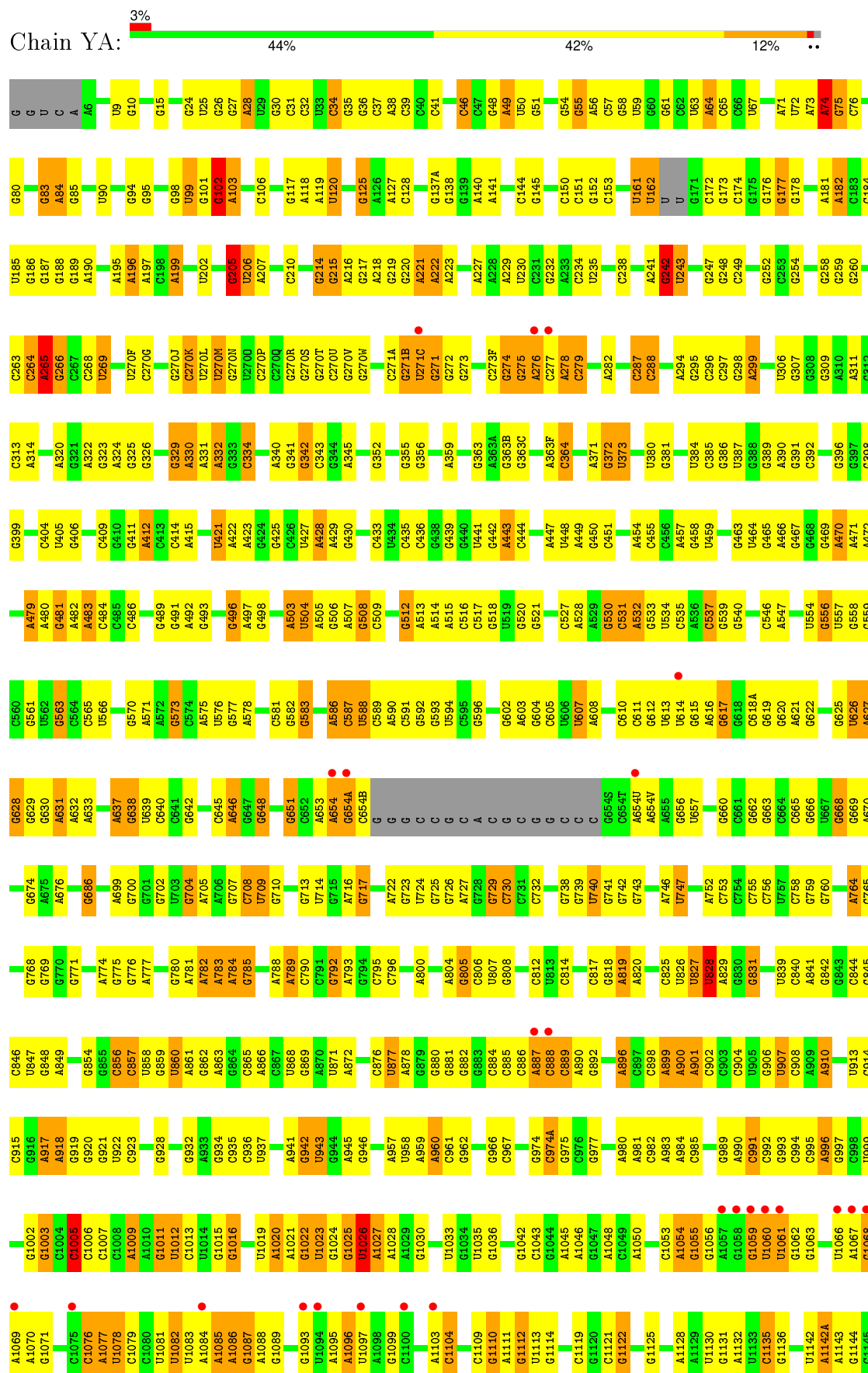
- Molecule 23: A-site ASL SufA6



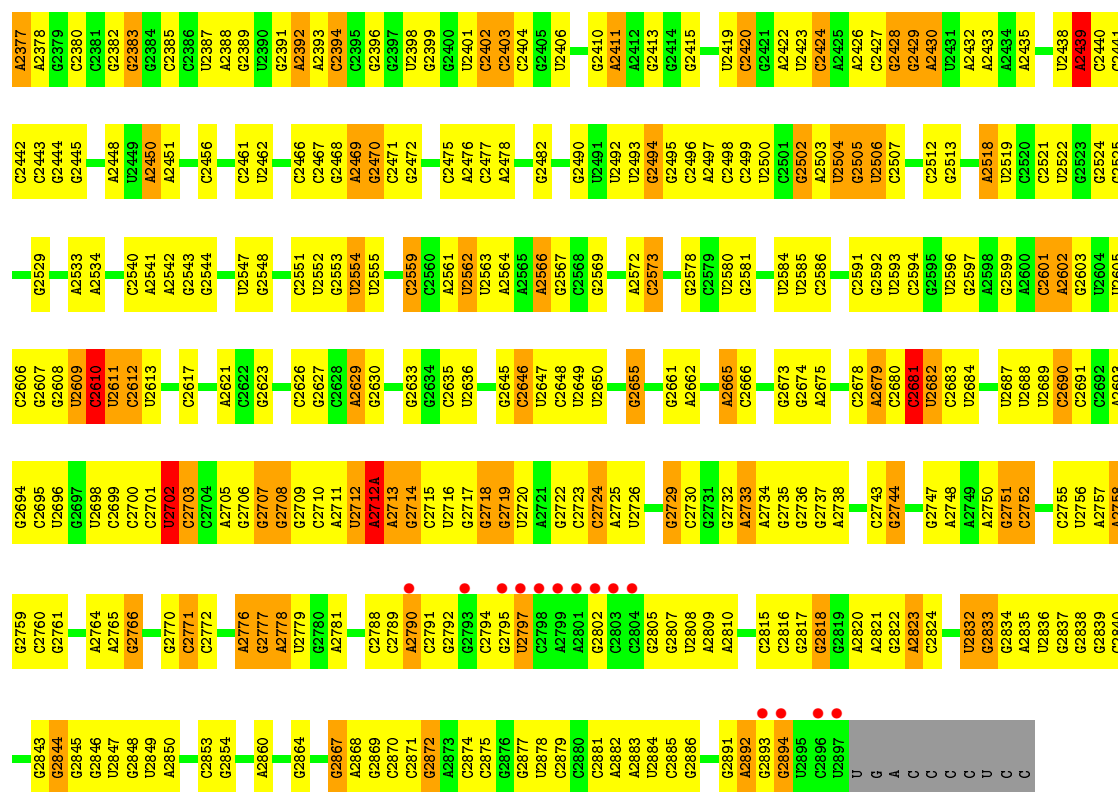
- Molecule 23: A-site ASL SufA6

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G1666	A1571	G1492	U1415	G1337	C1180	A1098	A1028	A959	G883	U803	A727	C	G598
G1667		G1493	U1283	U1283	C1181	A1099	A1029	A960	G884	A804	G728	C	G599
A1668	C1577	A1494	G1338	G1338	C1182	C1100	G1030	G961	G885	G805	G729	G	G600
A1669	U1578	A1495	A1285	A1285	G1183	U1101	G1031	G962	G886	C806	C730	C	C601
A1579	A1496	A1496	G1266	G1266	G1184	U1102	A1032	U963	A887	U807		A	G602
A1580		U1497	U1267	U1267	C1185	A1103	U1033	C964	C888	G808	A734	C	A603
	U1673		A1268	A1268	G1186	A1104	U1034		C889	G809	A735	G	G604
G1674			A1269	A1269	G1187	U1105	G1034	C971	A890	U810	A736	C	
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G1675	U1503		G1423	G1423	U1189	U1107	A1042	A973	C892	C812	G738	G	A608
A1587	A1504		A1270	A1270	G1190	G1110	G1043	G974	A896	U813	G739	C	A609
A1677	C1585		G1425	G1425		A1111	U1044	C974A	C897	C814	U740	C	G609A
A1678	C1586		A1426	A1426		G1112	A1045	G975	C898	C817	G741	C	C610
	C1598		A1428	G1356	A1276	U1113	A1046	C976	C899	G818	G742	C	C611
G1682	U1509		G1277	U1357	U1198	G1114	G1047	G977	A899	A819	G743	C	G612
C1600	C1510		C1430	G1358		G1115	A1048	G978	A900			C	U613
G1601	A1511		U1431	A1359	G1203		C1049	G979	A901		A746	C	U614
	G1512				U1204		A1050	A980	C902	G823	U747	C	G615
	U1513		A1434	C1363	U1205	C1123		A981	C903	A824	G748	C	A616
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C1504			G1436	A1365	C1207	A1126	G1055	A983	U905	U826	A751	C	G618
	U1515			A1366	C1208	A1127	A1056	A984	G906	U827	A752	C	C618A
C1607	U1516			A1367	G1209	A1128	A1057	C985	U907		C753	C	G619
A1608	G1517		G1441	A1367	G1209	A1128	A1057	C985	U907			C	G620
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A1610	G1519		A1444A	C1370	U1211	U1130	G1059	C987	A909		U757	C	G622
C1611	U1520		C1445	G1371	C1293	G1131	U1060		A910	G831	G758	C	G623
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A1614	G1522			U1372		C1135	G1062	C992		U839		C	C625
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A1616	A1529		A1449	A1378	C1217	G1137	C1064	C994	G916		G765	C	U626
C1617	G1530		G1449A	A1379	C1218	U1138	U1065	C995	A917			C	A627
A1618	A1618		C1450	G1380	G1219	G1139	U1066	A996	A918	G845	G768	C	G630
G1619					A1220	U1139	A1067	G997	G919	C846	G769	C	A631
	C1533		U1454	A1384	C1221	C1140	G1068	C998		U847	G770	C	A632
G1534	U1535		G1455	G1385		U1141	A1069	U999	U922	G843	G771	C	A633
A1536				C1386	G1224	U1142	A1070	A1000	C923			C	C634
C1537			G1459		A1308	A1424A	G1071	A1001	C924		A774	C	G635
G1538			A1460	U1390	G1228	A1143				G853	G775	C	C636
	U1639		G1461	U1391	G1231	G1151	C1076	C1005	G928	G854	G776	C	C637
A1640	C1640		C1462	A1392	G1232	C1152	A1077	C1006	G931	G855	G777	C	A638
A1641				A1393		C1153	U1078	C1007	G932		A777	C	G639
G1642			C1467		G1236	G1154	C1079	C1008	C932		G780	C	U639
	A1544		C1468	U1396	A1237	A1155	C1080	A1009	U858		A781	C	C640
C1752	A1545		A1469	C1397	G1238	A1156	U1081	A1010	C935		A782	C	C641
G1753	G1648		G1470	C1398	G1239		U1082	G1011	C936		G783	C	G642
A1755	G1649		A1471	A1399	U1240	C1161	U1083	U1012	U937	A861	A784	C	A643
G1756	G1650			G1400	A1241	G1162	A1084	C1013	G938	G862	G785	C	C644
	C1651				A1321	U1163	A1085	U1014	A863		G786	C	A645
A1759	A1652		C1474		G1322	G1164	A1086	G1015	A941		U787	C	A646
	G1653		A1477	C1403	U1323	G1169	G1087	G1016	C942		A788	C	G647
A1762	A1654		A1477	A1404	G1248	G1170	A1088	C1017	A945		A789	C	G651
G1763	C1655		G1479	U1405	G1249	G1171	G1089	U1018	U868		G790	C	C652
G1764	A1656		G1479	U1406	G1250	G1172	U1090	U1019	C946		C791	C	A653
C1657	C1657		G1480	C1407	C1251	G1173	U1091	A1020	G947		G792	C	A654
G1765	G1658		A1482	C1408	G1252	A1174	C1092	A1021	U871		A793	C	G654A
U1766	U1659		G1483	A1331	C1330	U1175	C1093	G1022	A953			C	G654B
C1767	C1660		G1484	G1410	A1254	U1176	U1094	U1023	A953		C796	C	G
	G1661		G1485	C1411	C1333	U1175	U1094	G1023	A953			C	G
G1771				A1567	C1334	A1177	A1095	U1026				C	G
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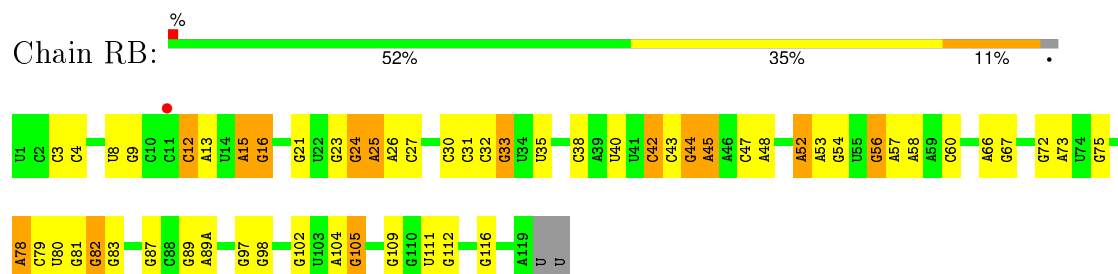
- Molecule 25: 23S rRNA



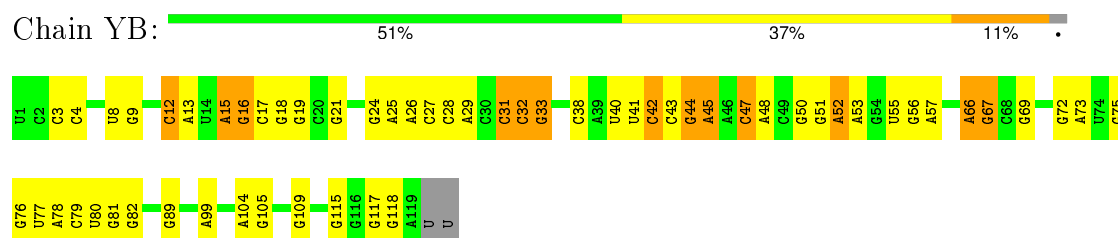
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A2298	A2225	C2143	G2061	G1898	G1811	U1730	C1647	A1555	U1485	U1317	G1226	G1150
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C2306	G2228	C2146	G2069	G1903	G1815	C1734	G1652	A1558	G1491	C1403	G1236	C1153
G2307	G2229	G2147	G2070	G1904	G1816	C1742	G1653	G1559	C1492	C1411	G1238	G1154
A2308	G2230	G2148	A2071	G1906	G1917	G1743	A1654	G1568	C1493	G1325	A1237	A1155
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G2358	G2282	G2191	G2037	G1965	A1870	C1790	A1701	C1617	G1538	C1366	G1287	A1210
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G2361	G2285	U2197	A2042	U1963	G1878	C1795	U1709	G1622	A1472	U1391	U1292	G1216
A2364	A2286	G2198	C2043	G1964	C1882	U1796	C1710	C1625	G1473	G1392	U1293	G1217
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G2366	G2288	G2129	A2051	A1966	A1884	U1798	C1712	G1638	G1475	A1394	A1301	G1219
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A2372	U2291	A2212	A2054	A1969	G1887	G1801	G1718	C1640	G1478	U1397	A1308	C1222
C2373	G2292	U2213	G2055	A1970	A1889	A1802	G1726	C1548	G1479	C1398	A1309	G1223
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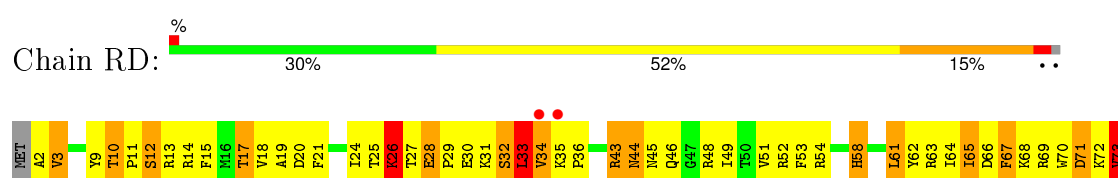
- Molecule 26: 5S rRNA

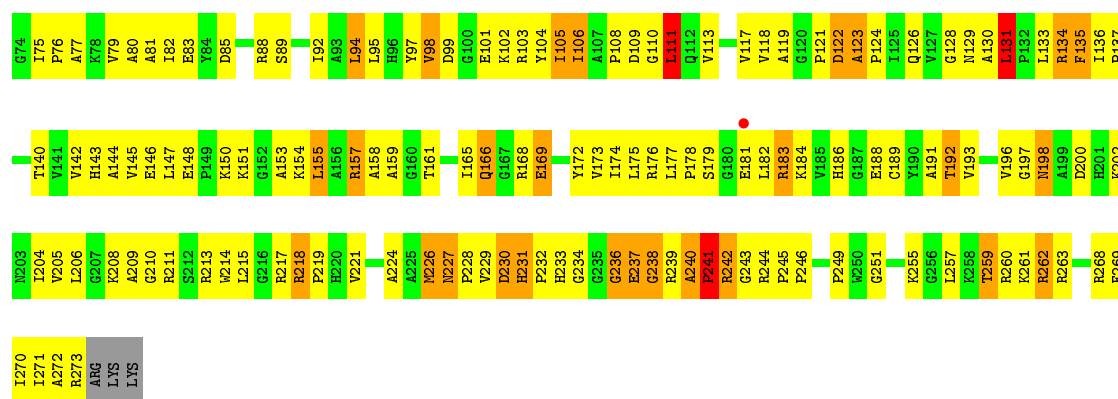


- Molecule 26: 5S rRNA

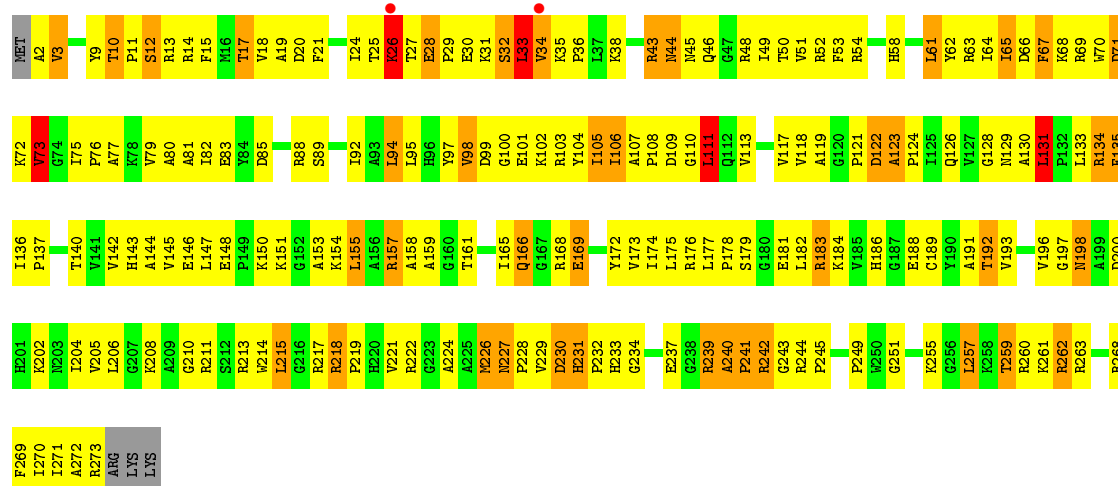


- Molecule 27: 50S ribosomal protein L2

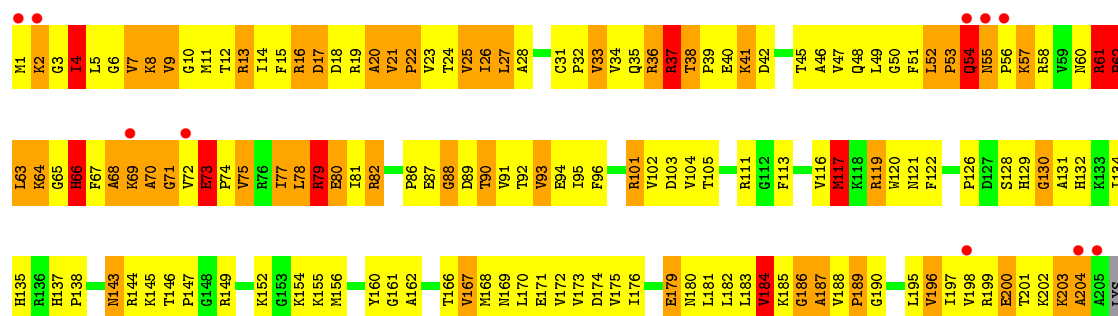




• Molecule 27: 50S ribosomal protein L2

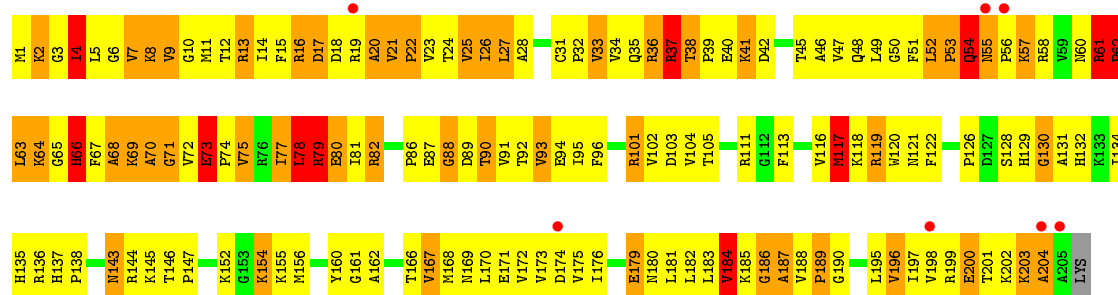


• Molecule 28: 50S ribosomal protein L3

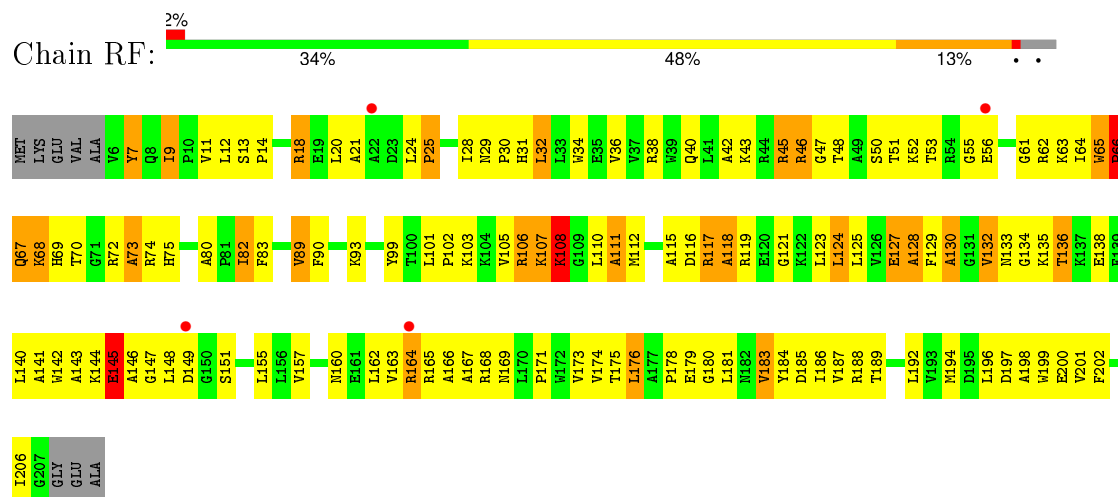


• Molecule 28: 50S ribosomal protein L3

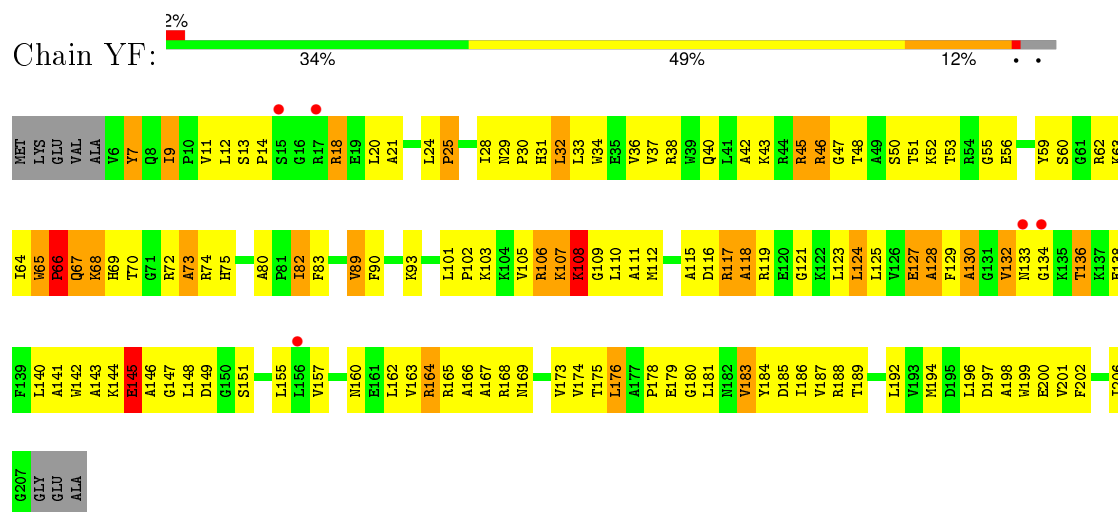




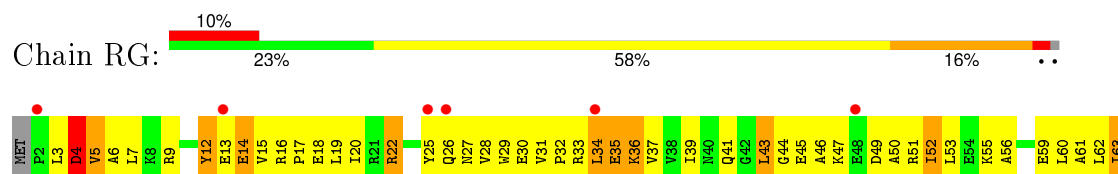
• Molecule 29: 50S ribosomal protein L4

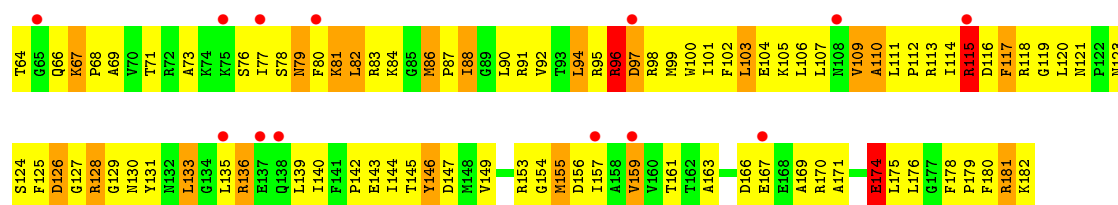


• Molecule 29: 50S ribosomal protein L4

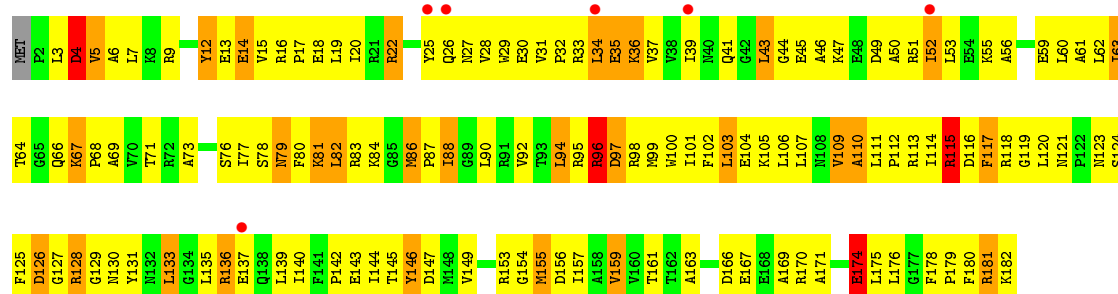


• Molecule 30: 50S ribosomal protein L5

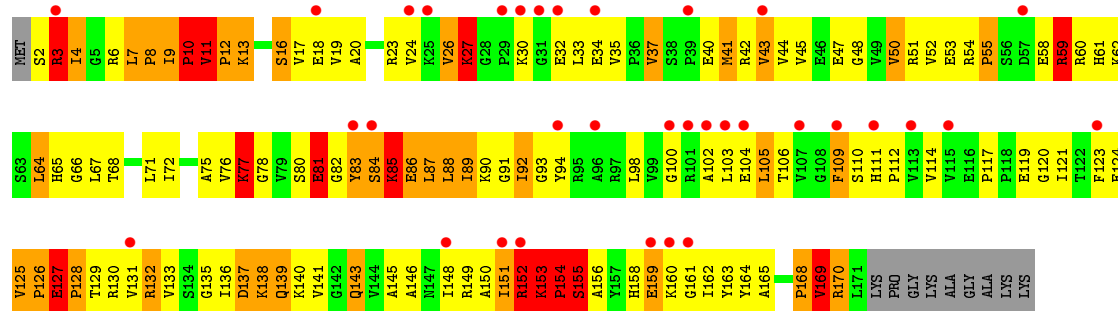
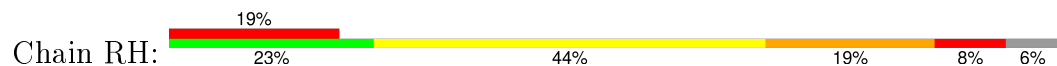




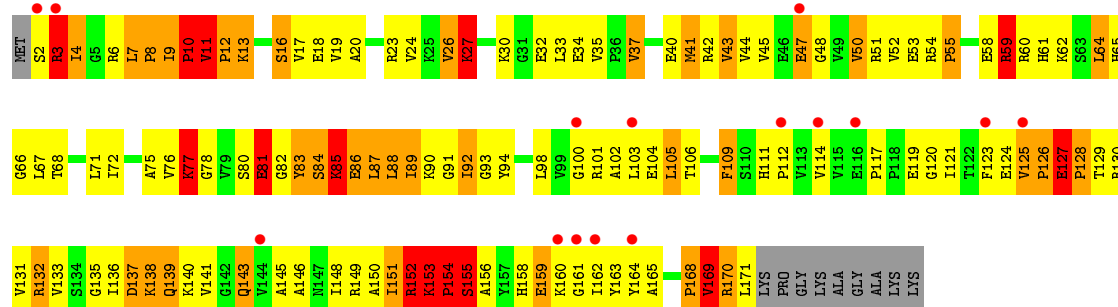
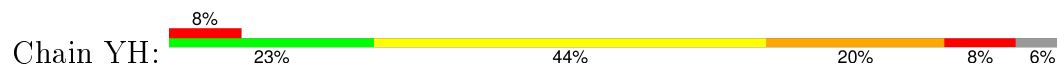
• Molecule 30: 50S ribosomal protein L5



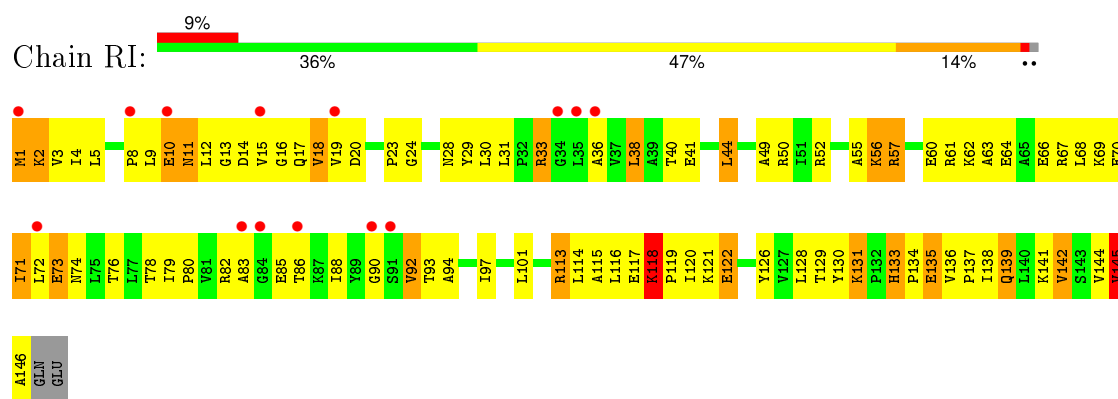
• Molecule 31: 50S ribosomal protein L6



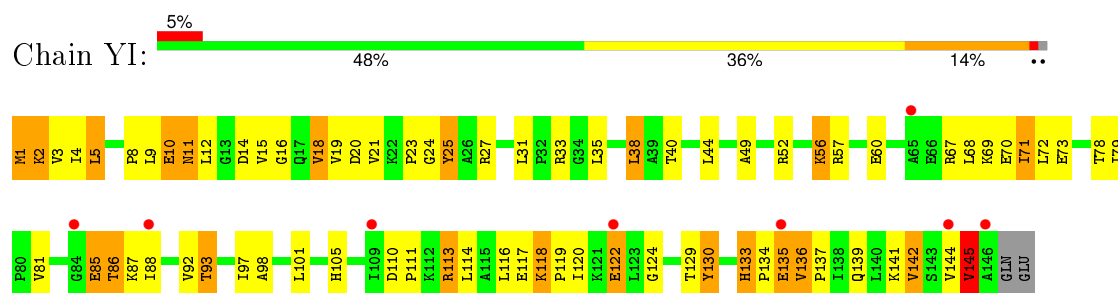
• Molecule 31: 50S ribosomal protein L6



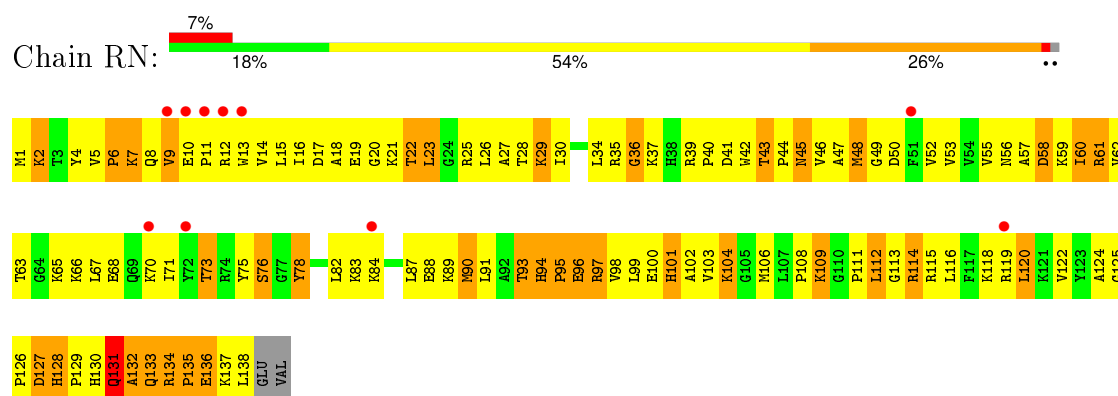
• Molecule 32: 50S ribosomal protein L9



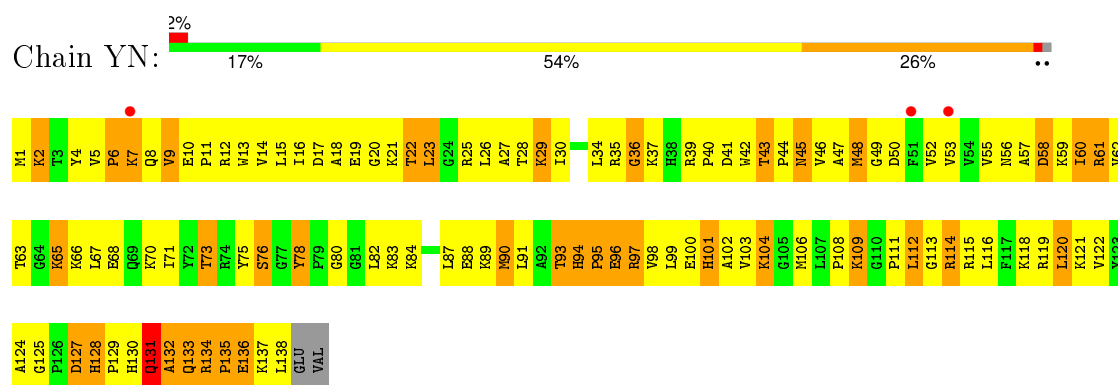
• Molecule 32: 50S ribosomal protein L9



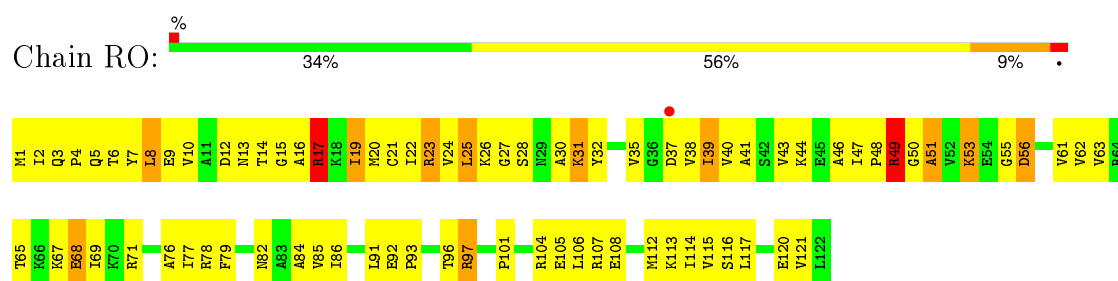
• Molecule 33: 50S ribosomal protein L13



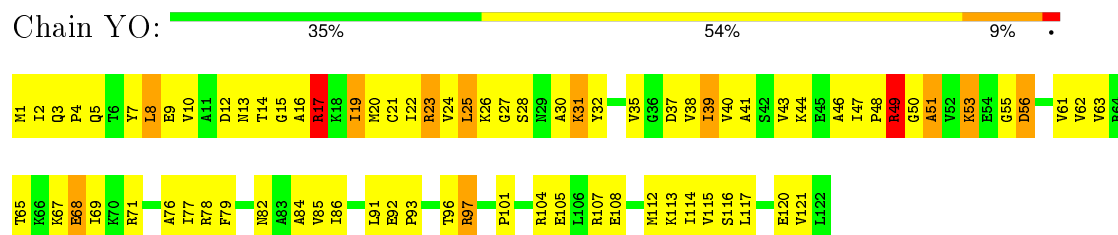
• Molecule 33: 50S ribosomal protein L13



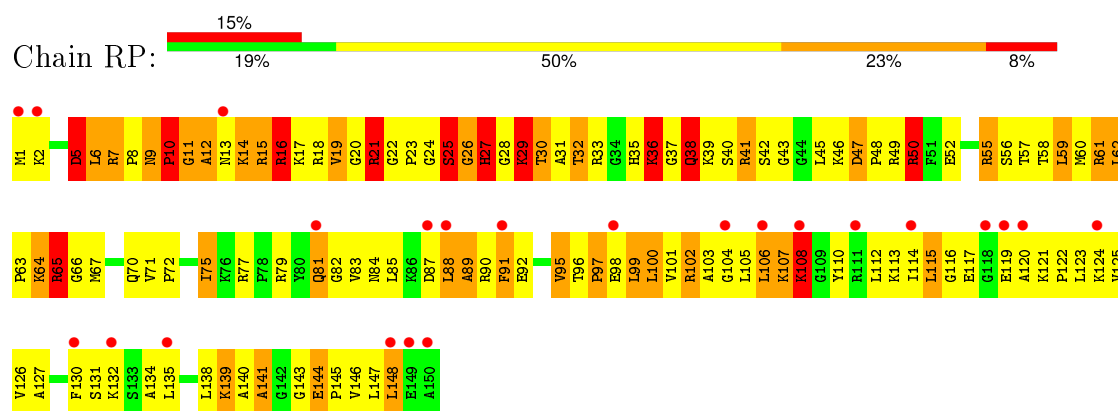
• Molecule 34: 50S ribosomal protein L14



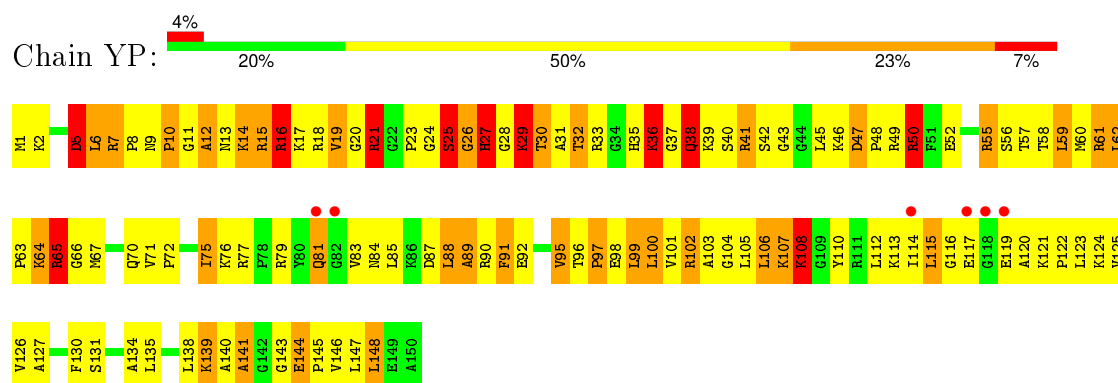
- Molecule 34: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L15

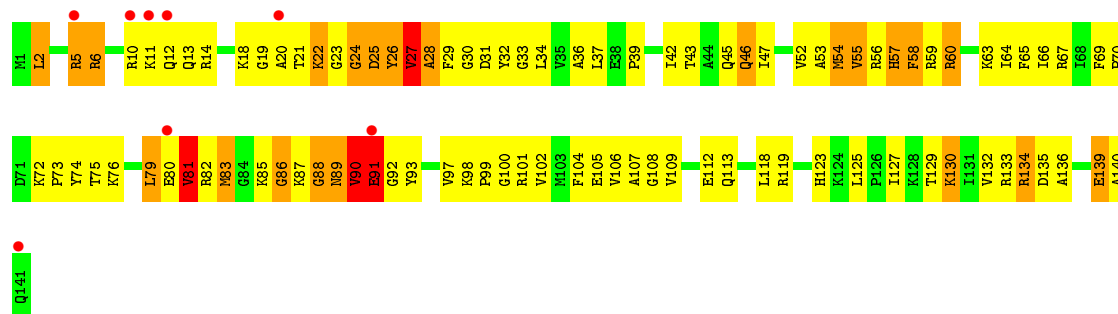


- Molecule 35: 50S ribosomal protein L15

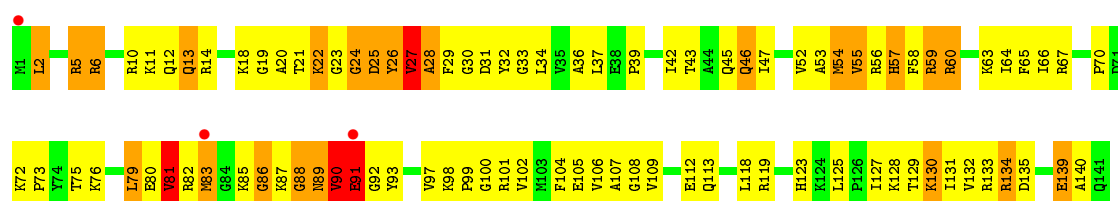


- Molecule 36: 50S ribosomal protein L16

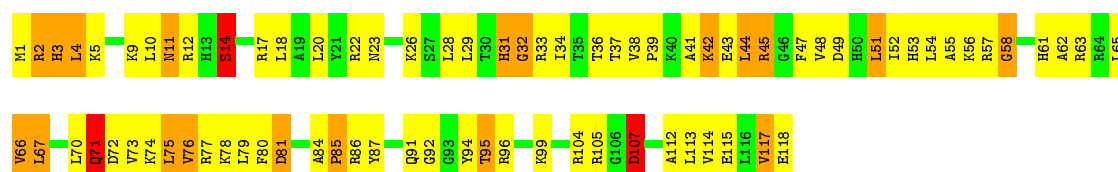
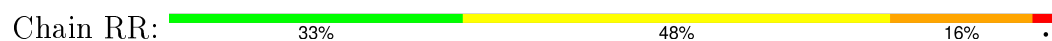




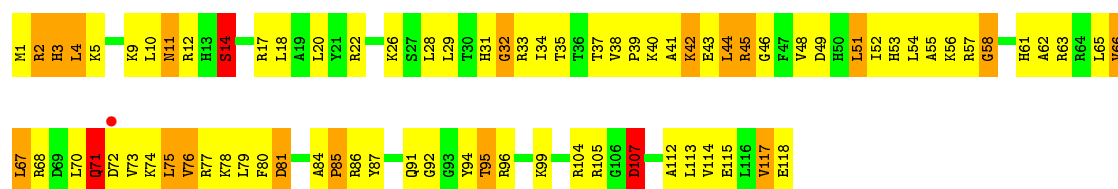
- Molecule 36: 50S ribosomal protein L16



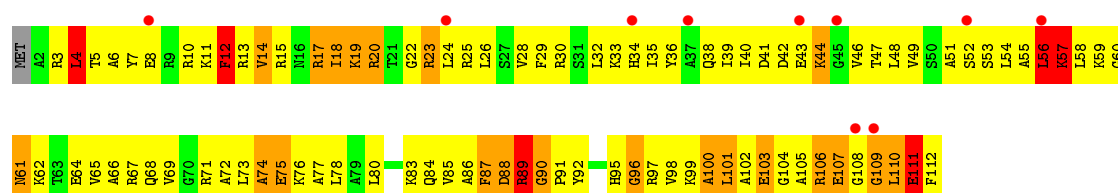
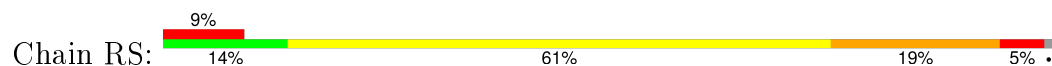
- Molecule 37: 50S ribosomal protein L17



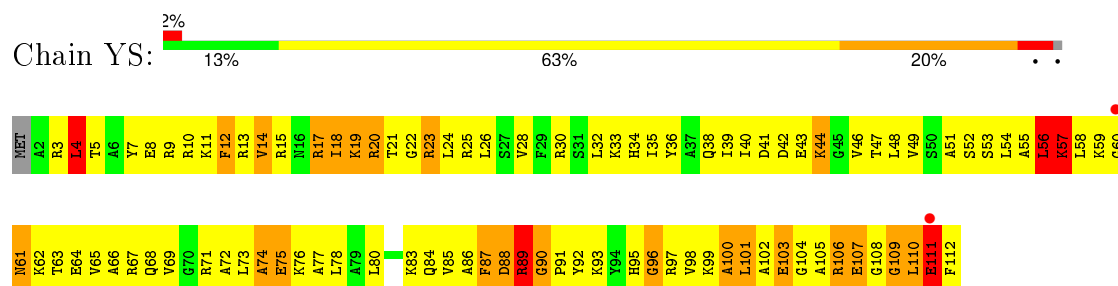
- Molecule 37: 50S ribosomal protein L17



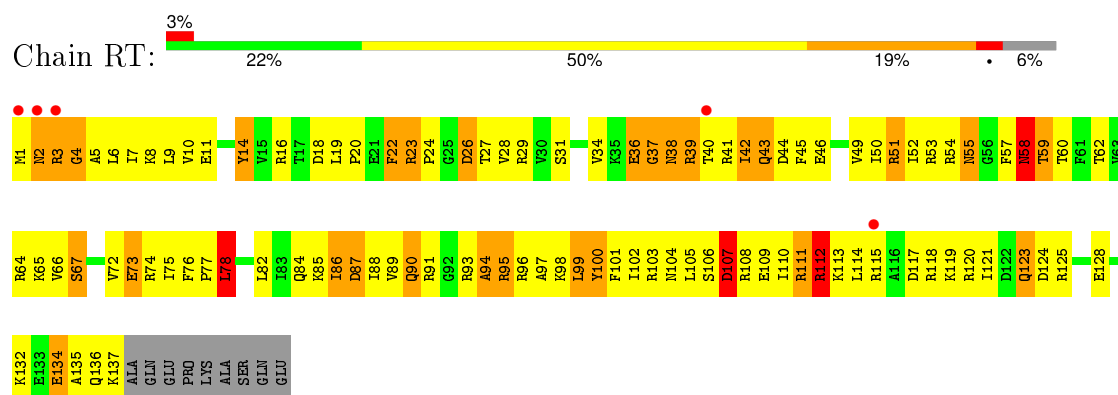
- Molecule 38: 50S ribosomal protein L18



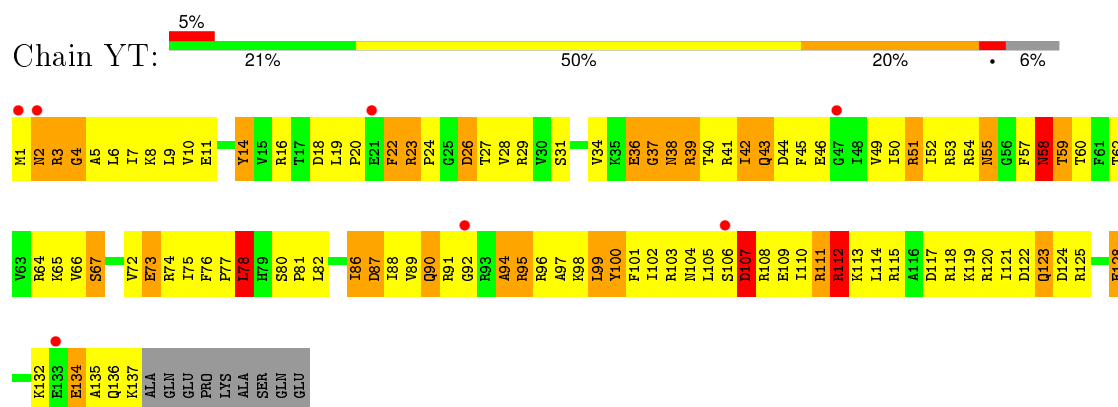
- Molecule 38: 50S ribosomal protein L18



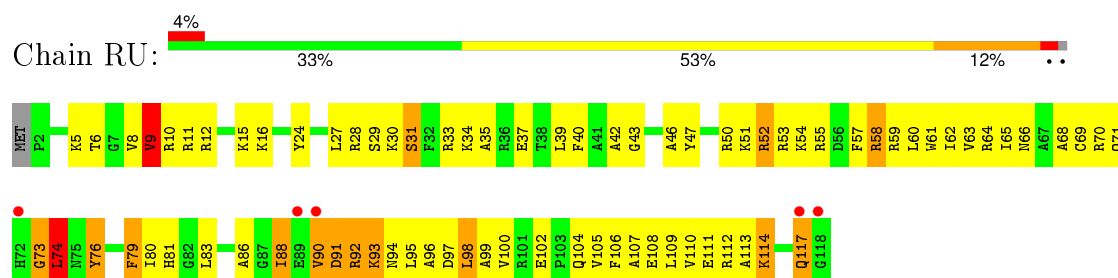
- Molecule 39: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L19

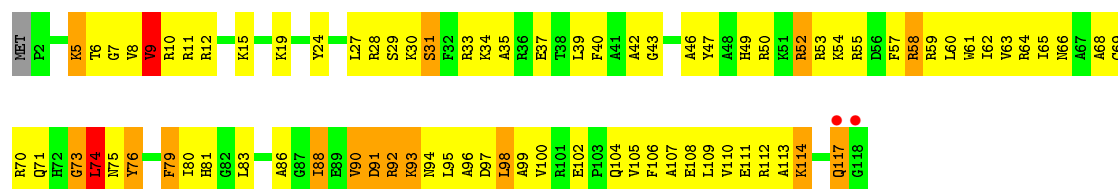


- Molecule 40: 50S ribosomal protein L20

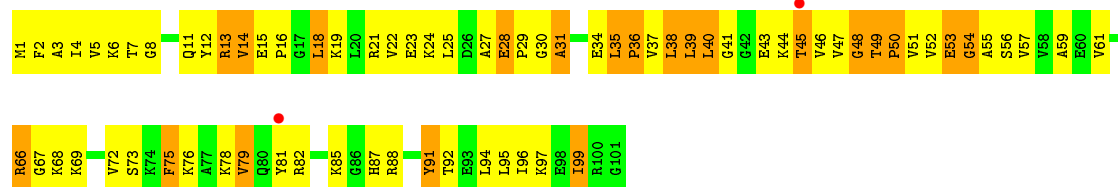


- Molecule 40: 50S ribosomal protein L20

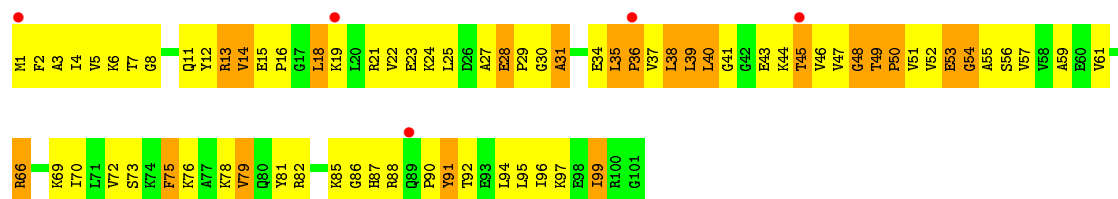




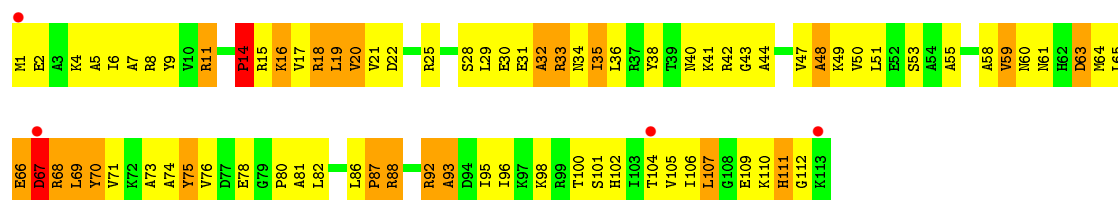
• Molecule 41: 50S ribosomal protein L21



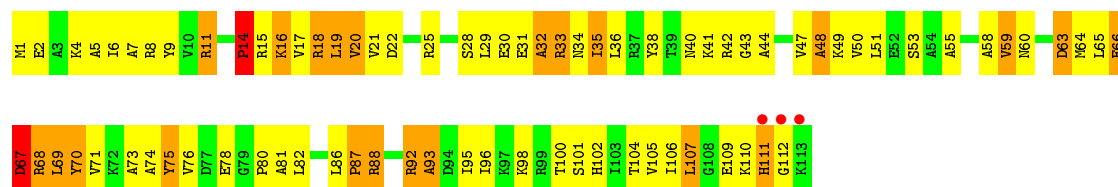
• Molecule 41: 50S ribosomal protein L21



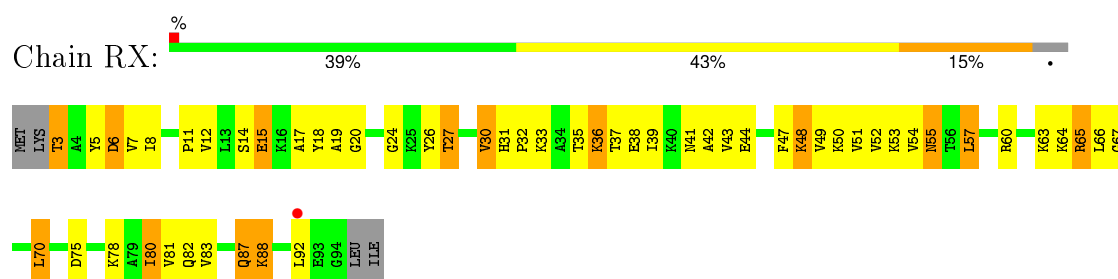
• Molecule 42: 50S ribosomal protein L22



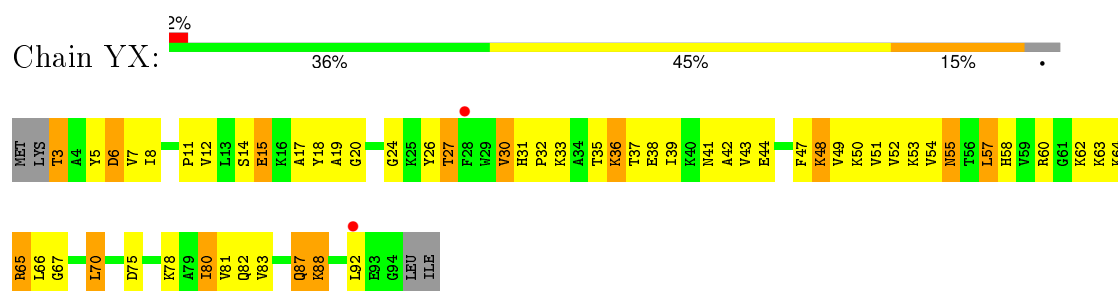
• Molecule 42: 50S ribosomal protein L22



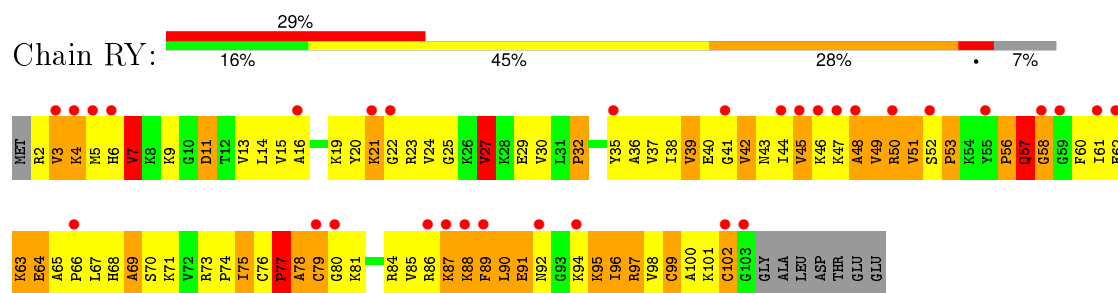
• Molecule 43: 50S ribosomal protein L23



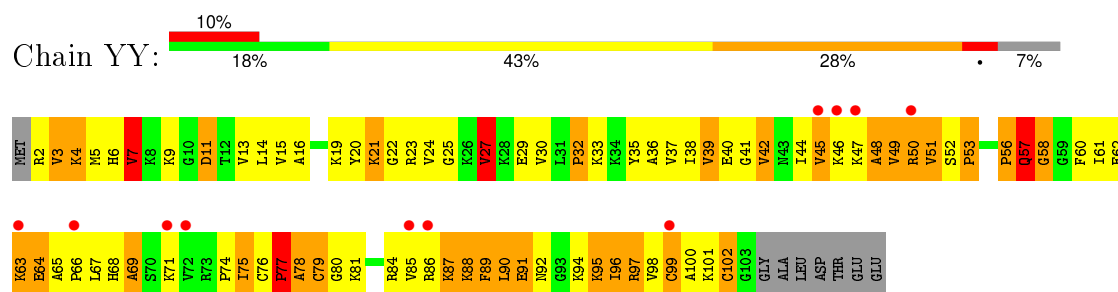
- Molecule 43: 50S ribosomal protein L23



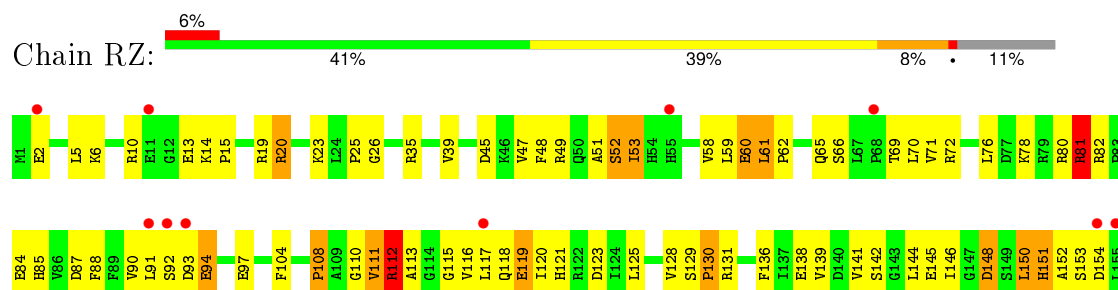
- Molecule 44: 50S ribosomal protein L24

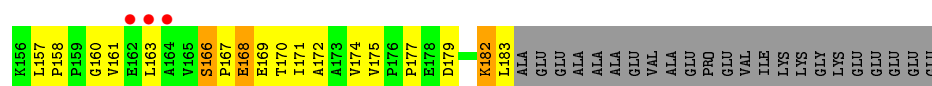


- Molecule 44: 50S ribosomal protein L24

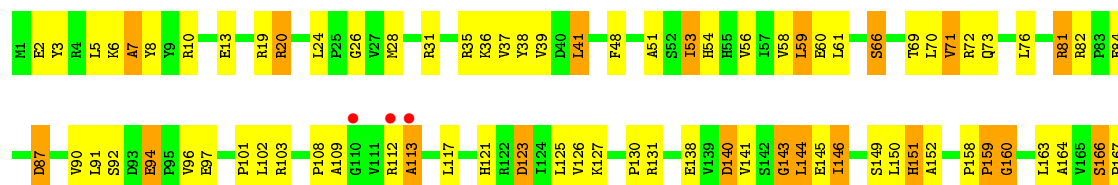


- Molecule 45: 50S ribosomal protein L25

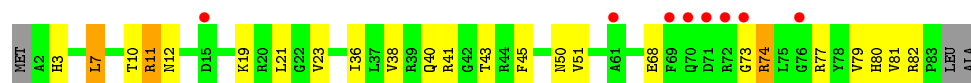




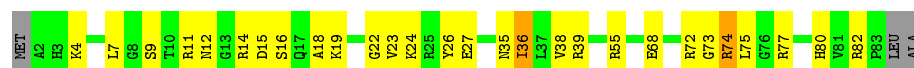
- Molecule 45: 50S ribosomal protein L25



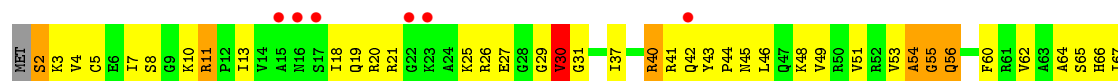
- Molecule 46: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



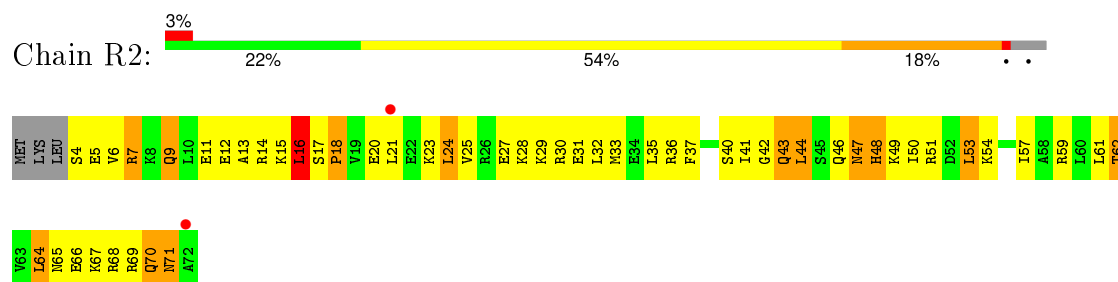
- Molecule 47: 50S ribosomal protein L28



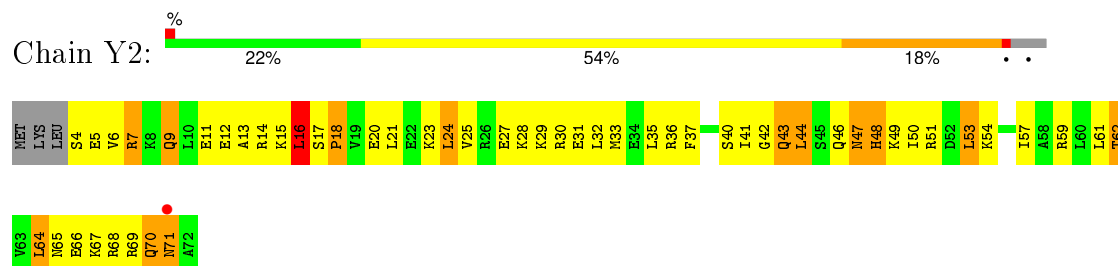
- Molecule 47: 50S ribosomal protein L28



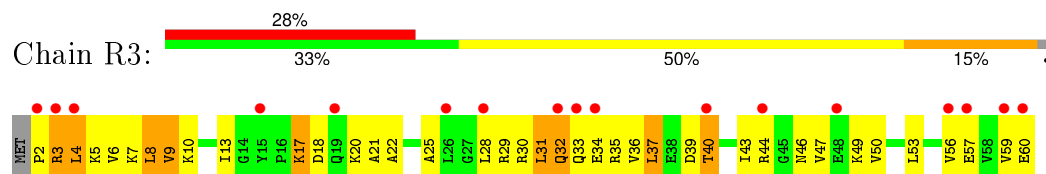
- Molecule 48: 50S ribosomal protein L29



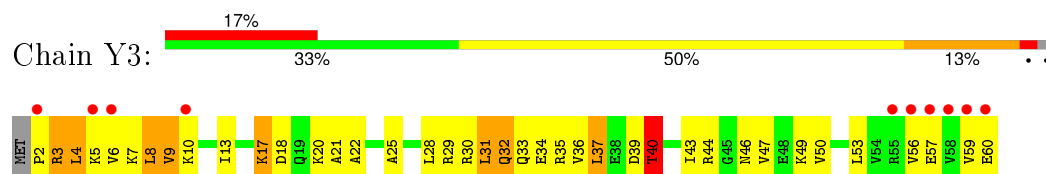
- Molecule 48: 50S ribosomal protein L29



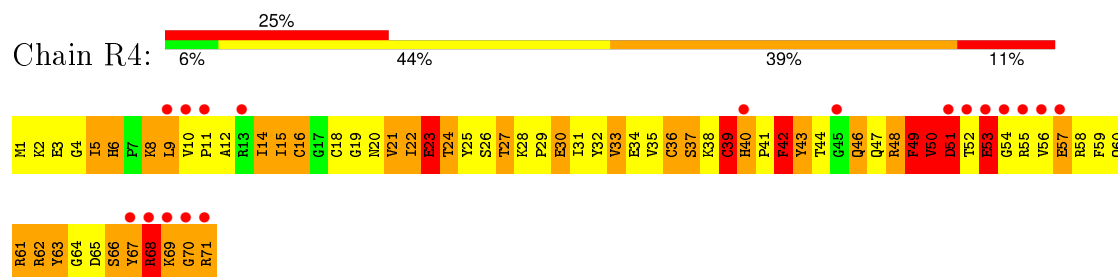
- Molecule 49: 50S ribosomal protein L30



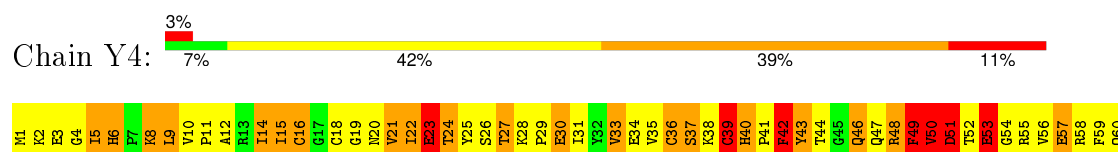
- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L31

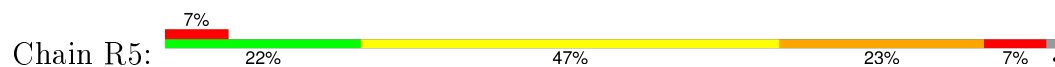


- Molecule 50: 50S ribosomal protein L31

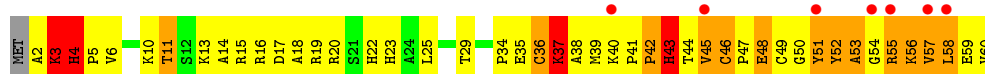




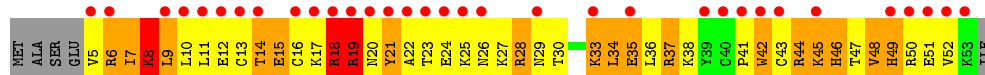
- Molecule 51: 50S ribosomal protein L32



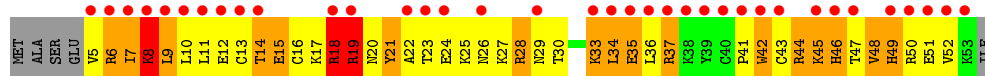
- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34

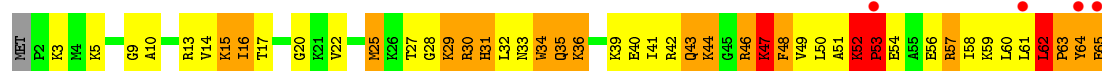


- Molecule 53: 50S ribosomal protein L34

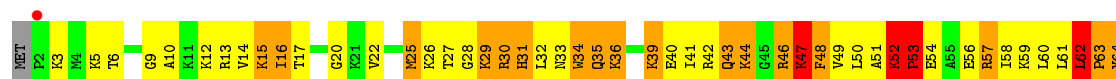
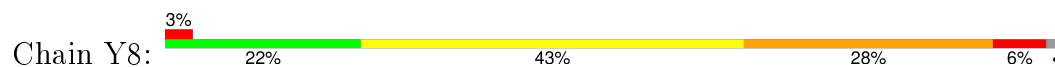


- Molecule 54: 50S ribosomal protein L35

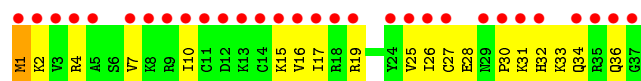
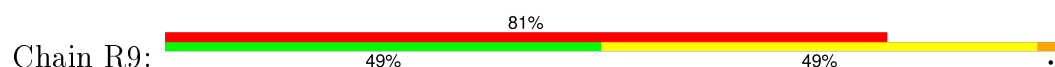




- Molecule 54: 50S ribosomal protein L35



- 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, α , β , γ	209.03Å 447.05Å 619.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 3.90 49.88 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.88-3.90) 97.9 (49.88-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.252 , 0.298 0.257 , 0.299	Depositor DCC
R_{free} test set	22786 reflections (4.65%)	DCC
Wilson B-factor (Å ²)	100.8	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 62.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 650647 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	291958	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 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	0.31	0/36098	0.87	34/56341 (0.1%)
1	XA	0.33	0/36101	0.89	31/56346 (0.1%)
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	0.37	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	0.61	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	0.36	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	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.46	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.34	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	0.39	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	0.52	0/1836	1.00	6/2859 (0.2%)
22	XV	0.52	0/1836	1.00	6/2859 (0.2%)
23	QX	0.32	0/193	0.83	0/299
23	XX	0.30	0/193	0.83	0/299
24	QY	0.66	2/311 (0.6%)	0.86	0/483
24	XY	0.66	2/311 (0.6%)	0.86	0/483
25	RA	0.37	0/69521	0.92	63/108529 (0.1%)
25	YA	0.39	0/69543	0.94	68/108563 (0.1%)
26	RB	0.31	0/2878	0.86	0/4490
26	YB	0.36	0/2878	0.91	1/4490 (0.0%)
27	RD	0.60	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	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	0.29	0/1151	0.55	0/1558
32	YI	0.27	0/1151	0.55	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	0.94	3/1544 (0.2%)
35	YP	0.50	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	0.89	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	0.78	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.27	0/1493	0.51	0/2026
45	YZ	0.29	0/1493	0.53	0/2026
46	R0	0.28	0/657	0.51	0/874
46	Y0	0.31	0/657	0.53	0/874
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	0.50	0/583	0.83	1/771 (0.1%)
48	Y2	0.51	0/583	0.83	1/771 (0.1%)
49	R3	0.47	0/474	0.72	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	0.50	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	0.60	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	1.80	1/60 (1.7%)
All	All	0.39	6/316339 (0.0%)	0.87	274/472939 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	RD	236	GLY	C-N	8.58	1.53	1.34
24	XY	34	C	C2-N3	7.54	1.41	1.35
24	QY	34	C	C2-N3	7.34	1.41	1.35
24	XY	34	C	C2-O2	6.60	1.30	1.24
24	QY	34	C	C2-O2	6.51	1.30	1.24

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	XL	47	LYS	C-N-CD	-20.47	75.57	120.60
12	QL	47	LYS	C-N-CD	-20.46	75.59	120.60
22	XV	17	C	C2-N1-C1'	11.76	131.74	118.80
22	QV	17	C	C2-N1-C1'	11.76	131.73	118.80
28	YE	21	VAL	C-N-CD	-10.09	98.41	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	630	0
1	XA	32249	0	16279	668	0
2	QB	1924	0	1975	286	0
2	XB	1924	0	1975	288	0
3	QC	1605	0	1668	225	0
3	XC	1605	0	1668	208	1
4	QD	1703	0	1765	276	0
4	XD	1703	0	1765	212	3
5	QE	1155	0	1213	144	0
5	XE	1155	0	1213	136	0
6	QF	843	0	857	93	0
6	XF	843	0	857	123	0
7	QG	1257	0	1296	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	138	0
8	QH	1116	0	1177	148	0
8	XH	1116	0	1177	154	0
9	QI	1010	0	1037	140	0
9	XI	1010	0	1037	149	0
10	QJ	801	0	849	150	0
10	XJ	801	0	849	132	0
11	QK	885	0	904	105	1
11	XK	885	0	904	123	0
12	QL	975	0	1062	103	0
12	XL	975	0	1062	103	0
13	QM	964	0	1034	157	0
13	XM	964	0	1034	161	0
14	QN	492	0	529	100	0
14	XN	492	0	529	96	0
15	QO	734	0	771	74	0
15	XO	734	0	771	73	0
16	QP	705	0	725	110	0
16	XP	705	0	725	110	0
17	QQ	834	0	904	80	0
17	XQ	834	0	904	80	0
18	QR	574	0	644	67	0
18	XR	574	0	644	68	0
19	QS	674	0	699	106	0
19	XS	674	0	699	129	0
20	QT	763	0	860	106	0
20	XT	763	0	861	101	0
21	QU	217	0	234	26	0
21	XU	217	0	234	27	0
22	QV	1644	0	836	29	0
22	XV	1644	0	836	28	0
23	QX	173	0	88	5	0
23	XX	173	0	88	2	0
24	QY	303	0	154	4	0
24	XY	303	0	154	5	0
25	RA	62071	0	31290	1129	0
25	YA	62091	0	31295	1166	0
26	RB	2573	0	1306	46	0
26	YB	2573	0	1306	41	0
27	RD	2115	0	2195	317	3
27	YD	2115	0	2195	336	0
28	RE	1568	0	1634	265	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	266	0
29	RF	1585	0	1632	178	0
29	YF	1585	0	1632	175	0
30	RG	1474	0	1535	194	0
30	YG	1474	0	1535	193	0
31	RH	1307	0	1382	224	0
31	YH	1307	0	1382	220	3
32	RI	1136	0	1223	57	0
32	YI	1136	0	1223	40	0
33	RN	1104	0	1180	194	0
33	YN	1104	0	1180	189	0
34	RO	933	0	996	124	0
34	YO	933	0	996	125	0
35	RP	1145	0	1228	243	0
35	YP	1145	0	1227	235	0
36	RQ	1122	0	1179	148	0
36	YQ	1122	0	1179	143	0
37	RR	968	0	1033	109	0
37	YR	968	0	1033	114	0
38	RS	882	0	943	153	0
38	YS	882	0	943	157	0
39	RT	1141	0	1202	156	0
39	YT	1141	0	1202	164	0
40	RU	964	0	1022	131	0
40	YU	964	0	1022	134	0
41	RV	779	0	852	130	0
41	YV	779	0	852	135	3
42	RW	900	0	964	95	0
42	YW	900	0	964	105	0
43	RX	725	0	778	68	0
43	YX	725	0	778	70	0
44	RY	785	0	878	160	0
44	YY	785	0	878	149	3
45	RZ	1461	0	1493	60	0
45	YZ	1461	0	1493	61	0
46	R0	648	0	671	19	0
46	Y0	648	0	672	23	0
47	R1	763	0	848	139	0
47	Y1	763	0	848	133	0
48	R2	581	0	629	81	0
48	Y2	581	0	629	71	0
49	R3	469	0	518	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	42	0
50	R4	581	0	574	154	0
50	Y4	581	0	574	169	0
51	R5	459	0	480	74	0
51	Y5	459	0	480	78	3
52	R6	424	0	450	88	0
52	Y6	424	0	450	90	0
53	R7	430	0	480	40	0
53	Y7	430	0	480	43	0
54	R8	517	0	582	97	0
54	Y8	517	0	582	105	0
55	R9	307	0	338	20	0
55	Y9	307	0	338	19	0
56	Z6	74	0	51	10	0
56	Z8	74	0	51	10	0
57	QA	65	0	0	0	0
57	QF	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	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	242	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	2	0	0	0	0
57	XA	70	0	0	0	0
57	XB	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	1	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	1	0	0	0	0
57	YA	267	0	0	0	0
57	YB	3	0	0	0	0
57	YD	2	0	0	0	0
57	YE	1	0	0	0	0
57	YP	1	0	0	0	0
58	QA	42	0	45	3	0
58	XA	42	0	45	2	0
59	QD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	291958	0	198347	15046	10

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 31.

The worst 5 of 15046 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	1.55
14:YN:32:SER:HB3	14:YN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.36	1.52
4:QD:167:GLY:HA2	27:YD:135:PHE:CZ	1.42	1.52
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52

The worst 5 of 10 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)
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.69	0.51
41:YV:50:PRO:CG	51:Y5:60:VAL:O[4_445]	1.99	0.21
31:YH:47:GLU:OE2	44:YY:79:CYS:CB[4_445]	2.03	0.17
41:YV:51:VAL:CB	51:Y5:60:VAL:OXT[4_445]	2.07	0.13
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	2.08	0.12

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	7
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	7
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	1	15
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	1	15
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	1	14
4	XD	206/209 (99%)	135 (66%)	48 (23%)	23 (11%)	0	10
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	1	13
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	11
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	16
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	16
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	1	14
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	16
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	10
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	10
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	7
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	7
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	1	16
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	1	12
11	QK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	24
11	XK	117/129 (91%)	86 (74%)	22 (19%)	9 (8%)	1	20
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	9
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	9
13	QM	119/126 (94%)	71 (60%)	28 (24%)	20 (17%)	0	4
13	XM	119/126 (94%)	72 (60%)	26 (22%)	21 (18%)	0	3
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	2
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	2
15	QO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	23
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	23
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	6
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	6
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	18
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	8
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	8
19	QS	82/93 (88%)	47 (57%)	17 (21%)	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	3
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	2
21	QU	23/27 (85%)	15 (65%)	4 (17%)	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	23
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	23
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%)	1	13
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	13
30	RG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0	9
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	9
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%)	105 (73%)	25 (17%)	14 (10%)	1	14
32	YI	144/148 (97%)	101 (70%)	29 (20%)	14 (10%)	1	14
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	5
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	5
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	21
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	21
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	2
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	2
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	13
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	13
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	8
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	8
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	63 (58%)	27 (25%)	19 (17%)	0	3
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	5
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	5
40	RU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	20
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	20
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	13
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	13
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	8
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	8
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	29
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	29
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%)	131 (72%)	32 (18%)	18 (10%)	1	14
45	YZ	181/206 (88%)	129 (71%)	33 (18%)	19 (10%)	1	11
46	R0	80/85 (94%)	67 (84%)	12 (15%)	1 (1%)	15	59
46	Y0	80/85 (94%)	70 (88%)	9 (11%)	1 (1%)	15	59
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	9
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	9
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	6
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	6
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	30
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	30
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
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%)	2	26
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	3
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	3
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%)	7661 (67%)	2332 (20%)	1477 (13%)	0	7

5 of 1477 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 ⓘ

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%)	7	35
2	XB	205/220 (93%)	181 (88%)	24 (12%)	7	35
3	QC	159/188 (85%)	143 (90%)	16 (10%)	9	41
3	XC	159/188 (85%)	143 (90%)	16 (10%)	9	41
4	QD	180/181 (99%)	160 (89%)	20 (11%)	8	38
4	XD	180/181 (99%)	165 (92%)	15 (8%)	14	51
5	QE	116/123 (94%)	107 (92%)	9 (8%)	16	54
5	XE	116/123 (94%)	108 (93%)	8 (7%)	19	59
6	QF	90/90 (100%)	76 (84%)	14 (16%)	3	24
6	XF	90/90 (100%)	76 (84%)	14 (16%)	3	24
7	QG	126/127 (99%)	115 (91%)	11 (9%)	13	49
7	XG	126/127 (99%)	115 (91%)	11 (9%)	13	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	106 (89%)	13 (11%)	8	39
8	XH	119/119 (100%)	106 (89%)	13 (11%)	8	39
9	QI	98/99 (99%)	87 (89%)	11 (11%)	7	37
9	XI	98/99 (99%)	87 (89%)	11 (11%)	7	37
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	12	47
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	12	47
11	QK	90/99 (91%)	81 (90%)	9 (10%)	9	42
11	XK	90/99 (91%)	81 (90%)	9 (10%)	9	42
12	QL	104/109 (95%)	90 (86%)	14 (14%)	5	30
12	XL	104/109 (95%)	90 (86%)	14 (14%)	5	30
13	QM	97/101 (96%)	81 (84%)	16 (16%)	3	21
13	XM	97/101 (96%)	81 (84%)	16 (16%)	3	21
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	16
14	XN	49/50 (98%)	44 (90%)	5 (10%)	9	41
15	QO	79/80 (99%)	73 (92%)	6 (8%)	16	55
15	XO	79/80 (99%)	73 (92%)	6 (8%)	16	55
16	QP	72/74 (97%)	63 (88%)	9 (12%)	6	32
16	XP	72/74 (97%)	63 (88%)	9 (12%)	6	32
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	22	61
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	22	61
18	QR	61/77 (79%)	54 (88%)	7 (12%)	7	36
18	XR	61/77 (79%)	54 (88%)	7 (12%)	7	36
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	25
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	25
20	QT	76/82 (93%)	68 (90%)	8 (10%)	8	40
20	XT	76/82 (93%)	68 (90%)	8 (10%)	8	40
21	QU	20/22 (91%)	19 (95%)	1 (5%)	30	68
21	XU	20/22 (91%)	19 (95%)	1 (5%)	30	68
27	RD	214/218 (98%)	176 (82%)	38 (18%)	2	18
27	YD	214/218 (98%)	176 (82%)	38 (18%)	2	18
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	8
29	RF	161/166 (97%)	140 (87%)	21 (13%)	5	31
29	YF	161/166 (97%)	140 (87%)	21 (13%)	5	31
30	RG	155/156 (99%)	130 (84%)	25 (16%)	3	22
30	YG	155/156 (99%)	130 (84%)	25 (16%)	3	22
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	13
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	13
32	RI	122/124 (98%)	100 (82%)	22 (18%)	2	17
32	YI	122/124 (98%)	98 (80%)	24 (20%)	1	13
33	RN	117/119 (98%)	98 (84%)	19 (16%)	3	22
33	YN	117/119 (98%)	98 (84%)	19 (16%)	3	22
34	RO	100/100 (100%)	90 (90%)	10 (10%)	9	42
34	YO	100/100 (100%)	90 (90%)	10 (10%)	9	42
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	8
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	8
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	3	22
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	3	22
37	RR	101/101 (100%)	84 (83%)	17 (17%)	2	20
37	YR	101/101 (100%)	84 (83%)	17 (17%)	2	20
38	RS	87/88 (99%)	74 (85%)	13 (15%)	4	26
38	YS	87/88 (99%)	74 (85%)	13 (15%)	4	26
39	RT	120/127 (94%)	97 (81%)	23 (19%)	2	14
39	YT	120/127 (94%)	97 (81%)	23 (19%)	2	14
40	RU	93/94 (99%)	80 (86%)	13 (14%)	4	29
40	YU	93/94 (99%)	80 (86%)	13 (14%)	4	29
41	RV	82/82 (100%)	71 (87%)	11 (13%)	5	30
41	YV	82/82 (100%)	71 (87%)	11 (13%)	5	30
42	RW	92/92 (100%)	77 (84%)	15 (16%)	3	22
42	YW	92/92 (100%)	77 (84%)	15 (16%)	3	22
43	RX	74/78 (95%)	63 (85%)	11 (15%)	4	26
43	YX	74/78 (95%)	63 (85%)	11 (15%)	4	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RY	85/91 (93%)	70 (82%)	15 (18%)	2	18
44	YY	85/91 (93%)	70 (82%)	15 (18%)	2	18
45	RZ	162/179 (90%)	140 (86%)	22 (14%)	5	29
45	YZ	162/179 (90%)	144 (89%)	18 (11%)	8	38
46	R0	65/67 (97%)	61 (94%)	4 (6%)	23	62
46	Y0	65/67 (97%)	61 (94%)	4 (6%)	23	62
47	R1	82/83 (99%)	67 (82%)	15 (18%)	2	16
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	2	16
48	R2	64/67 (96%)	57 (89%)	7 (11%)	8	39
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	8	39
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	10
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	10
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	4
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	4
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	8
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	8
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	11
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	11
53	R7	42/42 (100%)	39 (93%)	3 (7%)	18	58
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	18	58
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	4
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	4
55	R9	34/34 (100%)	32 (94%)	2 (6%)	24	64
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	24	64
All	All	9702/10066 (96%)	8303 (86%)	1399 (14%)	4	27

5 of 1399 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	R2	64	LEU
7	XG	12	LEU
45	YZ	87	ASP
50	R4	48	ARG
2	XB	33	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
48	R2	9	GLN
5	XE	72	GLN
41	YV	11	GLN
48	R2	47	ASN
2	XB	95	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	313 (20%)	45 (3%)
1	XA	1499/1522 (98%)	315 (21%)	47 (3%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	3 (42%)	2 (28%)
23	XX	7/25 (28%)	3 (42%)	2 (28%)
24	QY	13/18 (72%)	5 (38%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2879/2916 (98%)	667 (23%)	61 (2%)
25	YA	2880/2916 (98%)	675 (23%)	58 (2%)
26	RB	119/122 (97%)	24 (20%)	1 (0%)
26	YB	119/122 (97%)	26 (21%)	1 (0%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9189/9366 (98%)	2096 (22%)	221 (2%)

5 of 2096 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	9	G
1	QA	22	G
1	QA	32	A

5 of 221 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2439	A
1	XA	345	C
25	YA	1698	A

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Mol	Chain	Res	Type
25	RA	2566	A
1	XA	31	G

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

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	16,26,27	2.87	3 (18%)	19,39,42	1.53	4 (21%)
24	1MG	XY	37	24	16,26,27	2.89	3 (18%)	19,39,42	1.53	4 (21%)
56	PPU	Z6	76	25,56	30,40,41	2.59	5 (16%)	37,57,60	3.25	11 (29%)
56	PPU	Z8	76	25,56	30,40,41	2.57	5 (16%)	37,57,60	3.25	11 (29%)

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
56	PPU	Z6	76	25,56	-	0/21/43/44	0/4/4/4
56	PPU	Z8	76	25,56	-	0/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	C9-N6	-5.62	1.32	1.45
56	Z8	76	PPU	C9-N6	-5.57	1.32	1.45
56	Z6	76	PPU	C10-N6	-5.31	1.32	1.45
56	Z8	76	PPU	C10-N6	-5.31	1.32	1.45
24	XY	37	1MG	C6-C5	2.59	1.45	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z8	76	PPU	C2'-C1'-N9	-10.35	98.48	114.29
56	Z6	76	PPU	C2'-C1'-N9	-10.30	98.55	114.29
56	Z8	76	PPU	N3-C2-N1	-9.82	121.38	128.89
56	Z6	76	PPU	N3-C2-N1	-9.81	121.38	128.89
56	Z6	76	PPU	C3'-N3'-C	-8.28	110.13	123.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z6	76	PPU	9	0
56	Z8	76	PPU	8	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 676 ligands modelled in this entry, 674 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	PAR	QA	1666	-	45,45,45	1.41	9 (20%)	59,67,67	1.36	7 (11%)
58	PAR	XA	1671	-	45,45,45	1.56	9 (20%)	59,67,67	1.73	13 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	QA	1666	-	-	0/18/94/94	0/4/4/4
58	PAR	XA	1671	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1666	PAR	C44-C34	2.06	1.57	1.52
58	QA	1666	PAR	O54-C54	2.14	1.49	1.44
58	XA	1671	PAR	C44-C34	2.24	1.58	1.52
58	QA	1666	PAR	C44-C54	2.25	1.57	1.53
58	QA	1666	PAR	C62-C52	2.30	1.58	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1671	PAR	O34-C34-C24	-3.18	104.94	110.31
58	XA	1671	PAR	C31-C41-C51	-2.81	105.30	110.20
58	XA	1671	PAR	O62-C62-C12	-2.62	105.00	109.87
58	QA	1666	PAR	O33-C14-O54	-2.48	104.41	110.68
58	QA	1666	PAR	O11-C42-C32	-2.02	104.03	108.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1666	PAR	3	0
58	XA	1671	PAR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	0.11	33 (2%) 65 54	35, 87, 182, 299	0
1	XA	1500/1522 (98%)	-0.05	13 (0%) 85 79	21, 74, 169, 271	0
2	QB	237/256 (92%)	0.68	26 (10%) 7 5	84, 154, 204, 237	0
2	XB	237/256 (92%)	0.29	14 (5%) 26 17	51, 121, 182, 226	0
3	QC	205/239 (85%)	0.28	15 (7%) 18 12	57, 135, 182, 201	0
3	XC	205/239 (85%)	0.03	6 (2%) 55 42	32, 89, 145, 177	0
4	QD	208/209 (99%)	0.37	11 (5%) 30 22	38, 99, 165, 221	0
4	XD	208/209 (99%)	0.29	4 (1%) 70 59	27, 106, 160, 186	0
5	QE	151/162 (93%)	0.44	11 (7%) 18 12	36, 111, 158, 185	0
5	XE	151/162 (93%)	0.23	6 (3%) 42 31	3, 85, 142, 170	0
6	QF	101/101 (100%)	0.30	3 (2%) 54 40	33, 99, 158, 181	0
6	XF	101/101 (100%)	0.20	4 (3%) 42 31	25, 95, 145, 243	0
7	QG	155/156 (99%)	0.70	22 (14%) 4 3	55, 123, 179, 210	0
7	XG	155/156 (99%)	0.36	13 (8%) 14 9	42, 99, 156, 197	0
8	QH	138/138 (100%)	0.57	13 (9%) 11 7	61, 120, 167, 193	0
8	XH	138/138 (100%)	0.40	6 (4%) 39 28	20, 94, 147, 198	0
9	QI	127/128 (99%)	0.91	17 (13%) 4 4	67, 134, 193, 224	0
9	XI	127/128 (99%)	0.36	6 (4%) 35 26	29, 107, 165, 195	0
10	QJ	99/105 (94%)	1.39	22 (22%) 1 1	46, 149, 202, 222	0
10	XJ	99/105 (94%)	0.77	14 (14%) 4 3	35, 115, 175, 201	0
11	QK	119/129 (92%)	0.62	14 (11%) 6 5	42, 104, 158, 202	0
11	XK	119/129 (92%)	0.50	9 (7%) 17 11	27, 87, 148, 170	0
12	QL	125/132 (94%)	0.58	14 (11%) 7 5	21, 93, 142, 192	0
12	XL	125/132 (94%)	0.23	4 (3%) 51 38	20, 66, 131, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.47	13 (10%) 8 6	58, 122, 175, 214	0
13	XM	121/126 (96%)	0.22	4 (3%) 50 38	28, 92, 144, 180	0
14	QN	60/61 (98%)	0.88	8 (13%) 4 4	55, 129, 181, 204	0
14	XN	60/61 (98%)	0.28	3 (5%) 32 24	33, 82, 135, 170	0
15	QO	88/89 (98%)	0.27	4 (4%) 37 27	54, 105, 154, 178	0
15	XO	88/89 (98%)	0.18	2 (2%) 64 52	25, 91, 141, 171	0
16	QP	84/88 (95%)	0.79	11 (13%) 5 4	42, 86, 157, 171	0
16	XP	84/88 (95%)	0.77	10 (11%) 6 5	51, 101, 152, 235	0
17	QQ	100/105 (95%)	0.48	4 (4%) 42 31	33, 91, 144, 165	0
17	XQ	100/105 (95%)	0.58	8 (8%) 15 10	37, 95, 147, 200	0
18	QR	70/88 (79%)	0.81	8 (11%) 7 5	42, 110, 160, 212	0
18	XR	70/88 (79%)	0.49	4 (5%) 27 19	34, 86, 147, 168	0
19	QS	84/93 (90%)	0.95	15 (17%) 2 2	60, 131, 184, 190	0
19	XS	84/93 (90%)	0.46	4 (4%) 34 25	45, 97, 141, 220	0
20	QT	99/106 (93%)	0.33	2 (2%) 68 57	34, 91, 154, 181	0
20	XT	99/106 (93%)	0.59	8 (8%) 15 10	50, 112, 158, 181	0
21	QU	25/27 (92%)	2.58	14 (56%) 0 1	62, 132, 185, 206	0
21	XU	25/27 (92%)	1.47	6 (24%) 1 1	45, 89, 136, 166	0
22	QV	77/77 (100%)	0.07	1 (1%) 79 70	26, 99, 159, 205	0
22	XV	77/77 (100%)	-0.07	1 (1%) 79 70	28, 70, 121, 185	0
23	QX	8/25 (32%)	1.31	2 (25%) 1 1	70, 95, 129, 169	0
23	XX	8/25 (32%)	1.20	2 (25%) 1 1	36, 51, 102, 163	0
24	QY	13/18 (72%)	1.14	2 (15%) 3 3	104, 150, 249, 294	0
24	XY	13/18 (72%)	0.92	1 (7%) 16 11	70, 106, 221, 249	0
25	RA	2882/2916 (98%)	0.02	90 (3%) 52 40	14, 60, 203, 320	0
25	YA	2883/2916 (98%)	-0.08	80 (2%) 56 44	14, 50, 194, 329	0
26	RB	120/122 (98%)	0.17	1 (0%) 87 81	64, 113, 177, 203	0
26	YB	120/122 (98%)	-0.33	0 100 100	37, 69, 95, 158	0
27	RD	272/276 (98%)	0.11	3 (1%) 82 74	7, 56, 113, 177	0
27	YD	272/276 (98%)	0.14	2 (0%) 89 84	3, 49, 98, 152	0
28	RE	205/206 (99%)	0.37	10 (4%) 33 24	23, 73, 150, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.41	7 (3%) 49 37	15, 77, 151, 200	0
29	RF	202/210 (96%)	0.20	4 (1%) 68 57	4, 85, 151, 184	0
29	YF	202/210 (96%)	0.06	5 (2%) 61 48	8, 65, 124, 184	0
30	RG	181/182 (99%)	0.62	19 (10%) 8 6	52, 137, 205, 232	0
30	YG	181/182 (99%)	0.31	6 (3%) 50 38	25, 98, 166, 203	0
31	RH	170/180 (94%)	1.05	34 (20%) 1 1	69, 150, 202, 250	0
31	YH	170/180 (94%)	0.55	15 (8%) 12 8	32, 94, 152, 204	0
32	RI	146/148 (98%)	0.51	14 (9%) 10 7	29, 109, 161, 182	0
32	YI	146/148 (98%)	0.19	8 (5%) 29 20	18, 95, 158, 203	0
33	RN	138/140 (98%)	0.54	10 (7%) 18 12	33, 94, 152, 192	0
33	YN	138/140 (98%)	0.09	3 (2%) 65 54	19, 75, 132, 162	0
34	RO	122/122 (100%)	0.20	1 (0%) 87 81	6, 64, 120, 163	0
34	YO	122/122 (100%)	0.17	0 100 100	18, 61, 114, 144	0
35	RP	150/150 (100%)	0.72	23 (15%) 3 3	5, 87, 160, 191	0
35	YP	150/150 (100%)	0.38	6 (4%) 42 31	17, 75, 166, 203	0
36	RQ	141/141 (100%)	0.53	8 (5%) 27 19	25, 94, 140, 212	0
36	YQ	141/141 (100%)	0.18	3 (2%) 67 56	11, 61, 126, 169	0
37	RR	118/118 (100%)	0.06	0 100 100	12, 58, 116, 154	0
37	YR	118/118 (100%)	0.29	1 (0%) 87 81	24, 68, 127, 155	0
38	RS	111/112 (99%)	0.69	10 (9%) 12 8	40, 116, 169, 194	0
38	YS	111/112 (99%)	0.24	2 (1%) 71 61	9, 79, 133, 232	0
39	RT	137/146 (93%)	0.24	5 (3%) 46 35	19, 77, 171, 214	0
39	YT	137/146 (93%)	0.18	7 (5%) 32 23	30, 84, 164, 206	0
40	RU	117/118 (99%)	0.12	5 (4%) 39 28	17, 78, 154, 194	0
40	YU	117/118 (99%)	-0.04	2 (1%) 73 62	15, 65, 152, 189	0
41	RV	101/101 (100%)	0.30	2 (1%) 68 57	36, 105, 157, 216	0
41	YV	101/101 (100%)	0.36	5 (4%) 32 24	23, 84, 144, 243	0
42	RW	113/113 (100%)	0.41	4 (3%) 48 36	20, 65, 137, 216	0
42	YW	113/113 (100%)	0.16	3 (2%) 58 46	12, 56, 114, 193	0
43	RX	92/96 (95%)	0.18	1 (1%) 82 74	14, 69, 125, 158	0
43	YX	92/96 (95%)	0.29	2 (2%) 65 54	12, 56, 113, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	1.48	32 (31%) 1 1	36, 115, 175, 230	0
44	YY	102/110 (92%)	0.65	11 (10%) 8 6	24, 83, 156, 204	0
45	RZ	183/206 (88%)	0.41	13 (7%) 19 12	42, 122, 174, 213	0
45	YZ	183/206 (88%)	0.12	3 (1%) 74 64	23, 98, 153, 211	0
46	R0	82/85 (96%)	0.70	8 (9%) 10 7	13, 74, 111, 143	0
46	Y0	82/85 (96%)	0.48	0 100 100	11, 54, 85, 133	0
47	R1	97/98 (98%)	0.73	9 (9%) 11 7	11, 74, 170, 241	0
47	Y1	97/98 (98%)	0.49	6 (6%) 24 15	11, 64, 144, 205	0
48	R2	69/72 (95%)	0.18	2 (2%) 55 42	26, 101, 176, 197	0
48	Y2	69/72 (95%)	0.20	1 (1%) 78 68	26, 69, 141, 177	0
49	R3	59/60 (98%)	1.57	17 (28%) 1 1	19, 95, 150, 200	0
49	Y3	59/60 (98%)	0.79	10 (16%) 2 2	9, 70, 131, 166	0
50	R4	71/71 (100%)	1.05	18 (25%) 1 1	89, 171, 218, 267	0
50	Y4	71/71 (100%)	0.29	2 (2%) 56 44	69, 145, 208, 248	0
51	R5	59/60 (98%)	0.42	4 (6%) 20 13	13, 74, 179, 222	0
51	Y5	59/60 (98%)	0.47	7 (11%) 6 5	17, 78, 189, 225	0
52	R6	49/54 (90%)	3.37	33 (67%) 0 1	101, 150, 215, 233	0
52	Y6	49/54 (90%)	2.88	36 (73%) 0 0	73, 147, 211, 217	0
53	R7	49/49 (100%)	0.24	1 (2%) 68 57	17, 47, 108, 188	0
53	Y7	49/49 (100%)	0.33	4 (8%) 14 9	6, 40, 118, 133	0
54	R8	64/65 (98%)	0.52	4 (6%) 23 15	24, 80, 155, 197	0
54	Y8	64/65 (98%)	0.30	2 (3%) 52 40	6, 54, 120, 197	0
55	R9	37/37 (100%)	4.07	30 (81%) 0 0	94, 143, 197, 202	0
55	Y9	37/37 (100%)	4.78	36 (97%) 0 0	62, 123, 202, 228	0
56	Z6	2/3 (66%)	0.58	0 100 100	30, 30, 30, 75	0
56	Z8	2/3 (66%)	0.05	0 100 100	30, 30, 30, 47	0
All	All	20871/21494 (97%)	0.26	1127 (5%) 29 21	3, 80, 177, 329	0

The worst 5 of 1127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	R9	14	CYS	14.8
28	YE	205	ALA	12.3

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Mol	Chain	Res	Type	RSRZ
25	RA	2799	A	10.5
55	R9	11	CYS	10.4
55	Y9	34	GLN	9.5

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	PPU	Z6	76	37/38	0.93	0.26	-	41,41,41,41	0
56	PPU	Z8	76	37/38	0.92	0.29	-	38,38,38,38	0
24	1MG	XY	37	24/25	0.93	0.16	-	59,59,59,59	0
24	1MG	QY	37	24/25	0.90	0.24	-	99,99,99,99	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	YA	3109	1/1	0.86	1.51	77.90	80,80,80,80	0
57	MG	YA	3025	1/1	0.91	1.63	64.22	80,80,80,80	0
57	MG	RA	3098	1/1	0.92	0.94	58.11	80,80,80,80	0
57	MG	RA	3097	1/1	0.80	1.10	46.59	80,80,80,80	0
57	MG	YA	3031	1/1	0.91	1.20	40.73	80,80,80,80	0
57	MG	RA	3033	1/1	0.99	0.52	36.96	5,5,5,5	0
57	MG	YA	3035	1/1	0.90	0.85	32.02	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3261	1/1	0.81	0.99	29.67	8,8,8,8	0
57	MG	RA	3034	1/1	0.91	0.44	27.53	2,2,2,2	0
57	MG	RA	3024	1/1	0.95	0.44	26.32	28,28,28,28	0
57	MG	YA	3088	1/1	0.89	1.30	25.76	80,80,80,80	0
57	MG	YA	3047	1/1	0.95	0.48	25.38	14,14,14,14	0
57	MG	XA	1669	1/1	0.92	0.34	25.11	13,13,13,13	0
57	MG	YA	3248	1/1	0.73	0.56	24.35	17,17,17,17	0
57	MG	YA	3058	1/1	0.83	0.67	23.80	4,4,4,4	0
57	MG	RA	3062	1/1	0.85	0.73	23.26	1,1,1,1	0
57	MG	RA	3088	1/1	0.96	0.46	20.94	5,5,5,5	0
57	MG	RA	3063	1/1	0.97	0.61	20.84	0,0,0,0	0
57	MG	RA	3161	1/1	0.93	0.57	20.21	75,75,75,75	0
57	MG	YA	3229	1/1	0.56	0.61	20.03	30,30,30,30	0
57	MG	YA	3182	1/1	0.83	0.66	19.44	30,30,30,30	0
57	MG	RA	3124	1/1	0.70	0.58	19.12	35,35,35,35	0
57	MG	YA	3141	1/1	0.93	0.57	18.87	7,7,7,7	0
57	MG	RA	3002	1/1	0.81	0.50	17.69	4,4,4,4	0
57	MG	YA	3264	1/1	0.79	0.37	17.22	35,35,35,35	0
57	MG	RA	3004	1/1	0.94	0.50	17.17	13,13,13,13	0
57	MG	XA	1643	1/1	0.76	0.49	17.12	34,34,34,34	0
57	MG	YA	3009	1/1	0.94	0.43	17.06	0,0,0,0	0
57	MG	YA	3002	1/1	0.92	0.98	16.20	80,80,80,80	0
57	MG	RA	3089	1/1	0.96	0.48	14.92	2,2,2,2	0
57	MG	RA	3156	1/1	0.88	0.39	14.84	19,19,19,19	0
57	MG	RA	3174	1/1	0.91	0.45	14.84	17,17,17,17	0
57	MG	XA	1603	1/1	0.90	0.49	14.45	5,5,5,5	0
57	MG	YA	3254	1/1	0.93	0.52	14.42	1,1,1,1	0
57	MG	YA	3173	1/1	0.94	0.45	13.99	0,0,0,0	0
57	MG	QV	101	1/1	0.92	0.69	13.70	80,80,80,80	0
57	MG	YA	3155	1/1	0.81	0.55	13.52	38,38,38,38	0
57	MG	YA	3043	1/1	0.75	0.45	13.35	6,6,6,6	0
57	MG	YA	3049	1/1	0.97	0.47	12.77	6,6,6,6	0
57	MG	QA	1617	1/1	0.90	0.47	12.70	8,8,8,8	0
57	MG	YA	3106	1/1	0.85	0.22	12.16	84,84,84,84	0
57	MG	YA	3124	1/1	0.64	0.64	12.15	19,19,19,19	0
57	MG	YA	3081	1/1	0.88	0.56	12.12	0,0,0,0	0
57	MG	RA	3120	1/1	0.88	0.55	11.85	4,4,4,4	0
57	MG	YA	3095	1/1	0.91	0.47	11.75	1,1,1,1	0
57	MG	RA	3008	1/1	0.86	0.41	11.52	3,3,3,3	0
57	MG	XA	1604	1/1	0.91	0.85	10.54	13,13,13,13	0
57	MG	YA	3101	1/1	0.98	0.38	10.49	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3257	1/1	0.97	0.50	10.46	5,5,5,5	0
57	MG	RA	3184	1/1	0.79	0.37	10.30	13,13,13,13	0
57	MG	YA	3037	1/1	0.98	0.38	10.25	7,7,7,7	0
57	MG	RA	3026	1/1	0.73	1.19	10.17	80,80,80,80	0
57	MG	YA	3235	1/1	0.91	0.31	9.95	8,8,8,8	0
57	MG	RA	3049	1/1	0.91	0.40	9.80	4,4,4,4	0
57	MG	YA	3110	1/1	0.97	0.41	9.30	18,18,18,18	0
57	MG	YA	3145	1/1	0.78	0.29	9.18	16,16,16,16	0
57	MG	XA	1625	1/1	0.97	0.24	8.95	6,6,6,6	0
57	MG	YD	301	1/1	0.90	0.75	8.93	80,80,80,80	0
57	MG	YA	3207	1/1	0.68	0.29	8.78	20,20,20,20	0
57	MG	YA	3108	1/1	0.98	0.69	8.66	15,15,15,15	0
57	MG	YA	3102	1/1	0.94	0.49	8.54	3,3,3,3	0
57	MG	YA	3069	1/1	0.95	0.37	8.48	10,10,10,10	0
57	MG	YA	3033	1/1	0.97	0.62	8.24	5,5,5,5	0
57	MG	XA	1634	1/1	0.82	0.72	8.05	23,23,23,23	0
57	MG	QA	1658	1/1	0.63	0.25	8.01	90,90,90,90	0
57	MG	YA	3161	1/1	0.71	0.35	7.78	6,6,6,6	0
57	MG	YA	3116	1/1	0.91	0.52	7.75	80,80,80,80	0
57	MG	RA	3094	1/1	0.97	0.62	7.62	3,3,3,3	0
57	MG	RA	3009	1/1	0.75	0.49	7.08	84,84,84,84	0
57	MG	XA	1662	1/1	0.80	0.36	7.07	51,51,51,51	0
57	MG	RD	301	1/1	0.83	0.68	6.96	11,11,11,11	0
57	MG	RA	3077	1/1	0.97	0.41	6.81	19,19,19,19	0
57	MG	RA	3031	1/1	0.86	0.33	6.78	13,13,13,13	0
57	MG	RA	3036	1/1	0.90	0.47	6.70	2,2,2,2	0
57	MG	XA	1654	1/1	0.72	0.41	6.66	23,23,23,23	0
57	MG	RA	3021	1/1	0.97	0.24	6.58	5,5,5,5	0
57	MG	RA	3047	1/1	0.97	0.34	6.52	1,1,1,1	0
57	MG	YA	3023	1/1	0.97	0.38	6.45	6,6,6,6	0
57	MG	RA	3170	1/1	0.86	0.47	6.34	23,23,23,23	0
57	MG	YA	3263	1/1	0.94	0.24	6.33	7,7,7,7	0
57	MG	RA	3179	1/1	0.83	0.33	6.04	12,12,12,12	0
57	MG	YA	3240	1/1	0.87	0.38	5.96	23,23,23,23	0
57	MG	RA	3209	1/1	0.86	0.25	5.81	35,35,35,35	0
57	MG	RA	3054	1/1	0.96	0.26	5.74	41,41,41,41	0
57	MG	YA	3092	1/1	0.93	0.28	5.68	13,13,13,13	0
57	MG	RA	3019	1/1	0.93	0.35	5.64	14,14,14,14	0
57	MG	RA	3224	1/1	0.92	0.23	5.43	19,19,19,19	0
57	MG	YA	3011	1/1	0.97	0.28	5.31	2,2,2,2	0
57	MG	XA	1620	1/1	0.94	0.32	5.15	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3015	1/1	0.97	0.31	4.92	0,0,0,0	0
57	MG	RA	3222	1/1	0.66	0.37	4.84	45,45,45,45	0
57	MG	RA	3121	1/1	0.96	0.24	4.73	2,2,2,2	0
57	MG	YA	3170	1/1	0.95	0.25	4.73	26,26,26,26	0
57	MG	YA	3073	1/1	0.97	0.35	4.58	23,23,23,23	0
57	MG	YA	3252	1/1	0.90	0.46	4.55	16,16,16,16	0
57	MG	RA	3052	1/1	0.96	0.31	4.55	3,3,3,3	0
57	MG	RA	3058	1/1	0.87	0.37	4.33	9,9,9,9	0
57	MG	YA	3050	1/1	0.98	0.47	4.28	10,10,10,10	0
57	MG	QA	1647	1/1	0.82	0.56	4.21	29,29,29,29	0
57	MG	QA	1632	1/1	0.75	0.28	4.14	25,25,25,25	0
57	MG	RA	3035	1/1	0.97	0.38	4.05	1,1,1,1	0
57	MG	YA	3091	1/1	0.92	0.33	3.94	8,8,8,8	0
57	MG	YA	3036	1/1	0.96	0.24	3.82	7,7,7,7	0
57	MG	YA	3239	1/1	0.92	0.21	3.82	19,19,19,19	0
57	MG	RA	3012	1/1	0.98	0.49	3.72	7,7,7,7	0
57	MG	RA	3065	1/1	0.74	0.55	3.70	80,80,80,80	0
57	MG	RA	3099	1/1	0.89	0.25	3.68	6,6,6,6	0
57	MG	XA	1670	1/1	0.76	0.34	3.67	17,17,17,17	0
57	MG	YA	3096	1/1	0.97	0.55	3.63	2,2,2,2	0
57	MG	YA	3100	1/1	0.95	0.44	3.62	3,3,3,3	0
57	MG	RA	3101	1/1	0.71	0.21	3.61	32,32,32,32	0
57	MG	RA	3237	1/1	0.86	0.28	3.53	5,5,5,5	0
57	MG	YA	3013	1/1	0.98	0.41	3.52	1,1,1,1	0
57	MG	RA	3175	1/1	0.92	0.29	3.50	20,20,20,20	0
57	MG	YA	3005	1/1	0.95	0.24	3.41	68,68,68,68	0
57	MG	YA	3259	1/1	0.91	0.31	3.34	0,0,0,0	0
57	MG	YA	3206	1/1	0.95	0.25	3.16	25,25,25,25	0
57	MG	XA	1642	1/1	0.99	0.30	3.06	7,7,7,7	0
57	MG	RA	3225	1/1	0.75	0.32	3.05	18,18,18,18	0
57	MG	RA	3086	1/1	0.96	0.25	3.03	19,19,19,19	0
57	MG	YA	3034	1/1	0.91	0.36	2.98	4,4,4,4	0
57	MG	XA	1651	1/1	0.92	0.31	2.98	22,22,22,22	0
57	MG	YA	3218	1/1	0.89	0.19	2.97	2,2,2,2	0
57	MG	RP	202	1/1	0.44	0.52	2.94	65,65,65,65	0
57	MG	YA	3209	1/1	0.91	0.43	2.92	69,69,69,69	0
57	MG	YD	302	1/1	0.55	0.56	2.86	49,49,49,49	0
57	MG	XA	1611	1/1	0.97	0.37	2.76	3,3,3,3	0
57	MG	YA	3066	1/1	0.97	0.21	2.75	6,6,6,6	0
57	MG	YA	3041	1/1	0.87	0.38	2.73	10,10,10,10	0
58	PAR	XA	1671	42/42	0.91	0.26	2.66	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3112	1/1	0.93	0.22	2.55	11,11,11,11	0
57	MG	YA	3234	1/1	0.58	0.32	2.52	1,1,1,1	0
57	MG	RA	3022	1/1	0.94	0.27	2.40	1,1,1,1	0
57	MG	YA	3060	1/1	0.94	0.29	2.38	3,3,3,3	0
57	MG	QA	1660	1/1	0.92	0.25	2.26	26,26,26,26	0
57	MG	YA	3075	1/1	0.76	0.22	2.24	3,3,3,3	0
57	MG	YA	3027	1/1	0.99	0.25	2.22	3,3,3,3	0
57	MG	XA	1635	1/1	0.77	0.29	2.12	42,42,42,42	0
57	MG	YA	3016	1/1	0.98	0.27	2.06	2,2,2,2	0
57	MG	RA	3056	1/1	0.95	0.35	2.01	21,21,21,21	0
57	MG	YA	3186	1/1	0.89	0.27	1.83	4,4,4,4	0
57	MG	RA	3038	1/1	0.95	0.30	1.79	9,9,9,9	0
57	MG	YA	3080	1/1	0.92	0.26	1.78	9,9,9,9	0
57	MG	RA	3085	1/1	0.81	0.28	1.77	4,4,4,4	0
57	MG	XA	1618	1/1	0.96	0.24	1.76	26,26,26,26	0
57	MG	XA	1627	1/1	0.83	0.27	1.75	9,9,9,9	0
57	MG	YA	3172	1/1	0.88	0.21	1.67	41,41,41,41	0
57	MG	RA	3081	1/1	0.95	0.32	1.67	3,3,3,3	0
57	MG	XA	1644	1/1	0.96	0.17	1.62	3,3,3,3	0
57	MG	RA	3169	1/1	0.85	0.27	1.61	3,3,3,3	0
57	MG	XA	1658	1/1	0.93	0.21	1.58	0,0,0,0	0
57	MG	RA	3017	1/1	0.89	0.25	1.56	11,11,11,11	0
57	MG	RP	201	1/1	0.92	0.50	1.48	10,10,10,10	0
57	MG	YA	3038	1/1	0.97	0.22	1.46	5,5,5,5	0
57	MG	QA	1613	1/1	0.97	0.25	1.45	36,36,36,36	0
57	MG	RA	3027	1/1	0.96	0.25	1.39	4,4,4,4	0
57	MG	RA	3075	1/1	0.96	0.22	1.32	3,3,3,3	0
57	MG	YA	3024	1/1	0.95	0.29	1.28	17,17,17,17	0
57	MG	RA	3079	1/1	0.90	0.27	1.25	11,11,11,11	0
57	MG	YA	3057	1/1	0.96	0.27	1.23	27,27,27,27	0
57	MG	RA	3186	1/1	0.77	0.23	1.22	71,71,71,71	0
57	MG	RA	3057	1/1	0.93	0.27	1.19	8,8,8,8	0
57	MG	YA	3048	1/1	0.93	0.25	1.19	21,21,21,21	0
57	MG	YA	3079	1/1	0.91	0.28	1.19	22,22,22,22	0
57	MG	RA	3132	1/1	0.90	0.16	1.16	4,4,4,4	0
57	MG	RA	3045	1/1	0.94	0.18	1.13	23,23,23,23	0
57	MG	RA	3064	1/1	0.99	0.20	1.09	12,12,12,12	0
57	MG	RA	3177	1/1	0.82	0.21	1.02	3,3,3,3	0
57	MG	QA	1615	1/1	0.91	0.19	1.00	74,74,74,74	0
57	MG	YA	3168	1/1	0.96	0.23	0.93	18,18,18,18	0
57	MG	RA	3114	1/1	0.96	0.24	0.92	2,2,2,2	0
57	MG	RA	3206	1/1	0.94	0.26	0.91	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3068	1/1	0.94	0.22	0.89	68,68,68,68	0
57	MG	YA	3119	1/1	0.85	0.21	0.85	2,2,2,2	0
57	MG	YA	3238	1/1	0.77	0.19	0.82	11,11,11,11	0
57	MG	YA	3006	1/1	0.95	0.30	0.81	2,2,2,2	0
57	MG	RA	3106	1/1	0.98	0.23	0.78	3,3,3,3	0
58	PAR	QA	1666	42/42	0.92	0.23	0.76	58,58,58,58	0
57	MG	YA	3138	1/1	0.88	0.18	0.76	1,1,1,1	0
57	MG	XA	1617	1/1	0.89	0.28	0.74	2,2,2,2	0
57	MG	XA	1619	1/1	0.94	0.29	0.71	13,13,13,13	0
57	MG	YA	3059	1/1	0.99	0.25	0.57	3,3,3,3	0
57	MG	YA	3139	1/1	0.96	0.16	0.53	19,19,19,19	0
57	MG	QA	1612	1/1	0.84	0.25	0.43	5,5,5,5	0
57	MG	RA	3149	1/1	0.86	0.15	0.41	15,15,15,15	0
57	MG	RA	3241	1/1	0.97	0.32	0.40	29,29,29,29	0
57	MG	RA	3059	1/1	0.97	0.24	0.40	4,4,4,4	0
57	MG	YA	3212	1/1	0.95	0.14	0.39	17,17,17,17	0
57	MG	XA	1614	1/1	0.73	0.23	0.38	2,2,2,2	0
57	MG	RA	3104	1/1	0.91	0.19	0.37	5,5,5,5	0
57	MG	XA	1659	1/1	0.82	0.17	0.36	54,54,54,54	0
57	MG	RA	3164	1/1	0.97	0.16	0.36	34,34,34,34	0
57	MG	YA	3133	1/1	0.92	0.12	0.34	8,8,8,8	0
57	MG	QA	1626	1/1	0.72	0.21	0.32	10,10,10,10	0
57	MG	QA	1662	1/1	0.89	0.14	0.32	30,30,30,30	0
57	MG	RA	3159	1/1	0.93	0.18	0.29	0,0,0,0	0
57	MG	QA	1619	1/1	0.90	0.21	0.28	40,40,40,40	0
57	MG	RA	3195	1/1	0.88	0.27	0.23	8,8,8,8	0
57	MG	RB	201	1/1	0.84	0.19	0.23	30,30,30,30	0
57	MG	RE	302	1/1	0.97	0.27	0.20	10,10,10,10	0
57	MG	RA	3136	1/1	0.95	0.22	0.20	7,7,7,7	0
57	MG	RA	3135	1/1	0.95	0.17	0.09	7,7,7,7	0
57	MG	RA	3198	1/1	0.98	0.20	0.09	7,7,7,7	0
57	MG	YA	3042	1/1	0.97	0.23	0.08	2,2,2,2	0
57	MG	QA	1629	1/1	0.95	0.17	0.06	29,29,29,29	0
57	MG	YA	3113	1/1	0.98	0.19	0.02	2,2,2,2	0
57	MG	YA	3115	1/1	0.82	0.25	-0.00	31,31,31,31	0
57	MG	YA	3062	1/1	0.95	0.19	-0.06	5,5,5,5	0
57	MG	XV	101	1/1	0.97	0.22	-0.06	3,3,3,3	0
57	MG	XA	1636	1/1	0.98	0.19	-0.08	5,5,5,5	0
57	MG	RA	3087	1/1	0.94	0.22	-0.09	1,1,1,1	0
57	MG	XX	101	1/1	0.86	0.22	-0.09	11,11,11,11	0
57	MG	XA	1632	1/1	0.96	0.17	-0.10	36,36,36,36	0
57	MG	RA	3162	1/1	0.91	0.19	-0.10	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1621	1/1	0.97	0.22	-0.10	7,7,7,7	0
57	MG	RA	3207	1/1	0.95	0.20	-0.13	96,96,96,96	0
57	MG	YA	3187	1/1	0.82	0.12	-0.14	55,55,55,55	0
57	MG	RA	3150	1/1	0.93	0.17	-0.17	25,25,25,25	0
57	MG	RA	3131	1/1	0.93	0.21	-0.22	0,0,0,0	0
57	MG	RA	3042	1/1	0.98	0.19	-0.25	14,14,14,14	0
57	MG	RA	3074	1/1	0.91	0.17	-0.28	10,10,10,10	0
57	MG	RA	3072	1/1	0.98	0.18	-0.28	3,3,3,3	0
57	MG	XA	1622	1/1	0.98	0.21	-0.30	9,9,9,9	0
57	MG	XB	301	1/1	0.84	0.21	-0.34	26,26,26,26	0
59	ZN	XD	301	1/1	0.94	0.22	-0.50	5,5,5,5	0
57	MG	YA	3127	1/1	0.95	0.20	-0.51	11,11,11,11	0
57	MG	QA	1610	1/1	0.94	0.21	-0.53	3,3,3,3	0
57	MG	QA	1655	1/1	0.96	0.17	-0.55	6,6,6,6	0
57	MG	RA	3127	1/1	0.97	0.20	-0.61	10,10,10,10	0
57	MG	QA	1649	1/1	0.90	0.14	-0.61	2,2,2,2	0
57	MG	RA	3154	1/1	0.71	0.15	-0.64	17,17,17,17	0
57	MG	YA	3093	1/1	0.98	0.15	-0.66	8,8,8,8	0
57	MG	QA	1616	1/1	0.96	0.18	-0.68	10,10,10,10	0
57	MG	RA	3141	1/1	0.92	0.14	-0.69	3,3,3,3	0
57	MG	YA	3198	1/1	0.95	0.15	-0.70	16,16,16,16	0
57	MG	YA	3219	1/1	0.93	0.14	-0.74	17,17,17,17	0
57	MG	QA	1640	1/1	0.91	0.16	-0.79	46,46,46,46	0
59	ZN	XN	101	1/1	0.95	0.20	-0.81	82,82,82,82	0
59	ZN	QD	301	1/1	0.97	0.20	-0.82	21,21,21,21	0
57	MG	YA	3154	1/1	0.92	0.14	-0.85	8,8,8,8	0
57	MG	RA	3020	1/1	0.98	0.18	-0.87	5,5,5,5	0
57	MG	XA	1663	1/1	0.94	0.11	-0.95	29,29,29,29	0
57	MG	RA	3025	1/1	0.95	0.17	-0.95	66,66,66,66	0
57	MG	YA	3184	1/1	0.96	0.17	-0.97	51,51,51,51	0
57	MG	RA	3128	1/1	0.97	0.11	-1.00	2,2,2,2	0
57	MG	YA	3072	1/1	0.46	0.17	-1.05	7,7,7,7	0
57	MG	YA	3008	1/1	0.94	0.14	-1.06	1,1,1,1	0
57	MG	XA	1624	1/1	0.97	0.17	-1.10	23,23,23,23	0
57	MG	QA	1657	1/1	0.83	0.13	-1.10	65,65,65,65	0
57	MG	YP	201	1/1	0.93	0.14	-1.16	8,8,8,8	0
57	MG	XA	1657	1/1	0.97	0.15	-1.18	27,27,27,27	0
57	MG	RA	3218	1/1	0.75	0.14	-1.20	4,4,4,4	0
57	MG	XA	1668	1/1	0.92	0.14	-1.27	31,31,31,31	0
57	MG	YA	3262	1/1	0.97	0.15	-1.29	5,5,5,5	0
57	MG	RA	3014	1/1	0.92	0.15	-1.32	2,2,2,2	0
57	MG	RA	3111	1/1	0.96	0.12	-1.33	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YB	203	1/1	0.92	0.14	-1.35	33,33,33,33	0
57	MG	RA	3158	1/1	0.92	0.13	-1.42	12,12,12,12	0
57	MG	YA	3071	1/1	0.95	0.13	-1.49	40,40,40,40	0
57	MG	RF	301	1/1	0.78	0.20	-1.56	49,49,49,49	0
57	MG	XA	1647	1/1	0.89	0.12	-1.56	44,44,44,44	0
57	MG	YA	3180	1/1	0.97	0.13	-1.57	7,7,7,7	0
57	MG	YA	3191	1/1	0.89	0.12	-1.57	23,23,23,23	0
57	MG	YA	3216	1/1	0.95	0.16	-1.58	38,38,38,38	0
57	MG	RA	3160	1/1	0.88	0.15	-1.59	10,10,10,10	0
59	ZN	QN	101	1/1	0.78	0.12	-1.68	102,102,102,102	0
57	MG	YA	3144	1/1	0.93	0.13	-1.86	25,25,25,25	0
57	MG	YA	3083	1/1	0.91	0.14	-1.88	7,7,7,7	0
57	MG	XA	1649	1/1	0.94	0.13	-2.12	33,33,33,33	0
57	MG	XM	201	1/1	0.96	0.08	-2.13	26,26,26,26	0
57	MG	XA	1628	1/1	0.77	0.10	-2.17	28,28,28,28	0
57	MG	QM	201	1/1	0.97	0.10	-2.21	25,25,25,25	0
57	MG	QA	1636	1/1	0.98	0.12	-2.26	13,13,13,13	0
57	MG	XA	1612	1/1	0.97	0.13	-2.26	7,7,7,7	0
57	MG	XA	1610	1/1	0.98	0.10	-2.27	6,6,6,6	0
57	MG	YA	3166	1/1	0.98	0.13	-2.28	45,45,45,45	0
57	MG	YA	3114	1/1	0.92	0.15	-2.39	29,29,29,29	0
57	MG	RA	3183	1/1	0.98	0.13	-2.45	12,12,12,12	0
57	MG	RA	3122	1/1	0.93	0.08	-2.50	5,5,5,5	0
57	MG	QA	1606	1/1	0.96	0.12	-2.56	5,5,5,5	0
57	MG	XA	1637	1/1	0.89	0.10	-3.03	28,28,28,28	0
57	MG	YA	3169	1/1	0.94	0.11	-3.25	3,3,3,3	0
57	MG	YA	3179	1/1	0.98	0.05	-3.45	4,4,4,4	0
57	MG	QA	1650	1/1	0.95	0.11	-3.54	13,13,13,13	0
57	MG	YA	3130	1/1	0.99	0.08	-3.67	7,7,7,7	0
57	MG	YA	3136	1/1	0.95	0.09	-3.73	14,14,14,14	0
57	MG	QA	1644	1/1	0.90	0.07	-3.77	34,34,34,34	0
57	MG	RA	3115	1/1	0.98	0.10	-4.12	11,11,11,11	0
57	MG	QA	1609	1/1	0.98	0.06	-4.12	9,9,9,9	0
57	MG	YA	3255	1/1	0.99	0.13	-4.99	19,19,19,19	0
57	MG	YA	3015	1/1	0.84	0.11	-5.76	4,4,4,4	0
57	MG	QA	1604	1/1	0.95	0.16	-6.86	17,17,17,17	0
57	MG	RA	3110	1/1	0.89	0.64	-	12,12,12,12	0
57	MG	YA	3012	1/1	0.65	1.29	-	80,80,80,80	0
57	MG	YA	3078	1/1	0.93	0.44	-	0,0,0,0	0
57	MG	YA	3237	1/1	0.87	0.27	-	38,38,38,38	0
57	MG	YE	301	1/1	0.88	0.30	-	55,55,55,55	0
57	MG	XA	1660	1/1	0.80	0.57	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3151	1/1	0.98	0.28	-	10,10,10,10	0
57	MG	YA	3241	1/1	0.54	0.29	-	34,34,34,34	0
57	MG	YA	3140	1/1	0.96	0.22	-	8,8,8,8	0
57	MG	RA	3118	1/1	0.94	0.33	-	13,13,13,13	0
57	MG	YA	3244	1/1	0.95	0.10	-	0,0,0,0	0
57	MG	YA	3065	1/1	0.96	0.30	-	38,38,38,38	0
57	MG	YA	3067	1/1	0.89	0.60	-	5,5,5,5	0
57	MG	YA	3053	1/1	0.99	0.30	-	1,1,1,1	0
57	MG	RA	3007	1/1	0.86	0.64	-	26,26,26,26	0
57	MG	XA	1667	1/1	0.95	0.14	-	32,32,32,32	0
57	MG	YA	3156	1/1	0.81	0.22	-	6,6,6,6	0
57	MG	RA	3119	1/1	0.96	0.25	-	18,18,18,18	0
57	MG	RA	3006	1/1	0.78	1.49	-	80,80,80,80	0
57	MG	RA	3041	1/1	0.98	0.37	-	13,13,13,13	0
57	MG	RA	3125	1/1	0.85	0.25	-	37,37,37,37	0
57	MG	XA	1665	1/1	0.85	0.51	-	38,38,38,38	0
57	MG	YA	3018	1/1	0.91	0.75	-	80,80,80,80	0
57	MG	YA	3152	1/1	0.95	0.71	-	3,3,3,3	0
57	MG	YA	3167	1/1	0.71	0.33	-	49,49,49,49	0
57	MG	RA	3130	1/1	0.90	0.38	-	30,30,30,30	0
57	MG	YA	3045	1/1	0.79	0.36	-	20,20,20,20	0
57	MG	RA	3165	1/1	0.93	0.16	-	25,25,25,25	0
57	MG	QA	1661	1/1	0.79	0.62	-	9,9,9,9	0
57	MG	XA	1607	1/1	0.86	0.39	-	15,15,15,15	0
57	MG	YA	3046	1/1	0.95	0.45	-	0,0,0,0	0
57	MG	QA	1656	1/1	0.86	0.35	-	25,25,25,25	0
57	MG	YA	3122	1/1	0.77	0.36	-	8,8,8,8	0
57	MG	QA	1665	1/1	0.73	0.37	-	27,27,27,27	0
57	MG	RA	3053	1/1	0.98	0.32	-	4,4,4,4	0
57	MG	QA	1611	1/1	0.85	0.23	-	2,2,2,2	0
57	MG	RA	3217	1/1	0.73	0.23	-	18,18,18,18	0
57	MG	RA	3232	1/1	0.48	1.04	-	80,80,80,80	0
57	MG	QA	1602	1/1	0.87	0.49	-	9,9,9,9	0
57	MG	YA	3183	1/1	0.85	0.31	-	10,10,10,10	0
57	MG	YA	3157	1/1	0.91	0.46	-	18,18,18,18	0
57	MG	YA	3142	1/1	0.93	0.18	-	28,28,28,28	0
57	MG	RA	3090	1/1	0.96	0.45	-	3,3,3,3	0
57	MG	RA	3116	1/1	0.94	0.08	-	2,2,2,2	0
57	MG	YA	3223	1/1	0.78	0.40	-	27,27,27,27	0
57	MG	XA	1609	1/1	0.86	0.35	-	12,12,12,12	0
57	MG	YA	3188	1/1	0.95	0.13	-	4,4,4,4	0
57	MG	YA	3230	1/1	0.89	0.20	-	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1622	1/1	0.88	0.40	-	44,44,44,44	0
57	MG	RA	3201	1/1	0.88	0.41	-	1,1,1,1	0
57	MG	RA	3210	1/1	0.92	0.20	-	27,27,27,27	0
57	MG	RA	3230	1/1	0.75	0.35	-	2,2,2,2	0
57	MG	YA	3224	1/1	0.92	0.37	-	5,5,5,5	0
57	MG	XA	1641	1/1	0.91	0.27	-	2,2,2,2	0
57	MG	RA	3146	1/1	0.92	0.15	-	3,3,3,3	0
57	MG	YA	3266	1/1	0.96	0.35	-	1,1,1,1	0
57	MG	QA	1642	1/1	0.97	0.13	-	20,20,20,20	0
57	MG	RA	3142	1/1	0.98	0.10	-	28,28,28,28	0
57	MG	RE	301	1/1	0.92	0.20	-	18,18,18,18	0
57	MG	RA	3001	1/1	0.91	0.73	-	8,8,8,8	0
57	MG	YA	3250	1/1	0.93	0.51	-	6,6,6,6	0
57	MG	YA	3177	1/1	0.98	0.30	-	5,5,5,5	0
57	MG	YA	3253	1/1	0.89	0.49	-	5,5,5,5	0
57	MG	XA	1633	1/1	0.78	0.47	-	33,33,33,33	0
57	MG	RA	3123	1/1	0.95	0.22	-	24,24,24,24	0
57	MG	YA	3243	1/1	0.80	0.29	-	0,0,0,0	0
57	MG	RA	3103	1/1	0.98	0.19	-	1,1,1,1	0
57	MG	YA	3070	1/1	0.97	0.25	-	5,5,5,5	0
57	MG	YA	3258	1/1	0.68	1.75	-	80,80,80,80	0
57	MG	YA	3247	1/1	0.96	0.54	-	32,32,32,32	0
57	MG	YA	3260	1/1	0.94	0.29	-	2,2,2,2	0
57	MG	QA	1641	1/1	0.79	0.21	-	6,6,6,6	0
57	MG	QA	1601	1/1	0.82	0.32	-	12,12,12,12	0
57	MG	RA	3197	1/1	0.91	0.07	-	12,12,12,12	0
57	MG	YA	3143	1/1	0.91	0.26	-	10,10,10,10	0
57	MG	YA	3076	1/1	0.75	0.38	-	2,2,2,2	0
57	MG	YA	3204	1/1	0.95	0.15	-	23,23,23,23	0
57	MG	YA	3085	1/1	0.78	0.36	-	37,37,37,37	0
57	MG	YA	3146	1/1	0.91	0.32	-	4,4,4,4	0
57	MG	YB	201	1/1	0.82	0.43	-	48,48,48,48	0
57	MG	YA	3162	1/1	0.96	0.21	-	49,49,49,49	0
57	MG	QA	1635	1/1	0.96	0.18	-	8,8,8,8	0
57	MG	R5	101	1/1	0.84	0.21	-	33,33,33,33	0
57	MG	XA	1640	1/1	0.87	0.32	-	25,25,25,25	0
57	MG	QA	1648	1/1	0.88	0.34	-	30,30,30,30	0
57	MG	YA	3007	1/1	0.99	0.18	-	4,4,4,4	0
57	MG	RA	3066	1/1	0.95	0.53	-	8,8,8,8	0
57	MG	YA	3052	1/1	0.85	0.33	-	3,3,3,3	0
57	MG	YA	3245	1/1	0.91	0.33	-	3,3,3,3	0
57	MG	RA	3147	1/1	0.98	0.24	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3194	1/1	0.22	0.28	-	54,54,54,54	0
57	MG	RA	3216	1/1	0.43	0.81	-	39,39,39,39	0
57	MG	YA	3090	1/1	0.99	0.22	-	14,14,14,14	0
57	MG	YA	3099	1/1	0.89	0.28	-	2,2,2,2	0
57	MG	QA	1637	1/1	0.91	0.20	-	46,46,46,46	0
57	MG	YA	3236	1/1	0.68	0.16	-	24,24,24,24	0
57	MG	RA	3178	1/1	0.85	0.86	-	4,4,4,4	0
57	MG	XA	1661	1/1	0.85	0.52	-	32,32,32,32	0
57	MG	RA	3078	1/1	0.91	0.12	-	5,5,5,5	0
57	MG	YB	202	1/1	0.66	0.54	-	21,21,21,21	0
57	MG	RA	3166	1/1	0.89	0.23	-	20,20,20,20	0
57	MG	XA	1630	1/1	0.92	0.15	-	4,4,4,4	0
57	MG	YA	3228	1/1	0.93	0.26	-	9,9,9,9	0
57	MG	RA	3023	1/1	0.97	0.13	-	0,0,0,0	0
57	MG	RA	3182	1/1	0.80	0.45	-	23,23,23,23	0
57	MG	YA	3190	1/1	0.82	0.13	-	22,22,22,22	0
57	MG	YA	3021	1/1	0.96	0.46	-	15,15,15,15	0
57	MG	XA	1664	1/1	0.72	0.25	-	8,8,8,8	0
57	MG	YA	3265	1/1	0.94	0.45	-	1,1,1,1	0
57	MG	RA	3050	1/1	0.93	0.28	-	3,3,3,3	0
57	MG	YA	3151	1/1	0.95	0.09	-	26,26,26,26	0
57	MG	RA	3213	1/1	0.90	0.21	-	42,42,42,42	0
57	MG	RA	3043	1/1	0.96	0.23	-	6,6,6,6	0
57	MG	RA	3138	1/1	0.76	0.40	-	51,51,51,51	0
57	MG	YA	3017	1/1	0.93	0.45	-	8,8,8,8	0
57	MG	RA	3084	1/1	0.94	0.19	-	1,1,1,1	0
57	MG	YA	3087	1/1	0.98	0.38	-	8,8,8,8	0
57	MG	YA	3063	1/1	0.92	0.27	-	11,11,11,11	0
57	MG	YA	3118	1/1	0.92	0.36	-	63,63,63,63	0
57	MG	RA	3016	1/1	0.91	0.11	-	1,1,1,1	0
57	MG	XA	1648	1/1	0.63	0.41	-	28,28,28,28	0
57	MG	YA	3176	1/1	0.92	0.18	-	28,28,28,28	0
57	MG	YA	3175	1/1	0.85	0.28	-	43,43,43,43	0
57	MG	YA	3171	1/1	0.89	0.23	-	24,24,24,24	0
57	MG	XA	1621	1/1	0.97	0.12	-	23,23,23,23	0
57	MG	RA	3231	1/1	0.90	0.50	-	7,7,7,7	0
57	MG	YA	3217	1/1	0.88	0.21	-	14,14,14,14	0
57	MG	RA	3117	1/1	0.87	0.26	-	58,58,58,58	0
57	MG	YA	3213	1/1	0.98	0.29	-	17,17,17,17	0
57	MG	QA	1638	1/1	0.89	0.62	-	27,27,27,27	0
57	MG	RA	3108	1/1	0.90	0.31	-	3,3,3,3	0
57	MG	YA	3193	1/1	0.89	0.25	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3210	1/1	0.92	0.26	-	39,39,39,39	0
57	MG	YA	3227	1/1	0.98	0.24	-	0,0,0,0	0
57	MG	YA	3256	1/1	0.88	0.55	-	8,8,8,8	0
57	MG	YA	3107	1/1	0.85	0.32	-	22,22,22,22	0
57	MG	RA	3126	1/1	0.97	0.12	-	8,8,8,8	0
57	MG	YA	3120	1/1	0.96	0.38	-	0,0,0,0	0
57	MG	QA	1625	1/1	0.84	0.14	-	25,25,25,25	0
57	MG	YA	3135	1/1	0.93	0.23	-	1,1,1,1	0
57	MG	QA	1614	1/1	0.90	0.21	-	26,26,26,26	0
57	MG	YA	3097	1/1	0.86	0.34	-	11,11,11,11	0
57	MG	RA	3143	1/1	0.94	0.28	-	14,14,14,14	0
57	MG	RA	3187	1/1	0.96	0.14	-	10,10,10,10	0
57	MG	RA	3029	1/1	0.97	0.31	-	1,1,1,1	0
57	MG	YA	3077	1/1	0.94	0.43	-	3,3,3,3	0
57	MG	RA	3069	1/1	0.94	0.56	-	2,2,2,2	0
57	MG	RA	3144	1/1	0.93	0.30	-	2,2,2,2	0
57	MG	XA	1656	1/1	0.80	0.20	-	10,10,10,10	0
57	MG	YA	3001	1/1	0.98	0.53	-	0,0,0,0	0
57	MG	XA	1608	1/1	0.96	0.18	-	81,81,81,81	0
57	MG	YA	3129	1/1	0.94	0.27	-	0,0,0,0	0
57	MG	RA	3095	1/1	0.92	0.47	-	2,2,2,2	0
57	MG	YA	3089	1/1	0.79	0.54	-	4,4,4,4	0
57	MG	YA	3086	1/1	0.92	0.29	-	6,6,6,6	0
57	MG	RA	3157	1/1	0.97	0.26	-	1,1,1,1	0
57	MG	RA	3239	1/1	0.89	0.19	-	3,3,3,3	0
57	MG	RA	3005	1/1	0.94	0.34	-	6,6,6,6	0
57	MG	RA	3171	1/1	0.92	0.21	-	15,15,15,15	0
57	MG	RA	3228	1/1	0.88	0.23	-	43,43,43,43	0
57	MG	YA	3159	1/1	0.96	0.34	-	12,12,12,12	0
57	MG	RA	3242	1/1	0.62	0.36	-	7,7,7,7	0
57	MG	QA	1631	1/1	0.82	0.35	-	15,15,15,15	0
57	MG	RA	3234	1/1	0.78	0.50	-	7,7,7,7	0
57	MG	RA	3018	1/1	0.91	0.72	-	8,8,8,8	0
57	MG	YA	3051	1/1	0.98	0.26	-	3,3,3,3	0
57	MG	YA	3026	1/1	0.83	0.51	-	32,32,32,32	0
57	MG	RA	3003	1/1	0.91	0.36	-	4,4,4,4	0
57	MG	YA	3148	1/1	0.94	0.14	-	42,42,42,42	0
57	MG	RA	3048	1/1	0.83	0.24	-	20,20,20,20	0
57	MG	YA	3231	1/1	0.95	0.15	-	2,2,2,2	0
57	MG	YA	3222	1/1	0.88	0.29	-	3,3,3,3	0
57	MG	YA	3199	1/1	0.84	0.51	-	60,60,60,60	0
57	MG	YA	3125	1/1	0.87	0.21	-	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1615	1/1	0.94	0.41	-	2,2,2,2	0
57	MG	R8	101	1/1	0.85	0.29	-	19,19,19,19	0
57	MG	QA	1607	1/1	0.95	0.16	-	5,5,5,5	0
57	MG	YA	3022	1/1	0.98	0.23	-	2,2,2,2	0
57	MG	YA	3121	1/1	0.95	0.38	-	9,9,9,9	0
57	MG	RA	3192	1/1	0.73	0.17	-	0,0,0,0	0
57	MG	RA	3100	1/1	0.95	0.55	-	36,36,36,36	0
57	MG	QA	1654	1/1	0.93	0.10	-	55,55,55,55	0
57	MG	YA	3189	1/1	0.95	0.36	-	0,0,0,0	0
57	MG	RA	3152	1/1	0.93	0.17	-	3,3,3,3	0
57	MG	RA	3112	1/1	0.97	0.27	-	5,5,5,5	0
57	MG	YA	3104	1/1	0.89	0.10	-	3,3,3,3	0
57	MG	RA	3032	1/1	0.89	1.58	-	80,80,80,80	0
57	MG	RA	3039	1/1	0.93	0.21	-	2,2,2,2	0
57	MG	YA	3249	1/1	0.92	0.36	-	3,3,3,3	0
57	MG	XA	1616	1/1	0.93	0.22	-	10,10,10,10	0
57	MG	RA	3080	1/1	0.99	0.26	-	2,2,2,2	0
57	MG	QA	1630	1/1	0.75	0.45	-	54,54,54,54	0
57	MG	RA	3205	1/1	0.84	0.28	-	7,7,7,7	0
57	MG	QA	1628	1/1	0.85	0.54	-	62,62,62,62	0
57	MG	YA	3131	1/1	0.90	0.17	-	7,7,7,7	0
57	MG	XA	1605	1/1	0.59	0.65	-	18,18,18,18	0
57	MG	YA	3267	1/1	0.84	0.47	-	19,19,19,19	0
57	MG	RA	3203	1/1	0.85	0.42	-	30,30,30,30	0
57	MG	YA	3208	1/1	0.76	0.16	-	43,43,43,43	0
57	MG	RA	3073	1/1	0.97	0.28	-	37,37,37,37	0
57	MG	RA	3208	1/1	0.78	0.40	-	29,29,29,29	0
57	MG	RA	3236	1/1	0.88	0.59	-	4,4,4,4	0
57	MG	YA	3068	1/1	0.98	0.23	-	3,3,3,3	0
57	MG	RA	3140	1/1	0.93	0.29	-	17,17,17,17	0
57	MG	RA	3235	1/1	0.87	0.16	-	11,11,11,11	0
57	MG	RA	3172	1/1	0.90	0.14	-	4,4,4,4	0
57	MG	RA	3030	1/1	0.98	0.40	-	2,2,2,2	0
57	MG	RA	3060	1/1	0.98	0.41	-	65,65,65,65	0
57	MG	RA	3010	1/1	0.89	0.51	-	4,4,4,4	0
57	MG	YA	3153	1/1	0.91	0.51	-	21,21,21,21	0
57	MG	YA	3030	1/1	0.87	0.37	-	6,6,6,6	0
57	MG	RA	3096	1/1	0.96	0.44	-	2,2,2,2	0
57	MG	XA	1623	1/1	0.93	0.33	-	4,4,4,4	0
57	MG	QA	1623	1/1	0.56	0.86	-	41,41,41,41	0
57	MG	RA	3067	1/1	0.81	0.24	-	57,57,57,57	0
57	MG	QA	1652	1/1	0.95	0.18	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3188	1/1	0.90	0.16	-	11,11,11,11	0
57	MG	YA	3164	1/1	0.83	0.26	-	8,8,8,8	0
57	MG	QA	1605	1/1	0.93	0.49	-	5,5,5,5	0
57	MG	QA	1646	1/1	0.96	0.20	-	36,36,36,36	0
57	MG	YA	3202	1/1	0.88	0.30	-	4,4,4,4	0
57	MG	QA	1608	1/1	0.98	0.09	-	11,11,11,11	0
57	MG	YA	3158	1/1	0.95	0.26	-	23,23,23,23	0
57	MG	RA	3153	1/1	0.83	0.19	-	24,24,24,24	0
57	MG	RA	3044	1/1	0.93	0.36	-	2,2,2,2	0
57	MG	XA	1606	1/1	0.72	0.53	-	29,29,29,29	0
57	MG	YA	3040	1/1	0.96	0.61	-	0,0,0,0	0
57	MG	RA	3220	1/1	0.61	0.53	-	1,1,1,1	0
57	MG	YA	3134	1/1	0.89	0.20	-	11,11,11,11	0
57	MG	RA	3214	1/1	0.96	0.22	-	12,12,12,12	0
57	MG	RA	3190	1/1	0.83	0.37	-	8,8,8,8	0
57	MG	QA	1663	1/1	0.93	0.07	-	33,33,33,33	0
57	MG	XA	1631	1/1	0.94	0.33	-	0,0,0,0	0
57	MG	RA	3200	1/1	0.94	0.39	-	4,4,4,4	0
57	MG	QA	1639	1/1	0.90	0.16	-	18,18,18,18	0
57	MG	QA	1653	1/1	0.98	0.24	-	16,16,16,16	0
57	MG	RA	3185	1/1	0.96	0.18	-	16,16,16,16	0
57	MG	RA	3093	1/1	0.97	0.21	-	1,1,1,1	0
57	MG	RB	202	1/1	0.95	0.19	-	2,2,2,2	0
57	MG	RA	3051	1/1	0.94	0.45	-	3,3,3,3	0
57	MG	XA	1629	1/1	0.91	0.19	-	3,3,3,3	0
57	MG	RA	3202	1/1	0.92	0.22	-	9,9,9,9	0
57	MG	RA	3211	1/1	0.97	0.09	-	6,6,6,6	0
57	MG	YA	3192	1/1	0.90	0.10	-	6,6,6,6	0
57	MG	YA	3205	1/1	0.78	0.37	-	38,38,38,38	0
57	MG	RA	3129	1/1	0.82	0.24	-	21,21,21,21	0
57	MG	XA	1650	1/1	0.98	0.09	-	27,27,27,27	0
57	MG	YA	3064	1/1	0.81	0.25	-	4,4,4,4	0
57	MG	RA	3199	1/1	0.84	0.44	-	60,60,60,60	0
57	MG	YA	3126	1/1	0.97	0.37	-	5,5,5,5	0
57	MG	YA	3195	1/1	0.95	0.11	-	0,0,0,0	0
57	MG	RA	3219	1/1	0.91	0.11	-	4,4,4,4	0
57	MG	RA	3212	1/1	0.87	0.52	-	10,10,10,10	0
57	MG	YA	3165	1/1	0.94	0.31	-	7,7,7,7	0
57	MG	QA	1627	1/1	0.77	0.27	-	22,22,22,22	0
57	MG	QA	1645	1/1	0.84	0.11	-	5,5,5,5	0
57	MG	RA	3180	1/1	0.76	0.52	-	21,21,21,21	0
57	MG	RA	3083	1/1	0.95	0.27	-	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3011	1/1	0.98	0.18	-	5,5,5,5	0
57	MG	QA	1620	1/1	0.92	0.16	-	22,22,22,22	0
57	MG	RA	3070	1/1	0.90	0.33	-	6,6,6,6	0
57	MG	R0	101	1/1	0.03	0.77	-	29,29,29,29	0
57	MG	YA	3221	1/1	0.98	0.29	-	42,42,42,42	0
57	MG	YA	3178	1/1	0.97	0.37	-	2,2,2,2	0
57	MG	RA	3134	1/1	0.65	0.46	-	24,24,24,24	0
57	MG	RA	3105	1/1	0.96	0.18	-	6,6,6,6	0
57	MG	QA	1643	1/1	0.94	0.10	-	1,1,1,1	0
57	MG	QA	1659	1/1	0.94	0.24	-	11,11,11,11	0
57	MG	YA	3044	1/1	0.95	0.16	-	75,75,75,75	0
57	MG	XA	1653	1/1	0.88	0.39	-	13,13,13,13	0
57	MG	RA	3238	1/1	0.92	0.48	-	7,7,7,7	0
57	MG	RA	3137	1/1	0.95	0.34	-	2,2,2,2	0
57	MG	RA	3145	1/1	0.92	0.23	-	5,5,5,5	0
57	MG	YA	3020	1/1	0.97	0.28	-	12,12,12,12	0
57	MG	RA	3204	1/1	0.84	0.20	-	33,33,33,33	0
57	MG	RA	3076	1/1	0.96	0.38	-	13,13,13,13	0
57	MG	YA	3056	1/1	0.93	0.23	-	0,0,0,0	0
57	MG	RA	3223	1/1	0.92	0.17	-	11,11,11,11	0
57	MG	YA	3242	1/1	0.97	0.14	-	7,7,7,7	0
57	MG	YA	3117	1/1	0.94	0.30	-	11,11,11,11	0
57	MG	YA	3220	1/1	0.95	0.29	-	2,2,2,2	0
57	MG	QA	1664	1/1	0.87	0.14	-	24,24,24,24	0
57	MG	YA	3211	1/1	0.97	0.18	-	1,1,1,1	0
57	MG	RA	3221	1/1	0.70	0.76	-	15,15,15,15	0
57	MG	QA	1651	1/1	0.93	0.29	-	6,6,6,6	0
57	MG	YA	3225	1/1	0.91	0.39	-	34,34,34,34	0
57	MG	XA	1645	1/1	0.94	0.31	-	2,2,2,2	0
57	MG	RA	3189	1/1	0.67	0.42	-	55,55,55,55	0
57	MG	RA	3233	1/1	0.88	0.17	-	17,17,17,17	0
57	MG	YA	3251	1/1	0.86	0.52	-	6,6,6,6	0
57	MG	YA	3019	1/1	0.91	0.70	-	10,10,10,10	0
57	MG	YA	3094	1/1	0.96	0.28	-	0,0,0,0	0
57	MG	QA	1634	1/1	0.83	0.46	-	6,6,6,6	0
57	MG	RA	3193	1/1	0.90	0.18	-	17,17,17,17	0
57	MG	RA	3167	1/1	0.95	0.23	-	6,6,6,6	0
57	MG	QA	1633	1/1	0.91	0.28	-	35,35,35,35	0
57	MG	YA	3163	1/1	0.73	0.24	-	41,41,41,41	0
57	MG	YA	3003	1/1	0.97	0.19	-	9,9,9,9	0
57	MG	YA	3032	1/1	0.92	0.49	-	8,8,8,8	0
57	MG	YA	3105	1/1	0.98	0.49	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3061	1/1	0.90	0.15	-	32,32,32,32	0
57	MG	YA	3061	1/1	0.98	0.31	-	2,2,2,2	0
57	MG	YA	3197	1/1	0.91	0.36	-	1,1,1,1	0
57	MG	YA	3039	1/1	0.98	0.18	-	0,0,0,0	0
57	MG	RA	3071	1/1	0.95	0.57	-	23,23,23,23	0
57	MG	RA	3113	1/1	0.84	0.41	-	3,3,3,3	0
57	MG	XA	1601	1/1	0.92	1.45	-	80,80,80,80	0
57	MG	RA	3148	1/1	0.96	0.18	-	39,39,39,39	0
57	MG	YA	3028	1/1	0.97	0.27	-	1,1,1,1	0
57	MG	XA	1646	1/1	0.84	0.24	-	6,6,6,6	0
57	MG	YA	3215	1/1	0.98	0.14	-	25,25,25,25	0
57	MG	RA	3037	1/1	0.97	0.15	-	15,15,15,15	0
57	MG	RA	3176	1/1	0.94	0.36	-	14,14,14,14	0
57	MG	XA	1613	1/1	0.99	0.08	-	0,0,0,0	0
57	MG	YA	3149	1/1	0.88	0.22	-	17,17,17,17	0
57	MG	QF	201	1/1	0.90	0.39	-	1,1,1,1	0
57	MG	YA	3074	1/1	0.98	0.29	-	0,0,0,0	0
57	MG	YA	3132	1/1	0.92	0.09	-	31,31,31,31	0
57	MG	RA	3013	1/1	0.91	0.50	-	5,5,5,5	0
57	MG	YA	3082	1/1	0.88	0.51	-	0,0,0,0	0
57	MG	RA	3092	1/1	0.96	0.34	-	1,1,1,1	0
57	MG	YA	3098	1/1	0.94	0.18	-	2,2,2,2	0
57	MG	QA	1624	1/1	0.86	0.46	-	49,49,49,49	0
57	MG	XA	1655	1/1	0.68	0.70	-	40,40,40,40	0
57	MG	RA	3155	1/1	0.92	0.27	-	24,24,24,24	0
57	MG	YA	3014	1/1	0.94	0.41	-	2,2,2,2	0
57	MG	RA	3227	1/1	0.86	0.26	-	16,16,16,16	0
57	MG	YA	3123	1/1	0.92	0.24	-	24,24,24,24	0
57	MG	XA	1626	1/1	0.76	0.33	-	11,11,11,11	0
57	MG	YA	3150	1/1	0.87	0.22	-	11,11,11,11	0
57	MG	YA	3128	1/1	0.53	0.68	-	25,25,25,25	0
57	MG	XA	1666	1/1	0.94	0.15	-	16,16,16,16	0
57	MG	YA	3160	1/1	0.78	0.74	-	51,51,51,51	0
57	MG	YA	3226	1/1	0.93	0.50	-	4,4,4,4	0
57	MG	RA	3181	1/1	0.83	0.60	-	28,28,28,28	0
57	MG	RA	3040	1/1	0.98	0.31	-	11,11,11,11	0
57	MG	RA	3196	1/1	0.92	0.30	-	8,8,8,8	0
57	MG	RA	3173	1/1	0.93	0.33	-	54,54,54,54	0
57	MG	YA	3185	1/1	0.49	0.36	-	14,14,14,14	0
57	MG	RA	3055	1/1	0.96	0.49	-	1,1,1,1	0
57	MG	RA	3102	1/1	0.97	0.09	-	4,4,4,4	0
57	MG	RA	3215	1/1	0.96	0.18	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3174	1/1	0.62	0.41	-	47,47,47,47	0
57	MG	RA	3091	1/1	0.97	0.30	-	1,1,1,1	0
57	MG	RA	3082	1/1	0.97	0.39	-	18,18,18,18	0
57	MG	YA	3004	1/1	0.99	0.33	-	18,18,18,18	0
57	MG	YA	3200	1/1	0.93	0.42	-	10,10,10,10	0
57	MG	YA	3055	1/1	0.92	0.39	-	4,4,4,4	0
57	MG	Y0	101	1/1	0.91	0.26	-	3,3,3,3	0
57	MG	QA	1603	1/1	0.82	1.09	-	27,27,27,27	0
57	MG	XA	1638	1/1	0.91	0.18	-	37,37,37,37	0
57	MG	RA	3168	1/1	0.84	0.78	-	55,55,55,55	0
57	MG	RA	3240	1/1	0.87	0.32	-	2,2,2,2	0
57	MG	XA	1639	1/1	0.86	0.25	-	13,13,13,13	0
57	MG	RA	3163	1/1	0.77	0.91	-	13,13,13,13	0
57	MG	YA	3029	1/1	0.97	0.19	-	0,0,0,0	0
57	MG	YA	3111	1/1	0.95	0.22	-	19,19,19,19	0
57	MG	YA	3233	1/1	0.90	0.39	-	68,68,68,68	0
57	MG	RA	3226	1/1	0.83	0.24	-	26,26,26,26	0
57	MG	YA	3232	1/1	0.98	0.33	-	5,5,5,5	0
57	MG	YA	3137	1/1	0.95	0.14	-	2,2,2,2	0
57	MG	RA	3046	1/1	0.94	0.41	-	1,1,1,1	0
57	MG	YA	3196	1/1	0.94	0.69	-	6,6,6,6	0
57	MG	RA	3139	1/1	0.96	0.25	-	12,12,12,12	0
57	MG	YA	3181	1/1	0.97	0.19	-	4,4,4,4	0
57	MG	YA	3214	1/1	0.97	0.12	-	7,7,7,7	0
57	MG	YA	3103	1/1	0.95	1.26	-	80,80,80,80	0
57	MG	RA	3107	1/1	0.98	0.08	-	3,3,3,3	0
57	MG	RA	3133	1/1	0.91	0.18	-	33,33,33,33	0
57	MG	XA	1652	1/1	0.95	0.13	-	1,1,1,1	0
57	MG	RA	3028	1/1	0.96	0.19	-	2,2,2,2	0
57	MG	YA	3203	1/1	0.85	0.33	-	21,21,21,21	0
57	MG	YA	3084	1/1	0.98	0.46	-	17,17,17,17	0
57	MG	YA	3194	1/1	0.96	0.25	-	13,13,13,13	0
57	MG	YA	3054	1/1	0.66	0.83	-	80,80,80,80	0
57	MG	YA	3147	1/1	0.87	0.61	-	27,27,27,27	0
57	MG	RA	3229	1/1	0.83	0.33	-	9,9,9,9	0
57	MG	XA	1602	1/1	0.97	0.30	-	2,2,2,2	0
57	MG	RA	3191	1/1	0.84	0.16	-	26,26,26,26	0
57	MG	YA	3010	1/1	0.95	0.35	-	0,0,0,0	0
57	MG	YA	3201	1/1	0.70	0.39	-	2,2,2,2	0
57	MG	YA	3246	1/1	0.72	0.21	-	7,7,7,7	0
57	MG	QA	1618	1/1	0.71	0.43	-	49,49,49,49	0
57	MG	RA	3109	1/1	0.89	0.42	-	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.