



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 05:44 PM EST

PDB ID : 4P70
Title : Crystal Structure of Unmodified tRNA Proline (CGG) Bound to Codon CCG on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : unknown
Resolution : 3.68 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

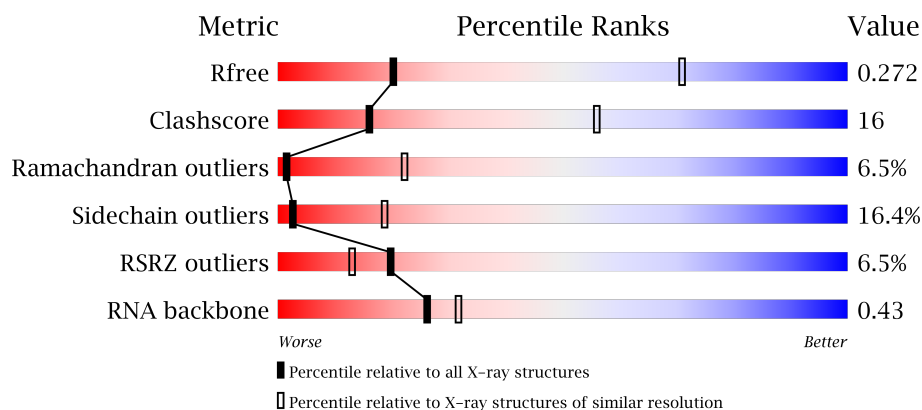
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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}	100719	1161 (3.86-3.50)
Clashscore	112137	1295 (3.86-3.50)
Ramachandran outliers	110173	1245 (3.86-3.50)
Sidechain outliers	110143	1242 (3.86-3.50)
RSRZ outliers	101464	1188 (3.86-3.50)
RNA backbone	2435	1005 (4.46-2.90)

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>5%</div> <div> <div></div> <div>35%</div> <div>47%</div> <div>14%</div> <div>..</div> </div> </div>
1	XA	1522	<div> <div>5%</div> <div> <div></div> <div>33%</div> <div>48%</div> <div>15%</div> <div>..</div> </div> </div>
2	QB	256	<div> <div>4%</div> <div> <div></div> <div>49%</div> <div>36%</div> <div>7%</div> <div>7%</div> </div> </div>
2	XB	256	<div> <div></div> <div> <div></div> <div>46%</div> <div>36%</div> <div>9%</div> <div>7%</div> </div> </div>



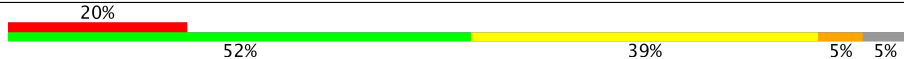
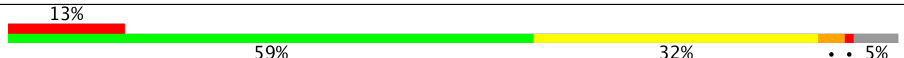
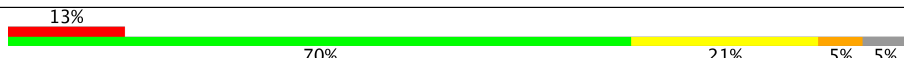

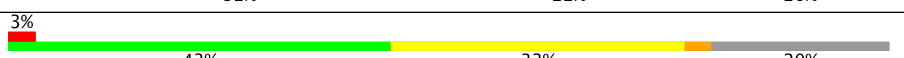
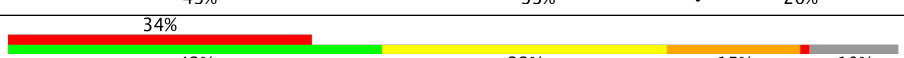
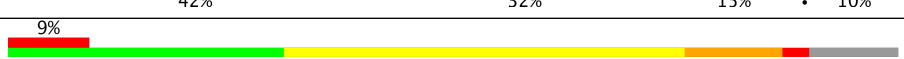
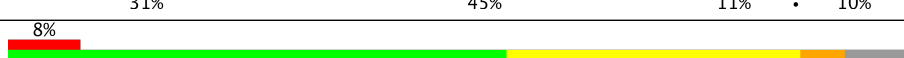
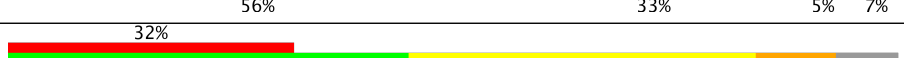




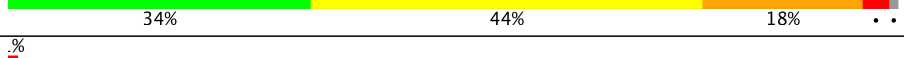
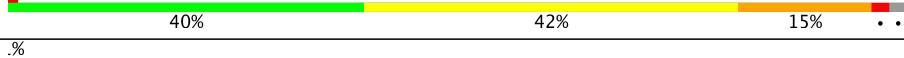
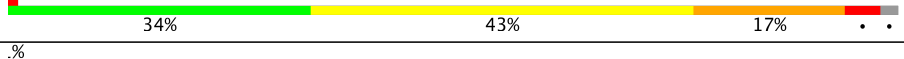

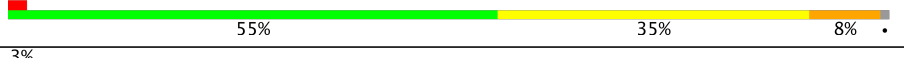

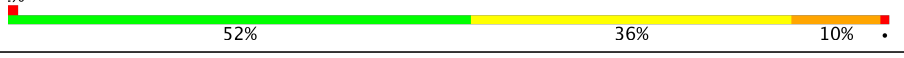



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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
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	RA	2916	
22	YA	2916	
23	RB	122	
23	YB	122	
24	RD	276	
24	YD	276	
25	RE	206	
25	YE	206	
26	RF	210	
26	YF	210	
27	RG	182	
27	YG	182	

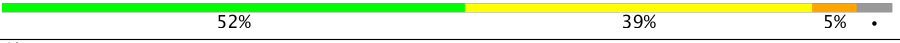
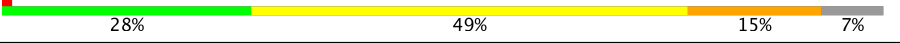
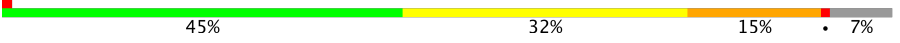
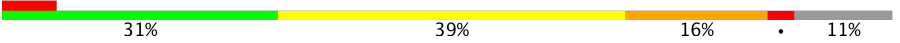
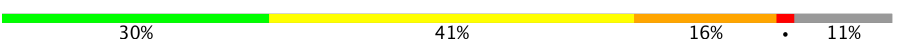

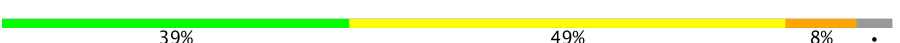



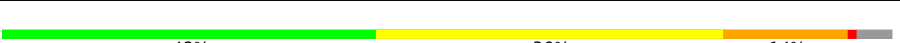
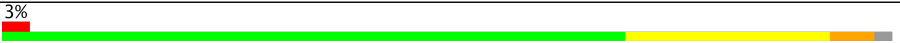

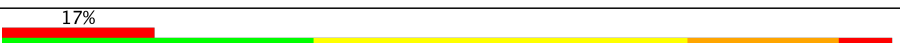
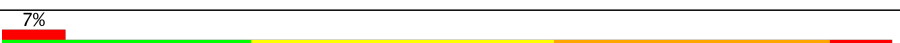

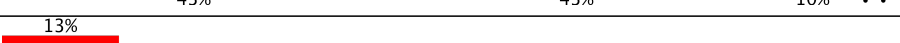


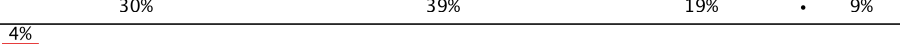

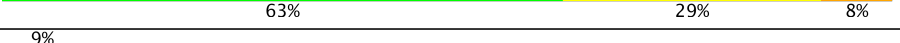

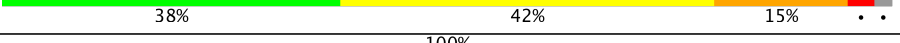
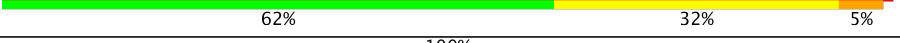
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Mol	Chain	Length	Quality of chain
28	RH	180	
28	YH	180	
29	RI	148	
29	YI	148	
30	RN	140	
30	YN	140	
31	RO	122	
31	YO	122	
32	RP	150	
32	YP	150	
33	RQ	141	
33	YQ	141	
34	RR	118	
34	YR	118	
35	RS	112	
35	YS	112	
36	RT	146	
36	YT	146	
37	RU	118	
37	YU	118	
38	RV	101	
38	YV	101	
39	RW	113	
39	YW	113	
40	RX	96	

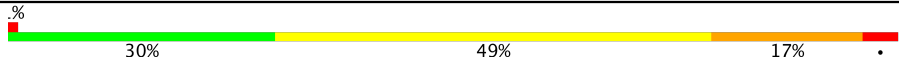




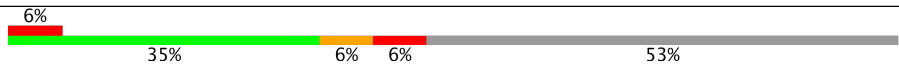


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Mol	Chain	Length	Quality of chain
40	YX	96	
41	RY	110	
41	YY	110	
42	RZ	206	
42	YZ	206	
43	R0	85	
43	Y0	85	
44	R1	98	
44	Y1	98	
45	R2	72	
45	Y2	72	
46	R3	60	
46	Y3	60	
47	R4	71	
47	Y4	71	
48	R5	60	
48	Y5	60	
49	R6	54	
49	Y6	54	
50	R7	49	
50	Y7	49	
51	R8	65	
51	Y8	65	
52	R9	37	
52	Y9	37	

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Mol	Chain	Length	Quality of chain
53	QV	77	
53	XV	77	
54	QX	25	
54	XX	25	
55	QY	17	
55	XY	17	
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	PAR	QA	1601	-	-	-	X
57	PAR	XA	1601	-	-	-	X
58	MG	QA	1634	-	-	-	X
58	MG	RA	3007	-	-	-	X
58	MG	RA	3009	-	-	-	X
58	MG	RA	3033	-	-	-	X
58	MG	RA	3036	-	-	-	X
58	MG	RA	3039	-	-	-	X
58	MG	RA	3067	-	-	-	X
58	MG	RA	3080	-	-	-	X
58	MG	RA	3093	-	-	-	X
58	MG	RA	3094	-	-	-	X
58	MG	RA	3096	-	-	-	X
58	MG	RA	3102	-	-	-	X
58	MG	RA	3125	-	-	-	X
58	MG	RA	3138	-	-	-	X
58	MG	RA	3141	-	-	-	X
58	MG	RA	3142	-	-	-	X
58	MG	RA	3144	-	-	-	X
58	MG	RA	3151	-	-	-	X
58	MG	RA	3164	-	-	-	X
58	MG	RA	3169	-	-	-	X
58	MG	RA	3175	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	RA	3183	-	-	-	X
58	MG	RA	3188	-	-	-	X
58	MG	RA	3196	-	-	-	X
58	MG	RA	3225	-	-	-	X
58	MG	RA	3227	-	-	-	X
58	MG	RA	3229	-	-	-	X
58	MG	RA	3235	-	-	-	X
58	MG	RP	201	-	-	-	X
58	MG	RP	202	-	-	-	X
58	MG	XA	1620	-	-	-	X
58	MG	XA	1666	-	-	-	X
58	MG	XA	1671	-	-	-	X
58	MG	XA	1675	-	-	-	X
58	MG	Y0	101	-	-	-	X
58	MG	YA	3003	-	-	-	X
58	MG	YA	3010	-	-	-	X
58	MG	YA	3014	-	-	-	X
58	MG	YA	3015	-	-	-	X
58	MG	YA	3035	-	-	-	X
58	MG	YA	3038	-	-	-	X
58	MG	YA	3047	-	-	-	X
58	MG	YA	3049	-	-	-	X
58	MG	YA	3080	-	-	-	X
58	MG	YA	3090	-	-	-	X
58	MG	YA	3099	-	-	-	X
58	MG	YA	3140	-	-	-	X
58	MG	YA	3142	-	-	-	X
58	MG	YA	3154	-	-	-	X
58	MG	YA	3161	-	-	-	X
58	MG	YA	3164	-	-	-	X
58	MG	YA	3165	-	-	-	X
58	MG	YA	3170	-	-	-	X
58	MG	YA	3180	-	-	-	X
58	MG	YA	3184	-	-	-	X
58	MG	YA	3197	-	-	-	X
58	MG	YA	3199	-	-	-	X
58	MG	YA	3204	-	-	-	X
58	MG	YA	3205	-	-	-	X
58	MG	YA	3206	-	-	-	X
58	MG	YA	3207	-	-	-	X
58	MG	YA	3216	-	-	-	X
58	MG	YA	3218	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	YA	3227	-	-	-	X
58	MG	YA	3237	-	-	-	X
58	MG	YA	3255	-	-	-	X
58	MG	YA	3258	-	-	-	X
58	MG	YA	3260	-	-	-	X
58	MG	YA	3261	-	-	-	X
58	MG	YD	301	-	-	-	X
58	MG	YP	201	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291730 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 type Z.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
22	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called 50S ribosomal protein L16.

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

- Molecule 34 is a protein called 50S ribosomal protein L17.

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

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

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

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L31.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a RNA chain called P-site tRNA fMET.

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

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	QX	8	Total 173	C 77	N 33	O 55	P 8	0	0	0
54	XX	8	Total 173	C 77	N 33	O 55	P 8	0	0	0

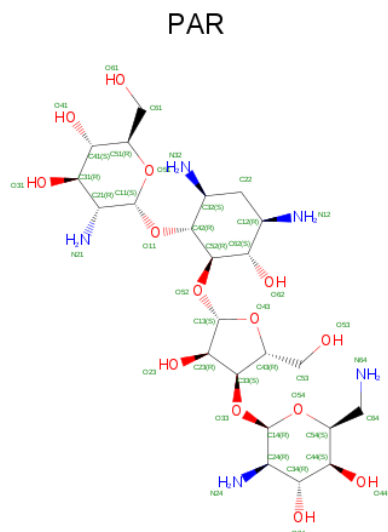
- Molecule 55 is a RNA chain called A site ASL of tRNA-Proline CGG (unmodified).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	QY	8	Total 174	C 77	N 33	O 56	P 8	0	0	0
55	XY	8	Total 174	C 77	N 33	O 56	P 8	0	0	0

- Molecule 56 is a RNA chain called tRNA acceptor end mimic.

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

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	QA	76	Total 76	Mg 76	0	0
58	RP	2	Total 2	Mg 2	0	0
58	YA	265	Total 265	Mg 265	0	0
58	QM	1	Total 1	Mg 1	0	0
58	YD	2	Total 2	Mg 2	0	0
58	QV	1	Total 1	Mg 1	0	0
58	XA	82	Total 82	Mg 82	0	0
58	R0	1	Total 1	Mg 1	0	0
58	Y0	1	Total 1	Mg 1	0	0
58	YQ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	R8	2	Total 2	Mg 2	0	0
58	YX	1	Total 1	Mg 1	0	0
58	RD	1	Total 1	Mg 1	0	0
58	XB	1	Total 1	Mg 1	0	0
58	QF	1	Total 1	Mg 1	0	0
58	R5	1	Total 1	Mg 1	0	0
58	RA	247	Total 247	Mg 247	0	0
58	YP	2	Total 2	Mg 2	0	0
58	Y5	1	Total 1	Mg 1	0	0
58	RE	2	Total 2	Mg 2	0	0
58	YB	3	Total 3	Mg 3	0	0
58	XV	2	Total 2	Mg 2	0	0
58	RB	2	Total 2	Mg 2	0	0
58	RF	1	Total 1	Mg 1	0	0
58	XM	1	Total 1	Mg 1	0	0

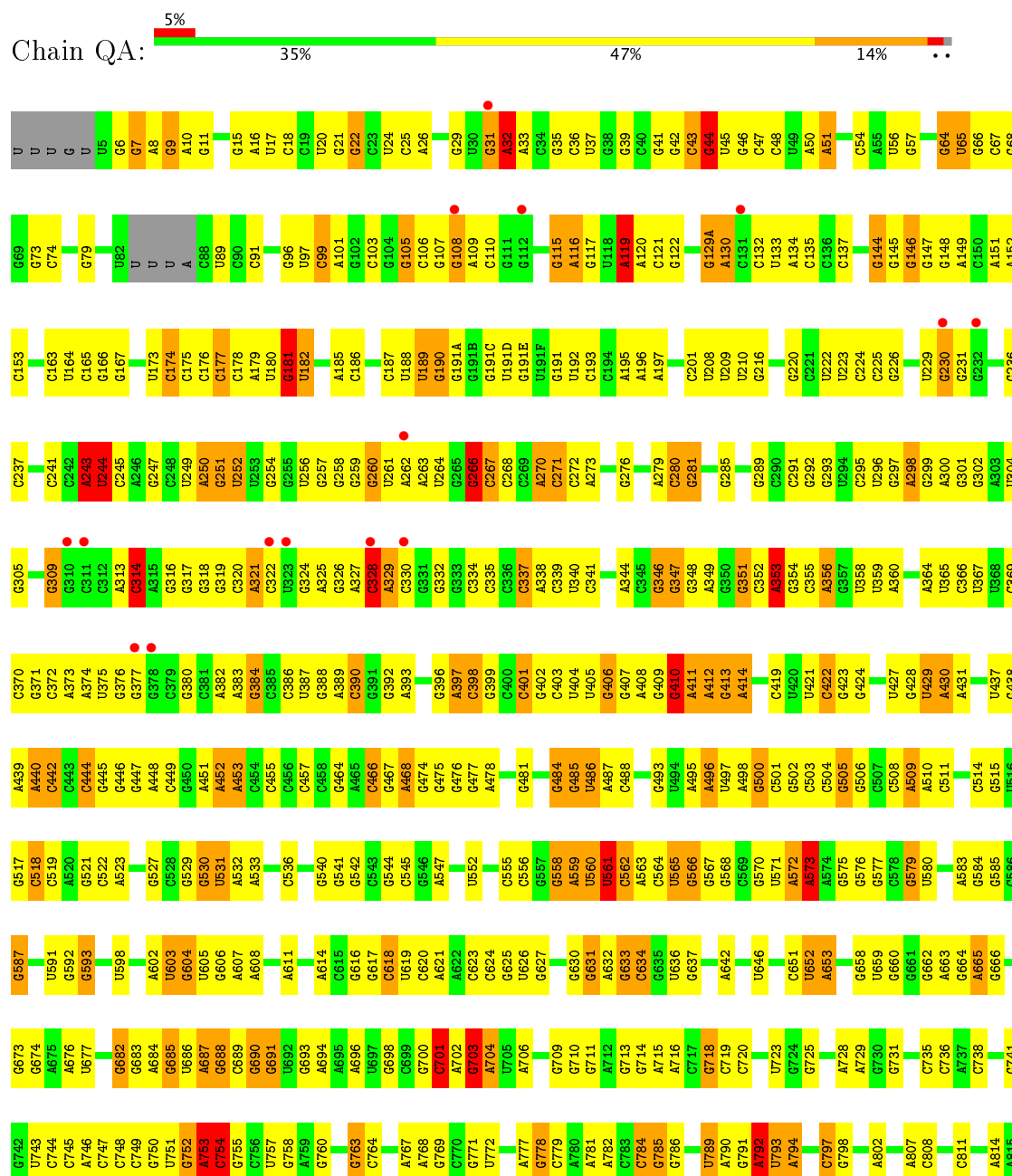
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

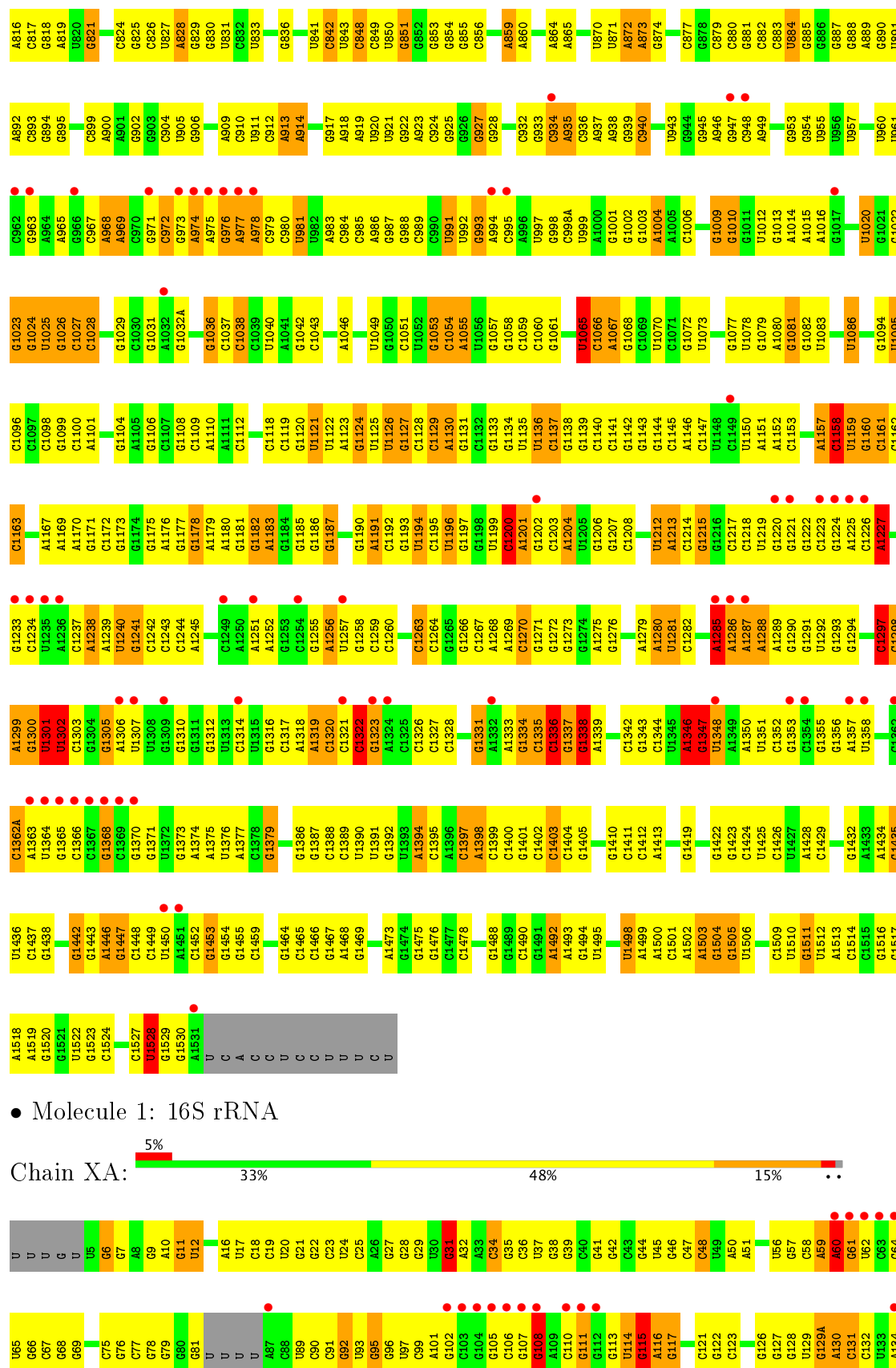
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	XD	1	Total 1	Zn 1	0	0
59	QD	1	Total 1	Zn 1	0	0
59	QN	1	Total 1	Zn 1	0	0
59	XN	1	Total 1	Zn 1	0	0

3 Residue-property plots

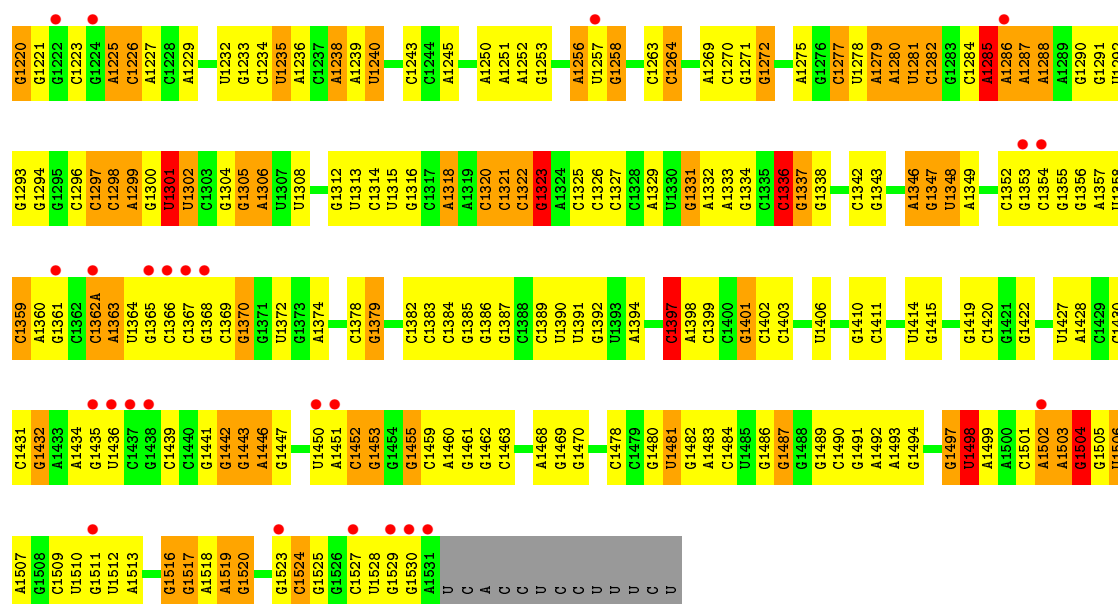
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA

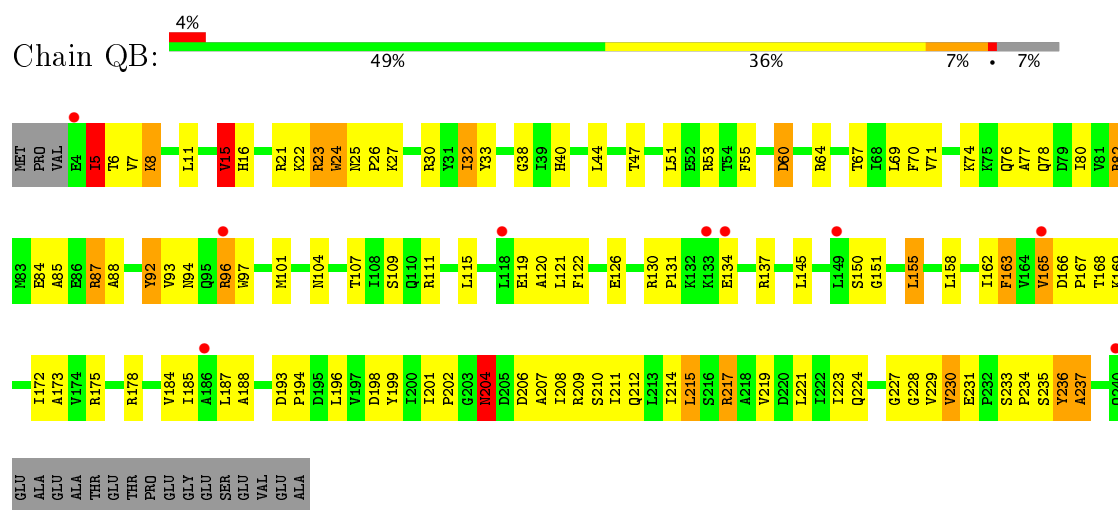




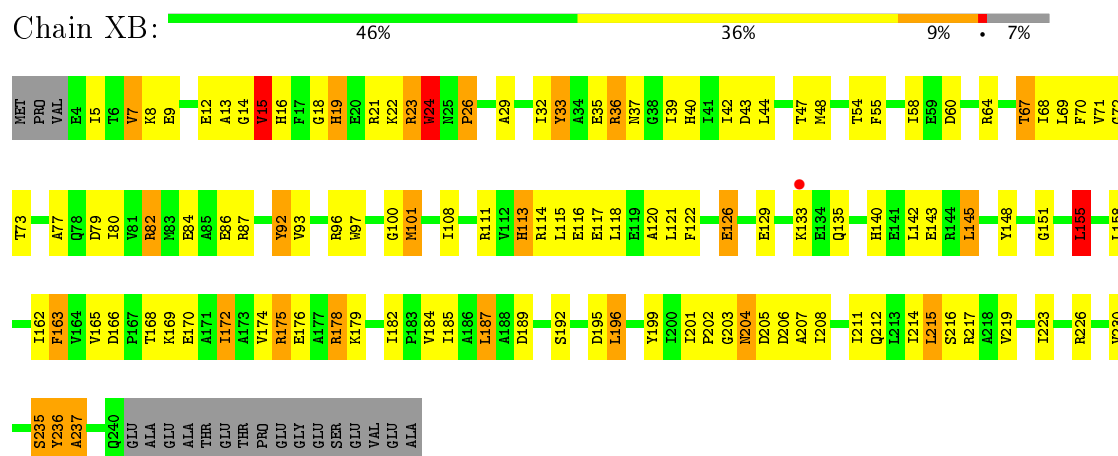
U1148	U1085	G1021	U957	C883	G807	G721	G638	G558	G491	C413	C347	C280	G200	C135
C1149	U1086	G1022	A958	U884	A807	G724	G639	A559	G492	A414	G348	G281	C201	C136
A1150	G1087	G1023	A959	G890	C808	G725	A640	U560	G493	U420	A349	A282	U209	C137
A1152	G1088	G1024	U960	G891	C809	G726	C643	U561	U494	U421	G350	G283	U210	G138
C1153	U1025	U1025	U961	U891	C810	A729	C644	C562	A495	C422	G351	G284	G216	A143
A1154	G1026	G1026	C962	A892	C811	G730	G645	A563	A496	G421	C352	G285	C217	A144
G1155	C1027	C1027	G963	C893	G812	G731	C647	C564	U497	G423	A353	G286	C218	G145
G1156	A1028	G1028	A964	G894	U813	G732	A648	U565	G500	G424	C354	G289	C219	G146
A1157	G1029	G1029	G966	C895	A814	G733	A649	U571	G501	G425	C355	G290	G220	G147
C1158	C1030	C1030	C967	C896	A815	A733	C651	A572	G502	G426	A356	G291	G221	G148
U1159	U1095	G1031	C968	C897	A816	G734	U652	A573	C501	G427	G357	G292	U222	A149
G1160	G1032	A1032	A969	C898	C817	G735	A653	A573	C504	G428	U358	G293		
C1161	G1032A	G1032A	C970	G902	A818	G736	A653	G576	C504	G429	U359	G293		
C1162	G1032B	G1032B	C971	G903	A819	A737		G577	G505	A430	A360	U294		
C1163	G1033	G1033	C972	C904	U820	G738		G578		A431		U295	G226	C154
A1101	G973	G973	C973	C904	U821	G739		G579	A509	A432	U365	U296	G227	G157
A1102	A974	A974	G974	A908	C822	U740		G580	C511	A433	U366	U297	U229	G158
C1103	G1036	G1036	A975	A909	G825	G741		G581	U512	U434	U367	A298	G230	G159
G1171	C1037	C1037	G976	C910	C826	G742		G585	C513		U368	G299	G231	A161
A1105	C1038	C1038	A977	C911	C827	G743		G588	C514	U437	G371	A300	G232	A162
C1106	C1039	C1039	A978	C912	C828	G744		G589	C515	G438	C372	G301	C233	C163
G1107	U1040	U1040	C979	A913	A828	G745		G590	U516	A440	A373	G302	C234	U164
C1108	G1042	G1042	U982	A915	G829	G750		C591	U517		A374	G303	C235	C165
G1177	C1043	C1043	A983	G917	U833	G755		C592	C518	G444	U375	G306	G236	G166
G1178	A1044	A1044	A986	G918	C834	G756		U591	C519	G445	G376	G309	C237	G167
C1112	G1045	G1045	A987	A919	U835	G757		G592	C522	A448	G377	G310	C240	G168
C1114	U1049	U1049	G987	G919	G836	G758		G595	A523	A449	C379	C311	C242	A171
G1117	G1050	G1050	G988	G922	G837	A759		G596	C527	G450	G380	G312	A243	A172
C1118	G1053	G1053	U991	A923	U841	G761		G597	C528	A451	C381	A313	U244	U173
G1119	C1054	C1054	U992	C924	C842	G762		U598	C529	A452	A382	G314	C245	C174
A1188	U1055	U1055	A994	G925	C843	G763		C600	U531	A453	A383	A315	A246	
G1190	U1056	U1056	A995	G926	C844	G764		A601	G530	C454	G384	G316	G247	
U1122	G1057	G1057	C995	G927	C849	G765		A602	U531	C455	U387	G317	G247	C177
A1123	G1058	G1058	A996	G931	U853	A766		A606	A532	C456	U388	G318	A250	A179
G1124	C1059	C1059	U997	C932	C857	A767		A607	A533	C457	A389	G319	G251	U180
U1125	G1060	G1060	G998	G933	G858	A768		G606	A534	C458	G390	G320	U252	G181
C1126	G1061	G1061	G999	C934	A859	G769		G607	G537	A465	G391	A321	G253	U182
G1127	U1062	U1062	A1000	A935	G864	G775		G617	A538	C466	G392	G322	G254	C186
C1128	C1063	C1063	G1001	C936	A865	A776		U619	A539	A467	A393	U323	U255	C186A
G1129	G1064	G1064	G1002	A937	A866	G777		C620	G540	A468	G396	A324	G256	G257
A1130	U1065	U1065	G1003	A938	A867	G778		A621	C541	A474	A397	G325	G258	U188
G1131	C1066	C1066	A1004	G939	A868	G779		A622	G542	G475	C398	A327	G259	U189
C1132	G1068	G1068	U1005	C940	C868	A780		A623	C543	G476	C399	G328	G260	G190
G1133	U1069	U1069	G1006	G941	G869	A781		C624	C544	A477	G400	G329	U261	G191A
U1136	C1070	C1070	C1007	G945	U870	U789		G625	C545	A478	C401	G330	A262	G191B
C1137	G1071	G1071	G1008	G946	A872	A790		U626	C546	C479	G402	G331	A263	G191C
G1138	U1074	U1074	G1010	A946	A873	G791		G627	A547	G481	G403	G332	U264	U191D
U1139	C1075	C1075	G1011	G947	G874	U793		G628	C548	A482	U404	G333	G265	G191E
C1140	U1076	U1076	A1014	C948	G875	A794		G629	C549	C483	U405	G337	G266	U191F
G1142	G1077	G1077	A1015	U950	G876	G795		G630	U551	G484	G406	A338	C267	G191
C1143	U1078	U1078	A1016	G951	C877	C796		G631	U552	G485	G407	A339	C268	U192
G1144	A1080	A1080	G1017	U952	G878	G799		A632	C553	U486	A408	U340	C269	A195
C1145	G1081	G1081	C1018	G953	C879	G803		G633	C554	A487	G409		C271	A196
A1146	U1084	U1084	U1020	U954	C880	U804		G634	C555	C488	G410	A344	A273	A197
C1147				U956	C882			G637	G557	C489	A412	G345	G199	G198
										G490		G346		



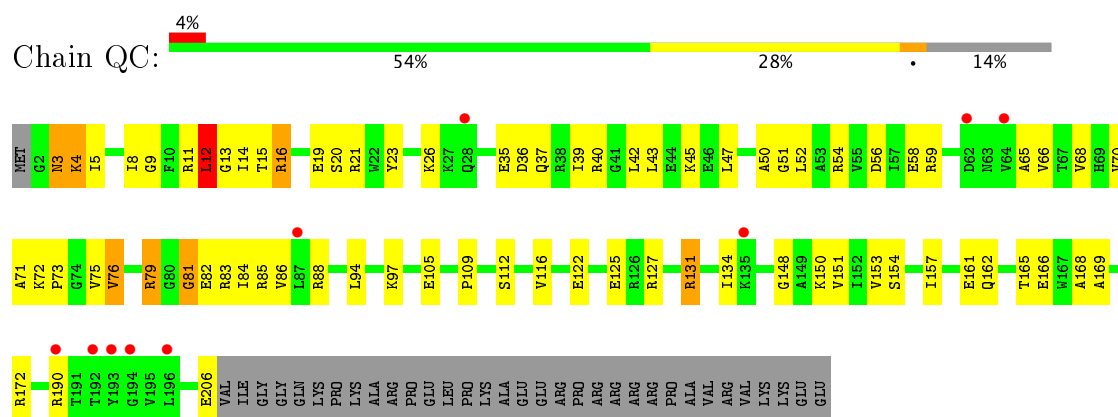
• Molecule 2: 30S ribosomal protein S2



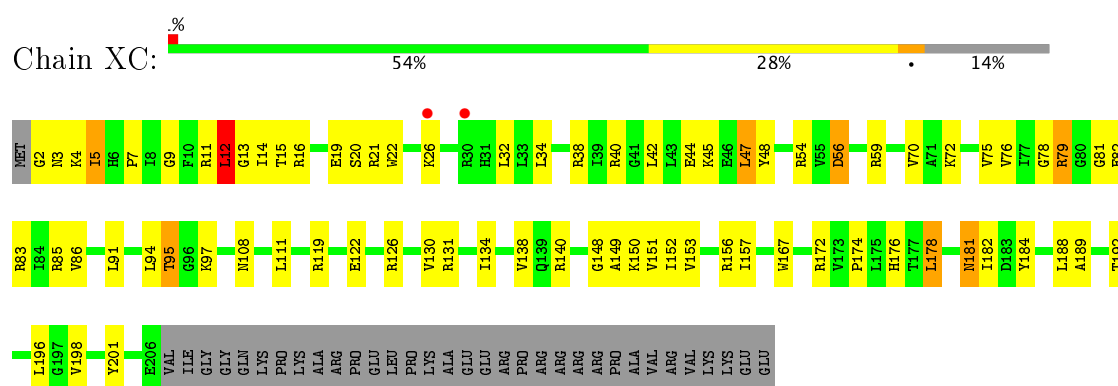
• Molecule 2: 30S ribosomal protein S2



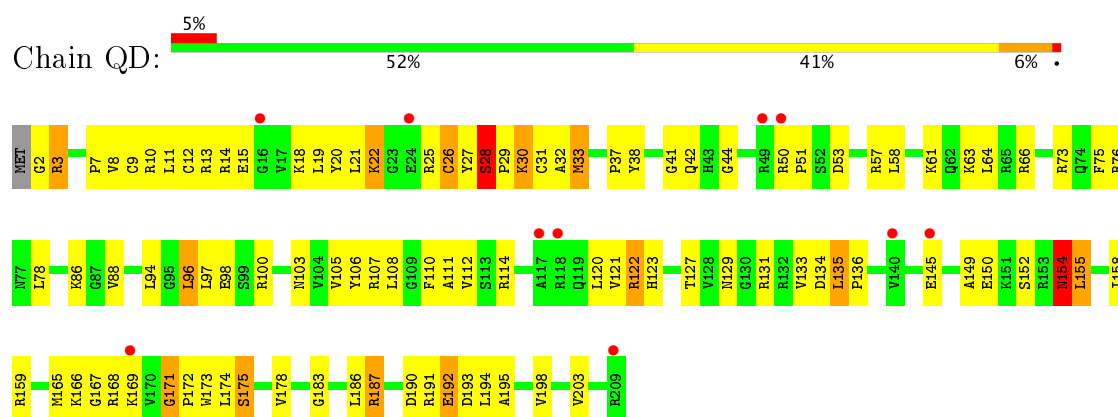
- Molecule 3: 30S ribosomal protein S3



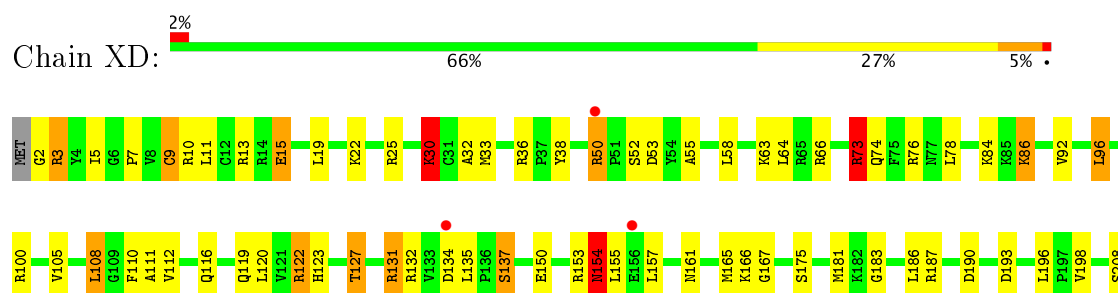
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4



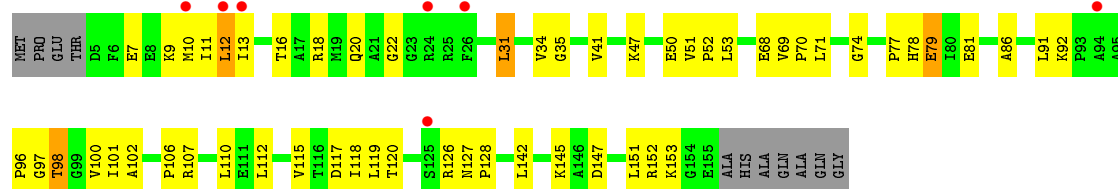
- Molecule 4: 30S ribosomal protein S4



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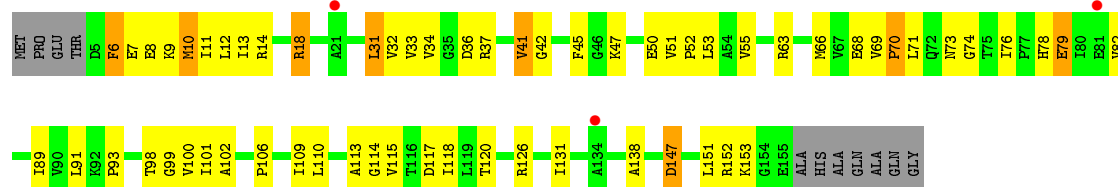
- Molecule 5: 30S ribosomal protein S5

Chain QE: 4% 59% 31% 7%



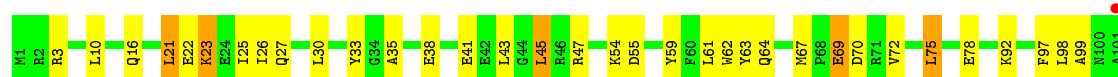
- Molecule 5: 30S ribosomal protein S5

Chain XE: 2% 56% 33% 5% 7%



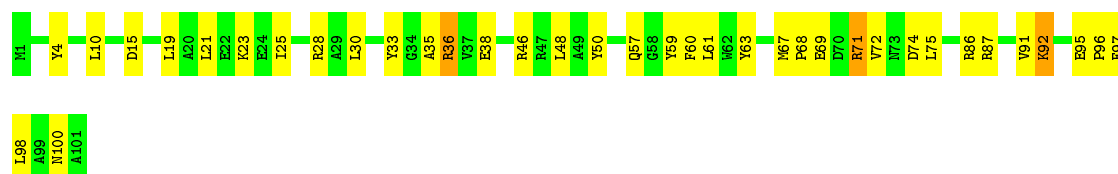
- Molecule 6: 30S ribosomal protein S6

Chain QF: % 66% 29% 5%



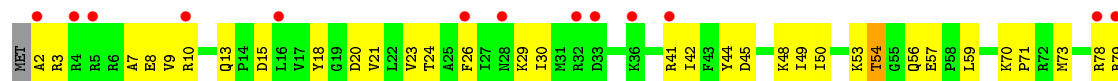
- Molecule 6: 30S ribosomal protein S6

Chain XF: 63% 34%



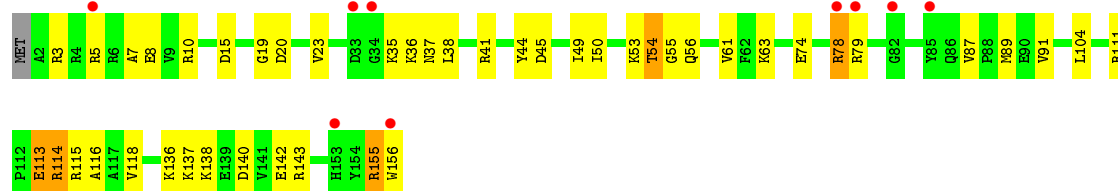
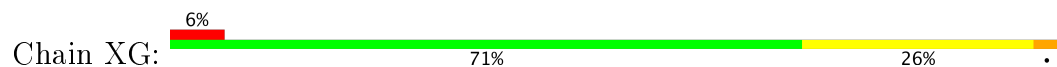
- Molecule 7: 30S ribosomal protein S7

Chain QG: 14% 64% 32%

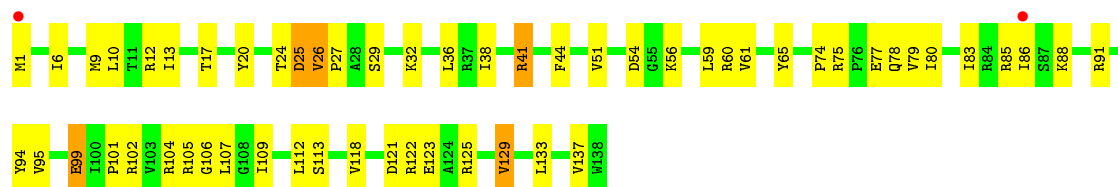




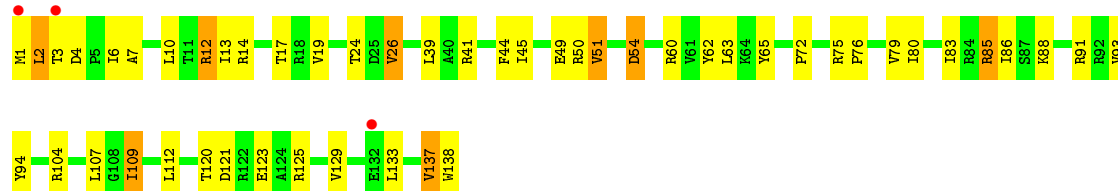
• Molecule 7: 30S ribosomal protein S7



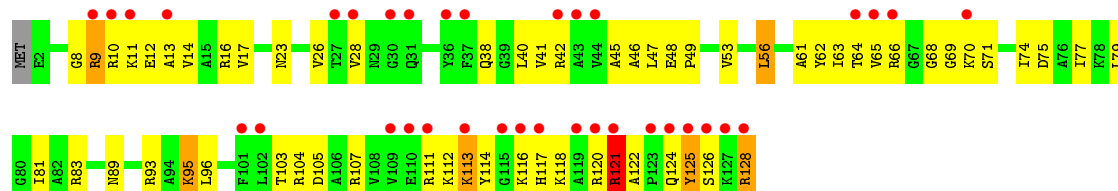
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

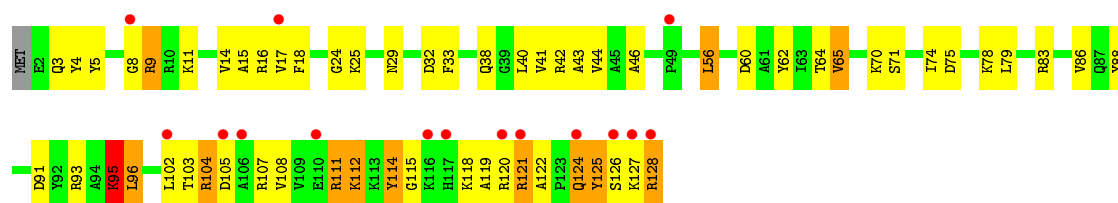


• Molecule 9: 30S ribosomal protein S9

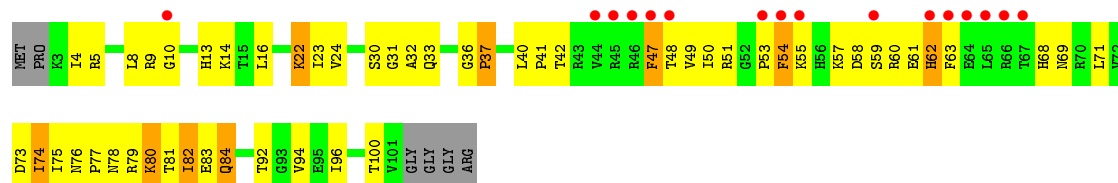


• Molecule 9: 30S ribosomal protein S9

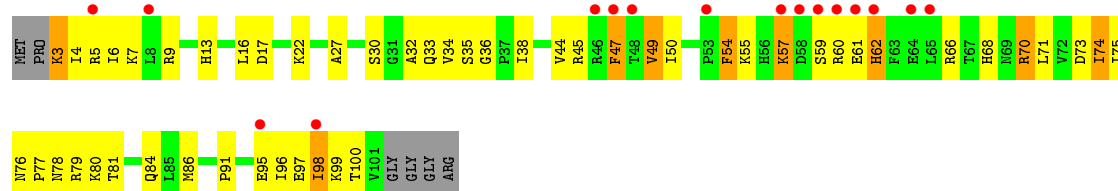




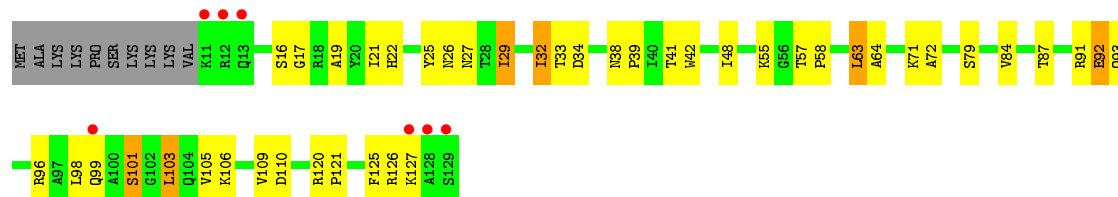
• Molecule 10: 30S ribosomal protein S10



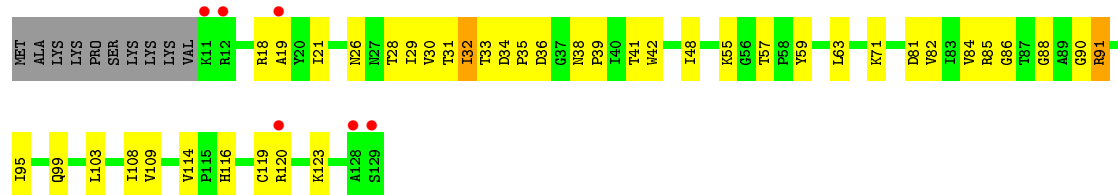
• Molecule 10: 30S ribosomal protein S10



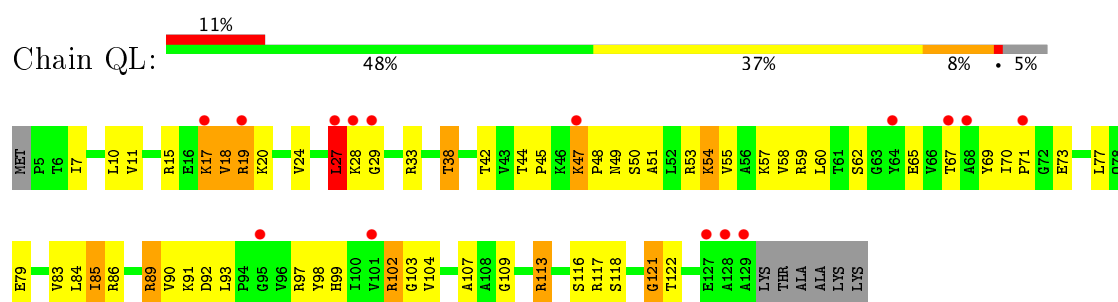
• Molecule 11: 30S ribosomal protein S11



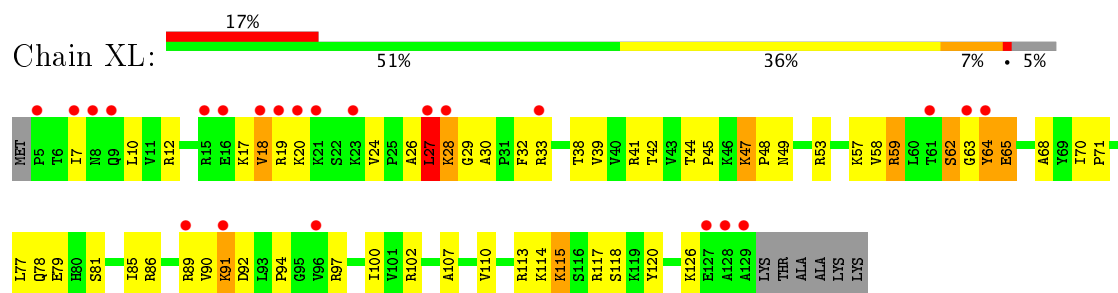
• Molecule 11: 30S ribosomal protein S11



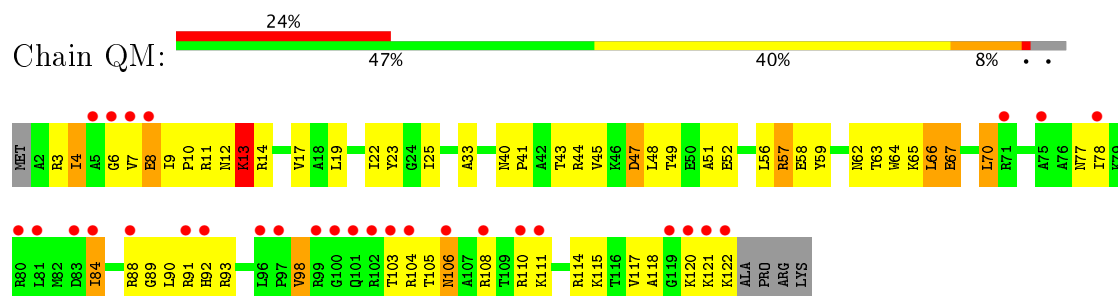
• Molecule 12: 30S ribosomal protein S12



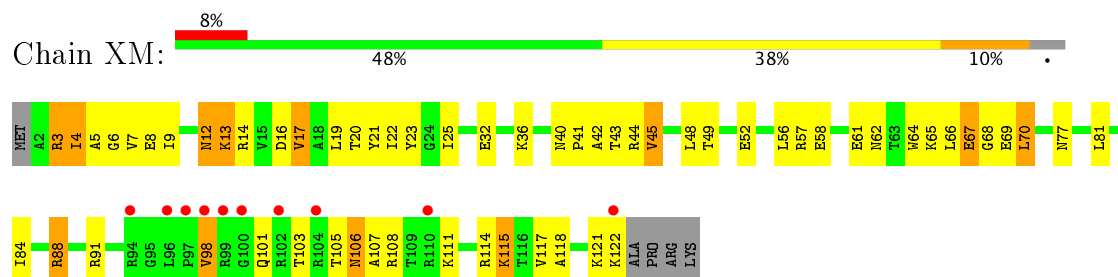
- Molecule 12: 30S ribosomal protein S12



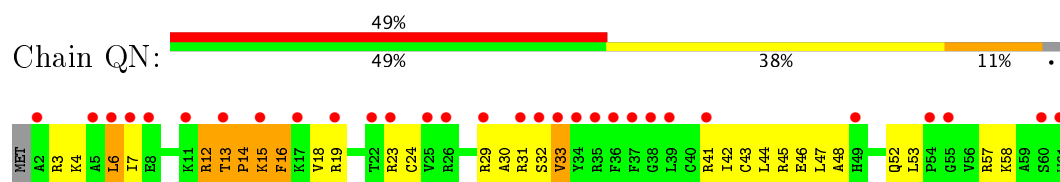
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13

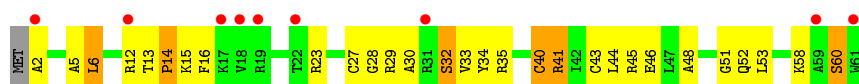


- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z





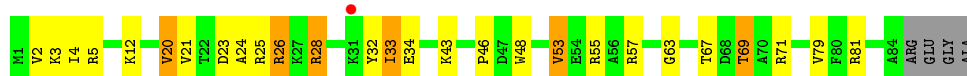
- Molecule 15: 30S ribosomal protein S15



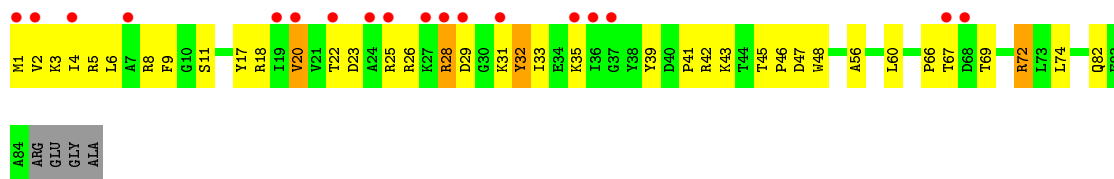
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



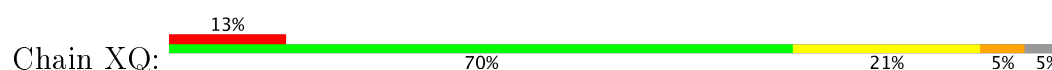
- Molecule 16: 30S ribosomal protein S16

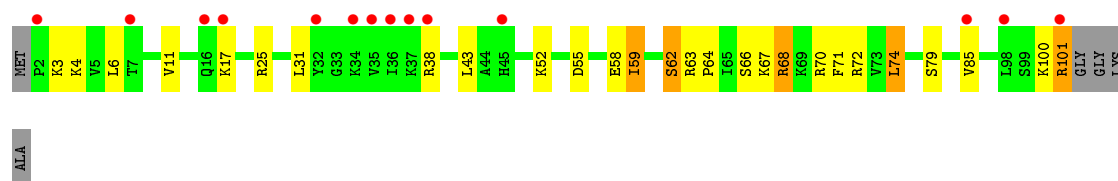


- Molecule 17: 30S ribosomal protein S17

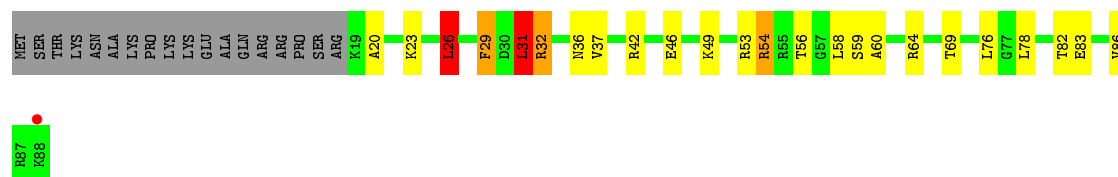


- Molecule 17: 30S ribosomal protein S17

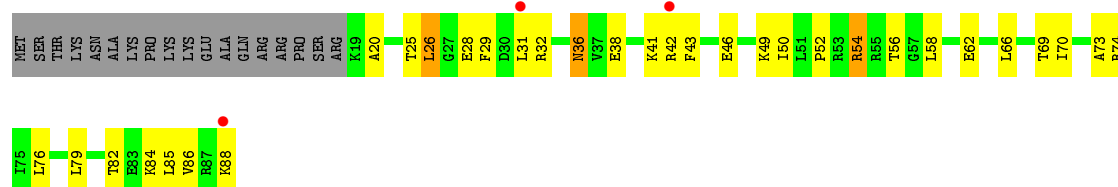
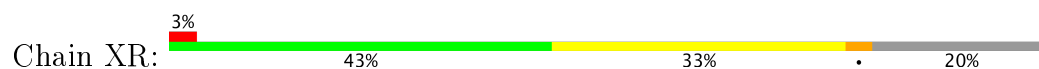




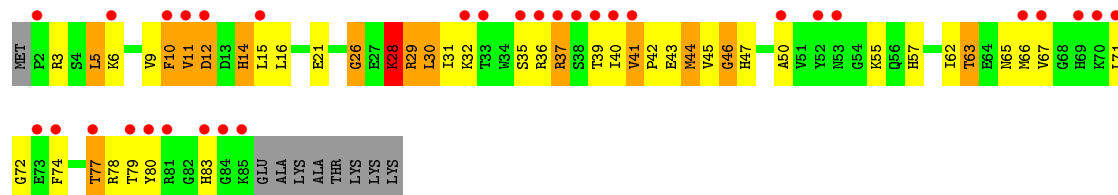
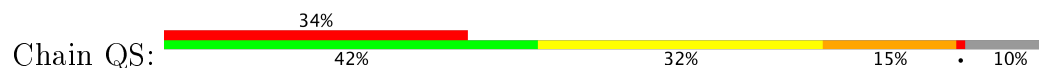
- Molecule 18: 30S ribosomal protein S18



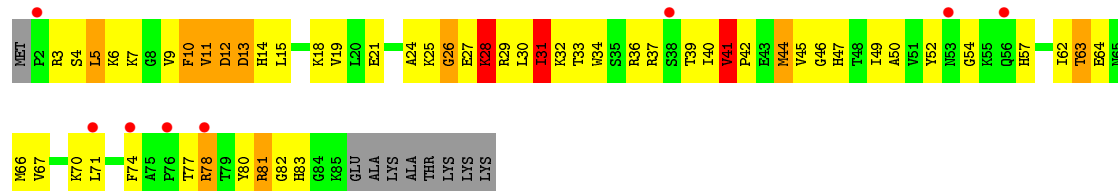
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

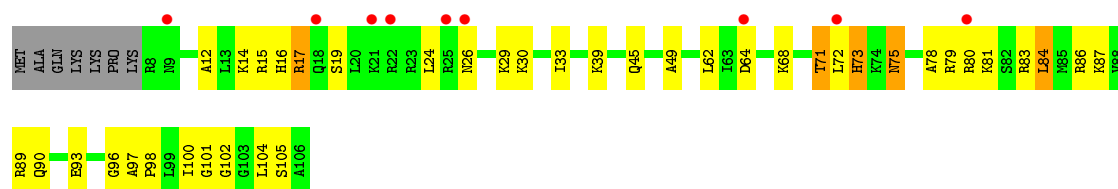


- Molecule 19: 30S ribosomal protein S19

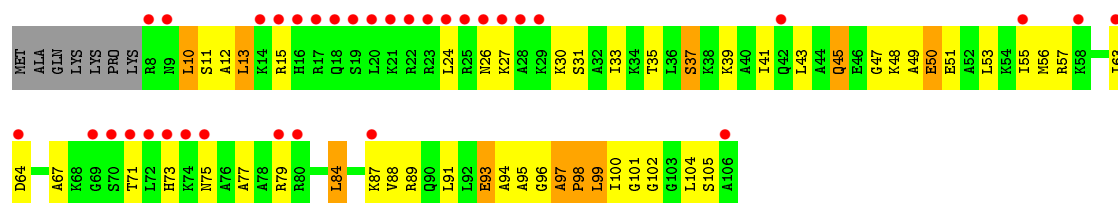


- Molecule 20: 30S ribosomal protein S20

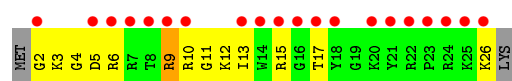
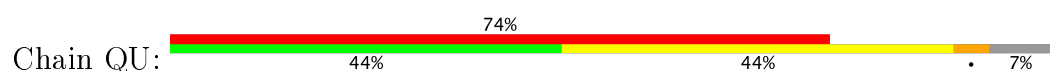




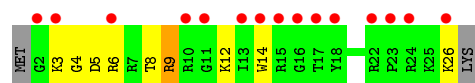
• Molecule 20: 30S ribosomal protein S20



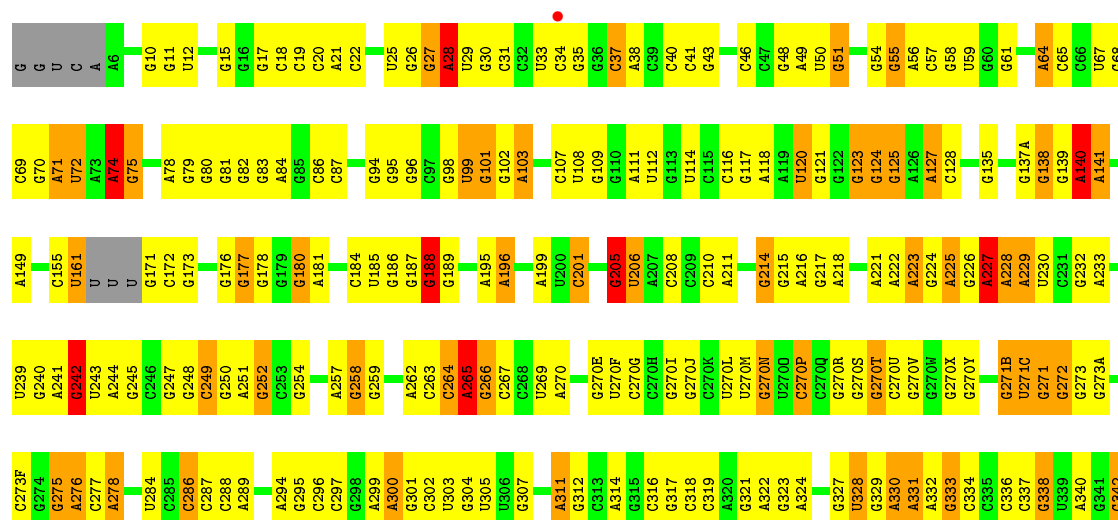
• Molecule 21: 30S ribosomal protein Thx



• Molecule 21: 30S ribosomal protein Thx



• Molecule 22: 23S rRNA



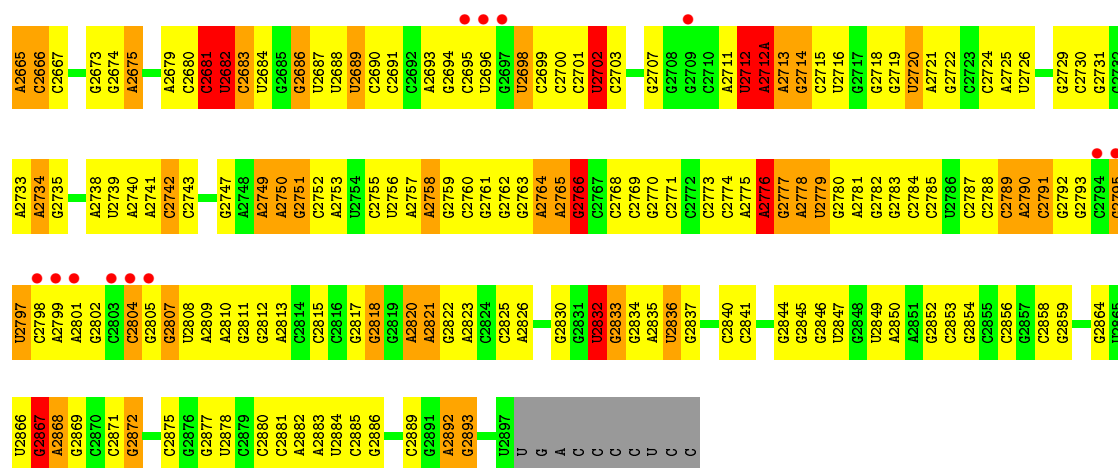
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A1284	A1210	G1136	A1069	A1070	U943	G873	G805	G739	C672	A628	C560	A423	A345
G1285	U1211	G1137	A1071	A1010	G945	G879	U807	G741	C673	G629	G563	U427	A346
A1286	G1212	G1138	C1072	G1011	G946	G880	G808	G742	A675	G630	C564	A428	G347
A1287	A1213	G1139	A1073	U1012	G947	G881	G809	G743	A676	A631	C565	A429	G348
U1288	A1214	G1140	A1074	G1013	G948	G882	U810	A746	C679	A632	U566	G430	G352
G1289	G1215	U1141	G1075	U1014	G948	G883	U811	U747	G680	A633	A497	G431	A357
C1290	U1142	A1142A	C1076	G1015	G952	G884	U812	A750	G681	C634	U499	U434	G360
C1291	A1143	A1143	A1077	G1016	G954	G885	U813	A751	G682	C635	G500	G361	U362
U1292	A1144	A1144	C1078	G1017	G955	C886	C814	A752	A685	A636	A572	G438	U363
C1293	A1145	A1145	C1079	U1018	G956	A887	C815	A753	G686	A637	A573	G439	A363A
C1297	A1146	A1146	C1080	U1019	G957	C888	C816	A754	U687	U638	A574	G440	G364
G1298	G1149	G1149	U1081	A1020	A957	C889	C817	C755	A688	U639	A575	G441	G370
C1299	C1223	G1150	U1082	A1021	U958	C890	U818	A756	C687	U640	A576	G442	A371
U1300	C1225	G1151	U1083	U1022	A959	A890	U819	C755	U689	G642	U576	G443	U372
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G1303	G1228	G1154	A1086	G1025	G962	A896	G823	C758	C691	A647	C580	G446	U375
C1306	G1229A	C1155	A1087	U1026	U963	C897	G824	G759	C692	G648	C581	G447	U376
G1309	G1236	C1156	U1088	A1027	C964	C898	U825	A761	C693	G651	G582	G448	U377
G1310	A1237	G1161	U1089	A1028	G965	C899	U826	U762	U694	C652	A514	A449	U380
G1311	G1238	G1162	C1082	G1030	C967	A900	U828	A763	G695	A653	A515	A450	G381
U1312	G1239	U1167	U1093	U1033	G968	A901	A829	C766	A699	A654	A586	G451	G382
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A1247	G1247	G1172	A1098	G1038	A973	G906	C834	G771	G704	C	C591	A456	G387
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G1260	G1260	G1184	G1112	C1049	A984	G920	U847	A782	A718	C	A536	A466	G400
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G1344	A1272	G1201	U1061	G997	G997	G934	A861	C797	G731	C664	G618	A482	A415
A1349	U1273	G1202	A1126	G1062	A1000	C936	G862	G798	C732	G665	U553	A483	C416
U1352	A1278	G1203	U1063	G1063	A1001	G937	A863	G799	A735	G666	U554	C484	C419
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C2248	U2249	C2250	G2251	C2254	G2257	C2258	G2259	C2260	C2261	C2262	C2263	A2266	A2267	A2268	A2269	A2273	C2274	G2275	G2276	G2277	G2278	G2279	G2280	C2281	G2282	C2283	C2284	G2285	A2286	A2287	A2288	U2291	C2292	C2293	C2297	A2298	G2299	C2301	C2302	G2303	C2306	C2307	G2308	C2309	A2310	A2311	C2318	G2319	C2320	C2321	C2322	C2323	C2324	C2325	C2326	C2327	C2328	C2329	C2330	C2331	C2332	C2333	C2334	C2335	C2336	C2343	U2344	G2345	A2346	C2347	C2350	G2351	A2352	G2353	G2354	C2355	G2358	C2359	A2360	C2364	G2365	A2366	A2367	G2371	G2372	G2373	A2376	C2377	A2378	G2379	G2383	C2384	C2385	C2386	U2387	C2391	A2392	G2397	U2398	G2399	G2400	U2401	A2402	C2403	C2404	C2405																																																																																																																																																																																																																																												
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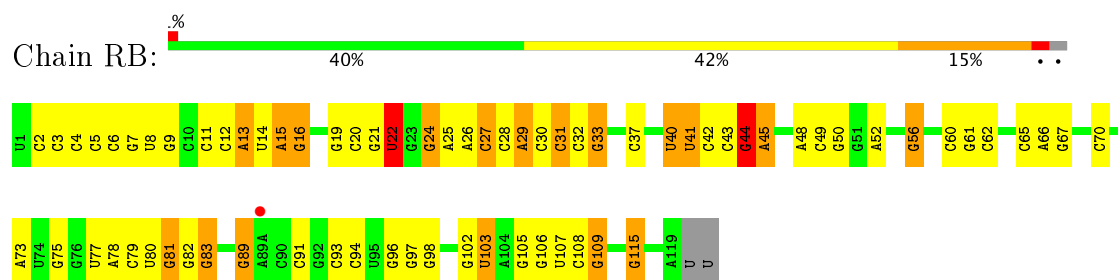


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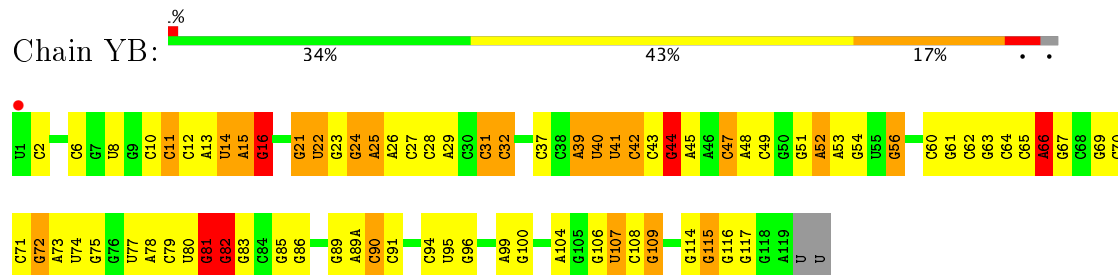
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U2655	C2507	C2507	G2369	G2369	G2305	G2239	G2165	C2106	C1964	A1900	G1895	G1738	U1659
U2656	G2508	G2508	A2370	A2370	A2241	G2240	G2166	G2107	C1965	A1901	C1896	C1739	C1662
U2657	C2509	C2509	C2371	C2371	U2242	G2241	U2167	C2108	G2037	A1966	C1897	G1742	
U2658	U2510	U2510	G2372	G2372	U2243	U2242	G2168	U2109	G2038	C1967	C1898	G1743	
U2659	G2512	G2512	C2373	C2373	U2244	U2243	A2169	G2110	G2039	C1968	G1899	G1744	
U2660	G2513	G2513	A2374	A2374	U2245	U2244	A2170	G2111	G2040	A1969	C1899	G1745	
U2661	U2514	U2514	G2375	G2375	G2246	G2245	G2171	C2112	U2041	A1970	A1901	G1750	
U2662	C2515	C2515	C2376	C2376	A2247	A2246	U2172	G2113	G2042	A1971	A1902	C1751	
U2663	A2516	A2516	G2377	G2377	C2312	C2311	G2173	G2114	A2043	A1972	G1903	C1752	
U2664	G2517	G2517	C2378	C2378	C2313	C2312	C2174	G2115	C2044	G1973	G1904	C1753	
U2665	U2518	U2518	C2379	C2379	G2314	G2313	C2175	G2116	U2045	C1974	C1905	C1754	
U2666	C2519	C2519	G2380	G2380	G2315	G2314	C2176	G2117	G2046	G1975	C1906	C1755	
U2667	U2520	U2520	A2381	A2381	G2316	G2315	A2177	G2118	U2047	C1976	G1907	U1757	
U2668	G2521	G2521	C2382	C2382	C2317	C2316	C2178		G2048	U1976			
U2669	A2522	A2522	G2383	G2383	C2318	C2317							
U2670	U2523	U2523	A2384	A2384	C2319	C2318							
U2671	C2524	C2524	C2385	C2385	C2320	C2319							
U2672	U2525	U2525	G2386	G2386	C2321	C2320							
U2673	G2526	G2526	A2387	A2387	C2322	C2321							
U2674	U2527	U2527	C2388	C2388	C2323	C2322							
U2675	C2528	C2528	G2389	G2389	C2324	C2323							
U2676	U2529	U2529	A2390	A2390	C2325	C2324							
U2677	G2530	G2530	C2391	C2391	C2326	C2325							
U2678	U2531	U2531	U2392	U2392	C2327	C2326							
U2679	C2532	C2532	A2393	A2393	C2328	C2327							
U2680	U2533	U2533	G2394	G2394	C2329	C2328							
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U2682	U2535	U2535	G2396	G2396	C2331	C2330							
U2683	C2536	C2536	A2397	A2397	C2332	C2331							
U2684	U2537	U2537	U2398	U2398	C2333	C2332							
U2685	G2538	G2538	C2399	C2399	C2334	C2333							
U2686	U2539	U2539	G2400	G2400	C2335	C2334							
U2687	C2540	C2540	A2401	A2401	C2336	C2335							
U2688	U2541	U2541	C2402	C2402	C2337	C2336							
U2689	G2542	G2542	C2403	C2403	C2338	C2337							
U2690	U2543	U2543	C2404	C2404	C2339	C2338							
U2691	C2544	C2544	G2405	G2405	C2340	C2339							
U2692	U2545	U2545	A2406	A2406	C2341	C2340							
U2693	G2546	G2546	C2407	C2407	C2342	C2341							
U2694	U2547	U2547	U2408	U2408	C2343	C2342							
U2695	C2548	C2548	C2409	C2409	C2344	C2343							
U2696	U2549	U2549	G2410	G2410	C2345	C2344							
U2697	G2550	G2550	A2411	A2411	C2346	C2345							
U2698	C2551	C2551	C2412	C2412	C2347	C2346							
U2699	U2552	U2552	C2413	C2413	C2348	C2347							
U2700	G2553	G2553	G2414	G2414	C2349	C2348							
U2701	U2554	U2554	C2415	C2415	C2350	C2349							
U2702	C2555	C2555	A2416	A2416	C2351	C2350							
U2703	G2556	G2556	G2417	G2417	C2352	C2351							
U2704	U2557	U2557	C2418	C2418	C2353	C2352							
U2705	C2558	C2558	A2419	A2419	C2354	C2353							
U2706	U2559	U2559	G2420	G2420	C2355	C2354							
U2707	G2560	G2560	C2421	C2421	C2356	C2355							
U2708	U2561	U2561	A2422	A2422	C2357	C2356							
U2709	C2562	C2562	G2423	G2423	C2358	C2357							
U2710	U2563	U2563	C2424	C2424	C2359	C2358							
U2711	G2564	G2564	A2425	A2425	C2360	C2359							
U2712	U2565	U2565	C2426	C2426	C2361	C2360							
U2713	C2566	C2566	G2427	G2427	C2362	C2361							
U2714	U2567	U2567	A2428	A2428	C2363	C2362							
U2715	G2568	G2568	C2429	C2429	C2364	C2363							
U2716	U2569	U2569	U2430	U2430	C2365	C2364							



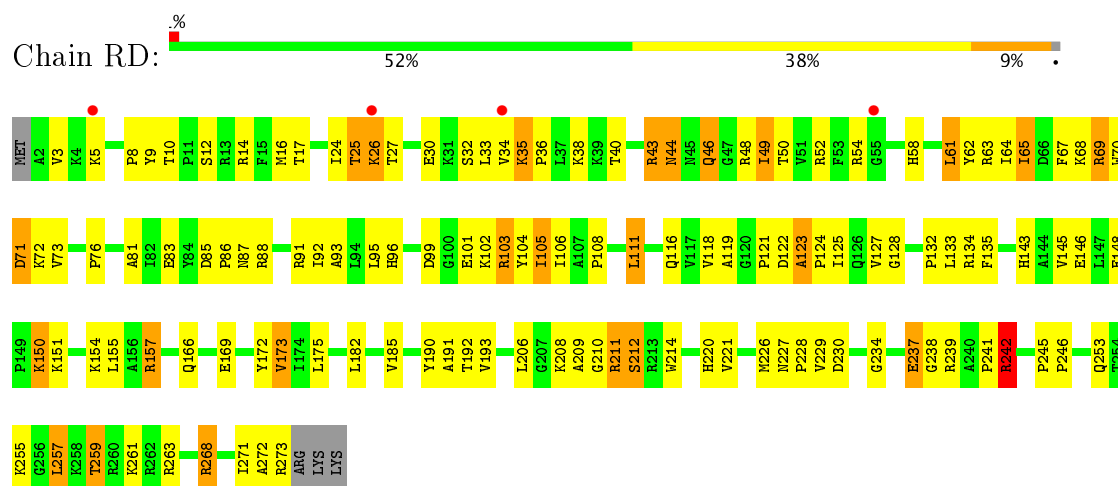
- Molecule 23: 5S rRNA



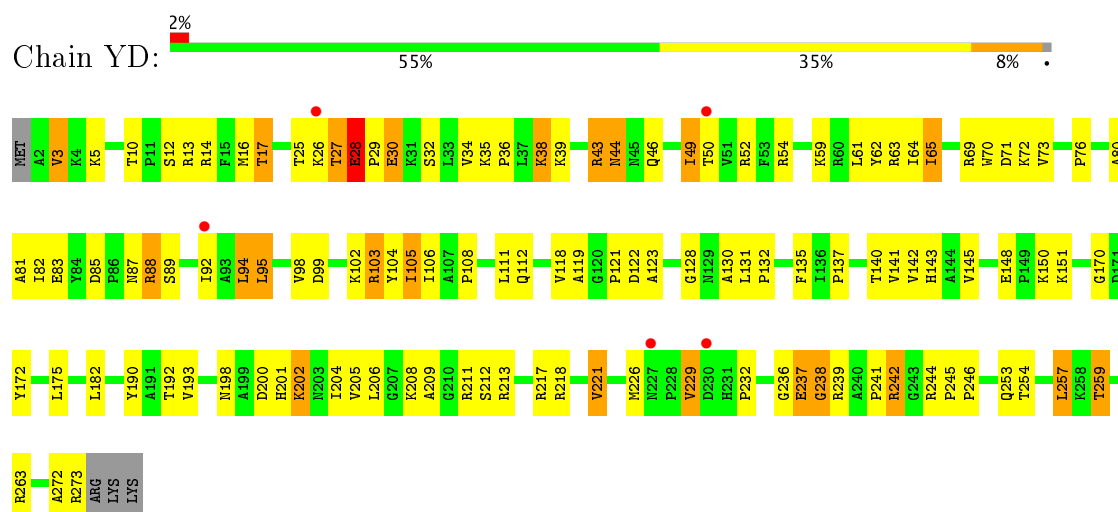
- Molecule 23: 5S rRNA



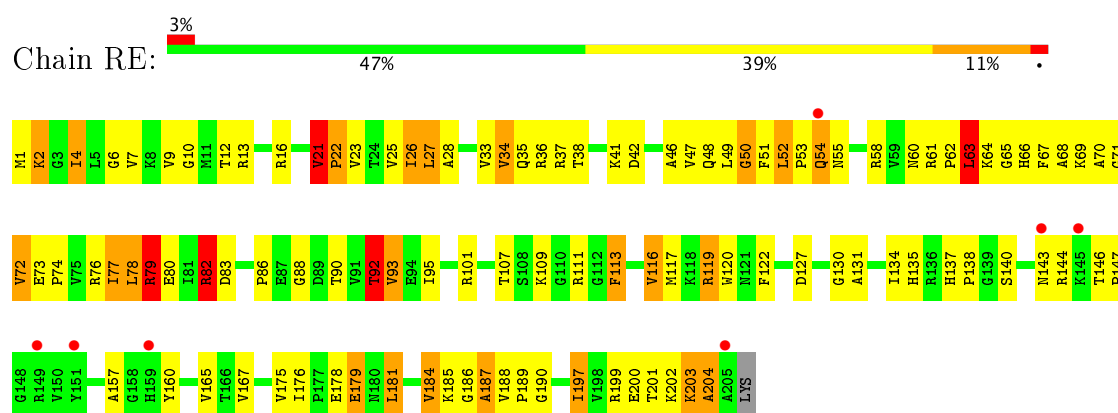
- Molecule 24: 50S ribosomal protein L2



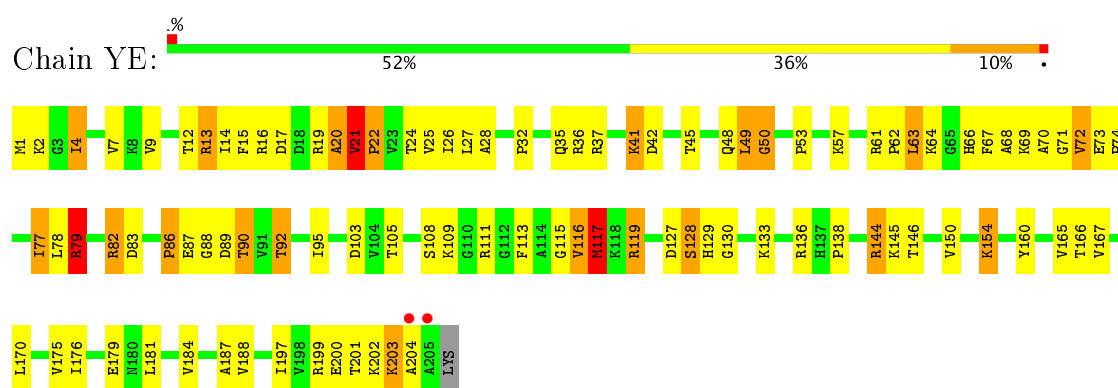
- Molecule 24: 50S ribosomal protein L2



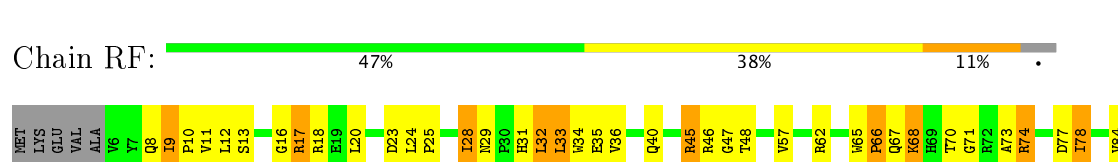
- Molecule 25: 50S ribosomal protein L3

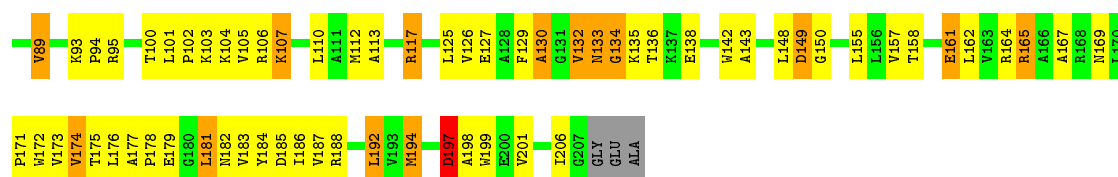


- Molecule 25: 50S ribosomal protein L3



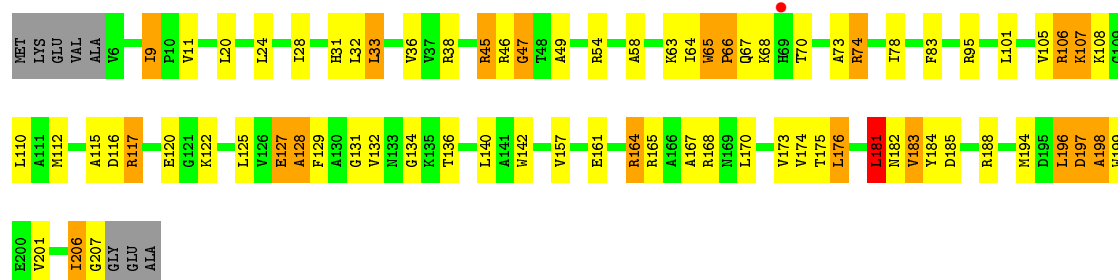
- Molecule 26: 50S ribosomal protein L4





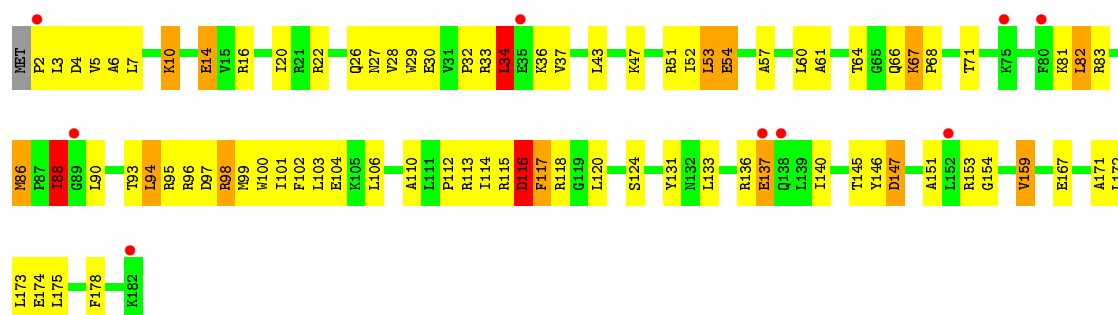
• Molecule 26: 50S ribosomal protein L4

Chain YF: 60% 26% 9%



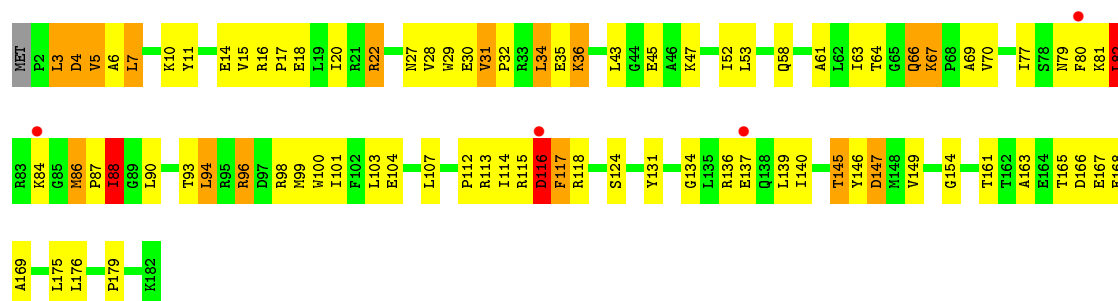
• Molecule 27: 50S ribosomal protein L5

Chain RG: 5% 54% 37% 7%



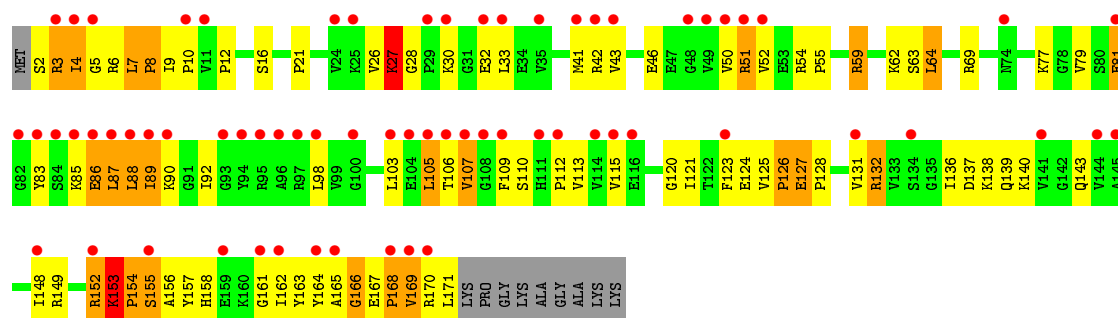
• Molecule 27: 50S ribosomal protein L5

Chain YG: 2% 53% 36% 9%

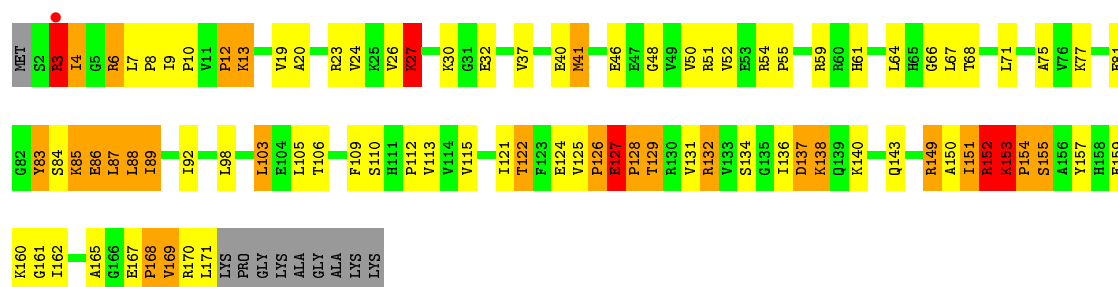


• Molecule 28: 50S ribosomal protein L6

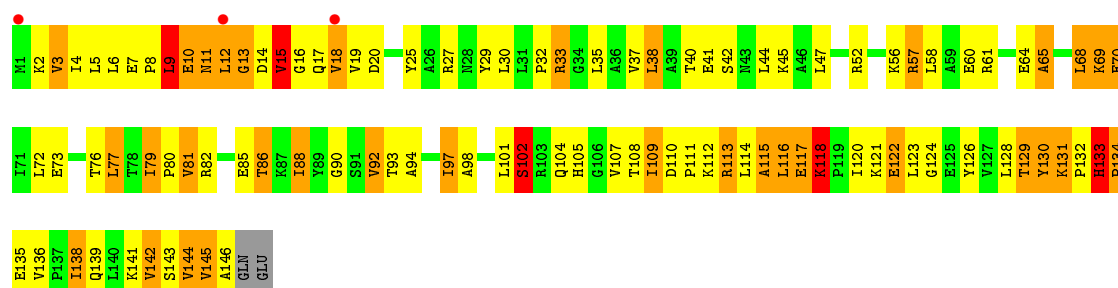
Chain RH: 37% 45% 36% 13% 6%

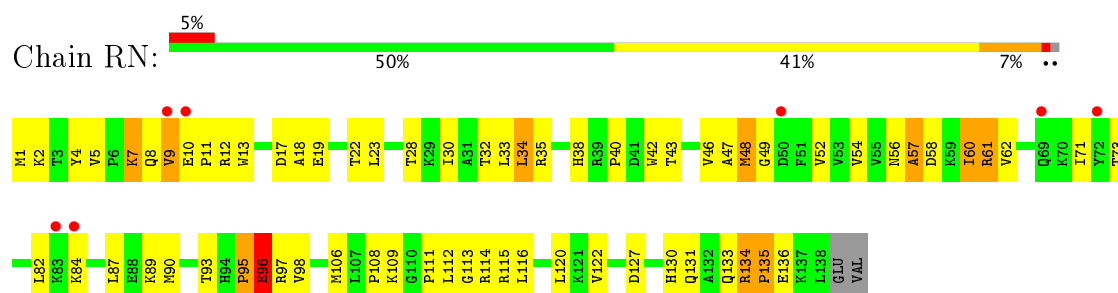


- Molecule 28: 50S ribosomal protein L6

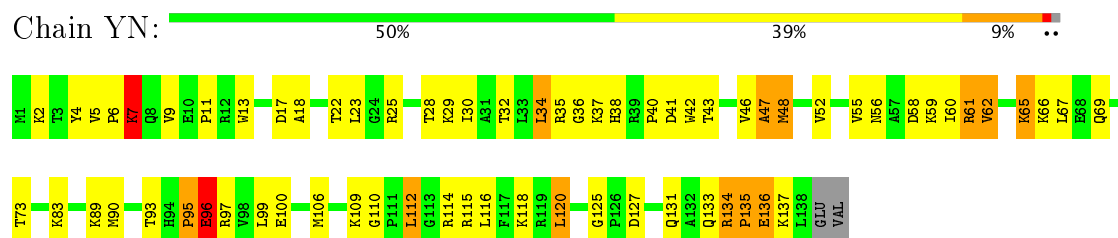


- Molecule 29: 50S ribosomal protein L9

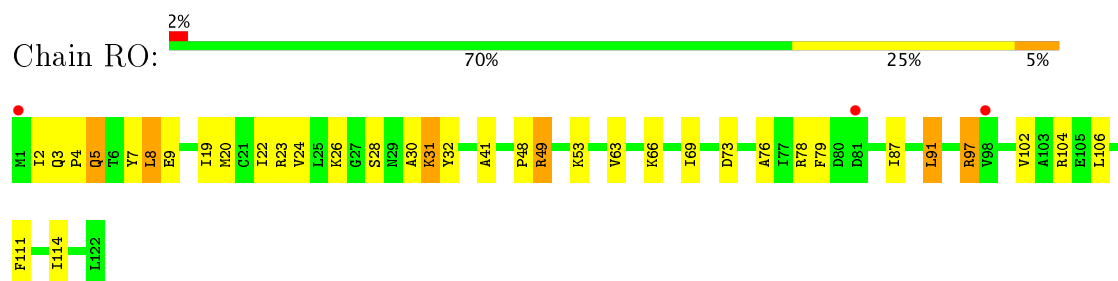




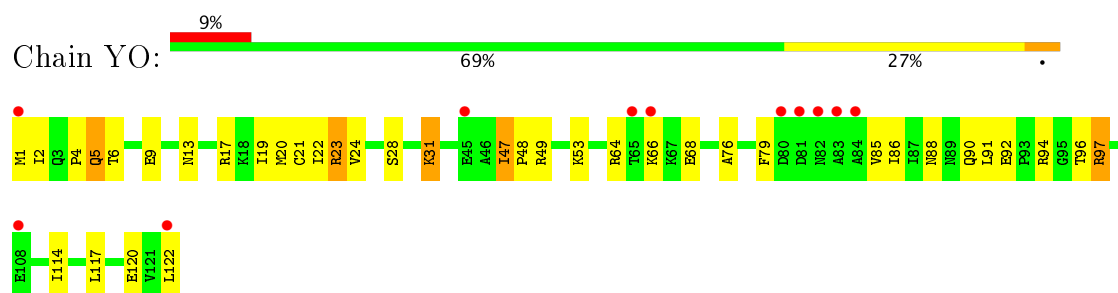
• Molecule 30: 50S ribosomal protein L13



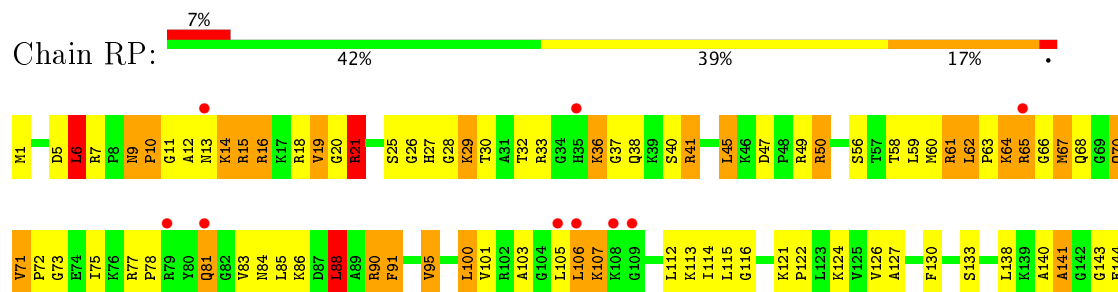
• Molecule 31: 50S ribosomal protein L14

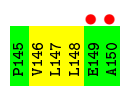


• Molecule 31: 50S ribosomal protein L14

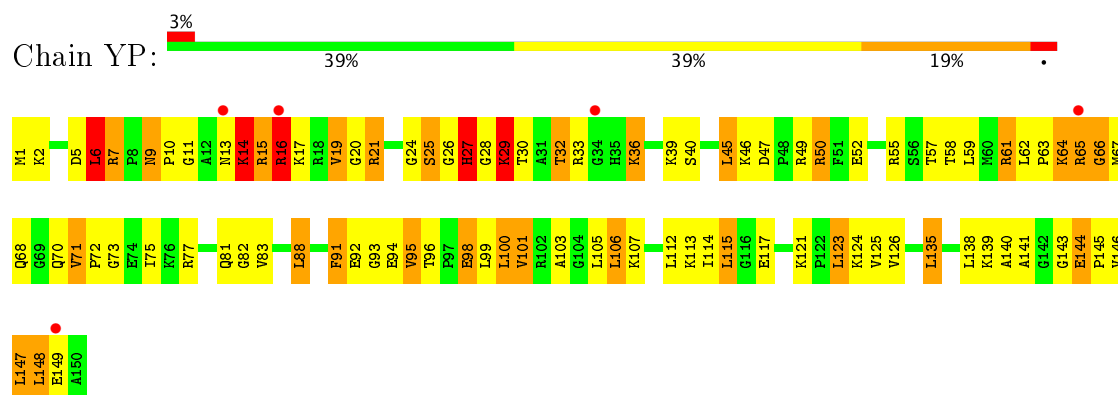


• Molecule 32: 50S ribosomal protein L15

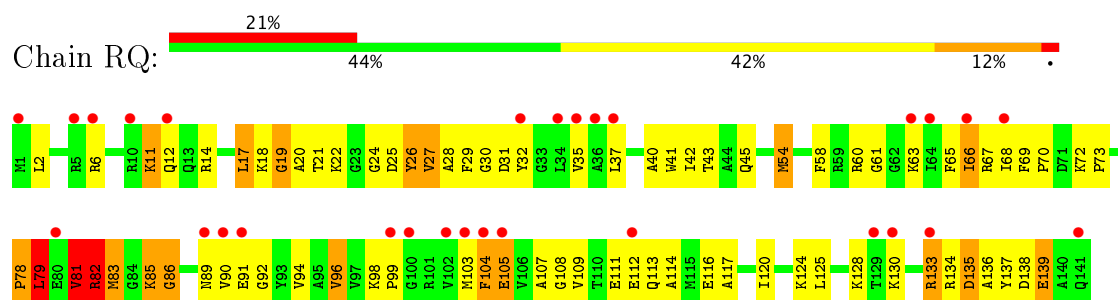




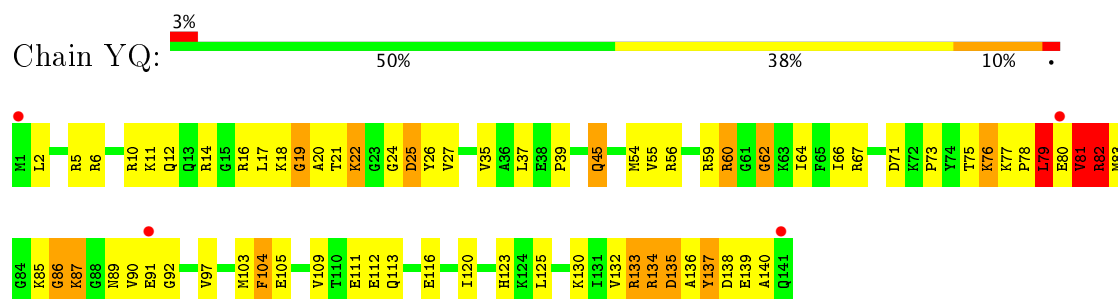
- Molecule 32: 50S ribosomal protein L15



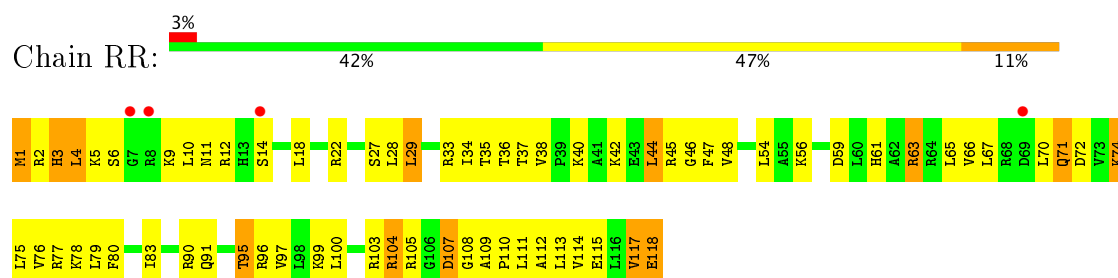
- Molecule 33: 50S ribosomal protein L16



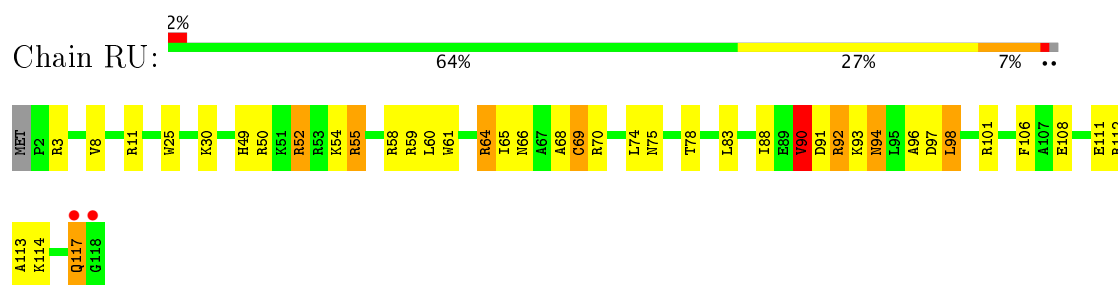
- Molecule 33: 50S ribosomal protein L16



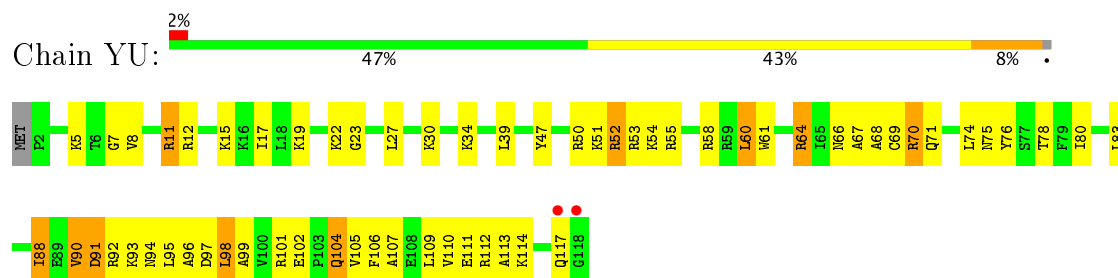
- Molecule 34: 50S ribosomal protein L17



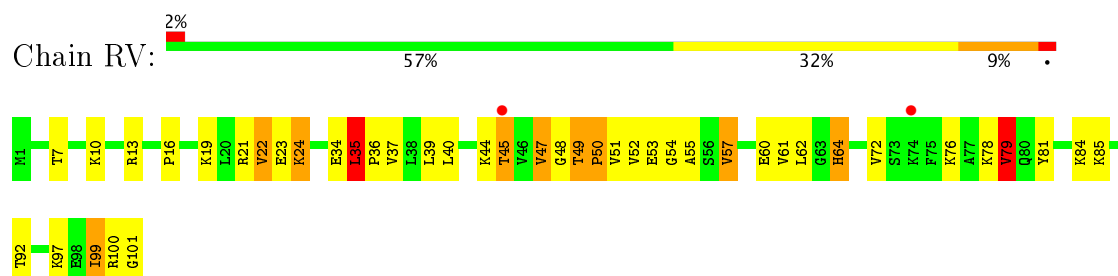
- Molecule 34: 50S ribosomal protein L17



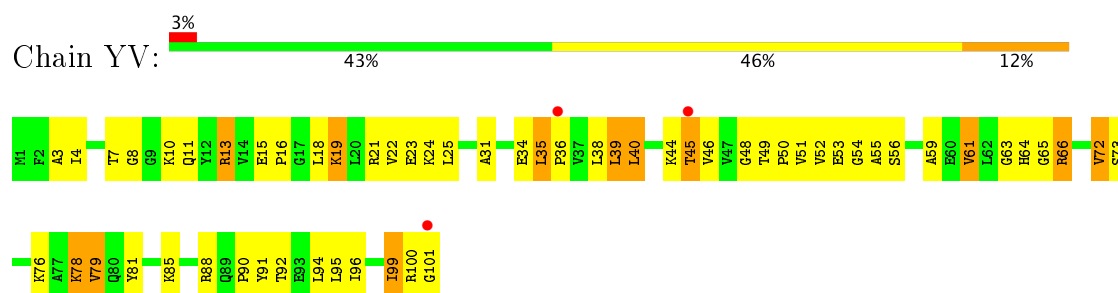
- Molecule 37: 50S ribosomal protein L20



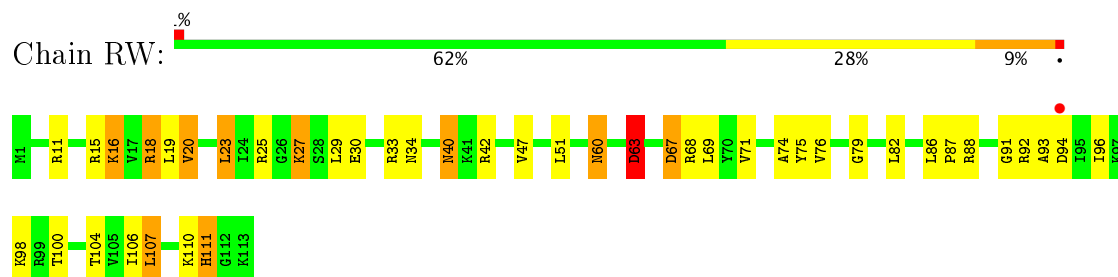
- Molecule 38: 50S ribosomal protein L21



- Molecule 38: 50S ribosomal protein L21



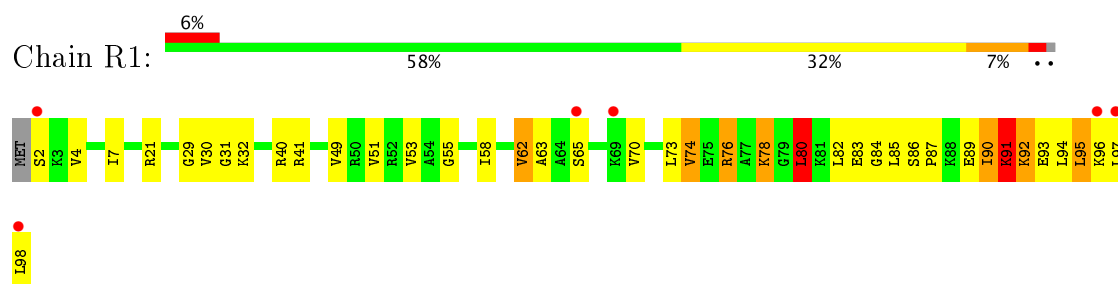
- Molecule 39: 50S ribosomal protein L22



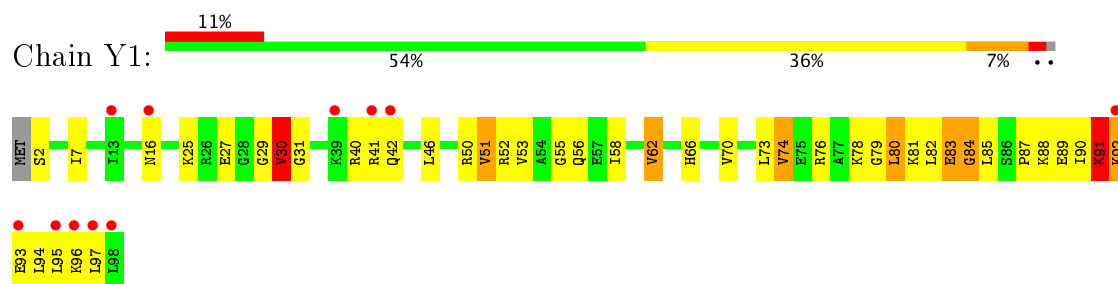
- Molecule 39: 50S ribosomal protein L22



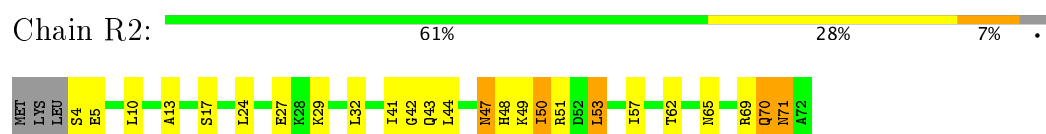
- Molecule 44: 50S ribosomal protein L28



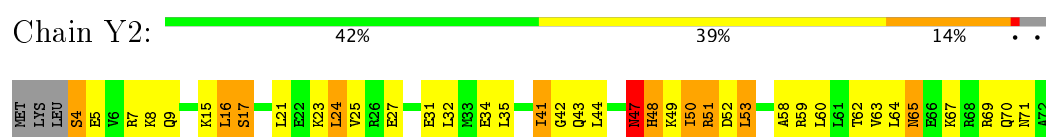
- Molecule 44: 50S ribosomal protein L28



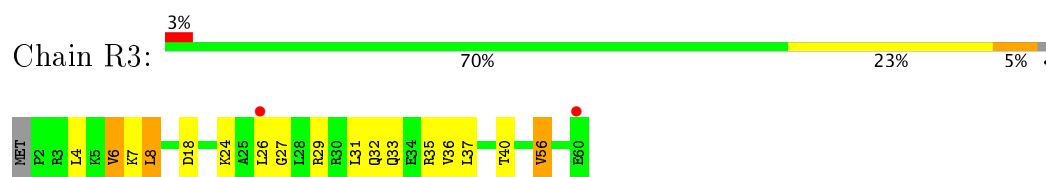
- Molecule 45: 50S ribosomal protein L29



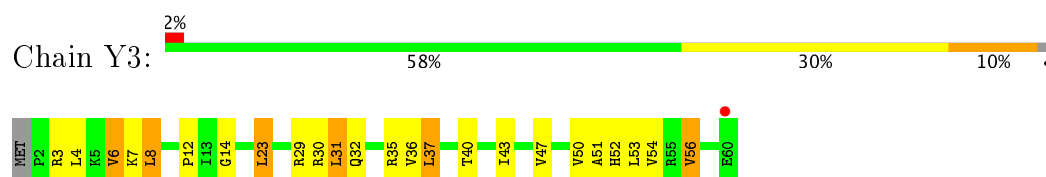
- Molecule 45: 50S ribosomal protein L29



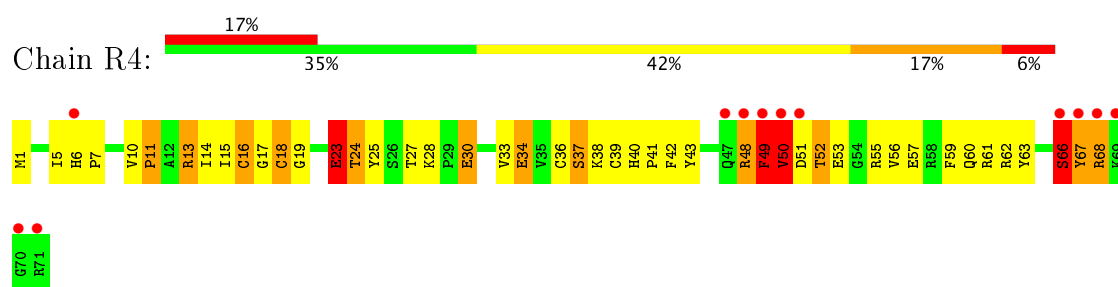
- Molecule 46: 50S ribosomal protein L30



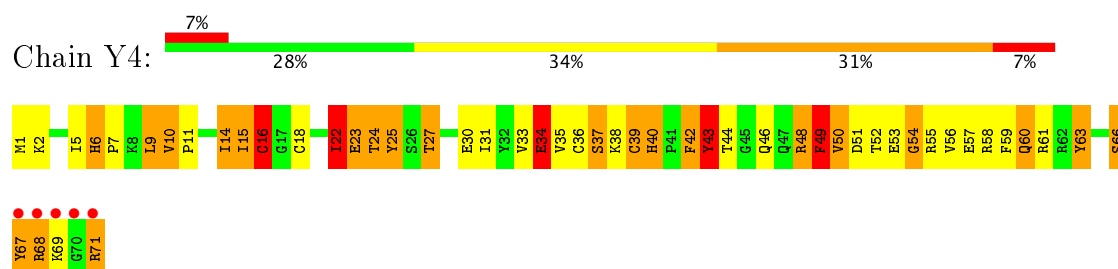
- Molecule 46: 50S ribosomal protein L30



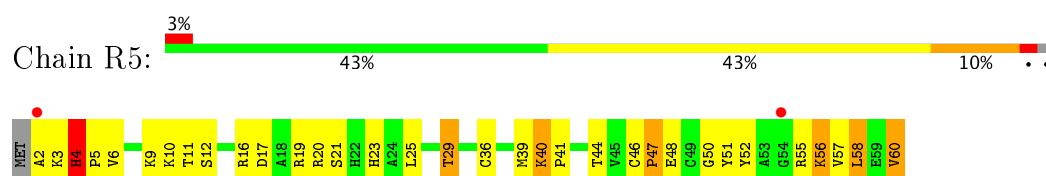
- Molecule 47: 50S ribosomal protein L31



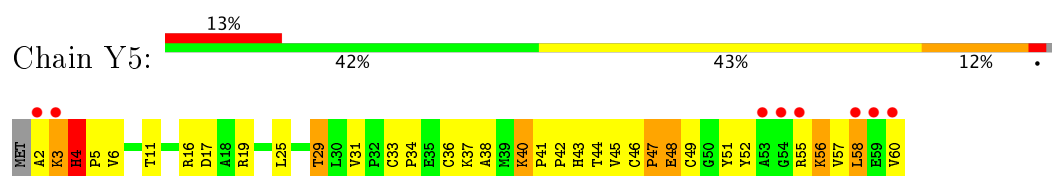
- Molecule 47: 50S ribosomal protein L31



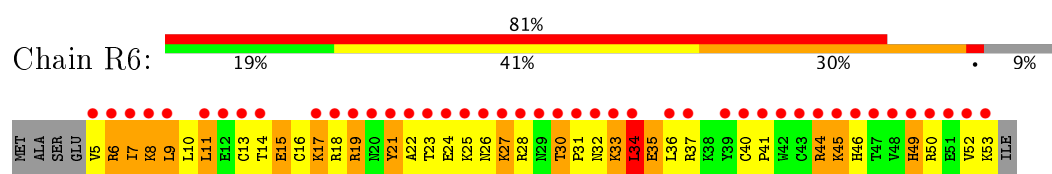
- Molecule 48: 50S ribosomal protein L32



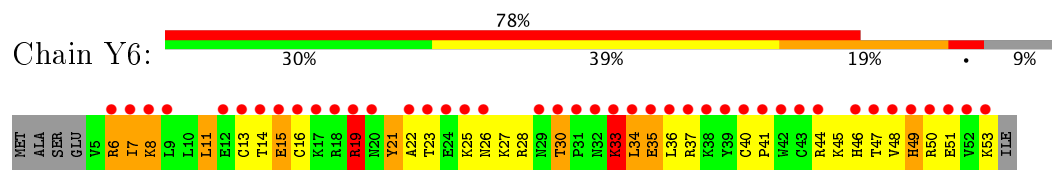
- Molecule 48: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L33

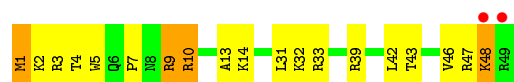


- Molecule 49: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L34

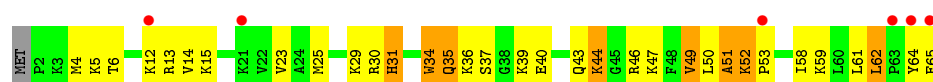




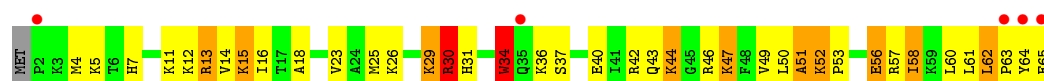
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35



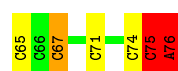
- Molecule 52: 50S ribosomal protein L36



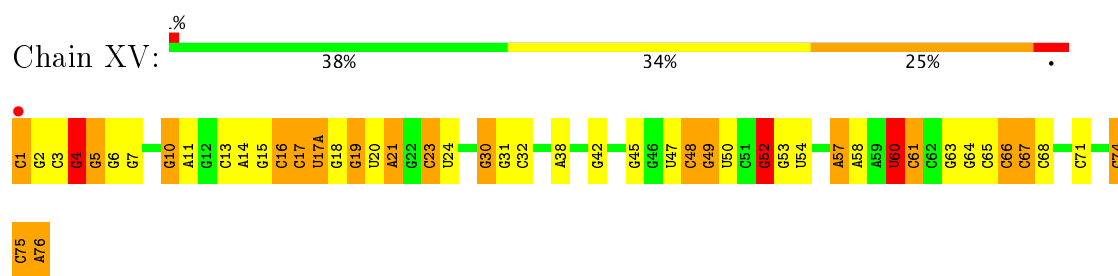
- Molecule 52: 50S ribosomal protein L36



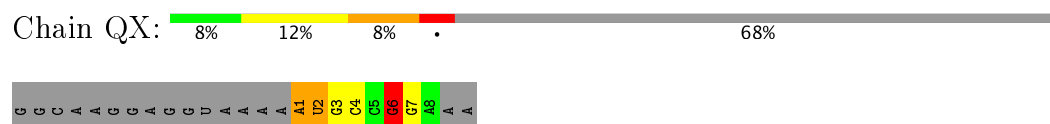
- Molecule 53: P-site tRNA fMET



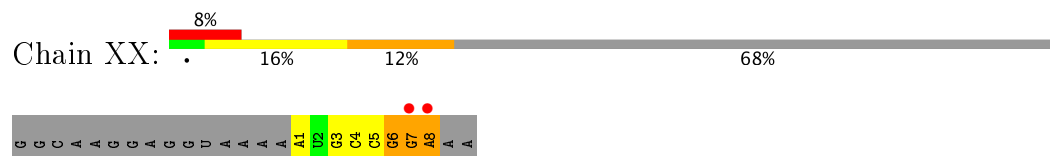
- Molecule 53: P-site tRNA fMET



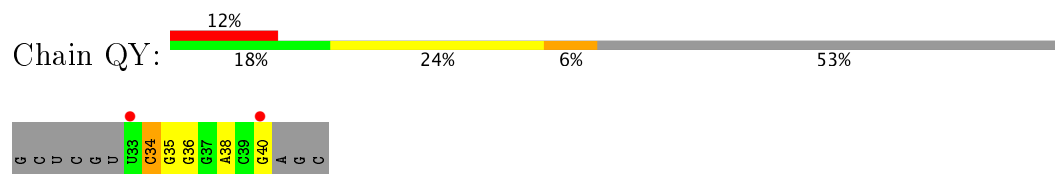
- Molecule 54: mRNA



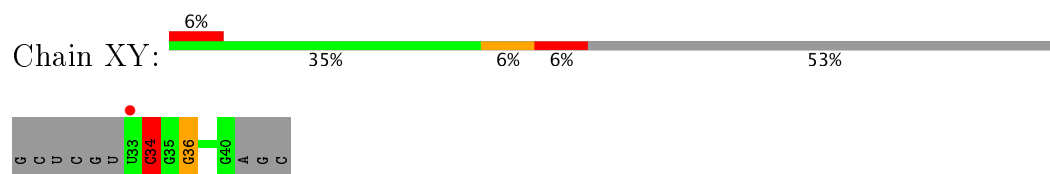
- Molecule 54: mRNA



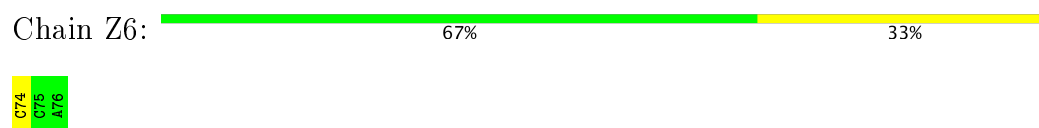
- Molecule 55: A site ASL of tRNA-Proline CGG (unmodified)



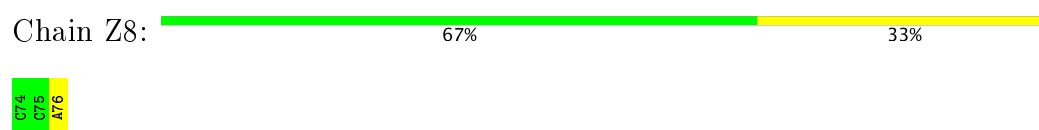
- Molecule 55: A site ASL of tRNA-Proline CGG (unmodified)



- 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	209.82Å 447.39Å 619.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	187.58 – 3.68 189.96 – 3.54	Depositor EDS
% Data completeness (in resolution range)	99.1 (187.58-3.68) 99.2 (189.96-3.54)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.212 , 0.272 0.212 , 0.272	Depositor DCC
R_{free} test set	27977 reflections (4.51%)	DCC
Wilson B-factor (Å ²)	83.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 77.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	291730	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 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	0.59	3/36098 (0.0%)	1.21	155/56341 (0.3%)
1	XA	0.65	1/36101 (0.0%)	1.27	208/56346 (0.4%)
2	QB	0.31	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.31	0/1629	0.53	0/2195
3	XC	0.37	0/1629	0.56	0/2195
4	QD	0.38	0/1733	0.58	1/2318 (0.0%)
4	XD	0.40	0/1733	0.60	0/2318
5	QE	0.35	0/1171	0.56	0/1576
5	XE	0.39	0/1171	0.59	0/1576
6	QF	0.38	0/856	0.54	0/1154
6	XF	0.38	0/856	0.58	0/1154
7	QG	0.33	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.50	0/1709
8	QH	0.33	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.55	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.33	0/814	0.54	0/1095
10	XJ	0.35	0/814	0.60	0/1095
11	QK	0.36	0/900	0.57	0/1213
11	XK	0.39	0/900	0.58	0/1213
12	QL	0.37	0/991	0.61	0/1327
12	XL	0.45	0/991	0.74	1/1327 (0.1%)
13	QM	0.32	0/974	0.59	0/1303
13	XM	0.37	0/974	0.63	0/1303
14	QN	0.41	0/501	0.60	0/664
14	XN	0.42	0/501	0.66	0/664
15	QO	0.35	0/745	0.54	0/992
15	XO	0.39	0/745	0.54	0/992
16	QP	0.36	0/721	0.57	0/970
16	XP	0.35	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.35	0/847	0.54	0/1131
17	XQ	0.35	0/847	0.54	0/1131
18	QR	0.35	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.59	0/768
19	QS	0.33	0/689	0.61	0/926
19	XS	0.38	0/689	0.69	1/926 (0.1%)
20	QT	0.36	0/765	0.64	0/1007
20	XT	0.31	0/765	0.59	0/1007
21	QU	0.31	0/221	0.54	0/288
21	XU	0.31	0/221	0.62	0/288
22	RA	0.72	8/69521 (0.0%)	1.34	555/108529 (0.5%)
22	YA	0.80	28/69543 (0.0%)	1.43	823/108563 (0.8%)
23	RB	0.58	0/2878	1.22	15/4490 (0.3%)
23	YB	0.63	0/2878	1.28	17/4490 (0.4%)
24	RD	0.51	0/2165	0.70	0/2919
24	YD	0.58	0/2165	0.78	1/2919 (0.0%)
25	RE	0.43	0/1601	0.73	3/2160 (0.1%)
25	YE	0.46	0/1601	0.75	2/2160 (0.1%)
26	RF	0.42	0/1620	0.62	0/2194
26	YF	0.48	0/1620	0.71	1/2194 (0.0%)
27	RG	0.31	0/1499	0.57	1/2016 (0.0%)
27	YG	0.40	0/1499	0.60	0/2016
28	RH	0.29	0/1332	0.58	0/1802
28	YH	0.45	0/1332	0.73	0/1802
29	RI	0.52	0/1151	0.79	1/1558 (0.1%)
29	YI	0.55	0/1151	0.80	0/1558
30	RN	0.41	0/1131	0.62	0/1525
30	YN	0.43	0/1131	0.64	0/1525
31	RO	0.41	0/943	0.62	1/1269 (0.1%)
31	YO	0.50	0/943	0.65	0/1269
32	RP	0.44	0/1162	0.81	1/1544 (0.1%)
32	YP	0.49	0/1162	0.90	2/1544 (0.1%)
33	RQ	0.47	0/1143	0.74	2/1527 (0.1%)
33	YQ	0.57	0/1143	0.80	1/1527 (0.1%)
34	RR	0.42	0/982	0.69	0/1312
34	YR	0.44	0/982	0.73	0/1312
35	RS	0.36	0/892	0.65	0/1187
35	YS	0.40	0/892	0.75	1/1187 (0.1%)
36	RT	0.42	0/1155	0.63	0/1542
36	YT	0.44	0/1155	0.67	0/1542
37	RU	0.40	0/982	0.65	0/1306
37	YU	0.50	0/982	0.68	0/1306
38	RV	0.38	0/790	0.61	1/1057 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YV	0.45	0/790	0.73	1/1057 (0.1%)
39	RW	0.49	0/911	0.67	0/1220
39	YW	0.45	0/911	0.68	0/1220
40	RX	0.47	0/739	0.62	0/993
40	YX	0.49	0/739	0.66	0/993
41	RY	0.44	0/798	0.68	0/1064
41	YY	0.46	0/798	0.70	0/1064
42	RZ	0.58	1/1493 (0.1%)	0.77	0/2026
42	YZ	0.56	0/1493	0.79	1/2026 (0.0%)
43	R0	0.65	0/657	0.80	0/874
43	Y0	0.74	1/657 (0.2%)	0.90	1/874 (0.1%)
44	R1	0.44	0/770	0.66	0/1022
44	Y1	0.46	0/770	0.69	0/1022
45	R2	0.39	0/583	0.65	0/771
45	Y2	0.52	0/583	0.73	0/771
46	R3	0.35	0/474	0.57	0/635
46	Y3	0.41	0/474	0.59	0/635
47	R4	0.33	0/594	0.68	0/795
47	Y4	0.37	0/594	0.68	0/795
48	R5	0.44	0/473	0.73	0/639
48	Y5	0.43	0/473	0.77	1/639 (0.2%)
49	R6	0.35	0/431	0.69	0/575
49	Y6	0.37	0/431	0.67	0/575
50	R7	0.49	0/438	0.68	0/575
50	Y7	0.57	0/438	0.71	0/575
51	R8	0.55	0/525	0.79	0/691
51	Y8	0.58	0/525	0.82	0/691
52	R9	0.26	0/310	0.45	0/407
52	Y9	0.32	0/310	0.48	0/407
53	QV	0.85	1/1836 (0.1%)	1.45	24/2859 (0.8%)
53	XV	0.89	1/1836 (0.1%)	1.54	25/2859 (0.9%)
54	QX	0.95	0/193	1.91	7/299 (2.3%)
54	XX	1.12	0/193	1.83	4/299 (1.3%)
55	QY	0.68	0/194	1.53	0/301
55	XY	0.72	0/194	1.25	1/301 (0.3%)
56	Z6	0.74	0/40	1.58	1/60 (1.7%)
56	Z8	0.92	0/40	1.50	0/60
All	All	0.64	44/316105 (0.0%)	1.20	1861/472575 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	QL	0	1
12	XL	0	1
25	RE	0	1
25	YE	0	1
26	YF	0	1
28	RH	0	2
28	YH	0	2
29	RI	0	1
35	YS	0	1
42	YZ	0	2
45	Y2	0	1
47	R4	0	1
51	R8	0	2
51	Y8	0	2
All	All	0	19

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	QV	1	C	OP3-P	-10.81	1.48	1.61
53	XV	1	C	OP3-P	-10.09	1.49	1.61
22	YA	783	A	N9-C4	-8.12	1.32	1.37
22	YA	2542	A	N9-C4	-7.43	1.33	1.37
22	YA	1966	A	N9-C4	-7.42	1.33	1.37

The worst 5 of 1861 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	QV	75	C	O5'-P-OP2	-13.28	93.75	105.70
22	YA	774	A	C2-N3-C4	-12.25	104.47	110.60
22	RA	1931	U	N3-C2-O2	-12.05	113.77	122.20
22	YA	1332	G	C6-C5-N7	-11.94	123.24	130.40
22	YA	450	G	C5-C6-N1	-11.37	105.81	111.50

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	QL	47	LYS	Peptide
25	RE	21	VAL	Peptide
28	RH	127	GLU	Peptide
28	RH	153	LYS	Peptide

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Mol	Chain	Res	Type	Group
29	RI	134	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16277	775	0
1	XA	32249	0	16279	824	0
2	QB	1924	0	1975	64	0
2	XB	1924	0	1975	83	0
3	QC	1605	0	1668	50	0
3	XC	1605	0	1668	63	0
4	QD	1703	0	1763	68	0
4	XD	1703	0	1764	48	0
5	QE	1155	0	1213	36	0
5	XE	1155	0	1213	43	0
6	QF	843	0	857	20	0
6	XF	843	0	857	23	0
7	QG	1257	0	1296	41	0
7	XG	1257	0	1296	30	0
8	QH	1116	0	1177	40	0
8	XH	1116	0	1177	32	0
9	QI	1010	0	1037	43	0
9	XI	1010	0	1037	60	0
10	QJ	801	0	849	50	0
10	XJ	801	0	849	40	0
11	QK	885	0	904	29	0
11	XK	885	0	904	33	0
12	QL	975	0	1062	43	0
12	XL	975	0	1062	47	0
13	QM	964	0	1034	46	0
13	XM	964	0	1034	62	0
14	QN	492	0	529	27	0
14	XN	492	0	529	23	0
15	QO	734	0	771	23	0
15	XO	734	0	771	22	0
16	QP	705	0	725	21	0
16	XP	705	0	725	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	QQ	834	0	904	26	0
17	XQ	834	0	904	20	0
18	QR	574	0	644	13	0
18	XR	574	0	644	21	0
19	QS	674	0	699	39	0
19	XS	674	0	699	55	0
20	QT	763	0	861	25	0
20	XT	763	0	861	40	0
21	QU	217	0	234	12	0
21	XU	217	0	234	8	0
22	RA	62071	0	31292	1370	0
22	YA	62091	0	31301	1336	1
23	RB	2573	0	1306	57	0
23	YB	2573	0	1306	64	1
24	RD	2115	0	2195	107	0
24	YD	2115	0	2195	106	0
25	RE	1568	0	1634	67	0
25	YE	1568	0	1634	68	0
26	RF	1585	0	1632	76	0
26	YF	1585	0	1632	64	0
27	RG	1474	0	1535	62	0
27	YG	1474	0	1535	69	0
28	RH	1307	0	1382	67	0
28	YH	1307	0	1382	62	0
29	RI	1136	0	1223	84	0
29	YI	1136	0	1223	73	0
30	RN	1104	0	1180	38	0
30	YN	1104	0	1180	51	0
31	RO	933	0	996	23	0
31	YO	933	0	996	25	0
32	RP	1145	0	1227	79	0
32	YP	1145	0	1228	95	0
33	RQ	1122	0	1179	58	0
33	YQ	1122	0	1179	49	0
34	RR	968	0	1033	48	0
34	YR	968	0	1033	37	0
35	RS	882	0	943	45	0
35	YS	882	0	943	43	0
36	RT	1141	0	1202	51	0
36	YT	1141	0	1202	56	0
37	RU	964	0	1022	36	0
37	YU	964	0	1022	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	RV	779	0	852	24	0
38	YV	779	0	852	43	0
39	RW	900	0	964	28	0
39	YW	900	0	964	26	0
40	RX	725	0	778	31	0
40	YX	725	0	778	24	0
41	RY	785	0	878	52	0
41	YY	785	0	878	43	0
42	RZ	1461	0	1493	96	0
42	YZ	1461	0	1493	104	0
43	R0	648	0	671	37	0
43	Y0	648	0	672	41	0
44	R1	763	0	848	32	0
44	Y1	763	0	848	36	0
45	R2	581	0	629	14	0
45	Y2	581	0	629	23	0
46	R3	469	0	518	7	0
46	Y3	469	0	518	15	0
47	R4	581	0	574	30	0
47	Y4	581	0	574	76	0
48	R5	459	0	480	30	0
48	Y5	459	0	480	31	0
49	R6	424	0	450	30	0
49	Y6	424	0	450	29	0
50	R7	430	0	480	17	0
50	Y7	430	0	480	19	0
51	R8	517	0	582	36	0
51	Y8	517	0	582	43	0
52	R9	307	0	338	14	0
52	Y9	307	0	338	17	0
53	QV	1644	0	836	29	0
53	XV	1644	0	836	36	0
54	QX	173	0	88	3	0
54	XX	173	0	88	3	0
55	QY	174	0	88	4	0
55	XY	174	0	88	2	0
56	Z6	74	0	51	0	0
56	Z8	74	0	51	4	0
57	QA	42	0	45	1	0
57	XA	42	0	45	2	0
58	QA	76	0	0	0	0
58	QF	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	QM	1	0	0	0	0
58	QV	1	0	0	0	0
58	R0	1	0	0	0	0
58	R5	1	0	0	0	0
58	R8	2	0	0	0	0
58	RA	247	0	0	0	0
58	RB	2	0	0	0	0
58	RD	1	0	0	0	0
58	RE	2	0	0	0	0
58	RF	1	0	0	0	0
58	RP	2	0	0	0	0
58	XA	82	0	0	0	0
58	XB	1	0	0	0	0
58	XM	1	0	0	0	0
58	XV	2	0	0	0	0
58	Y0	1	0	0	0	0
58	Y5	1	0	0	0	0
58	YA	265	0	0	0	0
58	YB	3	0	0	0	0
58	YD	2	0	0	0	0
58	YP	2	0	0	0	0
58	YQ	1	0	0	0	0
58	YX	1	0	0	0	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	291730	0	198220	7613	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 7613 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)
22:RA:2701:C:H3'	22:RA:2702:U:H5''	1.27	1.07
1:XA:963:G:N3	10:XJ:55:LYS:NZ	2.02	1.07
24:YD:43:ARG:NH1	24:YD:44:ASN:OD1	1.86	1.06
22:YA:2701:C:H3'	22:YA:2702:U:H5''	1.38	1.05
22:YA:1138:G:H21	30:YN:106:MET:HE3	1.22	1.04

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:YA:1593:G:O2'	23:YB:54:G:OP1[1_655]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	174 (74%)	44 (19%)	17 (7%)	1	19
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1	23
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	5	41
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	12	54
4	QD	206/209 (99%)	176 (85%)	24 (12%)	6 (3%)	5	42
4	XD	206/209 (99%)	177 (86%)	24 (12%)	5 (2%)	7	46
5	QE	149/162 (92%)	136 (91%)	8 (5%)	5 (3%)	4	39
5	XE	149/162 (92%)	133 (89%)	13 (9%)	3 (2%)	9	49
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	14	57
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	14	57
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	25	68
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	5	42
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3	34
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	5	40
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	5	41
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	27
11	QK	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	6	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	11	52
12	QL	123/132 (93%)	98 (80%)	18 (15%)	7 (6%)	2	25
12	XL	123/132 (93%)	98 (80%)	15 (12%)	10 (8%)	1	15
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	17
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	17
14	QN	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	20
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	10
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	15	58
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	7	47
16	QP	82/88 (93%)	74 (90%)	7 (8%)	1 (1%)	15	58
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	15	58
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	9	49
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	3	31
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	12	54
19	QS	82/93 (88%)	56 (68%)	15 (18%)	11 (13%)	0	5
19	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	5
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	2	23
20	XT	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	2	23
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	3	32
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	3	32
24	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	3	31
24	YD	270/276 (98%)	227 (84%)	34 (13%)	9 (3%)	4	39
25	RE	203/206 (98%)	147 (72%)	36 (18%)	20 (10%)	1	11
25	YE	203/206 (98%)	142 (70%)	41 (20%)	20 (10%)	1	11
26	RF	200/210 (95%)	167 (84%)	20 (10%)	13 (6%)	1	22
26	YF	200/210 (95%)	167 (84%)	25 (12%)	8 (4%)	3	34
27	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	16
27	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	21
28	RH	168/180 (93%)	114 (68%)	33 (20%)	21 (12%)	0	7
28	YH	168/180 (93%)	121 (72%)	23 (14%)	24 (14%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	RI	144/148 (97%)	94 (65%)	31 (22%)	19 (13%)	0	6
29	YI	144/148 (97%)	100 (69%)	23 (16%)	21 (15%)	0	5
30	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	13
30	YN	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	0	10
31	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	11	52
31	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	11	52
32	RP	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	1	12
32	YP	148/150 (99%)	108 (73%)	23 (16%)	17 (12%)	0	7
33	RQ	139/141 (99%)	99 (71%)	22 (16%)	18 (13%)	0	6
33	YQ	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	5
34	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	3	32
34	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2	27
35	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	1	11
35	YS	109/112 (97%)	78 (72%)	18 (16%)	13 (12%)	0	7
36	RT	135/146 (92%)	106 (78%)	17 (13%)	12 (9%)	1	13
36	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	18
37	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	4	38
37	YU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	4	38
38	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	2	23
38	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	15
39	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	4	37
39	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	10	51
40	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	8	47
40	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	8	47
41	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	4
41	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	7
42	RZ	181/206 (88%)	118 (65%)	35 (19%)	28 (16%)	0	4
42	YZ	181/206 (88%)	113 (62%)	46 (25%)	22 (12%)	0	7
43	R0	80/85 (94%)	61 (76%)	15 (19%)	4 (5%)	2	28
43	Y0	80/85 (94%)	66 (82%)	13 (16%)	1 (1%)	14	57
44	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	23
45	R2	67/72 (93%)	53 (79%)	9 (13%)	5 (8%)	1	17
45	Y2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	1	13
46	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	4	38
46	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	10	51
47	R4	69/71 (97%)	35 (51%)	18 (26%)	16 (23%)	0	1
47	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
48	R5	57/60 (95%)	44 (77%)	11 (19%)	2 (4%)	4	38
48	Y5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	4	38
49	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	1
49	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	3
50	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	8	48
50	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	8	48
51	R8	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1	15
51	Y8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	22
52	R9	35/37 (95%)	35 (100%)	0	0	100	100
52	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	9180 (80%)	1546 (14%)	744 (6%)	1	22

5 of 744 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	28	SER
13	QM	67	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	172 (84%)	33 (16%)	3	20
2	XB	205/220 (93%)	180 (88%)	25 (12%)	6	32
3	QC	159/188 (85%)	145 (91%)	14 (9%)	12	47
3	XC	159/188 (85%)	146 (92%)	13 (8%)	13	50
4	QD	180/181 (99%)	157 (87%)	23 (13%)	5	30
4	XD	180/181 (99%)	154 (86%)	26 (14%)	4	25
5	QE	116/123 (94%)	104 (90%)	12 (10%)	8	39
5	XE	116/123 (94%)	104 (90%)	12 (10%)	8	39
6	QF	90/90 (100%)	78 (87%)	12 (13%)	4	29
6	XF	90/90 (100%)	82 (91%)	8 (9%)	11	47
7	QG	126/127 (99%)	114 (90%)	12 (10%)	10	44
7	XG	126/127 (99%)	114 (90%)	12 (10%)	10	44
8	QH	119/119 (100%)	109 (92%)	10 (8%)	13	49
8	XH	119/119 (100%)	106 (89%)	13 (11%)	7	37
9	QI	98/99 (99%)	81 (83%)	17 (17%)	2	16
9	XI	98/99 (99%)	80 (82%)	18 (18%)	2	13
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4	28
10	XJ	89/92 (97%)	74 (83%)	15 (17%)	2	17
11	QK	90/99 (91%)	81 (90%)	9 (10%)	9	41
11	XK	90/99 (91%)	82 (91%)	8 (9%)	11	47
12	QL	104/109 (95%)	87 (84%)	17 (16%)	3	19
12	XL	104/109 (95%)	93 (89%)	11 (11%)	8	38
13	QM	97/101 (96%)	73 (75%)	24 (25%)	1	6
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	11
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	13
14	XN	49/50 (98%)	42 (86%)	7 (14%)	4	26
15	QO	79/80 (99%)	72 (91%)	7 (9%)	11	47
15	XO	79/80 (99%)	69 (87%)	10 (13%)	5	30
16	QP	72/74 (97%)	63 (88%)	9 (12%)	5	31
16	XP	72/74 (97%)	63 (88%)	9 (12%)	5	31
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	13	49
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	21	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	QR	61/77 (79%)	50 (82%)	11 (18%)	2	14
18	XR	61/77 (79%)	52 (85%)	9 (15%)	3	24
19	QS	73/80 (91%)	59 (81%)	14 (19%)	1	11
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	8
20	QT	76/82 (93%)	67 (88%)	9 (12%)	6	33
20	XT	76/82 (93%)	66 (87%)	10 (13%)	5	29
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	28	66
24	RD	214/218 (98%)	174 (81%)	40 (19%)	2	12
24	YD	214/218 (98%)	181 (85%)	33 (15%)	3	22
25	RE	165/166 (99%)	126 (76%)	39 (24%)	1	6
25	YE	165/166 (99%)	137 (83%)	28 (17%)	2	17
26	RF	161/166 (97%)	132 (82%)	29 (18%)	2	14
26	YF	161/166 (97%)	137 (85%)	24 (15%)	3	24
27	RG	155/156 (99%)	134 (86%)	21 (14%)	4	28
27	YG	155/156 (99%)	133 (86%)	22 (14%)	4	26
28	RH	142/148 (96%)	120 (84%)	22 (16%)	3	22
28	YH	142/148 (96%)	117 (82%)	25 (18%)	2	15
29	RI	122/124 (98%)	86 (70%)	36 (30%)	0	3
29	YI	122/124 (98%)	85 (70%)	37 (30%)	0	3
30	RN	117/119 (98%)	97 (83%)	20 (17%)	2	17
30	YN	117/119 (98%)	96 (82%)	21 (18%)	2	14
31	RO	100/100 (100%)	90 (90%)	10 (10%)	9	41
31	YO	100/100 (100%)	88 (88%)	12 (12%)	6	32
32	RP	116/116 (100%)	85 (73%)	31 (27%)	0	4
32	YP	116/116 (100%)	82 (71%)	34 (29%)	0	3
33	RQ	111/111 (100%)	95 (86%)	16 (14%)	4	25
33	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	17
34	RR	101/101 (100%)	83 (82%)	18 (18%)	2	14
34	YR	101/101 (100%)	81 (80%)	20 (20%)	1	10
35	RS	87/88 (99%)	69 (79%)	18 (21%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	YS	87/88 (99%)	68 (78%)	19 (22%)	1	8
36	RT	120/127 (94%)	102 (85%)	18 (15%)	3	23
36	YT	120/127 (94%)	98 (82%)	22 (18%)	2	13
37	RU	93/94 (99%)	78 (84%)	15 (16%)	3	20
37	YU	93/94 (99%)	77 (83%)	16 (17%)	2	16
38	RV	82/82 (100%)	66 (80%)	16 (20%)	1	11
38	YV	82/82 (100%)	67 (82%)	15 (18%)	2	13
39	RW	92/92 (100%)	73 (79%)	19 (21%)	1	9
39	YW	92/92 (100%)	76 (83%)	16 (17%)	2	15
40	RX	74/78 (95%)	64 (86%)	10 (14%)	4	28
40	YX	74/78 (95%)	60 (81%)	14 (19%)	2	12
41	RY	85/91 (93%)	63 (74%)	22 (26%)	0	5
41	YY	85/91 (93%)	64 (75%)	21 (25%)	1	6
42	RZ	162/179 (90%)	131 (81%)	31 (19%)	2	11
42	YZ	162/179 (90%)	121 (75%)	41 (25%)	0	5
43	R0	65/67 (97%)	56 (86%)	9 (14%)	4	27
43	Y0	65/67 (97%)	53 (82%)	12 (18%)	2	12
44	R1	82/83 (99%)	73 (89%)	9 (11%)	7	37
44	Y1	82/83 (99%)	70 (85%)	12 (15%)	3	25
45	R2	64/67 (96%)	57 (89%)	7 (11%)	7	37
45	Y2	64/67 (96%)	47 (73%)	17 (27%)	0	4
46	R3	51/52 (98%)	45 (88%)	6 (12%)	6	33
46	Y3	51/52 (98%)	43 (84%)	8 (16%)	3	21
47	R4	63/63 (100%)	45 (71%)	18 (29%)	0	3
47	Y4	63/63 (100%)	43 (68%)	20 (32%)	0	2
48	R5	51/52 (98%)	37 (72%)	14 (28%)	0	4
48	Y5	51/52 (98%)	37 (72%)	14 (28%)	0	4
49	R6	48/52 (92%)	35 (73%)	13 (27%)	0	4
49	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	9
50	R7	42/42 (100%)	34 (81%)	8 (19%)	2	12
50	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	R8	54/55 (98%)	44 (82%)	10 (18%)	2	12
51	Y8	54/55 (98%)	41 (76%)	13 (24%)	1	6
52	R9	34/34 (100%)	32 (94%)	2 (6%)	23	62
52	Y9	34/34 (100%)	32 (94%)	2 (6%)	23	62
All	All	9702/10066 (96%)	8111 (84%)	1591 (16%)	2	19

5 of 1591 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	R3	8	LEU
8	XH	41	ARG
42	YZ	153	SER
47	R4	67	TYR
2	XB	178	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
28	RH	147	ASN
29	RI	104	GLN
2	XB	204	ASN
25	RE	143	ASN
28	RH	143	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	341 (22%)	49 (3%)
1	XA	1498/1522 (98%)	352 (23%)	40 (2%)
22	RA	2879/2916 (98%)	747 (25%)	65 (2%)
22	YA	2880/2916 (98%)	734 (25%)	57 (1%)
23	RB	119/122 (97%)	29 (24%)	2 (1%)
23	YB	119/122 (97%)	32 (26%)	1 (0%)
53	QV	76/77 (98%)	22 (28%)	1 (1%)
53	XV	76/77 (98%)	24 (31%)	3 (3%)
54	QX	7/25 (28%)	4 (57%)	1 (14%)
54	XX	7/25 (28%)	3 (42%)	1 (14%)
55	QY	7/17 (41%)	3 (42%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	XY	7/17 (41%)	2 (28%)	0
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9175/9364 (97%)	2293 (24%)	220 (2%)

5 of 2293 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	7	G
1	QA	9	G
1	QA	22	G
1	QA	32	A
1	QA	39	G

5 of 220 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	RA	2351	G
1	XA	244	U
22	YA	2422	A
22	RA	2439	A
22	RA	2776	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PPU	Z6	76	56,22	31,40,41	1.02	1 (3%)	34,57,60	2.28	11 (32%)
56	PPU	Z8	76	56,22	31,40,41	1.05	2 (6%)	34,57,60	1.93	10 (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
56	PPU	Z6	76	56,22	-	0/21/43/44	0/4/4/4
56	PPU	Z8	76	56,22	-	0/21/43/44	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	C2'-C3'	-2.41	1.49	1.53
56	Z8	76	PPU	C5-C4	2.71	1.46	1.40
56	Z6	76	PPU	C5-C4	3.02	1.47	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-5.98	114.20	123.21
56	Z6	76	PPU	N3-C2-N1	-4.89	124.60	128.86
56	Z8	76	PPU	N3-C2-N1	-4.37	125.05	128.86
56	Z6	76	PPU	C10-N6-C6	-3.29	109.56	119.51
56	Z8	76	PPU	O2'-C2'-C3'	-3.05	103.55	111.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z8	76	PPU	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 706 ligands modelled in this entry, 704 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
57	PAR	QA	1601	-	45,45,45	1.33	7 (15%)	60,67,67	1.42	8 (13%)
57	PAR	XA	1601	-	45,45,45	1.37	6 (13%)	60,67,67	1.36	5 (8%)

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
57	PAR	QA	1601	-	-	0/18/94/94	0/4/4/4
57	PAR	XA	1601	-	-	0/18/94/94	0/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	QA	1601	PAR	C31-C21	2.03	1.56	1.53
57	QA	1601	PAR	C14-C24	2.05	1.56	1.52
57	XA	1601	PAR	C14-C24	2.16	1.56	1.52
57	QA	1601	PAR	C11-C21	2.33	1.57	1.52
57	QA	1601	PAR	O51-C11	2.41	1.47	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	QA	1601	PAR	O11-C42-C32	-3.13	101.71	108.96
57	QA	1601	PAR	O54-C54-C44	-2.07	105.85	109.66
57	QA	1601	PAR	C22-C32-C42	2.04	114.77	109.54
57	XA	1601	PAR	C11-O51-C51	2.66	118.72	113.72
57	XA	1601	PAR	O54-C54-C64	2.82	111.35	106.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	QA	1601	PAR	1	0
57	XA	1601	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%)	0.42	76 (5%) 29 20	28, 70, 146, 264	0
1	XA	1500/1522 (98%)	0.54	83 (5%) 26 17	18, 64, 151, 247	0
2	QB	237/256 (92%)	0.13	9 (3%) 41 29	48, 115, 166, 191	0
2	XB	237/256 (92%)	-0.23	1 (0%) 92 87	35, 98, 150, 194	0
3	QC	205/239 (85%)	0.52	10 (4%) 30 21	45, 105, 149, 166	0
3	XC	205/239 (85%)	0.15	2 (0%) 82 71	35, 78, 130, 168	0
4	QD	208/209 (99%)	0.46	10 (4%) 31 21	27, 79, 119, 169	0
4	XD	208/209 (99%)	0.30	4 (1%) 67 53	34, 75, 127, 151	0
5	QE	151/162 (93%)	0.45	7 (4%) 33 23	37, 88, 135, 167	0
5	XE	151/162 (93%)	0.29	3 (1%) 65 51	29, 65, 115, 148	0
6	QF	101/101 (100%)	-0.20	1 (0%) 82 71	21, 76, 112, 185	0
6	XF	101/101 (100%)	0.21	0 100 100	32, 72, 115, 153	0
7	QG	155/156 (99%)	0.57	22 (14%) 3 3	46, 96, 152, 185	0
7	XG	155/156 (99%)	0.31	9 (5%) 24 16	40, 87, 145, 167	0
8	QH	138/138 (100%)	0.29	2 (1%) 75 62	41, 90, 125, 153	0
8	XH	138/138 (100%)	0.28	3 (2%) 62 48	33, 72, 108, 149	0
9	QI	127/128 (99%)	1.38	35 (27%) 1 1	67, 109, 148, 172	0
9	XI	127/128 (99%)	0.65	15 (11%) 5 5	28, 99, 147, 164	0
10	QJ	99/105 (94%)	0.96	16 (16%) 2 2	59, 114, 165, 205	0
10	XJ	99/105 (94%)	0.90	16 (16%) 2 2	41, 103, 147, 171	0
11	QK	119/129 (92%)	0.54	7 (5%) 23 15	35, 79, 130, 177	0
11	XK	119/129 (92%)	0.68	6 (5%) 30 20	24, 71, 125, 182	0
12	QL	125/132 (94%)	1.06	15 (12%) 5 5	30, 70, 120, 182	0
12	XL	125/132 (94%)	0.91	23 (18%) 1 1	15, 58, 120, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	1.20	30 (24%) 1 1	36, 106, 144, 196	0
13	XM	121/126 (96%)	0.53	10 (8%) 12 9	38, 88, 137, 187	0
14	QN	60/61 (98%)	2.07	30 (50%) 0 1	58, 97, 124, 142	0
14	XN	60/61 (98%)	1.09	9 (15%) 3 2	34, 75, 109, 125	0
15	QO	88/89 (98%)	0.01	0 100 100	30, 79, 123, 154	0
15	XO	88/89 (98%)	0.25	1 (1%) 80 68	28, 73, 108, 124	0
16	QP	84/88 (95%)	0.44	1 (1%) 79 66	35, 69, 107, 152	0
16	XP	84/88 (95%)	1.13	18 (21%) 1 1	34, 74, 129, 163	0
17	QQ	100/105 (95%)	1.01	14 (14%) 3 3	24, 83, 122, 140	0
17	XQ	100/105 (95%)	0.98	14 (14%) 3 3	39, 78, 113, 165	0
18	QR	70/88 (79%)	0.06	1 (1%) 75 62	26, 78, 137, 167	0
18	XR	70/88 (79%)	0.31	3 (4%) 36 24	24, 70, 120, 147	0
19	QS	84/93 (90%)	1.70	32 (38%) 0 1	68, 111, 151, 176	0
19	XS	84/93 (90%)	0.60	8 (9%) 9 7	32, 97, 148, 177	0
20	QT	99/106 (93%)	0.91	9 (9%) 10 7	34, 79, 133, 144	0
20	XT	99/106 (93%)	1.62	34 (34%) 0 1	44, 88, 140, 174	0
21	QU	25/27 (92%)	3.32	20 (80%) 0 0	36, 102, 144, 147	0
21	XU	25/27 (92%)	2.34	15 (60%) 0 1	67, 92, 119, 132	0
22	RA	2882/2916 (98%)	0.47	146 (5%) 29 20	14, 51, 198, 261	0
22	YA	2883/2916 (98%)	0.41	106 (3%) 42 30	8, 43, 187, 292	0
23	RB	120/122 (98%)	-0.05	1 (0%) 86 76	53, 81, 118, 144	0
23	YB	120/122 (98%)	-0.03	1 (0%) 86 76	36, 67, 98, 136	0
24	RD	272/276 (98%)	0.33	4 (1%) 74 61	9, 50, 100, 155	0
24	YD	272/276 (98%)	0.59	5 (1%) 69 55	2, 42, 86, 187	0
25	RE	205/206 (99%)	0.38	7 (3%) 46 33	17, 61, 126, 193	0
25	YE	205/206 (99%)	0.19	2 (0%) 82 71	3, 56, 124, 170	0
26	RF	202/210 (96%)	-0.04	0 100 100	9, 61, 124, 182	0
26	YF	202/210 (96%)	0.01	1 (0%) 90 84	10, 53, 113, 148	0
27	RG	181/182 (99%)	0.49	9 (4%) 30 20	42, 97, 145, 178	0
27	YG	181/182 (99%)	0.13	4 (2%) 62 48	40, 80, 130, 201	0
28	RH	170/180 (94%)	1.84	67 (39%) 0 1	67, 134, 177, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YH	170/180 (94%)	-0.05	1 (0%) 89 82	24, 76, 126, 177	0
29	RI	146/148 (98%)	0.05	3 (2%) 64 50	24, 87, 130, 181	0
29	YI	146/148 (98%)	-0.03	3 (2%) 64 50	19, 86, 127, 152	0
30	RN	138/140 (98%)	0.44	7 (5%) 29 20	29, 68, 121, 174	0
30	YN	138/140 (98%)	0.11	0 100 100	13, 56, 111, 173	0
31	RO	122/122 (100%)	0.53	3 (2%) 58 43	11, 55, 102, 158	0
31	YO	122/122 (100%)	0.90	11 (9%) 10 7	9, 51, 88, 123	0
32	RP	150/150 (100%)	0.63	11 (7%) 16 11	13, 69, 133, 176	0
32	YP	150/150 (100%)	0.41	5 (3%) 47 34	12, 61, 122, 182	0
33	RQ	141/141 (100%)	1.22	29 (20%) 1 1	29, 71, 124, 164	0
33	YQ	141/141 (100%)	0.43	4 (2%) 53 39	16, 56, 115, 152	0
34	RR	118/118 (100%)	0.43	4 (3%) 46 33	3, 55, 102, 136	0
34	YR	118/118 (100%)	0.76	5 (4%) 37 25	27, 57, 95, 140	0
35	RS	111/112 (99%)	0.66	10 (9%) 10 7	34, 80, 124, 162	0
35	YS	111/112 (99%)	0.17	2 (1%) 69 55	27, 73, 113, 138	0
36	RT	137/146 (93%)	0.53	7 (5%) 29 20	27, 67, 143, 169	0
36	YT	137/146 (93%)	0.53	4 (2%) 52 38	19, 65, 135, 172	0
37	RU	117/118 (99%)	0.21	2 (1%) 70 57	12, 62, 111, 167	0
37	YU	117/118 (99%)	0.36	2 (1%) 70 57	13, 45, 111, 172	0
38	RV	101/101 (100%)	0.03	2 (1%) 65 51	16, 78, 131, 186	0
38	YV	101/101 (100%)	0.34	3 (2%) 51 36	21, 68, 139, 214	0
39	RW	113/113 (100%)	0.29	1 (0%) 84 73	15, 47, 106, 158	0
39	YW	113/113 (100%)	0.26	2 (1%) 69 55	16, 46, 106, 168	0
40	RX	92/96 (95%)	0.34	0 100 100	17, 56, 103, 130	0
40	YX	92/96 (95%)	0.09	0 100 100	9, 42, 86, 138	0
41	RY	102/110 (92%)	0.41	1 (0%) 82 71	28, 86, 142, 176	0
41	YY	102/110 (92%)	0.08	1 (0%) 82 71	30, 73, 138, 185	0
42	RZ	183/206 (88%)	0.42	12 (6%) 19 13	45, 92, 141, 160	0
42	YZ	183/206 (88%)	-0.18	1 (0%) 90 84	21, 82, 136, 178	0
43	R0	82/85 (96%)	0.98	7 (8%) 11 9	9, 51, 88, 102	0
43	Y0	82/85 (96%)	0.35	0 100 100	20, 48, 73, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	R1	97/98 (98%)	0.82	6 (6%) 21 14	13, 60, 144, 182	0
44	Y1	97/98 (98%)	1.05	11 (11%) 6 5	7, 53, 136, 172	0
45	R2	69/72 (95%)	-0.06	0 100 100	36, 77, 136, 164	0
45	Y2	69/72 (95%)	-0.06	0 100 100	18, 57, 116, 159	0
46	R3	59/60 (98%)	0.80	2 (3%) 46 33	33, 76, 118, 142	0
46	Y3	59/60 (98%)	0.03	1 (1%) 70 57	19, 57, 109, 169	0
47	R4	71/71 (100%)	0.87	12 (16%) 2 2	61, 142, 196, 236	0
47	Y4	71/71 (100%)	0.14	5 (7%) 17 12	58, 131, 182, 223	0
48	R5	59/60 (98%)	0.42	2 (3%) 46 33	12, 66, 149, 160	0
48	Y5	59/60 (98%)	0.85	8 (13%) 3 3	17, 64, 166, 185	0
49	R6	49/54 (90%)	4.51	44 (89%) 0 0	101, 159, 184, 200	0
49	Y6	49/54 (90%)	3.64	42 (85%) 0 0	95, 152, 182, 209	0
50	R7	49/49 (100%)	0.39	2 (4%) 38 26	11, 41, 95, 153	0
50	Y7	49/49 (100%)	0.42	4 (8%) 12 9	6, 33, 78, 135	0
51	R8	64/65 (98%)	0.83	6 (9%) 9 7	18, 59, 121, 163	0
51	Y8	64/65 (98%)	0.74	5 (7%) 14 10	16, 52, 108, 164	0
52	R9	37/37 (100%)	8.38	37 (100%) 0 0	92, 141, 184, 204	0
52	Y9	37/37 (100%)	5.98	37 (100%) 0 0	102, 132, 168, 182	0
53	QV	77/77 (100%)	-0.12	1 (1%) 77 64	35, 82, 137, 160	0
53	XV	77/77 (100%)	-0.07	1 (1%) 77 64	11, 71, 111, 159	0
54	QX	8/25 (32%)	0.84	0 100 100	44, 56, 107, 137	0
54	XX	8/25 (32%)	1.21	2 (25%) 1 1	37, 46, 104, 148	0
55	QY	8/17 (47%)	1.51	2 (25%) 1 1	62, 74, 124, 144	0
55	XY	8/17 (47%)	0.50	1 (12%) 4 4	54, 71, 109, 122	0
56	Z6	2/3 (66%)	0.81	0 100 100	45, 45, 45, 52	0
56	Z8	2/3 (66%)	1.45	0 100 100	30, 30, 30, 32	0
All	All	20861/21492 (97%)	0.50	1351 (6%) 20 13	2, 66, 150, 292	0

The worst 5 of 1351 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	R9	11	CYS	18.9
52	R9	37	GLY	15.5

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Mol	Chain	Res	Type	RSRZ
52	R9	14	CYS	15.0
52	Y9	1	MET	14.0
52	R9	36	GLN	14.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	0.96	0.40	-	37,37,37,37	0
56	PPU	Z8	76	37/38	0.96	0.40	-	30,30,30,30	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
58	MG	YA	3197	1/1	0.90	1.19	46.62	42,42,42,42	0
58	MG	YA	3218	1/1	0.84	0.82	40.60	59,59,59,59	0
58	MG	RA	3141	1/1	0.92	0.59	39.29	40,40,40,40	0
58	MG	YA	3142	1/1	0.91	0.61	28.37	31,31,31,31	0
58	MG	RA	3067	1/1	0.77	0.94	22.20	74,74,74,74	0
58	MG	YA	3099	1/1	0.85	0.58	21.74	74,74,74,74	0
58	MG	RA	3227	1/1	0.32	0.47	19.65	60,60,60,60	0
58	MG	YA	3080	1/1	0.83	0.56	16.33	74,74,74,74	0
58	MG	YA	3227	1/1	0.93	0.40	16.32	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	YA	3261	1/1	0.96	0.49	15.80	16,16,16,16	0
58	MG	RA	3009	1/1	0.95	0.94	15.45	74,74,74,74	0
58	MG	YA	3204	1/1	0.97	0.59	14.60	42,42,42,42	0
58	MG	RA	3036	1/1	0.93	0.48	14.10	18,18,18,18	0
58	MG	YA	3260	1/1	0.94	0.71	12.96	74,74,74,74	0
58	MG	YA	3154	1/1	0.93	0.44	12.64	11,11,11,11	0
58	MG	YA	3216	1/1	0.87	0.34	10.65	55,55,55,55	0
58	MG	YA	3015	1/1	0.96	0.52	9.86	74,74,74,74	0
58	MG	RA	3007	1/1	0.96	0.42	8.62	8,8,8,8	0
58	MG	YA	3140	1/1	0.92	0.34	8.53	8,8,8,8	0
58	MG	RA	3033	1/1	0.92	0.37	8.43	6,6,6,6	0
58	MG	YA	3205	1/1	0.70	0.37	8.39	62,62,62,62	0
58	MG	RA	3188	1/1	0.87	0.48	8.05	48,48,48,48	0
58	MG	RA	3196	1/1	0.78	0.26	7.38	63,63,63,63	0
58	MG	YP	201	1/1	0.98	1.20	7.10	54,54,54,54	0
58	MG	YA	3049	1/1	0.93	0.39	6.44	74,74,74,74	0
58	MG	YA	3255	1/1	0.92	0.38	6.31	12,12,12,12	0
58	MG	YA	3090	1/1	0.91	0.27	6.02	26,26,26,26	0
58	MG	YA	3207	1/1	0.85	0.34	5.83	55,55,55,55	0
58	MG	YA	3258	1/1	0.95	0.34	5.42	4,4,4,4	0
58	MG	YA	3206	1/1	0.92	0.27	5.40	52,52,52,52	0
58	MG	RA	3144	1/1	0.73	0.33	5.38	32,32,32,32	0
58	MG	RA	3142	1/1	0.93	0.38	5.08	20,20,20,20	0
58	MG	RP	201	1/1	0.98	0.92	4.96	118,118,118,118	0
58	MG	RA	3094	1/1	0.90	0.28	4.53	16,16,16,16	0
58	MG	XA	1620	1/1	0.91	0.33	4.49	15,15,15,15	0
58	MG	XA	1675	1/1	0.92	0.32	4.44	14,14,14,14	0
58	MG	RA	3151	1/1	0.99	0.38	4.42	3,3,3,3	0
58	MG	YA	3047	1/1	0.95	0.31	4.39	3,3,3,3	0
58	MG	RA	3225	1/1	0.74	0.39	4.28	33,33,33,33	0
58	MG	RA	3125	1/1	0.93	0.30	4.27	19,19,19,19	0
58	MG	RA	3183	1/1	0.84	0.29	4.08	11,11,11,11	0
58	MG	RA	3096	1/1	0.98	0.30	4.08	17,17,17,17	0
58	MG	RA	3138	1/1	0.76	0.28	4.07	38,38,38,38	0
58	MG	RA	3102	1/1	0.95	0.33	3.95	21,21,21,21	0
58	MG	YA	3165	1/1	0.83	0.22	3.77	1,1,1,1	0
58	MG	YA	3035	1/1	0.91	0.33	3.75	12,12,12,12	0
58	MG	YA	3170	1/1	0.67	0.33	3.72	33,33,33,33	0
57	PAR	QA	1601	42/42	0.92	0.35	3.64	42,42,42,42	0
58	MG	RA	3235	1/1	0.88	0.47	3.53	74,74,74,74	0
58	MG	RA	3169	1/1	0.96	0.20	3.35	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	QA	1634	1/1	0.95	0.42	3.34	23,23,23,23	0
58	MG	RA	3039	1/1	0.96	0.29	3.09	7,7,7,7	0
58	MG	YA	3164	1/1	0.81	0.39	3.04	44,44,44,44	0
58	MG	YA	3180	1/1	0.99	0.24	3.01	19,19,19,19	0
58	MG	YA	3184	1/1	0.87	0.20	2.90	23,23,23,23	0
58	MG	YA	3199	1/1	0.90	0.25	2.89	12,12,12,12	0
58	MG	RA	3175	1/1	0.95	0.27	2.85	14,14,14,14	0
58	MG	Y0	101	1/1	0.80	0.42	2.82	74,74,74,74	0
58	MG	RA	3093	1/1	0.97	0.24	2.76	12,12,12,12	0
58	MG	YA	3010	1/1	0.98	0.28	2.69	15,15,15,15	0
58	MG	XA	1671	1/1	0.94	0.38	2.64	33,33,33,33	0
58	MG	RA	3229	1/1	0.81	0.24	2.50	23,23,23,23	0
58	MG	RA	3164	1/1	0.78	0.30	2.30	45,45,45,45	0
58	MG	YA	3161	1/1	0.90	0.26	2.29	23,23,23,23	0
58	MG	YA	3038	1/1	0.97	0.33	2.28	16,16,16,16	0
57	PAR	XA	1601	42/42	0.93	0.30	2.22	38,38,38,38	0
58	MG	YA	3237	1/1	0.93	0.32	2.04	36,36,36,36	0
58	MG	YA	3003	1/1	0.94	0.42	2.04	74,74,74,74	0
58	MG	RA	3080	1/1	0.99	0.25	2.00	10,10,10,10	0
58	MG	QA	1605	1/1	0.97	0.28	1.97	6,6,6,6	0
58	MG	YA	3252	1/1	0.94	0.36	1.89	1,1,1,1	0
58	MG	RA	3024	1/1	0.97	0.29	1.85	11,11,11,11	0
58	MG	YA	3023	1/1	0.98	0.29	1.83	18,18,18,18	0
58	MG	QA	1675	1/1	0.87	0.26	1.83	32,32,32,32	0
58	MG	RA	3238	1/1	0.90	0.24	1.79	32,32,32,32	0
58	MG	YA	3098	1/1	0.98	0.33	1.77	8,8,8,8	0
58	MG	XA	1651	1/1	0.86	0.28	1.71	33,33,33,33	0
58	MG	RA	3147	1/1	0.94	0.37	1.49	32,32,32,32	0
58	MG	QA	1617	1/1	0.92	0.18	1.48	46,46,46,46	0
58	MG	RA	3031	1/1	0.92	0.36	1.47	9,9,9,9	0
58	MG	YA	3250	1/1	0.84	0.33	1.42	15,15,15,15	0
58	MG	YA	3012	1/1	0.90	0.29	1.41	10,10,10,10	0
58	MG	YA	3244	1/1	0.88	0.25	1.40	0,0,0,0	0
58	MG	RA	3032	1/1	0.96	0.25	1.35	14,14,14,14	0
58	MG	XA	1665	1/1	0.90	0.15	1.35	33,33,33,33	0
58	MG	RA	3158	1/1	0.87	0.22	1.35	15,15,15,15	0
58	MG	RA	3129	1/1	0.92	0.23	1.35	21,21,21,21	0
58	MG	QA	1656	1/1	0.98	0.27	1.34	44,44,44,44	0
58	MG	RA	3092	1/1	0.92	0.32	1.34	0,0,0,0	0
58	MG	RA	3017	1/1	0.90	0.34	1.33	18,18,18,18	0
58	MG	YA	3192	1/1	0.94	0.30	1.31	21,21,21,21	0
58	MG	RA	3029	1/1	0.97	0.23	1.22	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	YA	3014	1/1	0.87	0.46	1.22	74,74,74,74	0
58	MG	YA	3108	1/1	0.94	0.30	1.12	7,7,7,7	0
58	MG	XA	1605	1/1	0.96	0.35	1.11	15,15,15,15	0
58	MG	RP	202	1/1	0.98	0.43	1.08	76,76,76,76	0
58	MG	RA	3099	1/1	0.97	0.31	1.05	11,11,11,11	0
58	MG	YD	301	1/1	0.85	0.46	0.98	74,74,74,74	0
58	MG	RA	3163	1/1	0.94	0.26	0.80	34,34,34,34	0
58	MG	YA	3119	1/1	0.94	0.24	0.77	9,9,9,9	0
58	MG	RA	3154	1/1	0.89	0.20	0.74	59,59,59,59	0
58	MG	RD	301	1/1	0.94	0.33	0.72	12,12,12,12	0
58	MG	RA	3130	1/1	0.86	0.20	0.67	15,15,15,15	0
58	MG	QA	1619	1/1	0.95	0.25	0.65	12,12,12,12	0
58	MG	RA	3202	1/1	0.89	0.29	0.65	0,0,0,0	0
58	MG	XA	1653	1/1	0.96	0.37	0.61	42,42,42,42	0
58	MG	RA	3137	1/1	0.96	0.25	0.52	14,14,14,14	0
58	MG	RA	3059	1/1	0.97	0.23	0.47	8,8,8,8	0
58	MG	YA	3026	1/1	0.96	0.26	0.39	5,5,5,5	0
58	MG	RA	3026	1/1	0.96	0.24	0.38	7,7,7,7	0
58	MG	YA	3162	1/1	0.86	0.35	0.37	11,11,11,11	0
58	MG	RA	3134	1/1	0.96	0.26	0.34	17,17,17,17	0
58	MG	RA	3054	1/1	0.95	0.25	0.25	18,18,18,18	0
58	MG	XA	1666	1/1	0.96	0.52	0.22	85,85,85,85	0
58	MG	RA	3043	1/1	0.95	0.27	0.19	10,10,10,10	0
59	ZN	XD	301	1/1	1.00	0.29	0.12	10,10,10,10	0
58	MG	RA	3219	1/1	0.95	0.24	0.09	8,8,8,8	0
58	MG	RA	3041	1/1	0.96	0.26	0.07	9,9,9,9	0
58	MG	RA	3085	1/1	0.97	0.23	0.06	7,7,7,7	0
58	MG	YA	3223	1/1	0.88	0.21	0.05	34,34,34,34	0
58	MG	RA	3161	1/1	0.85	0.23	0.04	10,10,10,10	0
58	MG	QA	1612	1/1	0.92	0.28	0.04	15,15,15,15	0
58	MG	YA	3132	1/1	0.83	0.17	0.01	7,7,7,7	0
58	MG	YA	3072	1/1	0.90	0.21	-0.01	22,22,22,22	0
58	MG	YA	3091	1/1	0.98	0.22	-0.02	29,29,29,29	0
58	MG	RA	3001	1/1	0.92	0.27	-0.02	16,16,16,16	0
58	MG	YA	3182	1/1	0.76	0.24	-0.15	3,3,3,3	0
58	MG	YA	3115	1/1	0.92	0.22	-0.21	17,17,17,17	0
58	MG	YA	3238	1/1	0.99	0.27	-0.26	76,76,76,76	0
58	MG	RA	3243	1/1	0.87	0.26	-0.28	1,1,1,1	0
58	MG	YA	3233	1/1	0.84	0.22	-0.30	34,34,34,34	0
58	MG	RA	3014	1/1	0.89	0.19	-0.32	28,28,28,28	0
58	MG	QA	1664	1/1	0.87	0.16	-0.34	56,56,56,56	0
58	MG	RA	3086	1/1	0.93	0.22	-0.37	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	YA	3135	1/1	0.90	0.22	-0.39	6,6,6,6	0
58	MG	YA	3259	1/1	0.84	0.27	-0.39	5,5,5,5	0
58	MG	YA	3089	1/1	0.98	0.26	-0.45	13,13,13,13	0
58	MG	RA	3192	1/1	0.97	0.24	-0.46	17,17,17,17	0
58	MG	RA	3126	1/1	0.80	0.22	-0.47	16,16,16,16	0
58	MG	RA	3064	1/1	0.96	0.24	-0.49	4,4,4,4	0
58	MG	XA	1634	1/1	0.93	0.17	-0.50	7,7,7,7	0
59	ZN	QD	301	1/1	1.00	0.23	-0.58	27,27,27,27	0
58	MG	RA	3073	1/1	0.89	0.21	-0.60	10,10,10,10	0
58	MG	YA	3210	1/1	0.90	0.20	-0.60	17,17,17,17	0
58	MG	YA	3103	1/1	0.94	0.25	-0.61	8,8,8,8	0
58	MG	YA	3027	1/1	0.99	0.22	-0.61	21,21,21,21	0
58	MG	XB	301	1/1	0.88	0.17	-0.61	41,41,41,41	0
58	MG	RA	3146	1/1	0.91	0.16	-0.65	25,25,25,25	0
58	MG	YA	3042	1/1	0.97	0.23	-0.67	15,15,15,15	0
58	MG	RA	3038	1/1	0.96	0.22	-0.69	4,4,4,4	0
58	MG	QA	1610	1/1	0.96	0.22	-0.70	21,21,21,21	0
58	MG	XA	1639	1/1	0.90	0.21	-0.72	45,45,45,45	0
58	MG	YA	3053	1/1	0.94	0.22	-0.72	8,8,8,8	0
58	MG	QA	1603	1/1	0.81	0.23	-0.73	11,11,11,11	0
58	MG	YA	3114	1/1	0.97	0.22	-0.73	6,6,6,6	0
58	MG	QA	1669	1/1	0.95	0.20	-0.76	18,18,18,18	0
58	MG	RA	3197	1/1	0.96	0.18	-0.77	81,81,81,81	0
58	MG	YA	3257	1/1	0.91	0.26	-0.79	14,14,14,14	0
58	MG	YD	302	1/1	0.89	0.21	-0.80	5,5,5,5	0
58	MG	YA	3024	1/1	0.94	0.24	-0.82	10,10,10,10	0
58	MG	RA	3063	1/1	0.92	0.24	-0.85	19,19,19,19	0
58	MG	YA	3100	1/1	0.98	0.23	-0.85	8,8,8,8	0
58	MG	RA	3210	1/1	0.97	0.22	-0.87	8,8,8,8	0
58	MG	RE	302	1/1	0.98	0.22	-0.92	15,15,15,15	0
58	MG	RA	3022	1/1	0.94	0.20	-0.93	24,24,24,24	0
58	MG	RF	301	1/1	0.89	0.22	-1.00	13,13,13,13	0
58	MG	QA	1618	1/1	0.92	0.09	-1.00	17,17,17,17	0
58	MG	XA	1622	1/1	0.95	0.23	-1.01	6,6,6,6	0
58	MG	RA	3068	1/1	0.90	0.25	-1.01	13,13,13,13	0
58	MG	RA	3111	1/1	0.96	0.20	-1.03	12,12,12,12	0
58	MG	YA	3034	1/1	0.96	0.22	-1.05	7,7,7,7	0
58	MG	XA	1638	1/1	0.97	0.15	-1.05	4,4,4,4	0
58	MG	R8	102	1/1	0.97	0.20	-1.07	2,2,2,2	0
58	MG	XA	1619	1/1	0.93	0.24	-1.08	5,5,5,5	0
58	MG	YA	3050	1/1	0.97	0.23	-1.10	5,5,5,5	0
58	MG	YA	3088	1/1	0.97	0.20	-1.13	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	RA	3025	1/1	0.96	0.23	-1.18	3,3,3,3	0
58	MG	QA	1615	1/1	0.95	0.21	-1.19	9,9,9,9	0
58	MG	QA	1642	1/1	0.94	0.18	-1.19	38,38,38,38	0
58	MG	XA	1621	1/1	0.89	0.10	-1.26	19,19,19,19	0
58	MG	RA	3107	1/1	0.94	0.17	-1.26	2,2,2,2	0
58	MG	YA	3169	1/1	0.76	0.15	-1.28	16,16,16,16	0
58	MG	YA	3065	1/1	0.95	0.22	-1.28	31,31,31,31	0
58	MG	QA	1641	1/1	0.94	0.14	-1.35	43,43,43,43	0
58	MG	RA	3149	1/1	0.94	0.25	-1.38	4,4,4,4	0
58	MG	QA	1649	1/1	0.95	0.14	-1.39	32,32,32,32	0
58	MG	XA	1630	1/1	0.84	0.16	-1.40	15,15,15,15	0
58	MG	RA	3133	1/1	0.96	0.16	-1.41	7,7,7,7	0
58	MG	YA	3094	1/1	0.96	0.17	-1.49	12,12,12,12	0
58	MG	YA	3078	1/1	0.93	0.17	-1.50	9,9,9,9	0
58	MG	RA	3195	1/1	0.95	0.14	-1.52	7,7,7,7	0
58	MG	RA	3246	1/1	0.97	0.17	-1.54	33,33,33,33	0
58	MG	YX	101	1/1	0.96	0.19	-1.55	47,47,47,47	0
58	MG	QA	1632	1/1	0.89	0.17	-1.56	42,42,42,42	0
59	ZN	QN	101	1/1	0.99	0.07	-1.58	86,86,86,86	0
58	MG	QA	1622	1/1	0.93	0.09	-1.59	12,12,12,12	0
58	MG	YA	3058	1/1	0.93	0.17	-1.59	20,20,20,20	0
58	MG	RA	3232	1/1	0.82	0.11	-1.61	15,15,15,15	0
58	MG	YA	3110	1/1	0.97	0.14	-1.61	4,4,4,4	0
58	MG	YA	3124	1/1	0.94	0.23	-1.63	6,6,6,6	0
58	MG	RA	3211	1/1	0.97	0.20	-1.64	16,16,16,16	0
58	MG	YA	3044	1/1	0.97	0.24	-1.64	2,2,2,2	0
58	MG	YB	203	1/1	0.97	0.14	-1.65	4,4,4,4	0
58	MG	RA	3104	1/1	0.92	0.18	-1.65	11,11,11,11	0
58	MG	QA	1676	1/1	0.93	0.14	-1.66	13,13,13,13	0
58	MG	YA	3056	1/1	0.91	0.22	-1.68	5,5,5,5	0
58	MG	RA	3117	1/1	0.97	0.12	-1.70	11,11,11,11	0
58	MG	RA	3213	1/1	0.96	0.13	-1.71	9,9,9,9	0
58	MG	YA	3007	1/1	0.95	0.16	-1.72	8,8,8,8	0
58	MG	RA	3077	1/1	0.97	0.19	-1.76	6,6,6,6	0
58	MG	RA	3082	1/1	0.98	0.18	-1.77	10,10,10,10	0
58	MG	XA	1627	1/1	0.94	0.17	-1.77	12,12,12,12	0
58	MG	XA	1660	1/1	0.95	0.19	-1.78	22,22,22,22	0
58	MG	RA	3127	1/1	0.94	0.16	-1.79	22,22,22,22	0
58	MG	YA	3153	1/1	0.93	0.11	-1.79	14,14,14,14	0
58	MG	XA	1636	1/1	0.88	0.18	-1.83	8,8,8,8	0
58	MG	XA	1672	1/1	0.87	0.19	-1.88	16,16,16,16	0
58	MG	YA	3068	1/1	0.97	0.19	-1.92	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	RA	3215	1/1	0.90	0.09	-1.92	13,13,13,13	0
59	ZN	XN	101	1/1	0.98	0.12	-1.93	70,70,70,70	0
58	MG	RA	3155	1/1	0.91	0.16	-2.00	54,54,54,54	0
58	MG	YP	202	1/1	0.92	0.10	-2.04	1,1,1,1	0
58	MG	QA	1621	1/1	0.74	0.21	-2.05	38,38,38,38	0
58	MG	XA	1656	1/1	0.86	0.20	-2.06	17,17,17,17	0
58	MG	QA	1646	1/1	0.95	0.16	-2.09	28,28,28,28	0
58	MG	YA	3086	1/1	0.97	0.20	-2.11	3,3,3,3	0
58	MG	YA	3136	1/1	0.94	0.17	-2.13	0,0,0,0	0
58	MG	XA	1609	1/1	0.92	0.09	-2.14	51,51,51,51	0
58	MG	QA	1657	1/1	0.96	0.12	-2.14	19,19,19,19	0
58	MG	RA	3166	1/1	0.96	0.23	-2.20	5,5,5,5	0
58	MG	XA	1616	1/1	0.97	0.18	-2.20	5,5,5,5	0
58	MG	QA	1662	1/1	0.95	0.12	-2.21	0,0,0,0	0
58	MG	YA	3241	1/1	0.95	0.17	-2.21	18,18,18,18	0
58	MG	RB	201	1/1	0.95	0.08	-2.23	16,16,16,16	0
58	MG	RA	3019	1/1	0.95	0.11	-2.25	8,8,8,8	0
58	MG	YA	3006	1/1	0.97	0.16	-2.26	26,26,26,26	0
58	MG	YA	3025	1/1	0.97	0.13	-2.28	16,16,16,16	0
58	MG	YA	3113	1/1	0.96	0.22	-2.29	17,17,17,17	0
58	MG	RA	3040	1/1	0.98	0.20	-2.33	13,13,13,13	0
58	MG	YA	3032	1/1	0.94	0.22	-2.41	1,1,1,1	0
58	MG	YA	3073	1/1	0.98	0.10	-2.43	4,4,4,4	0
58	MG	QV	101	1/1	0.98	0.20	-2.44	22,22,22,22	0
58	MG	XA	1629	1/1	0.95	0.23	-2.46	4,4,4,4	0
58	MG	XA	1683	1/1	0.94	0.10	-2.46	10,10,10,10	0
58	MG	RA	3090	1/1	0.95	0.20	-2.57	6,6,6,6	0
58	MG	QA	1616	1/1	0.92	0.14	-2.57	52,52,52,52	0
58	MG	RA	3128	1/1	0.98	0.11	-2.59	9,9,9,9	0
58	MG	XA	1642	1/1	0.90	0.16	-2.67	47,47,47,47	0
58	MG	RA	3189	1/1	0.96	0.12	-2.69	14,14,14,14	0
58	MG	XA	1649	1/1	0.96	0.13	-2.70	17,17,17,17	0
58	MG	RA	3136	1/1	0.90	0.20	-2.74	5,5,5,5	0
58	MG	QM	201	1/1	0.94	0.06	-2.75	51,51,51,51	0
58	MG	RA	3070	1/1	0.96	0.17	-2.79	4,4,4,4	0
58	MG	RA	3069	1/1	0.97	0.17	-2.85	19,19,19,19	0
58	MG	QA	1648	1/1	0.96	0.12	-2.85	43,43,43,43	0
58	MG	QA	1614	1/1	0.98	0.13	-2.86	2,2,2,2	0
58	MG	RA	3179	1/1	0.95	0.14	-2.87	4,4,4,4	0
58	MG	YA	3129	1/1	0.97	0.16	-2.90	20,20,20,20	0
58	MG	YA	3028	1/1	0.91	0.19	-2.93	15,15,15,15	0
58	MG	XA	1661	1/1	0.94	0.09	-2.93	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	RA	3112	1/1	0.97	0.18	-2.95	7,7,7,7	0
58	MG	YA	3183	1/1	0.86	0.12	-2.96	19,19,19,19	0
58	MG	YA	3033	1/1	0.97	0.17	-2.98	12,12,12,12	0
58	MG	RA	3027	1/1	0.95	0.21	-3.01	15,15,15,15	0
58	MG	RA	3121	1/1	0.92	0.17	-3.02	36,36,36,36	0
58	MG	YA	3039	1/1	0.97	0.17	-3.03	20,20,20,20	0
58	MG	RA	3060	1/1	0.96	0.20	-3.03	15,15,15,15	0
58	MG	XA	1637	1/1	0.92	0.16	-3.04	14,14,14,14	0
58	MG	YA	3137	1/1	0.91	0.11	-3.04	10,10,10,10	0
58	MG	RA	3174	1/1	0.99	0.06	-3.06	17,17,17,17	0
58	MG	RA	3167	1/1	0.96	0.18	-3.10	1,1,1,1	0
58	MG	RA	3084	1/1	0.96	0.20	-3.11	14,14,14,14	0
58	MG	XA	1611	1/1	0.92	0.15	-3.18	11,11,11,11	0
58	MG	YA	3176	1/1	0.90	0.13	-3.21	45,45,45,45	0
58	MG	YA	3112	1/1	0.91	0.17	-3.25	13,13,13,13	0
58	MG	RA	3061	1/1	0.97	0.16	-3.32	0,0,0,0	0
58	MG	YA	3009	1/1	0.98	0.17	-3.38	15,15,15,15	0
58	MG	RA	3159	1/1	0.87	0.12	-3.42	23,23,23,23	0
58	MG	YA	3125	1/1	0.97	0.14	-3.44	11,11,11,11	0
58	MG	RA	3052	1/1	0.97	0.17	-3.56	1,1,1,1	0
58	MG	YA	3144	1/1	0.77	0.15	-3.62	6,6,6,6	0
58	MG	YA	3167	1/1	0.97	0.12	-3.63	15,15,15,15	0
58	MG	YA	3074	1/1	0.94	0.12	-3.80	1,1,1,1	0
58	MG	XA	1644	1/1	0.99	0.13	-3.81	4,4,4,4	0
58	MG	YA	3070	1/1	0.94	0.20	-3.82	1,1,1,1	0
58	MG	RA	3050	1/1	0.97	0.18	-3.86	9,9,9,9	0
58	MG	XA	1626	1/1	0.94	0.13	-3.90	15,15,15,15	0
58	MG	RA	3057	1/1	0.97	0.14	-3.94	4,4,4,4	0
58	MG	YA	3159	1/1	0.93	0.15	-3.97	12,12,12,12	0
58	MG	YA	3017	1/1	0.98	0.14	-4.08	11,11,11,11	0
58	MG	QA	1607	1/1	0.98	0.15	-4.12	22,22,22,22	0
58	MG	XA	1613	1/1	0.93	0.12	-4.14	8,8,8,8	0
58	MG	XA	1635	1/1	0.82	0.17	-4.15	26,26,26,26	0
58	MG	RA	3135	1/1	0.91	0.13	-4.19	12,12,12,12	0
58	MG	YA	3138	1/1	0.98	0.18	-4.23	6,6,6,6	0
58	MG	QA	1611	1/1	0.98	0.11	-4.31	1,1,1,1	0
58	MG	RA	3120	1/1	0.89	0.18	-4.32	4,4,4,4	0
58	MG	YA	3166	1/1	0.97	0.12	-4.49	11,11,11,11	0
58	MG	YA	3106	1/1	0.94	0.15	-4.64	16,16,16,16	0
58	MG	QA	1623	1/1	0.98	0.13	-4.75	46,46,46,46	0
58	MG	RA	3217	1/1	0.96	0.09	-4.88	8,8,8,8	0
58	MG	QA	1652	1/1	0.96	0.10	-4.89	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	YA	3189	1/1	0.96	0.07	-4.93	30,30,30,30	0
58	MG	XA	1659	1/1	0.96	0.12	-5.11	36,36,36,36	0
58	MG	YA	3048	1/1	0.96	0.15	-5.13	4,4,4,4	0
58	MG	RA	3079	1/1	0.96	0.07	-5.24	25,25,25,25	0
58	MG	RA	3045	1/1	0.96	0.15	-5.36	2,2,2,2	0
58	MG	XA	1615	1/1	0.95	0.08	-5.78	19,19,19,19	0
58	MG	XA	1673	1/1	0.95	0.12	-5.93	6,6,6,6	0
58	MG	QA	1638	1/1	0.98	0.10	-6.08	14,14,14,14	0
58	MG	RA	3047	1/1	0.98	0.15	-6.16	19,19,19,19	0
58	MG	XV	101	1/1	0.98	0.12	-6.33	3,3,3,3	0
58	MG	YA	3174	1/1	0.75	0.12	-6.62	10,10,10,10	0
58	MG	YA	3016	1/1	0.94	0.10	-6.92	7,7,7,7	0
58	MG	XA	1623	1/1	0.96	0.05	-7.40	28,28,28,28	0
58	MG	YA	3117	1/1	0.96	0.11	-7.55	28,28,28,28	0
58	MG	QA	1608	1/1	0.98	0.06	-8.26	4,4,4,4	0
58	MG	RA	3190	1/1	0.94	0.07	-8.27	40,40,40,40	0
58	MG	YA	3104	1/1	0.97	0.09	-9.49	0,0,0,0	0
58	MG	YA	3212	1/1	0.96	0.09	-9.86	10,10,10,10	0
58	MG	YA	3107	1/1	0.98	0.17	-10.02	9,9,9,9	0
58	MG	YA	3111	1/1	0.99	0.08	-10.36	26,26,26,26	0
58	MG	QA	1665	1/1	0.94	0.09	-	37,37,37,37	0
58	MG	RA	3245	1/1	0.94	0.36	-	7,7,7,7	0
58	MG	YA	3043	1/1	0.96	0.28	-	5,5,5,5	0
58	MG	RA	3003	1/1	0.92	0.18	-	4,4,4,4	0
58	MG	RA	3097	1/1	0.96	0.21	-	5,5,5,5	0
58	MG	XA	1648	1/1	0.94	0.16	-	19,19,19,19	0
58	MG	RA	3062	1/1	0.93	0.36	-	21,21,21,21	0
58	MG	RA	3072	1/1	0.91	0.29	-	18,18,18,18	0
58	MG	YA	3105	1/1	0.86	0.19	-	19,19,19,19	0
58	MG	XA	1679	1/1	0.77	0.18	-	18,18,18,18	0
58	MG	XM	201	1/1	0.58	0.35	-	98,98,98,98	0
58	MG	YA	3102	1/1	0.88	0.10	-	8,8,8,8	0
58	MG	RA	3074	1/1	0.86	0.20	-	6,6,6,6	0
58	MG	XA	1657	1/1	0.97	0.18	-	19,19,19,19	0
58	MG	RA	3106	1/1	0.93	0.14	-	6,6,6,6	0
58	MG	RA	3098	1/1	0.98	0.12	-	10,10,10,10	0
58	MG	YA	3151	1/1	0.83	0.21	-	3,3,3,3	0
58	MG	RA	3005	1/1	0.86	0.22	-	24,24,24,24	0
58	MG	RA	3145	1/1	0.97	0.17	-	3,3,3,3	0
58	MG	YA	3126	1/1	0.78	0.15	-	0,0,0,0	0
58	MG	RA	3186	1/1	0.94	0.28	-	17,17,17,17	0
58	MG	YA	3030	1/1	0.95	0.61	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	RA	3110	1/1	0.98	0.13	-	19,19,19,19	0
58	MG	XA	1606	1/1	0.95	0.23	-	3,3,3,3	0
58	MG	XA	1617	1/1	0.90	0.36	-	74,74,74,74	0
58	MG	RA	3122	1/1	0.94	0.15	-	5,5,5,5	0
58	MG	QA	1653	1/1	0.87	0.17	-	0,0,0,0	0
58	MG	YA	3181	1/1	0.87	0.26	-	0,0,0,0	0
58	MG	RA	3204	1/1	0.71	0.24	-	50,50,50,50	0
58	MG	XA	1669	1/1	0.95	0.06	-	55,55,55,55	0
58	MG	RA	3208	1/1	0.91	0.16	-	30,30,30,30	0
58	MG	YA	3158	1/1	0.90	0.36	-	21,21,21,21	0
58	MG	RA	3244	1/1	0.97	0.17	-	0,0,0,0	0
58	MG	RA	3115	1/1	0.94	0.26	-	21,21,21,21	0
58	MG	RA	3184	1/1	0.92	0.35	-	23,23,23,23	0
58	MG	YA	3152	1/1	0.92	0.24	-	27,27,27,27	0
58	MG	YA	3020	1/1	0.94	0.40	-	8,8,8,8	0
58	MG	YA	3229	1/1	0.98	0.15	-	14,14,14,14	0
58	MG	RA	3173	1/1	0.93	0.28	-	35,35,35,35	0
58	MG	YA	3045	1/1	0.96	0.25	-	5,5,5,5	0
58	MG	RA	3220	1/1	0.85	0.15	-	13,13,13,13	0
58	MG	QA	1602	1/1	0.91	0.21	-	6,6,6,6	0
58	MG	YA	3188	1/1	0.92	0.13	-	13,13,13,13	0
58	MG	XA	1658	1/1	0.86	0.14	-	3,3,3,3	0
58	MG	YA	3156	1/1	0.89	0.56	-	29,29,29,29	0
58	MG	YA	3087	1/1	0.98	0.19	-	5,5,5,5	0
58	MG	RA	3200	1/1	0.98	0.12	-	9,9,9,9	0
58	MG	YA	3083	1/1	0.98	0.25	-	5,5,5,5	0
58	MG	YA	3254	1/1	0.79	0.29	-	16,16,16,16	0
58	MG	RA	3247	1/1	0.78	0.29	-	9,9,9,9	0
58	MG	YA	3214	1/1	0.66	0.68	-	50,50,50,50	0
58	MG	QA	1672	1/1	0.86	0.32	-	19,19,19,19	0
58	MG	YA	3209	1/1	0.97	0.14	-	7,7,7,7	0
58	MG	RA	3071	1/1	0.95	0.24	-	11,11,11,11	0
58	MG	QA	1626	1/1	0.92	0.11	-	17,17,17,17	0
58	MG	RA	3091	1/1	0.98	0.28	-	9,9,9,9	0
58	MG	YA	3093	1/1	0.92	0.27	-	10,10,10,10	0
58	MG	YA	3177	1/1	0.96	0.13	-	4,4,4,4	0
58	MG	YA	3008	1/1	0.95	0.24	-	8,8,8,8	0
58	MG	RA	3100	1/1	0.96	0.13	-	0,0,0,0	0
58	MG	RA	3182	1/1	0.73	0.39	-	22,22,22,22	0
58	MG	RA	3116	1/1	0.97	0.11	-	8,8,8,8	0
58	MG	XA	1647	1/1	0.92	0.12	-	22,22,22,22	0
58	MG	YA	3141	1/1	0.93	0.13	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	RA	3087	1/1	0.99	0.18	-	10,10,10,10	0
58	MG	XA	1667	1/1	0.84	0.21	-	34,34,34,34	0
58	MG	RA	3123	1/1	0.96	0.08	-	10,10,10,10	0
58	MG	YA	3095	1/1	0.97	0.20	-	19,19,19,19	0
58	MG	YA	3249	1/1	0.85	0.33	-	20,20,20,20	0
58	MG	YA	3067	1/1	0.96	0.27	-	17,17,17,17	0
58	MG	RA	3081	1/1	0.96	0.39	-	18,18,18,18	0
58	MG	YA	3163	1/1	0.89	0.29	-	21,21,21,21	0
58	MG	YA	3193	1/1	0.94	0.08	-	14,14,14,14	0
58	MG	YA	3077	1/1	0.96	0.25	-	6,6,6,6	0
58	MG	RA	3132	1/1	0.97	0.20	-	9,9,9,9	0
58	MG	RA	3046	1/1	0.96	0.36	-	24,24,24,24	0
58	MG	XA	1663	1/1	0.88	0.21	-	32,32,32,32	0
58	MG	YA	3148	1/1	0.99	0.12	-	15,15,15,15	0
58	MG	RA	3020	1/1	0.98	0.20	-	4,4,4,4	0
58	MG	YA	3051	1/1	0.92	0.25	-	13,13,13,13	0
58	MG	QA	1658	1/1	0.90	0.16	-	39,39,39,39	0
58	MG	YA	3054	1/1	0.91	0.26	-	14,14,14,14	0
58	MG	YA	3036	1/1	0.91	0.28	-	11,11,11,11	0
58	MG	QA	1637	1/1	0.96	0.09	-	17,17,17,17	0
58	MG	QA	1645	1/1	0.87	0.29	-	4,4,4,4	0
58	MG	QA	1628	1/1	0.94	0.26	-	10,10,10,10	0
58	MG	XA	1643	1/1	0.94	0.34	-	74,74,74,74	0
58	MG	RA	3037	1/1	0.98	0.88	-	74,74,74,74	0
58	MG	XA	1641	1/1	0.93	0.24	-	11,11,11,11	0
58	MG	YA	3243	1/1	0.93	0.21	-	13,13,13,13	0
58	MG	YA	3037	1/1	0.97	0.14	-	16,16,16,16	0
58	MG	XA	1668	1/1	0.98	0.13	-	0,0,0,0	0
58	MG	RA	3051	1/1	0.91	0.31	-	1,1,1,1	0
58	MG	YA	3226	1/1	0.89	0.14	-	11,11,11,11	0
58	MG	RA	3236	1/1	0.97	0.37	-	13,13,13,13	0
58	MG	RA	3176	1/1	0.97	0.06	-	21,21,21,21	0
58	MG	YB	201	1/1	0.89	0.25	-	33,33,33,33	0
58	MG	QA	1640	1/1	0.89	0.27	-	13,13,13,13	0
58	MG	YB	202	1/1	0.88	0.33	-	19,19,19,19	0
58	MG	RA	3089	1/1	0.96	0.16	-	6,6,6,6	0
58	MG	XA	1610	1/1	0.90	0.21	-	6,6,6,6	0
58	MG	YA	3005	1/1	0.96	0.22	-	26,26,26,26	0
58	MG	RA	3218	1/1	0.92	0.12	-	17,17,17,17	0
58	MG	QA	1673	1/1	0.91	0.24	-	9,9,9,9	0
58	MG	YA	3120	1/1	0.86	0.29	-	46,46,46,46	0
58	MG	YA	3222	1/1	0.81	0.19	-	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	RA	3105	1/1	0.83	0.15	-	14,14,14,14	0
58	MG	RA	3205	1/1	0.86	0.46	-	17,17,17,17	0
58	MG	YA	3234	1/1	0.85	0.22	-	17,17,17,17	0
58	MG	YA	3001	1/1	0.94	0.20	-	23,23,23,23	0
58	MG	YA	3046	1/1	0.94	0.50	-	74,74,74,74	0
58	MG	QA	1630	1/1	0.95	0.17	-	7,7,7,7	0
58	MG	RA	3049	1/1	0.97	0.23	-	12,12,12,12	0
58	MG	QA	1627	1/1	0.91	0.18	-	30,30,30,30	0
58	MG	RB	202	1/1	0.98	0.13	-	29,29,29,29	0
58	MG	YA	3168	1/1	0.99	0.26	-	3,3,3,3	0
58	MG	RA	3180	1/1	0.92	0.24	-	17,17,17,17	0
58	MG	XA	1640	1/1	0.93	0.26	-	27,27,27,27	0
58	MG	YA	3055	1/1	0.93	0.28	-	6,6,6,6	0
58	MG	RA	3053	1/1	0.97	0.10	-	2,2,2,2	0
58	MG	QA	1613	1/1	0.95	0.36	-	8,8,8,8	0
58	MG	RA	3185	1/1	0.93	0.22	-	16,16,16,16	0
58	MG	XA	1632	1/1	0.83	0.14	-	9,9,9,9	0
58	MG	YA	3264	1/1	0.91	0.35	-	5,5,5,5	0
58	MG	RA	3198	1/1	0.90	0.19	-	26,26,26,26	0
58	MG	YA	3019	1/1	0.95	0.34	-	13,13,13,13	0
58	MG	RA	3224	1/1	0.92	0.83	-	142,142,142,142	0
58	MG	RA	3231	1/1	0.93	0.17	-	16,16,16,16	0
58	MG	R0	101	1/1	0.93	0.09	-	2,2,2,2	0
58	MG	QA	1620	1/1	0.97	0.10	-	3,3,3,3	0
58	MG	RA	3021	1/1	0.98	0.22	-	18,18,18,18	0
58	MG	XA	1614	1/1	0.98	0.10	-	21,21,21,21	0
58	MG	RA	3075	1/1	0.93	0.14	-	9,9,9,9	0
58	MG	YA	3097	1/1	0.97	0.14	-	11,11,11,11	0
58	MG	YA	3031	1/1	0.94	0.18	-	5,5,5,5	0
58	MG	RA	3206	1/1	0.96	0.14	-	5,5,5,5	0
58	MG	RA	3233	1/1	0.79	0.22	-	42,42,42,42	0
58	MG	QA	1674	1/1	0.88	0.18	-	8,8,8,8	0
58	MG	QA	1677	1/1	0.83	0.19	-	47,47,47,47	0
58	MG	QA	1631	1/1	0.98	0.14	-	50,50,50,50	0
58	MG	YA	3133	1/1	0.84	0.25	-	32,32,32,32	0
58	MG	YA	3062	1/1	0.97	0.20	-	4,4,4,4	0
58	MG	YA	3203	1/1	0.78	0.18	-	18,18,18,18	0
58	MG	QA	1624	1/1	0.95	0.12	-	26,26,26,26	0
58	MG	XA	1645	1/1	0.97	0.18	-	5,5,5,5	0
58	MG	YA	3200	1/1	0.88	0.15	-	6,6,6,6	0
58	MG	RA	3095	1/1	0.93	0.25	-	18,18,18,18	0
58	MG	YA	3236	1/1	0.83	0.23	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	RA	3223	1/1	0.89	0.32	-	54,54,54,54	0
58	MG	RA	3239	1/1	0.98	0.23	-	0,0,0,0	0
58	MG	YA	3040	1/1	0.93	0.17	-	19,19,19,19	0
58	MG	XA	1681	1/1	0.84	0.20	-	31,31,31,31	0
58	MG	QA	1668	1/1	0.90	0.17	-	0,0,0,0	0
58	MG	RA	3140	1/1	0.92	0.32	-	34,34,34,34	0
58	MG	XA	1607	1/1	0.90	0.28	-	7,7,7,7	0
58	MG	RA	3168	1/1	0.96	0.19	-	3,3,3,3	0
58	MG	YA	3143	1/1	0.96	0.09	-	0,0,0,0	0
58	MG	QA	1629	1/1	0.94	0.20	-	11,11,11,11	0
58	MG	YA	3139	1/1	0.92	0.15	-	8,8,8,8	0
58	MG	RA	3241	1/1	0.91	0.13	-	8,8,8,8	0
58	MG	XA	1654	1/1	0.94	0.27	-	54,54,54,54	0
58	MG	RA	3016	1/1	0.99	0.18	-	8,8,8,8	0
58	MG	RA	3216	1/1	0.89	0.28	-	2,2,2,2	0
58	MG	RA	3181	1/1	0.93	0.33	-	21,21,21,21	0
58	MG	YA	3118	1/1	0.86	0.35	-	8,8,8,8	0
58	MG	XA	1646	1/1	0.87	0.14	-	21,21,21,21	0
58	MG	QA	1633	1/1	0.95	0.23	-	15,15,15,15	0
58	MG	YA	3085	1/1	0.97	0.25	-	17,17,17,17	0
58	MG	YA	3130	1/1	0.78	0.25	-	21,21,21,21	0
58	MG	YA	3131	1/1	0.98	0.14	-	16,16,16,16	0
58	MG	XA	1618	1/1	0.95	0.12	-	0,0,0,0	0
58	MG	RA	3118	1/1	0.98	0.24	-	16,16,16,16	0
58	MG	YA	3002	1/1	0.94	0.22	-	0,0,0,0	0
58	MG	XA	1664	1/1	0.92	0.19	-	22,22,22,22	0
58	MG	YA	3246	1/1	0.85	0.22	-	0,0,0,0	0
58	MG	YA	3011	1/1	0.91	0.20	-	9,9,9,9	0
58	MG	YA	3116	1/1	0.80	0.22	-	14,14,14,14	0
58	MG	YA	3219	1/1	0.91	0.42	-	22,22,22,22	0
58	MG	YA	3201	1/1	0.98	0.14	-	57,57,57,57	0
58	MG	YA	3109	1/1	0.97	0.08	-	10,10,10,10	0
58	MG	RA	3194	1/1	0.98	0.25	-	0,0,0,0	0
58	MG	YA	3220	1/1	0.94	0.16	-	1,1,1,1	0
58	MG	YA	3160	1/1	0.92	0.14	-	16,16,16,16	0
58	MG	RA	3160	1/1	0.92	0.19	-	19,19,19,19	0
58	MG	RA	3221	1/1	0.60	0.23	-	30,30,30,30	0
58	MG	YA	3194	1/1	0.90	0.26	-	36,36,36,36	0
58	MG	YA	3221	1/1	0.97	0.08	-	19,19,19,19	0
58	MG	YA	3004	1/1	0.96	0.15	-	11,11,11,11	0
58	MG	YA	3081	1/1	0.90	0.29	-	10,10,10,10	0
58	MG	YA	3075	1/1	0.89	0.15	-	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	RA	3042	1/1	0.95	0.23	-	1,1,1,1	0
58	MG	RA	3006	1/1	0.81	0.41	-	10,10,10,10	0
58	MG	RA	3209	1/1	0.73	0.25	-	47,47,47,47	0
58	MG	YA	3122	1/1	0.97	0.15	-	9,9,9,9	0
58	MG	RA	3242	1/1	0.90	0.32	-	13,13,13,13	0
58	MG	YA	3247	1/1	0.88	0.49	-	34,34,34,34	0
58	MG	QA	1644	1/1	0.96	0.11	-	26,26,26,26	0
58	MG	YA	3239	1/1	0.90	0.17	-	41,41,41,41	0
58	MG	RA	3162	1/1	0.92	0.52	-	18,18,18,18	0
58	MG	YA	3013	1/1	0.88	0.32	-	3,3,3,3	0
58	MG	RA	3114	1/1	0.95	0.16	-	10,10,10,10	0
58	MG	YQ	201	1/1	0.88	0.11	-	90,90,90,90	0
58	MG	YA	3101	1/1	0.98	0.32	-	5,5,5,5	0
58	MG	YA	3179	1/1	0.81	0.23	-	26,26,26,26	0
58	MG	XA	1625	1/1	0.97	0.11	-	5,5,5,5	0
58	MG	YA	3187	1/1	0.88	0.29	-	41,41,41,41	0
58	MG	RA	3030	1/1	0.97	0.19	-	8,8,8,8	0
58	MG	RA	3013	1/1	0.77	0.27	-	29,29,29,29	0
58	MG	YA	3190	1/1	0.92	0.15	-	8,8,8,8	0
58	MG	YA	3155	1/1	0.84	0.24	-	45,45,45,45	0
58	MG	QA	1647	1/1	0.92	0.32	-	38,38,38,38	0
58	MG	XA	1674	1/1	0.96	0.17	-	4,4,4,4	0
58	MG	QF	201	1/1	0.91	0.25	-	36,36,36,36	0
58	MG	RA	3139	1/1	0.98	0.19	-	12,12,12,12	0
58	MG	YA	3128	1/1	0.98	0.46	-	6,6,6,6	0
58	MG	RA	3153	1/1	0.96	0.12	-	0,0,0,0	0
58	MG	YA	3232	1/1	0.98	0.24	-	35,35,35,35	0
58	MG	YA	3231	1/1	0.93	0.20	-	34,34,34,34	0
58	MG	RA	3240	1/1	0.95	0.29	-	5,5,5,5	0
58	MG	YA	3079	1/1	0.96	0.19	-	22,22,22,22	0
58	MG	YA	3147	1/1	0.95	0.27	-	9,9,9,9	0
58	MG	QA	1661	1/1	0.98	0.16	-	50,50,50,50	0
58	MG	YA	3240	1/1	0.96	0.15	-	12,12,12,12	0
58	MG	YA	3052	1/1	0.96	0.16	-	12,12,12,12	0
58	MG	YA	3208	1/1	0.87	0.41	-	35,35,35,35	0
58	MG	XA	1662	1/1	0.95	0.14	-	12,12,12,12	0
58	MG	RA	3228	1/1	0.85	0.16	-	13,13,13,13	0
58	MG	RA	3203	1/1	0.84	0.18	-	15,15,15,15	0
58	MG	YA	3171	1/1	0.92	0.22	-	22,22,22,22	0
58	MG	YA	3092	1/1	0.98	0.14	-	28,28,28,28	0
58	MG	YA	3145	1/1	0.87	0.20	-	20,20,20,20	0
58	MG	RA	3234	1/1	0.68	0.33	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	YA	3066	1/1	0.98	0.31	-	6,6,6,6	0
58	MG	QA	1655	1/1	0.92	0.21	-	14,14,14,14	0
58	MG	RA	3143	1/1	0.76	0.14	-	5,5,5,5	0
58	MG	RA	3157	1/1	0.67	0.38	-	37,37,37,37	0
58	MG	RA	3214	1/1	0.89	0.26	-	24,24,24,24	0
58	MG	RA	3028	1/1	0.97	0.30	-	17,17,17,17	0
58	MG	YA	3186	1/1	0.95	0.24	-	25,25,25,25	0
58	MG	XA	1678	1/1	0.93	0.23	-	2,2,2,2	0
58	MG	XA	1603	1/1	0.95	0.11	-	1,1,1,1	0
58	MG	YA	3256	1/1	0.89	0.60	-	74,74,74,74	0
58	MG	YA	3235	1/1	0.90	0.21	-	26,26,26,26	0
58	MG	QA	1635	1/1	0.94	0.39	-	76,76,76,76	0
58	MG	RA	3101	1/1	0.91	0.18	-	18,18,18,18	0
58	MG	RA	3008	1/1	0.94	0.46	-	6,6,6,6	0
58	MG	RA	3113	1/1	0.97	0.13	-	1,1,1,1	0
58	MG	XA	1655	1/1	0.91	0.29	-	68,68,68,68	0
58	MG	YA	3071	1/1	0.91	0.21	-	1,1,1,1	0
58	MG	YA	3195	1/1	0.93	0.19	-	5,5,5,5	0
58	MG	XA	1652	1/1	0.97	0.07	-	32,32,32,32	0
58	MG	RA	3035	1/1	0.99	0.11	-	2,2,2,2	0
58	MG	QA	1663	1/1	0.94	0.21	-	19,19,19,19	0
58	MG	RA	3148	1/1	0.89	0.39	-	47,47,47,47	0
58	MG	QA	1660	1/1	0.88	0.10	-	36,36,36,36	0
58	MG	YA	3173	1/1	0.89	0.25	-	15,15,15,15	0
58	MG	RA	3034	1/1	0.96	0.27	-	6,6,6,6	0
58	MG	RA	3226	1/1	0.90	0.32	-	1,1,1,1	0
58	MG	QA	1659	1/1	0.99	0.09	-	42,42,42,42	0
58	MG	XV	102	1/1	0.90	0.18	-	2,2,2,2	0
58	MG	RA	3055	1/1	0.95	0.12	-	10,10,10,10	0
58	MG	RA	3088	1/1	0.90	0.16	-	7,7,7,7	0
58	MG	RA	3199	1/1	0.87	0.78	-	63,63,63,63	0
58	MG	YA	3185	1/1	0.98	0.28	-	22,22,22,22	0
58	MG	YA	3175	1/1	0.97	0.25	-	14,14,14,14	0
58	MG	RA	3178	1/1	0.94	0.13	-	25,25,25,25	0
58	MG	RA	3108	1/1	0.95	0.10	-	6,6,6,6	0
58	MG	RA	3065	1/1	0.98	0.19	-	0,0,0,0	0
58	MG	QA	1643	1/1	0.89	0.23	-	21,21,21,21	0
58	MG	YA	3198	1/1	0.94	0.27	-	18,18,18,18	0
58	MG	RA	3066	1/1	0.97	0.16	-	7,7,7,7	0
58	MG	RA	3004	1/1	0.83	0.43	-	40,40,40,40	0
58	MG	XA	1680	1/1	0.79	0.31	-	45,45,45,45	0
58	MG	RA	3172	1/1	0.88	0.24	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	QA	1606	1/1	0.95	0.43	-	10,10,10,10	0
58	MG	XA	1602	1/1	0.85	0.23	-	15,15,15,15	0
58	MG	RA	3056	1/1	0.81	0.54	-	74,74,74,74	0
58	MG	YA	3022	1/1	0.96	0.26	-	7,7,7,7	0
58	MG	QA	1670	1/1	0.93	0.34	-	5,5,5,5	0
58	MG	RA	3131	1/1	0.97	0.30	-	7,7,7,7	0
58	MG	YA	3149	1/1	0.95	0.21	-	16,16,16,16	0
58	MG	QA	1639	1/1	0.94	0.22	-	33,33,33,33	0
58	MG	YA	3041	1/1	0.88	0.56	-	74,74,74,74	0
58	MG	QA	1604	1/1	0.76	0.25	-	5,5,5,5	0
58	MG	QA	1651	1/1	0.97	0.11	-	5,5,5,5	0
58	MG	RA	3187	1/1	0.94	0.21	-	42,42,42,42	0
58	MG	YA	3215	1/1	0.94	0.13	-	42,42,42,42	0
58	MG	XA	1608	1/1	0.96	0.17	-	1,1,1,1	0
58	MG	RA	3010	1/1	0.91	0.47	-	14,14,14,14	0
58	MG	YA	3228	1/1	0.81	0.14	-	9,9,9,9	0
58	MG	RA	3119	1/1	0.96	0.16	-	20,20,20,20	0
58	MG	QA	1671	1/1	0.86	0.16	-	6,6,6,6	0
58	MG	YA	3061	1/1	0.98	0.14	-	15,15,15,15	0
58	MG	RA	3230	1/1	0.94	0.20	-	41,41,41,41	0
58	MG	RA	3156	1/1	0.91	0.17	-	9,9,9,9	0
58	MG	QA	1636	1/1	0.94	0.18	-	1,1,1,1	0
58	MG	R8	101	1/1	0.96	0.15	-	6,6,6,6	0
58	MG	XA	1628	1/1	0.86	0.14	-	18,18,18,18	0
58	MG	YA	3242	1/1	0.94	0.14	-	9,9,9,9	0
58	MG	RE	301	1/1	0.92	0.20	-	9,9,9,9	0
58	MG	RA	3109	1/1	0.96	0.20	-	0,0,0,0	0
58	MG	XA	1624	1/1	0.92	0.10	-	22,22,22,22	0
58	MG	YA	3265	1/1	0.95	0.17	-	24,24,24,24	0
58	MG	YA	3211	1/1	0.94	0.50	-	55,55,55,55	0
58	MG	YA	3225	1/1	0.97	0.14	-	12,12,12,12	0
58	MG	YA	3262	1/1	0.89	0.23	-	26,26,26,26	0
58	MG	RA	3193	1/1	0.88	0.23	-	47,47,47,47	0
58	MG	YA	3064	1/1	0.98	0.14	-	4,4,4,4	0
58	MG	RA	3237	1/1	0.91	0.38	-	6,6,6,6	0
58	MG	QA	1666	1/1	0.94	0.12	-	68,68,68,68	0
58	MG	YA	3157	1/1	0.98	0.17	-	0,0,0,0	0
58	MG	R5	101	1/1	0.93	0.32	-	11,11,11,11	0
58	MG	QA	1609	1/1	0.98	0.10	-	32,32,32,32	0
58	MG	YA	3191	1/1	0.87	0.28	-	9,9,9,9	0
58	MG	RA	3222	1/1	0.94	0.11	-	2,2,2,2	0
58	MG	YA	3150	1/1	0.89	0.30	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	RA	3044	1/1	0.95	0.21	-	8,8,8,8	0
58	MG	RA	3023	1/1	0.97	0.23	-	9,9,9,9	0
58	MG	RA	3170	1/1	0.97	0.09	-	9,9,9,9	0
58	MG	RA	3152	1/1	0.97	0.24	-	14,14,14,14	0
58	MG	RA	3177	1/1	0.86	0.35	-	15,15,15,15	0
58	MG	RA	3058	1/1	0.96	0.11	-	5,5,5,5	0
58	MG	RA	3191	1/1	0.90	0.17	-	46,46,46,46	0
58	MG	YA	3123	1/1	0.97	0.21	-	1,1,1,1	0
58	MG	YA	3245	1/1	0.87	0.18	-	33,33,33,33	0
58	MG	YA	3076	1/1	0.96	0.34	-	10,10,10,10	0
58	MG	YA	3134	1/1	0.94	0.13	-	19,19,19,19	0
58	MG	RA	3083	1/1	0.97	0.22	-	32,32,32,32	0
58	MG	YA	3248	1/1	0.86	0.20	-	8,8,8,8	0
58	MG	XA	1676	1/1	0.89	0.34	-	19,19,19,19	0
58	MG	XA	1677	1/1	0.92	0.16	-	2,2,2,2	0
58	MG	YA	3253	1/1	0.98	0.14	-	22,22,22,22	0
58	MG	XA	1631	1/1	0.94	0.21	-	4,4,4,4	0
58	MG	RA	3207	1/1	0.89	0.21	-	7,7,7,7	0
58	MG	YA	3230	1/1	0.92	0.15	-	42,42,42,42	0
58	MG	RA	3212	1/1	0.57	0.75	-	73,73,73,73	0
58	MG	RA	3048	1/1	0.99	0.16	-	2,2,2,2	0
58	MG	YA	3172	1/1	0.93	0.37	-	40,40,40,40	0
58	MG	YA	3178	1/1	0.94	0.26	-	17,17,17,17	0
58	MG	RA	3015	1/1	0.96	0.27	-	0,0,0,0	0
58	MG	YA	3202	1/1	0.97	0.21	-	38,38,38,38	0
58	MG	RA	3201	1/1	0.83	0.25	-	34,34,34,34	0
58	MG	RA	3018	1/1	0.95	0.26	-	5,5,5,5	0
58	MG	XA	1612	1/1	0.98	0.24	-	10,10,10,10	0
58	MG	YA	3029	1/1	0.95	0.22	-	12,12,12,12	0
58	MG	YA	3146	1/1	0.93	0.23	-	40,40,40,40	0
58	MG	QA	1667	1/1	0.66	0.24	-	35,35,35,35	0
58	MG	RA	3165	1/1	0.95	0.23	-	30,30,30,30	0
58	MG	RA	3171	1/1	0.77	0.29	-	31,31,31,31	0
58	MG	YA	3224	1/1	0.96	0.26	-	18,18,18,18	0
58	MG	YA	3096	1/1	0.92	0.20	-	6,6,6,6	0
58	MG	YA	3213	1/1	0.99	0.12	-	31,31,31,31	0
58	MG	RA	3150	1/1	0.96	0.22	-	27,27,27,27	0
58	MG	RA	3124	1/1	0.89	0.16	-	2,2,2,2	0
58	MG	YA	3084	1/1	0.95	0.15	-	12,12,12,12	0
58	MG	YA	3251	1/1	0.91	0.57	-	10,10,10,10	0
58	MG	RA	3103	1/1	0.97	0.28	-	5,5,5,5	0
58	MG	RA	3011	1/1	0.96	0.22	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	YA	3057	1/1	0.95	0.34	-	11,11,11,11	0
58	MG	QA	1650	1/1	0.98	0.17	-	53,53,53,53	0
58	MG	RA	3078	1/1	0.98	0.21	-	16,16,16,16	0
58	MG	RA	3012	1/1	0.91	0.40	-	31,31,31,31	0
58	MG	XA	1633	1/1	0.94	0.10	-	7,7,7,7	0
58	MG	YA	3196	1/1	0.96	0.11	-	41,41,41,41	0
58	MG	YA	3063	1/1	0.99	0.36	-	12,12,12,12	0
58	MG	YA	3217	1/1	0.87	0.13	-	18,18,18,18	0
58	MG	XA	1650	1/1	0.79	0.21	-	14,14,14,14	0
58	MG	YA	3069	1/1	0.97	0.26	-	12,12,12,12	0
58	MG	YA	3060	1/1	0.93	0.24	-	8,8,8,8	0
58	MG	RA	3076	1/1	0.93	0.15	-	7,7,7,7	0
58	MG	YA	3263	1/1	0.73	0.26	-	40,40,40,40	0
58	MG	QA	1654	1/1	0.97	0.14	-	12,12,12,12	0
58	MG	YA	3121	1/1	0.95	0.11	-	6,6,6,6	0
58	MG	RA	3002	1/1	0.76	0.46	-	30,30,30,30	0
58	MG	YA	3127	1/1	0.89	0.30	-	23,23,23,23	0
58	MG	YA	3082	1/1	0.98	0.13	-	17,17,17,17	0
58	MG	XA	1682	1/1	0.88	0.20	-	35,35,35,35	0
58	MG	XA	1670	1/1	0.91	0.19	-	27,27,27,27	0
58	MG	YA	3059	1/1	0.94	0.14	-	11,11,11,11	0
58	MG	XA	1604	1/1	0.90	0.29	-	9,9,9,9	0
58	MG	Y5	101	1/1	0.98	0.26	-	13,13,13,13	0
58	MG	YA	3021	1/1	0.99	0.26	-	8,8,8,8	0
58	MG	QA	1625	1/1	0.95	0.30	-	29,29,29,29	0
58	MG	YA	3018	1/1	0.79	0.77	-	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.