



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:37 PM UTC

PDB ID : 5VPO / pdb_00005vpo
Title : The 70S P-site ASL SufA6 complex
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Deposited on : 2017-05-05
Resolution : 3.34 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

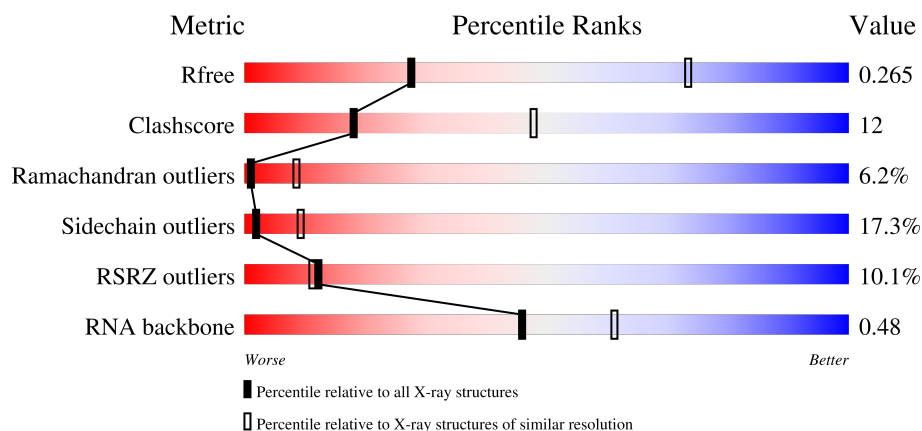
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)
RNA backbone	3983	1083 (3.68-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	QX	19	5% 16% 5% 79%
1	XX	19	5% 16% 5% 79%
2	QA	1521	5% 56% 34% 8%
2	XA	1521	4% 55% 34% 9%

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Mol	Chain	Length	Quality of chain
3	QB	256	
3	XB	256	
4	QC	239	
4	XC	239	
5	QD	209	
5	XD	209	
6	QE	162	
6	XE	162	
7	QF	101	
7	XF	101	
8	QG	156	
8	XG	156	
9	QH	138	
9	XH	138	
10	QI	128	
10	XI	128	
11	QJ	105	
11	XJ	105	
12	QK	129	
12	XK	129	
13	QL	132	
13	XL	132	
14	QM	126	
14	XM	126	
15	QN	61	

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Mol	Chain	Length	Quality of chain
15	XN	61	
16	QO	89	
16	XO	89	
17	QP	88	
17	XP	88	
18	QQ	105	
18	XQ	105	
19	QR	88	
19	XR	88	
20	QS	93	
20	XS	93	
21	QT	106	
21	XT	106	
22	QU	27	
22	XU	27	
23	RA	2915	
23	YA	2915	
24	RB	122	
24	YB	122	
25	RD	276	
25	YD	276	
26	RE	206	
26	YE	206	
27	RF	210	
27	YF	210	

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Mol	Chain	Length	Quality of chain
28	RG	182	
28	YG	182	
29	RH	180	
29	YH	180	
30	RI	148	
30	YI	148	
31	RN	140	
31	YN	140	
32	RO	122	
32	YO	122	
33	RP	150	
33	YP	150	
34	RQ	141	
34	YQ	141	
35	RR	118	
35	YR	118	
36	RS	112	
36	YS	112	
37	RT	146	
37	YT	146	
38	RU	118	
38	YU	118	
39	RV	101	
39	YV	101	
40	RW	113	

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Mol	Chain	Length	Quality of chain
40	YW	113	
41	RX	96	
41	YX	96	
42	RY	110	
42	YY	110	
43	RZ	206	
43	YZ	206	
44	R0	85	
44	Y0	85	
45	R1	98	
45	Y1	98	
46	R2	72	
46	Y2	72	
47	R3	60	
47	Y3	60	
48	R4	71	
48	Y4	71	
49	R5	60	
49	Y5	60	
50	R6	54	
50	Y6	54	
51	R7	49	
51	Y7	49	
52	R8	65	
52	Y8	65	

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Mol	Chain	Length	Quality of chain
53	R9	37	
53	Y9	37	
54	QV	18	
54	XV	18	

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
55	MG	QA	1603	-	-	-	X
55	MG	QA	1604	-	-	-	X
55	MG	QA	1613	-	-	-	X
55	MG	QA	1618	-	-	-	X
55	MG	QA	1619	-	-	-	X
55	MG	QA	1625	-	-	-	X
55	MG	QA	1631	-	-	-	X
55	MG	QA	1639	-	-	-	X
55	MG	QA	1641	-	-	-	X
55	MG	QA	1652	-	-	-	X
55	MG	QA	1665	-	-	-	X
55	MG	RA	3112	-	-	-	X
55	MG	RA	3122	-	-	-	X
55	MG	RA	3126	-	-	-	X
55	MG	RA	3152	-	-	-	X
55	MG	RA	3219	-	-	-	X
55	MG	RA	3220	-	-	-	X
55	MG	RA	3230	-	-	-	X
55	MG	RA	3242	-	-	-	X
55	MG	XA	1602	-	-	-	X
55	MG	XA	1609	-	-	-	X
55	MG	XA	1614	-	-	-	X
55	MG	XA	1617	-	-	-	X
55	MG	XA	1620	-	-	-	X
55	MG	XA	1623	-	-	-	X
55	MG	XA	1634	-	-	-	X
55	MG	XA	1635	-	-	-	X
55	MG	XA	1641	-	-	-	X
55	MG	XA	1645	-	-	-	X
55	MG	XA	1662	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	YA	3126	-	-	-	X
55	MG	YA	3131	-	-	-	X
55	MG	YP	202	-	-	-	X

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 288423 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 messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QX	4	Total	C	N	O	P	0	0	0
			80	36	11	29	4			
1	XX	4	Total	C	N	O	P	0	0	0
			80	36	11	29	4			

- Molecule 2 is a RNA chain called 16S rRNA.

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

- Molecule 3 is a protein called 30S ribosomal protein S2.

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

- Molecule 4 is a protein called 30S ribosomal protein S3.

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

- Molecule 5 is a protein called 30S ribosomal protein S4.

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

- Molecule 6 is a protein called 30S ribosomal protein S5.

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

- Molecule 7 is a protein called 30S ribosomal protein S6.

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

- Molecule 8 is a protein called 30S ribosomal protein S7.

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

- Molecule 9 is a protein called 30S ribosomal protein S8.

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

- Molecule 10 is a protein called 30S ribosomal protein S9.

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

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

- Molecule 11 is a protein called 30S ribosomal protein S10.

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

- Molecule 12 is a protein called 30S ribosomal protein S11.

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

- Molecule 13 is a protein called 30S ribosomal protein S12.

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

- Molecule 14 is a protein called 30S ribosomal protein S13.

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

- Molecule 15 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 16 is a protein called 30S ribosomal protein S15.

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

- Molecule 17 is a protein called 30S ribosomal protein S16.

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

- Molecule 18 is a protein called 30S ribosomal protein S17.

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

- Molecule 19 is a protein called 30S ribosomal protein S18.

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

- Molecule 20 is a protein called 30S ribosomal protein S19.

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

- Molecule 21 is a protein called 30S ribosomal protein S20.

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

- Molecule 22 is a protein called 30S ribosomal protein Thx.

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

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

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

- Molecule 24 is a RNA chain called 5S rRNA.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

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

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

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

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

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

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L31.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L35.

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

- Molecule 53 is a protein called 50S ribosomal protein L36.

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

- Molecule 54 is a RNA chain called P-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	XV	18	Total	C	N	O	P	0	0	0
			385	173	70	125	17			
54	QV	18	Total	C	N	O	P	0	0	0
			385	173	70	125	17			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	66	Total	Mg	0	0
			66	66		
55	QF	1	Total	Mg	0	0
			1	1		
55	QH	1	Total	Mg	0	0
			1	1		
55	QM	1	Total	Mg	0	0
			1	1		
55	RA	243	Total	Mg	0	0
			243	243		
55	RB	2	Total	Mg	0	0
			2	2		
55	RD	1	Total	Mg	0	0
			1	1		
55	RE	2	Total	Mg	0	0
			2	2		
55	RF	1	Total	Mg	0	0
			1	1		
55	RP	2	Total	Mg	0	0
			2	2		
55	RR	1	Total	Mg	0	0
			1	1		
55	R0	1	Total	Mg	0	0
			1	1		
55	R3	1	Total	Mg	0	0
			1	1		
55	R5	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	R8	1	Total 1	Mg 1	0	0
55	XA	71	Total 71	Mg 71	0	0
55	XB	1	Total 1	Mg 1	0	0
55	XL	1	Total 1	Mg 1	0	0
55	XM	1	Total 1	Mg 1	0	0
55	YA	267	Total 267	Mg 267	0	0
55	YB	4	Total 4	Mg 4	0	0
55	YD	2	Total 2	Mg 2	0	0
55	YE	1	Total 1	Mg 1	0	0
55	YP	2	Total 2	Mg 2	0	0
55	YX	1	Total 1	Mg 1	0	0
55	Y5	1	Total 1	Mg 1	0	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots [i](#)

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

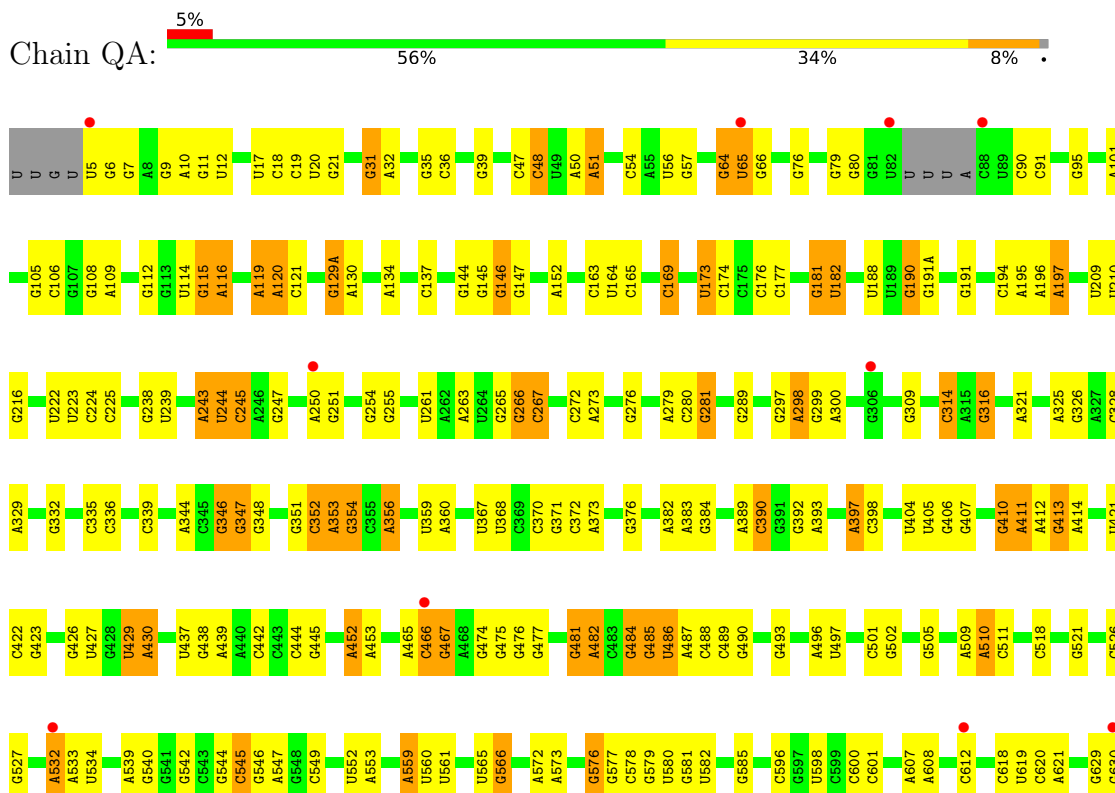
- Molecule 1: messenger RNA



- Molecule 1: messenger RNA



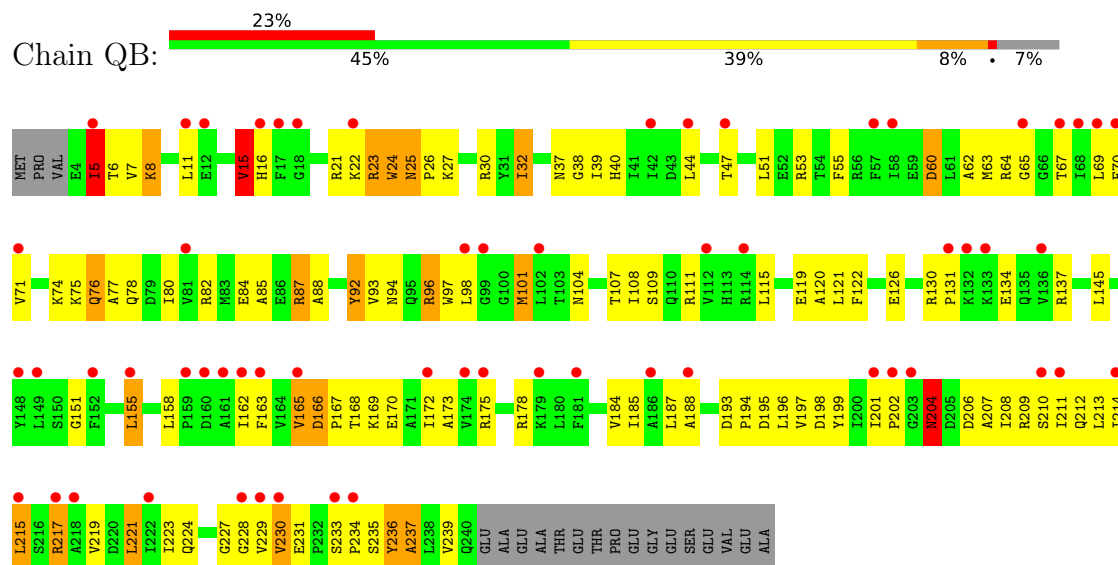
- Molecule 2: 16S rRNA



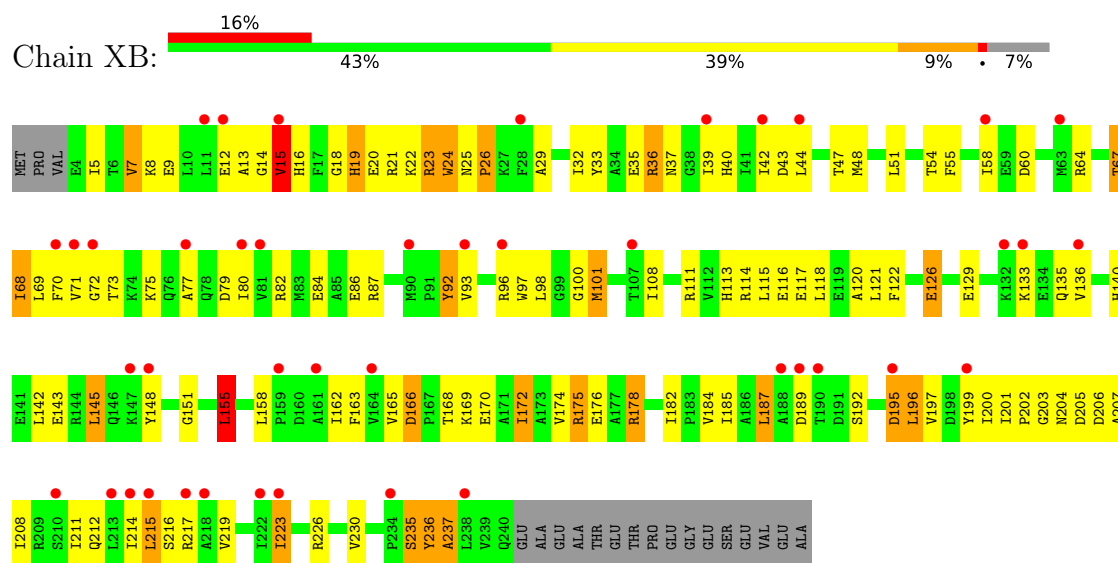


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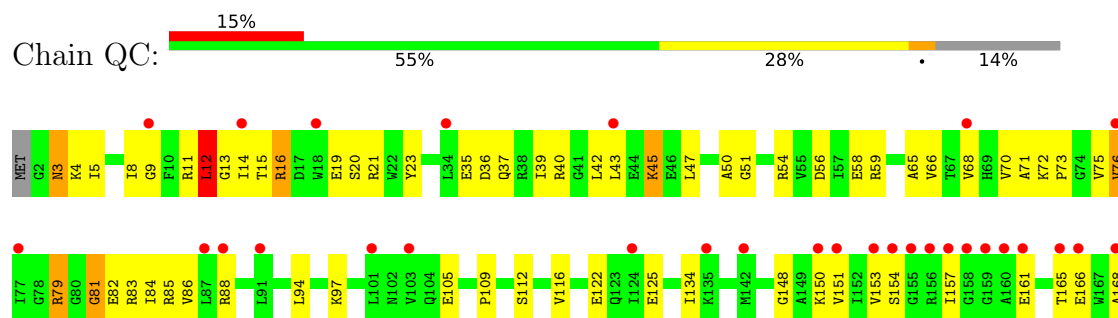
• Molecule 3: 30S ribosomal protein S2

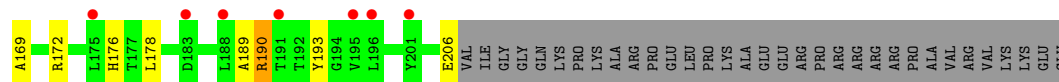


• Molecule 3: 30S ribosomal protein S2

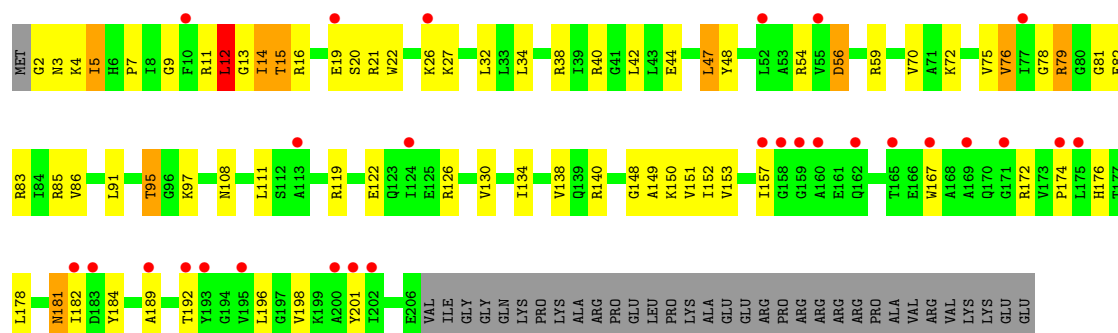


• Molecule 4: 30S ribosomal protein S3

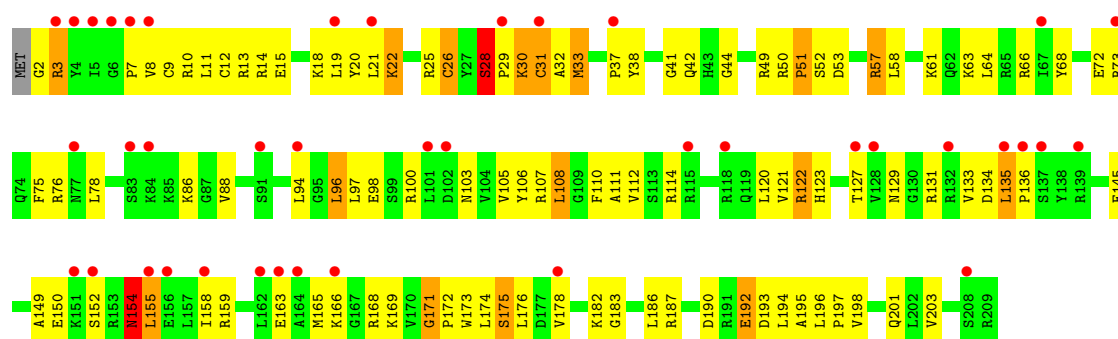




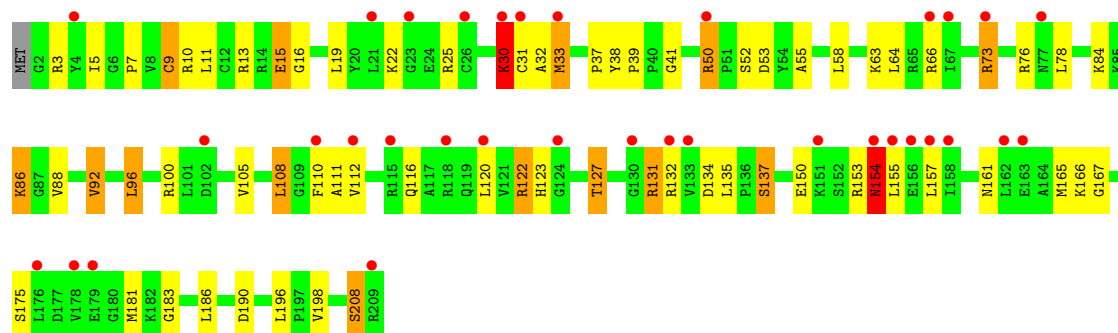
• Molecule 4: 30S ribosomal protein S3



• Molecule 5: 30S ribosomal protein S4

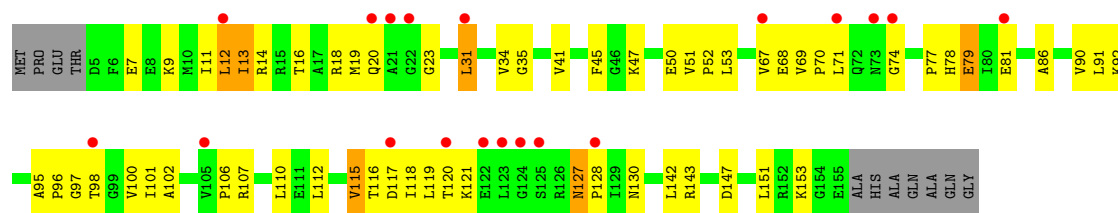


• Molecule 5: 30S ribosomal protein S4

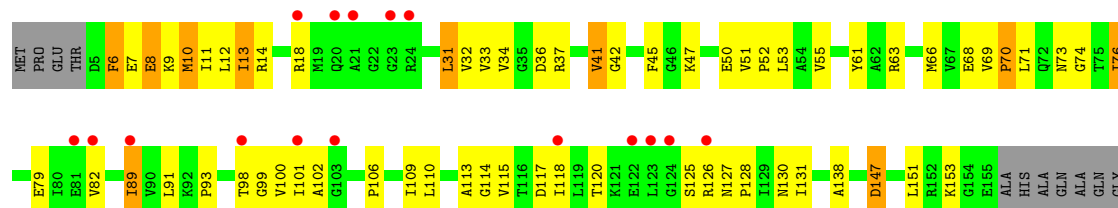


• Molecule 6: 30S ribosomal protein S5

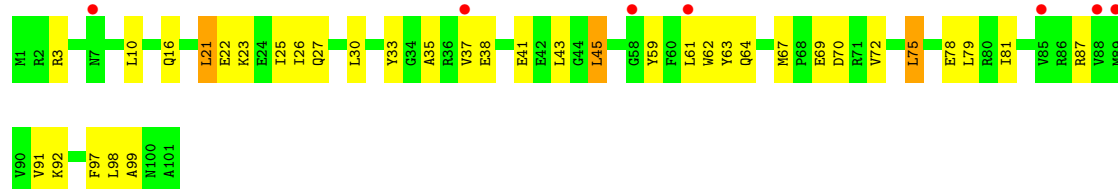




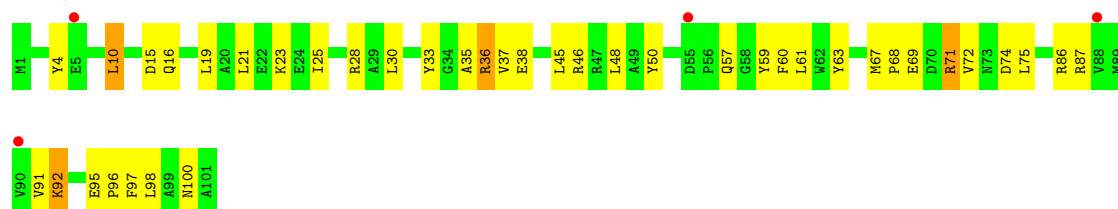
• Molecule 6: 30S ribosomal protein S5



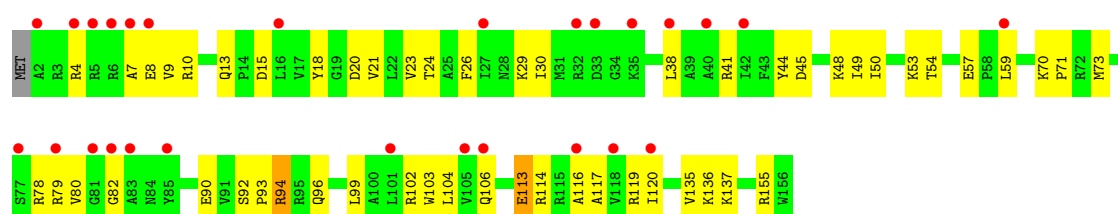
• Molecule 7: 30S ribosomal protein S6



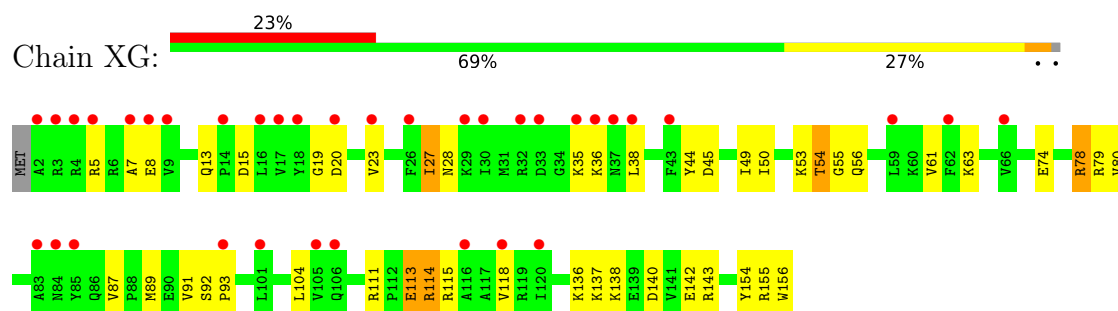
• Molecule 7: 30S ribosomal protein S6



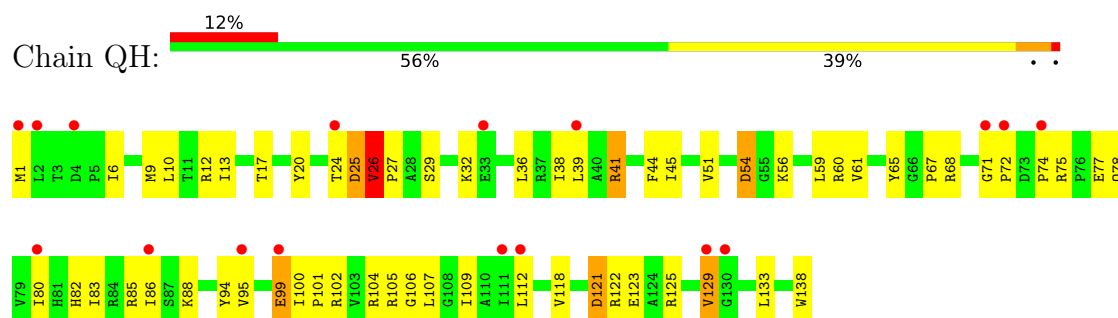
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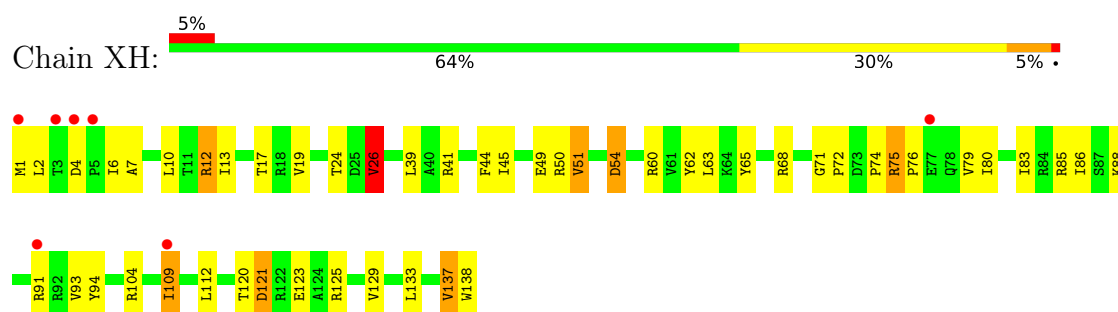
- Molecule 8: 30S ribosomal protein S7



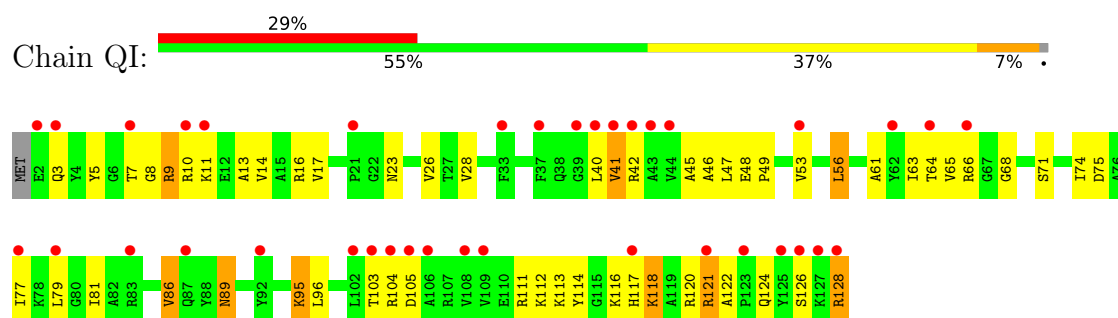
- Molecule 9: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S8

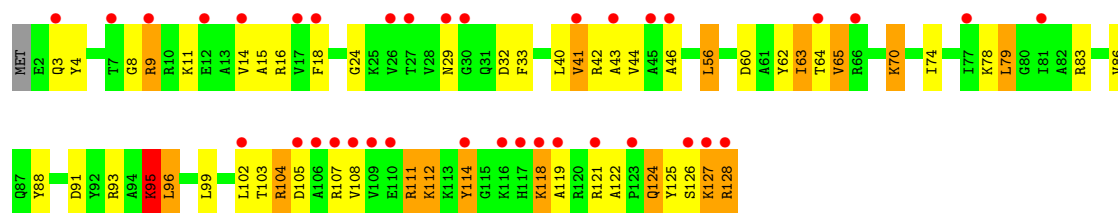


- Molecule 10: 30S ribosomal protein S9

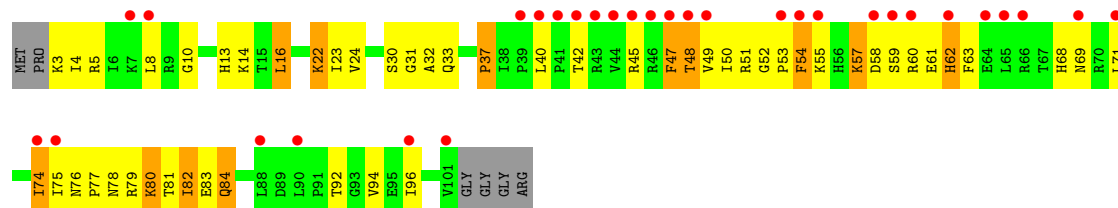


- Molecule 10: 30S ribosomal protein S9

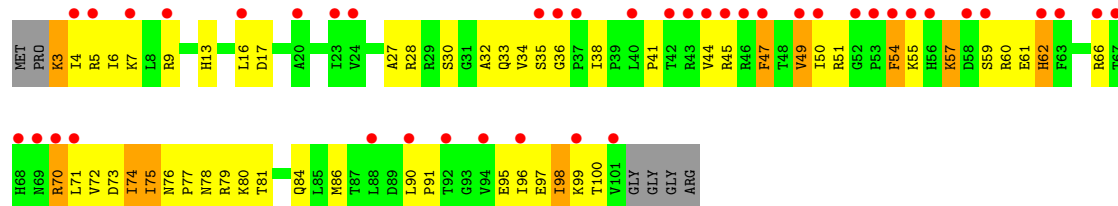
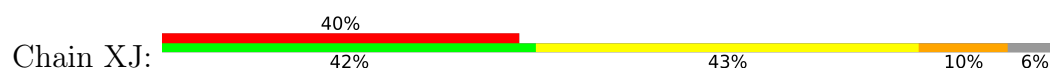




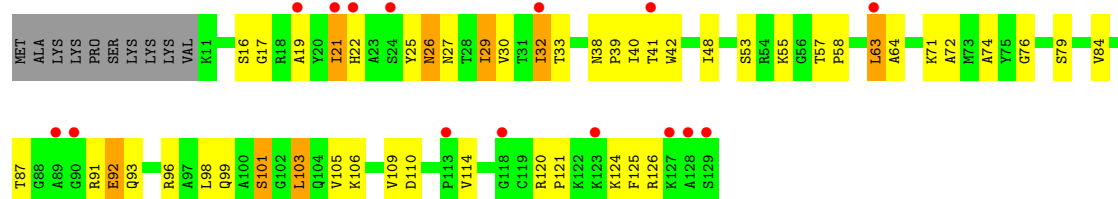
• Molecule 11: 30S ribosomal protein S10



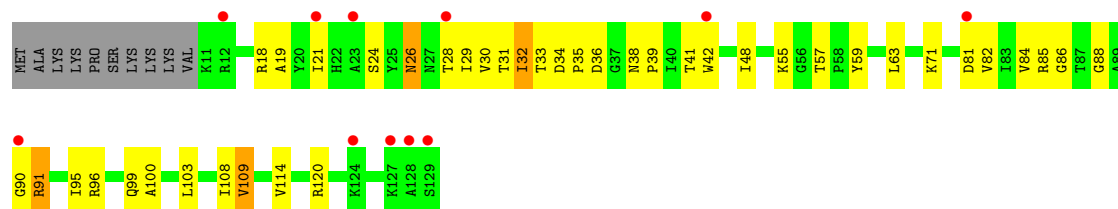
• Molecule 11: 30S ribosomal protein S10



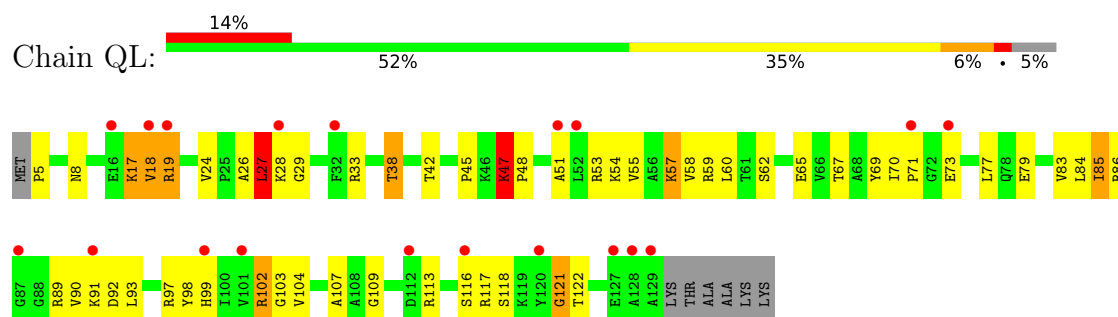
• Molecule 12: 30S ribosomal protein S11



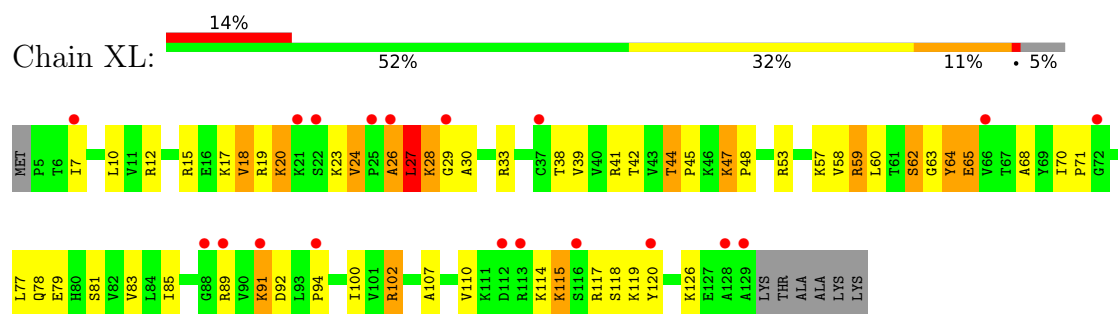
• Molecule 12: 30S ribosomal protein S11



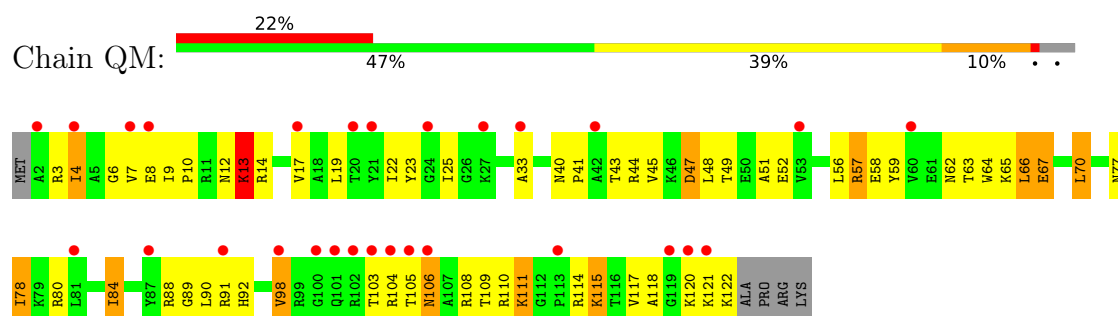
- Molecule 13: 30S ribosomal protein S12



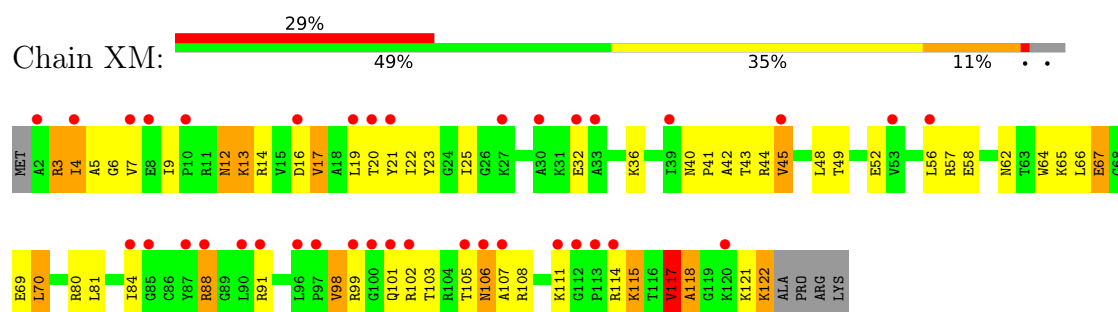
- Molecule 13: 30S ribosomal protein S12



- Molecule 14: 30S ribosomal protein S13

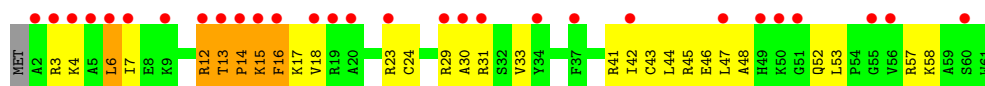


- Molecule 14: 30S ribosomal protein S13



- Molecule 15: 30S ribosomal protein S14 type Z

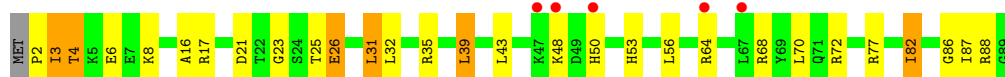




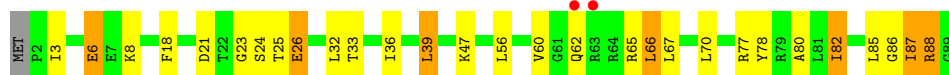
- Molecule 15: 30S ribosomal protein S14 type Z



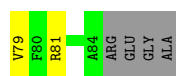
- Molecule 16: 30S ribosomal protein S15



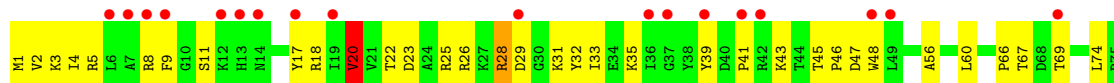
- Molecule 16: 30S ribosomal protein S15



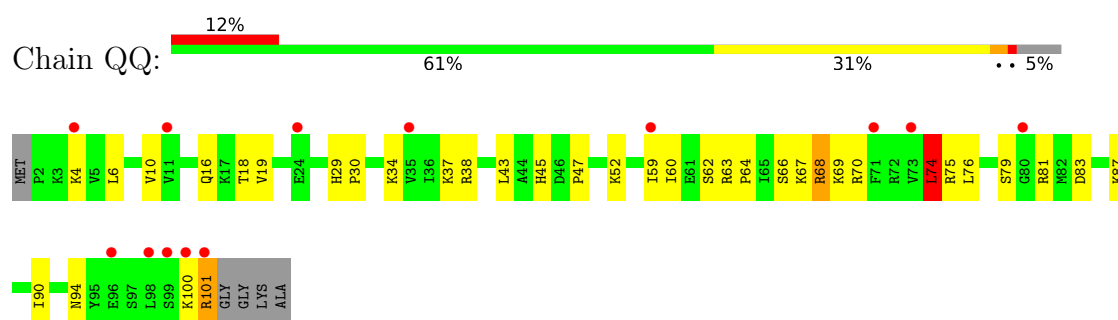
- Molecule 17: 30S ribosomal protein S16



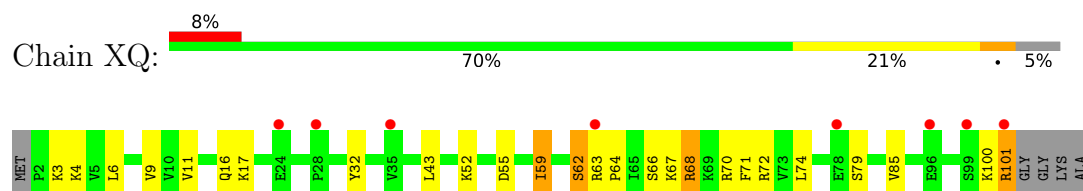
- Molecule 17: 30S ribosomal protein S16



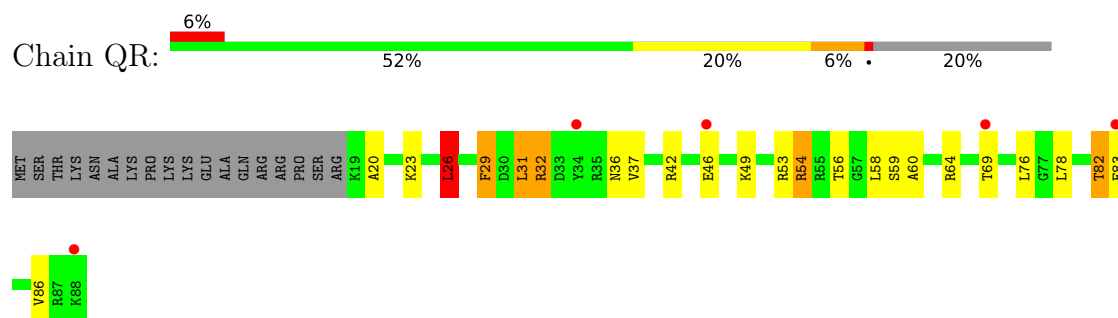
- Molecule 18: 30S ribosomal protein S17



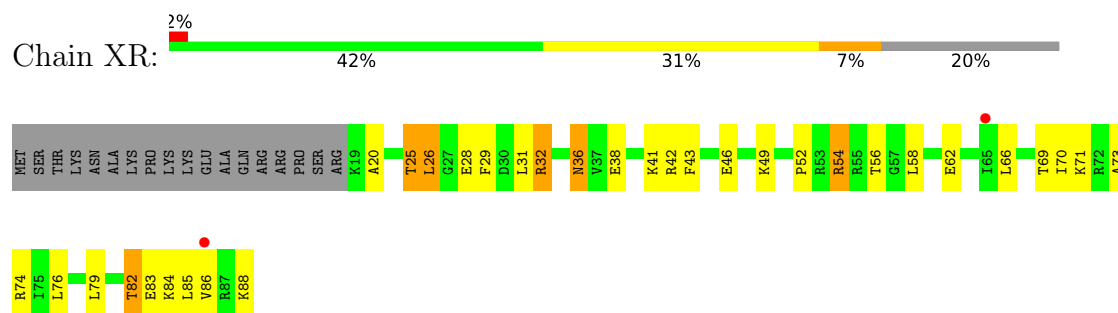
- Molecule 18: 30S ribosomal protein S17



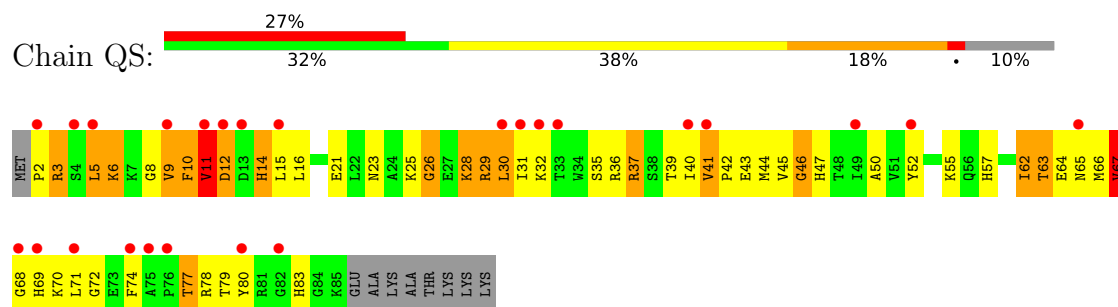
- Molecule 19: 30S ribosomal protein S18



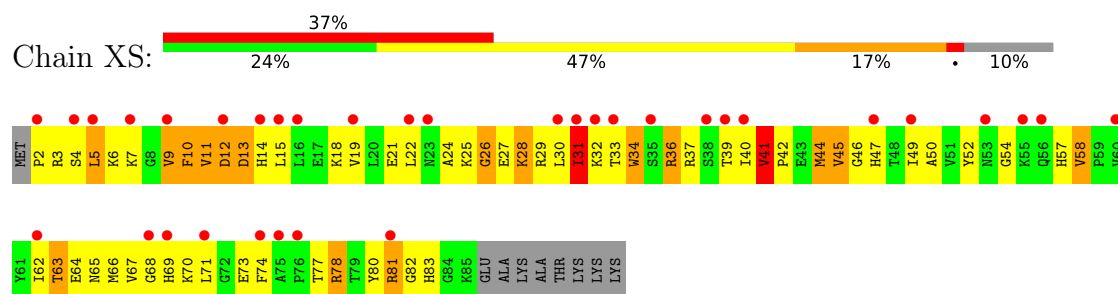
- Molecule 19: 30S ribosomal protein S18



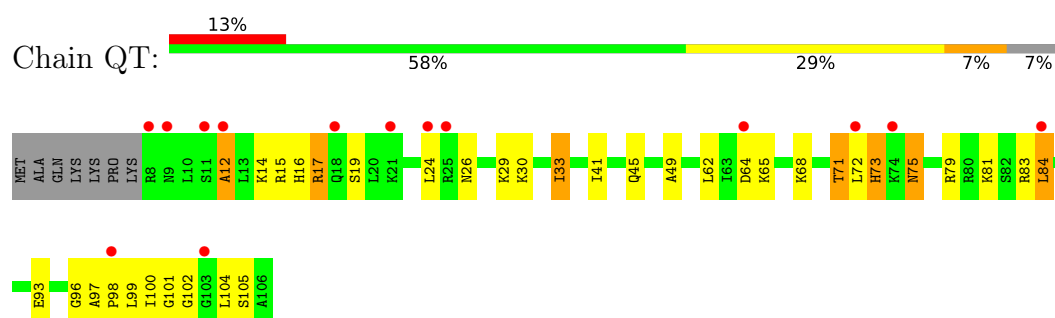
- Molecule 20: 30S ribosomal protein S19



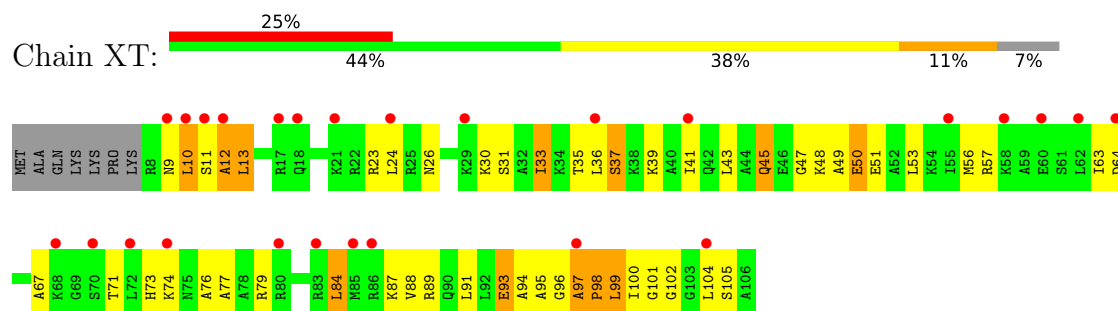
- Molecule 20: 30S ribosomal protein S19



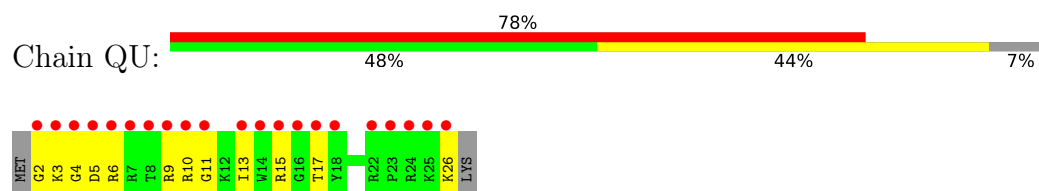
- Molecule 21: 30S ribosomal protein S20



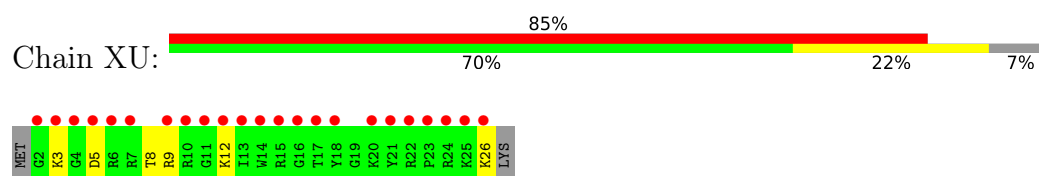
- Molecule 21: 30S ribosomal protein S20



- Molecule 22: 30S ribosomal protein Thx

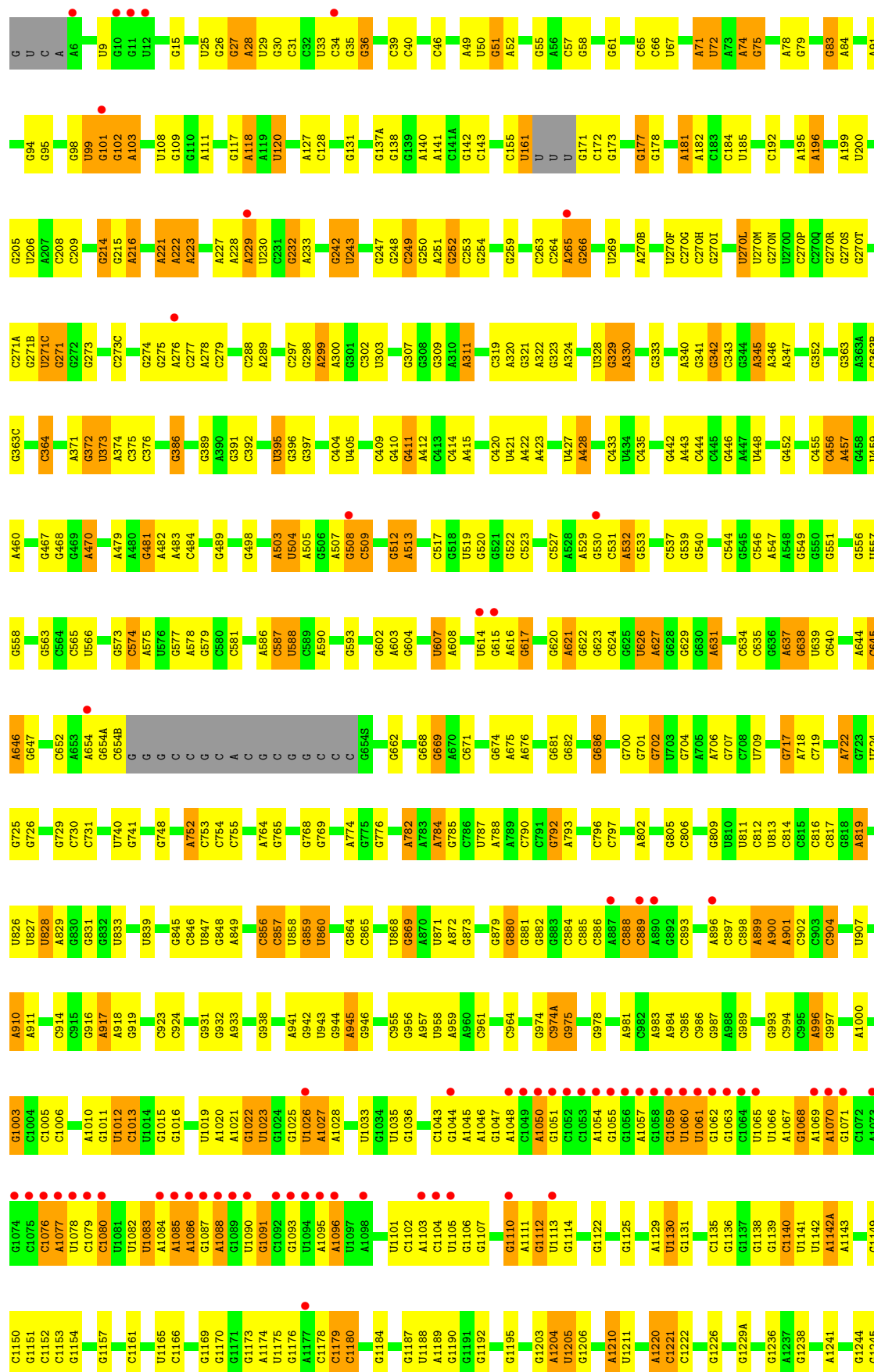


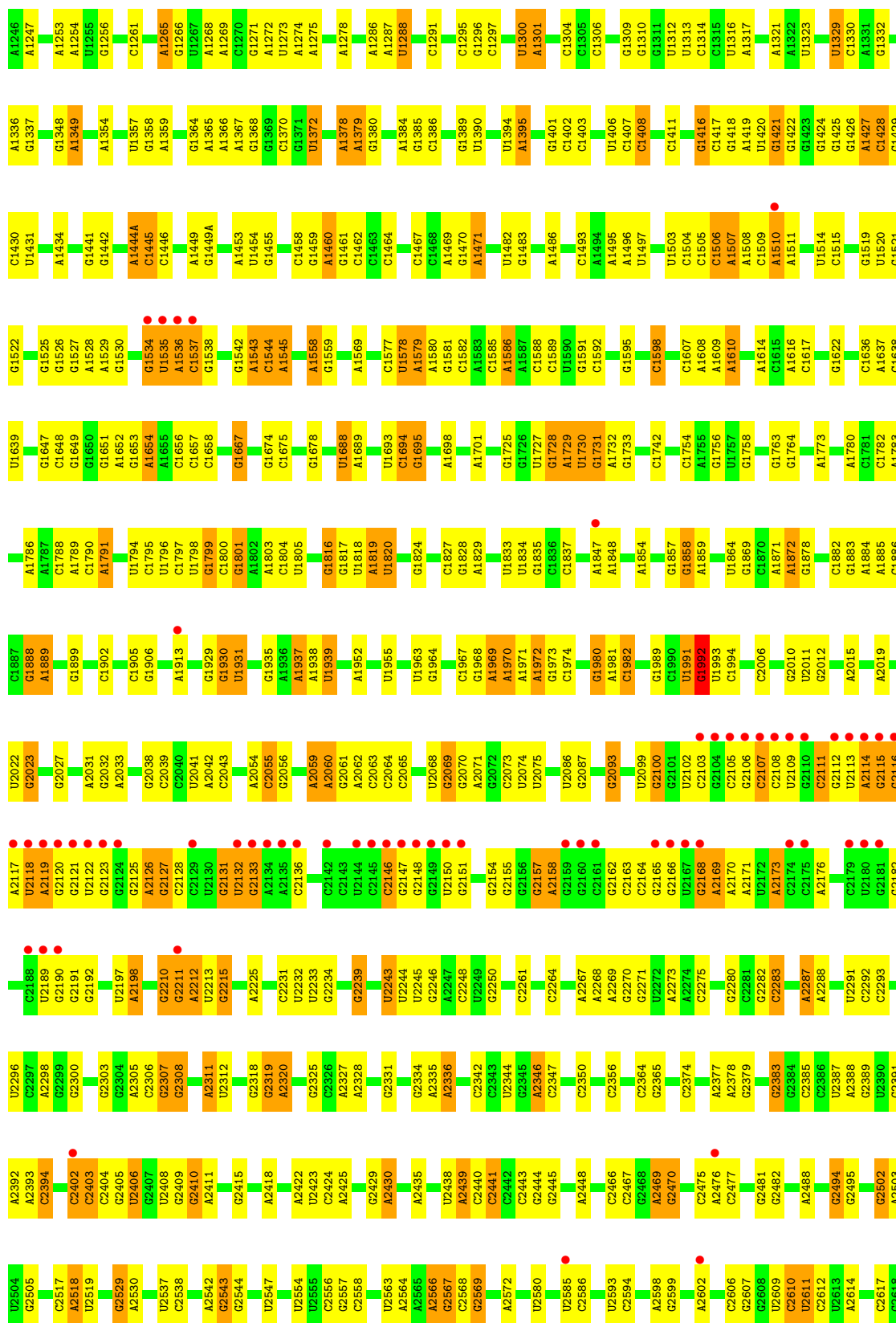
- Molecule 22: 30S ribosomal protein Thx

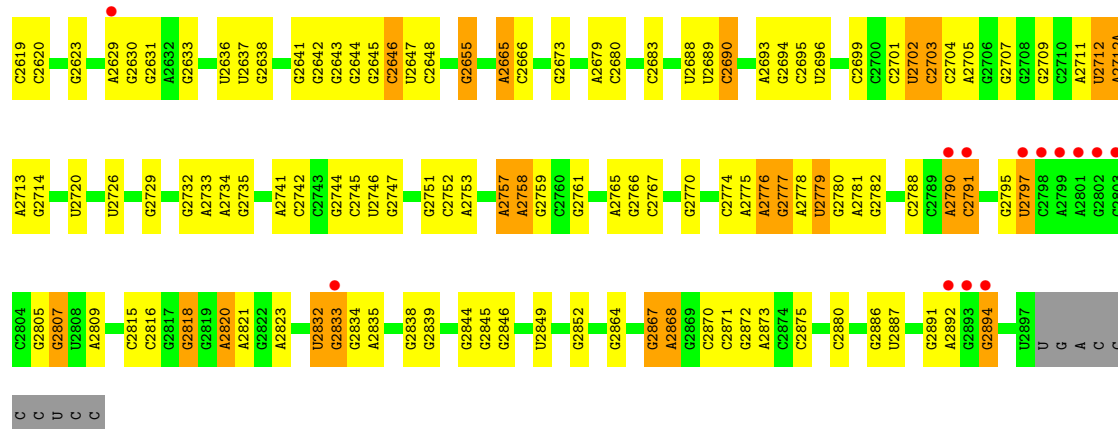


- Molecule 23: 23S rRNA

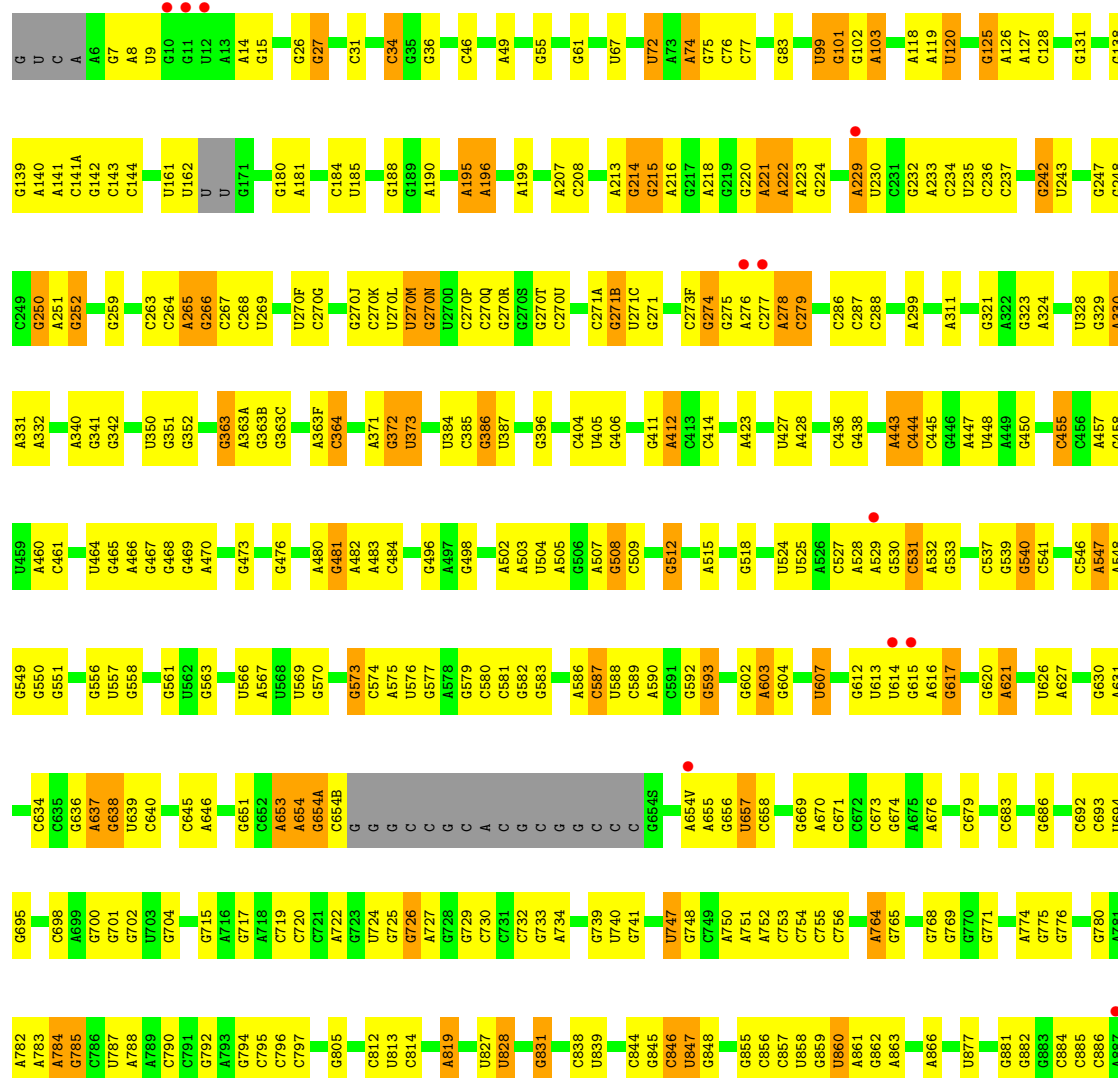




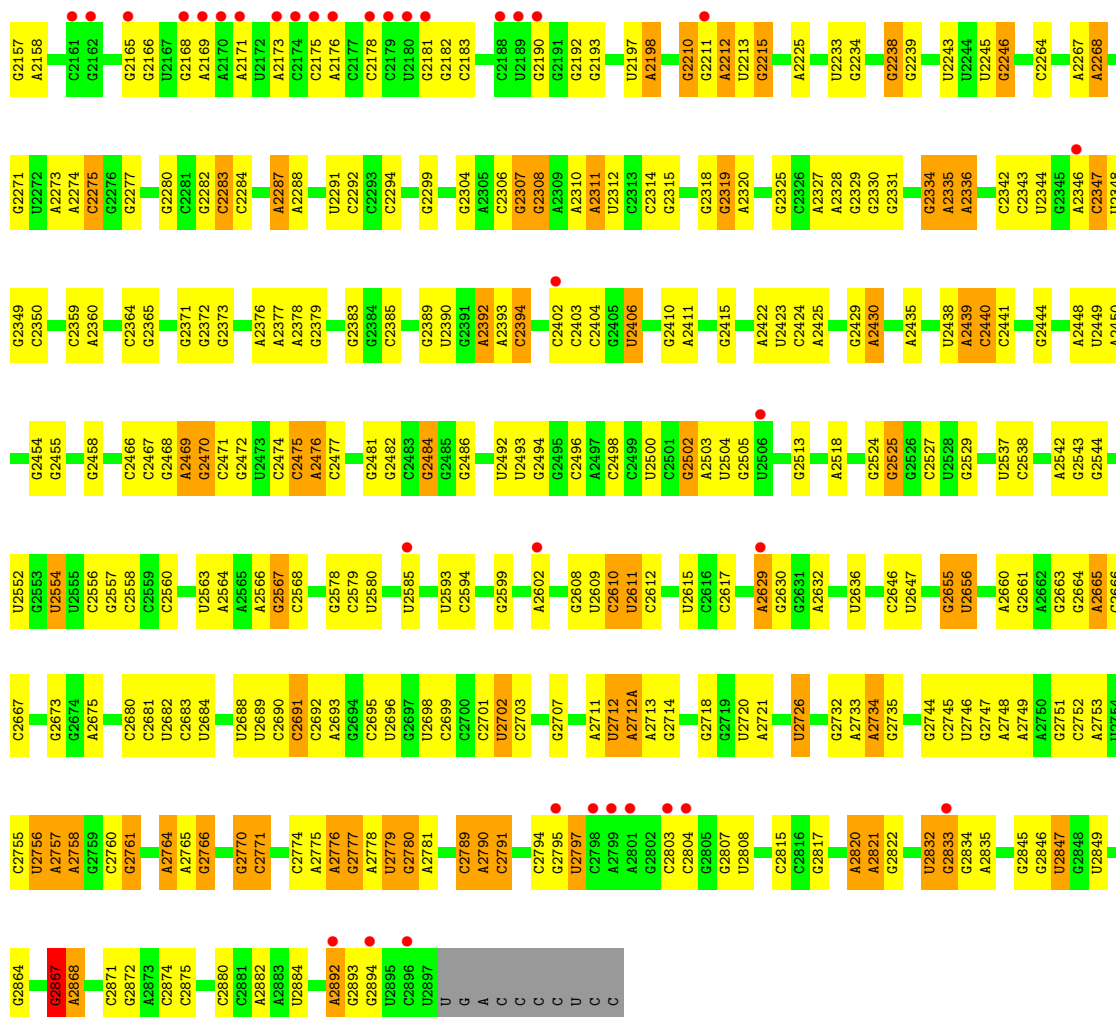




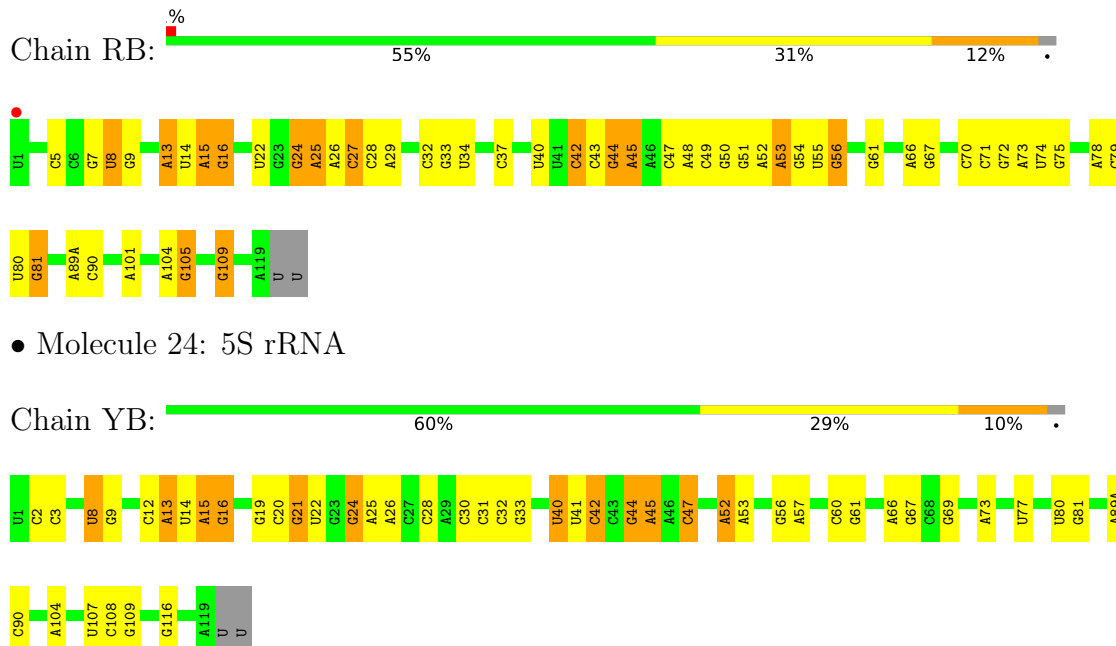
• Molecule 23: 23S rRNA



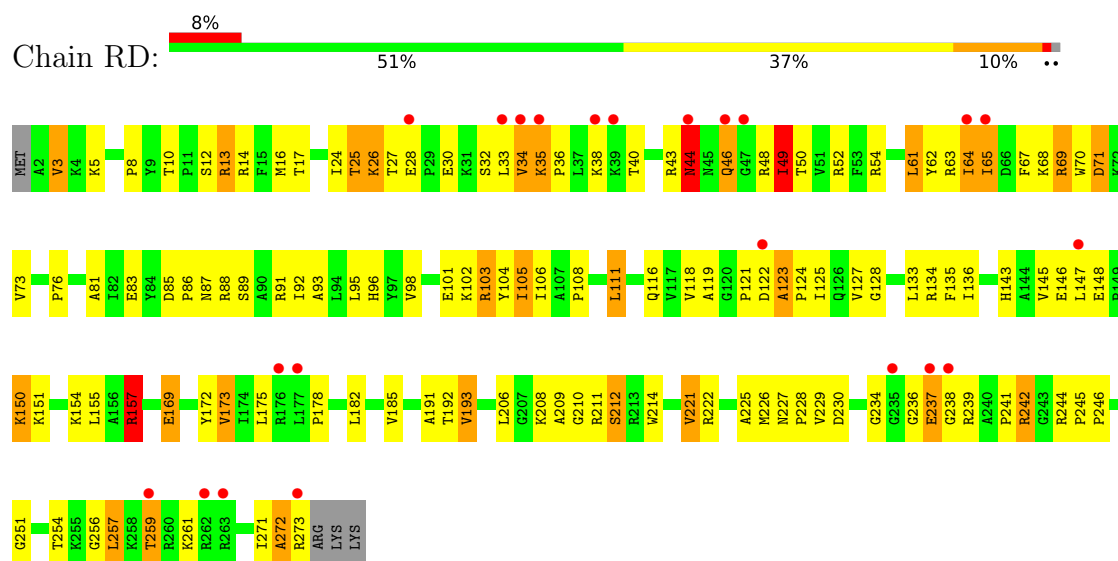
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G2093	A1981	A1871	G1758	G1647	U1535	A1444A	A1353	C1251	G1154	G1071	G992	C889
U2096	C1982	G1878	A1759	G1649	A1536	C1445	A1354	G1250	A1155	C1076	G993	A890
C2097	G1989	G1882	A1762	A1652	G1538	G1447	U1357	A1253	A1156	U1077	C995	G892
U2098	C1990	G1883	G1763	G1653	G1542	G1448	A1359	G1256	C1161	U1078	A996	A896
U2099	U1991	A1884	G1764	A1654	A1543	A1449A	A1360	C1257	G1162	C1079	C997	C897
G2100	G1992	A1888	C1765	A1654	A1544	G1450	G1365	G1264	G1163	U1081	C998	C898
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U2102	C1996	A1889	C1767	U1659	A1558	U1454	G1368	G1266	C1166	U1083	U907	
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G2106	A2013		A1780	G1668	A1568	G1459	U1372	A1269	G1171	G1011	A911	A911
C2107	A2014		C1781	A1668	G1568	A1460	G1378	G1270	G1173	U1089	C915	C915
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U2109				G1674	C1577		A1379	U1273	U1175		C1013	A917
G2110	A2020		A1786	C1675	U1578	C1467		U1278	G1176	G1093	G1016	A918
C2111	C2021		A1787	A1676	U1579	A1471	G1384	A1278	A1177	U1094		
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A2114	A2024		A1791	U1680			C1387	A1287	C1180	U1097	A1020	C923
G2115	C2025						G1388	C1291	G1187	G1098	A1021	G929
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A2117	C2027		C1795	U1689	A1586	U1482	U1394	C1293	A1189	C1100	G1024	G932
U2118	G2029		U1796	A1690	A1587	G1483	U1395	U1300	G1190	G1101	U1025	G938
G2119	A2030		C1797	C1691	G1591	G1484	A1396	A1301	G1191	A1103	U1026	
C2120	G2031		U1798		C1592	A1486	U1397			C1104	A1027	
G2121	A2032		G1799	C1694		G1487	C1398	C1306	G1195	U105	A1028	A941
U2122	G2033		C1800	G1695	G1595		C1399		C1201	G1106	U1033	G942
G2123			G1801	G1696		C1493	C1403	G1309	G1202	C1109	A1045	U943
C2124	U2040		A1936	G1697	C1598	A1494	G1404	G1310	G1203	G1110	A1046	A945
G2125	A2041		A1802	A1698	A1603	A1495	U1405	U1313	A1204	A1111	G1047	G946
A2126	C2042		C1804	G1699	C1604	U1497	U1406		U1205	G1112	A1048	
U2127	A2043		G1805	A1700			C1407	A1321	G1206	U1113	C1049	G956
C2128				A1701	C1607	C1506	C1408	A1322	G1209	G1122	A1050	U957
G2129	A2051		G1816	U1701	A1608	A1507	G1410	U1326	A1210	C1123	G1051	U958
U2130	C2055		G1824	G1717	A1609	A1508	C1409		U1211	G1224	C1053	A959
G2131	G2056		A1825	G1718	A1610	C1509	C1411	U1329	G1216	G1125	A1054	C961
C2132	U2057		G1826	G1725	A1614	A1511	G1416	C1330	C1217	G1055	G1056	G962
A2134	A2059		G1826	G1726	C1615		A1417	A1331	C1218	A1129	G1057	G968
G2135	A2060		A1829	U1727	C1616	U1514	G1418	G1332	G1219	U130	A1057	U969
C2136	A2061				C1617	U1520	A1419	U1335	C1221	G1131	G1058	G974
	C2063		U1834	G1731	A1618	G1521	U1420	A1336	C1222	G1135	U1060	C974A
G2141	A1960		C1835	A1732	G1622	G1522	G1421	G1337	G1235	G1136	U1061	G975
C2145	C2064		C1836	G1733	C1625	G1525	G1424	G1338	G1238	G1137	G1062	A980
G2146	C2065		U1847	C1743	G1626	A1528	A1427	G1339	G1239	G1139	G1063	A983
C2147	G2066		A1848	G1743	G1626	A1529	G1428	A1342	G1240	G1140	U1065	
G2148	C2067		G1858	G1750	A1637	G1530	G1429	U1240	U141	U1141	U1066	
U2149	U2068		A1859		G1638	G1531	C1430	G1348	A1241	U1142	A1067	G987
C2150	G2069		A1859	C1754	U1639	C1532	A1349	A1349	G1244	A1143	G1068	A990
G2151	A1969		A1859	A1755	C1640	C1533					A1069	
U2152	U2074		G1858	G1756								
G2153	U2075		A1859									
C2154	U2086		U1864									
G2155	G2087		G1869									
G2156												



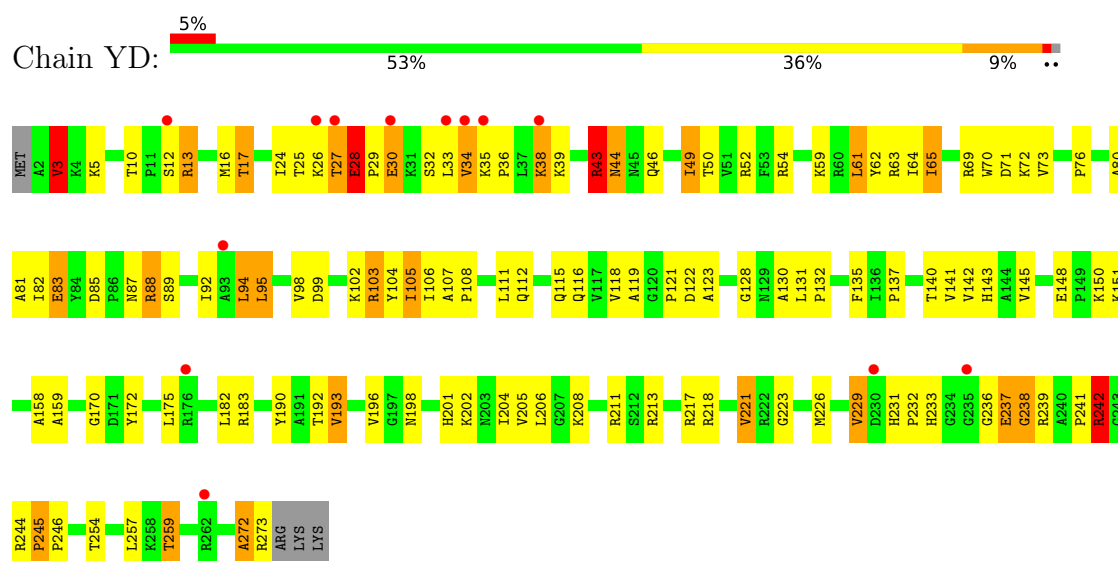
• Molecule 24: 5S rRNA



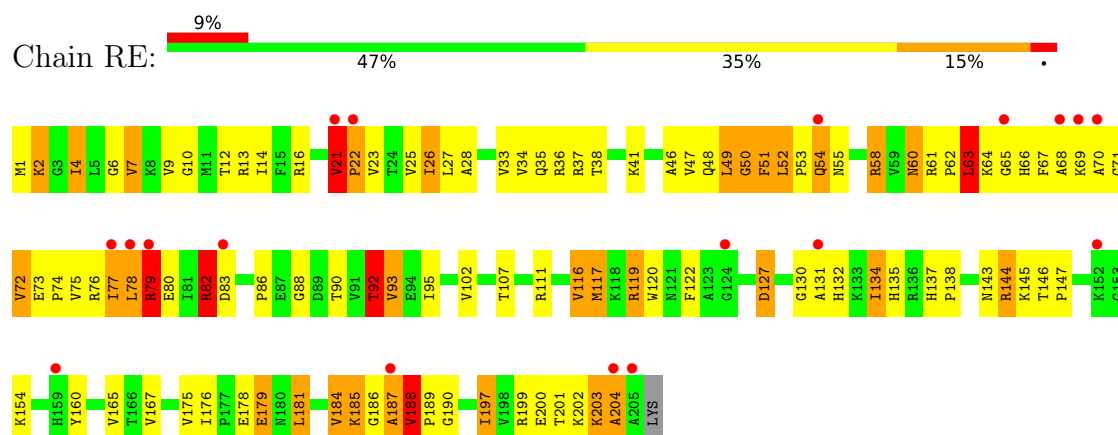
• Molecule 25: 50S ribosomal protein L2



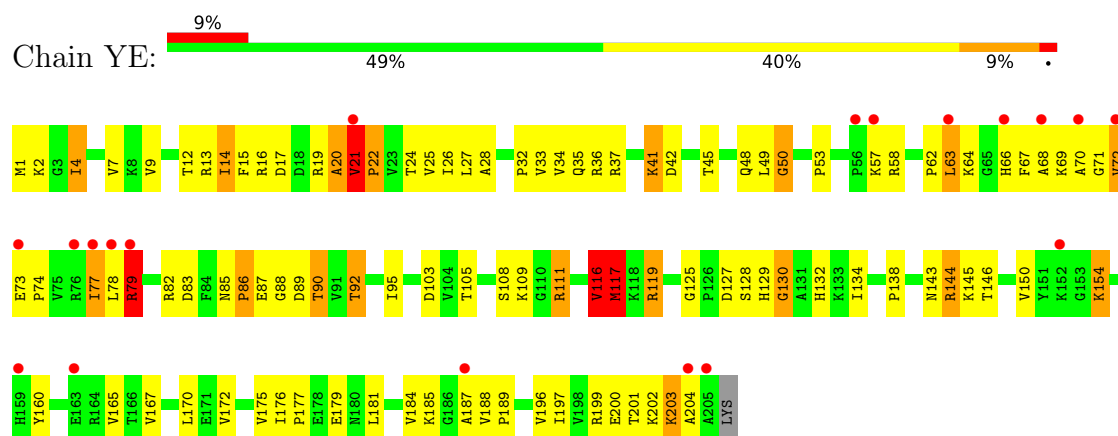
• Molecule 25: 50S ribosomal protein L2



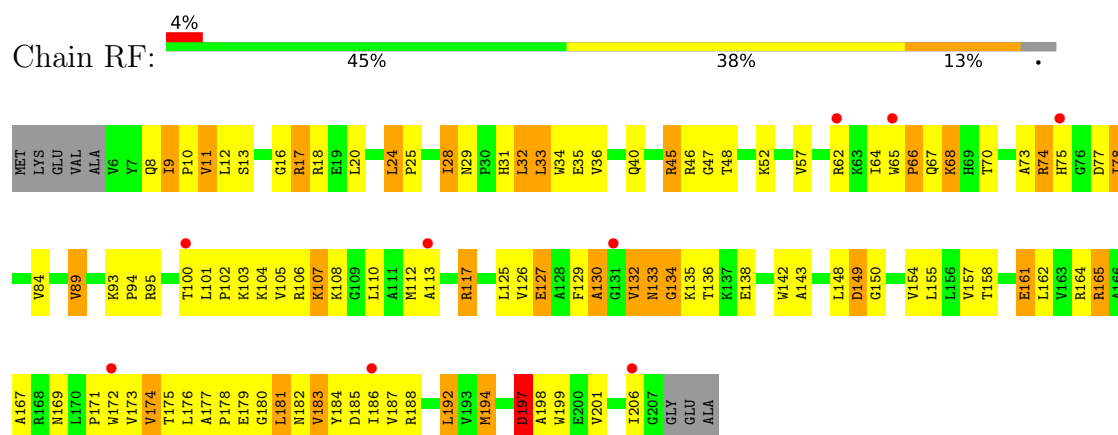
• Molecule 26: 50S ribosomal protein L3



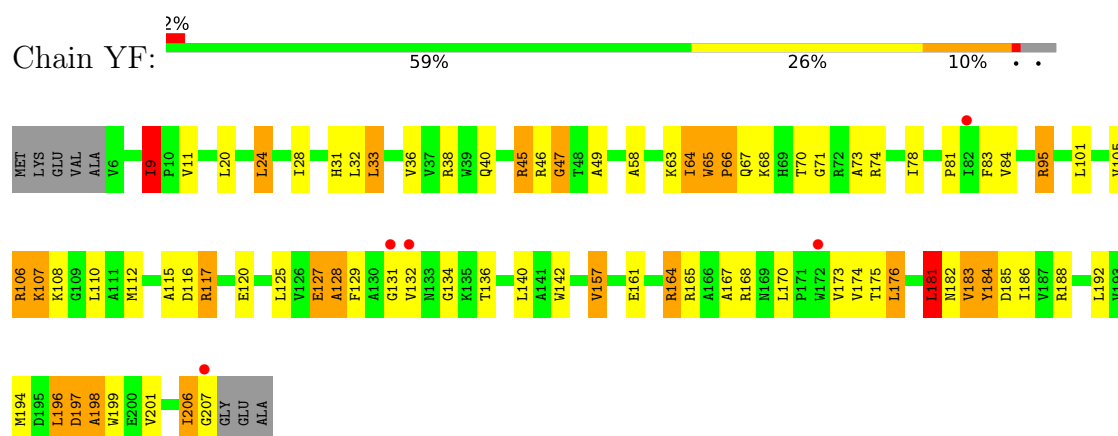
- Molecule 26: 50S ribosomal protein L3



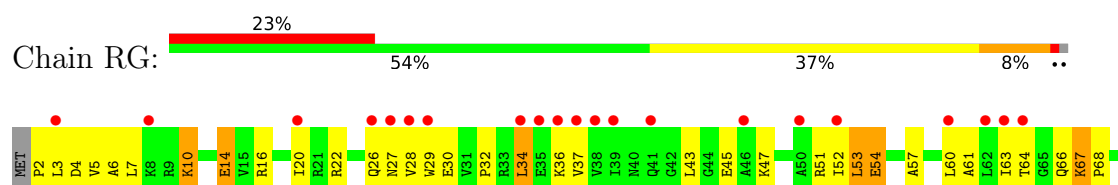
- Molecule 27: 50S ribosomal protein L4

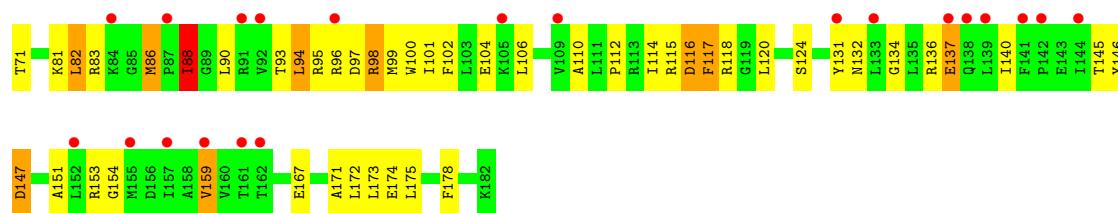


- Molecule 27: 50S ribosomal protein L4

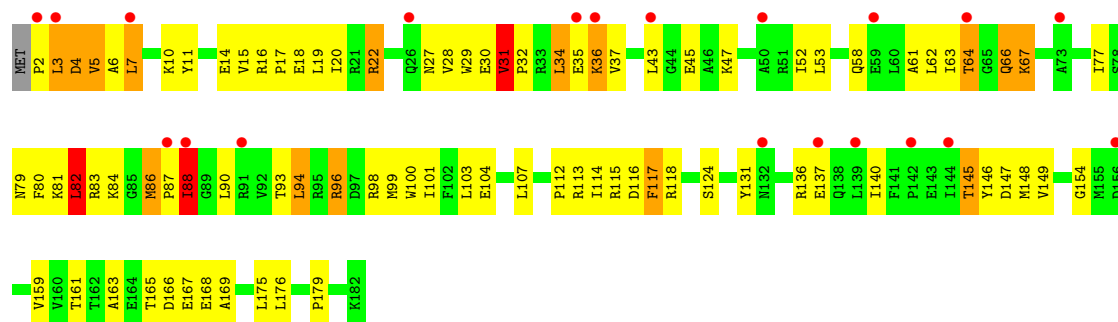


- Molecule 28: 50S ribosomal protein L5

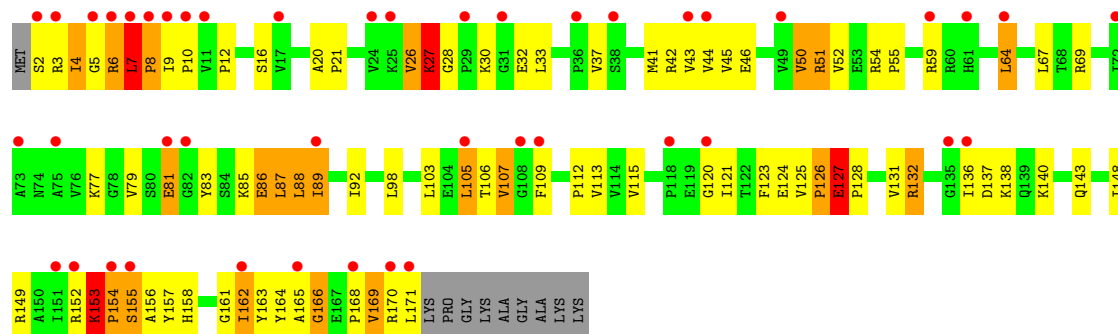




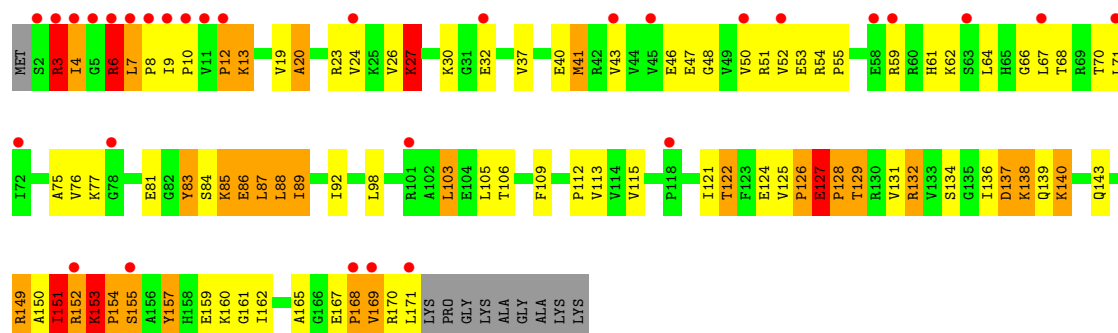
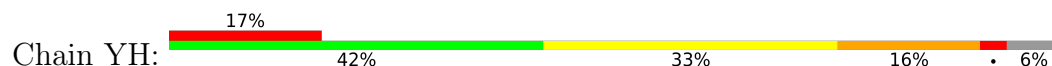
• Molecule 28: 50S ribosomal protein L5



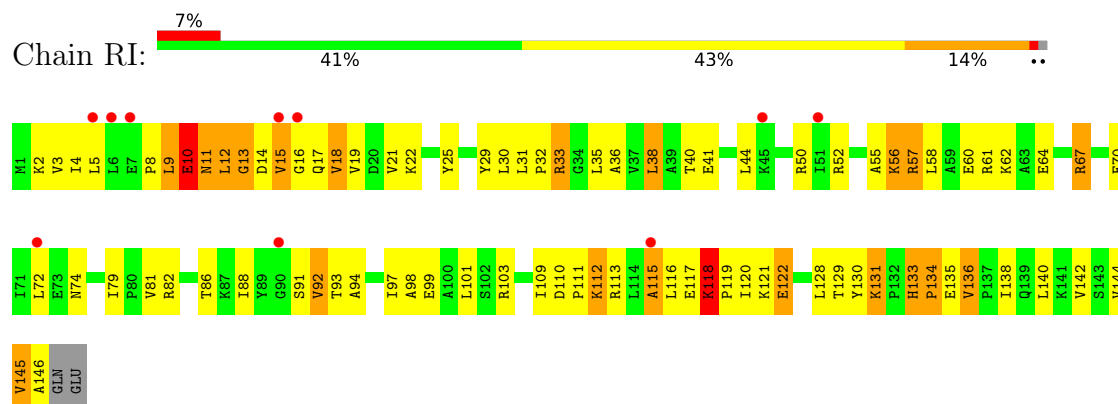
• Molecule 29: 50S ribosomal protein L6



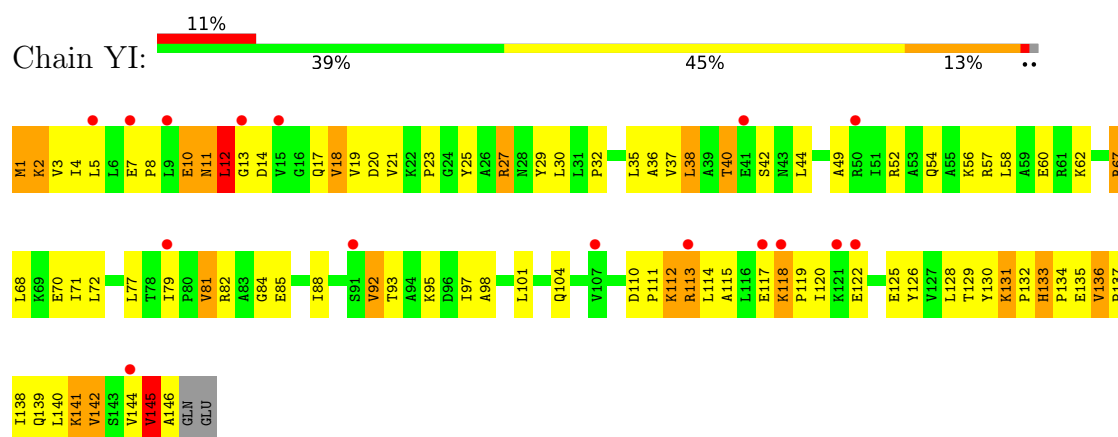
• Molecule 29: 50S ribosomal protein L6



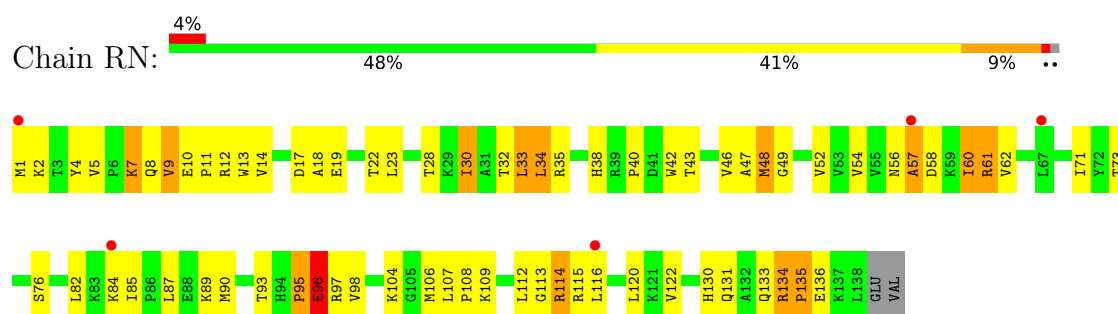
- Molecule 30: 50S ribosomal protein L9



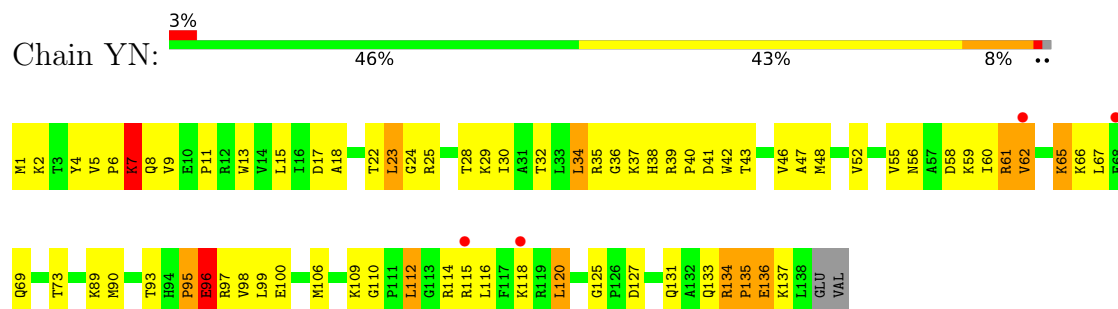
- Molecule 30: 50S ribosomal protein L9



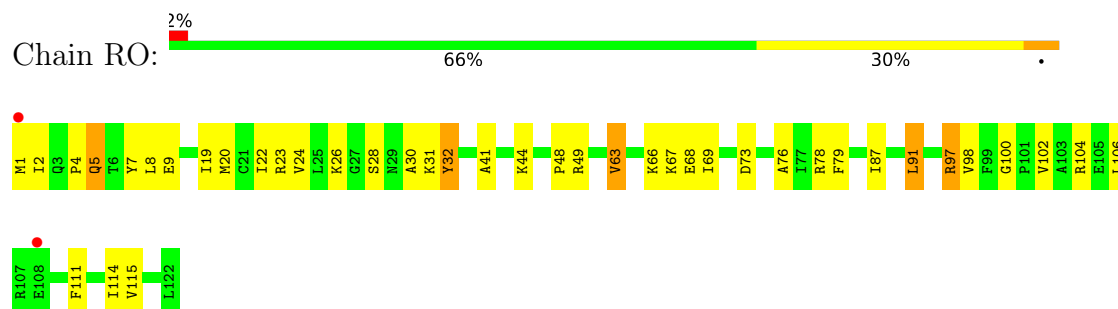
- Molecule 31: 50S ribosomal protein L13



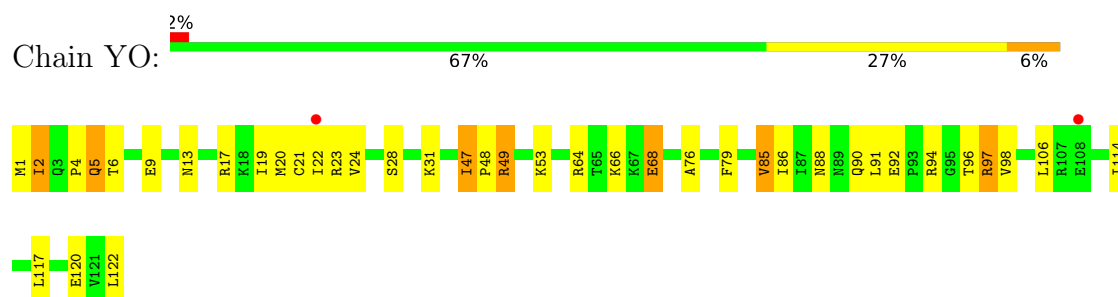
- Molecule 31: 50S ribosomal protein L13



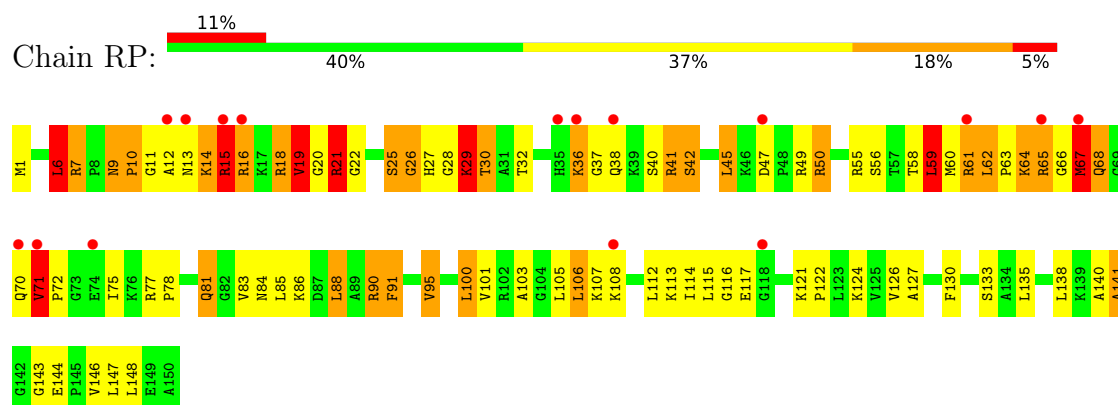
- Molecule 32: 50S ribosomal protein L14



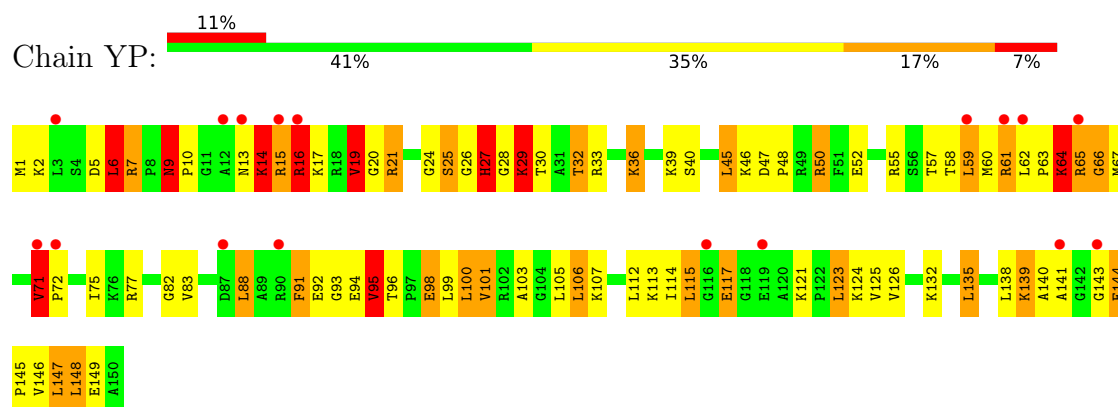
- Molecule 32: 50S ribosomal protein L14



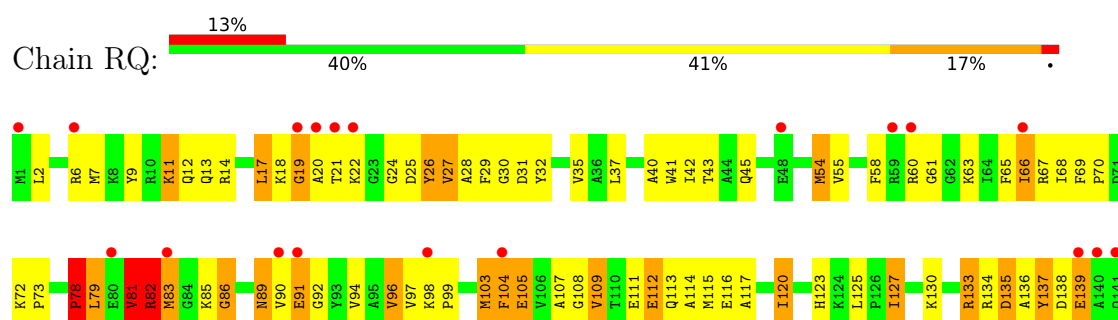
- Molecule 33: 50S ribosomal protein L15



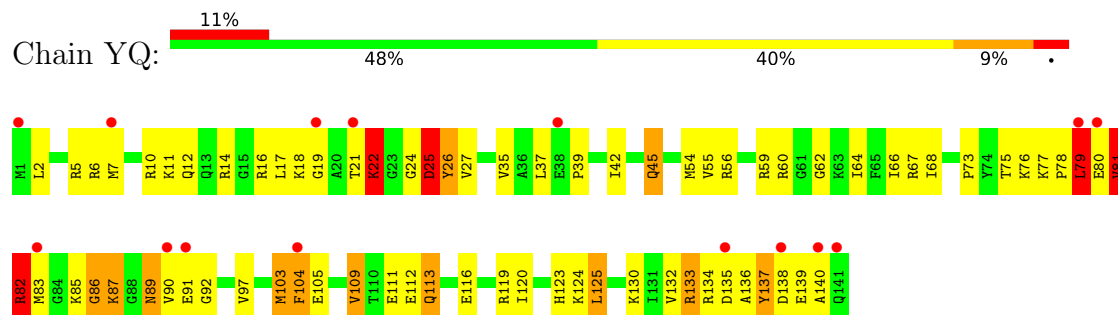
- Molecule 33: 50S ribosomal protein L15



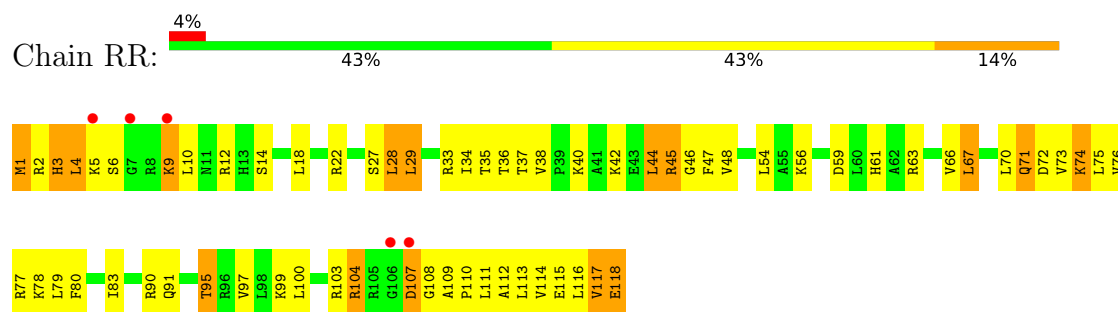
- Molecule 34: 50S ribosomal protein L16



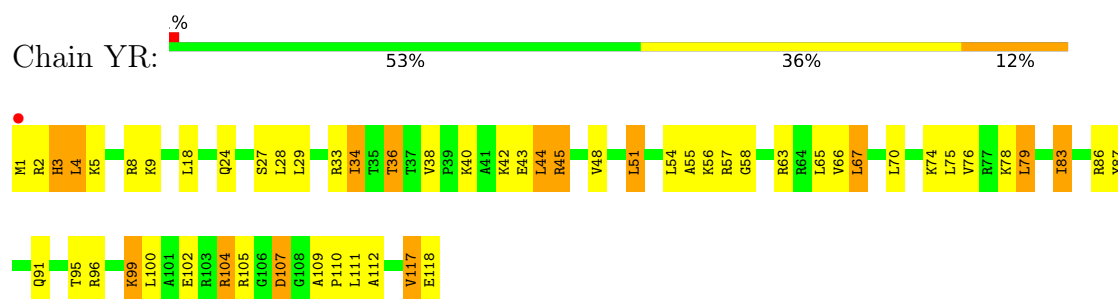
• Molecule 34: 50S ribosomal protein L16



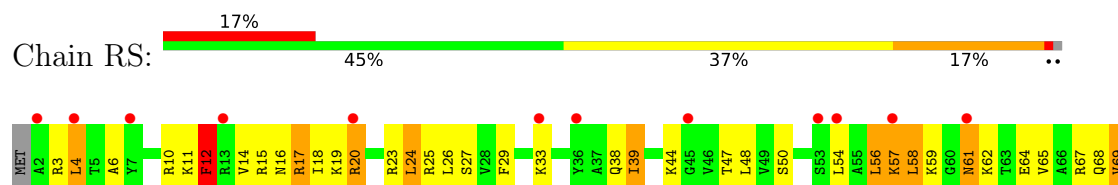
• Molecule 35: 50S ribosomal protein L17

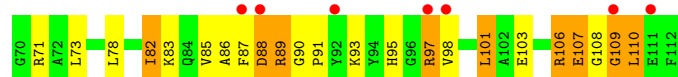


• Molecule 35: 50S ribosomal protein L17

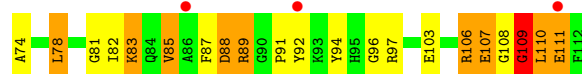
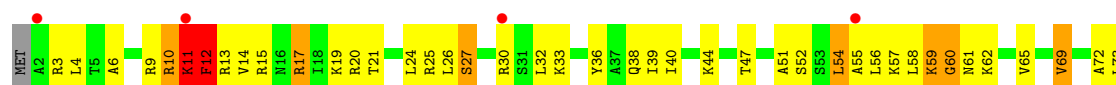


• Molecule 36: 50S ribosomal protein L18

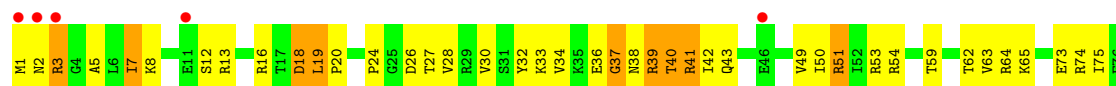
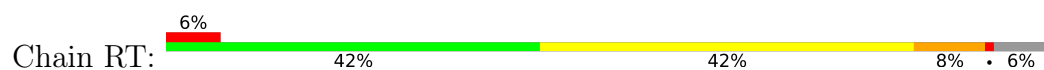




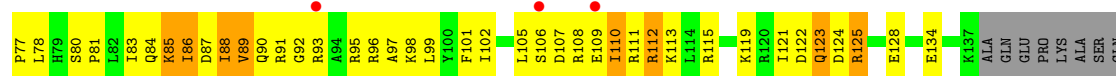
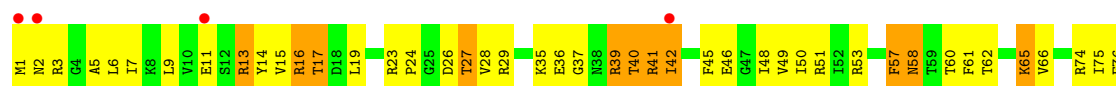
- Molecule 36: 50S ribosomal protein L18



- Molecule 37: 50S ribosomal protein L19

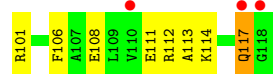
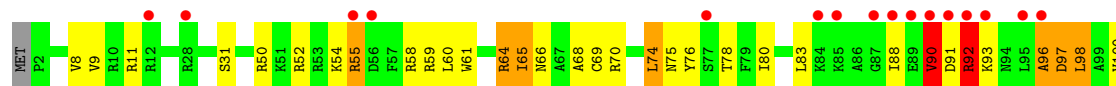


- Molecule 37: 50S ribosomal protein L19



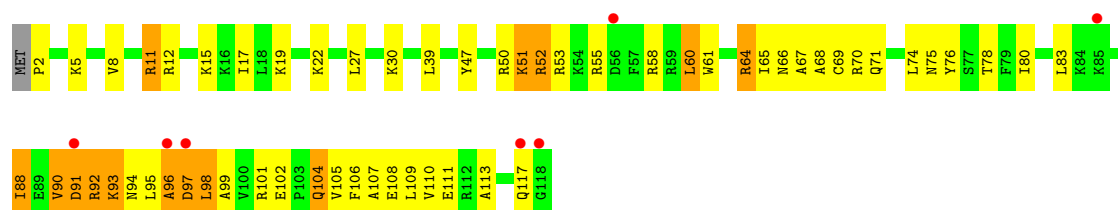
GLU

- Molecule 38: 50S ribosomal protein L20



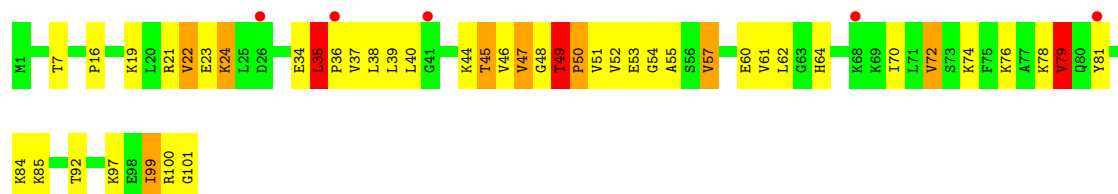
- Molecule 38: 50S ribosomal protein L20

Chain YU: 

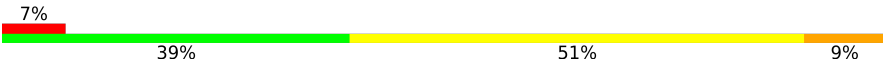


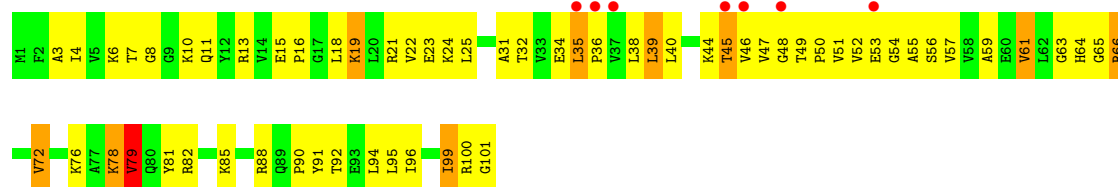
- Molecule 39: 50S ribosomal protein L21

Chain RV: 



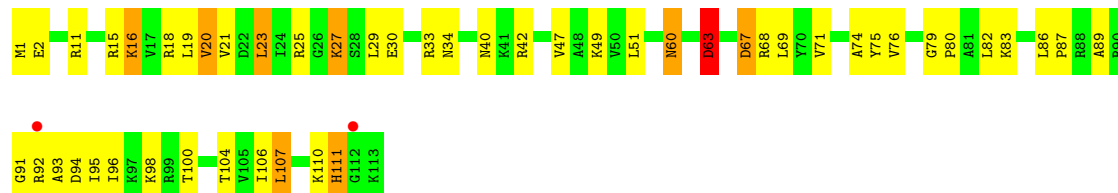
- Molecule 39: 50S ribosomal protein L21

Chain YV: 



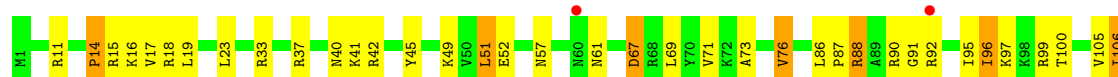
- Molecule 40: 50S ribosomal protein L22

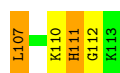
Chain RW: 



- Molecule 40: 50S ribosomal protein L22

Chain YW: 

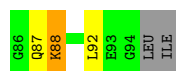




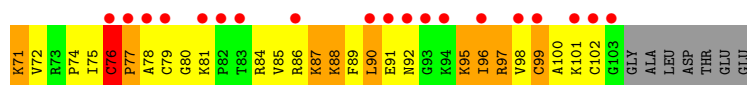
- Molecule 41: 50S ribosomal protein L23



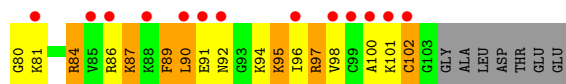
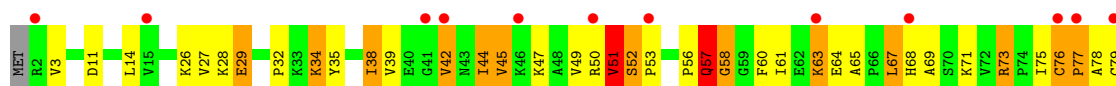
- Molecule 41: 50S ribosomal protein L23



- Molecule 42: 50S ribosomal protein L24

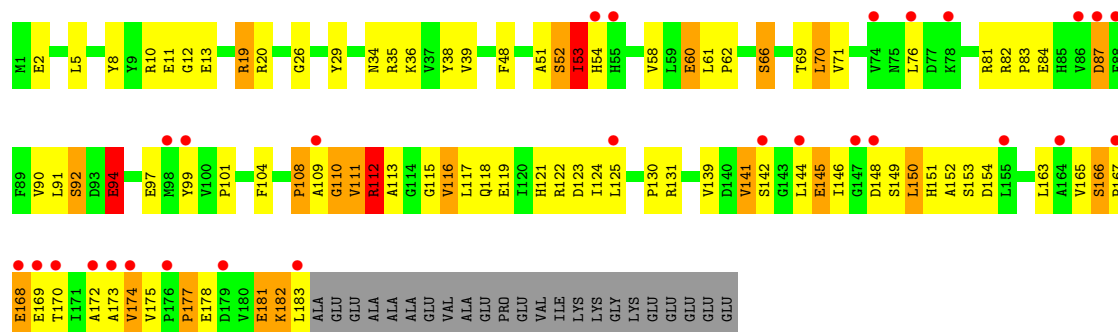


- Molecule 42: 50S ribosomal protein L24

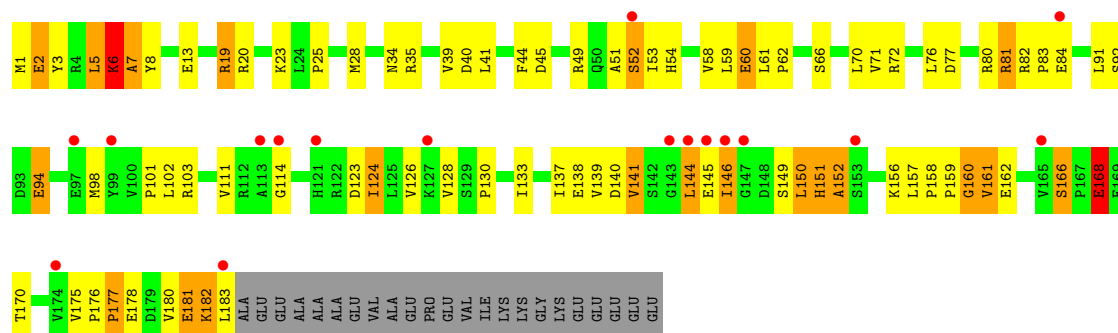


- Molecule 43: 50S ribosomal protein L25





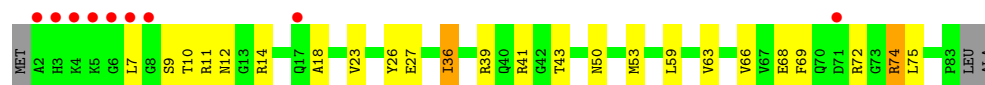
• Molecule 43: 50S ribosomal protein L25



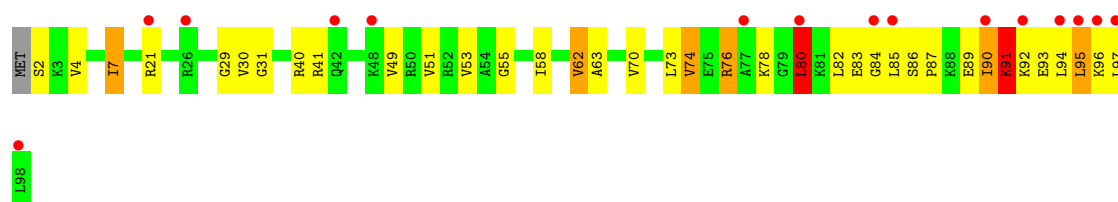
• Molecule 44: 50S ribosomal protein L27



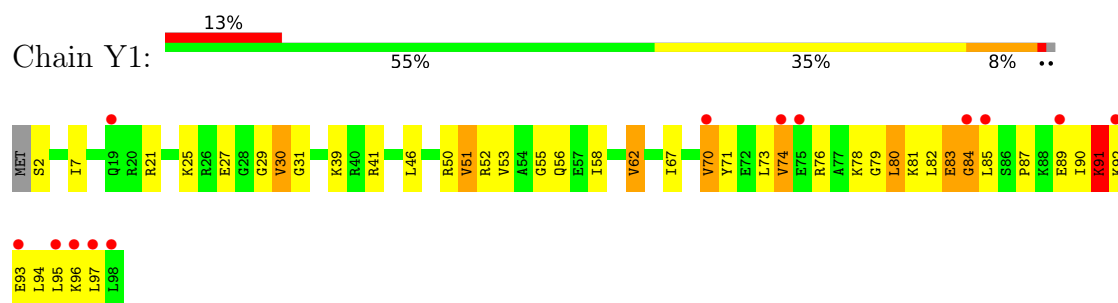
• Molecule 44: 50S ribosomal protein L27



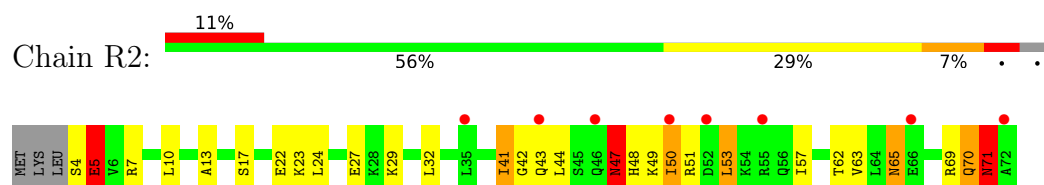
• Molecule 45: 50S ribosomal protein L28



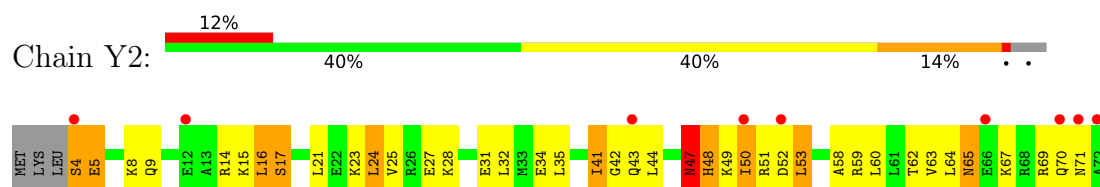
- Molecule 45: 50S ribosomal protein L28



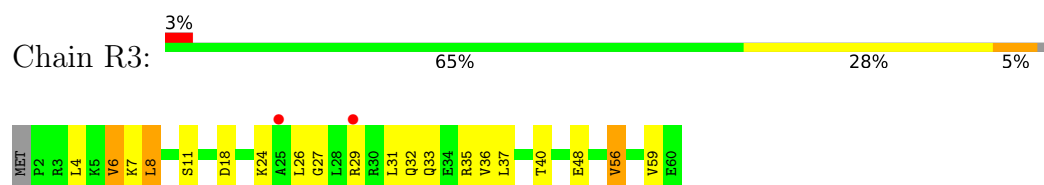
- Molecule 46: 50S ribosomal protein L29



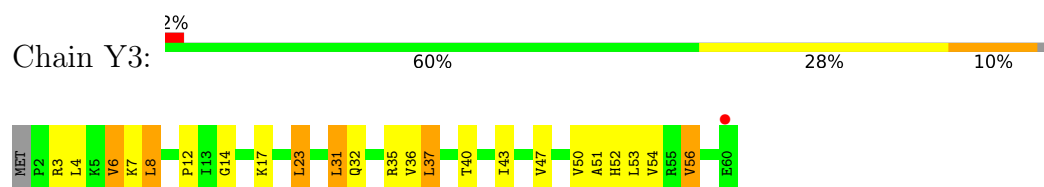
- Molecule 46: 50S ribosomal protein L29



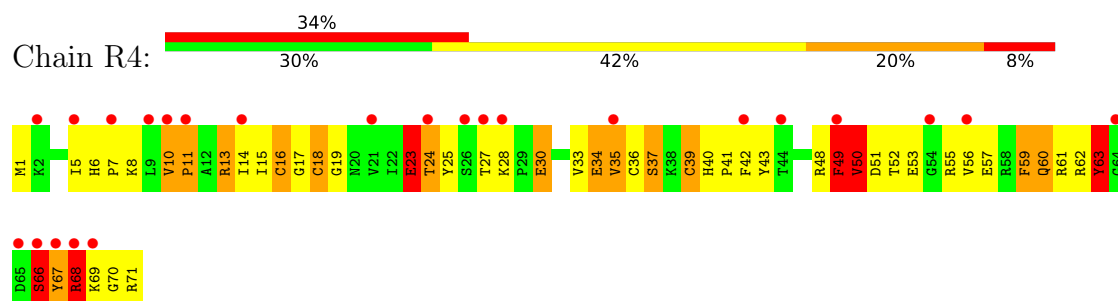
- Molecule 47: 50S ribosomal protein L30



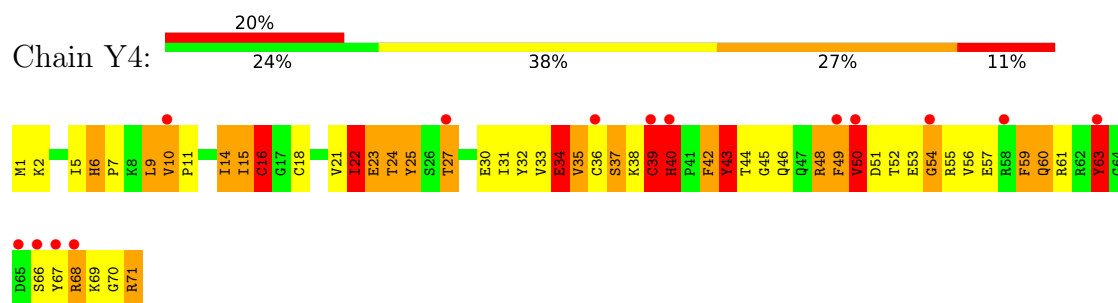
- Molecule 47: 50S ribosomal protein L30



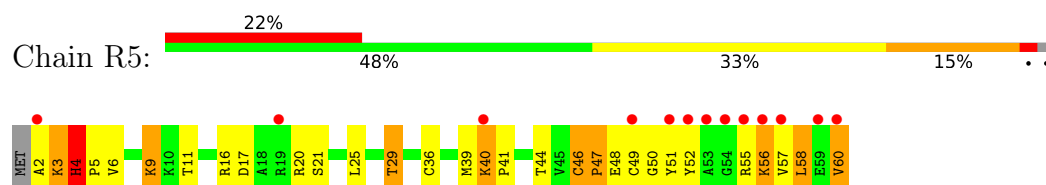
- Molecule 48: 50S ribosomal protein L31



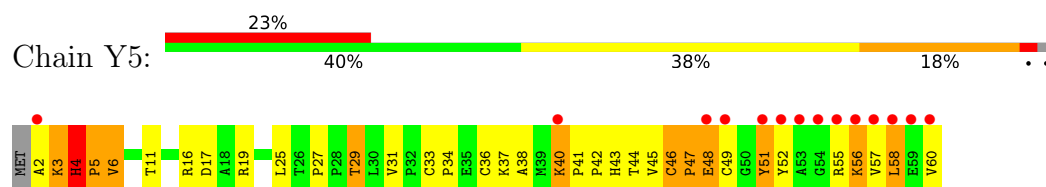
- Molecule 48: 50S ribosomal protein L31



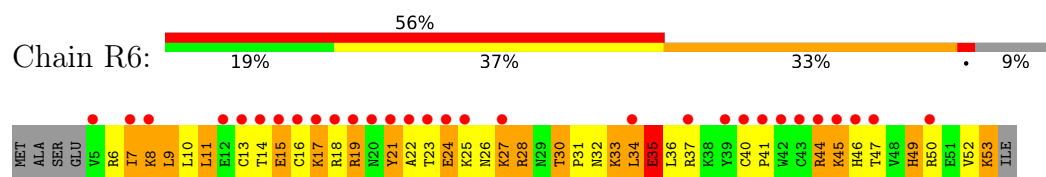
- Molecule 49: 50S ribosomal protein L32



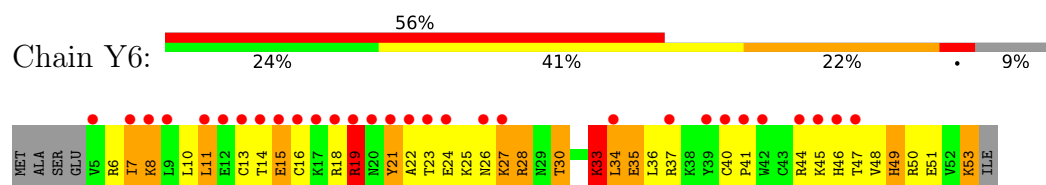
- Molecule 49: 50S ribosomal protein L32



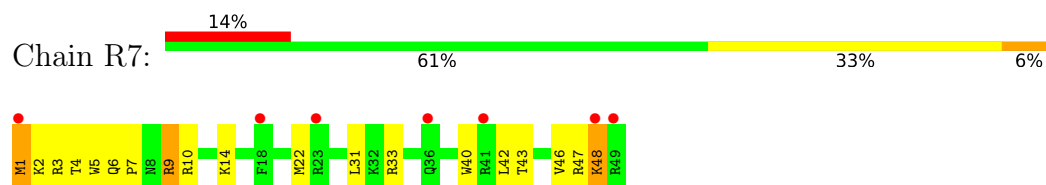
- Molecule 50: 50S ribosomal protein L33



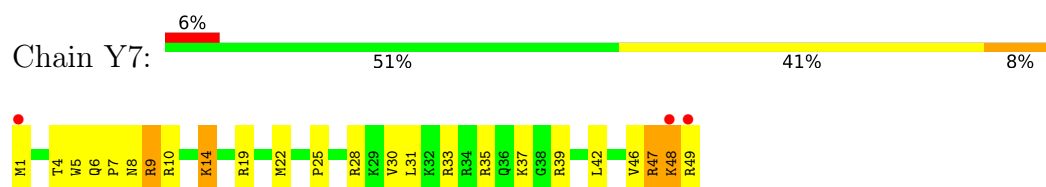
- Molecule 50: 50S ribosomal protein L33



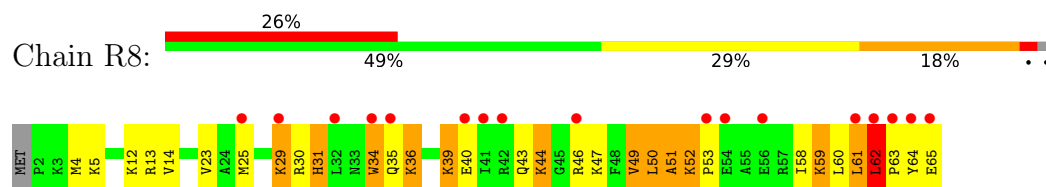
- Molecule 51: 50S ribosomal protein L34



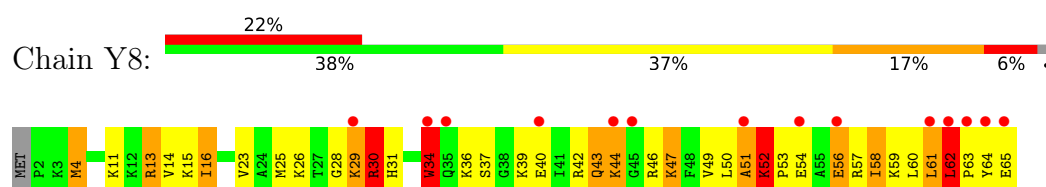
- Molecule 51: 50S ribosomal protein L34



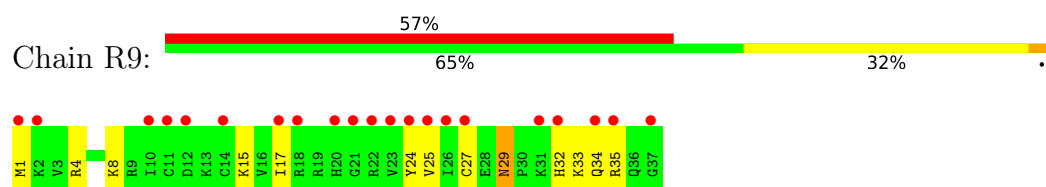
- Molecule 52: 50S ribosomal protein L35



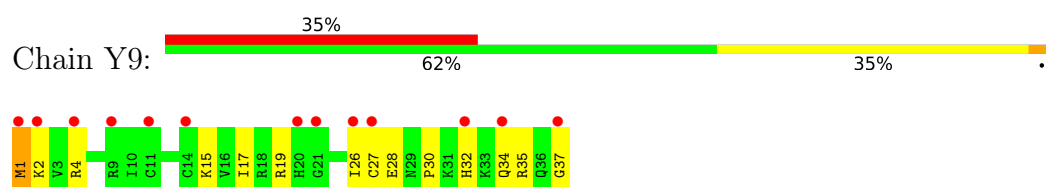
- Molecule 52: 50S ribosomal protein L35



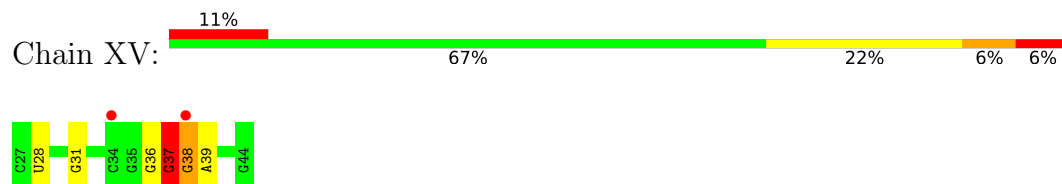
- Molecule 53: 50S ribosomal protein L36



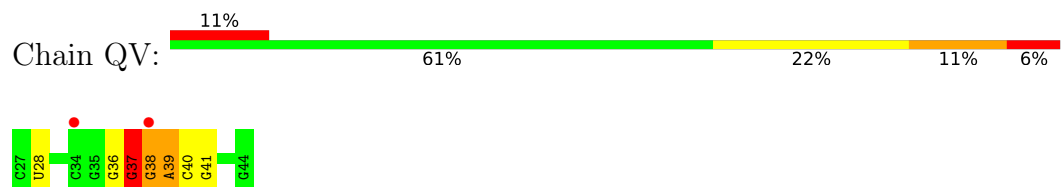
- Molecule 53: 50S ribosomal protein L36



- Molecule 54: P-site ASL SufA6



- Molecule 54: P-site ASL SufA6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.12Å 448.51Å 621.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.99 – 3.34 34.99 – 3.34	Depositor EDS
% Data completeness (in resolution range)	96.5 (34.99-3.34) 96.4 (34.99-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.237 , 0.267 0.236 , 0.265	Depositor DCC
R_{free} test set	43433 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	69.9	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	288423	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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: 1MG, MG, ZN

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	QX	0.30	0/87	0.66	0/132
1	XX	0.32	0/87	0.58	0/132
2	QA	0.17	0/36098	0.35	1/56341 (0.0%)
2	XA	0.18	0/36101	0.36	0/56346
3	QB	0.39	0/1959	0.86	4/2642 (0.2%)
3	XB	0.40	0/1959	0.89	4/2642 (0.2%)
4	QC	0.44	0/1629	0.86	0/2195
4	XC	0.48	0/1629	0.85	0/2195
5	QD	0.48	0/1733	0.97	3/2318 (0.1%)
5	XD	0.51	0/1733	0.97	5/2318 (0.2%)
6	QE	0.46	0/1171	0.95	6/1576 (0.4%)
6	XE	0.52	0/1171	0.94	0/1576
7	QF	0.45	0/856	0.80	0/1154
7	XF	0.51	0/856	0.88	0/1154
8	QG	0.43	0/1276	0.85	0/1709
8	XG	0.46	0/1276	0.86	1/1709 (0.1%)
9	QH	0.43	0/1136	0.93	2/1527 (0.1%)
9	XH	0.47	0/1136	0.92	4/1527 (0.3%)
10	QI	0.41	0/1029	0.90	3/1379 (0.2%)
10	XI	0.42	0/1029	0.89	1/1379 (0.1%)
11	QJ	0.43	0/814	0.92	2/1095 (0.2%)
11	XJ	0.48	0/814	1.00	3/1095 (0.3%)
12	QK	0.48	0/900	0.91	1/1213 (0.1%)
12	XK	0.51	0/900	0.94	0/1213
13	QL	0.47	0/991	0.96	3/1327 (0.2%)
13	XL	0.58	0/991	1.14	9/1327 (0.7%)
14	QM	0.42	0/974	0.98	0/1303
14	XM	0.47	0/974	0.98	1/1303 (0.1%)
15	QN	0.48	0/501	0.90	0/664
15	XN	0.57	0/501	1.04	3/664 (0.5%)
16	QO	0.45	0/745	0.80	0/992
16	XO	0.49	0/745	0.89	0/992

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QP	0.48	0/721	0.93	2/970 (0.2%)
17	XP	0.48	0/721	0.88	1/970 (0.1%)
18	QQ	0.42	0/847	0.85	0/1131
18	XQ	0.42	0/847	0.83	0/1131
19	QR	0.44	0/579	0.89	0/768
19	XR	0.47	0/579	0.85	1/768 (0.1%)
20	QS	0.45	0/689	0.99	3/926 (0.3%)
20	XS	0.47	0/689	1.01	6/926 (0.6%)
21	QT	0.46	0/765	0.96	2/1007 (0.2%)
21	XT	0.42	0/765	0.97	3/1007 (0.3%)
22	QU	0.36	0/221	0.79	0/288
22	XU	0.37	0/221	0.82	0/288
23	RA	0.21	0/69521	0.40	3/108529 (0.0%)
23	YA	0.26	0/69543	0.44	3/108563 (0.0%)
24	RB	0.18	0/2878	0.35	0/4490
24	YB	0.21	0/2878	0.41	0/4490
25	RD	0.63	0/2165	1.07	8/2919 (0.3%)
25	YD	0.73	0/2165	1.13	13/2919 (0.4%)
26	RE	0.57	0/1601	1.07	6/2160 (0.3%)
26	YE	0.60	0/1601	1.11	10/2160 (0.5%)
27	RF	0.53	0/1620	0.95	4/2194 (0.2%)
27	YF	0.60	0/1620	1.08	9/2194 (0.4%)
28	RG	0.41	0/1499	0.91	0/2016
28	YG	0.50	0/1499	0.91	2/2016 (0.1%)
29	RH	0.41	0/1332	1.02	9/1802 (0.5%)
29	YH	0.59	0/1332	1.10	7/1802 (0.4%)
30	RI	0.26	0/1151	0.58	0/1558
30	YI	0.27	0/1151	0.61	0/1558
31	RN	0.52	0/1131	1.01	2/1525 (0.1%)
31	YN	0.56	0/1131	0.94	1/1525 (0.1%)
32	RO	0.55	0/943	0.98	3/1269 (0.2%)
32	YO	0.60	0/943	0.97	0/1269
33	RP	0.61	0/1162	1.20	11/1544 (0.7%)
33	YP	0.67	0/1162	1.28	9/1544 (0.6%)
34	RQ	0.63	0/1143	1.09	4/1527 (0.3%)
34	YQ	0.74	1/1143 (0.1%)	1.13	8/1527 (0.5%)
35	RR	0.55	0/982	0.99	1/1312 (0.1%)
35	YR	0.56	0/982	1.04	3/1312 (0.2%)
36	RS	0.43	0/892	0.88	0/1187
36	YS	0.51	0/892	0.99	1/1187 (0.1%)
37	RT	0.53	0/1155	0.98	3/1542 (0.2%)
37	YT	0.58	0/1155	1.05	7/1542 (0.5%)
38	RU	0.54	0/982	1.04	6/1306 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YU	0.62	0/982	1.05	3/1306 (0.2%)
39	RV	0.47	0/790	0.97	5/1057 (0.5%)
39	YV	0.58	0/790	1.01	2/1057 (0.2%)
40	RW	0.64	0/911	0.98	0/1220
40	YW	0.60	0/911	1.00	0/1220
41	RX	0.59	0/739	0.96	4/993 (0.4%)
41	YX	0.61	0/739	1.00	2/993 (0.2%)
42	RY	0.54	0/798	1.07	6/1064 (0.6%)
42	YY	0.59	0/798	1.09	5/1064 (0.5%)
43	RZ	0.32	1/1493 (0.1%)	0.54	2/2026 (0.1%)
43	YZ	0.28	0/1493	0.54	0/2026
44	R0	0.45	1/657 (0.2%)	0.51	0/874
44	Y0	0.30	0/657	0.50	0/874
45	R1	0.55	0/770	0.97	0/1022
45	Y1	0.58	0/770	0.96	1/1022 (0.1%)
46	R2	0.46	0/583	1.01	1/771 (0.1%)
46	Y2	0.60	0/583	1.05	1/771 (0.1%)
47	R3	0.46	0/474	0.91	0/635
47	Y3	0.53	0/474	0.86	0/635
48	R4	0.45	0/594	1.18	8/795 (1.0%)
48	Y4	0.48	0/594	1.16	6/795 (0.8%)
49	R5	0.62	0/473	1.22	4/639 (0.6%)
49	Y5	0.64	0/473	1.33	9/639 (1.4%)
50	R6	0.53	0/431	1.01	2/575 (0.3%)
50	Y6	0.56	0/431	1.00	2/575 (0.3%)
51	R7	0.63	0/438	1.04	2/575 (0.3%)
51	Y7	0.70	0/438	1.02	3/575 (0.5%)
52	R8	0.69	0/525	1.17	4/691 (0.6%)
52	Y8	0.75	0/525	1.15	5/691 (0.7%)
53	R9	0.35	0/310	0.81	0/407
53	Y9	0.45	0/310	0.80	0/407
54	QV	0.36	1/403 (0.2%)	0.34	0/627
54	XV	0.33	1/403 (0.2%)	0.33	0/627
All	All	0.34	5/312559 (0.0%)	0.61	284/467055 (0.1%)

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
13	QL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	XL	0	1
26	RE	0	1
26	YE	0	1
27	YF	0	1
29	RH	0	2
29	YH	0	2
36	YS	0	1
43	YZ	0	1
46	Y2	0	1
52	R8	0	2
52	Y8	0	2
All	All	0	16

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	R0	12	ASN	CA-C	9.05	1.58	1.53
43	RZ	11	GLU	CA-C	7.50	1.62	1.52
54	QV	37	1MG	O3'-P	5.83	1.62	1.56
34	YQ	82	ARG	N-CA	5.51	1.51	1.46
54	XV	37	1MG	O3'-P	5.39	1.61	1.56

The worst 5 of 284 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RQ	82	ARG	N-CA-C	11.95	124.51	110.41
49	Y5	4	HIS	CA-C-N	-11.22	108.54	119.76
49	Y5	4	HIS	C-N-CA	-11.22	108.54	119.76
33	YP	59	LEU	N-CA-C	-10.61	99.87	112.92
5	QD	28	SER	CA-C-N	-10.42	108.88	120.45

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	QL	47	LYS	Peptide
52	R8	30	ARG	Peptide
26	RE	21	VAL	Peptide
29	RH	127	GLU	Peptide
29	RH	153	LYS	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	QX	80	0	44	1	0
1	XX	80	0	44	1	0
2	QA	32247	0	16278	443	0
2	XA	32249	0	16279	462	1
3	QB	1924	0	1975	83	0
3	XB	1924	0	1975	99	0
4	QC	1605	0	1668	61	0
4	XC	1605	0	1668	56	0
5	QD	1703	0	1763	75	0
5	XD	1703	0	1763	49	0
6	QE	1155	0	1213	39	0
6	XE	1155	0	1213	42	0
7	QF	843	0	857	21	0
7	XF	843	0	857	27	0
8	QG	1257	0	1296	38	0
8	XG	1257	0	1296	26	0
9	QH	1116	0	1177	55	0
9	XH	1116	0	1177	38	0
10	QI	1010	0	1037	37	0
10	XI	1010	0	1037	43	0
11	QJ	801	0	849	48	0
11	XJ	801	0	849	44	0
12	QK	885	0	904	30	0
12	XK	885	0	904	44	0
13	QL	975	0	1062	35	0
13	XL	975	0	1062	39	0
14	QM	964	0	1034	65	0
14	XM	964	0	1034	58	0
15	QN	492	0	529	22	0
15	XN	492	0	529	20	0
16	QO	734	0	771	21	0
16	XO	734	0	771	18	0
17	QP	705	0	725	16	0
17	XP	705	0	725	22	0
18	QQ	834	0	904	19	0
18	XQ	834	0	904	17	0
19	QR	574	0	644	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XR	574	0	644	22	0
20	QS	674	0	698	155	0
20	XS	674	0	698	147	0
21	QT	763	0	860	21	0
21	XT	763	0	861	42	0
22	QU	217	0	234	10	0
22	XU	217	0	234	4	0
23	RA	62071	0	31291	772	0
23	YA	62091	0	31298	753	0
24	RB	2573	0	1306	41	0
24	YB	2573	0	1306	29	0
25	RD	2115	0	2195	105	0
25	YD	2115	0	2195	101	0
26	RE	1568	0	1634	70	0
26	YE	1568	0	1634	61	0
27	RF	1585	0	1632	82	0
27	YF	1585	0	1632	69	0
28	RG	1474	0	1535	59	0
28	YG	1474	0	1535	61	0
29	RH	1307	0	1382	61	0
29	YH	1307	0	1382	70	0
30	RI	1136	0	1223	58	1
30	YI	1136	0	1223	47	0
31	RN	1104	0	1180	41	0
31	YN	1104	0	1180	52	0
32	RO	933	0	996	25	0
32	YO	933	0	996	29	0
33	RP	1145	0	1227	86	0
33	YP	1145	0	1228	89	0
34	RQ	1122	0	1179	60	0
34	YQ	1122	0	1179	46	0
35	RR	968	0	1033	48	0
35	YR	968	0	1033	38	0
36	RS	882	0	943	48	0
36	YS	882	0	943	41	0
37	RT	1141	0	1202	54	0
37	YT	1141	0	1202	52	0
38	RU	964	0	1022	30	0
38	YU	964	0	1022	57	0
39	RV	779	0	852	21	0
39	YV	779	0	852	45	0
40	RW	900	0	964	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YW	900	0	964	27	0
41	RX	725	0	778	30	0
41	YX	725	0	778	25	0
42	RY	785	0	878	53	0
42	YY	785	0	878	42	0
43	RZ	1461	0	1493	53	0
43	YZ	1461	0	1493	47	0
44	R0	648	0	672	19	0
44	Y0	648	0	672	20	0
45	R1	763	0	848	26	0
45	Y1	763	0	848	32	0
46	R2	581	0	629	17	0
46	Y2	581	0	629	25	0
47	R3	469	0	518	8	0
47	Y3	469	0	518	15	0
48	R4	581	0	574	161	0
48	Y4	581	0	569	167	0
49	R5	459	0	480	26	0
49	Y5	459	0	480	34	0
50	R6	424	0	450	26	0
50	Y6	424	0	450	31	0
51	R7	430	0	480	16	0
51	Y7	430	0	480	20	0
52	R8	517	0	582	32	0
52	Y8	517	0	582	48	0
53	R9	307	0	338	8	0
53	Y9	307	0	338	12	0
54	QV	385	0	198	6	0
54	XV	385	0	198	5	0
55	QA	66	0	0	0	0
55	QF	1	0	0	0	0
55	QH	1	0	0	0	0
55	QM	1	0	0	0	0
55	R0	1	0	0	0	0
55	R3	1	0	0	0	0
55	R5	1	0	0	0	0
55	R8	1	0	0	0	0
55	RA	243	0	0	0	0
55	RB	2	0	0	0	0
55	RD	1	0	0	0	0
55	RE	2	0	0	0	0
55	RF	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RP	2	0	0	0	0
55	RR	1	0	0	0	0
55	XA	71	0	0	0	0
55	XB	1	0	0	0	0
55	XL	1	0	0	0	0
55	XM	1	0	0	0	0
55	Y5	1	0	0	0	0
55	YA	267	0	0	0	0
55	YB	4	0	0	0	0
55	YD	2	0	0	0	0
55	YE	1	0	0	0	0
55	YP	2	0	0	0	0
55	YX	1	0	0	0	0
56	QD	1	0	0	0	0
56	QN	1	0	0	0	0
56	XD	1	0	0	0	0
56	XN	1	0	0	0	0
All	All	288423	0	196477	5800	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 12.

The worst 5 of 5800 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)
20:XS:68:GLY:CA	48:Y4:68:ARG:HB2	1.22	1.67
20:XS:68:GLY:HA2	48:Y4:68:ARG:CB	1.19	1.60
14:QM:80:ARG:HD3	48:R4:71:ARG:CZ	1.26	1.59
20:QS:67:VAL:N	48:R4:59:PHE:CZ	1.71	1.55
14:XM:80:ARG:HD3	48:Y4:71:ARG:CZ	1.09	1.53

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)
30:RI:91:SER:OG	2:XA:368:U:OP1[4_555]	2.13	0.07

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	
3	QB	235/256 (92%)	173 (74%)	45 (19%)	17 (7%)	1	6
3	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1	8
4	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	3	21
4	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	8	33
5	QD	206/209 (99%)	175 (85%)	25 (12%)	6 (3%)	3	21
5	XD	206/209 (99%)	177 (86%)	24 (12%)	5 (2%)	4	24
6	QE	149/162 (92%)	136 (91%)	8 (5%)	5 (3%)	3	19
6	XE	149/162 (92%)	133 (89%)	13 (9%)	3 (2%)	6	28
7	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
8	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	9	35
8	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	9	35
9	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	18	49
9	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	3	21
10	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	2	16
10	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	3	19
11	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	3	20
11	XJ	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	1	11
12	QK	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	4	23
12	XK	117/129 (91%)	100 (86%)	15 (13%)	2 (2%)	7	30
13	QL	123/132 (93%)	98 (80%)	18 (15%)	7 (6%)	1	9
13	XL	123/132 (93%)	98 (80%)	15 (12%)	10 (8%)	1	5
14	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	6
14	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	6
15	QN	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	2
16	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	37
16	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	25
17	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	10	37
17	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	10	37
18	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	6	28
18	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
19	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	14
19	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	8	33
20	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	1
20	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	1
21	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1	8
21	XT	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	1	8
22	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	14
22	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	14
25	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	14
25	YD	270/276 (98%)	227 (84%)	34 (13%)	9 (3%)	3	19
26	RE	203/206 (98%)	147 (72%)	36 (18%)	20 (10%)	0	3
26	YE	203/206 (98%)	142 (70%)	41 (20%)	20 (10%)	0	3
27	RF	200/210 (95%)	167 (84%)	20 (10%)	13 (6%)	1	8
27	YF	200/210 (95%)	167 (84%)	25 (12%)	8 (4%)	2	16
28	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	5
28	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	7
29	RH	168/180 (93%)	114 (68%)	33 (20%)	21 (12%)	0	1
29	YH	168/180 (93%)	121 (72%)	23 (14%)	24 (14%)	0	1
30	RI	144/148 (97%)	107 (74%)	25 (17%)	12 (8%)	0	5
30	YI	144/148 (97%)	108 (75%)	23 (16%)	13 (9%)	0	4
31	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	0	4
31	YN	136/140 (97%)	105 (77%)	17 (12%)	14 (10%)	0	2
32	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	7	30
32	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	RP	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	0	3
33	YP	148/150 (99%)	108 (73%)	23 (16%)	17 (12%)	0	2
34	RQ	139/141 (99%)	99 (71%)	22 (16%)	18 (13%)	0	1
34	YQ	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	1
35	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	14
35	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	1	11
36	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	3
36	YS	109/112 (97%)	78 (72%)	18 (16%)	13 (12%)	0	2
37	RT	135/146 (92%)	106 (78%)	17 (13%)	12 (9%)	0	4
37	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	6
38	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	18
38	YU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	18
39	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	9
39	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	5
40	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	2	18
40	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	6	30
41	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	5	26
41	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	5	26
42	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	1
42	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	2
43	RZ	181/206 (88%)	127 (70%)	37 (20%)	17 (9%)	0	3
43	YZ	181/206 (88%)	133 (74%)	31 (17%)	17 (9%)	0	3
44	R0	80/85 (94%)	70 (88%)	10 (12%)	0	100	100
44	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
45	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	3
45	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	8
46	R2	67/72 (93%)	53 (79%)	9 (13%)	5 (8%)	1	6
46	Y2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	0	4
47	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	18
47	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	6	30
48	R4	69/71 (97%)	35 (51%)	18 (26%)	16 (23%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
49	R5	57/60 (95%)	44 (77%)	11 (19%)	2 (4%)	3	18
49	Y5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	3	18
50	R6	47/54 (87%)	23 (49%)	14 (30%)	10 (21%)	0	0
50	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	0
51	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	5	27
51	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	5	27
52	R8	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1	5
52	Y8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	8
53	R9	35/37 (95%)	35 (100%)	0	0	100	100
53	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	9239 (80%)	1524 (13%)	707 (6%)	1	8

5 of 707 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	QB	236	TYR
4	QC	12	LEU
4	QC	190	ARG
5	QD	28	SER
14	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	
3	QB	205/220 (93%)	169 (82%)	36 (18%)	2	9
3	XB	205/220 (93%)	181 (88%)	24 (12%)	5	21
4	QC	159/188 (85%)	147 (92%)	12 (8%)	12	39
4	XC	159/188 (85%)	145 (91%)	14 (9%)	9	33
5	QD	180/181 (99%)	155 (86%)	25 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	XD	180/181 (99%)	155 (86%)	25 (14%)	3	15
6	QE	116/123 (94%)	102 (88%)	14 (12%)	5	20
6	XE	116/123 (94%)	100 (86%)	16 (14%)	3	15
7	QF	90/90 (100%)	79 (88%)	11 (12%)	5	20
7	XF	90/90 (100%)	79 (88%)	11 (12%)	5	20
8	QG	126/127 (99%)	115 (91%)	11 (9%)	9	33
8	XG	126/127 (99%)	112 (89%)	14 (11%)	6	23
9	QH	119/119 (100%)	105 (88%)	14 (12%)	5	21
9	XH	119/119 (100%)	106 (89%)	13 (11%)	6	24
10	QI	98/99 (99%)	80 (82%)	18 (18%)	1	7
10	XI	98/99 (99%)	77 (79%)	21 (21%)	1	5
11	QJ	89/92 (97%)	75 (84%)	14 (16%)	2	12
11	XJ	89/92 (97%)	74 (83%)	15 (17%)	2	10
12	QK	90/99 (91%)	79 (88%)	11 (12%)	5	20
12	XK	90/99 (91%)	81 (90%)	9 (10%)	7	28
13	QL	104/109 (95%)	91 (88%)	13 (12%)	4	19
13	XL	104/109 (95%)	90 (86%)	14 (14%)	4	16
14	QM	97/101 (96%)	73 (75%)	24 (25%)	1	3
14	XM	97/101 (96%)	79 (81%)	18 (19%)	1	7
15	QN	49/50 (98%)	40 (82%)	9 (18%)	1	7
15	XN	49/50 (98%)	42 (86%)	7 (14%)	3	14
16	QO	79/80 (99%)	72 (91%)	7 (9%)	9	32
16	XO	79/80 (99%)	68 (86%)	11 (14%)	3	15
17	QP	72/74 (97%)	62 (86%)	10 (14%)	3	15
17	XP	72/74 (97%)	66 (92%)	6 (8%)	10	35
18	QQ	95/97 (98%)	86 (90%)	9 (10%)	8	30
18	XQ	95/97 (98%)	88 (93%)	7 (7%)	13	39
19	QR	61/77 (79%)	50 (82%)	11 (18%)	2	8
19	XR	61/77 (79%)	50 (82%)	11 (18%)	2	8
20	QS	73/80 (91%)	59 (81%)	14 (19%)	1	6
20	XS	73/80 (91%)	56 (77%)	17 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	QT	76/82 (93%)	66 (87%)	10 (13%)	4	17
21	XT	76/82 (93%)	66 (87%)	10 (13%)	4	17
22	QU	20/22 (91%)	20 (100%)	0	100	100
22	XU	20/22 (91%)	20 (100%)	0	100	100
25	RD	214/218 (98%)	170 (79%)	44 (21%)	1	5
25	YD	214/218 (98%)	176 (82%)	38 (18%)	2	8
26	RE	165/166 (99%)	122 (74%)	43 (26%)	0	2
26	YE	165/166 (99%)	134 (81%)	31 (19%)	1	7
27	RF	161/166 (97%)	127 (79%)	34 (21%)	1	5
27	YF	161/166 (97%)	134 (83%)	27 (17%)	2	10
28	RG	155/156 (99%)	135 (87%)	20 (13%)	4	18
28	YG	155/156 (99%)	131 (84%)	24 (16%)	2	12
29	RH	142/148 (96%)	116 (82%)	26 (18%)	2	7
29	YH	142/148 (96%)	111 (78%)	31 (22%)	1	4
30	RI	122/124 (98%)	99 (81%)	23 (19%)	1	7
30	YI	122/124 (98%)	90 (74%)	32 (26%)	0	2
31	RN	117/119 (98%)	94 (80%)	23 (20%)	1	6
31	YN	117/119 (98%)	94 (80%)	23 (20%)	1	6
32	RO	100/100 (100%)	91 (91%)	9 (9%)	9	32
32	YO	100/100 (100%)	85 (85%)	15 (15%)	3	13
33	RP	116/116 (100%)	83 (72%)	33 (28%)	0	1
33	YP	116/116 (100%)	81 (70%)	35 (30%)	0	1
34	RQ	111/111 (100%)	90 (81%)	21 (19%)	1	7
34	YQ	111/111 (100%)	94 (85%)	17 (15%)	3	12
35	RR	101/101 (100%)	81 (80%)	20 (20%)	1	6
35	YR	101/101 (100%)	80 (79%)	21 (21%)	1	5
36	RS	87/88 (99%)	67 (77%)	20 (23%)	1	3
36	YS	87/88 (99%)	65 (75%)	22 (25%)	0	2
37	RT	120/127 (94%)	101 (84%)	19 (16%)	2	11
37	YT	120/127 (94%)	93 (78%)	27 (22%)	1	4
38	RU	93/94 (99%)	79 (85%)	14 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	YU	93/94 (99%)	79 (85%)	14 (15%)	3	13
39	RV	82/82 (100%)	63 (77%)	19 (23%)	1	3
39	YV	82/82 (100%)	66 (80%)	16 (20%)	1	6
40	RW	92/92 (100%)	73 (79%)	19 (21%)	1	5
40	YW	92/92 (100%)	76 (83%)	16 (17%)	2	9
41	RX	74/78 (95%)	61 (82%)	13 (18%)	2	9
41	YX	74/78 (95%)	59 (80%)	15 (20%)	1	5
42	RY	85/91 (93%)	56 (66%)	29 (34%)	0	1
42	YY	85/91 (93%)	62 (73%)	23 (27%)	0	2
43	RZ	162/179 (90%)	135 (83%)	27 (17%)	2	11
43	YZ	162/179 (90%)	131 (81%)	31 (19%)	1	6
44	R0	65/67 (97%)	57 (88%)	8 (12%)	4	20
44	Y0	65/67 (97%)	60 (92%)	5 (8%)	12	38
45	R1	82/83 (99%)	74 (90%)	8 (10%)	7	29
45	Y1	82/83 (99%)	69 (84%)	13 (16%)	2	11
46	R2	64/67 (96%)	49 (77%)	15 (23%)	1	3
46	Y2	64/67 (96%)	48 (75%)	16 (25%)	0	2
47	R3	51/52 (98%)	43 (84%)	8 (16%)	2	12
47	Y3	51/52 (98%)	44 (86%)	7 (14%)	3	16
48	R4	63/63 (100%)	44 (70%)	19 (30%)	0	1
48	Y4	63/63 (100%)	42 (67%)	21 (33%)	0	1
49	R5	51/52 (98%)	35 (69%)	16 (31%)	0	1
49	Y5	51/52 (98%)	37 (72%)	14 (28%)	0	2
50	R6	48/52 (92%)	32 (67%)	16 (33%)	0	1
50	Y6	48/52 (92%)	34 (71%)	14 (29%)	0	1
51	R7	42/42 (100%)	35 (83%)	7 (17%)	2	11
51	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	11
52	R8	54/55 (98%)	43 (80%)	11 (20%)	1	5
52	Y8	54/55 (98%)	37 (68%)	17 (32%)	0	1
53	R9	34/34 (100%)	30 (88%)	4 (12%)	5	21
53	Y9	34/34 (100%)	31 (91%)	3 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9702/10066 (96%)	8023 (83%)	1679 (17%)	2 9

5 of 1679 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	XF	71	ARG
26	YE	16	ARG
47	Y3	31	LEU
9	XH	80	ILE
7	XF	45	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
25	YD	96	HIS
44	Y0	29	GLN
26	YE	54	GLN
35	YR	71	GLN
31	RN	69	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QX	3/19 (15%)	1 (33%)	0
1	XX	3/19 (15%)	0	0
2	QA	1499/1521 (98%)	274 (18%)	46 (3%)
2	XA	1499/1521 (98%)	272 (18%)	40 (2%)
23	RA	2879/2915 (98%)	580 (20%)	62 (2%)
23	YA	2880/2915 (98%)	586 (20%)	62 (2%)
24	RB	119/122 (97%)	22 (18%)	2 (1%)
24	YB	119/122 (97%)	25 (21%)	2 (1%)
54	QV	17/18 (94%)	4 (23%)	1 (5%)
54	XV	17/18 (94%)	4 (23%)	1 (5%)
All	All	9035/9190 (98%)	1768 (19%)	216 (2%)

5 of 1768 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QX	1	C
2	QA	6	G

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Mol	Chain	Res	Type
2	QA	9	G
2	QA	32	A
2	QA	39	G

5 of 216 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	XA	89	U
2	XA	1200	C
23	YA	2126	A
2	XA	244	U
2	XA	509	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
54	1MG	XV	37	54	23,26,27	1.34	3 (13%)	33,39,42	1.74	4 (12%)
54	1MG	QV	37	54	23,26,27	1.36	3 (13%)	33,39,42	1.78	3 (9%)

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
54	1MG	XV	37	54	-	2/7/25/26	0/3/3/3
54	1MG	QV	37	54	-	2/7/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	XV	37	1MG	C5-C4	3.68	1.48	1.38
54	QV	37	1MG	C5-C4	3.65	1.48	1.38
54	QV	37	1MG	C2-N1	3.04	1.42	1.37
54	XV	37	1MG	C2-N1	2.78	1.42	1.37
54	XV	37	1MG	C5-N7	-2.28	1.34	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	XV	37	1MG	C5-C4-N3	-5.83	119.11	128.39
54	QV	37	1MG	C5-C4-N3	-5.82	119.13	128.39
54	QV	37	1MG	N9-C4-N3	4.75	135.44	125.95
54	XV	37	1MG	N9-C4-N3	4.51	134.98	125.95
54	QV	37	1MG	C2-N3-C4	4.35	121.75	111.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	XV	37	1MG	O4'-C4'-C5'-O5'
54	QV	37	1MG	O4'-C4'-C5'-O5'
54	XV	37	1MG	C3'-C4'-C5'-O5'
54	QV	37	1MG	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	XV	37	1MG	3	0
54	QV	37	1MG	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 681 ligands modelled in this entry, 681 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QX	4/19 (21%)	1.26	1 (25%) 2 2	111, 112, 113, 116	0
1	XX	4/19 (21%)	1.14	1 (25%) 2 2	97, 97, 99, 102	0
2	QA	1500/1521 (98%)	0.48	75 (5%) 34 23	68, 108, 190, 262	0
2	XA	1500/1521 (98%)	0.48	61 (4%) 41 27	54, 105, 188, 260	0
3	QB	237/256 (92%)	1.44	60 (25%) 1 2	139, 160, 171, 173	0
3	XB	237/256 (92%)	1.24	42 (17%) 4 4	123, 144, 157, 164	0
4	QC	205/239 (85%)	1.23	37 (18%) 3 4	136, 150, 164, 168	0
4	XC	205/239 (85%)	1.04	28 (13%) 6 6	129, 140, 155, 160	0
5	QD	208/209 (99%)	1.30	40 (19%) 3 3	106, 117, 124, 127	0
5	XD	208/209 (99%)	1.13	34 (16%) 4 5	96, 110, 119, 122	0
6	QE	151/162 (93%)	1.04	19 (12%) 8 7	99, 113, 122, 125	0
6	XE	151/162 (93%)	0.98	16 (10%) 11 10	88, 104, 117, 127	0
7	QF	101/101 (100%)	0.83	7 (6%) 23 16	97, 104, 109, 120	0
7	XF	101/101 (100%)	0.72	4 (3%) 42 28	89, 98, 108, 114	0
8	QG	155/156 (99%)	1.16	27 (17%) 4 4	137, 158, 164, 166	0
8	XG	155/156 (99%)	1.22	36 (23%) 2 2	124, 150, 160, 163	0
9	QH	138/138 (100%)	1.04	17 (12%) 8 8	97, 115, 130, 139	0
9	XH	138/138 (100%)	0.81	7 (5%) 33 23	87, 105, 116, 124	0
10	QI	127/128 (99%)	1.54	37 (29%) 1 1	138, 176, 181, 183	0
10	XI	127/128 (99%)	1.59	36 (28%) 1 1	129, 167, 174, 177	0
11	QJ	99/105 (94%)	1.66	31 (31%) 1 1	148, 174, 179, 181	0
11	XJ	99/105 (94%)	1.81	42 (42%) 0 0	140, 166, 173, 174	0
12	QK	119/129 (92%)	1.00	15 (12%) 8 7	86, 113, 124, 142	0
12	XK	119/129 (92%)	0.97	11 (9%) 14 12	75, 101, 116, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
13	QL	125/132 (94%)	1.17	19 (15%)	5	5	86, 94, 105, 125	0
13	XL	125/132 (94%)	1.18	19 (15%)	5	5	78, 92, 99, 125	0
14	QM	121/126 (96%)	1.48	28 (23%)	2	2	153, 176, 181, 183	0
14	XM	121/126 (96%)	1.66	37 (30%)	1	1	155, 177, 180, 184	0
15	QN	60/61 (98%)	2.30	29 (48%)	0	0	154, 160, 174, 177	0
15	XN	60/61 (98%)	1.91	21 (35%)	1	1	145, 152, 171, 172	0
16	QO	88/89 (98%)	0.80	5 (5%)	29	20	90, 109, 117, 118	0
16	XO	88/89 (98%)	0.68	2 (2%)	61	42	79, 95, 102, 103	0
17	QP	84/88 (95%)	1.25	18 (21%)	2	3	93, 102, 117, 139	0
17	XP	84/88 (95%)	1.24	19 (22%)	2	2	96, 112, 126, 151	0
18	QQ	100/105 (95%)	1.11	13 (13%)	7	7	90, 99, 105, 106	0
18	XQ	100/105 (95%)	0.97	8 (8%)	18	14	83, 98, 104, 105	0
19	QR	70/88 (79%)	0.78	5 (7%)	22	15	99, 109, 118, 121	0
19	XR	70/88 (79%)	0.70	2 (2%)	53	36	90, 101, 111, 113	0
20	QS	84/93 (90%)	1.45	25 (29%)	1	1	159, 181, 184, 185	0
20	XS	84/93 (90%)	1.76	34 (40%)	0	0	165, 185, 190, 191	0
21	QT	99/106 (93%)	1.15	14 (14%)	6	6	91, 104, 115, 118	0
21	XT	99/106 (93%)	1.47	26 (26%)	1	2	101, 117, 128, 131	0
22	QU	25/27 (92%)	3.60	21 (84%)	0	0	164, 170, 171, 173	0
22	XU	25/27 (92%)	3.44	23 (92%)	0	0	164, 169, 172, 173	0
23	RA	2882/2915 (98%)	0.07	144 (4%)	34	23	45, 71, 200, 279	0
23	YA	2883/2915 (98%)	-0.20	103 (3%)	46	31	29, 49, 175, 271	0
24	RB	120/122 (98%)	0.48	1 (0%)	82	69	82, 117, 139, 156	0
24	YB	120/122 (98%)	-0.09	0	100	100	50, 71, 89, 104	0
25	RD	272/276 (98%)	0.72	22 (8%)	18	14	46, 67, 79, 83	0
25	YD	272/276 (98%)	0.63	13 (4%)	35	24	33, 53, 65, 73	0
26	RE	205/206 (99%)	0.79	18 (8%)	15	13	47, 76, 96, 102	0
26	YE	205/206 (99%)	0.68	19 (9%)	14	12	34, 59, 80, 91	0
27	RF	202/210 (96%)	0.60	9 (4%)	38	25	48, 89, 108, 118	0
27	YF	202/210 (96%)	0.39	5 (2%)	58	40	31, 58, 82, 95	0
28	RG	181/182 (99%)	1.46	42 (23%)	2	2	134, 164, 177, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	YG	181/182 (99%)	1.00	20 (11%)	10 10	79, 114, 136, 149	0
29	RH	170/180 (94%)	1.45	44 (25%)	1 2	113, 136, 151, 182	0
29	YH	170/180 (94%)	1.24	31 (18%)	3 4	64, 75, 84, 135	0
30	RI	146/148 (98%)	0.72	10 (6%)	23 16	80, 117, 131, 133	0
30	YI	146/148 (98%)	0.84	16 (10%)	10 10	65, 108, 118, 121	0
31	RN	138/140 (98%)	0.66	5 (3%)	46 31	59, 82, 101, 108	0
31	YN	138/140 (98%)	0.48	4 (2%)	53 36	40, 54, 77, 82	0
32	RO	122/122 (100%)	0.27	2 (1%)	70 52	57, 71, 81, 84	0
32	YO	122/122 (100%)	0.30	2 (1%)	70 52	44, 57, 72, 77	0
33	RP	150/150 (100%)	0.92	16 (10%)	11 10	53, 85, 108, 123	0
33	YP	150/150 (100%)	0.89	17 (11%)	10 9	33, 59, 83, 104	0
34	RQ	141/141 (100%)	1.04	19 (13%)	7 6	66, 89, 104, 117	0
34	YQ	141/141 (100%)	0.87	15 (10%)	11 10	45, 59, 74, 86	0
35	RR	118/118 (100%)	0.54	5 (4%)	40 26	55, 68, 77, 80	0
35	YR	118/118 (100%)	0.43	1 (0%)	82 69	41, 54, 62, 66	0
36	RS	111/112 (99%)	1.18	19 (17%)	4 4	99, 115, 123, 126	0
36	YS	111/112 (99%)	0.73	7 (6%)	26 18	64, 73, 80, 84	0
37	RT	137/146 (93%)	0.66	9 (6%)	24 16	68, 79, 123, 139	0
37	YT	137/146 (93%)	0.63	7 (5%)	33 23	51, 64, 108, 131	0
38	RU	117/118 (99%)	0.93	19 (16%)	4 5	57, 78, 95, 108	0
38	YU	117/118 (99%)	0.56	7 (5%)	27 19	35, 46, 63, 75	0
39	RV	101/101 (100%)	0.75	5 (4%)	34 23	56, 96, 104, 108	0
39	YV	101/101 (100%)	0.55	7 (6%)	23 16	33, 63, 74, 80	0
40	RW	113/113 (100%)	0.32	2 (1%)	67 49	49, 62, 83, 105	0
40	YW	113/113 (100%)	0.10	2 (1%)	67 49	37, 45, 63, 93	0
41	RX	92/96 (95%)	0.82	6 (6%)	25 17	63, 74, 84, 88	0
41	YX	92/96 (95%)	0.26	2 (2%)	62 44	43, 49, 60, 62	0
42	RY	102/110 (92%)	1.70	34 (33%)	1 1	79, 89, 108, 115	0
42	YY	102/110 (92%)	1.21	25 (24%)	2 2	55, 63, 85, 93	0
43	RZ	183/206 (88%)	1.20	28 (15%)	5 5	98, 118, 129, 133	0
43	YZ	183/206 (88%)	0.76	17 (9%)	14 12	64, 83, 100, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	R0	82/85 (96%)	0.66	9 (10%)	10	10	66, 80, 88, 93	0
44	Y0	82/85 (96%)	0.23	9 (10%)	10	10	44, 52, 62, 65	0
45	R1	97/98 (98%)	0.99	15 (15%)	5	5	55, 71, 105, 108	0
45	Y1	97/98 (98%)	0.94	13 (13%)	7	7	40, 53, 90, 94	0
46	R2	69/72 (95%)	0.91	8 (11%)	9	9	81, 88, 95, 103	0
46	Y2	69/72 (95%)	0.81	9 (13%)	7	7	52, 59, 66, 78	0
47	R3	59/60 (98%)	0.61	2 (3%)	48	32	68, 81, 97, 104	0
47	Y3	59/60 (98%)	0.38	1 (1%)	69	51	42, 53, 70, 78	0
48	R4	71/71 (100%)	1.64	24 (33%)	1	1	154, 183, 185, 185	0
48	Y4	71/71 (100%)	1.25	14 (19%)	3	3	106, 147, 190, 191	0
49	R5	59/60 (98%)	1.17	13 (22%)	2	2	48, 72, 95, 106	0
49	Y5	59/60 (98%)	1.29	14 (23%)	2	2	32, 59, 84, 87	0
50	R6	49/54 (90%)	2.52	30 (61%)	0	0	84, 95, 102, 105	0
50	Y6	49/54 (90%)	2.90	30 (61%)	0	0	63, 74, 83, 88	0
51	R7	49/49 (100%)	0.93	7 (14%)	6	6	47, 52, 59, 70	0
51	Y7	49/49 (100%)	0.51	3 (6%)	27	19	33, 36, 46, 55	0
52	R8	64/65 (98%)	1.30	17 (26%)	1	2	63, 72, 80, 92	0
52	Y8	64/65 (98%)	1.01	14 (21%)	2	2	40, 49, 57, 66	0
53	R9	37/37 (100%)	2.27	21 (56%)	0	0	83, 96, 106, 108	0
53	Y9	37/37 (100%)	1.92	13 (35%)	1	1	54, 61, 67, 71	0
54	QV	17/18 (94%)	0.64	2 (11%)	9	9	124, 139, 156, 157	0
54	XV	17/18 (94%)	0.77	2 (11%)	9	9	112, 131, 151, 152	0
All	All	20713/21318 (97%)	0.62	2101 (10%)	12	11	29, 88, 176, 279	0

The worst 5 of 2101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	QU	2	GLY	12.0
15	QN	55	GLY	10.2
23	YA	2116	G	9.8
49	Y5	2	ALA	9.7
50	Y6	22	ALA	9.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	1MG	QV	37	24/25	0.58	0.14	127,127,127,127	0
54	1MG	XV	37	24/25	0.79	0.13	117,117,117,117	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	XA	1644	1/1	-0.36	0.38	155,155,155,155	0
55	MG	QA	1619	1/1	-0.19	0.47	146,146,146,146	0
55	MG	XA	1667	1/1	0.09	0.32	127,127,127,127	0
55	MG	XA	1634	1/1	0.11	0.46	154,154,154,154	0
55	MG	XA	1663	1/1	0.17	0.34	103,103,103,103	0
55	MG	XM	201	1/1	0.22	0.19	168,168,168,168	0
55	MG	XA	1671	1/1	0.28	0.19	94,94,94,94	0
55	MG	XA	1623	1/1	0.28	0.44	121,121,121,121	0
55	MG	XA	1629	1/1	0.31	0.23	129,129,129,129	0
55	MG	QA	1631	1/1	0.33	0.65	124,124,124,124	0
55	MG	QA	1647	1/1	0.35	0.36	156,156,156,156	0
55	MG	XA	1643	1/1	0.39	0.34	125,125,125,125	0
55	MG	XA	1625	1/1	0.39	0.29	143,143,143,143	0
55	MG	XA	1602	1/1	0.44	0.47	133,133,133,133	0
55	MG	QA	1603	1/1	0.46	0.46	83,83,83,83	0
55	MG	QA	1639	1/1	0.47	0.41	103,103,103,103	0
55	MG	QA	1622	1/1	0.52	0.20	140,140,140,140	0
55	MG	QA	1665	1/1	0.53	0.54	93,93,93,93	0
55	MG	QA	1625	1/1	0.53	0.59	92,92,92,92	0
55	MG	QA	1652	1/1	0.53	0.47	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1660	1/1	0.53	0.32	146,146,146,146	0
55	MG	XA	1624	1/1	0.54	0.23	133,133,133,133	0
55	MG	QA	1618	1/1	0.54	0.47	95,95,95,95	0
55	MG	XA	1637	1/1	0.55	0.19	85,85,85,85	0
55	MG	XA	1653	1/1	0.55	0.40	91,91,91,91	0
55	MG	XA	1652	1/1	0.56	0.18	101,101,101,101	0
55	MG	QA	1616	1/1	0.56	0.20	108,108,108,108	0
55	MG	XA	1622	1/1	0.56	0.26	130,130,130,130	0
55	MG	XA	1666	1/1	0.56	0.36	85,85,85,85	0
55	MG	QA	1644	1/1	0.56	0.29	108,108,108,108	0
55	MG	RA	3210	1/1	0.56	0.36	85,85,85,85	0
55	MG	RB	201	1/1	0.56	0.24	125,125,125,125	0
55	MG	XA	1641	1/1	0.57	0.72	146,146,146,146	0
55	MG	QA	1617	1/1	0.57	0.26	98,98,98,98	0
55	MG	QA	1662	1/1	0.58	0.25	118,118,118,118	0
55	MG	QA	1653	1/1	0.59	0.31	108,108,108,108	0
55	MG	QA	1613	1/1	0.59	0.70	76,76,76,76	0
55	MG	RB	202	1/1	0.59	0.19	123,123,123,123	0
55	MG	XA	1650	1/1	0.60	0.13	166,166,166,166	0
55	MG	QA	1626	1/1	0.60	0.28	102,102,102,102	0
55	MG	XA	1636	1/1	0.61	0.16	165,165,165,165	0
55	MG	XA	1661	1/1	0.62	0.23	108,108,108,108	0
55	MG	RA	3223	1/1	0.62	0.15	76,76,76,76	0
55	MG	RA	3111	1/1	0.62	0.30	77,77,77,77	0
55	MG	QA	1658	1/1	0.63	0.12	82,82,82,82	0
55	MG	XA	1662	1/1	0.64	0.48	85,85,85,85	0
55	MG	RA	3081	1/1	0.64	0.40	68,68,68,68	0
55	MG	QA	1604	1/1	0.65	0.44	74,74,74,74	0
55	MG	XA	1659	1/1	0.65	0.24	98,98,98,98	0
55	MG	RA	3230	1/1	0.65	0.51	72,72,72,72	0
55	MG	QA	1641	1/1	0.66	0.41	87,87,87,87	0
55	MG	QA	1657	1/1	0.66	0.23	160,160,160,160	0
55	MG	QA	1635	1/1	0.66	0.33	142,142,142,142	0
55	MG	QF	201	1/1	0.67	0.28	98,98,98,98	0
55	MG	RA	3154	1/1	0.67	0.32	65,65,65,65	0
55	MG	RA	3186	1/1	0.67	0.31	78,78,78,78	0
55	MG	XA	1635	1/1	0.67	0.58	79,79,79,79	0
55	MG	QA	1623	1/1	0.68	0.23	140,140,140,140	0
55	MG	RA	3152	1/1	0.68	0.46	62,62,62,62	0
55	MG	QA	1661	1/1	0.68	0.31	103,103,103,103	0
55	MG	XA	1645	1/1	0.69	0.40	92,92,92,92	0
55	MG	XA	1620	1/1	0.69	0.53	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	R0	101	1/1	0.69	0.18	62,62,62,62	0
55	MG	XA	1638	1/1	0.69	0.19	101,101,101,101	0
55	MG	YP	202	1/1	0.69	0.78	38,38,38,38	0
55	MG	RA	3216	1/1	0.70	0.29	70,70,70,70	0
55	MG	QM	201	1/1	0.70	0.12	170,170,170,170	0
55	MG	QH	201	1/1	0.71	0.33	92,92,92,92	0
55	MG	QA	1624	1/1	0.71	0.23	95,95,95,95	0
55	MG	RA	3227	1/1	0.71	0.36	68,68,68,68	0
55	MG	QA	1627	1/1	0.71	0.32	87,87,87,87	0
55	MG	YA	3178	1/1	0.71	0.30	59,59,59,59	0
55	MG	QA	1649	1/1	0.71	0.33	96,96,96,96	0
55	MG	QA	1630	1/1	0.72	0.28	80,80,80,80	0
55	MG	XA	1632	1/1	0.72	0.35	96,96,96,96	0
55	MG	XA	1668	1/1	0.72	0.21	91,91,91,91	0
55	MG	RA	3063	1/1	0.72	0.32	91,91,91,91	0
55	MG	RA	3218	1/1	0.72	0.24	68,68,68,68	0
55	MG	YA	3059	1/1	0.72	0.30	50,50,50,50	0
55	MG	RA	3162	1/1	0.72	0.29	55,55,55,55	0
55	MG	RA	3126	1/1	0.72	0.64	61,61,61,61	0
55	MG	RA	3121	1/1	0.73	0.29	55,55,55,55	0
55	MG	RA	3220	1/1	0.73	0.84	57,57,57,57	0
55	MG	XA	1664	1/1	0.73	0.21	166,166,166,166	0
55	MG	QA	1650	1/1	0.73	0.29	78,78,78,78	0
55	MG	XA	1627	1/1	0.73	0.18	63,63,63,63	0
55	MG	QA	1614	1/1	0.73	0.38	81,81,81,81	0
55	MG	XA	1608	1/1	0.73	0.21	105,105,105,105	0
55	MG	XA	1611	1/1	0.73	0.34	79,79,79,79	0
55	MG	XA	1619	1/1	0.73	0.24	76,76,76,76	0
55	MG	RA	3058	1/1	0.73	0.29	52,52,52,52	0
55	MG	RA	3242	1/1	0.73	0.40	52,52,52,52	0
55	MG	QA	1610	1/1	0.74	0.24	75,75,75,75	0
55	MG	XB	301	1/1	0.74	0.29	119,119,119,119	0
55	MG	XA	1647	1/1	0.75	0.24	101,101,101,101	0
55	MG	RA	3076	1/1	0.75	0.30	42,42,42,42	0
55	MG	QA	1645	1/1	0.75	0.33	70,70,70,70	0
55	MG	RA	3192	1/1	0.75	0.20	103,103,103,103	0
55	MG	QA	1663	1/1	0.75	0.17	105,105,105,105	0
55	MG	RA	3116	1/1	0.75	0.38	53,53,53,53	0
55	MG	QA	1637	1/1	0.76	0.29	71,71,71,71	0
55	MG	RA	3056	1/1	0.76	0.26	47,47,47,47	0
55	MG	QA	1642	1/1	0.76	0.38	84,84,84,84	0
55	MG	YA	3126	1/1	0.76	0.53	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1617	1/1	0.76	0.42	60,60,60,60	0
55	MG	YA	3216	1/1	0.76	0.24	51,51,51,51	0
55	MG	RA	3087	1/1	0.76	0.30	75,75,75,75	0
55	MG	RA	3009	1/1	0.77	0.27	53,53,53,53	0
55	MG	RA	3219	1/1	0.77	0.44	79,79,79,79	0
55	MG	RA	3010	1/1	0.77	0.37	64,64,64,64	0
55	MG	XA	1609	1/1	0.77	0.41	66,66,66,66	0
55	MG	RA	3165	1/1	0.77	0.30	80,80,80,80	0
55	MG	RA	3183	1/1	0.77	0.34	59,59,59,59	0
55	MG	QA	1609	1/1	0.77	0.14	104,104,104,104	0
55	MG	YA	3122	1/1	0.77	0.32	40,40,40,40	0
55	MG	RA	3234	1/1	0.77	0.32	56,56,56,56	0
55	MG	YA	3169	1/1	0.77	0.31	61,61,61,61	0
55	MG	QA	1656	1/1	0.77	0.33	79,79,79,79	0
55	MG	RA	3142	1/1	0.77	0.13	72,72,72,72	0
55	MG	YA	3236	1/1	0.77	0.25	53,53,53,53	0
55	MG	YB	204	1/1	0.77	0.23	71,71,71,71	0
55	MG	RA	3093	1/1	0.77	0.31	46,46,46,46	0
55	MG	XA	1614	1/1	0.78	0.47	54,54,54,54	0
55	MG	QA	1621	1/1	0.78	0.21	84,84,84,84	0
55	MG	XA	1651	1/1	0.78	0.24	89,89,89,89	0
55	MG	XA	1610	1/1	0.78	0.25	63,63,63,63	0
55	MG	RA	3228	1/1	0.78	0.21	69,69,69,69	0
55	MG	RA	3123	1/1	0.79	0.34	63,63,63,63	0
55	MG	YA	3131	1/1	0.79	0.45	62,62,62,62	0
55	MG	XA	1612	1/1	0.79	0.28	75,75,75,75	0
55	MG	RA	3112	1/1	0.79	0.44	73,73,73,73	0
55	MG	YA	3027	1/1	0.79	0.30	32,32,32,32	0
55	MG	YA	3221	1/1	0.79	0.17	53,53,53,53	0
55	MG	QA	1632	1/1	0.79	0.17	90,90,90,90	0
55	MG	YA	3089	1/1	0.79	0.31	28,28,28,28	0
55	MG	QA	1646	1/1	0.79	0.14	94,94,94,94	0
55	MG	XA	1628	1/1	0.80	0.11	66,66,66,66	0
55	MG	YA	3110	1/1	0.80	0.28	54,54,54,54	0
55	MG	RA	3196	1/1	0.80	0.21	72,72,72,72	0
55	MG	XA	1630	1/1	0.80	0.34	68,68,68,68	0
55	MG	RA	3017	1/1	0.80	0.29	44,44,44,44	0
55	MG	XA	1649	1/1	0.80	0.37	72,72,72,72	0
55	MG	RA	3139	1/1	0.80	0.37	68,68,68,68	0
55	MG	RA	3122	1/1	0.80	0.49	65,65,65,65	0
55	MG	RA	3151	1/1	0.80	0.28	56,56,56,56	0
55	MG	RA	3024	1/1	0.80	0.27	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3153	1/1	0.80	0.38	79,79,79,79	0
55	MG	RR	201	1/1	0.80	0.30	52,52,52,52	0
55	MG	RF	301	1/1	0.81	0.29	84,84,84,84	0
55	MG	RA	3184	1/1	0.81	0.14	54,54,54,54	0
55	MG	RA	3119	1/1	0.81	0.31	70,70,70,70	0
55	MG	RA	3048	1/1	0.81	0.37	46,46,46,46	0
55	MG	RA	3141	1/1	0.81	0.44	72,72,72,72	0
55	MG	RA	3051	1/1	0.81	0.37	52,52,52,52	0
55	MG	RA	3212	1/1	0.81	0.35	55,55,55,55	0
55	MG	RA	3145	1/1	0.81	0.36	56,56,56,56	0
55	MG	RA	3173	1/1	0.81	0.14	46,46,46,46	0
55	MG	YA	3050	1/1	0.81	0.32	27,27,27,27	0
55	MG	RA	3030	1/1	0.81	0.30	41,41,41,41	0
55	MG	YA	3068	1/1	0.81	0.37	45,45,45,45	0
55	MG	YA	3018	1/1	0.82	0.36	28,28,28,28	0
55	MG	QA	1612	1/1	0.82	0.37	62,62,62,62	0
55	MG	RA	3127	1/1	0.82	0.25	77,77,77,77	0
55	MG	R3	101	1/1	0.82	0.31	62,62,62,62	0
55	MG	RA	3171	1/1	0.82	0.35	61,61,61,61	0
55	MG	YA	3087	1/1	0.82	0.29	39,39,39,39	0
55	MG	RA	3060	1/1	0.82	0.31	45,45,45,45	0
55	MG	RA	3174	1/1	0.82	0.26	75,75,75,75	0
55	MG	YA	3121	1/1	0.82	0.36	49,49,49,49	0
55	MG	RA	3225	1/1	0.82	0.22	61,61,61,61	0
55	MG	RA	3032	1/1	0.82	0.29	47,47,47,47	0
55	MG	RA	3114	1/1	0.82	0.26	76,76,76,76	0
55	MG	YA	3140	1/1	0.82	0.30	38,38,38,38	0
55	MG	YA	3152	1/1	0.82	0.12	44,44,44,44	0
55	MG	RA	3229	1/1	0.82	0.11	61,61,61,61	0
55	MG	RA	3023	1/1	0.82	0.77	45,45,45,45	0
55	MG	RA	3079	1/1	0.82	0.24	60,60,60,60	0
55	MG	QA	1634	1/1	0.82	0.55	69,69,69,69	0
55	MG	YA	3234	1/1	0.82	0.34	66,66,66,66	0
55	MG	RA	3200	1/1	0.82	0.17	65,65,65,65	0
55	MG	RA	3084	1/1	0.82	0.28	56,56,56,56	0
55	MG	RA	3028	1/1	0.82	0.13	73,73,73,73	0
55	MG	RA	3103	1/1	0.83	0.18	58,58,58,58	0
55	MG	RA	3067	1/1	0.83	0.55	43,43,43,43	0
55	MG	YA	3117	1/1	0.83	0.21	36,36,36,36	0
55	MG	RA	3026	1/1	0.83	0.24	45,45,45,45	0
55	MG	RA	3130	1/1	0.83	0.17	69,69,69,69	0
55	MG	RA	3163	1/1	0.83	0.28	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1670	1/1	0.83	0.44	77,77,77,77	0
55	MG	RA	3133	1/1	0.83	0.20	67,67,67,67	0
55	MG	QA	1655	1/1	0.83	0.19	91,91,91,91	0
55	MG	YA	3165	1/1	0.83	0.39	50,50,50,50	0
55	MG	XA	1633	1/1	0.83	0.22	72,72,72,72	0
55	MG	RA	3172	1/1	0.83	0.23	54,54,54,54	0
55	MG	QA	1638	1/1	0.83	0.35	78,78,78,78	0
55	MG	XA	1658	1/1	0.83	0.16	88,88,88,88	0
55	MG	QA	1664	1/1	0.83	0.13	111,111,111,111	0
55	MG	YA	3064	1/1	0.83	0.27	38,38,38,38	0
55	MG	RA	3039	1/1	0.83	0.29	45,45,45,45	0
55	MG	RA	3044	1/1	0.83	0.30	49,49,49,49	0
55	MG	RA	3042	1/1	0.84	0.41	46,46,46,46	0
55	MG	YA	3023	1/1	0.84	0.52	27,27,27,27	0
55	MG	RA	3043	1/1	0.84	0.34	42,42,42,42	0
55	MG	RA	3239	1/1	0.84	0.26	47,47,47,47	0
55	MG	YA	3155	1/1	0.84	0.43	58,58,58,58	0
55	MG	RA	3202	1/1	0.84	0.12	53,53,53,53	0
55	MG	RA	3224	1/1	0.84	0.24	61,61,61,61	0
55	MG	QA	1608	1/1	0.84	0.19	91,91,91,91	0
55	MG	YA	3188	1/1	0.84	0.23	43,43,43,43	0
55	MG	YA	3201	1/1	0.84	0.14	46,46,46,46	0
55	MG	YA	3207	1/1	0.84	0.15	55,55,55,55	0
55	MG	QA	1651	1/1	0.84	0.38	81,81,81,81	0
55	MG	QA	1666	1/1	0.84	0.18	100,100,100,100	0
55	MG	XA	1616	1/1	0.84	0.36	68,68,68,68	0
55	MG	XL	201	1/1	0.84	0.14	97,97,97,97	0
55	MG	QA	1602	1/1	0.84	0.47	74,74,74,74	0
55	MG	YD	302	1/1	0.84	0.26	30,30,30,30	0
55	MG	YA	3016	1/1	0.84	0.28	30,30,30,30	0
55	MG	YA	3106	1/1	0.85	0.23	40,40,40,40	0
55	MG	XA	1618	1/1	0.85	0.23	72,72,72,72	0
55	MG	RA	3089	1/1	0.85	0.36	55,55,55,55	0
55	MG	RA	3075	1/1	0.85	0.27	62,62,62,62	0
55	MG	XA	1642	1/1	0.85	0.18	134,134,134,134	0
55	MG	RA	3168	1/1	0.85	0.16	59,59,59,59	0
55	MG	QA	1628	1/1	0.85	0.24	71,71,71,71	0
55	MG	YA	3136	1/1	0.85	0.29	39,39,39,39	0
55	MG	R8	101	1/1	0.85	0.43	57,57,57,57	0
55	MG	RA	3035	1/1	0.85	0.38	49,49,49,49	0
55	MG	XA	1648	1/1	0.85	0.36	85,85,85,85	0
55	MG	XA	1626	1/1	0.85	0.25	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1606	1/1	0.85	0.35	68,68,68,68	0
55	MG	YA	3172	1/1	0.85	0.26	67,67,67,67	0
55	MG	RA	3211	1/1	0.85	0.24	67,67,67,67	0
55	MG	RA	3125	1/1	0.85	0.29	75,75,75,75	0
55	MG	YA	3198	1/1	0.85	0.31	29,29,29,29	0
55	MG	RA	3231	1/1	0.85	0.23	54,54,54,54	0
55	MG	RA	3214	1/1	0.85	0.15	71,71,71,71	0
55	MG	YA	3063	1/1	0.85	0.29	35,35,35,35	0
55	MG	RA	3004	1/1	0.85	0.35	68,68,68,68	0
55	MG	RA	3113	1/1	0.85	0.50	70,70,70,70	0
55	MG	RA	3012	1/1	0.85	0.25	42,42,42,42	0
55	MG	RA	3054	1/1	0.85	0.33	44,44,44,44	0
55	MG	YA	3091	1/1	0.85	0.29	40,40,40,40	0
55	MG	YA	3094	1/1	0.85	0.34	39,39,39,39	0
55	MG	RA	3029	1/1	0.86	0.30	50,50,50,50	0
55	MG	YA	3015	1/1	0.86	0.16	28,28,28,28	0
55	MG	RA	3217	1/1	0.86	0.36	78,78,78,78	0
55	MG	QA	1605	1/1	0.86	0.58	71,71,71,71	0
55	MG	YA	3135	1/1	0.86	0.16	48,48,48,48	0
55	MG	RA	3014	1/1	0.86	0.30	39,39,39,39	0
55	MG	YA	3024	1/1	0.86	0.37	36,36,36,36	0
55	MG	XA	1615	1/1	0.86	0.37	56,56,56,56	0
55	MG	YA	3038	1/1	0.86	0.18	32,32,32,32	0
55	MG	YA	3049	1/1	0.86	0.37	37,37,37,37	0
55	MG	RA	3061	1/1	0.86	0.32	42,42,42,42	0
55	MG	RA	3222	1/1	0.86	0.18	53,53,53,53	0
55	MG	RP	201	1/1	0.86	0.93	60,60,60,60	0
55	MG	RA	3140	1/1	0.86	0.28	51,51,51,51	0
55	MG	YA	3192	1/1	0.86	0.35	48,48,48,48	0
55	MG	RA	3033	1/1	0.86	0.39	61,61,61,61	0
55	MG	YA	3079	1/1	0.86	0.25	34,34,34,34	0
55	MG	YA	3203	1/1	0.86	0.19	34,34,34,34	0
55	MG	RA	3170	1/1	0.86	0.11	66,66,66,66	0
55	MG	YA	3213	1/1	0.86	0.15	37,37,37,37	0
55	MG	RA	3204	1/1	0.86	0.18	61,61,61,61	0
55	MG	YA	3219	1/1	0.86	0.27	52,52,52,52	0
55	MG	RA	3050	1/1	0.86	0.28	47,47,47,47	0
55	MG	XA	1603	1/1	0.86	0.50	49,49,49,49	0
55	MG	QA	1615	1/1	0.86	0.34	70,70,70,70	0
55	MG	YA	3250	1/1	0.86	0.23	40,40,40,40	0
55	MG	YA	3258	1/1	0.86	0.31	42,42,42,42	0
55	MG	RA	3022	1/1	0.86	0.36	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YD	301	1/1	0.86	0.43	34,34,34,34	0
55	MG	YA	3114	1/1	0.86	0.29	38,38,38,38	0
55	MG	RA	3078	1/1	0.86	0.29	43,43,43,43	0
55	MG	RA	3181	1/1	0.87	0.15	60,60,60,60	0
55	MG	YA	3085	1/1	0.87	0.37	29,29,29,29	0
55	MG	RA	3073	1/1	0.87	0.20	51,51,51,51	0
55	MG	QA	1611	1/1	0.87	0.41	67,67,67,67	0
55	MG	XA	1654	1/1	0.87	0.37	69,69,69,69	0
55	MG	XA	1657	1/1	0.87	0.26	78,78,78,78	0
55	MG	YA	3102	1/1	0.87	0.30	52,52,52,52	0
55	MG	YA	3197	1/1	0.87	0.34	36,36,36,36	0
55	MG	XA	1605	1/1	0.87	0.51	76,76,76,76	0
55	MG	QA	1648	1/1	0.87	0.24	83,83,83,83	0
55	MG	YA	3113	1/1	0.87	0.29	31,31,31,31	0
55	MG	QA	1601	1/1	0.87	0.41	88,88,88,88	0
55	MG	RA	3193	1/1	0.87	0.34	77,77,77,77	0
55	MG	RA	3194	1/1	0.87	0.26	80,80,80,80	0
55	MG	YA	3045	1/1	0.87	0.30	29,29,29,29	0
55	MG	RA	3117	1/1	0.87	0.24	43,43,43,43	0
55	MG	RA	3146	1/1	0.87	0.29	69,69,69,69	0
55	MG	YA	3133	1/1	0.87	0.33	49,49,49,49	0
55	MG	RA	3150	1/1	0.87	0.24	63,63,63,63	0
55	MG	RA	3129	1/1	0.87	0.23	50,50,50,50	0
55	MG	RA	3020	1/1	0.87	0.27	42,42,42,42	0
55	MG	YA	3148	1/1	0.87	0.24	32,32,32,32	0
55	MG	RA	3069	1/1	0.87	0.36	56,56,56,56	0
55	MG	YA	3153	1/1	0.87	0.27	54,54,54,54	0
55	MG	RA	3083	1/1	0.88	0.26	44,44,44,44	0
55	MG	XA	1669	1/1	0.88	0.37	73,73,73,73	0
55	MG	QA	1606	1/1	0.88	0.20	89,89,89,89	0
55	MG	RA	3085	1/1	0.88	0.23	49,49,49,49	0
55	MG	XA	1640	1/1	0.88	0.40	56,56,56,56	0
55	MG	RA	3160	1/1	0.88	0.13	61,61,61,61	0
55	MG	RA	3086	1/1	0.88	0.33	49,49,49,49	0
55	MG	YA	3212	1/1	0.88	0.27	40,40,40,40	0
55	MG	YA	3069	1/1	0.88	0.23	34,34,34,34	0
55	MG	YA	3011	1/1	0.88	0.31	27,27,27,27	0
55	MG	YA	3137	1/1	0.88	0.29	41,41,41,41	0
55	MG	RA	3008	1/1	0.88	0.28	60,60,60,60	0
55	MG	YA	3230	1/1	0.88	0.21	39,39,39,39	0
55	MG	RA	3164	1/1	0.88	0.28	47,47,47,47	0
55	MG	YA	3235	1/1	0.88	0.08	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1631	1/1	0.88	0.35	63,63,63,63	0
55	MG	RA	3055	1/1	0.88	0.28	47,47,47,47	0
55	MG	RE	302	1/1	0.88	0.35	42,42,42,42	0
55	MG	QA	1607	1/1	0.88	0.18	101,101,101,101	0
55	MG	YA	3032	1/1	0.88	0.35	39,39,39,39	0
55	MG	RA	3082	1/1	0.88	0.26	72,72,72,72	0
55	MG	YA	3039	1/1	0.88	0.32	30,30,30,30	0
55	MG	YA	3040	1/1	0.89	0.34	25,25,25,25	0
55	MG	QA	1629	1/1	0.89	0.37	80,80,80,80	0
55	MG	RA	3148	1/1	0.89	0.30	55,55,55,55	0
55	MG	YA	3146	1/1	0.89	0.22	34,34,34,34	0
55	MG	RA	3149	1/1	0.89	0.14	60,60,60,60	0
55	MG	RA	3180	1/1	0.89	0.27	61,61,61,61	0
55	MG	RA	3091	1/1	0.89	0.33	44,44,44,44	0
55	MG	RA	3221	1/1	0.89	0.22	56,56,56,56	0
55	MG	YA	3161	1/1	0.89	0.36	47,47,47,47	0
55	MG	YA	3065	1/1	0.89	0.26	43,43,43,43	0
55	MG	RA	3047	1/1	0.89	0.27	52,52,52,52	0
55	MG	RA	3095	1/1	0.89	0.36	47,47,47,47	0
55	MG	YA	3176	1/1	0.89	0.24	59,59,59,59	0
55	MG	YA	3177	1/1	0.89	0.14	45,45,45,45	0
55	MG	YA	3074	1/1	0.89	0.22	38,38,38,38	0
55	MG	YA	3183	1/1	0.89	0.35	53,53,53,53	0
55	MG	YA	3184	1/1	0.89	0.21	53,53,53,53	0
55	MG	YA	3075	1/1	0.89	0.26	37,37,37,37	0
55	MG	YA	3189	1/1	0.89	0.23	47,47,47,47	0
55	MG	RA	3100	1/1	0.89	0.26	53,53,53,53	0
55	MG	RA	3019	1/1	0.89	0.28	40,40,40,40	0
55	MG	YA	3003	1/1	0.89	0.31	29,29,29,29	0
55	MG	YA	3009	1/1	0.89	0.38	34,34,34,34	0
55	MG	RA	3156	1/1	0.89	0.30	57,57,57,57	0
55	MG	RA	3158	1/1	0.89	0.27	51,51,51,51	0
55	MG	RA	3027	1/1	0.89	0.48	44,44,44,44	0
55	MG	QA	1643	1/1	0.89	0.40	72,72,72,72	0
55	MG	RA	3052	1/1	0.89	0.21	54,54,54,54	0
55	MG	RA	3053	1/1	0.89	0.43	40,40,40,40	0
55	MG	YA	3026	1/1	0.89	0.17	59,59,59,59	0
55	MG	YA	3222	1/1	0.89	0.20	56,56,56,56	0
55	MG	YA	3228	1/1	0.89	0.18	41,41,41,41	0
55	MG	YA	3115	1/1	0.89	0.18	35,35,35,35	0
55	MG	YA	3231	1/1	0.89	0.15	38,38,38,38	0
55	MG	RA	3115	1/1	0.89	0.21	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3031	1/1	0.89	0.38	33,33,33,33	0
55	MG	QA	1640	1/1	0.89	0.16	85,85,85,85	0
55	MG	YA	3239	1/1	0.89	0.12	51,51,51,51	0
55	MG	YA	3242	1/1	0.89	0.13	49,49,49,49	0
55	MG	YA	3243	1/1	0.89	0.10	50,50,50,50	0
55	MG	YA	3125	1/1	0.89	0.23	29,29,29,29	0
55	MG	YA	3033	1/1	0.89	0.32	31,31,31,31	0
55	MG	YA	3263	1/1	0.89	0.24	48,48,48,48	0
55	MG	YA	3129	1/1	0.89	0.38	44,44,44,44	0
55	MG	YA	3037	1/1	0.89	0.27	25,25,25,25	0
55	MG	RA	3074	1/1	0.89	0.23	51,51,51,51	0
55	MG	QA	1633	1/1	0.89	0.15	110,110,110,110	0
55	MG	RA	3203	1/1	0.90	0.25	58,58,58,58	0
55	MG	RD	301	1/1	0.90	0.21	47,47,47,47	0
55	MG	YA	3006	1/1	0.90	0.41	36,36,36,36	0
55	MG	YA	3211	1/1	0.90	0.18	29,29,29,29	0
55	MG	YA	3099	1/1	0.90	0.36	32,32,32,32	0
55	MG	YA	3007	1/1	0.90	0.28	28,28,28,28	0
55	MG	YA	3103	1/1	0.90	0.21	24,24,24,24	0
55	MG	YA	3217	1/1	0.90	0.13	39,39,39,39	0
55	MG	YA	3047	1/1	0.90	0.31	30,30,30,30	0
55	MG	YA	3220	1/1	0.90	0.26	37,37,37,37	0
55	MG	RA	3101	1/1	0.90	0.15	46,46,46,46	0
55	MG	YA	3164	1/1	0.90	0.14	59,59,59,59	0
55	MG	YA	3225	1/1	0.90	0.25	27,27,27,27	0
55	MG	RA	3206	1/1	0.90	0.30	46,46,46,46	0
55	MG	YA	3229	1/1	0.90	0.32	38,38,38,38	0
55	MG	RA	3102	1/1	0.90	0.18	51,51,51,51	0
55	MG	YA	3171	1/1	0.90	0.18	48,48,48,48	0
55	MG	RA	3001	1/1	0.90	0.30	58,58,58,58	0
55	MG	YA	3175	1/1	0.90	0.31	30,30,30,30	0
55	MG	RA	3187	1/1	0.90	0.26	59,59,59,59	0
55	MG	RA	3045	1/1	0.90	0.31	61,61,61,61	0
55	MG	YA	3067	1/1	0.90	0.22	37,37,37,37	0
55	MG	RA	3031	1/1	0.90	0.31	44,44,44,44	0
55	MG	RA	3021	1/1	0.90	0.30	44,44,44,44	0
55	MG	RA	3176	1/1	0.90	0.22	63,63,63,63	0
55	MG	RA	3199	1/1	0.90	0.17	70,70,70,70	0
55	MG	RA	3099	1/1	0.90	0.39	40,40,40,40	0
55	MG	RA	3015	1/1	0.90	0.17	44,44,44,44	0
55	MG	XA	1656	1/1	0.90	0.39	67,67,67,67	0
55	MG	YA	3200	1/1	0.90	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	ZN	QN	101	1/1	0.90	0.07	158,158,158,158	0
55	MG	RA	3107	1/1	0.91	0.18	52,52,52,52	0
55	MG	YA	3014	1/1	0.91	0.30	25,25,25,25	0
55	MG	YA	3160	1/1	0.91	0.26	37,37,37,37	0
55	MG	RA	3132	1/1	0.91	0.45	52,52,52,52	0
55	MG	YA	3052	1/1	0.91	0.22	33,33,33,33	0
55	MG	YA	3056	1/1	0.91	0.22	32,32,32,32	0
55	MG	RA	3068	1/1	0.91	0.31	44,44,44,44	0
55	MG	YA	3061	1/1	0.91	0.24	35,35,35,35	0
55	MG	RA	3137	1/1	0.91	0.41	46,46,46,46	0
55	MG	YA	3174	1/1	0.91	0.37	47,47,47,47	0
55	MG	RA	3036	1/1	0.91	0.35	47,47,47,47	0
55	MG	RA	3070	1/1	0.91	0.18	56,56,56,56	0
55	MG	RA	3124	1/1	0.91	0.38	56,56,56,56	0
55	MG	RA	3046	1/1	0.91	0.28	42,42,42,42	0
55	MG	YA	3179	1/1	0.91	0.25	33,33,33,33	0
55	MG	YA	3128	1/1	0.91	0.23	42,42,42,42	0
55	MG	YA	3029	1/1	0.91	0.37	26,26,26,26	0
55	MG	RA	3144	1/1	0.91	0.47	45,45,45,45	0
55	MG	QA	1620	1/1	0.91	0.19	76,76,76,76	0
55	MG	RA	3185	1/1	0.91	0.21	75,75,75,75	0
55	MG	RA	3041	1/1	0.91	0.28	44,44,44,44	0
55	MG	RA	3128	1/1	0.91	0.24	53,53,53,53	0
55	MG	YA	3199	1/1	0.91	0.30	44,44,44,44	0
55	MG	RA	3191	1/1	0.91	0.33	72,72,72,72	0
55	MG	RA	3092	1/1	0.91	0.22	50,50,50,50	0
55	MG	YA	3041	1/1	0.91	0.27	30,30,30,30	0
55	MG	YA	3206	1/1	0.91	0.31	45,45,45,45	0
55	MG	XA	1607	1/1	0.91	0.21	86,86,86,86	0
55	MG	YA	3001	1/1	0.92	0.28	27,27,27,27	0
55	MG	YA	3002	1/1	0.92	0.35	30,30,30,30	0
55	MG	YA	3202	1/1	0.92	0.06	44,44,44,44	0
55	MG	YA	3139	1/1	0.92	0.33	34,34,34,34	0
55	MG	YA	3204	1/1	0.92	0.09	43,43,43,43	0
55	MG	YA	3083	1/1	0.92	0.35	35,35,35,35	0
55	MG	YA	3143	1/1	0.92	0.23	43,43,43,43	0
55	MG	YA	3209	1/1	0.92	0.19	38,38,38,38	0
55	MG	YA	3084	1/1	0.92	0.27	29,29,29,29	0
55	MG	XA	1639	1/1	0.92	0.55	66,66,66,66	0
55	MG	RA	3205	1/1	0.92	0.17	60,60,60,60	0
55	MG	YA	3215	1/1	0.92	0.20	40,40,40,40	0
55	MG	RA	3104	1/1	0.92	0.25	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3008	1/1	0.92	0.26	36,36,36,36	0
55	MG	YA	3157	1/1	0.92	0.26	45,45,45,45	0
55	MG	YA	3044	1/1	0.92	0.42	28,28,28,28	0
55	MG	RE	301	1/1	0.92	0.22	37,37,37,37	0
55	MG	RA	3209	1/1	0.92	0.12	58,58,58,58	0
55	MG	YA	3224	1/1	0.92	0.10	25,25,25,25	0
55	MG	YA	3048	1/1	0.92	0.34	36,36,36,36	0
55	MG	YA	3105	1/1	0.92	0.33	32,32,32,32	0
55	MG	YA	3012	1/1	0.92	0.27	20,20,20,20	0
55	MG	RA	3105	1/1	0.92	0.25	50,50,50,50	0
55	MG	QA	1636	1/1	0.92	0.18	87,87,87,87	0
55	MG	YA	3055	1/1	0.92	0.33	31,31,31,31	0
55	MG	RA	3038	1/1	0.92	0.24	39,39,39,39	0
55	MG	RA	3197	1/1	0.92	0.27	67,67,67,67	0
55	MG	YA	3020	1/1	0.92	0.29	26,26,26,26	0
55	MG	YA	3062	1/1	0.92	0.22	30,30,30,30	0
55	MG	RA	3080	1/1	0.92	0.43	53,53,53,53	0
55	MG	R5	101	1/1	0.92	0.29	45,45,45,45	0
55	MG	YA	3254	1/1	0.92	0.29	35,35,35,35	0
55	MG	RA	3134	1/1	0.92	0.22	52,52,52,52	0
55	MG	RA	3201	1/1	0.92	0.38	58,58,58,58	0
55	MG	YB	201	1/1	0.92	0.13	63,63,63,63	0
55	MG	YA	3130	1/1	0.92	0.21	31,31,31,31	0
55	MG	YA	3195	1/1	0.92	0.20	54,54,54,54	0
55	MG	RA	3077	1/1	0.92	0.33	46,46,46,46	0
55	MG	RA	3190	1/1	0.92	0.38	64,64,64,64	0
55	MG	Y5	101	1/1	0.92	0.17	33,33,33,33	0
55	MG	RA	3178	1/1	0.92	0.16	47,47,47,47	0
55	MG	YA	3186	1/1	0.93	0.21	65,65,65,65	0
55	MG	RA	3006	1/1	0.93	0.38	46,46,46,46	0
55	MG	YA	3010	1/1	0.93	0.24	35,35,35,35	0
55	MG	XA	1655	1/1	0.93	0.41	69,69,69,69	0
55	MG	RA	3235	1/1	0.93	0.35	53,53,53,53	0
55	MG	YA	3013	1/1	0.93	0.33	27,27,27,27	0
55	MG	YA	3123	1/1	0.93	0.24	36,36,36,36	0
55	MG	YA	3124	1/1	0.93	0.39	27,27,27,27	0
55	MG	RA	3236	1/1	0.93	0.41	49,49,49,49	0
55	MG	RA	3237	1/1	0.93	0.48	56,56,56,56	0
55	MG	RA	3175	1/1	0.93	0.18	48,48,48,48	0
55	MG	XA	1660	1/1	0.93	0.36	66,66,66,66	0
55	MG	RA	3195	1/1	0.93	0.10	52,52,52,52	0
55	MG	RA	3159	1/1	0.93	0.30	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3132	1/1	0.93	0.12	60,60,60,60	0
55	MG	RA	3088	1/1	0.93	0.40	42,42,42,42	0
55	MG	XA	1613	1/1	0.93	0.13	75,75,75,75	0
55	MG	YA	3070	1/1	0.93	0.08	36,36,36,36	0
55	MG	YA	3071	1/1	0.93	0.07	47,47,47,47	0
55	MG	RA	3147	1/1	0.93	0.17	49,49,49,49	0
55	MG	YA	3028	1/1	0.93	0.18	29,29,29,29	0
55	MG	YA	3142	1/1	0.93	0.07	32,32,32,32	0
55	MG	YA	3078	1/1	0.93	0.27	31,31,31,31	0
55	MG	YA	3145	1/1	0.93	0.21	44,44,44,44	0
55	MG	RA	3097	1/1	0.93	0.28	48,48,48,48	0
55	MG	YA	3030	1/1	0.93	0.36	42,42,42,42	0
55	MG	YA	3223	1/1	0.93	0.26	55,55,55,55	0
55	MG	RA	3182	1/1	0.93	0.15	49,49,49,49	0
55	MG	RA	3066	1/1	0.93	0.22	51,51,51,51	0
55	MG	YA	3154	1/1	0.93	0.12	31,31,31,31	0
55	MG	RA	3138	1/1	0.93	0.26	44,44,44,44	0
55	MG	RA	3106	1/1	0.93	0.21	46,46,46,46	0
55	MG	RA	3169	1/1	0.93	0.20	50,50,50,50	0
55	MG	XA	1621	1/1	0.93	0.16	77,77,77,77	0
55	MG	YA	3163	1/1	0.93	0.25	43,43,43,43	0
55	MG	YA	3095	1/1	0.93	0.29	40,40,40,40	0
55	MG	YA	3097	1/1	0.93	0.20	35,35,35,35	0
55	MG	YA	3240	1/1	0.93	0.30	40,40,40,40	0
55	MG	YA	3166	1/1	0.93	0.10	41,41,41,41	0
55	MG	RA	3011	1/1	0.93	0.45	54,54,54,54	0
55	MG	YA	3244	1/1	0.93	0.34	39,39,39,39	0
55	MG	YA	3248	1/1	0.93	0.21	42,42,42,42	0
55	MG	YA	3100	1/1	0.93	0.28	26,26,26,26	0
55	MG	YA	3101	1/1	0.93	0.33	38,38,38,38	0
55	MG	RA	3208	1/1	0.93	0.12	73,73,73,73	0
55	MG	YA	3261	1/1	0.93	0.25	34,34,34,34	0
55	MG	RA	3110	1/1	0.93	0.08	50,50,50,50	0
55	MG	XA	1601	1/1	0.93	0.39	55,55,55,55	0
55	MG	RA	3120	1/1	0.93	0.31	48,48,48,48	0
55	MG	YA	3108	1/1	0.93	0.31	28,28,28,28	0
55	MG	RA	3040	1/1	0.93	0.27	45,45,45,45	0
55	MG	YA	3180	1/1	0.93	0.14	48,48,48,48	0
55	MG	YA	3112	1/1	0.93	0.24	44,44,44,44	0
55	MG	XA	1604	1/1	0.93	0.55	75,75,75,75	0
55	MG	RA	3025	1/1	0.94	0.20	43,43,43,43	0
55	MG	RA	3090	1/1	0.94	0.26	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3016	1/1	0.94	0.39	41,41,41,41	0
55	MG	RA	3049	1/1	0.94	0.25	41,41,41,41	0
55	MG	RA	3166	1/1	0.94	0.23	54,54,54,54	0
55	MG	RA	3167	1/1	0.94	0.13	56,56,56,56	0
55	MG	QA	1659	1/1	0.94	0.13	69,69,69,69	0
55	MG	RA	3226	1/1	0.94	0.14	62,62,62,62	0
55	MG	YA	3004	1/1	0.94	0.20	30,30,30,30	0
55	MG	YA	3118	1/1	0.94	0.41	33,33,33,33	0
55	MG	YA	3120	1/1	0.94	0.27	29,29,29,29	0
55	MG	RA	3094	1/1	0.94	0.23	45,45,45,45	0
55	MG	YA	3073	1/1	0.94	0.32	35,35,35,35	0
55	MG	YA	3226	1/1	0.94	0.39	40,40,40,40	0
55	MG	YA	3036	1/1	0.94	0.25	32,32,32,32	0
55	MG	RA	3189	1/1	0.94	0.13	58,58,58,58	0
55	MG	RA	3136	1/1	0.94	0.09	46,46,46,46	0
55	MG	RA	3057	1/1	0.94	0.46	40,40,40,40	0
55	MG	YA	3233	1/1	0.94	0.23	42,42,42,42	0
55	MG	YA	3082	1/1	0.94	0.32	31,31,31,31	0
55	MG	RA	3108	1/1	0.94	0.14	49,49,49,49	0
55	MG	YA	3182	1/1	0.94	0.26	38,38,38,38	0
55	MG	RA	3233	1/1	0.94	0.32	28,28,28,28	0
55	MG	RA	3109	1/1	0.94	0.17	48,48,48,48	0
55	MG	RA	3096	1/1	0.94	0.28	39,39,39,39	0
55	MG	YA	3088	1/1	0.94	0.28	34,34,34,34	0
55	MG	XA	1665	1/1	0.94	0.32	70,70,70,70	0
55	MG	YA	3247	1/1	0.94	0.15	39,39,39,39	0
55	MG	YA	3090	1/1	0.94	0.24	39,39,39,39	0
55	MG	QA	1654	1/1	0.94	0.07	98,98,98,98	0
55	MG	YA	3093	1/1	0.94	0.31	26,26,26,26	0
55	MG	YA	3256	1/1	0.94	0.36	28,28,28,28	0
55	MG	RA	3003	1/1	0.94	0.64	47,47,47,47	0
55	MG	YA	3017	1/1	0.94	0.35	31,31,31,31	0
55	MG	RA	3238	1/1	0.94	0.35	51,51,51,51	0
55	MG	YA	3266	1/1	0.94	0.47	39,39,39,39	0
55	MG	YA	3144	1/1	0.94	0.18	38,38,38,38	0
55	MG	YA	3053	1/1	0.94	0.28	25,25,25,25	0
55	MG	RA	3072	1/1	0.94	0.29	61,61,61,61	0
55	MG	YA	3021	1/1	0.94	0.26	28,28,28,28	0
55	MG	YA	3150	1/1	0.94	0.15	61,61,61,61	0
55	MG	YA	3022	1/1	0.94	0.26	30,30,30,30	0
55	MG	YA	3060	1/1	0.94	0.20	39,39,39,39	0
55	MG	RA	3177	1/1	0.95	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3191	1/1	0.95	0.24	42,42,42,42	0
55	MG	RA	3161	1/1	0.95	0.40	67,67,67,67	0
55	MG	YA	3193	1/1	0.95	0.17	39,39,39,39	0
55	MG	YA	3245	1/1	0.95	0.14	39,39,39,39	0
55	MG	YA	3035	1/1	0.95	0.27	26,26,26,26	0
55	MG	YA	3147	1/1	0.95	0.20	36,36,36,36	0
55	MG	YA	3092	1/1	0.95	0.21	35,35,35,35	0
55	MG	RA	3071	1/1	0.95	0.31	49,49,49,49	0
55	MG	YA	3134	1/1	0.95	0.20	42,42,42,42	0
55	MG	RA	3002	1/1	0.95	0.31	45,45,45,45	0
55	MG	YA	3107	1/1	0.95	0.29	32,32,32,32	0
55	MG	YA	3262	1/1	0.95	0.34	27,27,27,27	0
55	MG	YA	3046	1/1	0.95	0.32	24,24,24,24	0
55	MG	YA	3156	1/1	0.95	0.40	51,51,51,51	0
55	MG	YA	3138	1/1	0.95	0.14	39,39,39,39	0
55	MG	YB	202	1/1	0.95	0.30	49,49,49,49	0
55	MG	YB	203	1/1	0.95	0.24	45,45,45,45	0
55	MG	YA	3159	1/1	0.95	0.21	36,36,36,36	0
55	MG	YA	3109	1/1	0.95	0.12	33,33,33,33	0
55	MG	YA	3210	1/1	0.95	0.23	38,38,38,38	0
55	MG	YP	201	1/1	0.95	0.06	56,56,56,56	0
55	MG	RA	3157	1/1	0.95	0.22	43,43,43,43	0
55	MG	YX	101	1/1	0.95	0.09	53,53,53,53	0
55	MG	YA	3098	1/1	0.95	0.28	29,29,29,29	0
55	MG	YA	3066	1/1	0.95	0.32	34,34,34,34	0
55	MG	YA	3237	1/1	0.96	0.19	34,34,34,34	0
55	MG	YA	3043	1/1	0.96	0.27	32,32,32,32	0
55	MG	RA	3207	1/1	0.96	0.17	48,48,48,48	0
55	MG	YA	3241	1/1	0.96	0.25	47,47,47,47	0
55	MG	YA	3208	1/1	0.96	0.15	36,36,36,36	0
55	MG	RA	3018	1/1	0.96	0.18	50,50,50,50	0
55	MG	RP	202	1/1	0.96	0.07	62,62,62,62	0
55	MG	RA	3131	1/1	0.96	0.25	51,51,51,51	0
55	MG	RA	3241	1/1	0.96	0.38	48,48,48,48	0
55	MG	RA	3062	1/1	0.96	0.30	41,41,41,41	0
55	MG	YA	3111	1/1	0.96	0.08	38,38,38,38	0
55	MG	YA	3251	1/1	0.96	0.34	31,31,31,31	0
55	MG	YA	3252	1/1	0.96	0.31	23,23,23,23	0
55	MG	YA	3185	1/1	0.96	0.19	37,37,37,37	0
55	MG	YA	3158	1/1	0.96	0.22	43,43,43,43	0
55	MG	YA	3005	1/1	0.96	0.18	37,37,37,37	0
55	MG	YA	3259	1/1	0.96	0.33	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3260	1/1	0.96	0.07	40,40,40,40	0
55	MG	YA	3051	1/1	0.96	0.20	32,32,32,32	0
55	MG	YA	3019	1/1	0.96	0.35	25,25,25,25	0
55	MG	YA	3072	1/1	0.96	0.18	55,55,55,55	0
55	MG	YA	3264	1/1	0.96	0.30	29,29,29,29	0
55	MG	RA	3005	1/1	0.96	0.42	35,35,35,35	0
55	MG	YA	3267	1/1	0.96	0.21	37,37,37,37	0
55	MG	YA	3194	1/1	0.96	0.29	44,44,44,44	0
55	MG	YA	3096	1/1	0.96	0.23	30,30,30,30	0
55	MG	YA	3196	1/1	0.96	0.20	52,52,52,52	0
55	MG	RA	3013	1/1	0.96	0.16	47,47,47,47	0
55	MG	YA	3167	1/1	0.96	0.14	52,52,52,52	0
55	MG	YA	3168	1/1	0.96	0.25	38,38,38,38	0
55	MG	YE	301	1/1	0.96	0.24	32,32,32,32	0
55	MG	RA	3135	1/1	0.96	0.14	45,45,45,45	0
55	MG	YA	3077	1/1	0.96	0.26	32,32,32,32	0
55	MG	XA	1646	1/1	0.96	0.26	52,52,52,52	0
55	MG	RA	3007	1/1	0.96	0.32	39,39,39,39	0
55	MG	RA	3098	1/1	0.96	0.41	43,43,43,43	0
56	ZN	XN	101	1/1	0.96	0.05	152,152,152,152	0
55	MG	RA	3064	1/1	0.97	0.50	32,32,32,32	0
55	MG	RA	3198	1/1	0.97	0.15	49,49,49,49	0
55	MG	YA	3246	1/1	0.97	0.37	32,32,32,32	0
55	MG	YA	3214	1/1	0.97	0.08	42,42,42,42	0
55	MG	YA	3042	1/1	0.97	0.16	35,35,35,35	0
55	MG	RA	3065	1/1	0.97	0.53	47,47,47,47	0
55	MG	RA	3118	1/1	0.97	0.16	55,55,55,55	0
55	MG	YA	3218	1/1	0.97	0.17	38,38,38,38	0
55	MG	YA	3253	1/1	0.97	0.17	35,35,35,35	0
55	MG	YA	3190	1/1	0.97	0.22	43,43,43,43	0
55	MG	RA	3155	1/1	0.97	0.07	60,60,60,60	0
55	MG	YA	3257	1/1	0.97	0.40	28,28,28,28	0
55	MG	YA	3116	1/1	0.97	0.28	44,44,44,44	0
55	MG	RA	3037	1/1	0.97	0.22	41,41,41,41	0
55	MG	YA	3080	1/1	0.97	0.37	28,28,28,28	0
55	MG	YA	3119	1/1	0.97	0.27	45,45,45,45	0
55	MG	YA	3081	1/1	0.97	0.25	26,26,26,26	0
55	MG	RA	3188	1/1	0.97	0.15	50,50,50,50	0
55	MG	YA	3170	1/1	0.97	0.26	34,34,34,34	0
55	MG	YA	3034	1/1	0.97	0.36	31,31,31,31	0
55	MG	RA	3034	1/1	0.97	0.42	38,38,38,38	0
55	MG	YA	3173	1/1	0.97	0.24	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3232	1/1	0.97	0.11	45,45,45,45	0
55	MG	RA	3243	1/1	0.97	0.28	51,51,51,51	0
55	MG	YA	3104	1/1	0.97	0.27	30,30,30,30	0
55	MG	YA	3149	1/1	0.97	0.19	40,40,40,40	0
55	MG	YA	3205	1/1	0.97	0.28	40,40,40,40	0
55	MG	YA	3086	1/1	0.97	0.34	30,30,30,30	0
55	MG	YA	3238	1/1	0.97	0.10	36,36,36,36	0
55	MG	YA	3127	1/1	0.97	0.25	32,32,32,32	0
55	MG	RA	3232	1/1	0.97	0.34	37,37,37,37	0
55	MG	YA	3025	1/1	0.97	0.42	24,24,24,24	0
56	ZN	QD	301	1/1	0.97	0.09	116,116,116,116	0
55	MG	RA	3213	1/1	0.97	0.06	61,61,61,61	0
55	MG	YA	3054	1/1	0.97	0.21	41,41,41,41	0
55	MG	YA	3141	1/1	0.98	0.27	31,31,31,31	0
55	MG	RA	3215	1/1	0.98	0.20	52,52,52,52	0
55	MG	YA	3151	1/1	0.98	0.30	29,29,29,29	0
55	MG	YA	3255	1/1	0.98	0.30	30,30,30,30	0
55	MG	YA	3181	1/1	0.98	0.26	32,32,32,32	0
55	MG	RA	3240	1/1	0.98	0.21	51,51,51,51	0
55	MG	YA	3162	1/1	0.98	0.12	39,39,39,39	0
55	MG	RA	3179	1/1	0.98	0.06	45,45,45,45	0
55	MG	RA	3059	1/1	0.98	0.12	43,43,43,43	0
55	MG	YA	3057	1/1	0.98	0.31	38,38,38,38	0
55	MG	YA	3187	1/1	0.98	0.17	41,41,41,41	0
55	MG	YA	3249	1/1	0.98	0.25	26,26,26,26	0
55	MG	YA	3076	1/1	0.98	0.29	21,21,21,21	0
55	MG	YA	3265	1/1	0.98	0.21	35,35,35,35	0
55	MG	YA	3058	1/1	0.98	0.36	29,29,29,29	0
55	MG	RA	3143	1/1	0.99	0.12	51,51,51,51	0
56	ZN	XD	301	1/1	0.99	0.17	99,99,99,99	0
55	MG	YA	3227	1/1	0.99	0.09	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.