wwPDB X-ray Structure Validation Summary Report (i)

Mar 29, 2026 – 09:12 AM UTC

PDB ID	:	1VVJ / pdb_00001vvj
Title	:	Crystal Structure of Frameshift Suppressor tRNA SufA6 bound to Codon CCC-G on the Ribosome
Authors	:	Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on	:	2013-05-24
Resolution	:	3.44 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 (i) 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 (i)) were used in the production of this report:

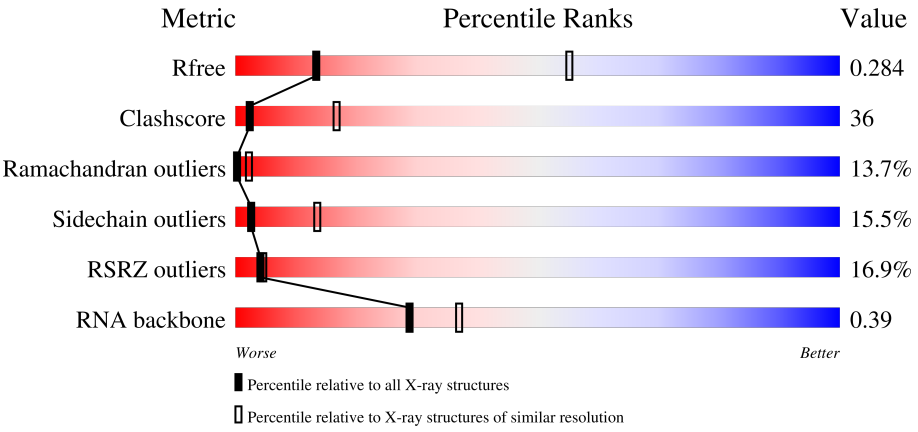
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)
RNA backbone	3983	1170 (3.88-3.00)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	QA	1522	6% 36% 48% 15% ·
1	XA	1522	4% 38% 46% 14% ·
2	QB	256	30% 16% 58% 17% · 7%
2	XB	256	20% 15% 60% 16% · 7%

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Mol	Chain	Length	Quality of chain
3	QC	239	16% 21% 54% 9% 14%
3	XC	239	14% 22% 53% 10% 14%
4	QD	209	27% 23% 56% 17%
4	XD	209	27% 23% 56% 17%
5	QE	162	30% 24% 50% 19% 7%
5	XE	162	11% 24% 49% 20% 7%
6	QF	101	13% 24% 58% 18%
6	XF	101	9% 21% 60% 19%
7	QG	156	17% 27% 60% 13%
7	XG	156	14% 26% 61% 12%
8	QH	138	25% 24% 59% 14%
8	XH	138	19% 21% 62% 14%
9	QI	128	27% 16% 62% 20%
9	XI	128	19% 18% 60% 20%
10	QJ	105	61% 17% 63% 13% 6%
10	XJ	105	36% 18% 62% 13% 6%
11	QK	129	32% 26% 53% 11% 8%
11	XK	129	24% 25% 54% 11% 8%
12	QL	132	27% 28% 44% 20% 5%
12	XL	132	23% 27% 45% 20% 5%
13	QM	126	26% 13% 57% 22%
13	XM	126	21% 13% 59% 20%
14	QN	61	49% 21% 54% 18% 5%
14	XN	61	21% 21% 49% 21% 7%
15	QO	89	25% 25% 56% 18%

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Mol	Chain	Length	Quality of chain
15	XO	89	16% 22% 58% 18%
16	QP	88	32% 10% 67% 16% 5%
16	XP	88	28% 13% 64% 17% 5%
17	QQ	105	32% 30% 50% 15% 5%
17	XQ	105	30% 28% 52% 15% 5%
18	QR	88	13% 16% 47% 16% 20%
18	XR	88	3% 16% 47% 16% 20%
19	QS	93	37% 22% 41% 24% 10%
19	XS	93	33% 23% 39% 25% 10%
20	QT	106	33% 20% 52% 22% 7%
20	XT	106	22% 17% 54% 23% 7%
21	QU	27	59% 19% 56% 19% 7%
21	XU	27	56% 11% 63% 19% 7%
22	QV	77	13% 27% 55% 18%
22	XV	77	12% 29% 52% 19%
23	QX	25	20% 24% 68%
23	XX	25	4% 20% 8% 68%
24	QY	18	17% 17% 39% 22% 22%
24	XY	18	22% 22% 33% 22% 22%
25	RA	2916	4% 40% 44% 15%
25	YA	2916	4% 39% 44% 15%
26	RB	122	3% 45% 37% 16%
26	YB	122	% 37% 44% 17%
27	RD	276	21% 26% 49% 19%
27	YD	276	16% 28% 46% 20%

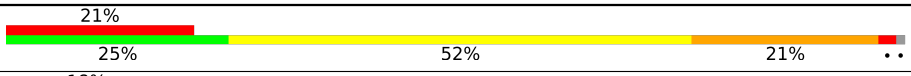
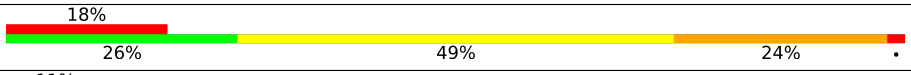
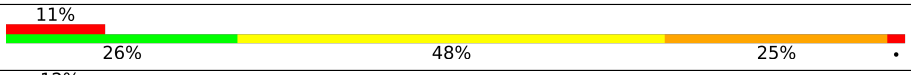
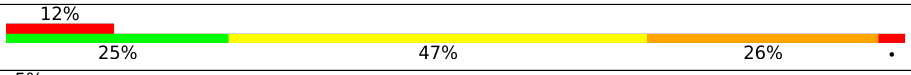
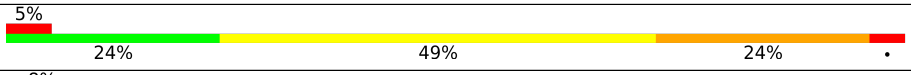
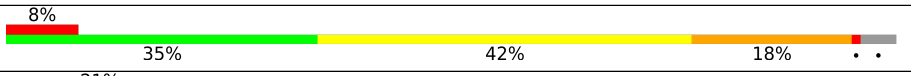
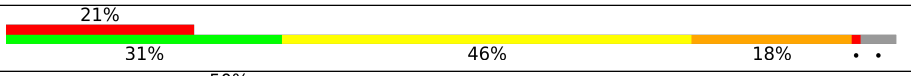
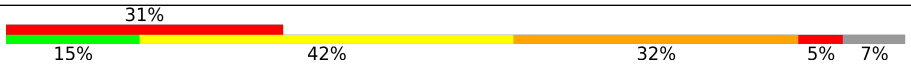
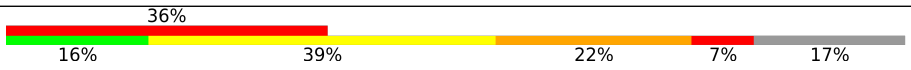
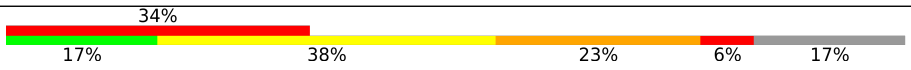
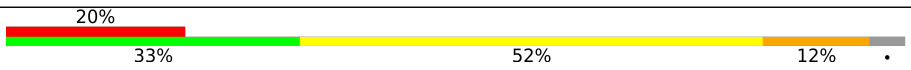
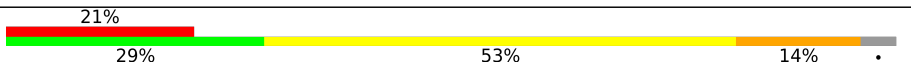
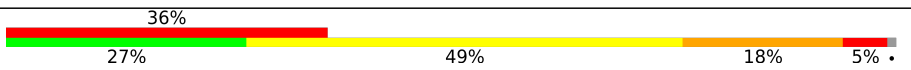
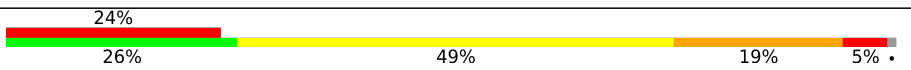
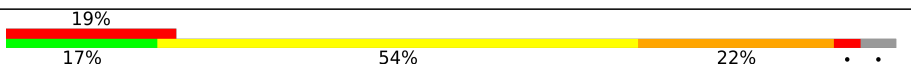
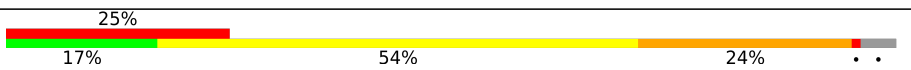
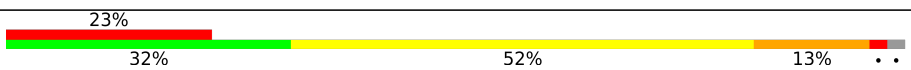
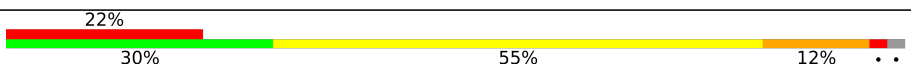
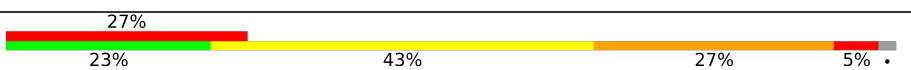
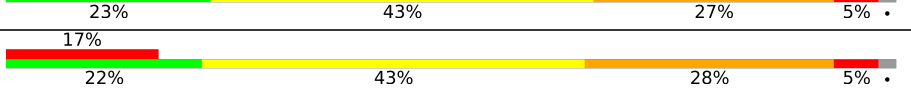
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Mol	Chain	Length	Quality of chain
28	RE	206	22% 20% 44% 28% 8%
28	YE	206	23% 21% 44% 27% 8%
29	RF	210	29% 30% 48% 15%
29	YF	210	22% 29% 50% 15%
30	RG	182	69% 22% 57% 19%
30	YG	182	54% 23% 56% 18%
31	RH	180	30% 21% 42% 23% 9% 6%
31	YH	180	36% 22% 42% 22% 9% 6%
32	RI	148	28% 17% 51% 27%
32	YI	148	17% 20% 47% 28%
33	RN	140	14% 15% 51% 31%
33	YN	140	13% 16% 50% 31%
34	RO	122	20% 29% 58% 11%
34	YO	122	22% 28% 59% 11%
35	RP	150	31% 17% 44% 30% 9%
35	YP	150	27% 19% 43% 31% 8%
36	RQ	141	33% 30% 46% 18% 6%
36	YQ	141	21% 28% 48% 18% 6%
37	RR	118	19% 31% 48% 16%
37	YR	118	19% 33% 48% 14%
38	RS	112	16% 13% 57% 22% 6%
38	YS	112	14% 11% 60% 22% 6%
39	RT	146	29% 19% 49% 23% 6%
39	YT	146	23% 18% 50% 23% 6%
40	RU	118	21% 26% 50% 21%

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

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Mol	Chain	Length	Quality of chain
53	R7	49	16% 35% 51% 14%
53	Y7	49	18% 33% 53% 14%
54	R8	65	42% 17% 45% 29% 8%
54	Y8	65	34% 14% 46% 31% 8%
55	Z6	3	67% 33%
55	Z8	3	67% 33%

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
56	MG	QA	1620	-	-	-	X
56	MG	RA	3027	-	-	-	X
56	MG	YA	3012	-	-	-	X

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 291123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1501	Total	C	N	O	P	0	0	0
			32269	14363	5986	10420	1500			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total 170	C 76	N 31	O 55	P 8	0	0	0
23	XX	8	Total 170	C 76	N 31	O 55	P 8	0	0	0

- Molecule 24 is a RNA chain called messenger RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	172	Total	C	N	O	S	0	0	0
			1378	879	248	248	3			
45	YZ	172	Total	C	N	O	S	0	0	0
			1378	879	248	248	3			

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

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

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

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

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

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

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

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

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

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called tRNA acceptor end mimic.

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

- Molecule 55 is a RNA chain called RNA (5'-R(*CP*CP*(PPU))-3').

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

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

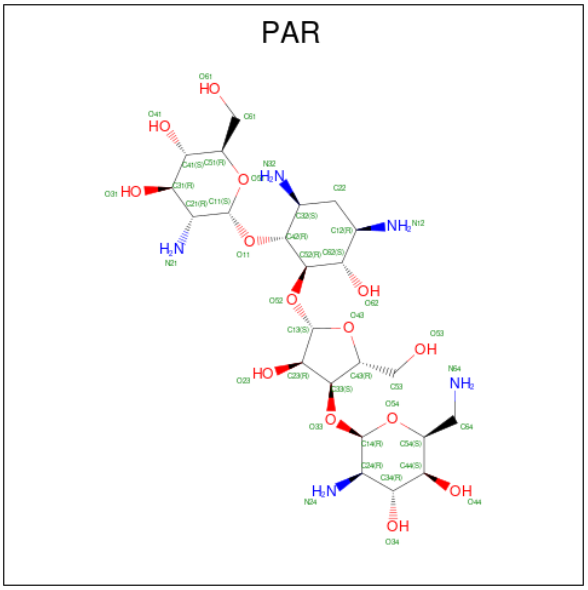
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	60	Total 60	Mg 60	0	0
56	QF	1	Total 1	Mg 1	0	0
56	QH	1	Total 1	Mg 1	0	0
56	QM	1	Total 1	Mg 1	0	0
56	QV	2	Total 2	Mg 2	0	0
56	QX	2	Total 2	Mg 2	0	0
56	RA	212	Total 212	Mg 212	0	0
56	RB	2	Total 2	Mg 2	0	0
56	RE	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RF	1	Total Mg 1 1	0	0
56	RP	1	Total Mg 1 1	0	0
56	R5	1	Total Mg 1 1	0	0
56	XA	63	Total Mg 63 63	0	0
56	XM	2	Total Mg 2 2	0	0
56	XV	2	Total Mg 2 2	0	0
56	YA	242	Total Mg 242 242	0	0
56	YB	2	Total Mg 2 2	0	0
56	YE	2	Total Mg 2 2	0	0
56	YX	1	Total Mg 1 1	0	0
56	Y5	1	Total Mg 1 1	0	0

- Molecule 57 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

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

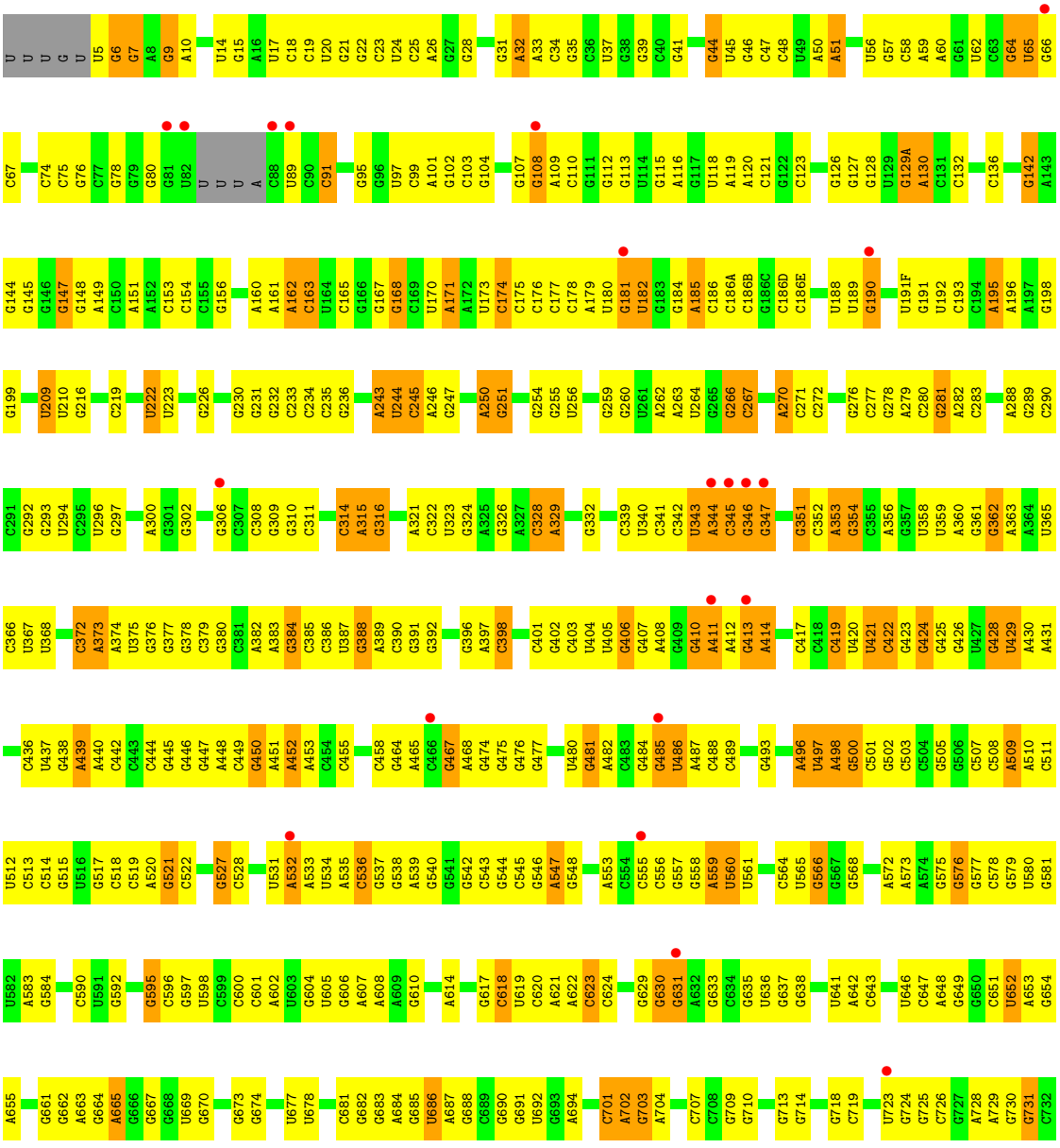
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	QD	1	Total Zn 1 1	0	0
58	QN	1	Total Zn 1 1	0	0
58	XD	1	Total Zn 1 1	0	0
58	XN	1	Total Zn 1 1	0	0

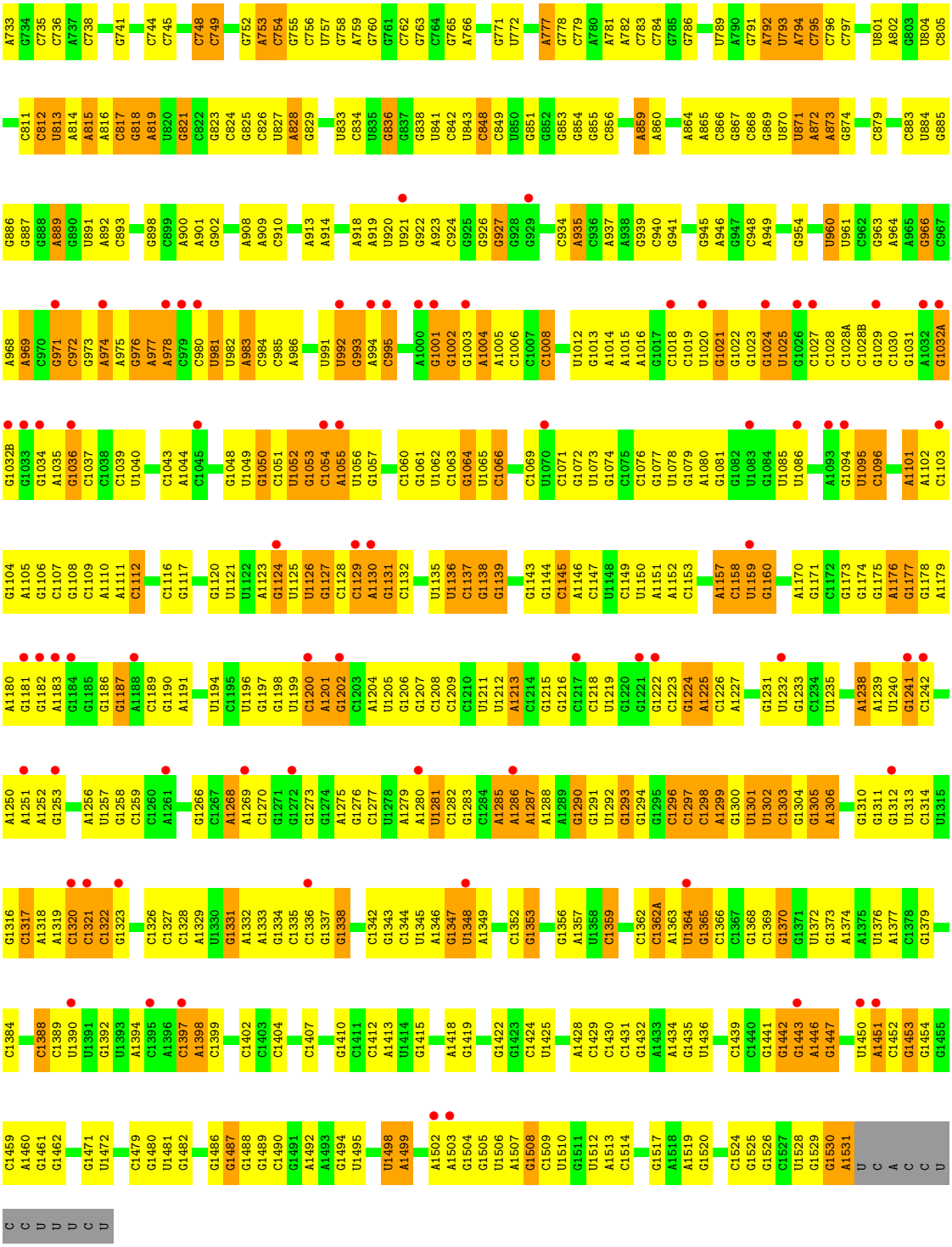
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

Chain QA: 

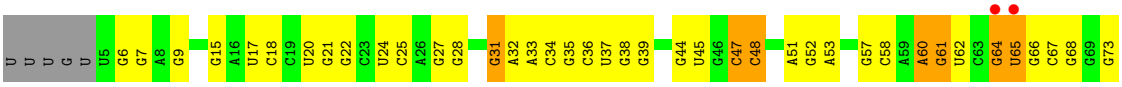


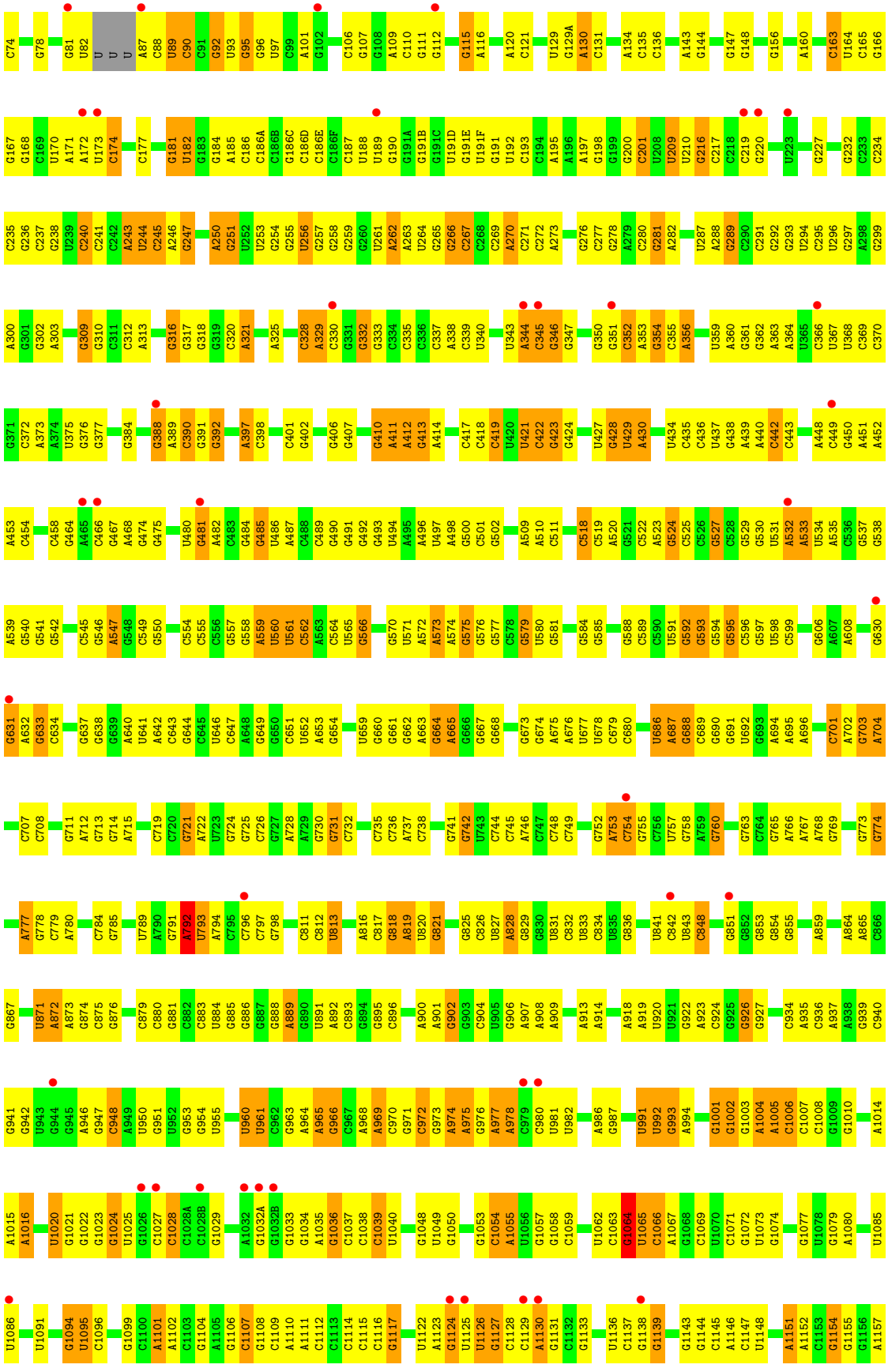


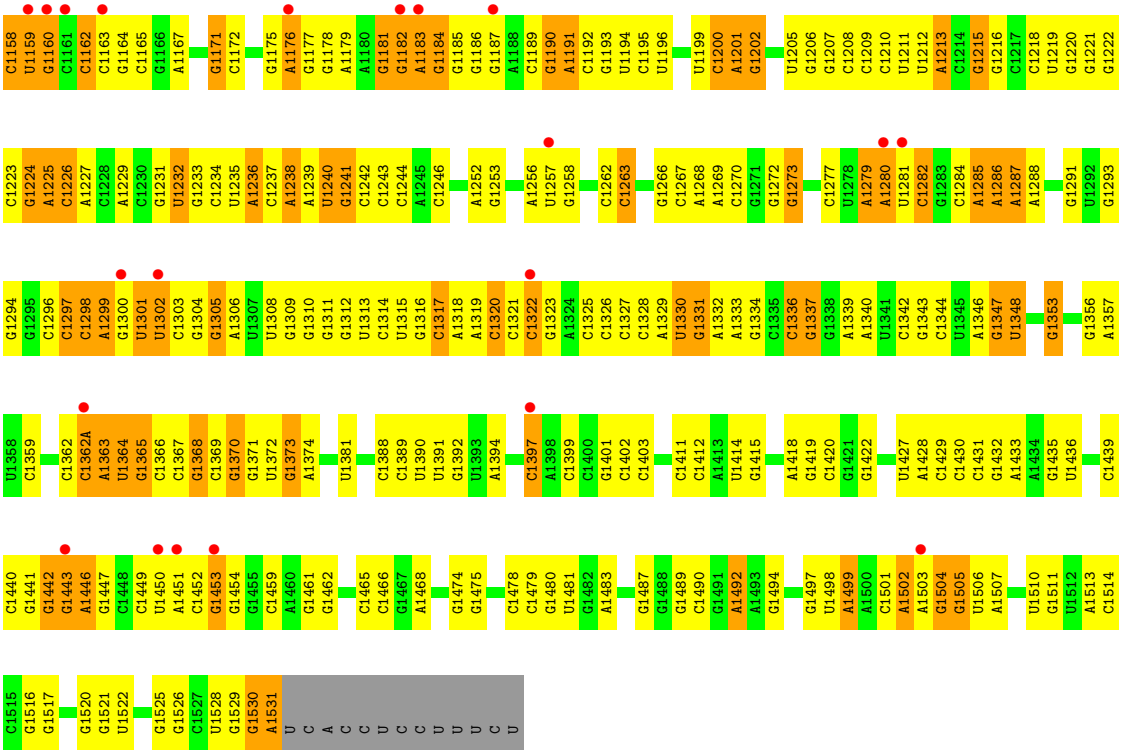
• Molecule 1: 16S rRNA

Chain XA:



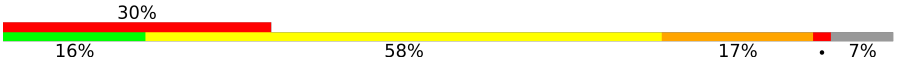


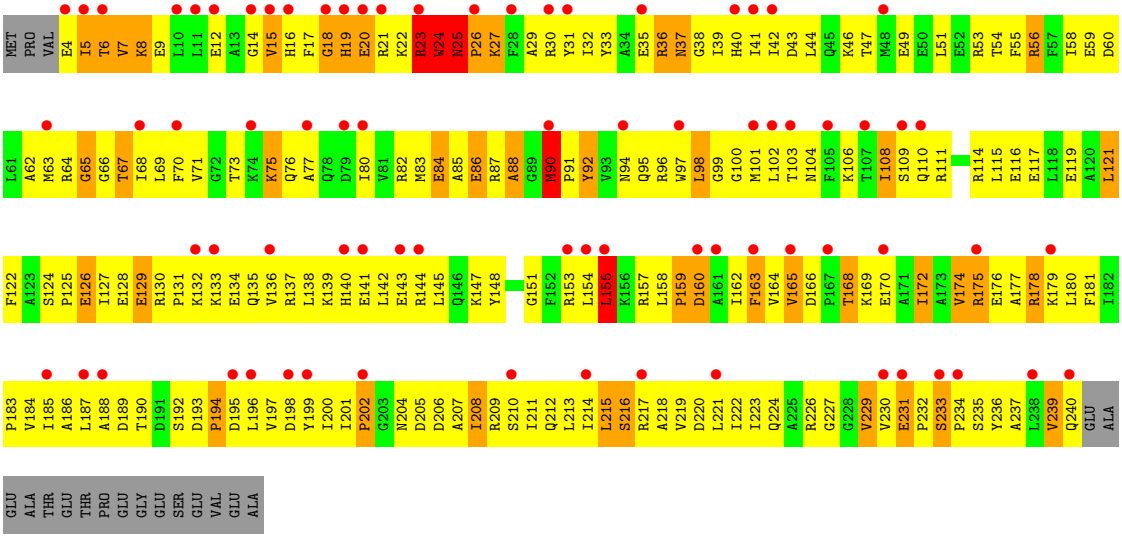




• Molecule 2: 30S ribosomal protein S2

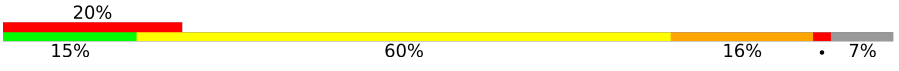
Chain QB:



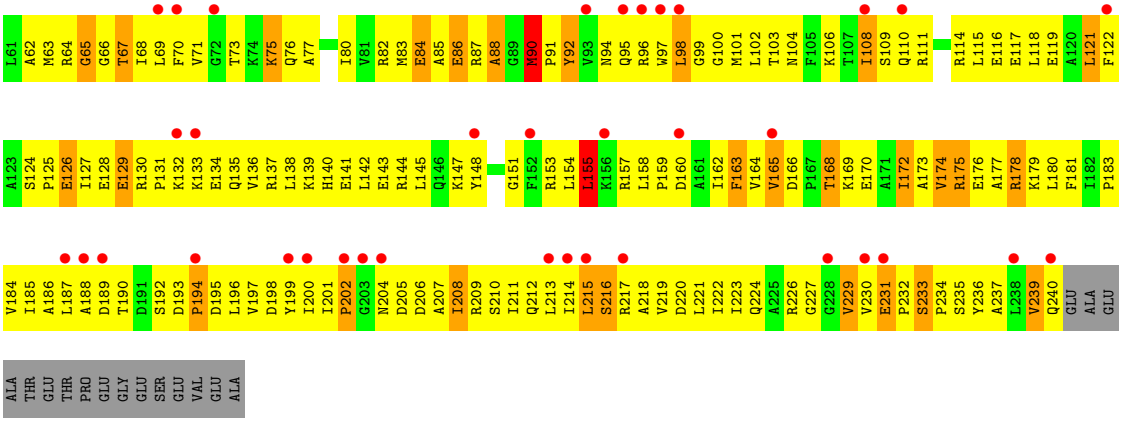


• Molecule 2: 30S ribosomal protein S2

Chain XB:

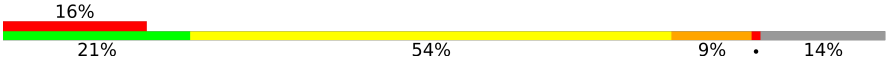


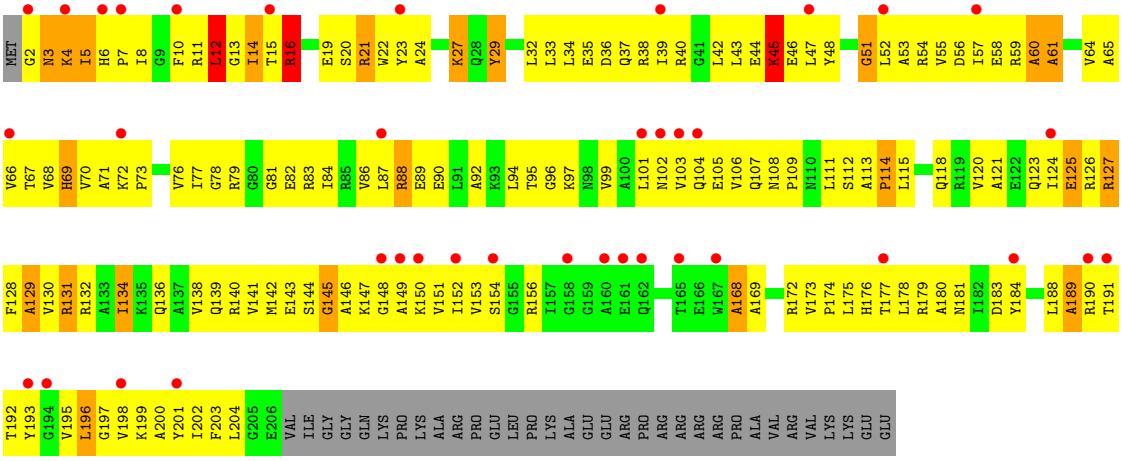




• Molecule 3: 30S ribosomal protein S3

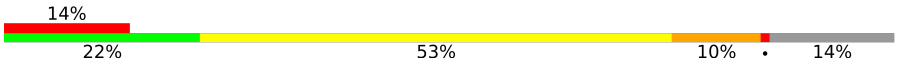
Chain QC:

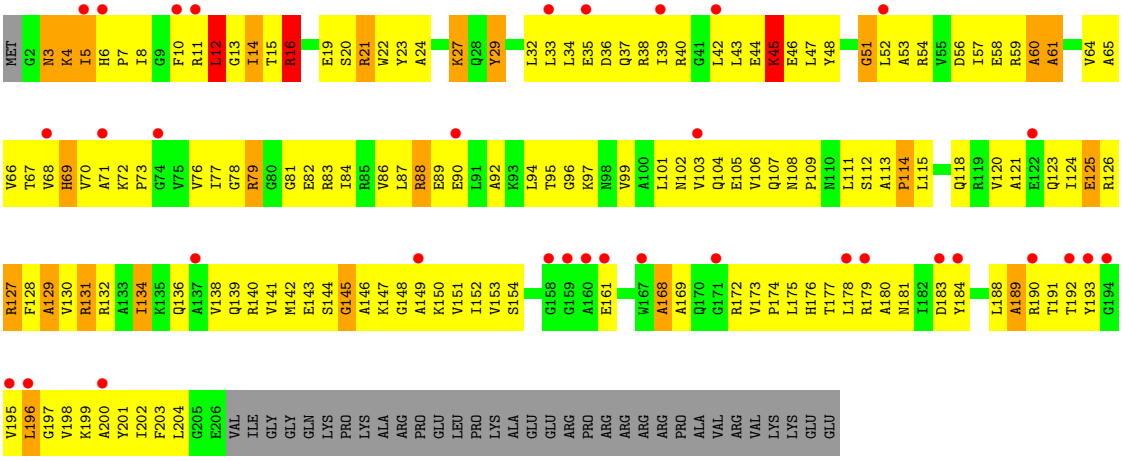




• Molecule 3: 30S ribosomal protein S3

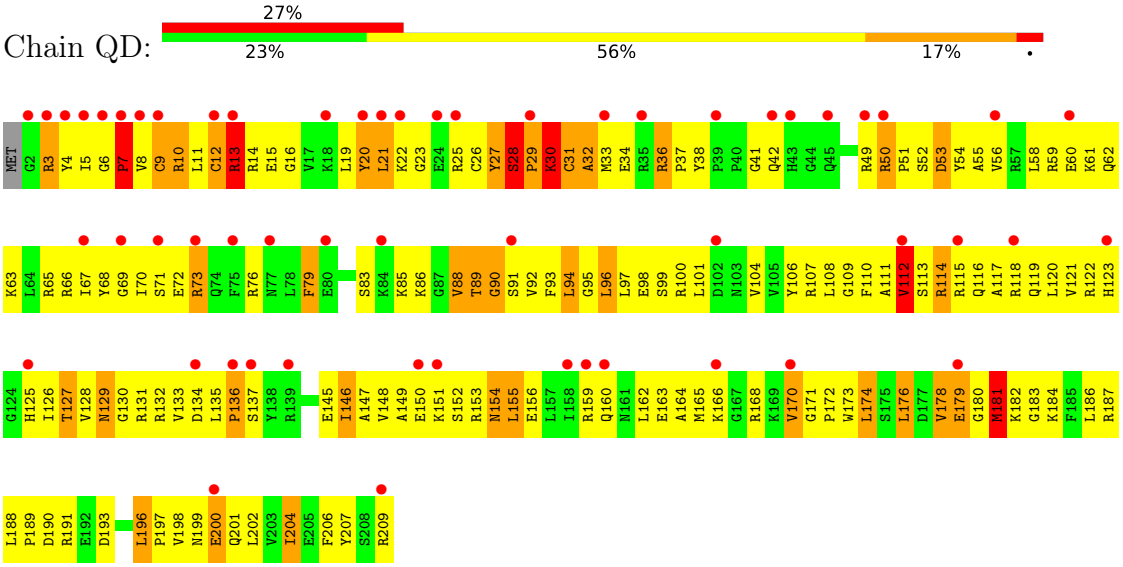
Chain XC:





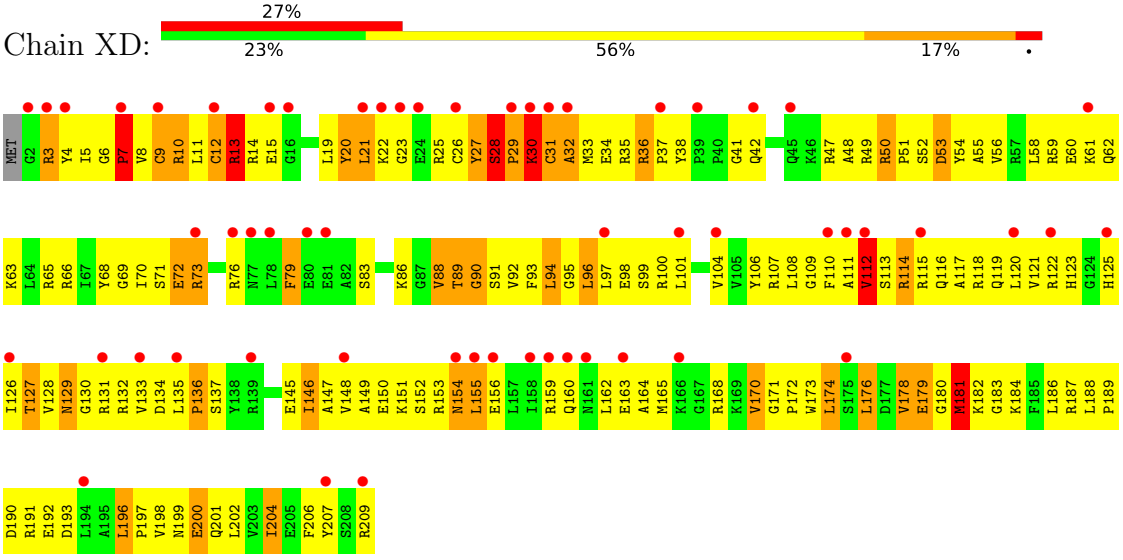
• Molecule 4: 30S ribosomal protein S4

Chain QD:



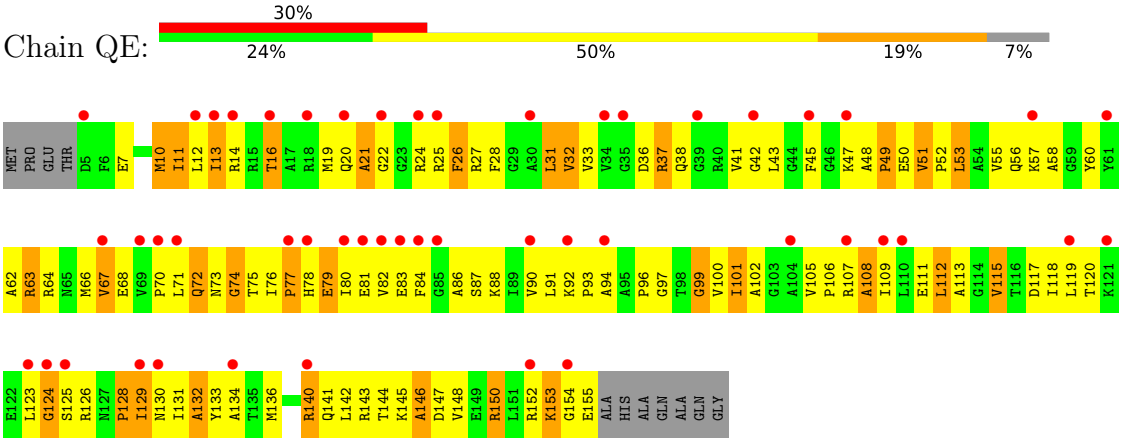
• Molecule 4: 30S ribosomal protein S4

Chain XD:



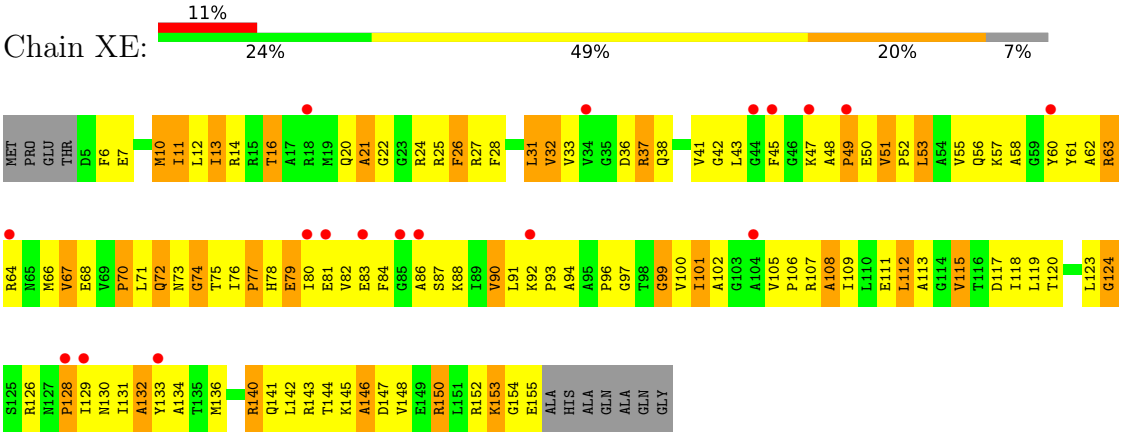
• Molecule 5: 30S ribosomal protein S5

Chain QE:



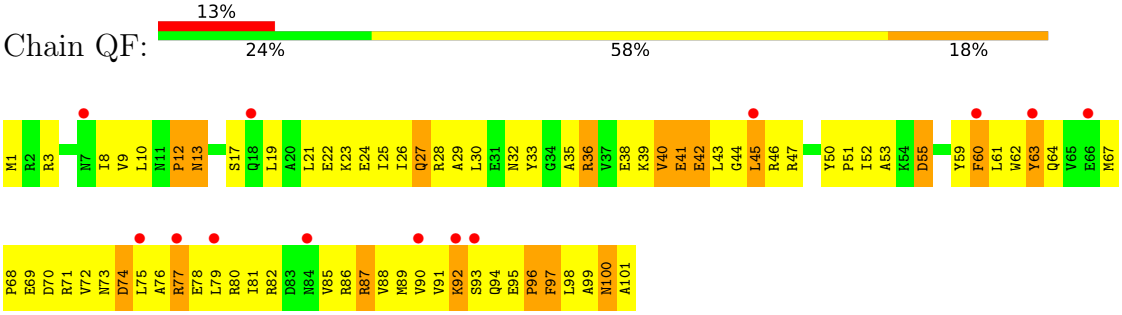
• Molecule 5: 30S ribosomal protein S5

Chain XE:



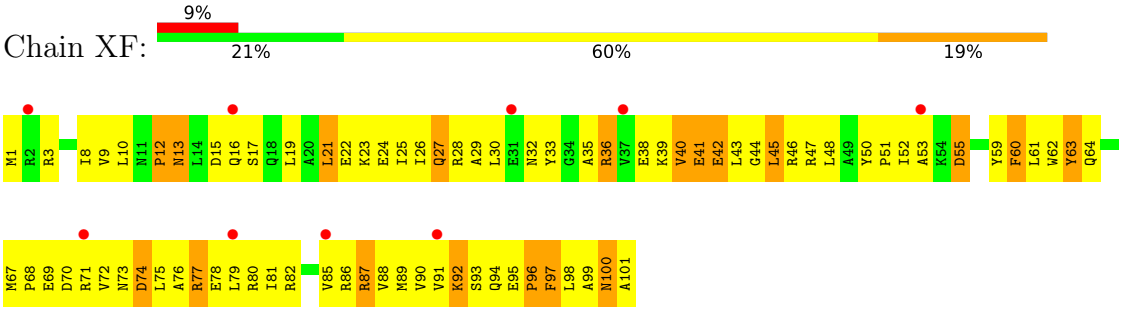
• Molecule 6: 30S ribosomal protein S6

Chain QF:



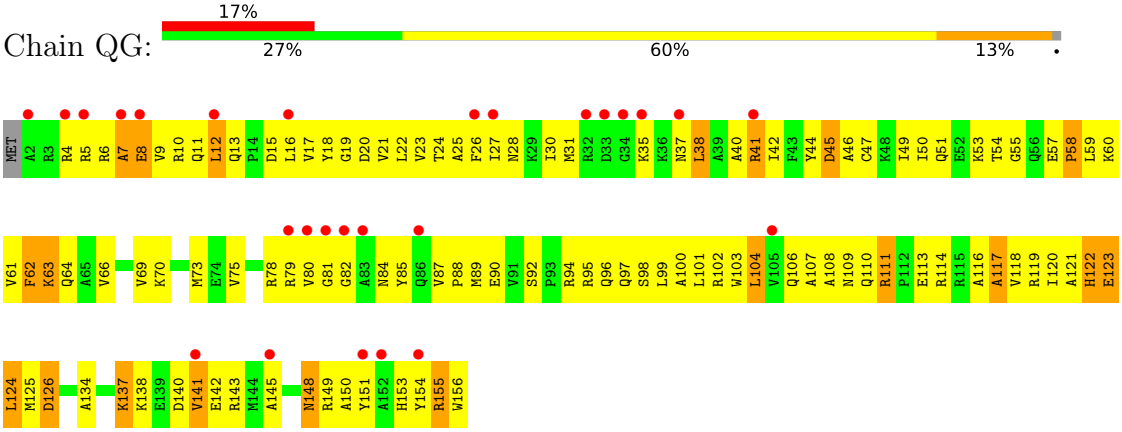
• Molecule 6: 30S ribosomal protein S6

Chain XF:



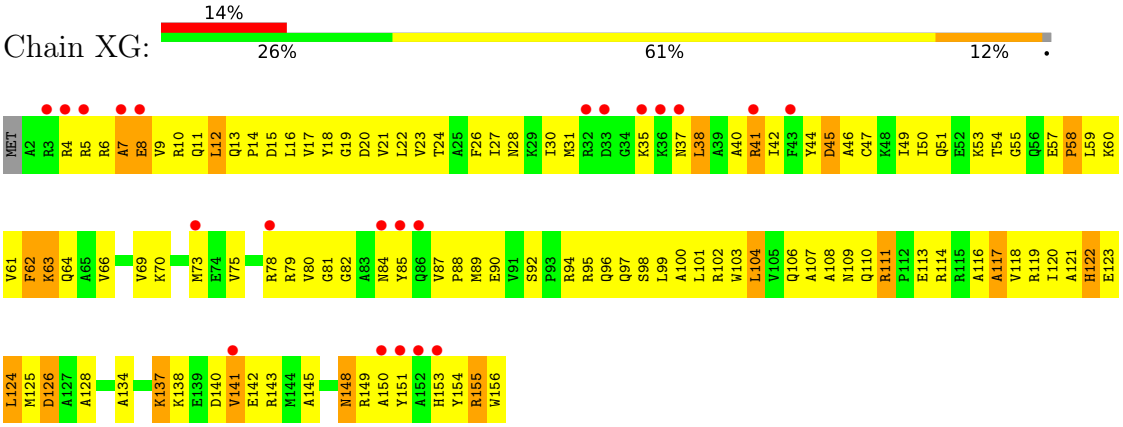
• Molecule 7: 30S ribosomal protein S7

Chain QG:



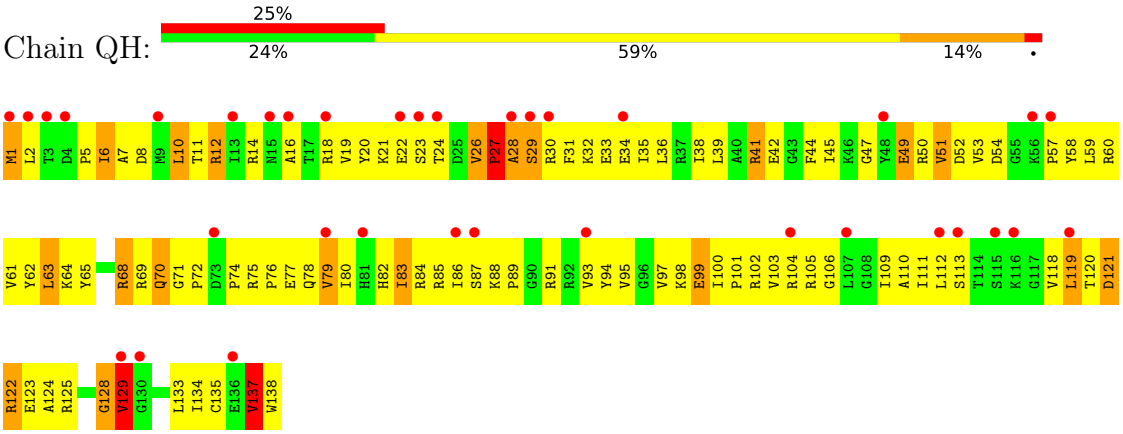
• Molecule 7: 30S ribosomal protein S7

Chain XG:



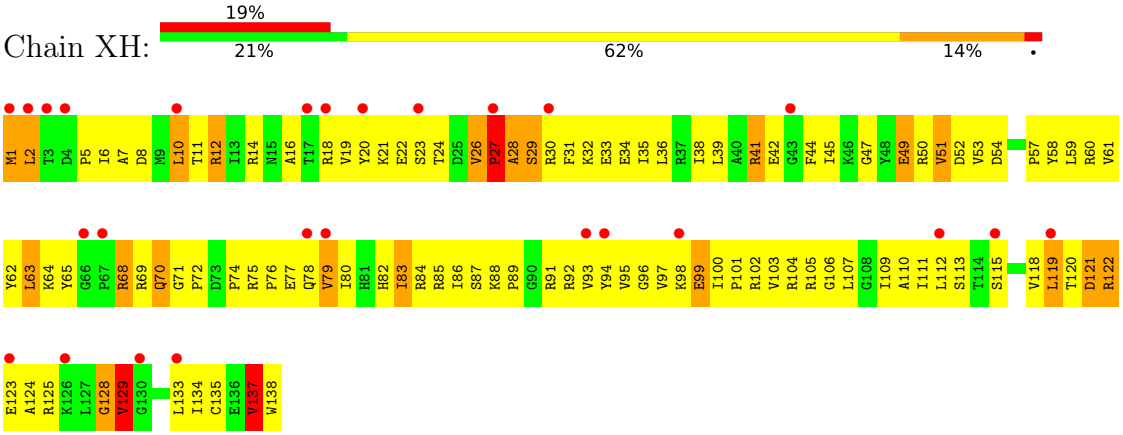
• Molecule 8: 30S ribosomal protein S8

Chain QH:



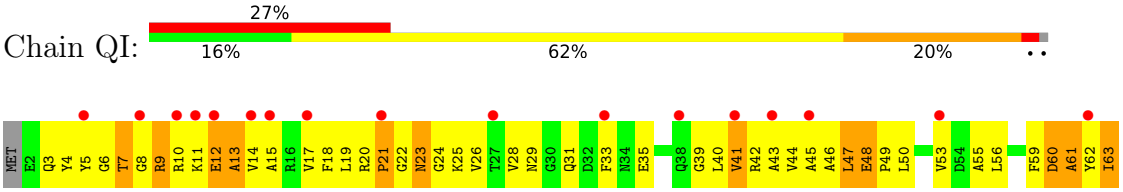
• Molecule 8: 30S ribosomal protein S8

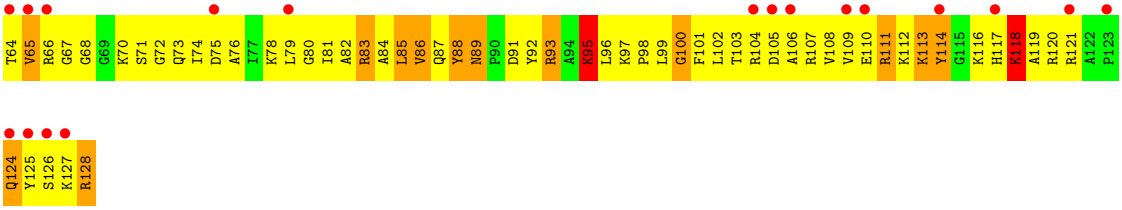
Chain XH:



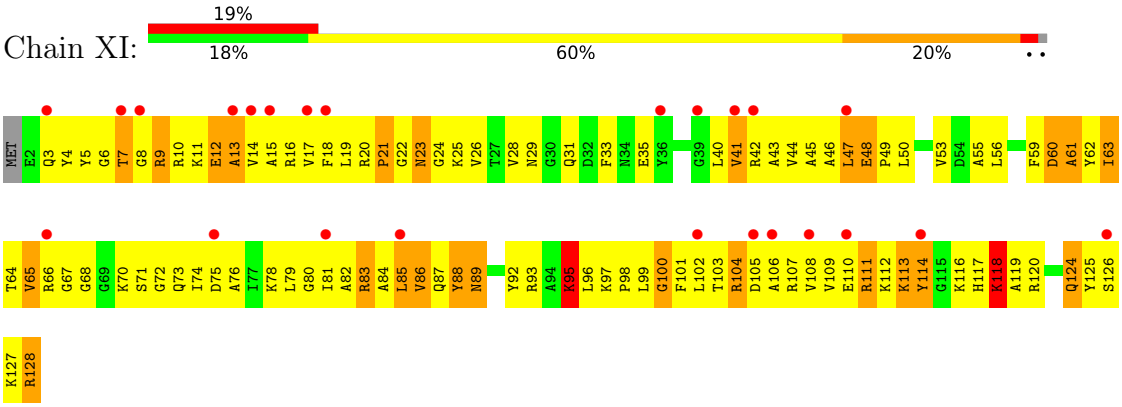
• Molecule 9: 30S ribosomal protein S9

Chain QI:

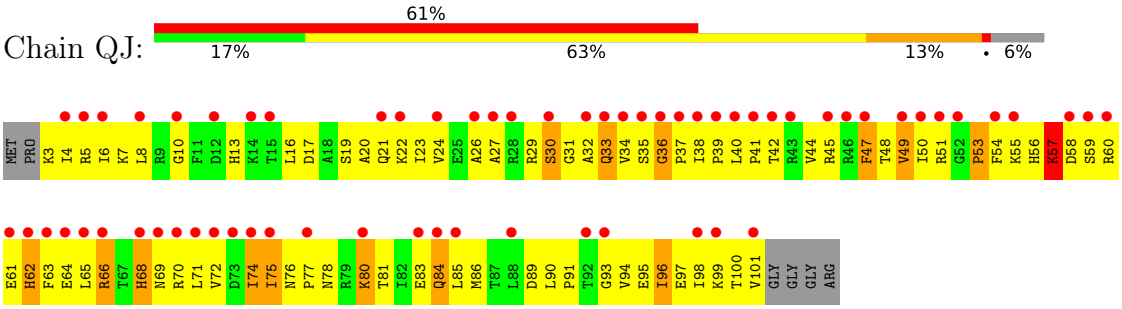




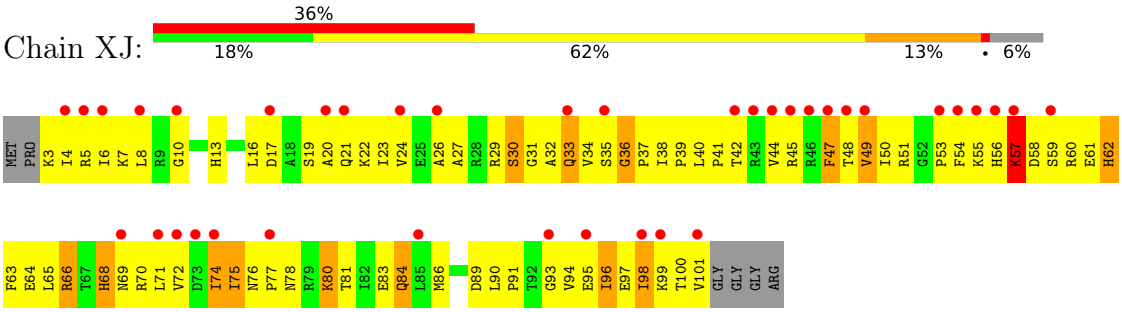
• Molecule 9: 30S ribosomal protein S9



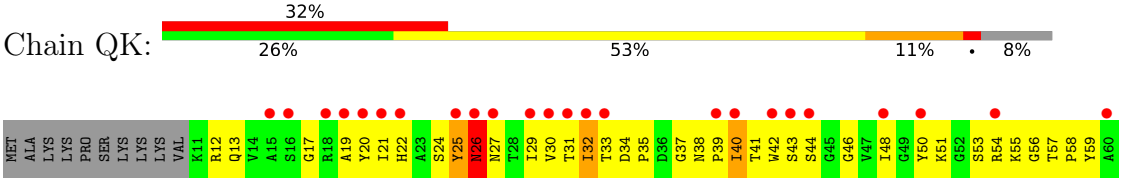
• Molecule 10: 30S ribosomal protein S10

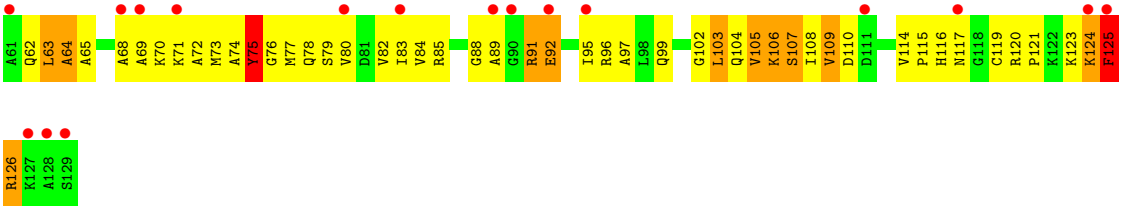


• Molecule 10: 30S ribosomal protein S10

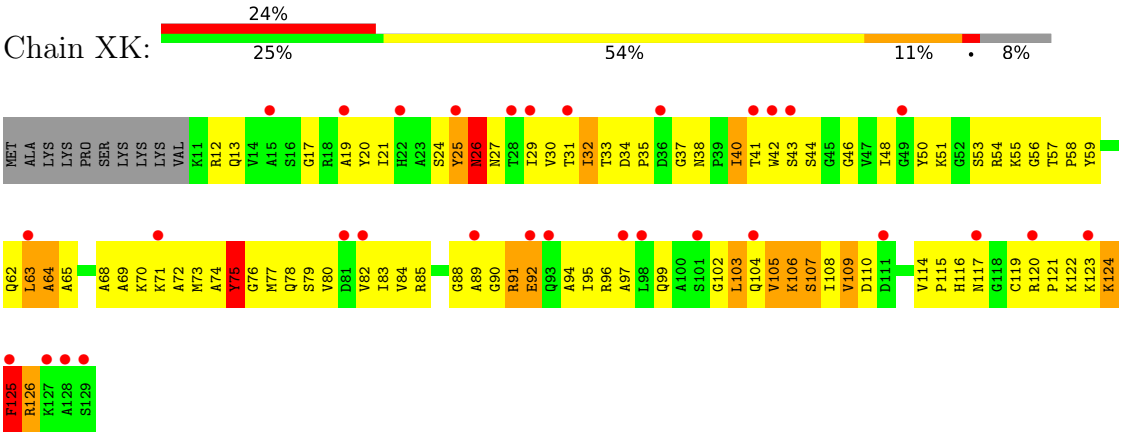


• Molecule 11: 30S ribosomal protein S11

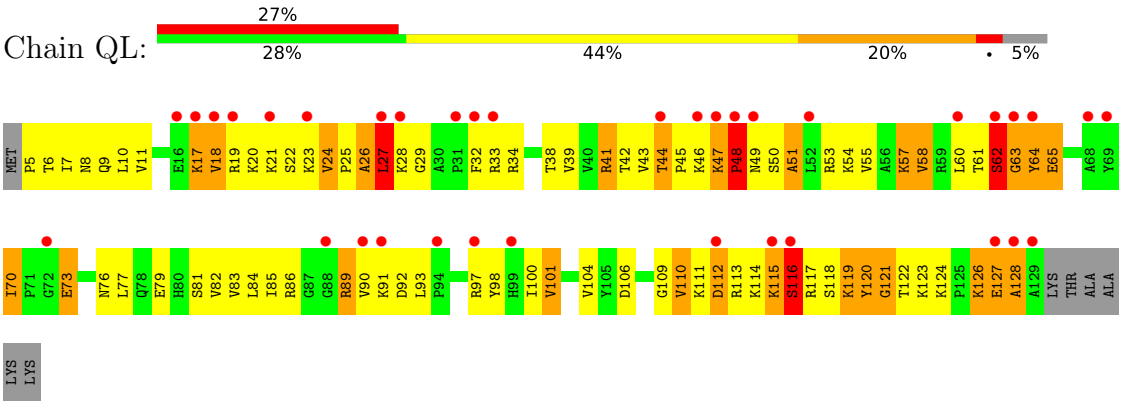




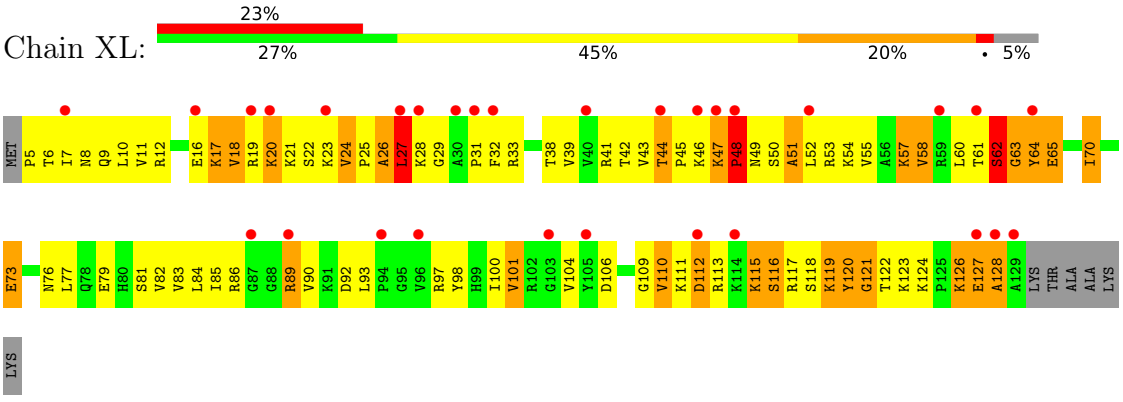
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12

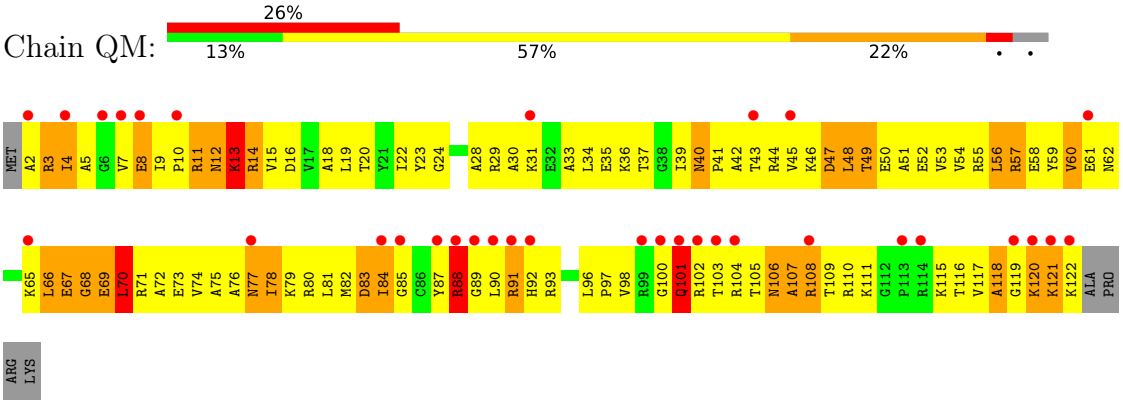


• Molecule 12: 30S ribosomal protein S12



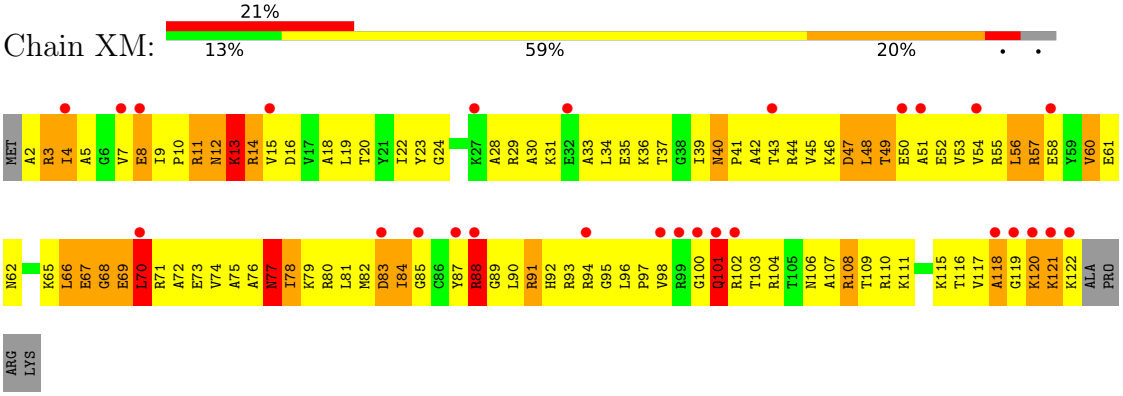
• Molecule 13: 30S ribosomal protein S13

Chain QM:



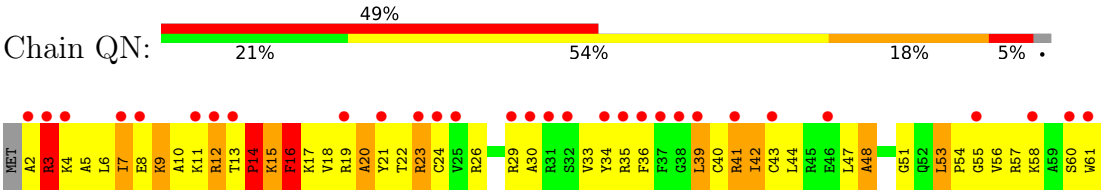
- Molecule 13: 30S ribosomal protein S13

Chain XM:



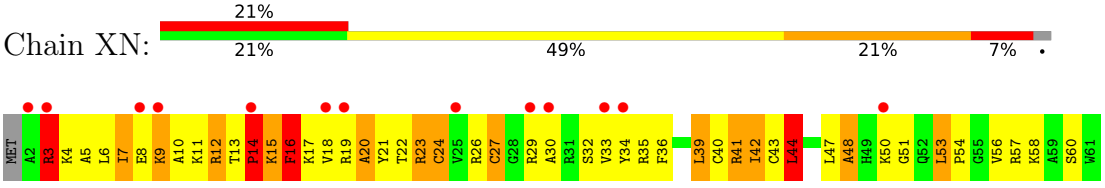
- Molecule 14: 30S ribosomal protein S14

Chain QN:



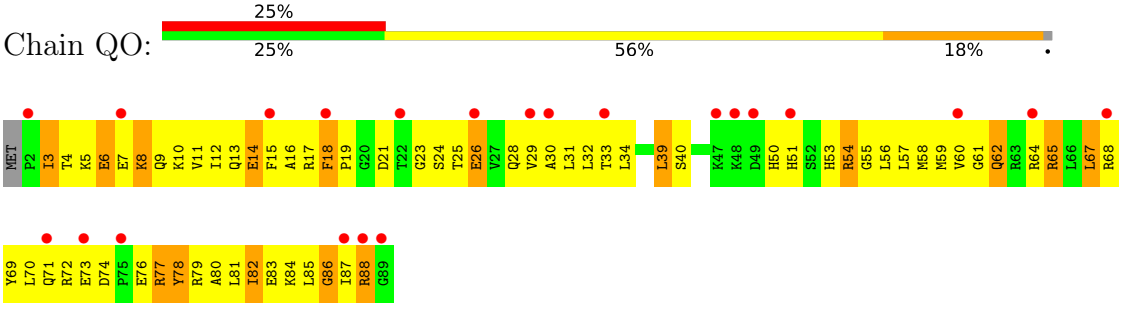
- Molecule 14: 30S ribosomal protein S14

Chain XN:



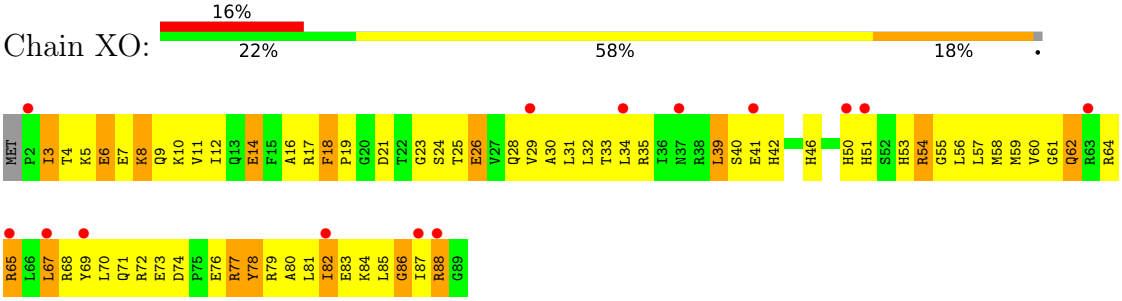
- Molecule 15: 30S ribosomal protein S15

Chain QO:



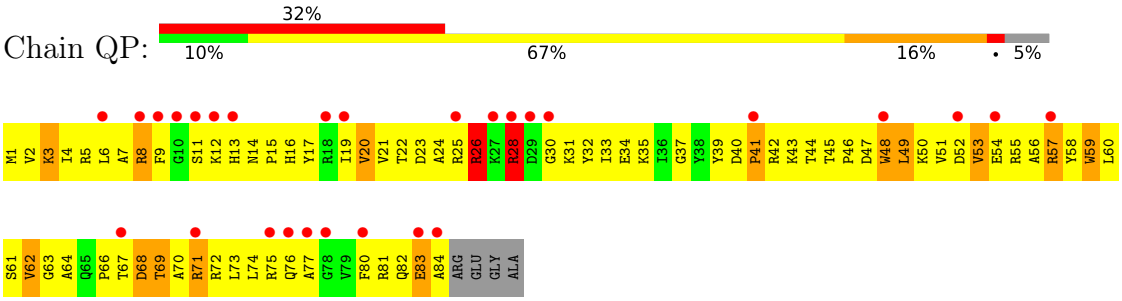
• Molecule 15: 30S ribosomal protein S15

Chain XO:



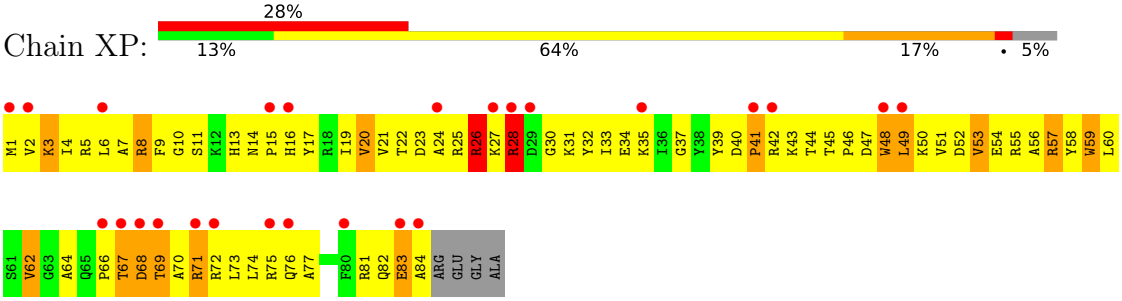
• Molecule 16: 30S ribosomal protein S16

Chain QP:



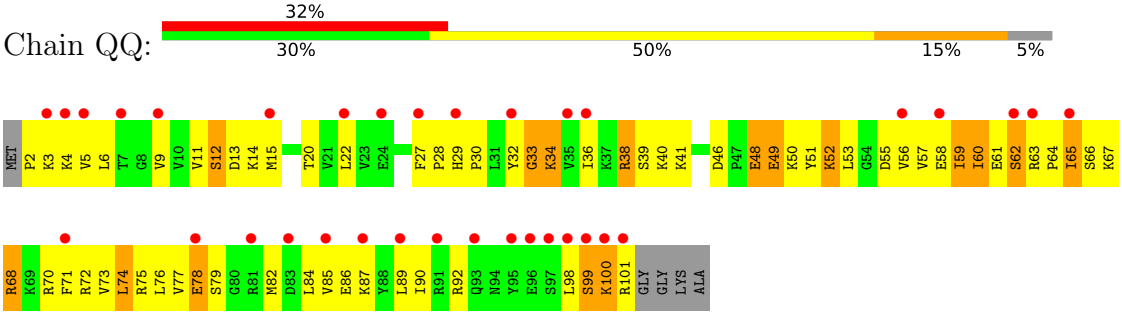
• Molecule 16: 30S ribosomal protein S16

Chain XP:



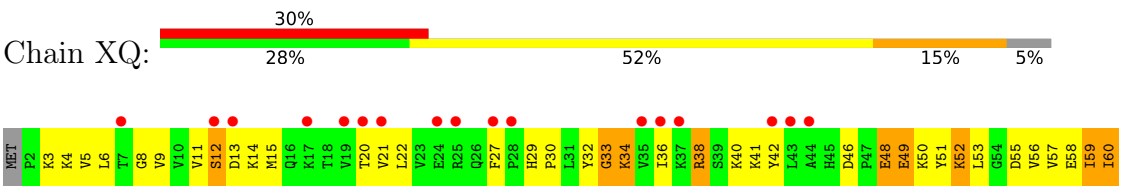
• Molecule 17: 30S ribosomal protein S17

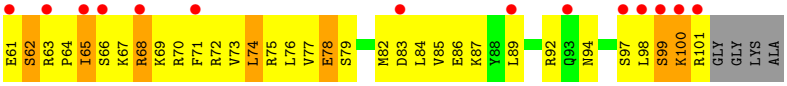
Chain QQ:



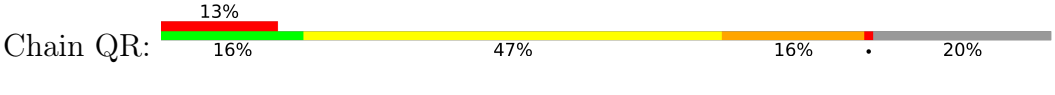
• Molecule 17: 30S ribosomal protein S17

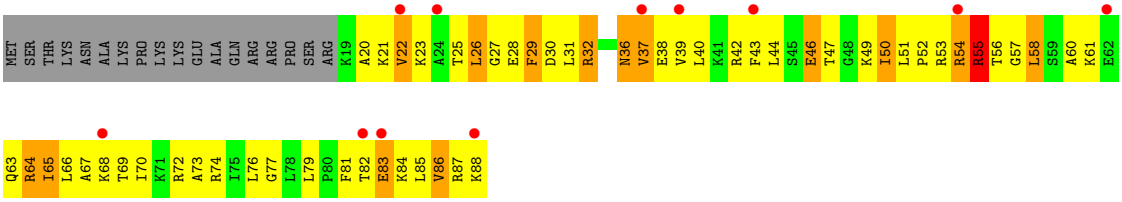
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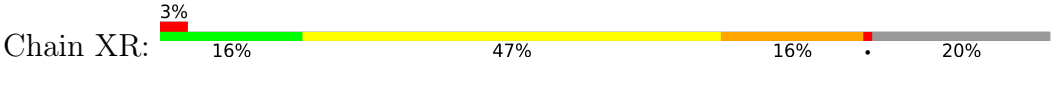


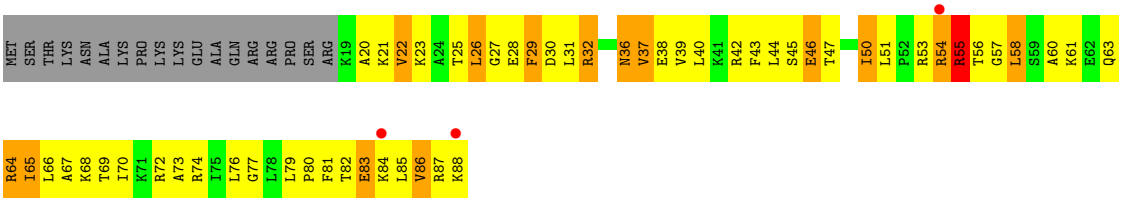
• Molecule 18: 30S ribosomal protein S18



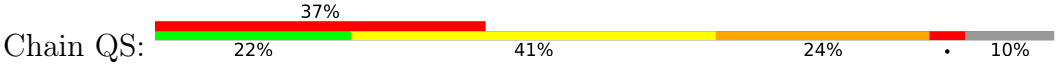


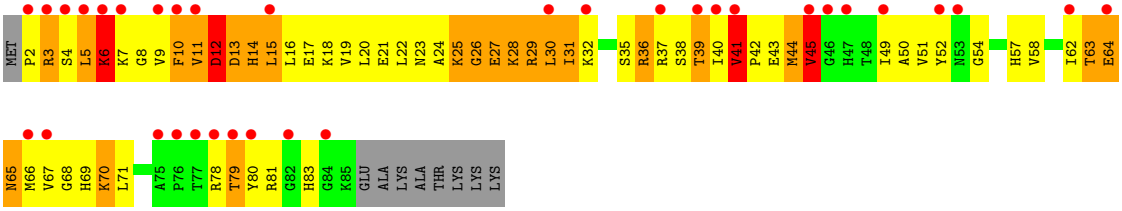
• Molecule 18: 30S ribosomal protein S18



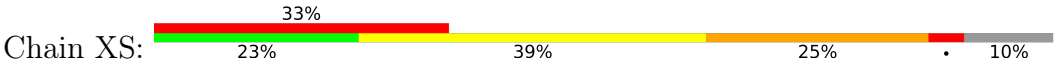


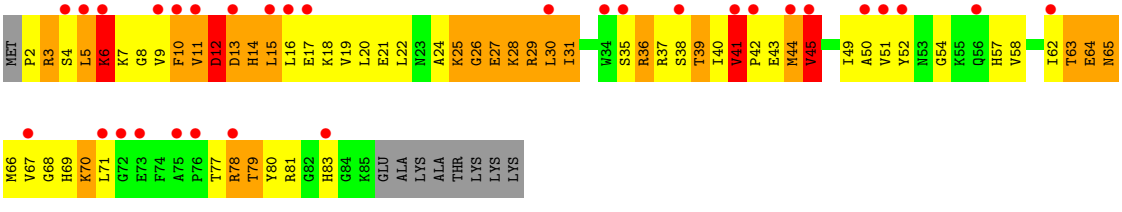
• Molecule 19: 30S ribosomal protein S19



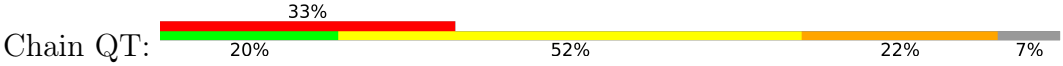


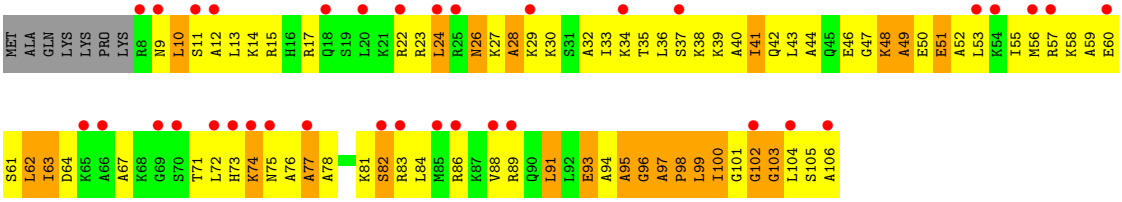
• Molecule 19: 30S ribosomal protein S19





• Molecule 20: 30S ribosomal protein S20

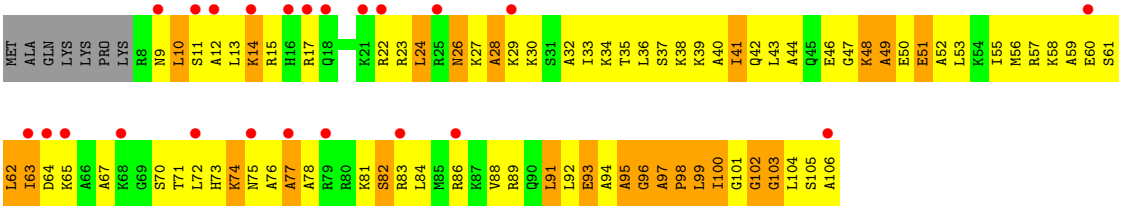




• Molecule 20: 30S ribosomal protein S20

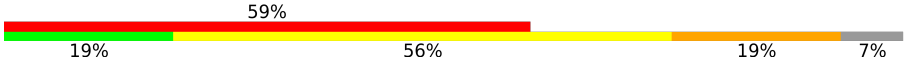
Chain XT:

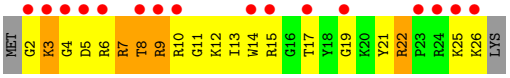




• Molecule 21: 30S ribosomal protein S21

Chain QU:





• Molecule 21: 30S ribosomal protein S21

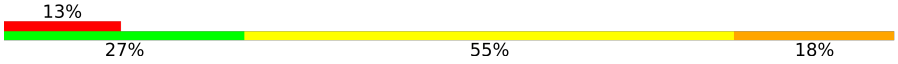
Chain XU:

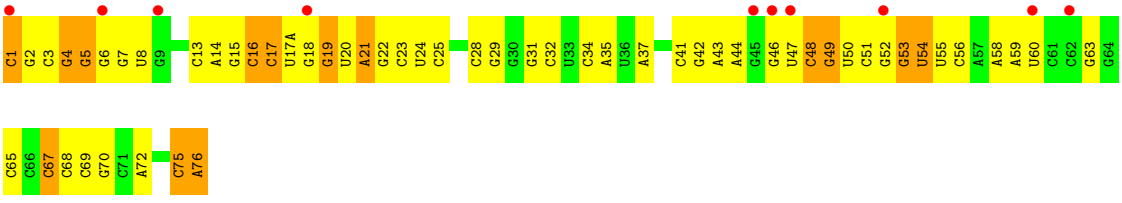




• Molecule 22: P-site tRNA fMet

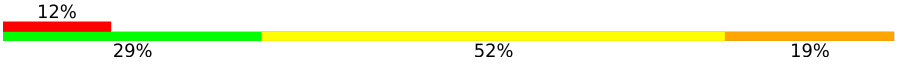
Chain QV:

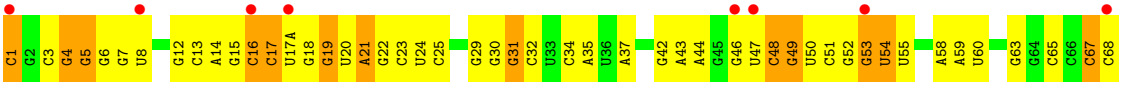


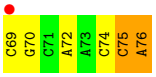


• Molecule 22: P-site tRNA fMet

Chain XV:







• Molecule 23: A-site ASL SufA6

Chain QX:





• Molecule 23: A-site ASL SufA6

Chain XX:

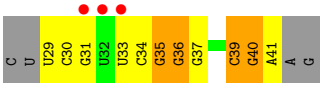




• Molecule 24: messenger RNA

Chain QY:

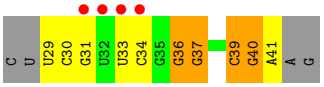




• Molecule 24: messenger RNA

Chain XY:

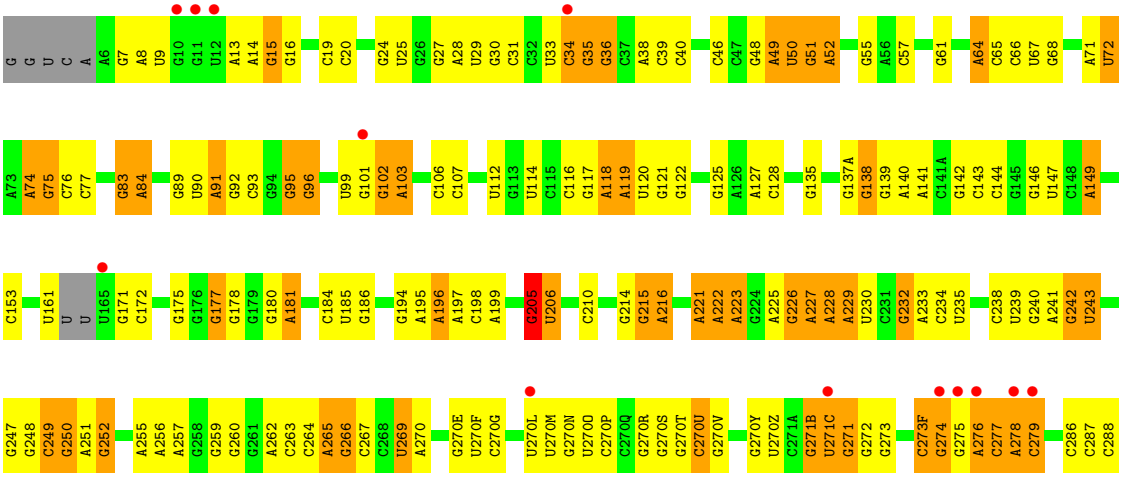


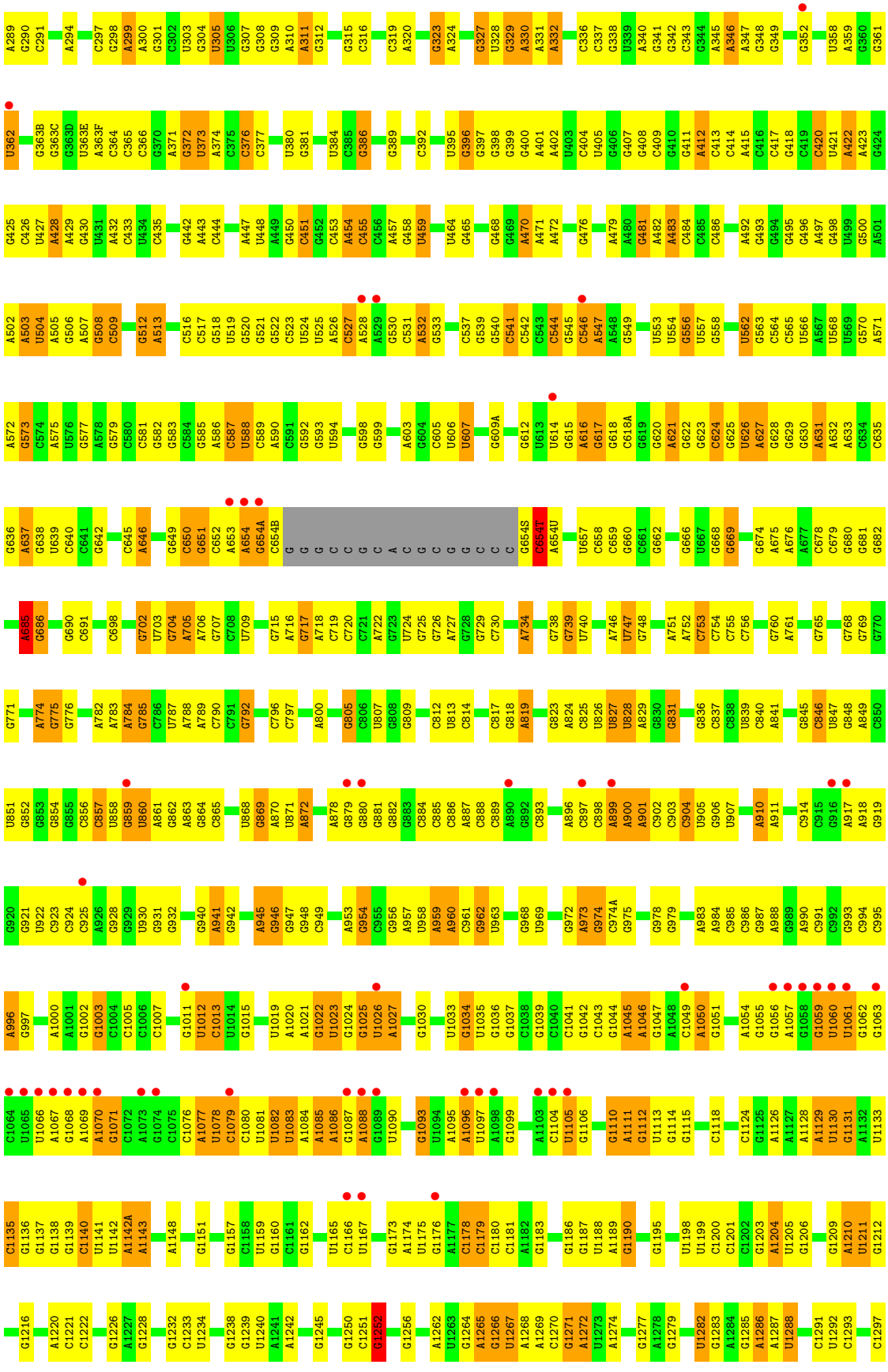


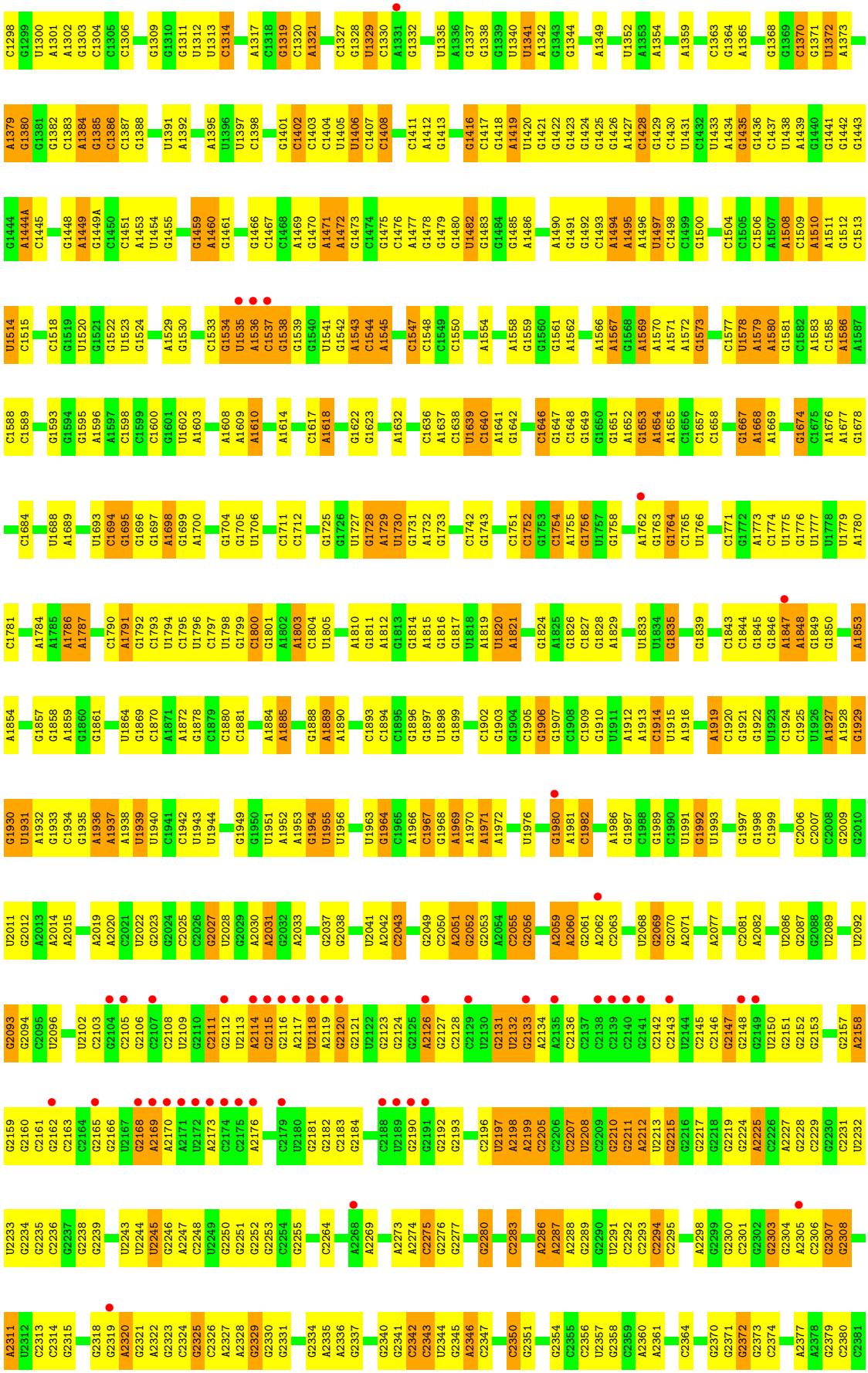
• Molecule 25: 23S rRNA

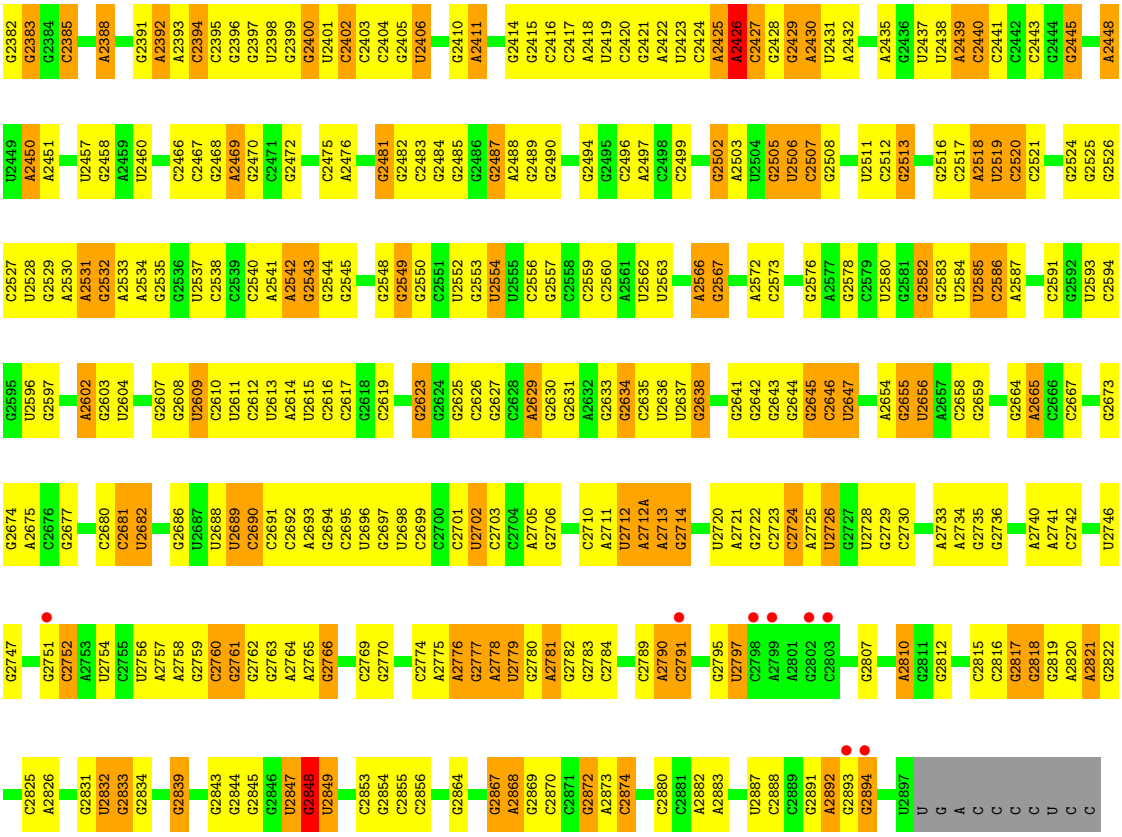
Chain RA:







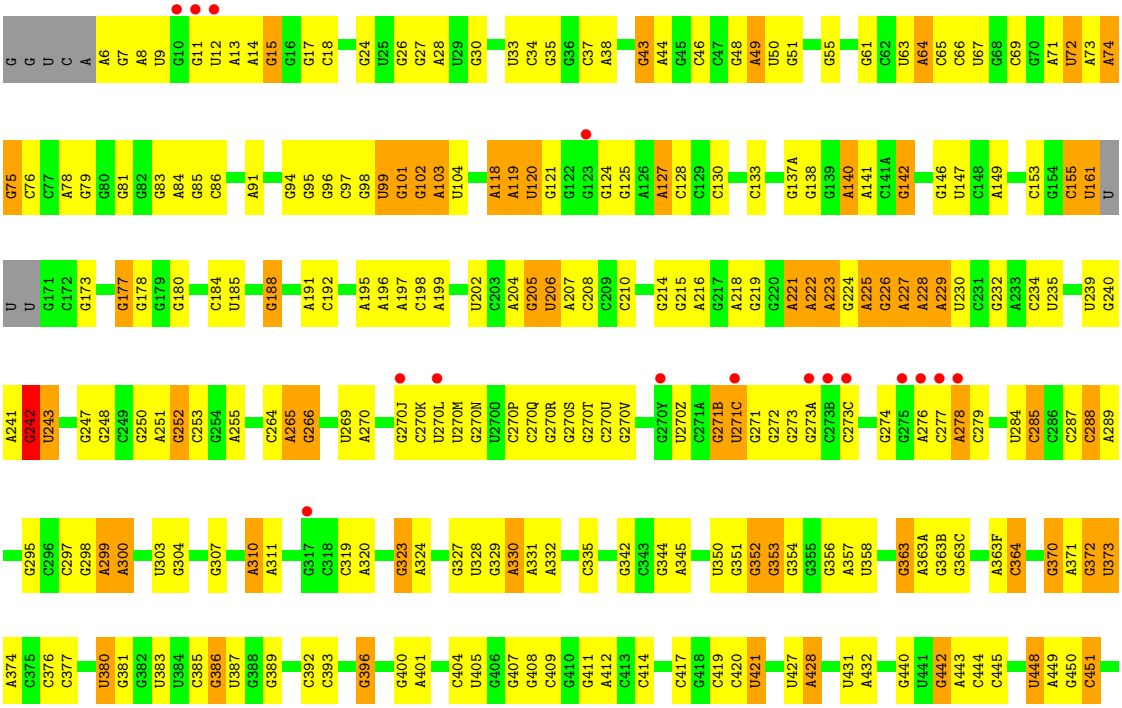


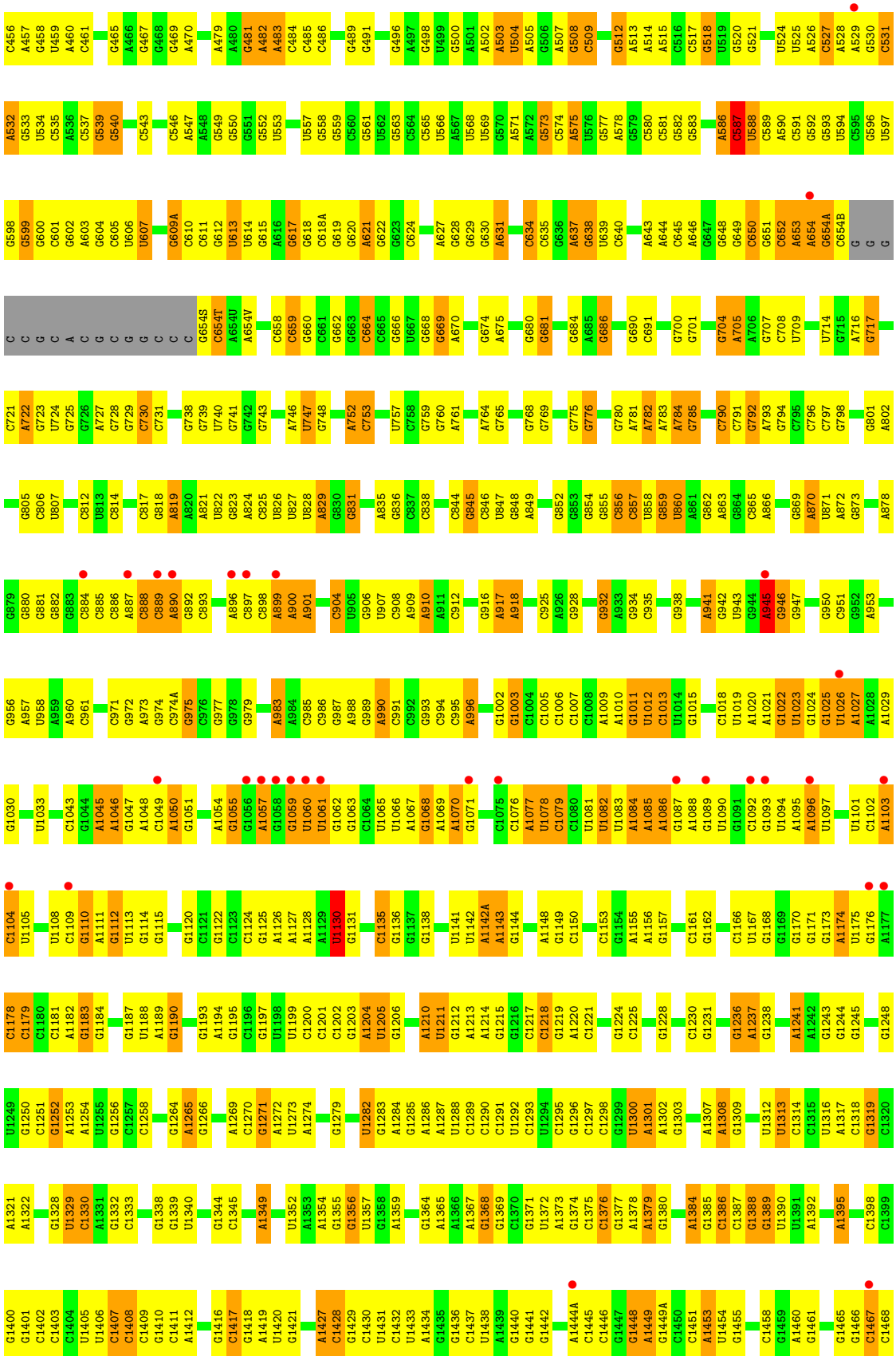


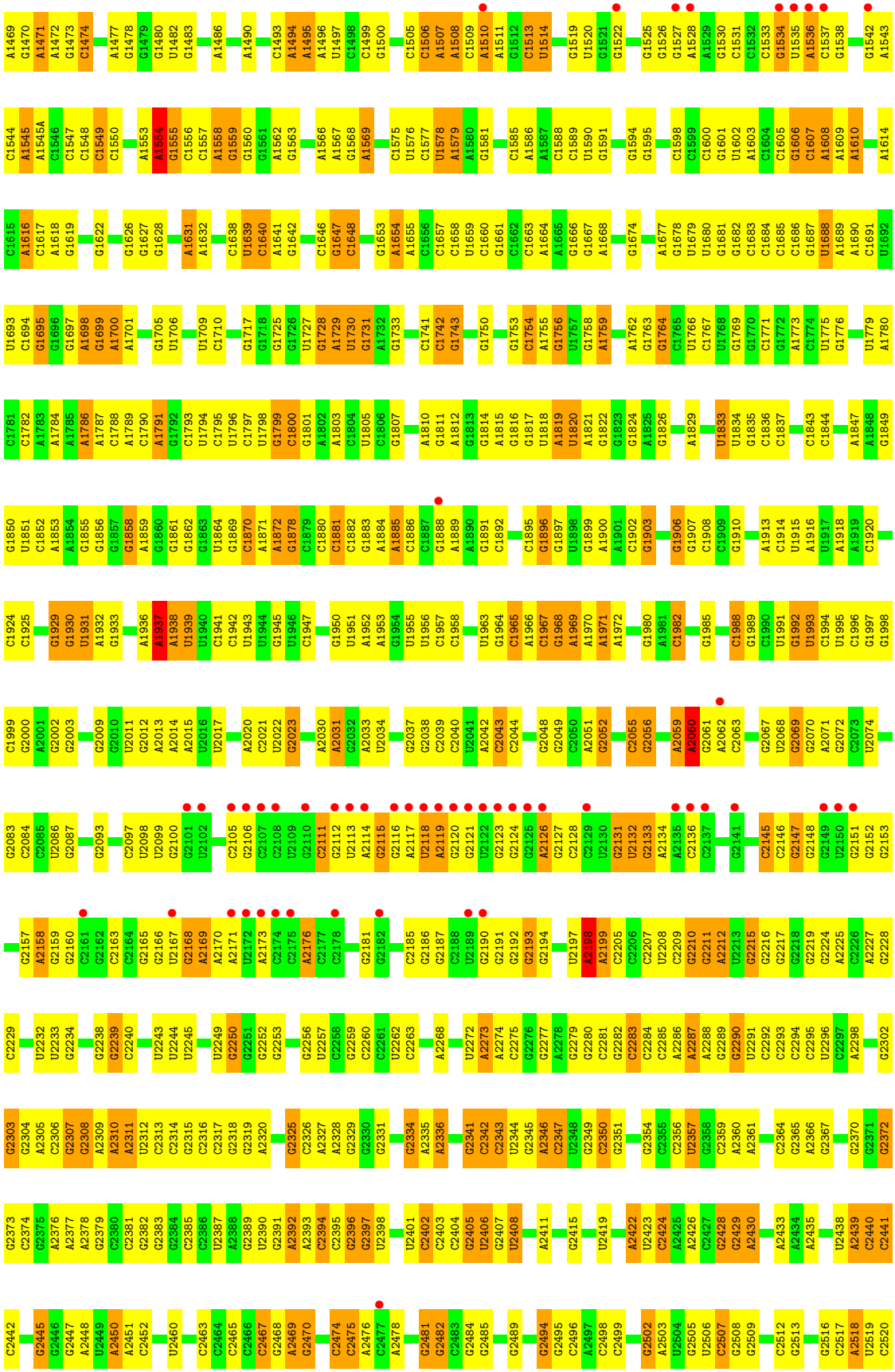
• Molecule 25: 23S rRNA

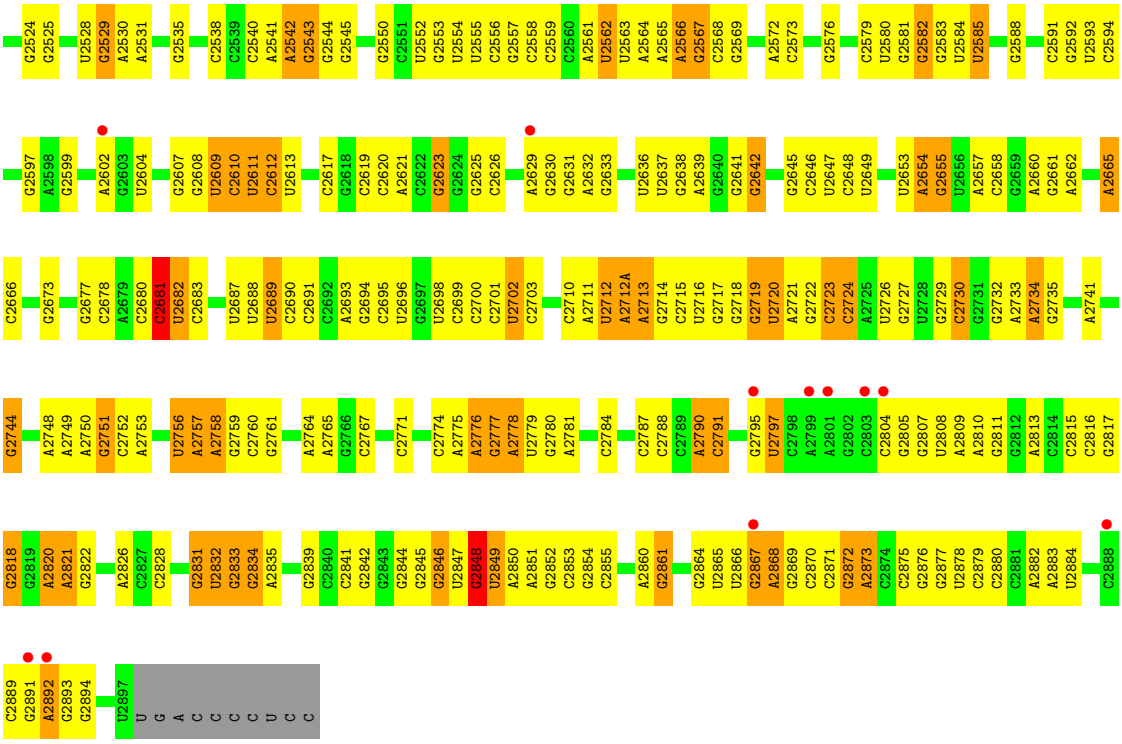
Chain YA:







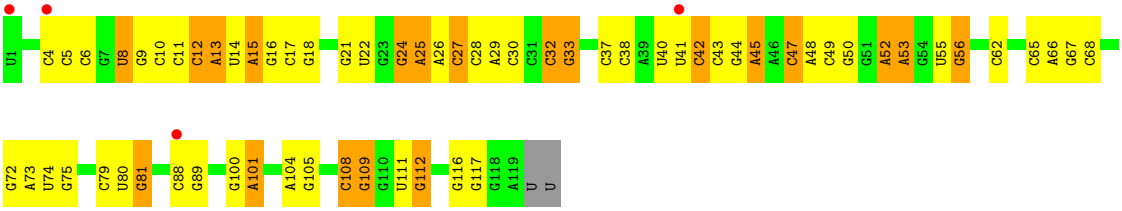




• Molecule 26: 5S rRNA

Chain RB:

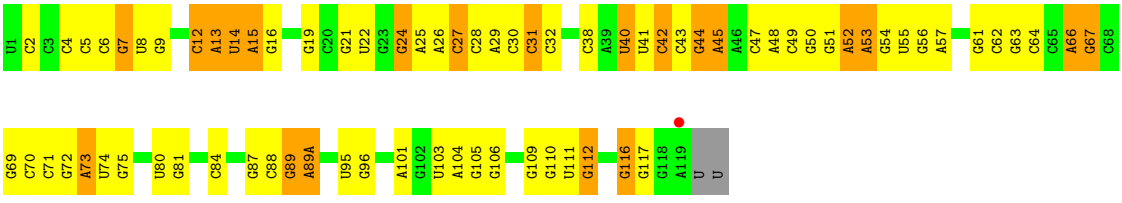




• Molecule 26: 5S rRNA

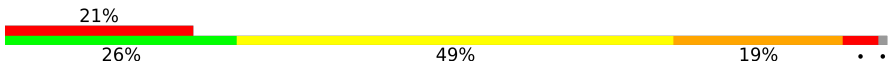
Chain YB:

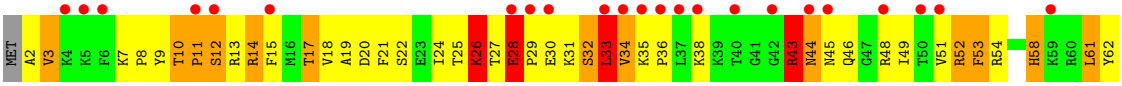


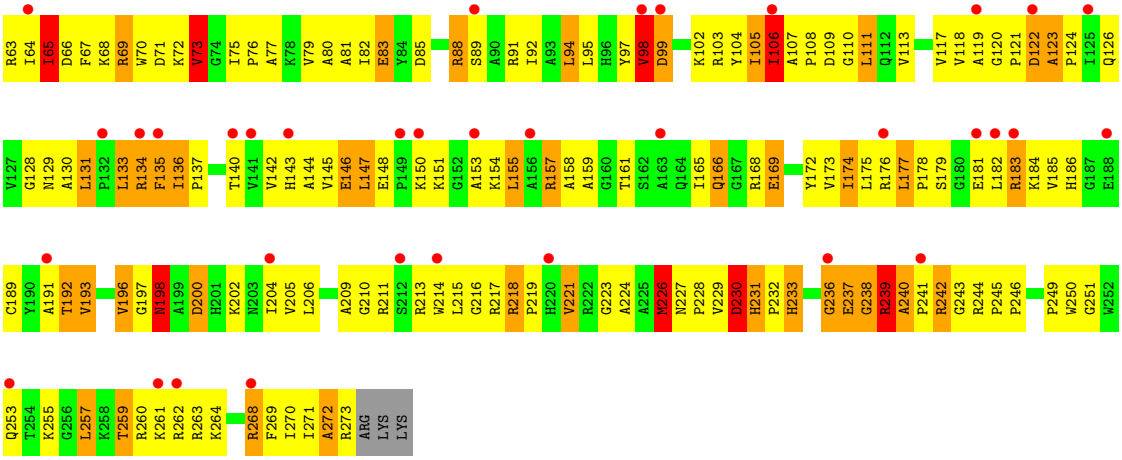


• Molecule 27: 50S ribosomal protein L2

Chain RD:

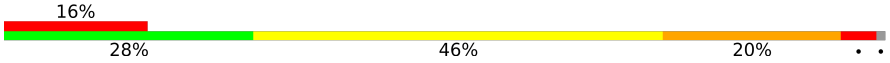


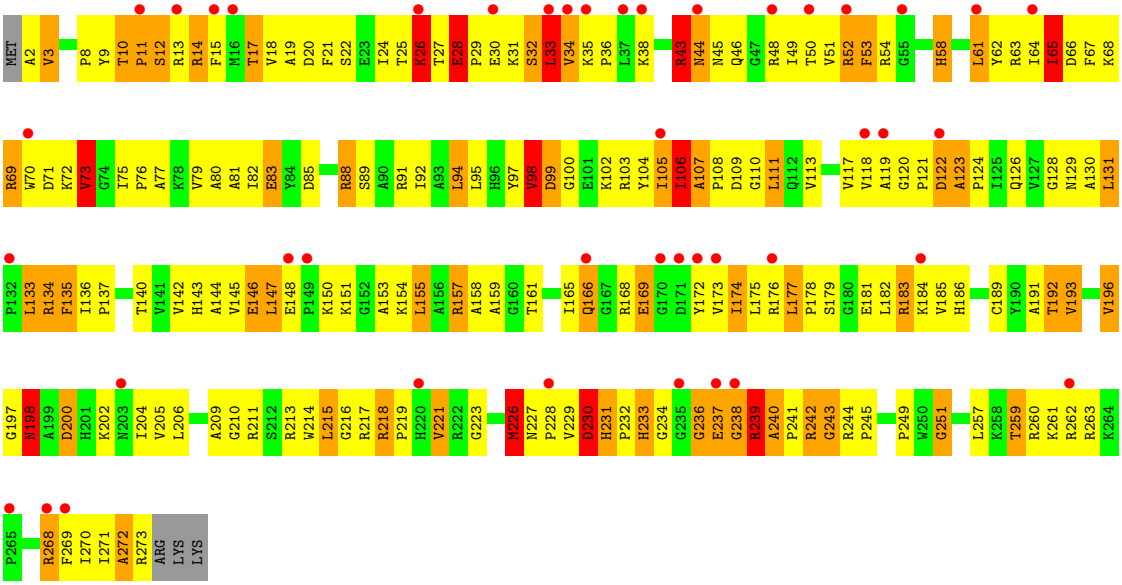




- Molecule 27: 50S ribosomal protein L2

Chain YD:

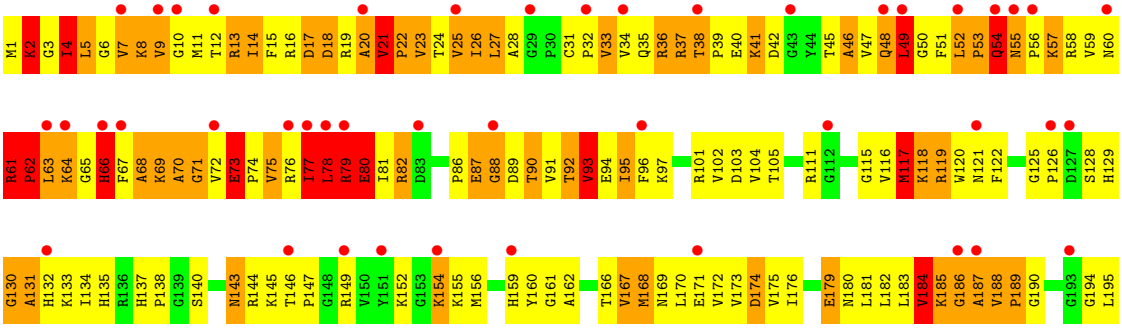




- Molecule 28: 50S ribosomal protein L3

Chain RE:



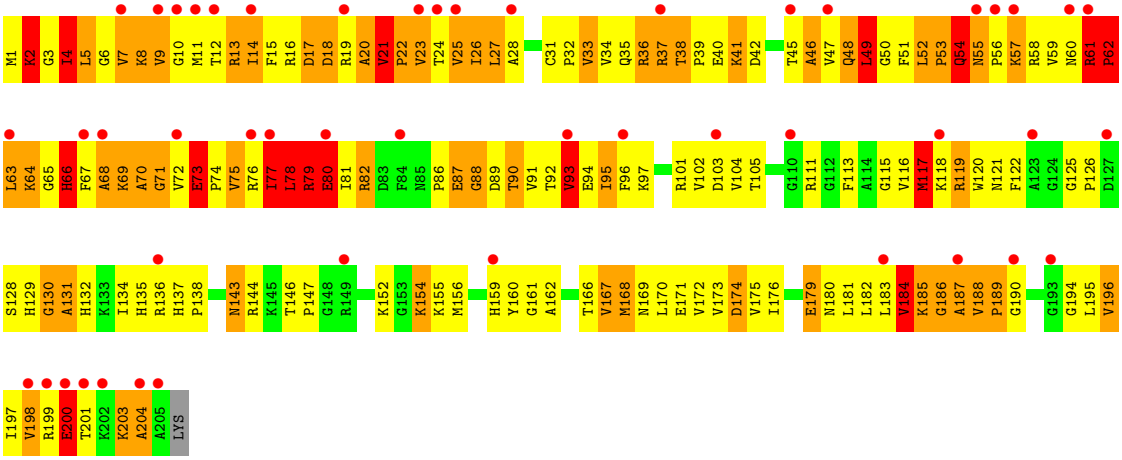




• Molecule 28: 50S ribosomal protein L3

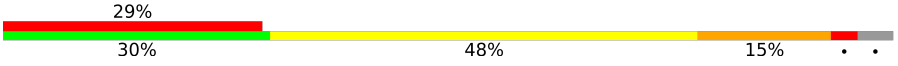
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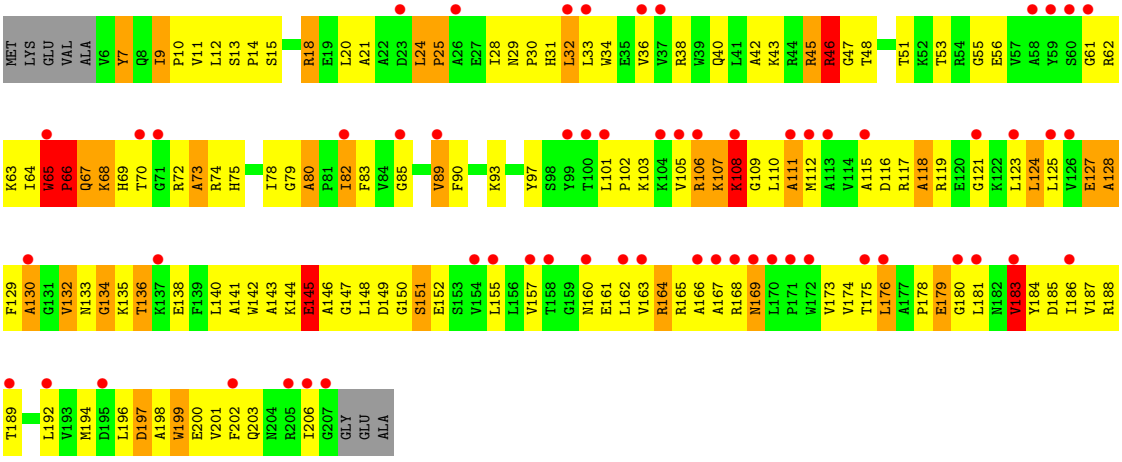




• Molecule 29: 50S ribosomal protein L4

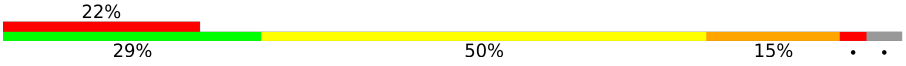
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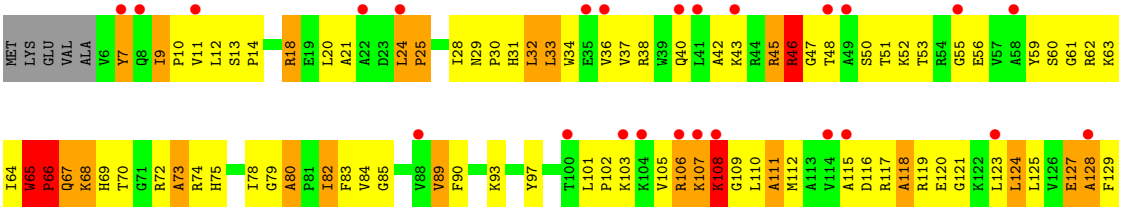


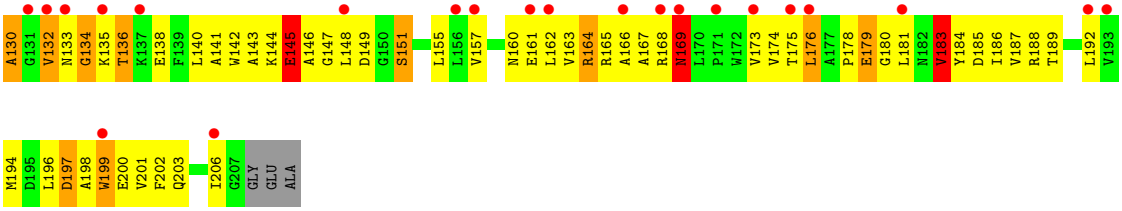


• Molecule 29: 50S ribosomal protein L4

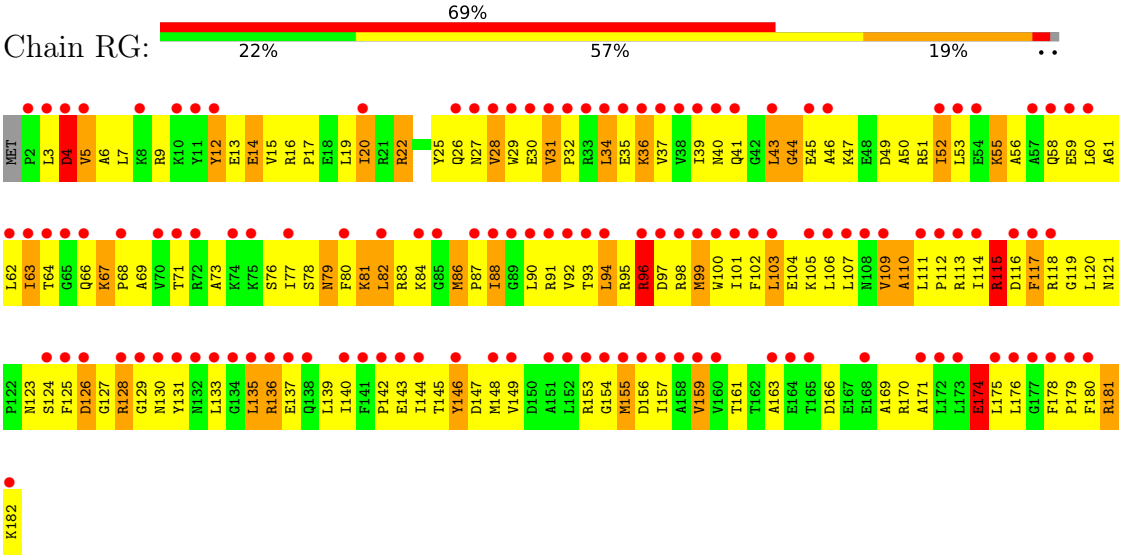
Chain YF:



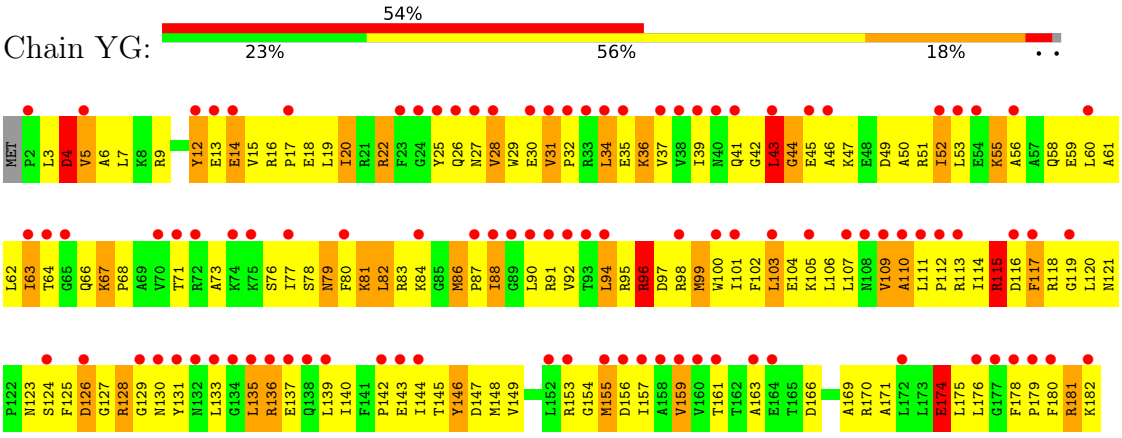




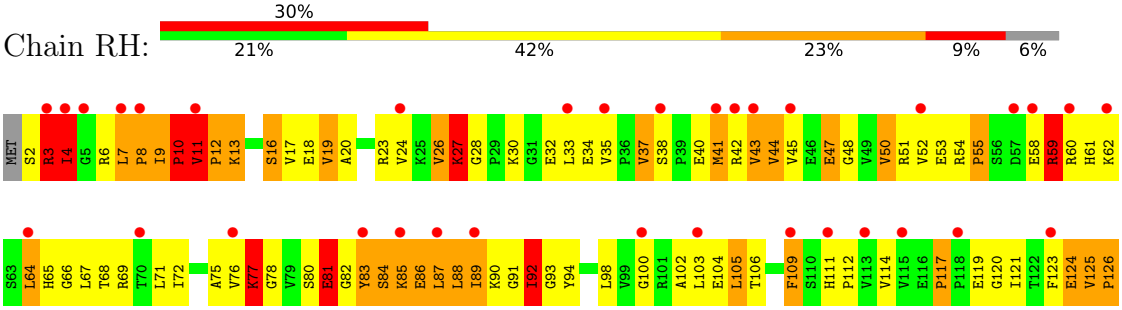
• Molecule 30: 50S ribosomal protein L5

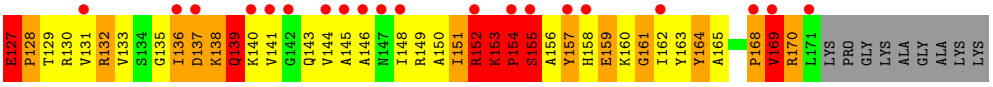


• Molecule 30: 50S ribosomal protein L5



• Molecule 31: 50S ribosomal protein L6

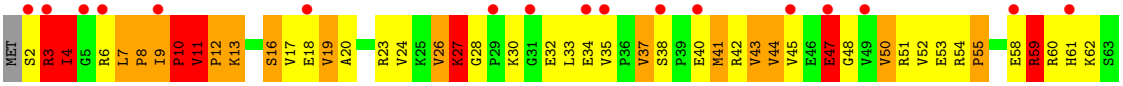


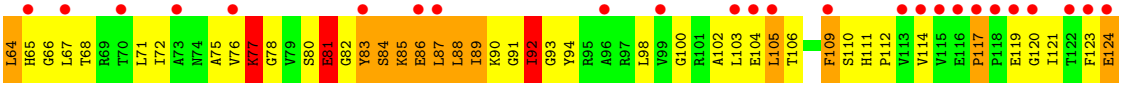


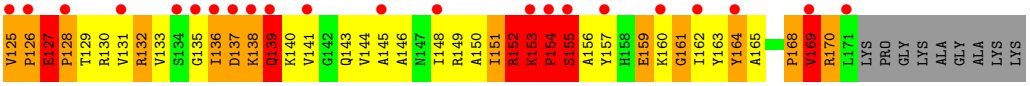
• Molecule 31: 50S ribosomal protein L6

Chain YH:





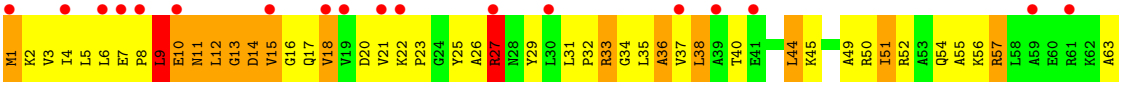


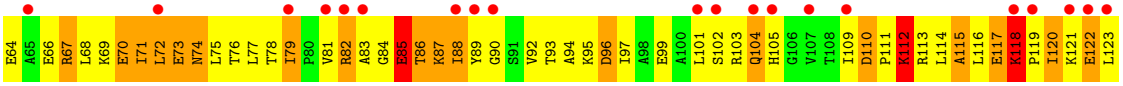


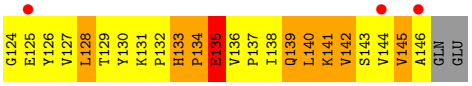
• Molecule 32: 50S ribosomal protein L9

Chain RI:





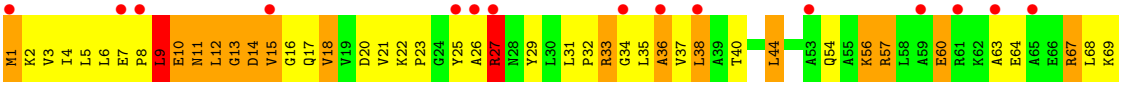


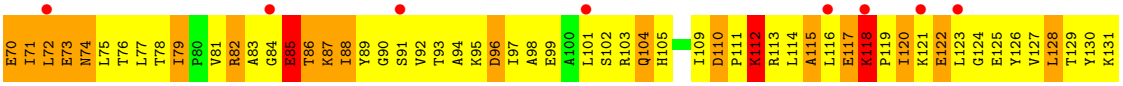


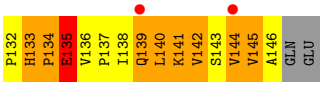
• Molecule 32: 50S ribosomal protein L9

Chain YI:





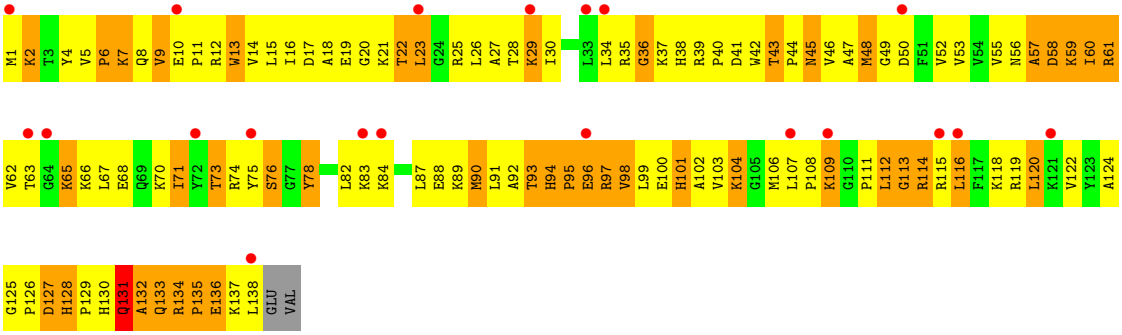




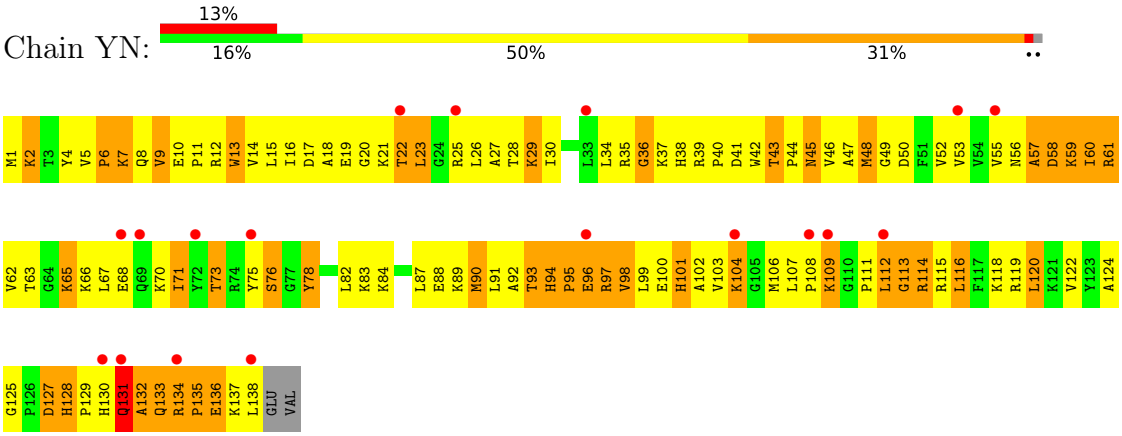
• Molecule 33: 50S ribosomal protein L13

Chain RN:

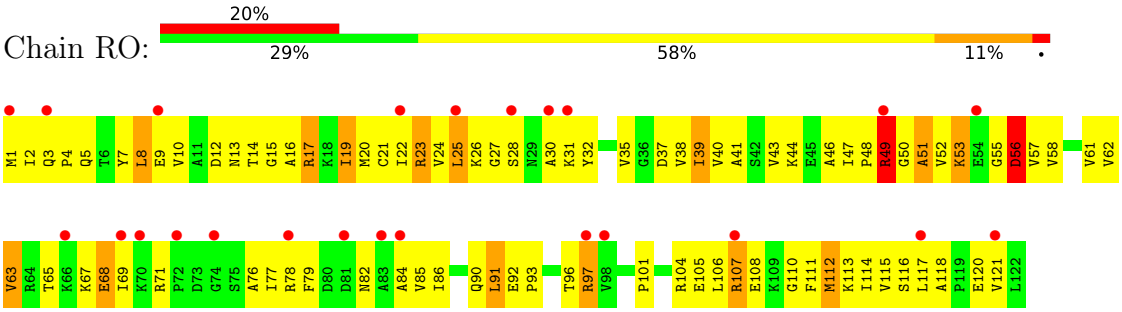




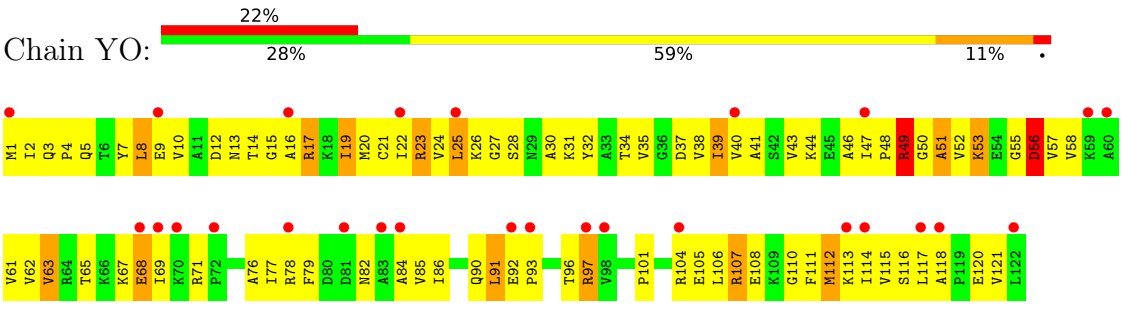
• Molecule 33: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L14

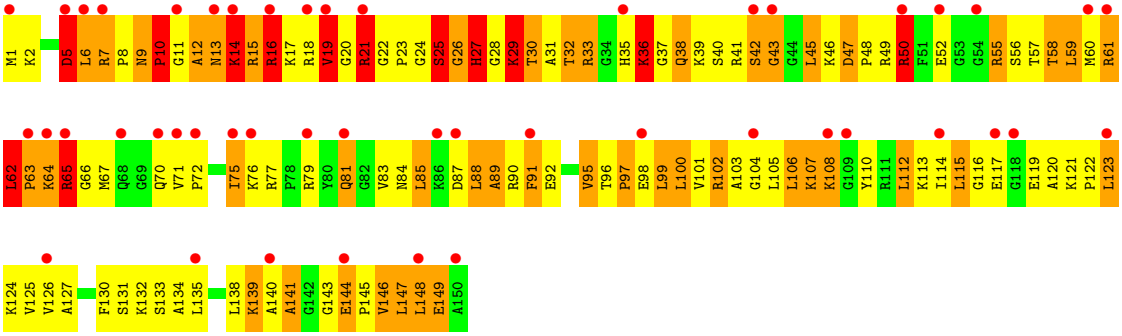


• Molecule 34: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L15

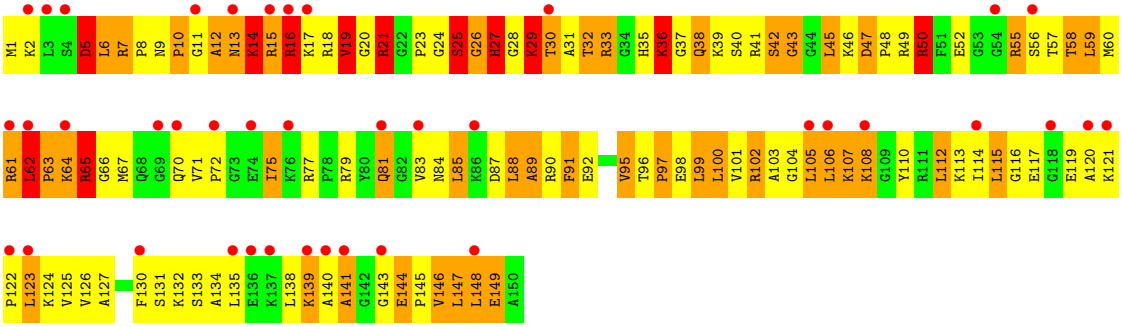




• Molecule 35: 50S ribosomal protein L15

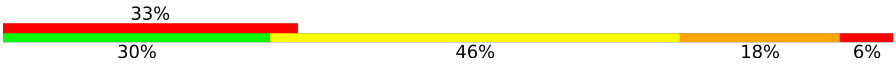
Chain YP:

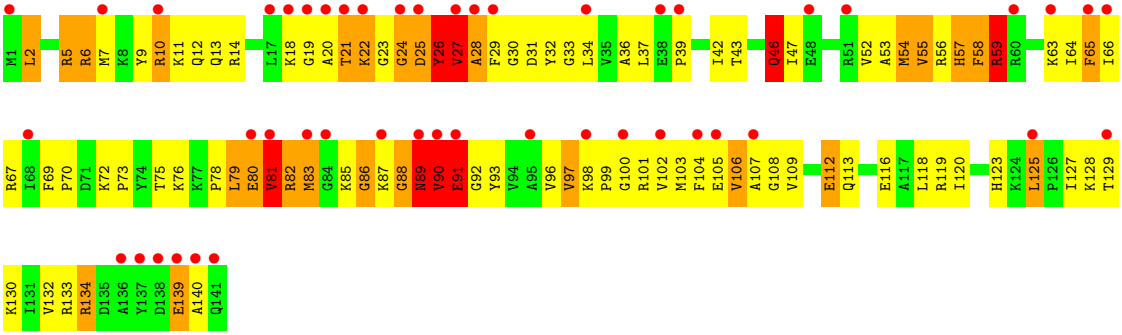




• Molecule 36: 50S ribosomal protein L16

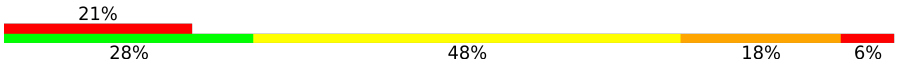
Chain RQ:

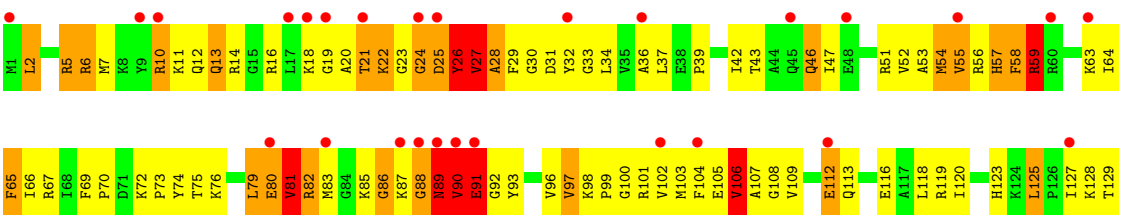


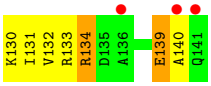


• Molecule 36: 50S ribosomal protein L16

Chain YQ:



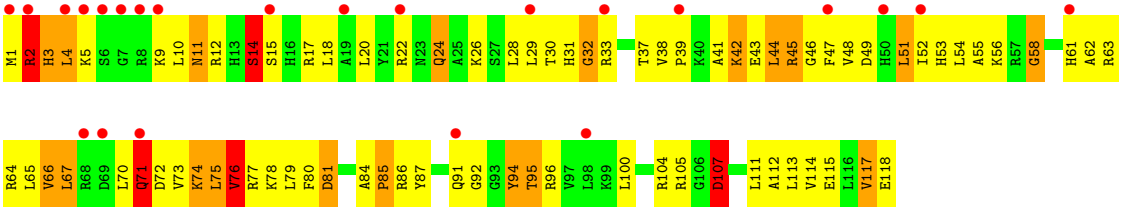




• Molecule 37: 50S ribosomal protein L17

Chain RR:

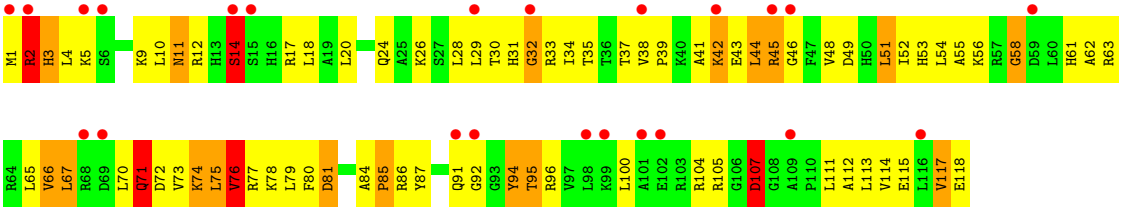




• Molecule 37: 50S ribosomal protein L17

Chain YR:

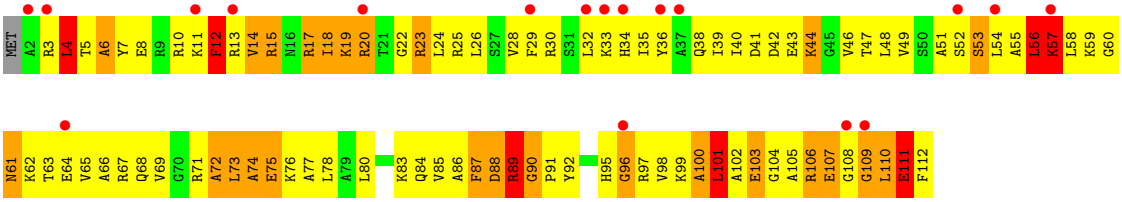




• Molecule 38: 50S ribosomal protein L18

Chain RS:

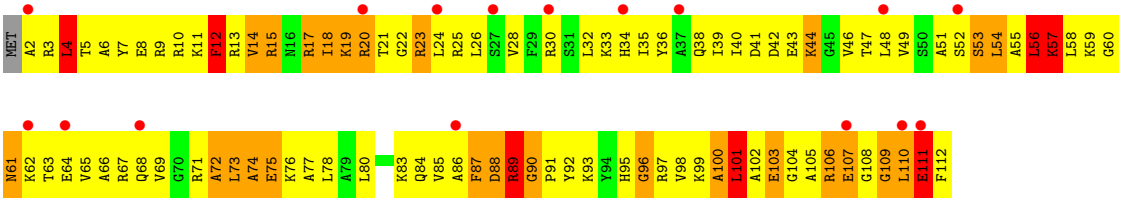




• Molecule 38: 50S ribosomal protein L18

Chain YS:

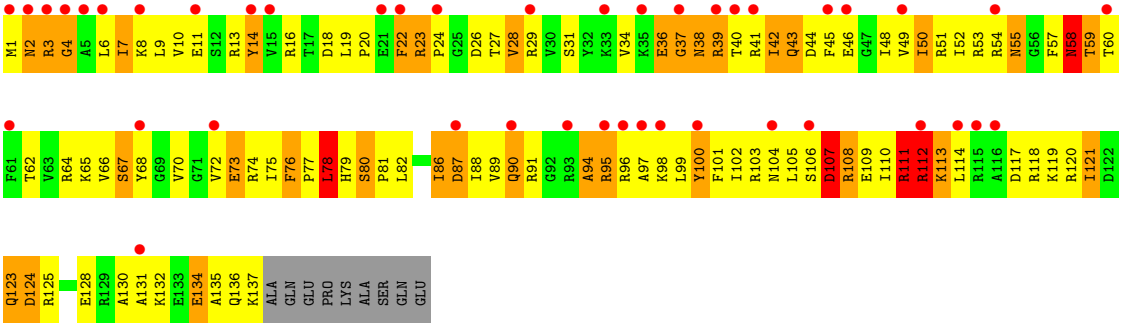




• Molecule 39: 50S ribosomal protein L19

Chain RT:

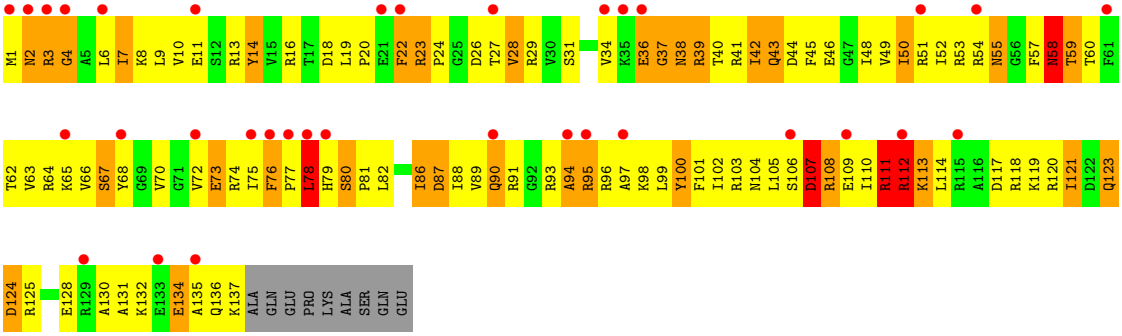




• Molecule 39: 50S ribosomal protein L19

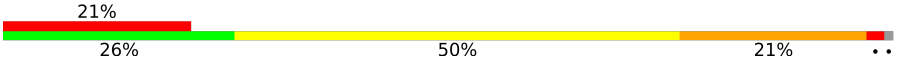
Chain YT:

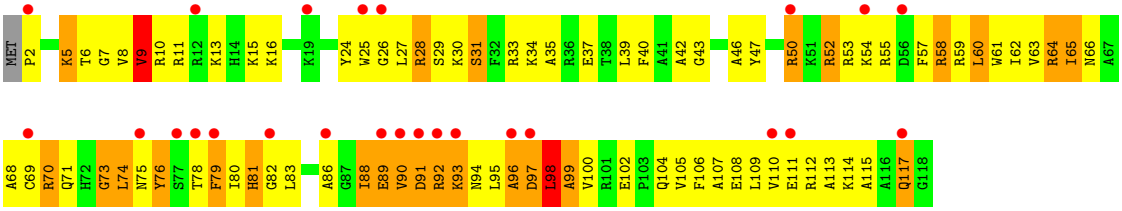




• Molecule 40: 50S ribosomal protein L20

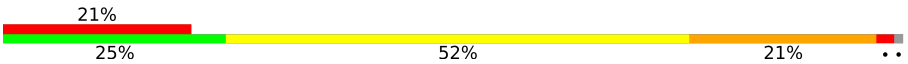
Chain RU:

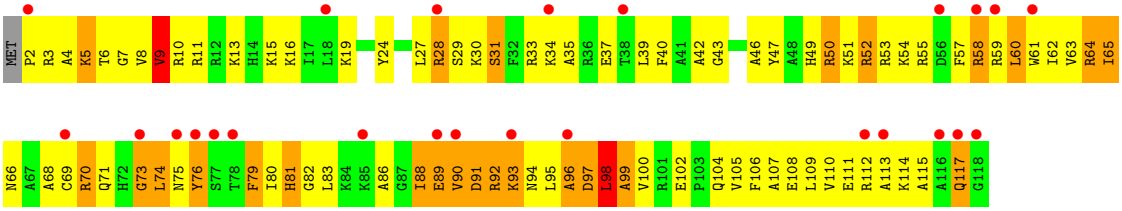




• Molecule 40: 50S ribosomal protein L20

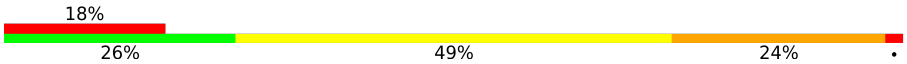
Chain YU:

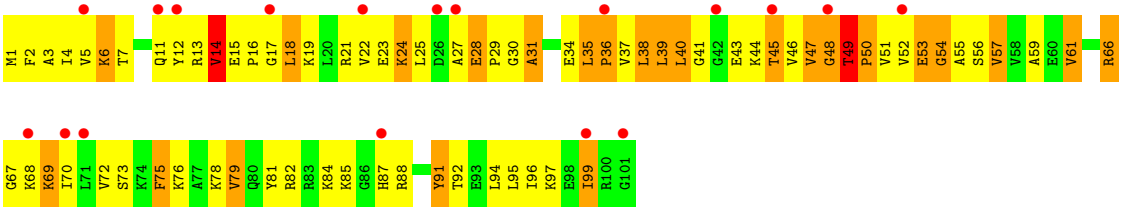




• Molecule 41: 50S ribosomal protein L21

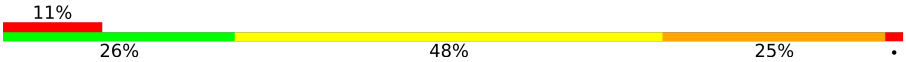
Chain RV:

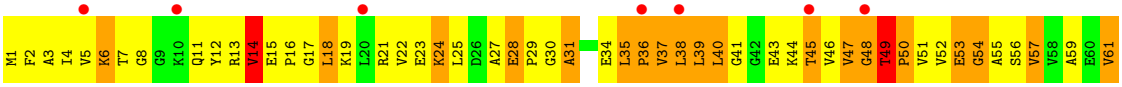


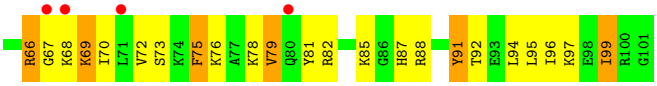


• Molecule 41: 50S ribosomal protein L21

Chain YV:

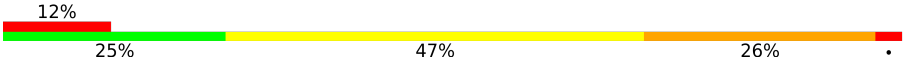




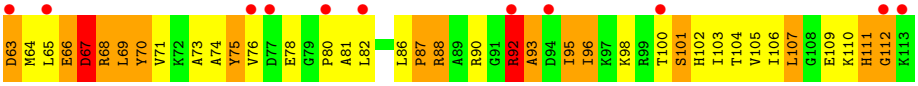


• Molecule 42: 50S ribosomal protein L22

Chain RW:

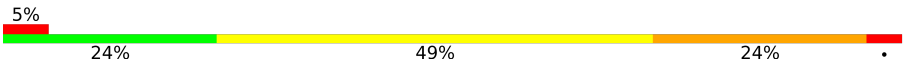


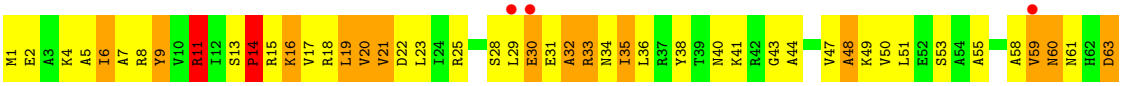


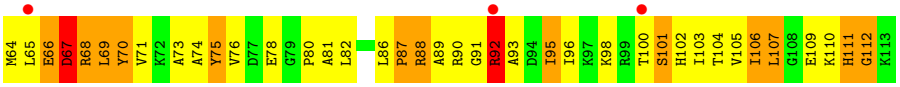


• Molecule 42: 50S ribosomal protein L22

Chain YW:





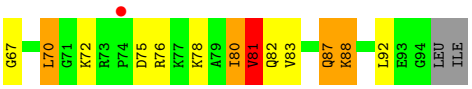


• Molecule 43: 50S ribosomal protein L23

Chain RX:

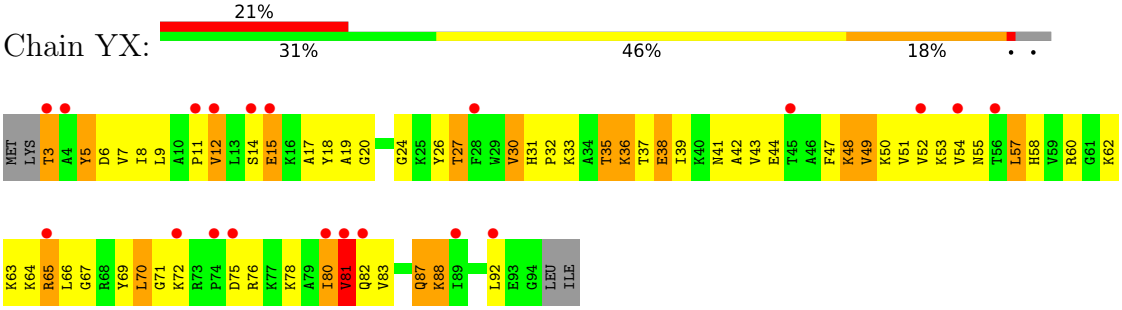






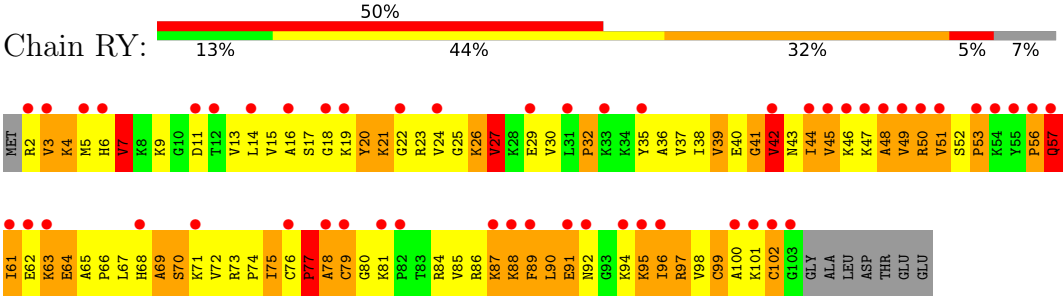
• Molecule 43: 50S ribosomal protein L23

Chain YX:



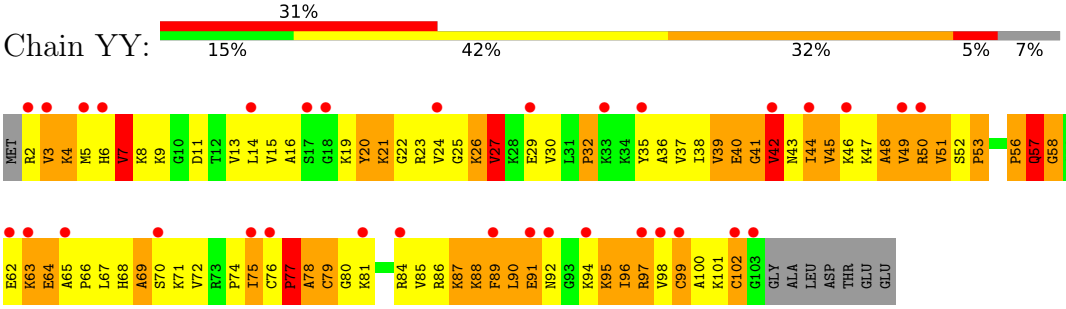
• Molecule 44: 50S ribosomal protein L24

Chain RY:



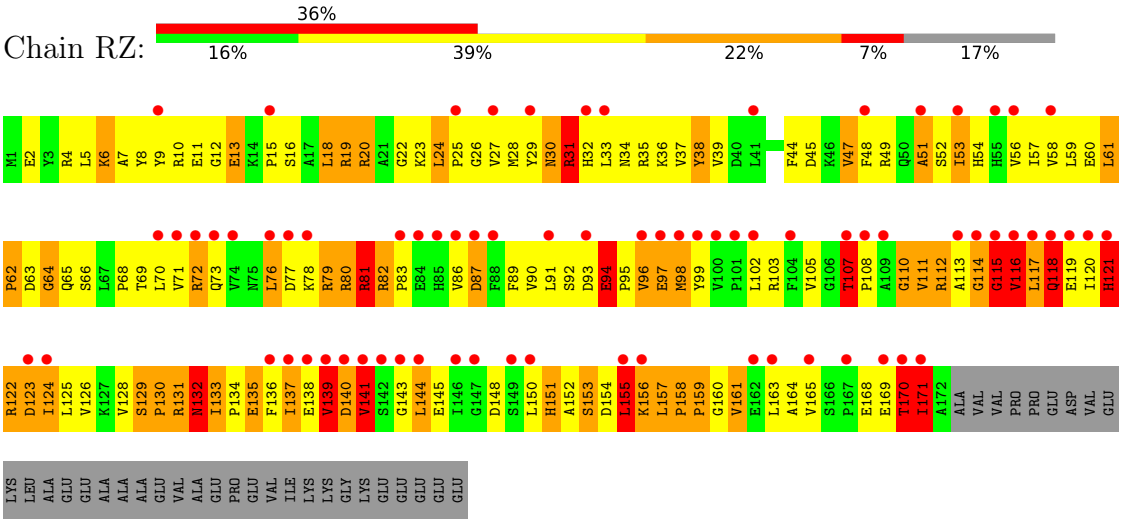
• Molecule 44: 50S ribosomal protein L24

Chain YY:



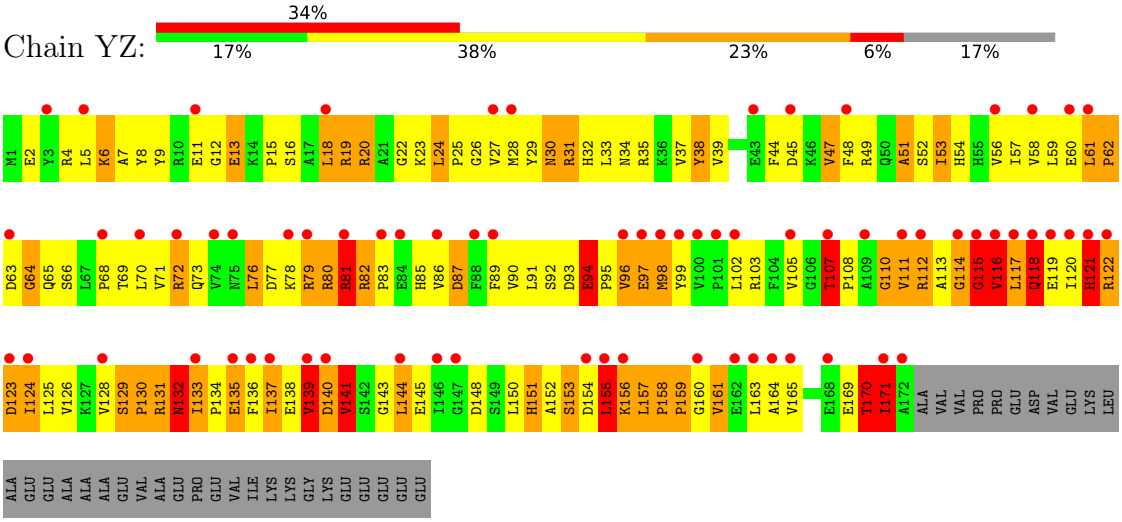
• Molecule 45: 50S ribosomal protein L25

Chain RZ:



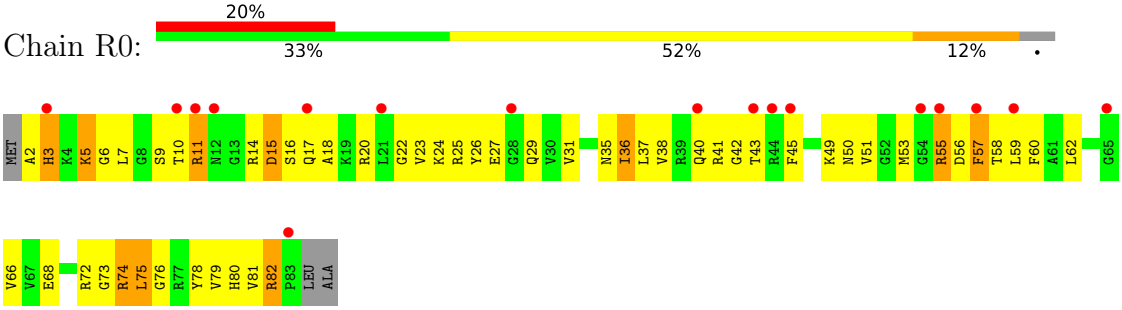
• Molecule 45: 50S ribosomal protein L25

Chain YZ:



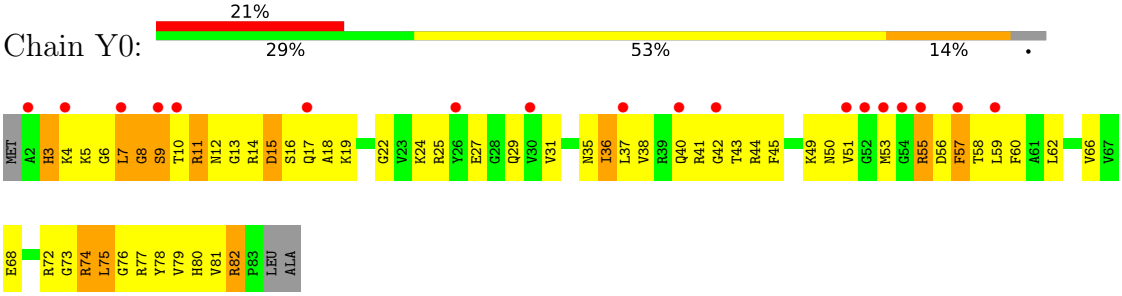
- Molecule 46: 50S ribosomal protein L27

Chain R0:



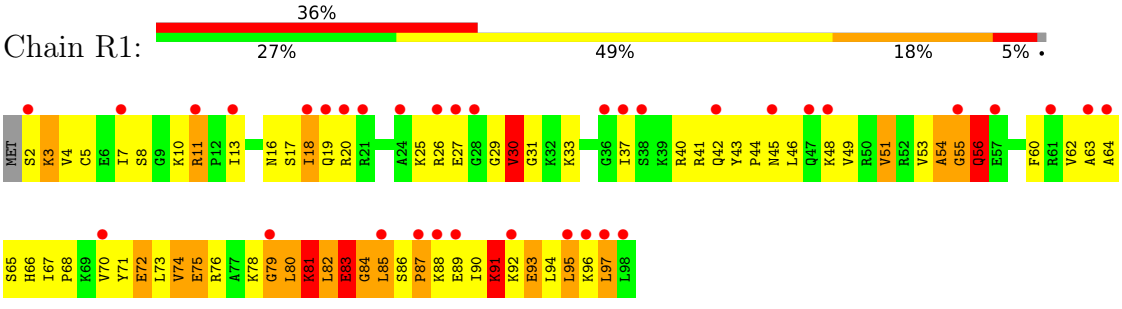
- Molecule 46: 50S ribosomal protein L27

Chain Y0:



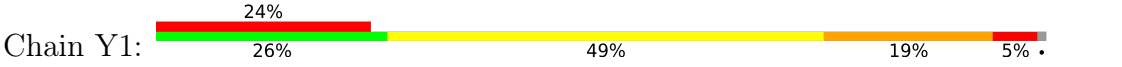
- Molecule 47: 50S ribosomal protein L28

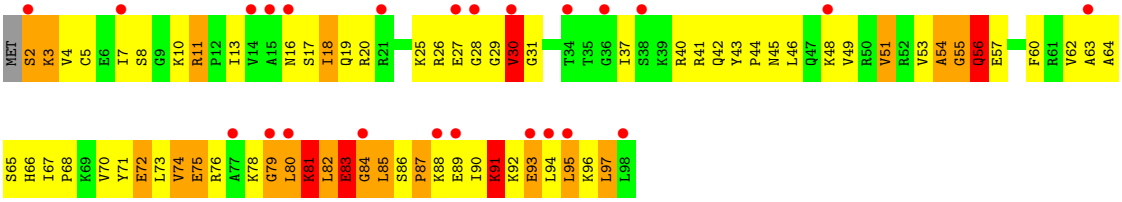
Chain R1:



- Molecule 47: 50S ribosomal protein L28

Chain Y1:

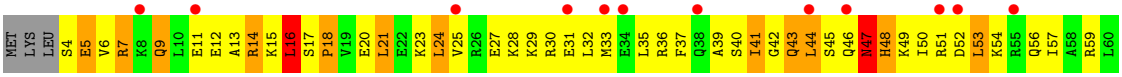




• Molecule 48: 50S ribosomal protein L29

Chain R2:







• Molecule 48: 50S ribosomal protein L29

Chain Y2:



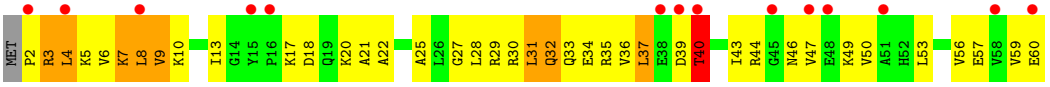




• Molecule 49: 50S ribosomal protein L30

Chain R3:

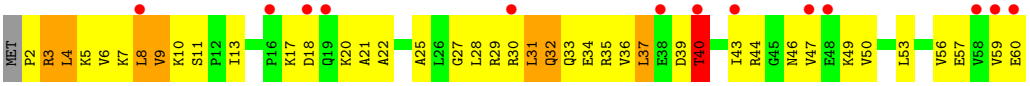




• Molecule 49: 50S ribosomal protein L30

Chain Y3:



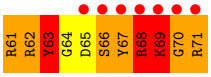


• Molecule 50: 50S ribosomal protein L32

Chain R4:



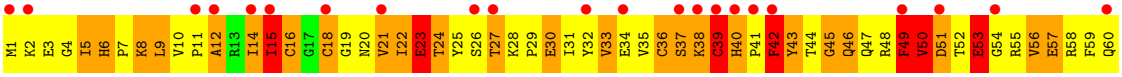


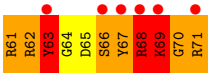


• Molecule 50: 50S ribosomal protein L32

Chain Y4:

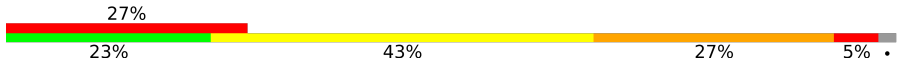


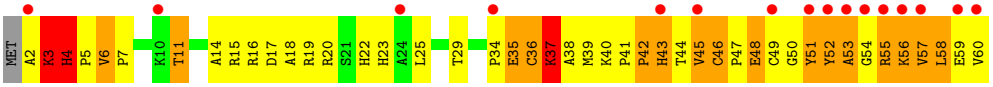




• Molecule 51: 50S ribosomal protein L33

Chain R5:

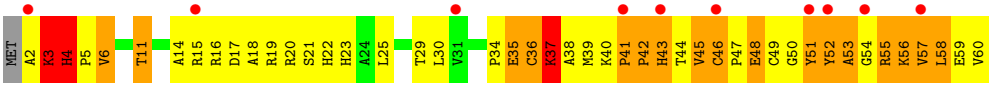




• Molecule 51: 50S ribosomal protein L33

Chain Y5:

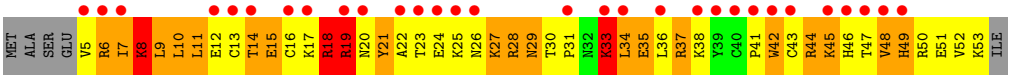




• Molecule 52: 50S ribosomal protein L34

Chain R6:

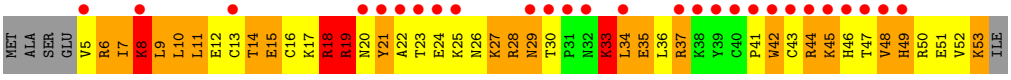




• Molecule 52: 50S ribosomal protein L34

Chain Y6:

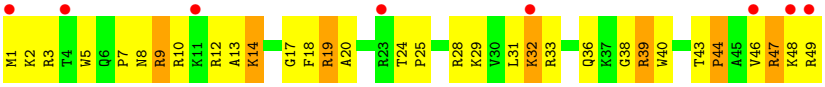




• Molecule 53: 50S ribosomal protein L35

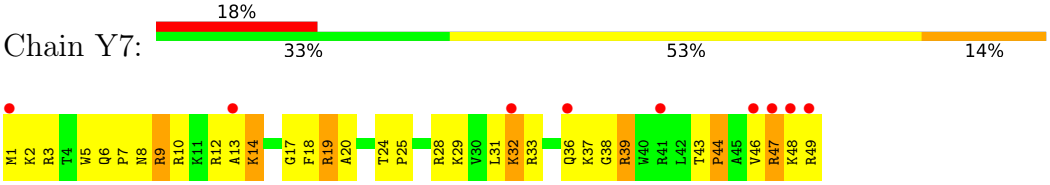
Chain R7:





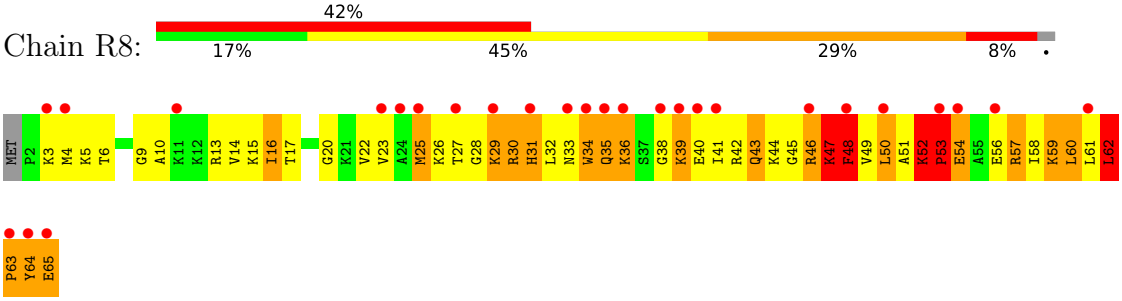
• Molecule 53: 50S ribosomal protein L35

Chain Y7:



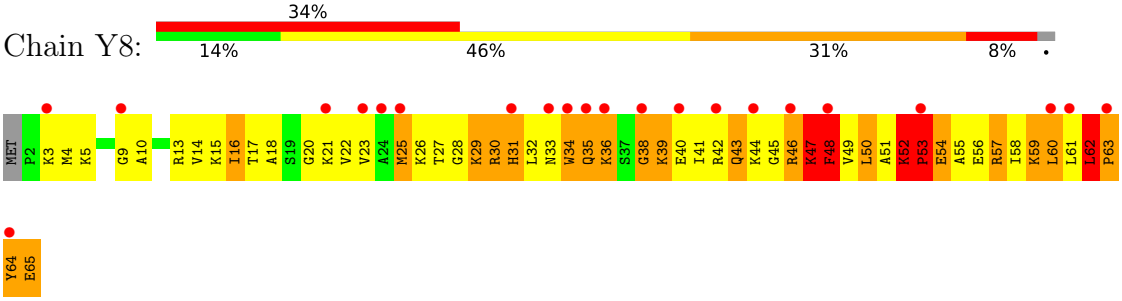
• Molecule 54: tRNA acceptor end mimic

Chain R8:



• Molecule 54: tRNA acceptor end mimic

Chain Y8:



• Molecule 55: RNA (5'-R(*CP*CP*(PPU))-3')

Chain Z6:



• Molecule 55: RNA (5'-R(*CP*CP*(PPU))-3')

Chain Z8:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.55Å 449.21Å 619.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.81 – 3.44 34.81 – 3.44	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.81-3.44) 98.6 (34.81-3.44)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.243 , 0.285 0.243 , 0.284	Depositor DCC
R_{free} test set	40944 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å^2)	65.0	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 68.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	291123	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 1MG, PAR, MG, PPU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	QA	0.24	0/36098	0.47	2/56341 (0.0%)
1	XA	0.26	0/36123	0.49	2/56380 (0.0%)
2	QB	0.42	0/1959	1.06	13/2642 (0.5%)
2	XB	0.42	0/1959	1.06	12/2642 (0.5%)
3	QC	0.43	0/1629	0.93	1/2195 (0.0%)
3	XC	0.44	0/1629	0.92	1/2195 (0.0%)
4	QD	0.50	0/1733	1.08	15/2318 (0.6%)
4	XD	0.50	0/1733	1.08	15/2318 (0.6%)
5	QE	0.45	0/1171	1.02	8/1576 (0.5%)
5	XE	0.45	0/1171	1.02	9/1576 (0.6%)
6	QF	0.50	0/856	0.97	3/1154 (0.3%)
6	XF	0.49	0/856	0.97	3/1154 (0.3%)
7	QG	0.43	0/1276	0.90	2/1709 (0.1%)
7	XG	0.42	0/1276	0.90	2/1709 (0.1%)
8	QH	0.50	0/1136	1.06	5/1527 (0.3%)
8	XH	0.50	0/1136	1.05	6/1527 (0.4%)
9	QI	0.40	0/1029	1.03	9/1379 (0.7%)
9	XI	0.40	0/1029	1.03	9/1379 (0.7%)
10	QJ	0.46	0/814	0.91	1/1095 (0.1%)
10	XJ	0.47	0/814	0.91	1/1095 (0.1%)
11	QK	0.47	0/900	1.04	6/1213 (0.5%)
11	XK	0.47	0/900	1.05	6/1213 (0.5%)
12	QL	0.55	0/991	1.73	11/1327 (0.8%)
12	XL	0.55	0/991	1.75	11/1327 (0.8%)
13	QM	0.43	0/974	1.04	9/1303 (0.7%)
13	XM	0.43	0/974	1.04	8/1303 (0.6%)
14	QN	0.51	0/501	1.10	5/664 (0.8%)
14	XN	0.50	0/501	1.10	5/664 (0.8%)
15	QO	0.48	0/745	0.99	3/992 (0.3%)
15	XO	0.48	0/745	1.00	3/992 (0.3%)
16	QP	0.46	0/721	1.03	4/970 (0.4%)
16	XP	0.46	0/721	1.03	4/970 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.43	0/847	1.06	7/1131 (0.6%)
17	XQ	0.43	0/847	1.07	6/1131 (0.5%)
18	QR	0.46	0/579	1.04	3/768 (0.4%)
18	XR	0.46	0/579	1.04	3/768 (0.4%)
19	QS	0.45	0/689	1.21	7/926 (0.8%)
19	XS	0.46	0/689	1.21	6/926 (0.6%)
20	QT	0.42	0/765	1.09	4/1007 (0.4%)
20	XT	0.42	0/765	1.09	5/1007 (0.5%)
21	QU	0.43	0/221	1.01	1/288 (0.3%)
21	XU	0.42	0/221	1.01	1/288 (0.3%)
22	QV	0.34	1/1836 (0.1%)	0.44	0/2859
22	XV	0.34	1/1836 (0.1%)	0.45	0/2859
23	QX	0.39	0/189	0.72	0/292
23	XX	0.54	0/189	0.95	2/292 (0.7%)
24	QY	0.41	0/311	0.57	0/483
24	XY	0.37	0/311	0.46	0/483
25	RA	0.29	1/69543 (0.0%)	0.51	9/108563 (0.0%)
25	YA	0.33	1/69521 (0.0%)	0.53	16/108529 (0.0%)
26	RB	0.25	0/2878	0.47	0/4490
26	YB	0.27	0/2878	0.48	0/4490
27	RD	0.84	3/2165 (0.1%)	1.30	32/2919 (1.1%)
27	YD	0.84	3/2165 (0.1%)	1.30	30/2919 (1.0%)
28	RE	0.62	0/1601	1.35	29/2160 (1.3%)
28	YE	0.62	0/1601	1.35	29/2160 (1.3%)
29	RF	0.62	0/1620	1.19	19/2194 (0.9%)
29	YF	0.62	0/1620	1.19	18/2194 (0.8%)
30	RG	0.47	0/1499	0.99	8/2016 (0.4%)
30	YG	0.47	0/1499	0.99	9/2016 (0.4%)
31	RH	0.57	0/1332	1.22	15/1802 (0.8%)
31	YH	0.57	0/1332	1.22	15/1802 (0.8%)
32	RI	0.53	0/1151	1.13	8/1558 (0.5%)
32	YI	0.53	0/1151	1.11	8/1558 (0.5%)
33	RN	0.55	0/1131	1.18	10/1525 (0.7%)
33	YN	0.55	0/1131	1.18	10/1525 (0.7%)
34	RO	0.64	0/943	1.03	5/1269 (0.4%)
34	YO	0.65	0/943	1.04	5/1269 (0.4%)
35	RP	0.63	1/1162 (0.1%)	1.37	17/1544 (1.1%)
35	YP	0.63	1/1162 (0.1%)	1.37	17/1544 (1.1%)
36	RQ	0.69	0/1143	1.34	19/1527 (1.2%)
36	YQ	0.69	0/1143	1.34	19/1527 (1.2%)
37	RR	0.55	0/982	1.17	10/1312 (0.8%)
37	YR	0.55	0/982	1.17	10/1312 (0.8%)
38	RS	0.52	0/892	1.19	8/1187 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YS	0.52	0/892	1.18	9/1187 (0.8%)
39	RT	0.56	0/1155	1.18	16/1542 (1.0%)
39	YT	0.56	0/1155	1.18	17/1542 (1.1%)
40	RU	0.59	0/982	1.21	10/1306 (0.8%)
40	YU	0.60	0/982	1.21	10/1306 (0.8%)
41	RV	0.56	0/790	1.10	6/1057 (0.6%)
41	YV	0.56	0/790	1.10	6/1057 (0.6%)
42	RW	0.58	0/911	1.18	13/1220 (1.1%)
42	YW	0.58	0/911	1.18	13/1220 (1.1%)
43	RX	0.62	0/739	1.14	5/993 (0.5%)
43	YX	0.62	0/739	1.13	5/993 (0.5%)
44	RY	0.64	0/798	1.16	3/1064 (0.3%)
44	YY	0.64	0/798	1.16	4/1064 (0.4%)
45	RZ	0.60	1/1408 (0.1%)	1.07	10/1908 (0.5%)
45	YZ	0.60	1/1408 (0.1%)	1.07	10/1908 (0.5%)
46	R0	0.73	0/657	1.16	6/874 (0.7%)
46	Y0	0.81	2/657 (0.3%)	1.19	6/874 (0.7%)
47	R1	0.58	0/770	1.20	9/1022 (0.9%)
47	Y1	0.58	0/770	1.20	9/1022 (0.9%)
48	R2	0.60	0/583	1.32	9/771 (1.2%)
48	Y2	0.60	0/583	1.32	9/771 (1.2%)
49	R3	0.53	0/474	1.04	1/635 (0.2%)
49	Y3	0.54	0/474	1.04	0/635
50	R4	0.47	0/594	1.24	10/795 (1.3%)
50	Y4	0.47	0/594	1.24	10/795 (1.3%)
51	R5	0.65	0/473	1.22	4/639 (0.6%)
51	Y5	0.65	0/473	1.22	7/639 (1.1%)
52	R6	0.53	0/431	1.06	3/575 (0.5%)
52	Y6	0.53	0/431	1.06	3/575 (0.5%)
53	R7	0.73	0/438	1.19	2/575 (0.3%)
53	Y7	0.74	0/438	1.19	2/575 (0.3%)
54	R8	0.79	0/525	1.41	9/691 (1.3%)
54	Y8	0.80	0/525	1.41	9/691 (1.3%)
55	Z6	0.47	0/40	0.62	0/60
55	Z8	0.46	0/40	0.62	0/60
All	All	0.39	16/315563 (0.0%)	0.73	859/471909 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	YD	236	GLY	C-N	14.38	1.53	1.33
27	RD	236	GLY	C-N	14.31	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	YD	239	ARG	CA-C	-13.01	1.35	1.52
27	RD	239	ARG	CA-C	-12.97	1.35	1.52
45	YZ	139	VAL	CA-C	6.83	1.60	1.52

The worst 5 of 859 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	QL	47	LYS	CA-C-N	31.21	158.85	119.84
12	QL	47	LYS	C-N-CA	31.21	158.85	119.84
12	XL	47	LYS	CA-C-N	31.17	158.80	119.84
12	XL	47	LYS	C-N-CA	31.17	158.80	119.84
35	YP	59	LEU	N-CA-C	-14.61	91.40	111.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16275	839	0
1	XA	32269	0	16289	818	0
2	QB	1924	0	1975	310	0
2	XB	1924	0	1975	317	0
3	QC	1605	0	1668	213	0
3	XC	1605	0	1668	212	1
4	QD	1703	0	1762	259	0
4	XD	1703	0	1763	234	0
5	QE	1155	0	1213	162	0
5	XE	1155	0	1213	153	0
6	QF	843	0	857	101	0
6	XF	843	0	857	107	0
7	QG	1257	0	1296	158	0
7	XG	1257	0	1296	154	0
8	QH	1116	0	1176	164	0
8	XH	1116	0	1177	173	0
9	QI	1010	0	1037	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	XI	1010	0	1037	165	0
10	QJ	801	0	849	139	0
10	XJ	801	0	849	138	0
11	QK	885	0	904	117	1
11	XK	885	0	904	119	0
12	QL	975	0	1062	115	0
12	XL	975	0	1062	118	0
13	QM	964	0	1034	181	0
13	XM	964	0	1034	188	0
14	QN	492	0	531	96	0
14	XN	492	0	529	93	0
15	QO	734	0	771	82	0
15	XO	734	0	771	82	0
16	QP	705	0	725	119	0
16	XP	705	0	725	118	0
17	QQ	834	0	904	85	0
17	XQ	834	0	904	86	0
18	QR	574	0	644	77	0
18	XR	574	0	644	74	0
19	QS	674	0	699	111	0
19	XS	674	0	699	147	0
20	QT	763	0	860	115	0
20	XT	763	0	861	113	0
21	QU	217	0	234	31	0
21	XU	217	0	234	29	0
22	QV	1644	0	836	41	0
22	XV	1644	0	836	40	0
23	QX	170	0	87	16	0
23	XX	170	0	88	10	0
24	QY	303	0	154	12	0
24	XY	303	0	154	17	0
25	RA	62091	0	31301	1410	0
25	YA	62071	0	31286	1362	0
26	RB	2573	0	1306	68	0
26	YB	2573	0	1306	61	0
27	RD	2115	0	2195	332	0
27	YD	2115	0	2195	354	0
28	RE	1568	0	1634	289	0
28	YE	1568	0	1634	280	0
29	RF	1585	0	1632	189	0
29	YF	1585	0	1632	197	0
30	RG	1474	0	1535	224	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	YG	1474	0	1535	219	0
31	RH	1307	0	1382	223	0
31	YH	1307	0	1382	226	1
32	RI	1136	0	1223	187	0
32	YI	1136	0	1223	184	0
33	RN	1104	0	1180	202	0
33	YN	1104	0	1180	194	0
34	RO	933	0	996	132	0
34	YO	933	0	996	134	0
35	RP	1145	0	1228	257	0
35	YP	1145	0	1228	257	0
36	RQ	1122	0	1179	174	0
36	YQ	1122	0	1179	177	0
37	RR	968	0	1033	120	0
37	YR	968	0	1033	116	0
38	RS	882	0	943	164	0
38	YS	882	0	943	166	0
39	RT	1141	0	1202	157	0
39	YT	1141	0	1202	161	0
40	RU	964	0	1022	144	0
40	YU	964	0	1022	148	0
41	RV	779	0	852	139	0
41	YV	779	0	852	136	1
42	RW	900	0	964	106	0
42	YW	900	0	964	112	0
43	RX	725	0	778	71	0
43	YX	725	0	778	82	0
44	RY	785	0	878	169	0
44	YY	785	0	878	162	1
45	RZ	1378	0	1407	242	0
45	YZ	1378	0	1407	237	0
46	R0	648	0	672	89	0
46	Y0	648	0	672	87	0
47	R1	763	0	848	145	0
47	Y1	763	0	848	150	0
48	R2	581	0	629	84	0
48	Y2	581	0	629	78	0
49	R3	469	0	518	43	0
49	Y3	469	0	518	43	0
50	R4	581	0	574	167	0
50	Y4	581	0	574	184	0
51	R5	459	0	480	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Y5	459	0	480	76	1
52	R6	424	0	450	92	0
52	Y6	424	0	450	90	0
53	R7	430	0	480	48	0
53	Y7	430	0	480	43	0
54	R8	517	0	582	108	0
54	Y8	517	0	582	106	0
55	Z6	74	0	51	10	0
55	Z8	74	0	51	4	0
56	QA	60	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	2	0	0	0	0
56	QX	2	0	0	0	0
56	R5	1	0	0	0	0
56	RA	212	0	0	0	0
56	RB	2	0	0	0	0
56	RE	2	0	0	0	0
56	RF	1	0	0	0	0
56	RP	1	0	0	0	0
56	XA	63	0	0	0	0
56	XM	2	0	0	0	0
56	XV	2	0	0	0	0
56	Y5	1	0	0	0	0
56	YA	242	0	0	0	0
56	YB	2	0	0	0	0
56	YE	2	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	4	0
57	XA	42	0	45	1	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
All	All	291123	0	197505	17274	3

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 36.

The worst 5 of 17274 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:QN:39:LEU:HD22	14:QN:43:CYS:SG	1.33	1.63
36:YQ:81:VAL:HG23	46:Y0:7:LEU:CD2	1.21	1.60
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.54
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.35	1.52
19:QS:5:LEU:HD22	50:R4:67:TYR:CE2	1.45	1.51

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.98	0.22
31:YH:47:GLU:OE2	44:YY:79:CYS:CB[4_445]	2.04	0.16
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	2.06	0.14

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	3
2	XB	235/256 (92%)	152 (65%)	53 (23%)	30 (13%)	0	3
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	5
3	XC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	5
4	QD	206/209 (99%)	133 (65%)	51 (25%)	22 (11%)	0	4
4	XD	206/209 (99%)	133 (65%)	50 (24%)	23 (11%)	0	4
5	QE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	4
5	XE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	5
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	0	5
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	0	5
7	QG	153/156 (98%)	102 (67%)	37 (24%)	14 (9%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	XG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0 5
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0 4
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0 4
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0 3
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0 3
10	QJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0 4
10	XJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0 5
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1 7
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1 7
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0 4
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0 4
13	QM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0 1
13	XM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0 1
14	QN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0 1
14	XN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0 1
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1 8
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1 8
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0 2
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0 2
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	0 6
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	0 6
18	QR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0 3
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0 3
19	QS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0 0
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0 0
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0 1
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0 1
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0 1
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0 1
27	RD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	1 7
27	YD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0 1
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0 1
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0 5
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0 5
30	RG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0 3
30	YG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0 3
31	RH	168/180 (93%)	94 (56%)	35 (21%)	39 (23%)	0 0
31	YH	168/180 (93%)	95 (56%)	35 (21%)	38 (23%)	0 0
32	RI	144/148 (97%)	83 (58%)	33 (23%)	28 (19%)	0 1
32	YI	144/148 (97%)	85 (59%)	32 (22%)	27 (19%)	0 1
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0 1
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0 1
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1 7
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1 7
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0 1
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0 1
36	RQ	139/141 (99%)	94 (68%)	30 (22%)	15 (11%)	0 4
36	YQ	139/141 (99%)	94 (68%)	30 (22%)	15 (11%)	0 4
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0 3
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0 3
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0 1
38	YS	109/112 (97%)	63 (58%)	27 (25%)	19 (17%)	0 1
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0 2
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0 2
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1 7
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1 7
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0 5
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0 5
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0 3
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0 3
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	1 12
44	RY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0 0
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0 0
45	RZ	170/206 (82%)	91 (54%)	40 (24%)	39 (23%)	0 0
45	YZ	170/206 (82%)	91 (54%)	40 (24%)	39 (23%)	0 0
46	R0	80/85 (94%)	61 (76%)	14 (18%)	5 (6%)	1 10
46	Y0	80/85 (94%)	62 (78%)	12 (15%)	6 (8%)	1 7
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0 3
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0 3
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0 2
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0 2
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	1 12
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	1 12
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0 0
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0 0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0 0
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0 0
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0 0
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0 0
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1 10
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1 10
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0 1
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0 1
All	All	11378/12054 (94%)	7461 (66%)	2359 (21%)	1558 (14%)	0 2

5 of 1558 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	182 (89%)	23 (11%)	6	24
2	XB	205/220 (93%)	182 (89%)	23 (11%)	6	24
3	QC	159/188 (85%)	142 (89%)	17 (11%)	6	26
3	XC	159/188 (85%)	142 (89%)	17 (11%)	6	26
4	QD	180/181 (99%)	161 (89%)	19 (11%)	6	26
4	XD	180/181 (99%)	161 (89%)	19 (11%)	6	26
5	QE	116/123 (94%)	106 (91%)	10 (9%)	10	33
5	XE	116/123 (94%)	106 (91%)	10 (9%)	10	33
6	QF	90/90 (100%)	77 (86%)	13 (14%)	3	16
6	XF	90/90 (100%)	77 (86%)	13 (14%)	3	16
7	QG	126/127 (99%)	112 (89%)	14 (11%)	6	24
7	XG	126/127 (99%)	112 (89%)	14 (11%)	6	24
8	QH	119/119 (100%)	105 (88%)	14 (12%)	5	22
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	25
9	QI	98/99 (99%)	85 (87%)	13 (13%)	4	19
9	XI	98/99 (99%)	85 (87%)	13 (13%)	4	19
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	9	32
10	XJ	89/92 (97%)	80 (90%)	9 (10%)	7	27
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	28
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	28
12	QL	104/109 (95%)	86 (83%)	18 (17%)	2	10
12	XL	104/109 (95%)	86 (83%)	18 (17%)	2	10
13	QM	97/101 (96%)	83 (86%)	14 (14%)	3	16
13	XM	97/101 (96%)	82 (84%)	15 (16%)	2	13
14	QN	49/50 (98%)	45 (92%)	4 (8%)	10	35
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	QO	79/80 (99%)	70 (89%)	9 (11%)	5 23
15	XO	79/80 (99%)	70 (89%)	9 (11%)	5 23
16	QP	72/74 (97%)	64 (89%)	8 (11%)	6 24
16	XP	72/74 (97%)	64 (89%)	8 (11%)	6 24
17	QQ	95/97 (98%)	86 (90%)	9 (10%)	8 30
17	XQ	95/97 (98%)	86 (90%)	9 (10%)	8 30
18	QR	61/77 (79%)	51 (84%)	10 (16%)	2 12
18	XR	61/77 (79%)	51 (84%)	10 (16%)	2 12
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3 14
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3 14
20	QT	76/82 (93%)	69 (91%)	7 (9%)	8 31
20	XT	76/82 (93%)	69 (91%)	7 (9%)	8 31
21	QU	20/22 (91%)	20 (100%)	0	100 100
21	XU	20/22 (91%)	20 (100%)	0	100 100
27	RD	214/218 (98%)	174 (81%)	40 (19%)	1 8
27	YD	214/218 (98%)	174 (81%)	40 (19%)	1 8
28	RE	165/166 (99%)	125 (76%)	40 (24%)	1 3
28	YE	165/166 (99%)	125 (76%)	40 (24%)	1 3
29	RF	161/166 (97%)	138 (86%)	23 (14%)	3 16
29	YF	161/166 (97%)	137 (85%)	24 (15%)	3 15
30	RG	155/156 (99%)	133 (86%)	22 (14%)	3 16
30	YG	155/156 (99%)	134 (86%)	21 (14%)	4 18
31	RH	142/148 (96%)	111 (78%)	31 (22%)	1 5
31	YH	142/148 (96%)	112 (79%)	30 (21%)	1 5
32	RI	122/124 (98%)	95 (78%)	27 (22%)	1 5
32	YI	122/124 (98%)	94 (77%)	28 (23%)	1 4
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2 11
33	YN	117/119 (98%)	97 (83%)	20 (17%)	2 11
34	RO	100/100 (100%)	88 (88%)	12 (12%)	5 22
34	YO	100/100 (100%)	88 (88%)	12 (12%)	5 22
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	YP	116/116 (100%)	88 (76%)	28 (24%)	1 3
36	RQ	111/111 (100%)	94 (85%)	17 (15%)	3 14
36	YQ	111/111 (100%)	94 (85%)	17 (15%)	3 14
37	RR	101/101 (100%)	85 (84%)	16 (16%)	2 13
37	YR	101/101 (100%)	85 (84%)	16 (16%)	2 13
38	RS	87/88 (99%)	73 (84%)	14 (16%)	2 12
38	YS	87/88 (99%)	73 (84%)	14 (16%)	2 12
39	RT	120/127 (94%)	99 (82%)	21 (18%)	2 10
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2 10
40	RU	93/94 (99%)	81 (87%)	12 (13%)	4 19
40	YU	93/94 (99%)	81 (87%)	12 (13%)	4 19
41	RV	82/82 (100%)	67 (82%)	15 (18%)	2 9
41	YV	82/82 (100%)	66 (80%)	16 (20%)	1 7
42	RW	92/92 (100%)	76 (83%)	16 (17%)	2 10
42	YW	92/92 (100%)	75 (82%)	17 (18%)	1 8
43	RX	74/78 (95%)	61 (82%)	13 (18%)	2 10
43	YX	74/78 (95%)	61 (82%)	13 (18%)	2 10
44	RY	85/91 (93%)	66 (78%)	19 (22%)	1 4
44	YY	85/91 (93%)	66 (78%)	19 (22%)	1 4
45	RZ	152/179 (85%)	121 (80%)	31 (20%)	1 6
45	YZ	152/179 (85%)	121 (80%)	31 (20%)	1 6
46	R0	65/67 (97%)	56 (86%)	9 (14%)	3 17
46	Y0	65/67 (97%)	58 (89%)	7 (11%)	6 25
47	R1	82/83 (99%)	70 (85%)	12 (15%)	3 15
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	3 15
48	R2	64/67 (96%)	56 (88%)	8 (12%)	4 20
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6 25
49	R3	51/52 (98%)	41 (80%)	10 (20%)	1 7
49	Y3	51/52 (98%)	41 (80%)	10 (20%)	1 7
50	R4	63/63 (100%)	46 (73%)	17 (27%)	0 2
50	Y4	63/63 (100%)	46 (73%)	17 (27%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	R5	51/52 (98%)	40 (78%)	11 (22%)	1 5
51	Y5	51/52 (98%)	40 (78%)	11 (22%)	1 5
52	R6	48/52 (92%)	36 (75%)	12 (25%)	0 3
52	Y6	48/52 (92%)	36 (75%)	12 (25%)	0 3
53	R7	42/42 (100%)	38 (90%)	4 (10%)	8 30
53	Y7	42/42 (100%)	38 (90%)	4 (10%)	8 30
54	R8	54/55 (98%)	40 (74%)	14 (26%)	0 3
54	Y8	54/55 (98%)	40 (74%)	14 (26%)	0 3
All	All	9614/9998 (96%)	8124 (84%)	1490 (16%)	2 13

5 of 1490 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	XO	26	GLU
32	YI	79	ILE
18	XR	46	GLU
15	XO	8	LYS
28	YE	75	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 151 such sidechains are listed below:

Mol	Chain	Res	Type
33	YN	130	HIS
47	Y1	66	HIS
35	YP	81	GLN
41	YV	87	HIS
54	Y8	33	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	343 (22%)	51 (3%)
1	XA	1499/1522 (98%)	335 (22%)	55 (3%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	6 (85%)	1 (14%)
23	XX	7/25 (28%)	2 (28%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	QY	13/18 (72%)	6 (46%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2880/2916 (98%)	739 (25%)	76 (2%)
25	YA	2879/2916 (98%)	751 (26%)	75 (2%)
26	RB	119/122 (97%)	30 (25%)	2 (1%)
26	YB	119/122 (97%)	38 (31%)	1 (0%)
55	Z6	1/3 (33%)	0	0
55	Z8	1/3 (33%)	0	0
All	All	9189/9366 (98%)	2315 (25%)	265 (2%)

5 of 2315 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	9	G
1	QA	32	A
1	QA	39	G

5 of 265 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	YA	1653	G
25	YA	1929	G
25	YA	2832	U
25	RA	1379	A
25	RA	1266	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	PPU	Z8	76	25,55	37,40,41	2.57	8 (21%)	47,57,60	2.55	15 (31%)
24	1MG	QY	37	24	23,26,27	2.65	4 (17%)	33,39,42	2.01	8 (24%)
24	1MG	XY	37	24	23,26,27	2.64	4 (17%)	33,39,42	2.03	8 (24%)
55	PPU	Z6	76	25,55	37,40,41	2.57	8 (21%)	47,57,60	2.55	15 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PPU	Z8	76	25,55	-	2/25/43/44	0/4/4/4
24	1MG	QY	37	24	-	0/7/25/26	0/3/3/3
24	1MG	XY	37	24	-	0/7/25/26	0/3/3/3
55	PPU	Z6	76	25,55	-	2/25/43/44	0/4/4/4

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Z6	76	PPU	O-C	9.54	1.41	1.23
55	Z8	76	PPU	O-C	9.53	1.41	1.23
24	QY	37	1MG	C2-N2	8.13	1.48	1.34
24	XY	37	1MG	C2-N2	8.09	1.48	1.34
24	QY	37	1MG	C4-N3	6.64	1.49	1.34

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	Z8	76	PPU	C3'-N3'-C	-8.50	110.27	123.20
55	Z6	76	PPU	C3'-N3'-C	-8.49	110.28	123.20
24	QY	37	1MG	N2-C2-N1	6.23	123.79	118.79
24	XY	37	1MG	N2-C2-N1	6.09	123.68	118.79
55	Z6	76	PPU	C2'-C1'-N9	-5.97	98.48	113.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	Z8	76	PPU	4	0
24	XY	37	1MG	1	0
55	Z6	76	PPU	10	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 607 ligands modelled in this entry, 605 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	PAR	QA	1661	-	44,45,45	1.25	6 (13%)	63,67,67	1.30	8 (12%)
57	PAR	XA	1664	-	44,45,45	1.29	6 (13%)	63,67,67	1.30	6 (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
57	PAR	QA	1661	-	-	6/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	XA	1664	-	-	3/18/94/94	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	XA	1664	PAR	C52-C42	3.04	1.58	1.52
57	QA	1661	PAR	C52-C42	2.99	1.58	1.52
57	XA	1664	PAR	C11-C21	2.99	1.58	1.52
57	QA	1661	PAR	O54-C14	2.87	1.49	1.41
57	XA	1664	PAR	O54-C14	2.68	1.48	1.41

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	XA	1664	PAR	O33-C14-C24	4.64	115.67	108.08
57	QA	1661	PAR	C14-O54-C54	4.21	121.94	113.72
57	QA	1661	PAR	O33-C14-C24	4.07	114.74	108.08
57	XA	1664	PAR	C14-O54-C54	4.06	121.65	113.72
57	QA	1661	PAR	O54-C54-C64	3.26	112.33	106.07

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1661	PAR	C44-C54-C64-N64
57	QA	1661	PAR	O54-C54-C64-N64
57	XA	1664	PAR	O51-C51-C61-O61
57	XA	1664	PAR	C41-C51-C61-O61
57	QA	1661	PAR	O51-C51-C61-O61

There are no ring outliers.

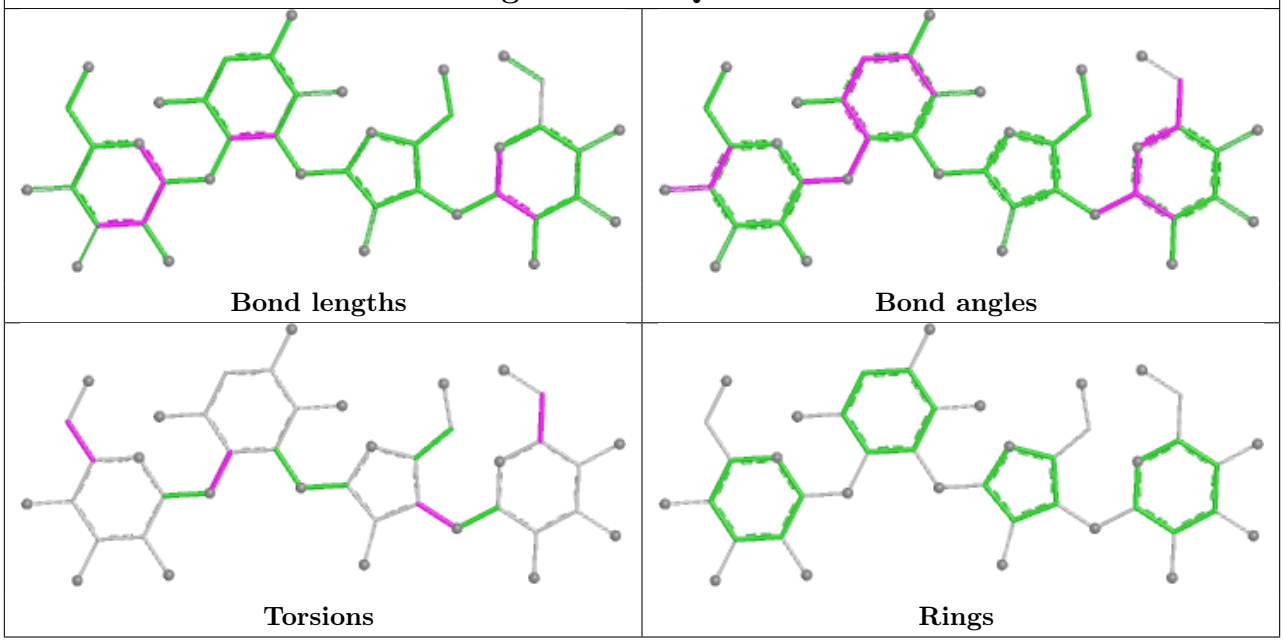
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	QA	1661	PAR	4	0
57	XA	1664	PAR	1	0

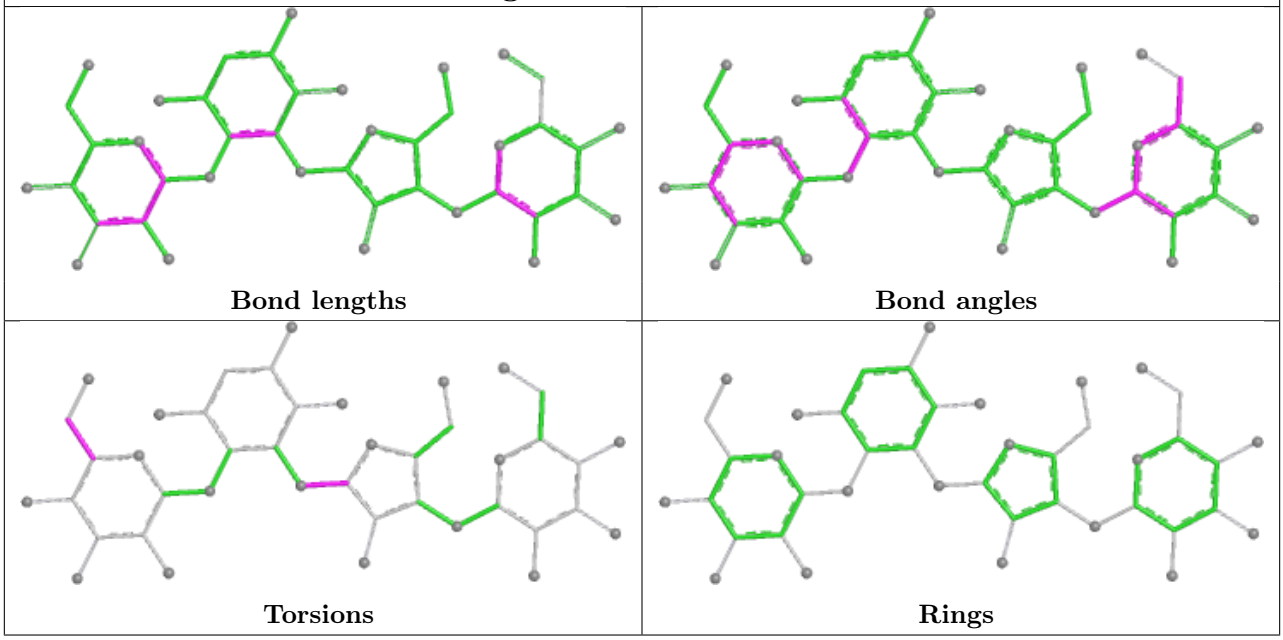
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PAR QA 1661



Ligand PAR XA 1664



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	QA	1500/1522 (98%)	0.54	94 (6%) 26 18	30, 83, 175, 356	0
1	XA	1501/1522 (98%)	0.37	65 (4%) 40 25	30, 76, 171, 324	0
2	QB	237/256 (92%)	1.62	76 (32%) 1 1	56, 138, 222, 266	0
2	XB	237/256 (92%)	1.32	52 (21%) 2 3	55, 126, 194, 238	0
3	QC	205/239 (85%)	1.17	38 (18%) 3 4	54, 122, 199, 216	0
3	XC	205/239 (85%)	0.97	34 (16%) 4 5	39, 95, 158, 217	0
4	QD	208/209 (99%)	1.28	56 (26%) 1 2	44, 92, 154, 184	0
4	XD	208/209 (99%)	1.41	57 (27%) 1 2	39, 95, 161, 234	0
5	QE	151/162 (93%)	1.59	49 (32%) 1 1	29, 104, 175, 237	0
5	XE	151/162 (93%)	0.91	18 (11%) 9 8	34, 79, 149, 229	0
6	QF	101/101 (100%)	1.00	13 (12%) 7 7	44, 86, 125, 222	0
6	XF	101/101 (100%)	0.80	9 (8%) 15 12	36, 86, 144, 209	0
7	QG	155/156 (99%)	1.22	27 (17%) 4 4	51, 106, 181, 215	0
7	XG	155/156 (99%)	1.06	22 (14%) 6 6	46, 103, 177, 230	0
8	QH	138/138 (100%)	1.44	35 (25%) 1 2	48, 108, 167, 204	0
8	XH	138/138 (100%)	1.29	26 (18%) 3 4	48, 96, 158, 208	0
9	QI	127/128 (99%)	1.59	35 (27%) 1 2	53, 124, 188, 214	0
9	XI	127/128 (99%)	1.39	24 (18%) 3 4	43, 116, 194, 219	0
10	QJ	99/105 (94%)	2.50	64 (64%) 0 0	67, 145, 212, 246	0
10	XJ	99/105 (94%)	1.80	38 (38%) 1 1	37, 119, 193, 210	0
11	QK	119/129 (92%)	1.70	41 (34%) 1 1	42, 92, 152, 199	0
11	XK	119/129 (92%)	1.42	31 (26%) 1 2	39, 89, 165, 204	0
12	QL	125/132 (94%)	1.56	36 (28%) 1 2	42, 84, 176, 269	0
12	XL	125/132 (94%)	1.25	30 (24%) 2 3	30, 66, 131, 242	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	QM	121/126 (96%)	1.49	33 (27%)	1	2	43, 124, 197, 254	0
13	XM	121/126 (96%)	1.36	27 (22%)	2	3	44, 98, 183, 264	0
14	QN	60/61 (98%)	2.26	30 (50%)	0	1	61, 128, 195, 227	0
14	XN	60/61 (98%)	1.40	13 (21%)	2	3	47, 87, 134, 161	0
15	QO	88/89 (98%)	1.36	22 (25%)	2	3	42, 97, 165, 235	0
15	XO	88/89 (98%)	0.97	14 (15%)	5	5	39, 79, 130, 178	0
16	QP	84/88 (95%)	1.55	28 (33%)	1	1	41, 79, 136, 206	0
16	XP	84/88 (95%)	1.64	25 (29%)	1	2	54, 92, 151, 203	0
17	QQ	100/105 (95%)	1.72	34 (34%)	1	1	53, 102, 165, 210	0
17	XQ	100/105 (95%)	1.64	31 (31%)	1	1	38, 101, 159, 213	0
18	QR	70/88 (79%)	1.05	11 (15%)	5	5	34, 90, 156, 213	0
18	XR	70/88 (79%)	0.83	3 (4%)	40	25	30, 88, 138, 206	0
19	QS	84/93 (90%)	1.91	34 (40%)	0	1	87, 149, 204, 237	0
19	XS	84/93 (90%)	1.57	31 (36%)	1	1	55, 105, 176, 244	0
20	QT	99/106 (93%)	1.66	35 (35%)	1	1	48, 101, 192, 233	0
20	XT	99/106 (93%)	1.38	23 (23%)	2	3	50, 107, 163, 197	0
21	QU	25/27 (92%)	2.62	16 (64%)	0	0	41, 100, 139, 189	0
21	XU	25/27 (92%)	2.33	15 (60%)	0	0	52, 96, 135, 165	0
22	QV	77/77 (100%)	1.15	10 (12%)	7	7	40, 91, 151, 170	0
22	XV	77/77 (100%)	0.76	9 (11%)	9	8	34, 77, 126, 180	0
23	QX	8/25 (32%)	2.22	5 (62%)	0	0	61, 82, 137, 169	0
23	XX	8/25 (32%)	1.40	1 (12%)	8	7	39, 67, 104, 175	0
24	QY	13/18 (72%)	1.96	3 (23%)	2	3	93, 213, 294, 312	0
24	XY	13/18 (72%)	1.71	4 (30%)	1	1	69, 188, 276, 278	0
25	RA	2883/2916 (98%)	0.17	120 (4%)	40	26	24, 57, 221, 389	0
25	YA	2882/2916 (98%)	0.04	111 (3%)	43	27	17, 48, 215, 377	0
26	RB	120/122 (98%)	0.54	4 (3%)	49	32	52, 91, 141, 150	0
26	YB	120/122 (98%)	0.27	1 (0%)	82	64	44, 74, 109, 158	0
27	RD	272/276 (98%)	1.30	58 (21%)	2	3	19, 60, 98, 243	0
27	YD	272/276 (98%)	0.95	43 (15%)	5	5	13, 50, 85, 221	0
28	RE	205/206 (99%)	1.34	45 (21%)	2	3	24, 78, 165, 260	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	YE	205/206 (99%)	1.38	48 (23%)	2	3	22, 76, 161, 238	0
29	RF	202/210 (96%)	1.53	60 (29%)	1	2	21, 82, 158, 250	0
29	YF	202/210 (96%)	1.17	47 (23%)	2	3	13, 64, 130, 197	0
30	RG	181/182 (99%)	3.27	125 (69%)	0	0	58, 164, 258, 303	0
30	YG	181/182 (99%)	2.28	99 (54%)	0	0	59, 108, 186, 248	0
31	RH	170/180 (94%)	1.63	54 (31%)	1	1	78, 171, 239, 267	0
31	YH	170/180 (94%)	1.81	64 (37%)	1	1	39, 100, 156, 260	0
32	RI	146/148 (98%)	1.55	41 (28%)	1	2	56, 118, 204, 240	0
32	YI	146/148 (98%)	1.07	25 (17%)	4	4	40, 104, 169, 214	0
33	RN	138/140 (98%)	1.14	20 (14%)	6	6	32, 84, 153, 194	0
33	YN	138/140 (98%)	0.99	18 (13%)	7	7	31, 78, 128, 166	0
34	RO	122/122 (100%)	1.18	24 (19%)	3	3	24, 71, 133, 170	0
34	YO	122/122 (100%)	1.27	27 (22%)	2	3	23, 66, 114, 153	0
35	RP	150/150 (100%)	1.61	47 (31%)	1	1	15, 79, 185, 232	0
35	YP	150/150 (100%)	1.47	40 (26%)	1	2	5, 68, 135, 230	0
36	RQ	141/141 (100%)	1.80	47 (33%)	1	1	38, 85, 149, 219	0
36	YQ	141/141 (100%)	1.34	30 (21%)	2	3	27, 66, 118, 196	0
37	RR	118/118 (100%)	1.08	23 (19%)	3	3	28, 68, 107, 171	0
37	YR	118/118 (100%)	1.18	23 (19%)	3	3	20, 64, 114, 153	0
38	RS	111/112 (99%)	1.20	18 (16%)	4	5	40, 90, 146, 203	0
38	YS	111/112 (99%)	0.99	16 (14%)	6	6	36, 77, 134, 207	0
39	RT	137/146 (93%)	1.59	43 (31%)	1	1	39, 90, 189, 221	0
39	YT	137/146 (93%)	1.46	34 (24%)	2	3	41, 78, 176, 220	0
40	RU	117/118 (99%)	1.33	25 (21%)	2	3	27, 73, 155, 249	0
40	YU	117/118 (99%)	1.09	25 (21%)	2	3	20, 59, 129, 212	0
41	RV	101/101 (100%)	1.26	18 (17%)	4	4	28, 88, 167, 278	0
41	YV	101/101 (100%)	0.96	11 (10%)	10	9	25, 82, 143, 255	0
42	RW	113/113 (100%)	0.91	14 (12%)	8	7	28, 63, 127, 241	0
42	YW	113/113 (100%)	0.67	6 (5%)	32	21	22, 60, 109, 204	0
43	RX	92/96 (95%)	0.90	8 (8%)	16	12	31, 65, 108, 137	0
43	YX	92/96 (95%)	1.15	20 (21%)	2	3	21, 50, 92, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	RY	102/110 (92%)	2.56	55 (53%)	0	0	46, 106, 214, 270	0
44	YY	102/110 (92%)	1.59	34 (33%)	1	1	25, 85, 144, 243	0
45	RZ	172/206 (83%)	1.95	74 (43%)	0	1	62, 130, 264, 332	0
45	YZ	172/206 (83%)	1.96	71 (41%)	0	1	33, 111, 243, 361	0
46	R0	82/85 (96%)	1.18	17 (20%)	2	3	35, 72, 104, 143	0
46	Y0	82/85 (96%)	1.18	18 (21%)	2	3	28, 63, 99, 116	0
47	R1	97/98 (98%)	1.61	35 (36%)	1	1	24, 67, 167, 259	0
47	Y1	97/98 (98%)	1.37	24 (24%)	2	3	20, 65, 161, 211	0
48	R2	69/72 (95%)	1.18	14 (20%)	3	3	34, 82, 149, 217	0
48	Y2	69/72 (95%)	1.64	18 (26%)	1	2	22, 72, 138, 203	0
49	R3	59/60 (98%)	1.21	14 (23%)	2	3	35, 81, 147, 173	0
49	Y3	59/60 (98%)	1.13	13 (22%)	2	3	33, 67, 108, 178	0
50	R4	71/71 (100%)	2.23	34 (47%)	0	1	102, 207, 282, 352	0
50	Y4	71/71 (100%)	2.11	28 (39%)	1	1	88, 160, 251, 277	0
51	R5	59/60 (98%)	1.49	16 (27%)	1	2	12, 64, 224, 264	0
51	Y5	59/60 (98%)	1.09	10 (16%)	4	4	20, 71, 220, 229	0
52	R6	49/54 (90%)	2.65	30 (61%)	0	0	119, 196, 290, 297	0
52	Y6	49/54 (90%)	2.56	27 (55%)	0	0	120, 182, 235, 265	0
53	R7	49/49 (100%)	1.17	8 (16%)	4	5	19, 44, 100, 216	0
53	Y7	49/49 (100%)	1.28	9 (18%)	3	4	15, 37, 100, 216	0
54	R8	64/65 (98%)	1.84	27 (42%)	0	1	18, 62, 156, 228	0
54	Y8	64/65 (98%)	1.79	22 (34%)	1	1	20, 61, 116, 173	0
55	Z6	2/3 (66%)	0.37	0	100	100	49, 49, 49, 51	0
55	Z8	2/3 (66%)	0.13	0	100	100	36, 36, 36, 37	0
All	All	20776/21420 (96%)	0.91	3507 (16%)	4	4	5, 78, 194, 389	0

The worst 5 of 3507 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	R6	42	TRP	11.0
14	XN	2	ALA	10.7
30	RG	155	MET	10.5
36	RQ	141	GLN	10.2
8	XH	1	MET	10.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
24	1MG	QY	37	24/25	0.77	0.16	124,124,124,124	0
24	1MG	XY	37	24/25	0.88	0.11	89,89,89,89	0
55	PPU	Z6	76	37/38	0.93	0.15	53,53,53,53	0
55	PPU	Z8	76	37/38	0.94	0.14	40,40,40,40	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3027	1/1	0.34	0.52	80,80,80,80	0
56	MG	XA	1605	1/1	0.35	0.26	126,126,126,126	0
56	MG	QH	201	1/1	0.37	0.11	124,124,124,124	0
56	MG	YA	3169	1/1	0.40	0.33	84,84,84,84	0
56	MG	RA	3203	1/1	0.51	0.20	73,73,73,73	0
56	MG	RA	3191	1/1	0.53	0.30	62,62,62,62	0
56	MG	YA	3012	1/1	0.59	0.87	80,80,80,80	0
56	MG	RA	3173	1/1	0.61	0.13	71,71,71,71	0
56	MG	YA	3039	1/1	0.62	0.19	30,30,30,30	0
56	MG	RA	3186	1/1	0.62	0.23	90,90,90,90	0
56	MG	YA	3186	1/1	0.62	0.28	50,50,50,50	0
56	MG	YA	3171	1/1	0.63	0.24	72,72,72,72	0
56	MG	YA	3120	1/1	0.66	0.20	36,36,36,36	0
56	MG	RA	3130	1/1	0.67	0.22	44,44,44,44	0
56	MG	XA	1638	1/1	0.67	0.29	55,55,55,55	0
56	MG	YA	3172	1/1	0.68	0.14	55,55,55,55	0
56	MG	QA	1639	1/1	0.68	0.19	44,44,44,44	0
56	MG	RA	3202	1/1	0.69	0.23	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	QA	1627	1/1	0.70	0.20	57,57,57,57	0
56	MG	YA	3151	1/1	0.70	0.30	26,26,26,26	0
56	MG	XA	1619	1/1	0.71	0.19	46,46,46,46	0
56	MG	RA	3175	1/1	0.71	0.27	99,99,99,99	0
56	MG	YA	3166	1/1	0.72	0.19	51,51,51,51	0
56	MG	RA	3033	1/1	0.73	0.26	62,62,62,62	0
56	MG	RA	3044	1/1	0.74	0.20	21,21,21,21	0
56	MG	YA	3084	1/1	0.74	0.17	23,23,23,23	0
56	MG	RA	3176	1/1	0.74	0.39	71,71,71,71	0
56	MG	YA	3181	1/1	0.75	0.23	51,51,51,51	0
56	MG	YA	3177	1/1	0.75	0.22	35,35,35,35	0
56	MG	YA	3190	1/1	0.75	0.31	51,51,51,51	0
56	MG	XA	1620	1/1	0.76	0.18	55,55,55,55	0
56	MG	RA	3141	1/1	0.76	0.27	43,43,43,43	0
56	MG	XA	1644	1/1	0.76	0.10	59,59,59,59	0
56	MG	QA	1620	1/1	0.76	0.42	40,40,40,40	0
56	MG	YA	3207	1/1	0.76	0.34	66,66,66,66	0
56	MG	YA	3105	1/1	0.77	0.17	16,16,16,16	0
56	MG	RA	3190	1/1	0.77	0.17	50,50,50,50	0
56	MG	YA	3214	1/1	0.77	0.19	42,42,42,42	0
56	MG	XA	1647	1/1	0.78	0.35	58,58,58,58	0
56	MG	YA	3152	1/1	0.78	0.23	38,38,38,38	0
56	MG	RA	3192	1/1	0.78	0.28	56,56,56,56	0
56	MG	QA	1621	1/1	0.78	0.14	48,48,48,48	0
56	MG	XA	1636	1/1	0.79	0.21	58,58,58,58	0
56	MG	YA	3156	1/1	0.79	0.17	33,33,33,33	0
56	MG	YA	3208	1/1	0.79	0.30	53,53,53,53	0
56	MG	RA	3164	1/1	0.79	0.31	52,52,52,52	0
56	MG	YA	3239	1/1	0.79	0.37	48,48,48,48	0
56	MG	YA	3173	1/1	0.80	0.13	43,43,43,43	0
56	MG	QA	1615	1/1	0.80	0.24	46,46,46,46	0
56	MG	YA	3122	1/1	0.80	0.15	35,35,35,35	0
56	MG	YA	3116	1/1	0.80	0.23	28,28,28,28	0
56	MG	YA	3228	1/1	0.80	0.14	45,45,45,45	0
56	MG	YA	3188	1/1	0.80	0.15	38,38,38,38	0
56	MG	RA	3201	1/1	0.81	0.14	22,22,22,22	0
56	MG	YA	3139	1/1	0.81	0.16	32,32,32,32	0
56	MG	RA	3206	1/1	0.81	0.25	38,38,38,38	0
56	MG	RA	3080	1/1	0.81	0.34	44,44,44,44	0
56	MG	RA	3196	1/1	0.82	0.28	53,53,53,53	0
56	MG	QX	102	1/1	0.82	0.12	42,42,42,42	0
56	MG	RA	3048	1/1	0.82	0.13	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3070	1/1	0.82	0.31	37,37,37,37	0
56	MG	YA	3096	1/1	0.82	0.25	15,15,15,15	0
56	MG	RA	3073	1/1	0.82	0.19	5,5,5,5	0
56	MG	RA	3210	1/1	0.82	0.26	38,38,38,38	0
56	MG	QA	1649	1/1	0.82	0.15	45,45,45,45	0
56	MG	RA	3185	1/1	0.82	0.08	44,44,44,44	0
56	MG	RA	3111	1/1	0.82	0.10	52,52,52,52	0
56	MG	XA	1627	1/1	0.82	0.30	31,31,31,31	0
56	MG	RA	3122	1/1	0.82	0.17	70,70,70,70	0
56	MG	QA	1625	1/1	0.82	0.20	66,66,66,66	0
56	MG	RA	3131	1/1	0.82	0.28	77,77,77,77	0
56	MG	RA	3208	1/1	0.83	0.17	47,47,47,47	0
56	MG	QA	1626	1/1	0.83	0.36	77,77,77,77	0
56	MG	XA	1642	1/1	0.83	0.11	49,49,49,49	0
56	MG	RA	3101	1/1	0.83	0.21	50,50,50,50	0
56	MG	RA	3127	1/1	0.83	0.15	47,47,47,47	0
56	MG	RA	3146	1/1	0.83	0.17	44,44,44,44	0
56	MG	XA	1621	1/1	0.83	0.11	22,22,22,22	0
56	MG	YA	3236	1/1	0.83	0.12	57,57,57,57	0
56	MG	RA	3179	1/1	0.83	0.18	22,22,22,22	0
56	MG	YA	3141	1/1	0.84	0.22	43,43,43,43	0
56	MG	RA	3200	1/1	0.84	0.23	58,58,58,58	0
56	MG	QA	1640	1/1	0.84	0.12	54,54,54,54	0
56	MG	XA	1641	1/1	0.84	0.13	24,24,24,24	0
56	MG	RA	3056	1/1	0.84	0.20	26,26,26,26	0
56	MG	RA	3124	1/1	0.84	0.28	21,21,21,21	0
56	MG	RA	3193	1/1	0.84	0.12	49,49,49,49	0
56	MG	RA	3188	1/1	0.84	0.21	58,58,58,58	0
56	MG	YA	3130	1/1	0.84	0.13	16,16,16,16	0
56	MG	YA	3018	1/1	0.84	0.29	24,24,24,24	0
56	MG	YA	3240	1/1	0.84	0.17	45,45,45,45	0
56	MG	YA	3200	1/1	0.85	0.08	15,15,15,15	0
56	MG	QA	1637	1/1	0.85	0.31	49,49,49,49	0
56	MG	XM	201	1/1	0.85	0.07	28,28,28,28	0
56	MG	YA	3165	1/1	0.85	0.19	42,42,42,42	0
56	MG	XA	1610	1/1	0.85	0.22	37,37,37,37	0
56	MG	XA	1618	1/1	0.85	0.20	24,24,24,24	0
56	MG	YA	3170	1/1	0.85	0.28	10,10,10,10	0
56	MG	RA	3155	1/1	0.85	0.14	12,12,12,12	0
56	MG	YE	302	1/1	0.85	0.23	13,13,13,13	0
56	MG	RA	3140	1/1	0.86	0.26	45,45,45,45	0
56	MG	XA	1658	1/1	0.86	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	QA	1653	1/1	0.86	0.34	39,39,39,39	0
56	MG	XM	202	1/1	0.86	0.11	43,43,43,43	0
56	MG	RA	3187	1/1	0.86	0.44	68,68,68,68	0
56	MG	RA	3145	1/1	0.86	0.21	37,37,37,37	0
56	MG	QF	201	1/1	0.86	0.10	56,56,56,56	0
56	MG	YA	3045	1/1	0.86	0.22	22,22,22,22	0
56	MG	RA	3153	1/1	0.86	0.15	36,36,36,36	0
56	MG	QA	1631	1/1	0.86	0.11	55,55,55,55	0
56	MG	RA	3159	1/1	0.86	0.31	26,26,26,26	0
56	MG	YA	3106	1/1	0.86	0.34	32,32,32,32	0
56	MG	XA	1625	1/1	0.86	0.12	20,20,20,20	0
56	MG	YA	3199	1/1	0.86	0.28	42,42,42,42	0
56	MG	QA	1622	1/1	0.86	0.12	60,60,60,60	0
56	MG	XA	1631	1/1	0.86	0.19	45,45,45,45	0
56	MG	YA	3128	1/1	0.86	0.21	23,23,23,23	0
56	MG	RA	3069	1/1	0.86	0.21	43,43,43,43	0
56	MG	RA	3015	1/1	0.86	0.14	15,15,15,15	0
56	MG	QA	1638	1/1	0.86	0.18	53,53,53,53	0
56	MG	RA	3076	1/1	0.86	0.25	22,22,22,22	0
56	MG	RA	3183	1/1	0.86	0.15	49,49,49,49	0
56	MG	YA	3153	1/1	0.86	0.13	26,26,26,26	0
58	ZN	QN	101	1/1	0.86	0.09	155,155,155,155	0
56	MG	QA	1657	1/1	0.87	0.10	76,76,76,76	0
56	MG	RA	3199	1/1	0.87	0.24	47,47,47,47	0
56	MG	RA	3181	1/1	0.87	0.11	34,34,34,34	0
56	MG	RA	3012	1/1	0.87	0.35	26,26,26,26	0
56	MG	RA	3119	1/1	0.87	0.18	34,34,34,34	0
56	MG	YA	3019	1/1	0.87	0.29	21,21,21,21	0
56	MG	RA	3059	1/1	0.87	0.22	21,21,21,21	0
56	MG	RA	3123	1/1	0.87	0.16	32,32,32,32	0
56	MG	QA	1659	1/1	0.87	0.18	79,79,79,79	0
56	MG	YA	3085	1/1	0.87	0.30	41,41,41,41	0
56	MG	YA	3220	1/1	0.87	0.08	18,18,18,18	0
56	MG	RA	3092	1/1	0.87	0.14	18,18,18,18	0
56	MG	RA	3093	1/1	0.87	0.14	24,24,24,24	0
56	MG	RA	3095	1/1	0.87	0.17	31,31,31,31	0
56	MG	RA	3096	1/1	0.87	0.14	8,8,8,8	0
56	MG	YA	3119	1/1	0.87	0.31	35,35,35,35	0
56	MG	XA	1648	1/1	0.87	0.20	25,25,25,25	0
56	MG	QA	1635	1/1	0.88	0.17	31,31,31,31	0
56	MG	QA	1651	1/1	0.88	0.14	70,70,70,70	0
56	MG	YA	3124	1/1	0.88	0.23	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	QA	1652	1/1	0.88	0.07	36,36,36,36	0
56	MG	XA	1622	1/1	0.88	0.12	40,40,40,40	0
56	MG	YA	3016	1/1	0.88	0.12	19,19,19,19	0
56	MG	YA	3197	1/1	0.88	0.11	33,33,33,33	0
56	MG	RA	3180	1/1	0.88	0.10	28,28,28,28	0
56	MG	YA	3149	1/1	0.88	0.21	26,26,26,26	0
56	MG	QA	1601	1/1	0.88	0.25	27,27,27,27	0
56	MG	RA	3103	1/1	0.88	0.43	48,48,48,48	0
56	MG	QA	1655	1/1	0.88	0.15	50,50,50,50	0
56	MG	RA	3115	1/1	0.88	0.22	59,59,59,59	0
56	MG	QA	1617	1/1	0.88	0.17	41,41,41,41	0
56	MG	RA	3079	1/1	0.88	0.16	32,32,32,32	0
56	MG	QA	1614	1/1	0.88	0.22	38,38,38,38	0
56	MG	QA	1632	1/1	0.88	0.17	41,41,41,41	0
56	MG	RA	3126	1/1	0.88	0.20	27,27,27,27	0
56	MG	XA	1650	1/1	0.88	0.21	39,39,39,39	0
56	MG	RA	3116	1/1	0.89	0.15	69,69,69,69	0
56	MG	RA	3068	1/1	0.89	0.17	16,16,16,16	0
56	MG	RA	3046	1/1	0.89	0.16	31,31,31,31	0
56	MG	RA	3136	1/1	0.89	0.24	49,49,49,49	0
56	MG	RA	3161	1/1	0.89	0.17	32,32,32,32	0
56	MG	YA	3198	1/1	0.89	0.29	32,32,32,32	0
56	MG	YA	3070	1/1	0.89	0.13	22,22,22,22	0
56	MG	QA	1634	1/1	0.89	0.08	48,48,48,48	0
56	MG	XA	1649	1/1	0.89	0.26	28,28,28,28	0
56	MG	QA	1623	1/1	0.89	0.19	28,28,28,28	0
56	MG	XA	1652	1/1	0.89	0.08	64,64,64,64	0
56	MG	RA	3143	1/1	0.89	0.30	16,16,16,16	0
56	MG	XA	1662	1/1	0.89	0.18	27,27,27,27	0
56	MG	RA	3144	1/1	0.89	0.14	36,36,36,36	0
56	MG	RA	3209	1/1	0.89	0.19	49,49,49,49	0
56	MG	XV	102	1/1	0.89	0.11	22,22,22,22	0
56	MG	QA	1630	1/1	0.89	0.17	66,66,66,66	0
57	PAR	QA	1661	42/42	0.89	0.20	75,75,75,75	0
56	MG	YA	3127	1/1	0.89	0.23	44,44,44,44	0
56	MG	YA	3168	1/1	0.90	0.30	65,65,65,65	0
56	MG	RA	3102	1/1	0.90	0.26	32,32,32,32	0
56	MG	RA	3074	1/1	0.90	0.18	8,8,8,8	0
56	MG	YA	3098	1/1	0.90	0.15	49,49,49,49	0
56	MG	XA	1656	1/1	0.90	0.09	37,37,37,37	0
56	MG	RA	3106	1/1	0.90	0.38	24,24,24,24	0
56	MG	RA	3008	1/1	0.90	0.17	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1663	1/1	0.90	0.14	85,85,85,85	0
56	MG	RA	3077	1/1	0.90	0.27	14,14,14,14	0
56	MG	QA	1643	1/1	0.90	0.19	24,24,24,24	0
56	MG	RA	3117	1/1	0.90	0.26	42,42,42,42	0
56	MG	YA	3196	1/1	0.90	0.15	33,33,33,33	0
56	MG	YA	3009	1/1	0.90	0.29	27,27,27,27	0
56	MG	XA	1637	1/1	0.90	0.22	39,39,39,39	0
56	MG	QA	1644	1/1	0.90	0.19	23,23,23,23	0
56	MG	YA	3133	1/1	0.90	0.29	43,43,43,43	0
56	MG	YA	3201	1/1	0.90	0.09	122,122,122,122	0
56	MG	RA	3066	1/1	0.90	0.10	12,12,12,12	0
56	MG	QA	1619	1/1	0.90	0.21	48,48,48,48	0
56	MG	YA	3209	1/1	0.90	0.22	41,41,41,41	0
56	MG	YA	3034	1/1	0.90	0.26	3,3,3,3	0
56	MG	YA	3215	1/1	0.90	0.20	51,51,51,51	0
56	MG	QA	1610	1/1	0.90	0.10	33,33,33,33	0
56	MG	QA	1629	1/1	0.90	0.21	68,68,68,68	0
56	MG	YA	3231	1/1	0.90	0.23	32,32,32,32	0
56	MG	YA	3049	1/1	0.90	0.29	15,15,15,15	0
56	MG	RA	3097	1/1	0.90	0.14	24,24,24,24	0
56	MG	YA	3159	1/1	0.90	0.27	43,43,43,43	0
56	MG	YA	3241	1/1	0.90	0.28	33,33,33,33	0
56	MG	YA	3162	1/1	0.90	0.10	34,34,34,34	0
56	MG	YA	3082	1/1	0.90	0.14	13,13,13,13	0
56	MG	QA	1609	1/1	0.90	0.24	34,34,34,34	0
56	MG	RA	3129	1/1	0.91	0.23	26,26,26,26	0
56	MG	YA	3099	1/1	0.91	0.30	11,11,11,11	0
56	MG	RA	3162	1/1	0.91	0.24	56,56,56,56	0
56	MG	QA	1633	1/1	0.91	0.26	50,50,50,50	0
56	MG	YA	3113	1/1	0.91	0.16	21,21,21,21	0
56	MG	YA	3183	1/1	0.91	0.23	36,36,36,36	0
56	MG	RA	3112	1/1	0.91	0.28	50,50,50,50	0
56	MG	RA	3197	1/1	0.91	0.25	50,50,50,50	0
56	MG	RA	3113	1/1	0.91	0.26	24,24,24,24	0
56	MG	QA	1660	1/1	0.91	0.14	45,45,45,45	0
56	MG	RA	3178	1/1	0.91	0.10	62,62,62,62	0
56	MG	RA	3011	1/1	0.91	0.15	30,30,30,30	0
56	MG	RA	3078	1/1	0.91	0.15	15,15,15,15	0
56	MG	QA	1613	1/1	0.91	0.32	56,56,56,56	0
56	MG	YA	3029	1/1	0.91	0.28	17,17,17,17	0
56	MG	YA	3032	1/1	0.91	0.21	9,9,9,9	0
56	MG	QA	1618	1/1	0.91	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3081	1/1	0.91	0.20	28,28,28,28	0
56	MG	YA	3213	1/1	0.91	0.07	41,41,41,41	0
56	MG	XA	1645	1/1	0.91	0.12	31,31,31,31	0
56	MG	RA	3150	1/1	0.91	0.16	26,26,26,26	0
56	MG	YA	3218	1/1	0.91	0.14	19,19,19,19	0
56	MG	YA	3063	1/1	0.91	0.11	6,6,6,6	0
56	MG	RA	3105	1/1	0.91	0.19	50,50,50,50	0
56	MG	YA	3158	1/1	0.91	0.11	20,20,20,20	0
56	MG	YA	3074	1/1	0.91	0.14	28,28,28,28	0
56	MG	YA	3079	1/1	0.91	0.18	18,18,18,18	0
56	MG	XA	1609	1/1	0.91	0.23	15,15,15,15	0
56	MG	RA	3024	1/1	0.91	0.27	4,4,4,4	0
56	MG	XA	1615	1/1	0.91	0.16	19,19,19,19	0
56	MG	Y5	101	1/1	0.91	0.17	25,25,25,25	0
56	MG	YA	3094	1/1	0.91	0.22	10,10,10,10	0
57	PAR	XA	1664	42/42	0.91	0.16	57,57,57,57	0
56	MG	RA	3108	1/1	0.91	0.17	26,26,26,26	0
56	MG	RA	3061	1/1	0.92	0.11	28,28,28,28	0
56	MG	XA	1659	1/1	0.92	0.14	60,60,60,60	0
56	MG	RA	3091	1/1	0.92	0.06	21,21,21,21	0
56	MG	RA	3151	1/1	0.92	0.08	23,23,23,23	0
56	MG	YA	3081	1/1	0.92	0.14	18,18,18,18	0
56	MG	RA	3098	1/1	0.92	0.14	11,11,11,11	0
56	MG	XA	1639	1/1	0.92	0.22	32,32,32,32	0
56	MG	XA	1640	1/1	0.92	0.14	47,47,47,47	0
56	MG	YA	3001	1/1	0.92	0.25	13,13,13,13	0
56	MG	RA	3036	1/1	0.92	0.25	10,10,10,10	0
56	MG	QA	1604	1/1	0.92	0.11	33,33,33,33	0
56	MG	RA	3160	1/1	0.92	0.08	25,25,25,25	0
56	MG	RA	3025	1/1	0.92	0.08	9,9,9,9	0
56	MG	RA	3114	1/1	0.92	0.10	30,30,30,30	0
56	MG	YA	3219	1/1	0.92	0.17	29,29,29,29	0
56	MG	RA	3104	1/1	0.92	0.21	44,44,44,44	0
56	MG	YA	3227	1/1	0.92	0.12	22,22,22,22	0
56	MG	YA	3115	1/1	0.92	0.10	21,21,21,21	0
56	MG	YA	3229	1/1	0.92	0.17	52,52,52,52	0
56	MG	YA	3030	1/1	0.92	0.27	24,24,24,24	0
56	MG	RA	3205	1/1	0.92	0.20	54,54,54,54	0
56	MG	RA	3166	1/1	0.92	0.35	56,56,56,56	0
56	MG	XA	1626	1/1	0.92	0.25	27,27,27,27	0
56	MG	YA	3178	1/1	0.92	0.33	68,68,68,68	0
56	MG	YA	3040	1/1	0.92	0.12	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3182	1/1	0.92	0.29	30,30,30,30	0
56	MG	XA	1654	1/1	0.92	0.11	50,50,50,50	0
56	MG	RA	3128	1/1	0.92	0.16	27,27,27,27	0
56	MG	YA	3055	1/1	0.92	0.18	16,16,16,16	0
56	MG	RA	3172	1/1	0.93	0.16	29,29,29,29	0
56	MG	RA	3062	1/1	0.93	0.28	21,21,21,21	0
56	MG	YA	3126	1/1	0.93	0.09	27,27,27,27	0
56	MG	RA	3174	1/1	0.93	0.30	68,68,68,68	0
56	MG	YA	3192	1/1	0.93	0.20	40,40,40,40	0
56	MG	YA	3194	1/1	0.93	0.37	42,42,42,42	0
56	MG	RA	3121	1/1	0.93	0.27	35,35,35,35	0
56	MG	YA	3047	1/1	0.93	0.14	6,6,6,6	0
56	MG	XA	1655	1/1	0.93	0.21	33,33,33,33	0
56	MG	YA	3052	1/1	0.93	0.20	17,17,17,17	0
56	MG	YA	3140	1/1	0.93	0.17	2,2,2,2	0
56	MG	RA	3063	1/1	0.93	0.16	27,27,27,27	0
56	MG	YA	3148	1/1	0.93	0.07	25,25,25,25	0
56	MG	RA	3177	1/1	0.93	0.13	59,59,59,59	0
56	MG	RA	3039	1/1	0.93	0.22	18,18,18,18	0
56	MG	XA	1660	1/1	0.93	0.13	61,61,61,61	0
56	MG	RA	3083	1/1	0.93	0.11	26,26,26,26	0
56	MG	XA	1629	1/1	0.93	0.17	49,49,49,49	0
56	MG	QA	1656	1/1	0.93	0.14	53,53,53,53	0
56	MG	QA	1607	1/1	0.93	0.24	22,22,22,22	0
56	MG	RA	3031	1/1	0.93	0.19	26,26,26,26	0
56	MG	YA	3164	1/1	0.93	0.20	25,25,25,25	0
56	MG	YA	3088	1/1	0.93	0.24	20,20,20,20	0
56	MG	RA	3094	1/1	0.93	0.13	19,19,19,19	0
56	MG	RA	3054	1/1	0.93	0.20	5,5,5,5	0
56	MG	RA	3020	1/1	0.93	0.14	29,29,29,29	0
56	MG	YA	3237	1/1	0.93	0.14	15,15,15,15	0
56	MG	YA	3014	1/1	0.93	0.28	12,12,12,12	0
56	MG	RF	301	1/1	0.93	0.11	45,45,45,45	0
56	MG	R5	101	1/1	0.93	0.09	27,27,27,27	0
56	MG	RA	3034	1/1	0.93	0.22	16,16,16,16	0
56	MG	YX	101	1/1	0.93	0.06	28,28,28,28	0
56	MG	YA	3024	1/1	0.93	0.31	10,10,10,10	0
56	MG	RA	3189	1/1	0.93	0.07	34,34,34,34	0
56	MG	RA	3060	1/1	0.93	0.12	25,25,25,25	0
56	MG	QV	102	1/1	0.93	0.16	8,8,8,8	0
56	MG	YA	3044	1/1	0.94	0.24	9,9,9,9	0
56	MG	RA	3072	1/1	0.94	0.09	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3160	1/1	0.94	0.07	37,37,37,37	0
56	MG	XA	1646	1/1	0.94	0.10	23,23,23,23	0
56	MG	RA	3029	1/1	0.94	0.16	2,2,2,2	0
56	MG	RA	3120	1/1	0.94	0.08	10,10,10,10	0
56	MG	RA	3147	1/1	0.94	0.35	49,49,49,49	0
56	MG	YA	3056	1/1	0.94	0.07	9,9,9,9	0
56	MG	YA	3058	1/1	0.94	0.22	16,16,16,16	0
56	MG	XA	1606	1/1	0.94	0.23	17,17,17,17	0
56	MG	XA	1651	1/1	0.94	0.09	18,18,18,18	0
56	MG	RA	3148	1/1	0.94	0.17	21,21,21,21	0
56	MG	YA	3075	1/1	0.94	0.14	14,14,14,14	0
56	MG	XA	1653	1/1	0.94	0.35	44,44,44,44	0
56	MG	RA	3149	1/1	0.94	0.10	48,48,48,48	0
56	MG	YA	3179	1/1	0.94	0.24	31,31,31,31	0
56	MG	XA	1612	1/1	0.94	0.24	21,21,21,21	0
56	MG	YA	3083	1/1	0.94	0.19	21,21,21,21	0
56	MG	XA	1614	1/1	0.94	0.12	14,14,14,14	0
56	MG	QA	1616	1/1	0.94	0.09	42,42,42,42	0
56	MG	YA	3187	1/1	0.94	0.14	58,58,58,58	0
56	MG	RA	3057	1/1	0.94	0.09	22,22,22,22	0
56	MG	QX	101	1/1	0.94	0.07	24,24,24,24	0
56	MG	RA	3016	1/1	0.94	0.23	2,2,2,2	0
56	MG	YA	3097	1/1	0.94	0.21	19,19,19,19	0
56	MG	YA	3195	1/1	0.94	0.10	55,55,55,55	0
56	MG	RA	3156	1/1	0.94	0.18	22,22,22,22	0
56	MG	QA	1650	1/1	0.94	0.10	36,36,36,36	0
56	MG	XA	1623	1/1	0.94	0.22	31,31,31,31	0
56	MG	XA	1624	1/1	0.94	0.15	35,35,35,35	0
56	MG	YA	3107	1/1	0.94	0.12	25,25,25,25	0
56	MG	RA	3021	1/1	0.94	0.30	27,27,27,27	0
56	MG	YA	3203	1/1	0.94	0.06	24,24,24,24	0
56	MG	YA	3003	1/1	0.94	0.13	13,13,13,13	0
56	MG	YA	3008	1/1	0.94	0.21	17,17,17,17	0
56	MG	YA	3117	1/1	0.94	0.28	60,60,60,60	0
56	MG	RA	3043	1/1	0.94	0.11	30,30,30,30	0
56	MG	YA	3011	1/1	0.94	0.23	13,13,13,13	0
56	MG	YA	3121	1/1	0.94	0.15	23,23,23,23	0
56	MG	RA	3064	1/1	0.94	0.17	25,25,25,25	0
56	MG	RA	3087	1/1	0.94	0.11	9,9,9,9	0
56	MG	YA	3015	1/1	0.94	0.23	10,10,10,10	0
56	MG	YA	3224	1/1	0.94	0.15	18,18,18,18	0
56	MG	YA	3225	1/1	0.94	0.20	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	QA	1612	1/1	0.94	0.06	37,37,37,37	0
56	MG	XA	1635	1/1	0.94	0.10	36,36,36,36	0
56	MG	RA	3167	1/1	0.94	0.06	35,35,35,35	0
56	MG	YA	3131	1/1	0.94	0.07	20,20,20,20	0
56	MG	YA	3021	1/1	0.94	0.13	12,12,12,12	0
56	MG	RA	3171	1/1	0.94	0.20	49,49,49,49	0
56	MG	RA	3134	1/1	0.94	0.18	18,18,18,18	0
56	MG	RA	3010	1/1	0.94	0.24	4,4,4,4	0
56	MG	RA	3137	1/1	0.94	0.13	36,36,36,36	0
56	MG	YB	202	1/1	0.94	0.05	42,42,42,42	0
56	MG	YA	3033	1/1	0.94	0.23	6,6,6,6	0
56	MG	YA	3150	1/1	0.94	0.05	54,54,54,54	0
56	MG	QA	1605	1/1	0.94	0.09	51,51,51,51	0
56	MG	RA	3053	1/1	0.94	0.20	5,5,5,5	0
56	MG	RA	3071	1/1	0.94	0.10	32,32,32,32	0
56	MG	YA	3041	1/1	0.94	0.23	6,6,6,6	0
56	MG	RA	3075	1/1	0.95	0.20	4,4,4,4	0
56	MG	YA	3136	1/1	0.95	0.17	4,4,4,4	0
56	MG	YA	3191	1/1	0.95	0.12	24,24,24,24	0
56	MG	QA	1608	1/1	0.95	0.21	27,27,27,27	0
56	MG	RA	3169	1/1	0.95	0.07	23,23,23,23	0
56	MG	RA	3018	1/1	0.95	0.18	6,6,6,6	0
56	MG	YA	3145	1/1	0.95	0.25	42,42,42,42	0
56	MG	YA	3146	1/1	0.95	0.17	50,50,50,50	0
56	MG	YA	3090	1/1	0.95	0.18	11,11,11,11	0
56	MG	RA	3030	1/1	0.95	0.16	15,15,15,15	0
56	MG	RA	3139	1/1	0.95	0.13	31,31,31,31	0
56	MG	QA	1624	1/1	0.95	0.24	24,24,24,24	0
56	MG	RB	202	1/1	0.95	0.09	31,31,31,31	0
56	MG	YA	3204	1/1	0.95	0.14	43,43,43,43	0
56	MG	YA	3205	1/1	0.95	0.12	28,28,28,28	0
56	MG	YA	3006	1/1	0.95	0.20	0,0,0,0	0
56	MG	YA	3102	1/1	0.95	0.17	5,5,5,5	0
56	MG	RA	3047	1/1	0.95	0.14	7,7,7,7	0
56	MG	YA	3210	1/1	0.95	0.05	35,35,35,35	0
56	MG	YA	3211	1/1	0.95	0.11	42,42,42,42	0
56	MG	YA	3212	1/1	0.95	0.05	21,21,21,21	0
56	MG	QA	1603	1/1	0.95	0.07	28,28,28,28	0
56	MG	XA	1602	1/1	0.95	0.12	15,15,15,15	0
56	MG	YA	3109	1/1	0.95	0.30	25,25,25,25	0
56	MG	YA	3163	1/1	0.95	0.17	40,40,40,40	0
56	MG	RA	3002	1/1	0.95	0.16	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3114	1/1	0.95	0.19	6,6,6,6	0
56	MG	YA	3221	1/1	0.95	0.10	26,26,26,26	0
56	MG	XA	1630	1/1	0.95	0.10	39,39,39,39	0
56	MG	RA	3084	1/1	0.95	0.24	17,17,17,17	0
56	MG	XA	1633	1/1	0.95	0.18	32,32,32,32	0
56	MG	YA	3118	1/1	0.95	0.23	12,12,12,12	0
56	MG	YA	3066	1/1	0.95	0.30	18,18,18,18	0
56	MG	YA	3068	1/1	0.95	0.23	12,12,12,12	0
56	MG	RA	3003	1/1	0.95	0.18	17,17,17,17	0
56	MG	YA	3175	1/1	0.95	0.08	12,12,12,12	0
56	MG	YA	3071	1/1	0.95	0.08	18,18,18,18	0
56	MG	RA	3163	1/1	0.95	0.16	38,38,38,38	0
56	MG	XA	1657	1/1	0.95	0.20	28,28,28,28	0
56	MG	YA	3180	1/1	0.95	0.17	53,53,53,53	0
56	MG	YA	3078	1/1	0.95	0.22	25,25,25,25	0
56	MG	YA	3022	1/1	0.95	0.21	6,6,6,6	0
56	MG	RA	3089	1/1	0.95	0.19	26,26,26,26	0
56	MG	YA	3185	1/1	0.95	0.09	10,10,10,10	0
56	MG	RA	3182	1/1	0.95	0.24	25,25,25,25	0
56	MG	YA	3132	1/1	0.95	0.09	13,13,13,13	0
58	ZN	XN	101	1/1	0.95	0.05	107,107,107,107	0
56	MG	YA	3087	1/1	0.96	0.17	7,7,7,7	0
56	MG	YA	3193	1/1	0.96	0.12	39,39,39,39	0
56	MG	YA	3142	1/1	0.96	0.10	30,30,30,30	0
56	MG	YA	3144	1/1	0.96	0.12	13,13,13,13	0
56	MG	YA	3031	1/1	0.96	0.22	6,6,6,6	0
56	MG	XA	1632	1/1	0.96	0.16	11,11,11,11	0
56	MG	RA	3088	1/1	0.96	0.05	24,24,24,24	0
56	MG	RA	3009	1/1	0.96	0.16	21,21,21,21	0
56	MG	RA	3125	1/1	0.96	0.13	24,24,24,24	0
56	MG	RA	3107	1/1	0.96	0.19	21,21,21,21	0
56	MG	RA	3195	1/1	0.96	0.22	28,28,28,28	0
56	MG	YA	3101	1/1	0.96	0.20	5,5,5,5	0
56	MG	YA	3155	1/1	0.96	0.14	22,22,22,22	0
56	MG	YA	3206	1/1	0.96	0.17	24,24,24,24	0
56	MG	XA	1611	1/1	0.96	0.13	29,29,29,29	0
56	MG	RA	3026	1/1	0.96	0.14	6,6,6,6	0
56	MG	XA	1613	1/1	0.96	0.10	45,45,45,45	0
56	MG	YA	3048	1/1	0.96	0.18	4,4,4,4	0
56	MG	YA	3161	1/1	0.96	0.17	30,30,30,30	0
56	MG	RA	3019	1/1	0.96	0.17	10,10,10,10	0
56	MG	YA	3111	1/1	0.96	0.16	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3050	1/1	0.96	0.23	2,2,2,2	0
56	MG	XA	1643	1/1	0.96	0.08	47,47,47,47	0
56	MG	RA	3051	1/1	0.96	0.35	1,1,1,1	0
56	MG	RA	3038	1/1	0.96	0.07	14,14,14,14	0
56	MG	RA	3014	1/1	0.96	0.15	10,10,10,10	0
56	MG	YA	3059	1/1	0.96	0.14	74,74,74,74	0
56	MG	RA	3132	1/1	0.96	0.13	12,12,12,12	0
56	MG	YA	3065	1/1	0.96	0.08	12,12,12,12	0
56	MG	YA	3226	1/1	0.96	0.15	14,14,14,14	0
56	MG	YA	3013	1/1	0.96	0.14	3,3,3,3	0
56	MG	YA	3174	1/1	0.96	0.20	29,29,29,29	0
56	MG	RA	3133	1/1	0.96	0.13	32,32,32,32	0
56	MG	YA	3176	1/1	0.96	0.09	54,54,54,54	0
56	MG	YA	3232	1/1	0.96	0.27	43,43,43,43	0
56	MG	YA	3233	1/1	0.96	0.07	44,44,44,44	0
56	MG	YA	3234	1/1	0.96	0.13	34,34,34,34	0
56	MG	YA	3235	1/1	0.96	0.21	26,26,26,26	0
56	MG	RA	3042	1/1	0.96	0.18	11,11,11,11	0
56	MG	RA	3135	1/1	0.96	0.19	32,32,32,32	0
56	MG	YA	3238	1/1	0.96	0.20	34,34,34,34	0
56	MG	QA	1642	1/1	0.96	0.05	49,49,49,49	0
56	MG	RA	3058	1/1	0.96	0.17	13,13,13,13	0
56	MG	YA	3129	1/1	0.96	0.10	22,22,22,22	0
56	MG	YA	3242	1/1	0.96	0.26	34,34,34,34	0
56	MG	YA	3020	1/1	0.96	0.22	8,8,8,8	0
56	MG	QA	1645	1/1	0.96	0.14	22,22,22,22	0
56	MG	RA	3085	1/1	0.96	0.07	15,15,15,15	0
56	MG	RE	301	1/1	0.96	0.10	22,22,22,22	0
56	MG	YA	3135	1/1	0.96	0.15	33,33,33,33	0
56	MG	YA	3027	1/1	0.96	0.14	5,5,5,5	0
56	MG	RA	3086	1/1	0.96	0.17	33,33,33,33	0
56	MG	RA	3045	1/1	0.96	0.21	12,12,12,12	0
56	MG	YA	3025	1/1	0.97	0.10	6,6,6,6	0
56	MG	YA	3080	1/1	0.97	0.24	3,3,3,3	0
56	MG	QA	1606	1/1	0.97	0.15	7,7,7,7	0
56	MG	YA	3028	1/1	0.97	0.12	23,23,23,23	0
56	MG	YA	3143	1/1	0.97	0.13	33,33,33,33	0
56	MG	QA	1641	1/1	0.97	0.17	25,25,25,25	0
56	MG	XA	1661	1/1	0.97	0.08	38,38,38,38	0
56	MG	YA	3202	1/1	0.97	0.04	21,21,21,21	0
56	MG	RA	3118	1/1	0.97	0.15	14,14,14,14	0
56	MG	YA	3086	1/1	0.97	0.10	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3082	1/1	0.97	0.06	13,13,13,13	0
56	MG	RA	3055	1/1	0.97	0.11	12,12,12,12	0
56	MG	RA	3184	1/1	0.97	0.17	33,33,33,33	0
56	MG	YA	3091	1/1	0.97	0.14	23,23,23,23	0
56	MG	YA	3092	1/1	0.97	0.10	11,11,11,11	0
56	MG	YA	3093	1/1	0.97	0.07	18,18,18,18	0
56	MG	YA	3038	1/1	0.97	0.10	12,12,12,12	0
56	MG	XV	101	1/1	0.97	0.14	14,14,14,14	0
56	MG	RA	3023	1/1	0.97	0.26	24,24,24,24	0
56	MG	XA	1617	1/1	0.97	0.14	26,26,26,26	0
56	MG	YA	3042	1/1	0.97	0.16	28,28,28,28	0
56	MG	YA	3217	1/1	0.97	0.06	35,35,35,35	0
56	MG	YA	3100	1/1	0.97	0.20	1,1,1,1	0
56	MG	YA	3002	1/1	0.97	0.23	15,15,15,15	0
56	MG	RA	3168	1/1	0.97	0.14	31,31,31,31	0
56	MG	YA	3004	1/1	0.97	0.11	13,13,13,13	0
56	MG	YA	3222	1/1	0.97	0.06	9,9,9,9	0
56	MG	YA	3223	1/1	0.97	0.05	30,30,30,30	0
56	MG	YA	3005	1/1	0.97	0.11	19,19,19,19	0
56	MG	RA	3207	1/1	0.97	0.13	51,51,51,51	0
56	MG	YA	3007	1/1	0.97	0.13	6,6,6,6	0
56	MG	RA	3065	1/1	0.97	0.17	21,21,21,21	0
56	MG	YA	3054	1/1	0.97	0.11	14,14,14,14	0
56	MG	RA	3110	1/1	0.97	0.08	51,51,51,51	0
56	MG	YA	3230	1/1	0.97	0.19	43,43,43,43	0
56	MG	RA	3152	1/1	0.97	0.09	26,26,26,26	0
56	MG	RA	3211	1/1	0.97	0.24	13,13,13,13	0
56	MG	RA	3037	1/1	0.97	0.07	10,10,10,10	0
56	MG	YA	3061	1/1	0.97	0.08	35,35,35,35	0
56	MG	YA	3062	1/1	0.97	0.09	6,6,6,6	0
56	MG	QA	1628	1/1	0.97	0.22	14,14,14,14	0
56	MG	YA	3064	1/1	0.97	0.07	23,23,23,23	0
56	MG	RA	3100	1/1	0.97	0.06	44,44,44,44	0
56	MG	RP	201	1/1	0.97	0.35	37,37,37,37	0
56	MG	YA	3125	1/1	0.97	0.05	18,18,18,18	0
56	MG	XA	1628	1/1	0.97	0.11	24,24,24,24	0
56	MG	YA	3069	1/1	0.97	0.14	16,16,16,16	0
56	MG	YB	201	1/1	0.97	0.18	21,21,21,21	0
56	MG	RA	3157	1/1	0.97	0.07	20,20,20,20	0
56	MG	YE	301	1/1	0.97	0.07	1,1,1,1	0
56	MG	RA	3194	1/1	0.97	0.10	14,14,14,14	0
56	MG	YA	3072	1/1	0.97	0.11	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3073	1/1	0.97	0.26	24,24,24,24	0
56	MG	XA	1603	1/1	0.97	0.12	23,23,23,23	0
56	MG	RA	3001	1/1	0.97	0.11	36,36,36,36	0
56	MG	YA	3077	1/1	0.97	0.18	8,8,8,8	0
56	MG	RA	3032	1/1	0.97	0.13	17,17,17,17	0
56	MG	RA	3142	1/1	0.98	0.09	15,15,15,15	0
56	MG	RA	3013	1/1	0.98	0.15	10,10,10,10	0
56	MG	YA	3057	1/1	0.98	0.27	22,22,22,22	0
56	MG	YA	3017	1/1	0.98	0.06	16,16,16,16	0
56	MG	RA	3165	1/1	0.98	0.03	5,5,5,5	0
56	MG	YA	3154	1/1	0.98	0.08	15,15,15,15	0
56	MG	YA	3103	1/1	0.98	0.07	12,12,12,12	0
56	MG	YA	3104	1/1	0.98	0.17	6,6,6,6	0
56	MG	YA	3157	1/1	0.98	0.16	29,29,29,29	0
56	MG	YA	3060	1/1	0.98	0.13	13,13,13,13	0
56	MG	RA	3212	1/1	0.98	0.23	18,18,18,18	0
56	MG	QA	1646	1/1	0.98	0.06	14,14,14,14	0
56	MG	RA	3090	1/1	0.98	0.11	14,14,14,14	0
56	MG	RE	302	1/1	0.98	0.24	22,22,22,22	0
56	MG	YA	3112	1/1	0.98	0.05	41,41,41,41	0
56	MG	QA	1647	1/1	0.98	0.07	41,41,41,41	0
56	MG	RA	3041	1/1	0.98	0.12	5,5,5,5	0
56	MG	YA	3026	1/1	0.98	0.30	9,9,9,9	0
56	MG	RA	3170	1/1	0.98	0.04	41,41,41,41	0
56	MG	XA	1601	1/1	0.98	0.07	15,15,15,15	0
56	MG	RA	3006	1/1	0.98	0.12	3,3,3,3	0
56	MG	RA	3028	1/1	0.98	0.12	12,12,12,12	0
56	MG	RA	3017	1/1	0.98	0.10	13,13,13,13	0
56	MG	QM	201	1/1	0.98	0.07	34,34,34,34	0
56	MG	XA	1607	1/1	0.98	0.16	5,5,5,5	0
56	MG	YA	3123	1/1	0.98	0.09	15,15,15,15	0
56	MG	QA	1648	1/1	0.98	0.04	100,100,100,100	0
56	MG	YA	3035	1/1	0.98	0.11	10,10,10,10	0
56	MG	YA	3036	1/1	0.98	0.14	3,3,3,3	0
56	MG	RA	3198	1/1	0.98	0.04	53,53,53,53	0
56	MG	QA	1658	1/1	0.98	0.04	68,68,68,68	0
56	MG	QA	1602	1/1	0.98	0.27	19,19,19,19	0
56	MG	RA	3050	1/1	0.98	0.12	0,0,0,0	0
56	MG	RA	3022	1/1	0.98	0.25	3,3,3,3	0
56	MG	YA	3184	1/1	0.98	0.13	33,33,33,33	0
56	MG	RA	3158	1/1	0.98	0.13	14,14,14,14	0
56	MG	XA	1616	1/1	0.98	0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3046	1/1	0.98	0.10	4,4,4,4	0
56	MG	RA	3204	1/1	0.98	0.04	30,30,30,30	0
56	MG	YA	3189	1/1	0.98	0.07	31,31,31,31	0
56	MG	YA	3137	1/1	0.98	0.07	15,15,15,15	0
56	MG	YA	3089	1/1	0.98	0.15	2,2,2,2	0
56	MG	YA	3010	1/1	0.98	0.11	3,3,3,3	0
56	MG	RA	3138	1/1	0.98	0.07	21,21,21,21	0
56	MG	RA	3052	1/1	0.98	0.37	24,24,24,24	0
56	MG	YA	3051	1/1	0.98	0.15	4,4,4,4	0
56	MG	RA	3035	1/1	0.98	0.11	21,21,21,21	0
56	MG	YA	3095	1/1	0.98	0.13	5,5,5,5	0
56	MG	YA	3053	1/1	0.98	0.20	4,4,4,4	0
56	MG	YA	3147	1/1	0.98	0.14	11,11,11,11	0
56	MG	QA	1654	1/1	0.98	0.13	14,14,14,14	0
56	MG	RA	3040	1/1	0.99	0.06	9,9,9,9	0
56	MG	RA	3004	1/1	0.99	0.06	5,5,5,5	0
56	MG	YA	3037	1/1	0.99	0.12	3,3,3,3	0
56	MG	RA	3049	1/1	0.99	0.10	10,10,10,10	0
56	MG	YA	3167	1/1	0.99	0.03	12,12,12,12	0
56	MG	XA	1634	1/1	0.99	0.06	28,28,28,28	0
56	MG	XA	1608	1/1	0.99	0.09	7,7,7,7	0
56	MG	YA	3108	1/1	0.99	0.10	5,5,5,5	0
56	MG	RA	3005	1/1	0.99	0.10	8,8,8,8	0
56	MG	YA	3216	1/1	0.99	0.04	42,42,42,42	0
56	MG	YA	3110	1/1	0.99	0.03	10,10,10,10	0
56	MG	RA	3067	1/1	0.99	0.05	7,7,7,7	0
56	MG	YA	3076	1/1	0.99	0.24	7,7,7,7	0
56	MG	YA	3043	1/1	0.99	0.26	9,9,9,9	0
56	MG	QA	1636	1/1	0.99	0.07	15,15,15,15	0
56	MG	YA	3134	1/1	0.99	0.09	29,29,29,29	0
56	MG	RA	3007	1/1	0.99	0.10	8,8,8,8	0
56	MG	QA	1611	1/1	0.99	0.04	32,32,32,32	0
56	MG	QV	101	1/1	0.99	0.12	17,17,17,17	0
56	MG	YA	3138	1/1	0.99	0.15	15,15,15,15	0
56	MG	RA	3109	1/1	0.99	0.06	26,26,26,26	0
58	ZN	QD	301	1/1	0.99	0.10	59,59,59,59	0
56	MG	RA	3099	1/1	0.99	0.07	21,21,21,21	0
56	MG	XA	1604	1/1	0.99	0.06	31,31,31,31	0
56	MG	RB	201	1/1	1.00	0.03	13,13,13,13	0
56	MG	YA	3067	1/1	1.00	0.06	15,15,15,15	0
56	MG	RA	3154	1/1	1.00	0.02	12,12,12,12	0
58	ZN	XD	301	1/1	1.00	0.14	49,49,49,49	0

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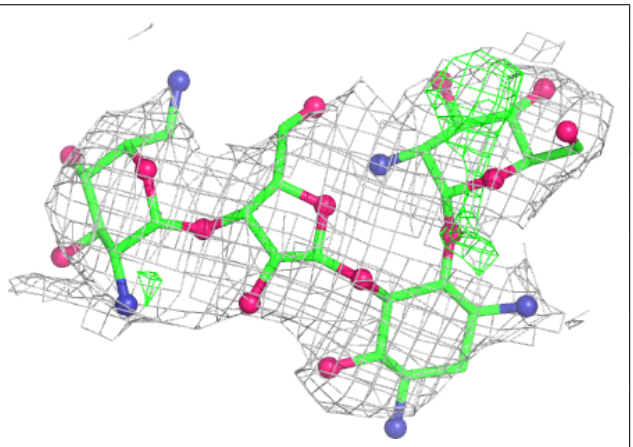
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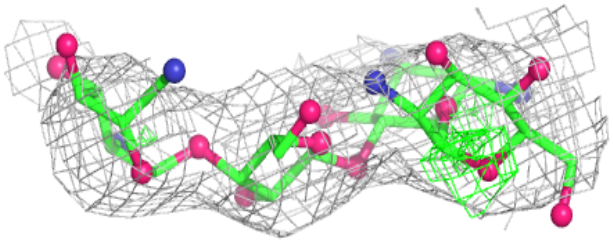
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3023	1/1	1.00	0.13	4,4,4,4	0

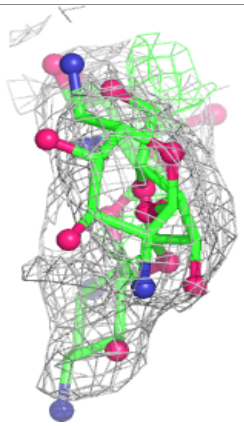
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR QA 1661:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

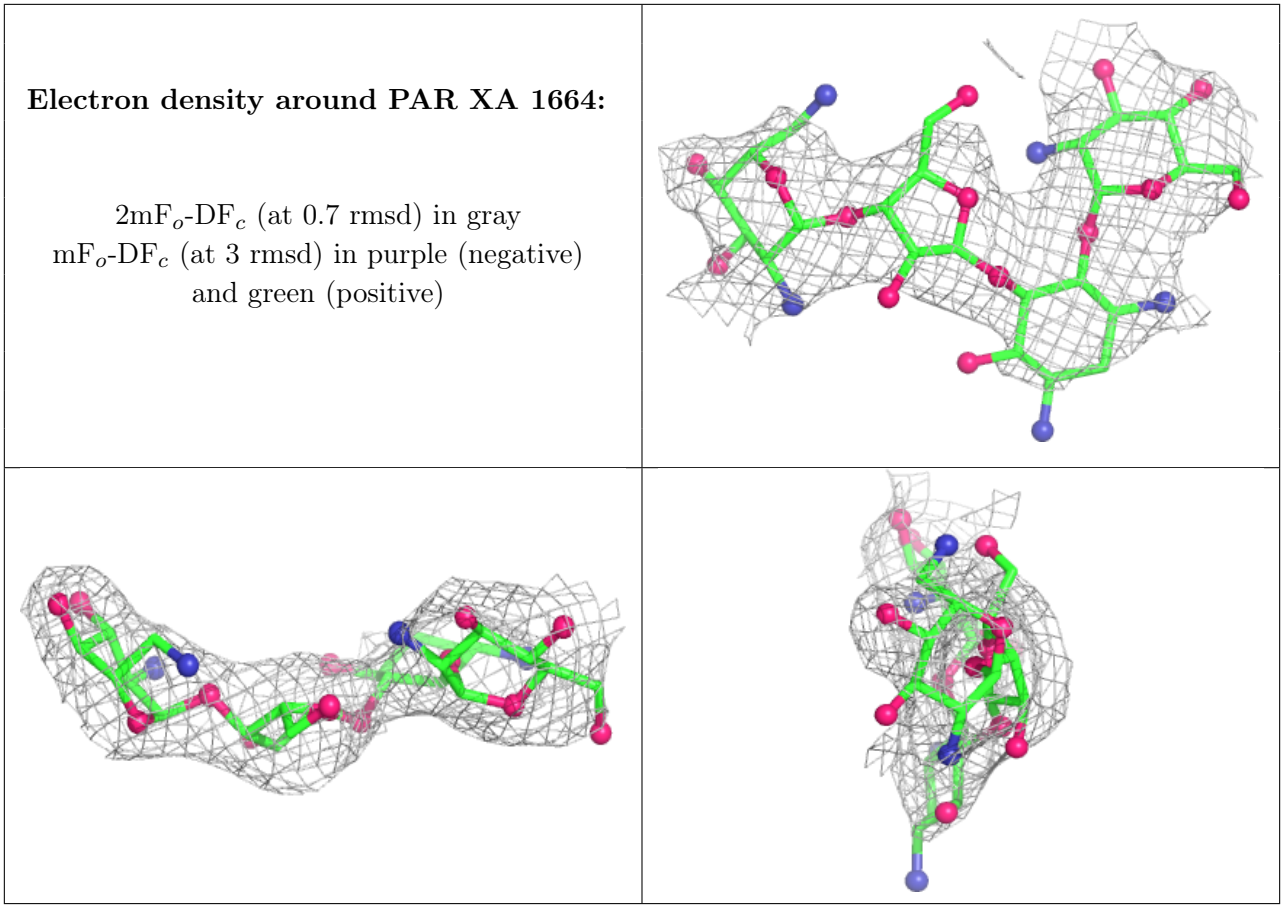






Electron density around PAR XA 1664:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.