wwPDB X-ray Structure Validation Summary Report (i)

Oct 1, 2023 – 01:02 PM EDT

PDB ID	:	4LSK
Title	:	Crystal Structure of tRNA Proline (CGG) Bound to Codon CCG-G on the Ribosome
Authors	:	Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on	:	2013-07-22
Resolution	:	3.48 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:

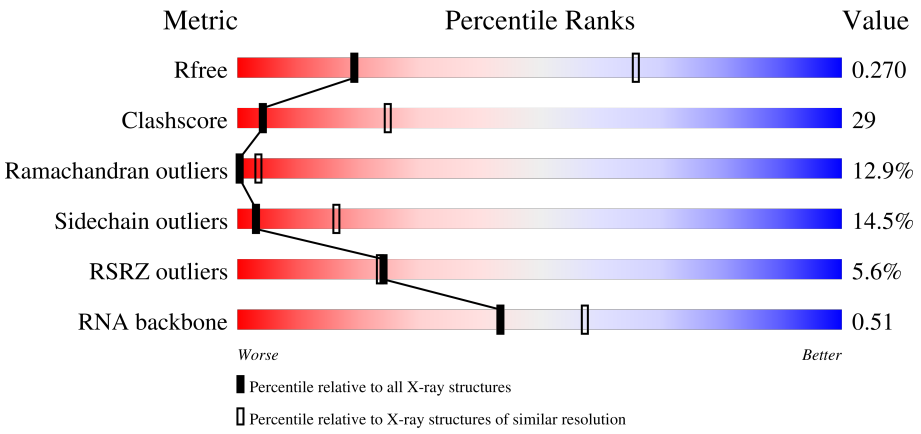
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.48 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)
RNA backbone	3102	1054 (4.00-2.96)

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	3% 52% 36% 9% ••
1	XA	1522	2% 51% 36% 10% ••
2	QB	256	11% 17% 59% 16% • 7%
2	XB	256	7% 17% 59% 16% • 7%

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Mol	Chain	Length	Quality of chain
3	QC	239	5% 23% 53% 9% 14%
3	XC	239	% 23% 53% 9% 14%
4	QD	209	2% 25% 59% 13%
4	XD	209	3% 27% 60% 11%
5	QE	162	3% 29% 52% 12% 7%
5	XE	162	3% 30% 52% 12% 7%
6	QF	101	2% 25% 59% 15%
6	XF	101	3% 23% 60% 16%
7	QG	156	10% 28% 62% 10%
7	XG	156	8% 29% 60% 10%
8	QH	138	2% 28% 59% 12%
8	XH	138	27% 60% 12%
9	QI	128	13% 21% 64% 13%
9	XI	128	5% 20% 66% 13%
10	QJ	105	32% 18% 63% 12% 6%
10	XJ	105	12% 16% 65% 12% 6%
11	QK	129	7% 33% 49% 9% 8%
11	XK	129	5% 32% 49% 11% 8%
12	QL	132	6% 30% 48% 14% 5%
12	XL	132	4% 30% 49% 14% 5%
13	QM	126	12% 21% 52% 21%
13	XM	126	5% 21% 52% 21%
14	QN	61	15% 16% 59% 15% 8%
14	XN	61	5% 15% 61% 18% 5%
15	QO	89	6% 33% 55% 11%

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Mol	Chain	Length	Quality of chain
15	XO	89	3% 30% 57% 11% •
16	QP	88	3% 18% 60% 15% • 5%
16	XP	88	2% 19% 59% 15% • 5%
17	QQ	105	4% 36% 48% 11% 5%
17	XQ	105	2% 35% 49% 11% 5%
18	QR	88	5% 24% 43% 11% • 20%
18	XR	88	% 22% 45% 11% • 20%
19	QS	93	18% 25% 40% 23% • 10%
19	XS	93	3% 25% 39% 23% • 10%
20	QT	106	4% 24% 50% 19% • 7%
20	XT	106	4% 25% 49% 19% • 7%
21	QU	27	33% 26% 48% 19% 7%
21	XU	27	15% 30% 44% 19% 7%
22	QV	77	6% 30% 53% 16% •
22	XV	77	3% 30% 53% 16% •
23	QY	17	12% 24% 41% 24% 12%
23	XY	17	12% 24% 29% 35% 12%
24	QX	25	8% 8% • 12% 8% 68%
24	XX	25	8% 8% • 12% 8% 68%
25	RA	2916	5% 54% 34% 10% ••
25	YA	2916	4% 54% 34% 10% ••
26	RB	122	2% 52% 32% 15% •
26	YB	122	63% 25% 10% •
27	RD	276	31% 51% 14% ••
27	YD	276	% 30% 53% 14% ••

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Mol	Chain	Length	Quality of chain
28	RE	206	3% 23% 48% 24% 5%
28	YE	206	2% 24% 46% 24% 5%
29	RF	210	2% 35% 47% 13%
29	YF	210	35% 48% 12%
30	RG	182	46% 21% 59% 16%
30	YG	182	18% 21% 60% 16%
31	RH	180	22% 23% 44% 19% 8% 6%
31	YH	180	5% 24% 43% 19% 8% 6%
32	RI	148	8% 46% 41% 11%
32	YI	148	4% 43% 38% 17%
33	RN	140	3% 18% 54% 26%
33	YN	140	% 19% 53% 26%
34	RO	122	% 35% 54% 9%
34	YO	122	34% 56% 9%
35	RP	150	8% 19% 51% 23% 8%
35	YP	150	3% 19% 51% 23% 7%
36	RQ	141	6% 31% 50% 16%
36	YQ	141	2% 31% 50% 16%
37	RR	118	% 32% 48% 17%
37	YR	118	35% 46% 17%
38	RS	112	3% 12% 63% 19% 5%
38	YS	112	2% 12% 62% 20%
39	RT	146	9% 21% 51% 19% 6%
39	YT	146	3% 21% 51% 20% 6%
40	RU	118	2% 34% 53% 11%

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Mol	Chain	Length	Quality of chain
40	YU	118	3% 30% 55% 13%
41	RV	101	3% 27% 52% 21%
41	YV	101	4% 28% 51% 21%
42	RW	113	2% 28% 50% 19%
42	YW	113	% 29% 50% 19%
43	RX	96	% 39% 43% 15%
43	YX	96	38% 44% 15%
44	RY	110	18% 17% 44% 28% 7%
44	YY	110	7% 19% 42% 28% 7%
45	RZ	206	10% 49% 31% 8% 11%
45	YZ	206	6% 50% 31% 8% 11%
46	R0	85	% 65% 27%
46	Y0	85	71% 22%
47	R1	98	7% 30% 48% 18%
47	Y1	98	7% 30% 48% 18%
48	R2	72	22% 54% 18%
48	Y2	72	% 22% 54% 18%
49	R3	60	10% 32% 52% 15%
49	Y3	60	3% 32% 52% 13%
50	R4	71	42% 7% 42% 39% 11%
50	Y4	71	30% 6% 44% 39% 11%
51	R5	60	18% 23% 47% 22% 7%
51	Y5	60	12% 22% 48% 22% 7%
52	R6	54	41% 7% 46% 31% 6% 9%
52	Y6	54	39% 7% 46% 31% 6% 9%

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Mol	Chain	Length	Quality of chain
53	R7	49	2% 37% 55% 8%
53	Y7	49	4% 35% 57% 8%
54	R8	65	5% 22% 43% 28% 6%
54	Y8	65	5% 20% 45% 28% 6%
55	R9	37	22% 46% 51%
55	Y9	37	11% 59% 35% 5%
56	Z6	3	33% 33% 33%
56	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
57	MG	QF	201	-	-	-	X
57	MG	RA	3091	-	-	-	X
57	MG	RA	3139	-	-	-	X
57	MG	RA	3199	-	-	-	X
57	MG	RA	3221	-	-	-	X
57	MG	RA	3223	-	-	-	X
57	MG	RA	3228	-	-	-	X
57	MG	XA	1657	-	-	-	X
57	MG	XA	1658	-	-	-	X
57	MG	XA	1673	-	-	-	X
57	MG	YA	3085	-	-	-	X
57	MG	YA	3122	-	-	-	X
57	MG	YA	3166	-	-	-	X
57	MG	YA	3177	-	-	-	X
57	MG	YA	3206	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 292002 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	QY	15	323	144	58	106	15	0	0	0
23	XY	15	323	144	58	106	15	0	0	0

- Molecule 24 is a RNA chain called A-site ASL SufA6.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	QA	65	65	65	0	0
57	QF	1	1	1	0	0
57	QH	1	1	1	0	0
57	QM	1	1	1	0	0
57	QV	1	1	1	0	0

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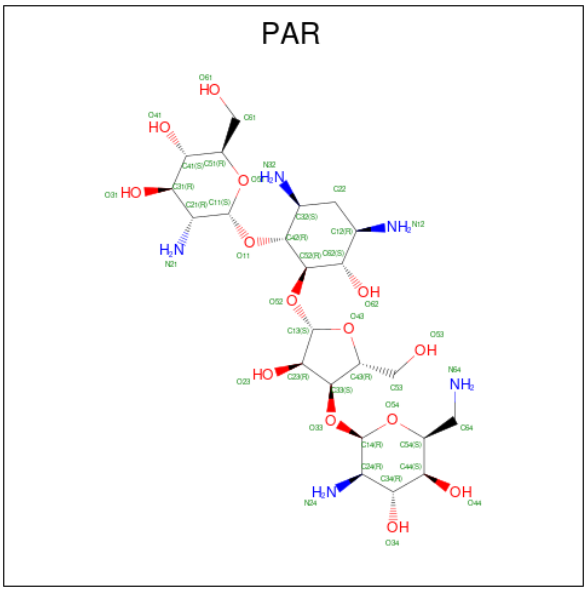
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	QX	1	1	1	0	0
57	RA	241	241	241	0	0
57	RB	2	2	2	0	0
57	RD	1	1	1	0	0
57	RE	2	2	2	0	0
57	RF	1	1	1	0	0
57	RR	2	2	2	0	0
57	R0	1	1	1	0	0
57	R5	1	1	1	0	0
57	XA	74	74	74	0	0
57	YA	268	268	268	0	0
57	YB	4	4	4	0	0
57	YE	1	1	1	0	0
57	YP	2	2	2	0	0
57	Y0	1	1	1	0	0
57	Y5	1	1	1	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

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

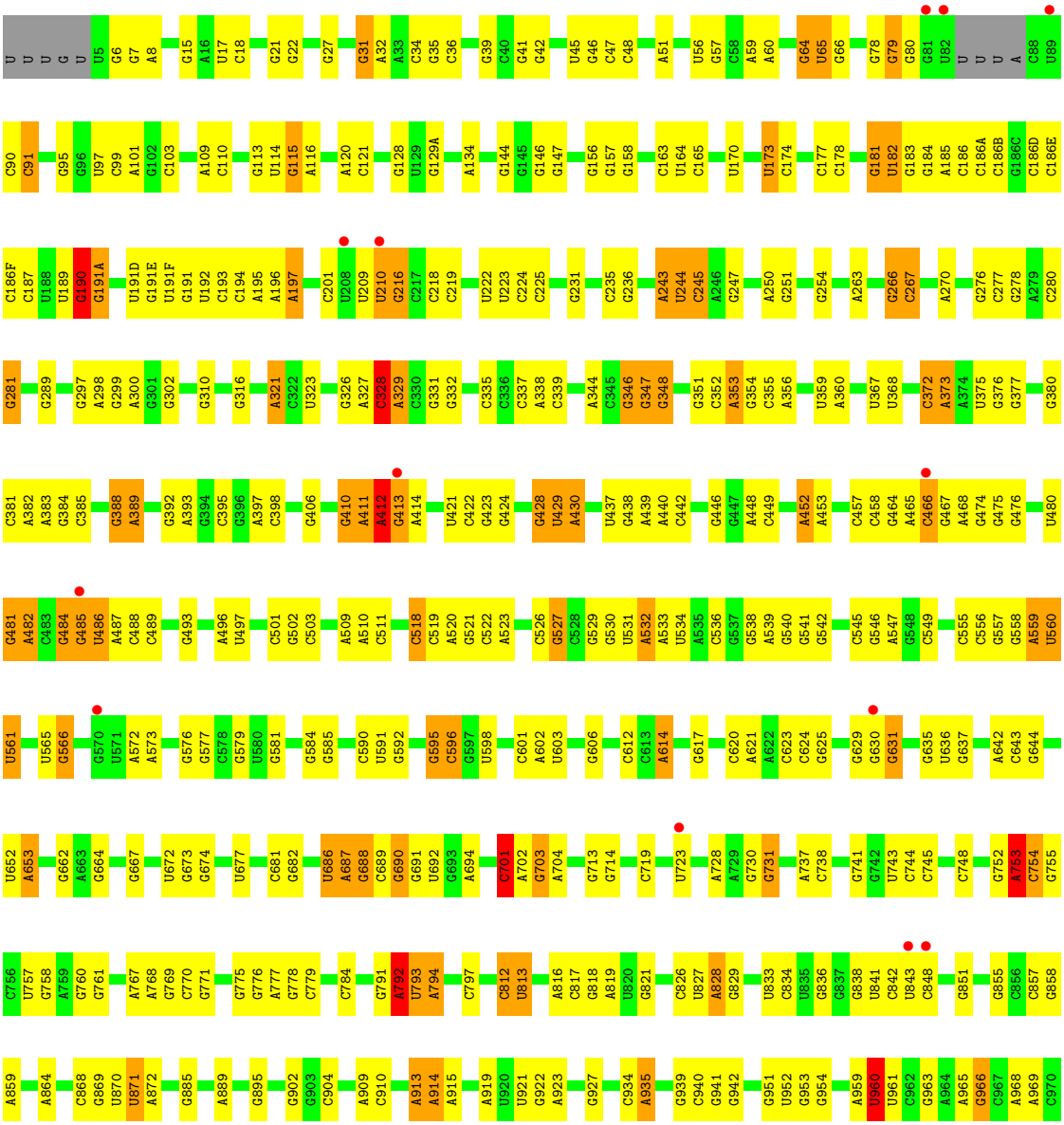
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
59	QD	1	1	1	0	0
			Total	Zn		
59	QN	1	1	1	0	0
			Total	Zn		
59	R9	1	1	1	0	0
			Total	Zn		
59	XD	1	1	1	0	0
			Total	Zn		
59	XN	1	1	1	0	0
			Total	Zn		
59	Y9	1	1	1	0	0

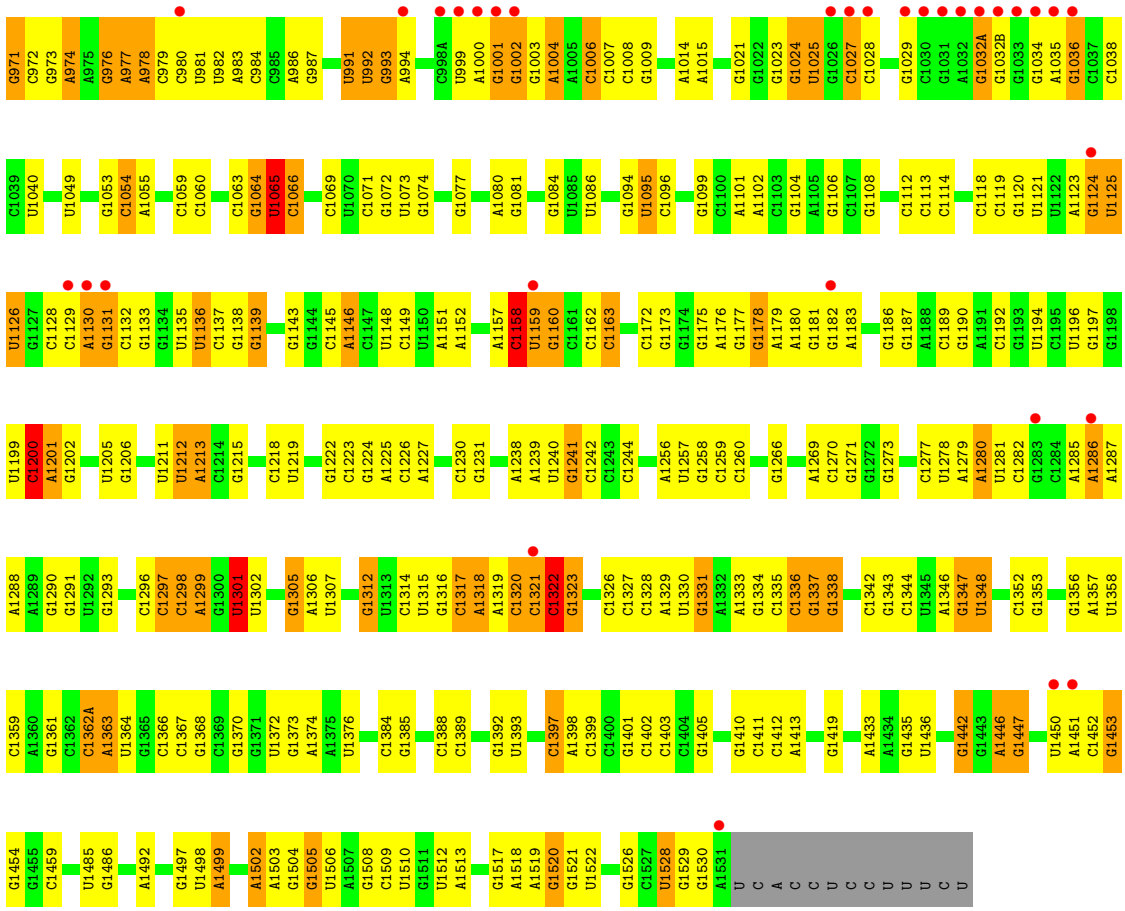
3 Residue-property plots (i)

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

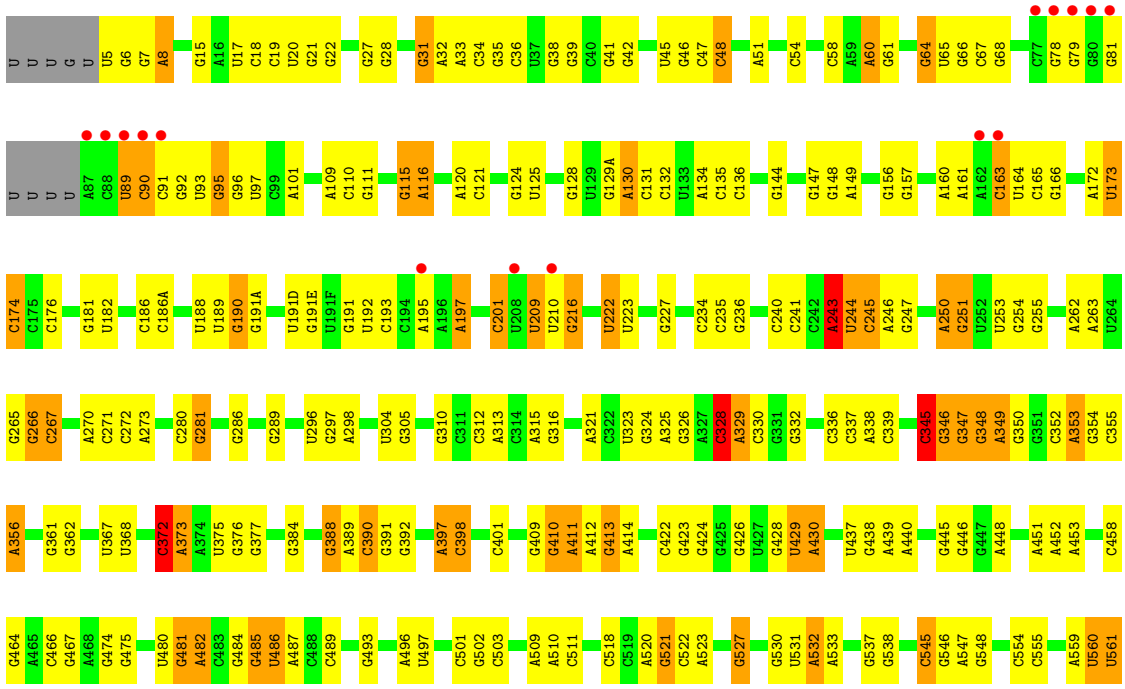
Chain QA: 3% 52% 36% 9%

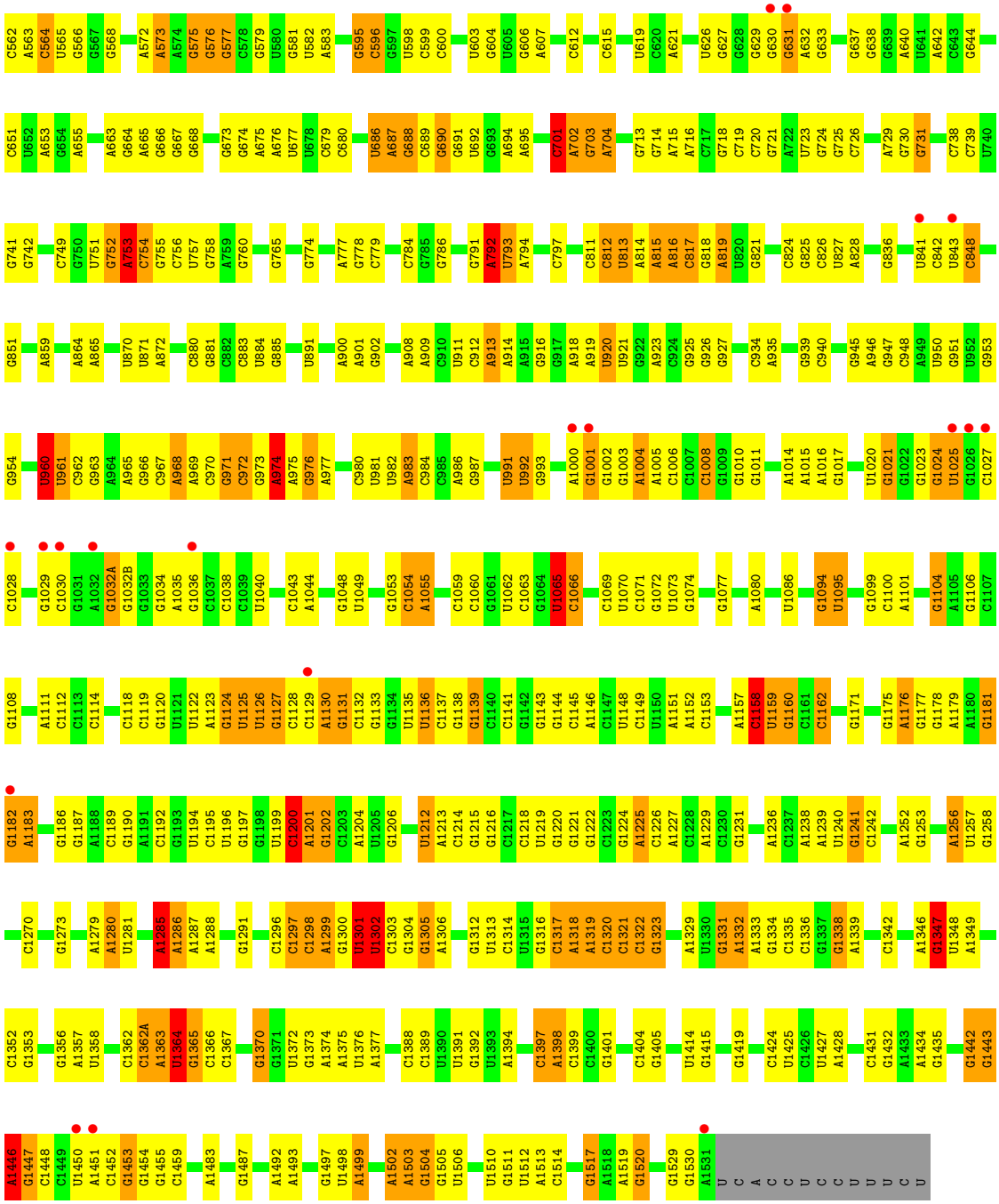




• Molecule 1: 16S rRNA

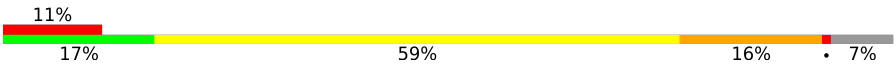
Chain XA:

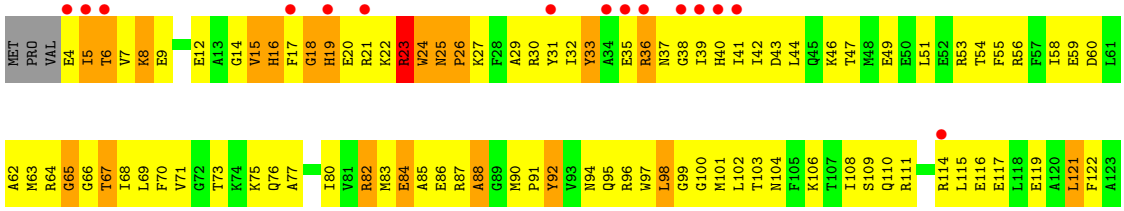


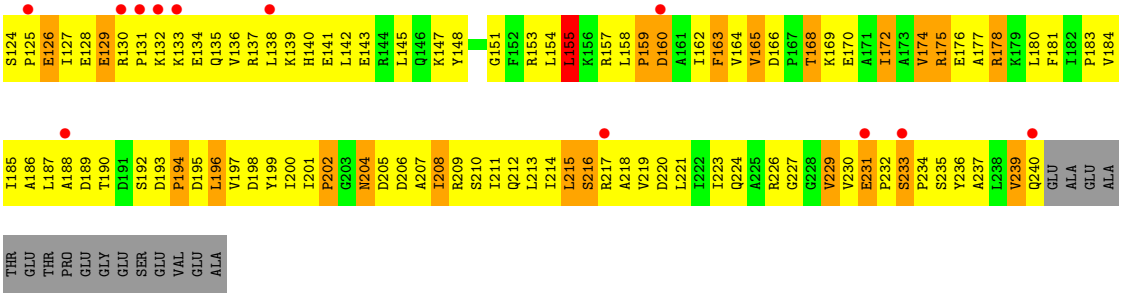


• Molecule 2: 30S ribosomal protein S2

Chain QB:

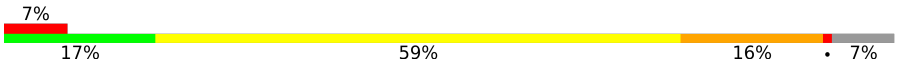


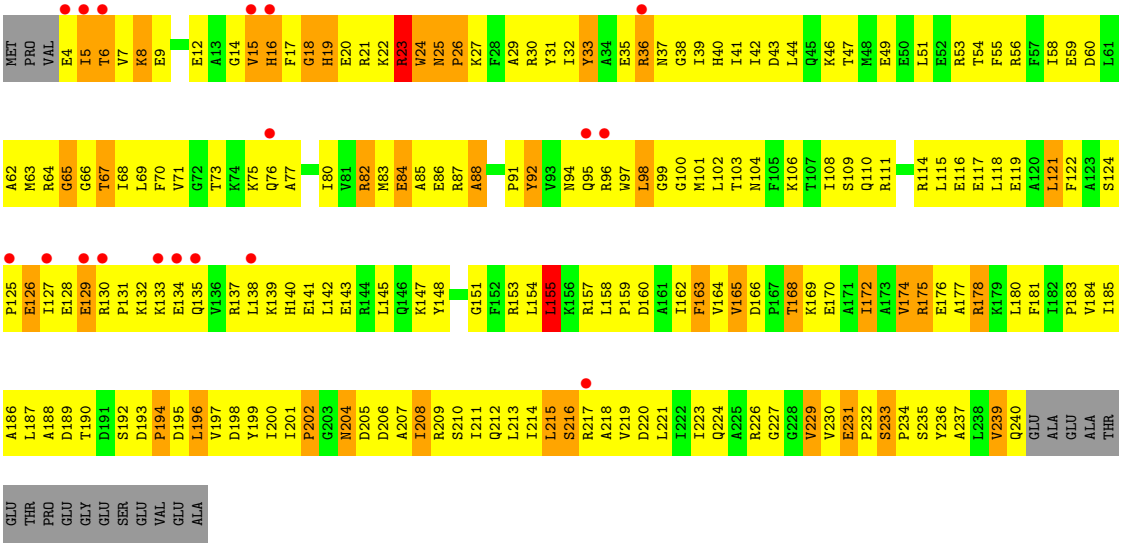




- Molecule 2: 30S ribosomal protein S2

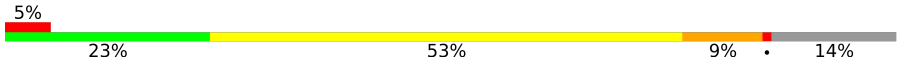
Chain XB:

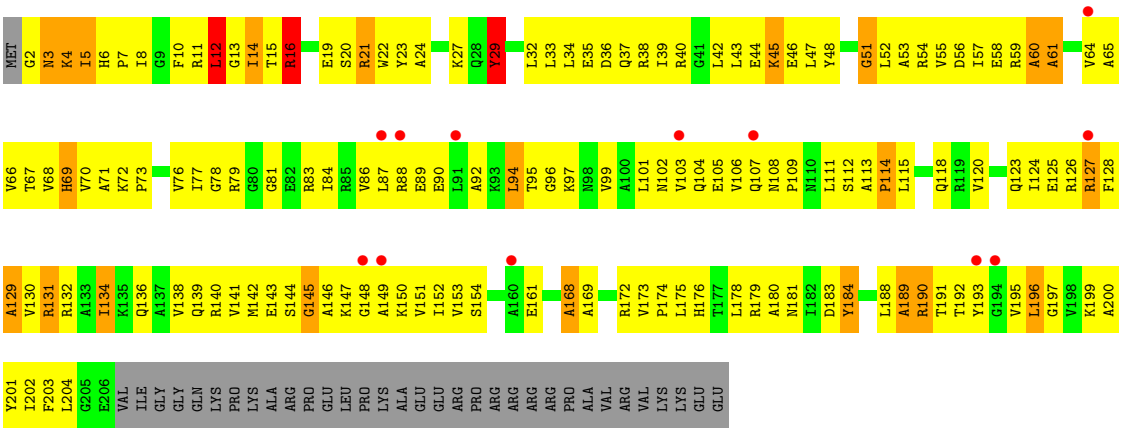




- Molecule 3: 30S ribosomal protein S3

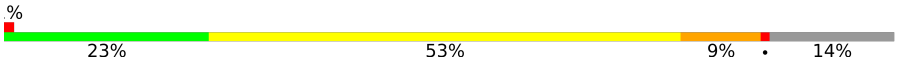
Chain QC:

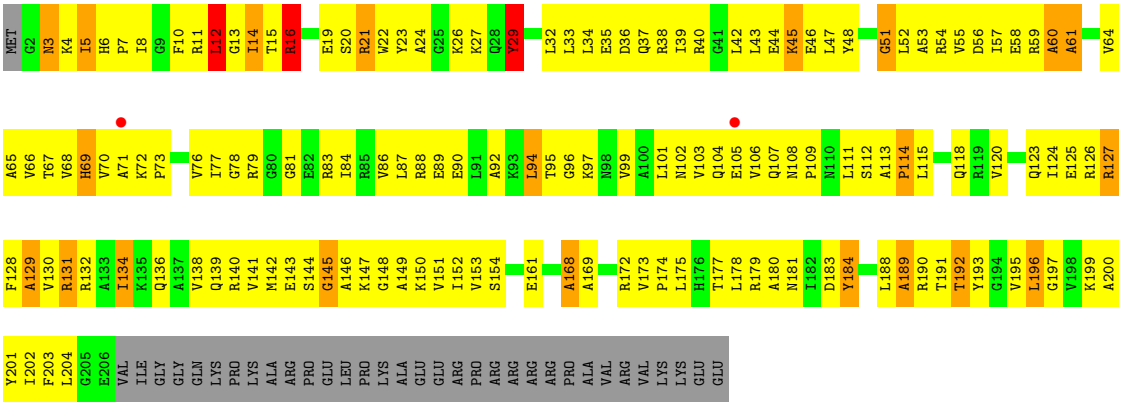




- Molecule 3: 30S ribosomal protein S3

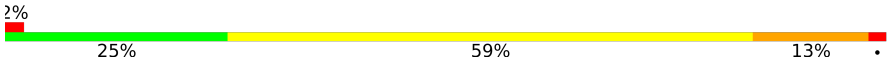
Chain XC:

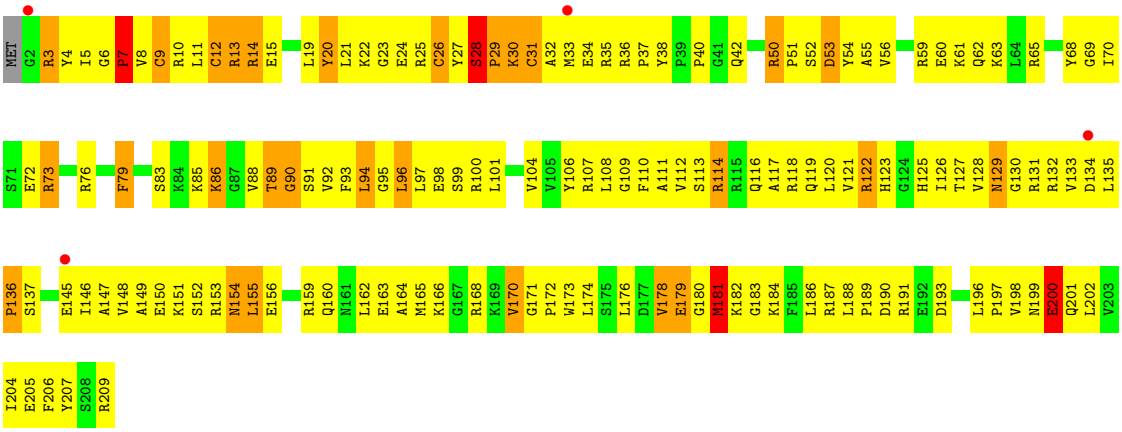




• Molecule 4: 30S ribosomal protein S4

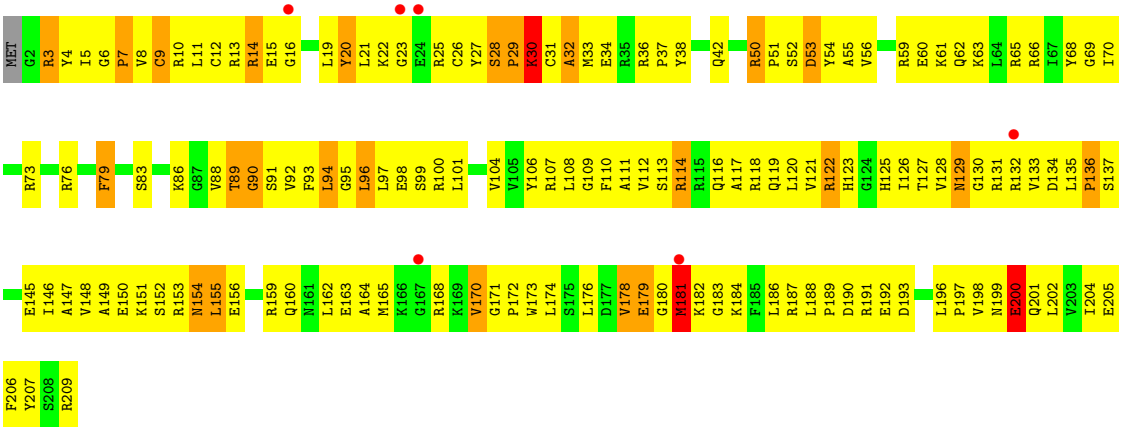
Chain QD:





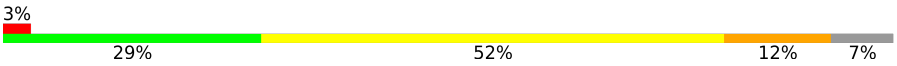
• Molecule 4: 30S ribosomal protein S4

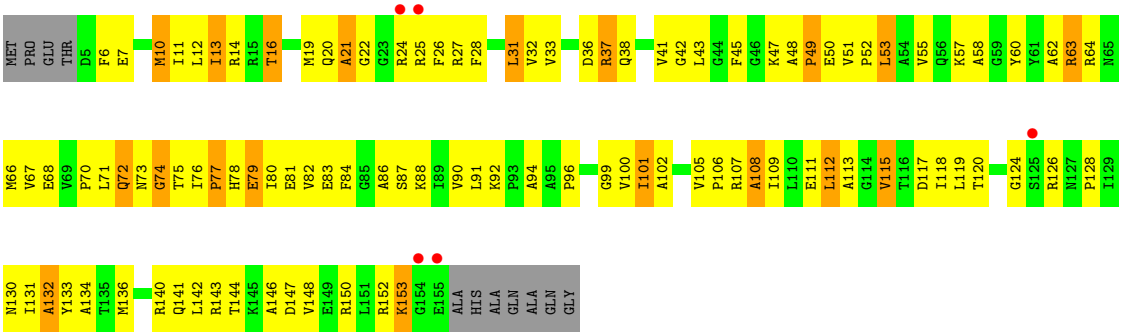
Chain XD:



• Molecule 5: 30S ribosomal protein S5

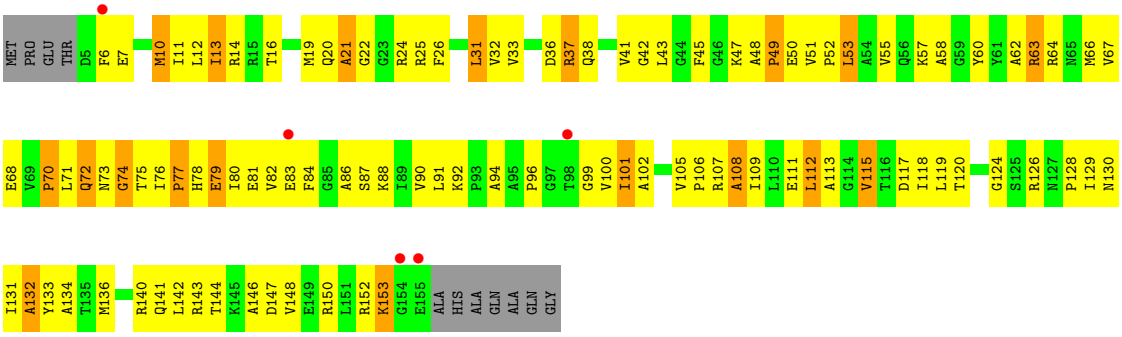
Chain QE:





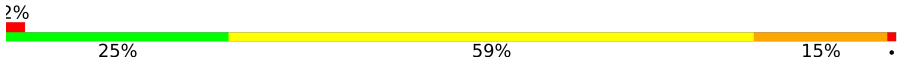
• Molecule 5: 30S ribosomal protein S5

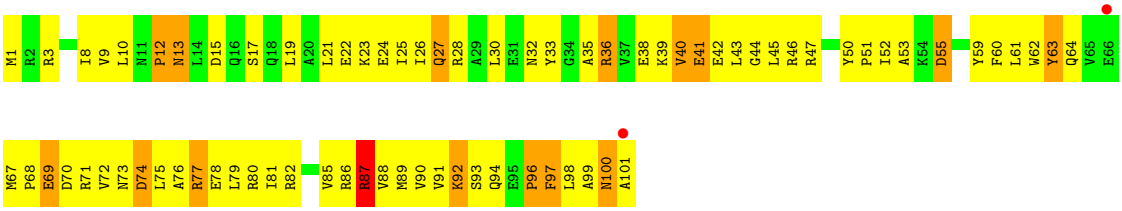
Chain XE:



• Molecule 6: 30S ribosomal protein S6

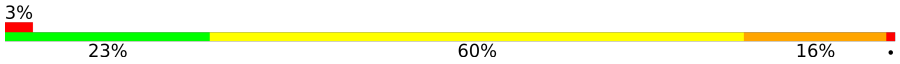
Chain QF:

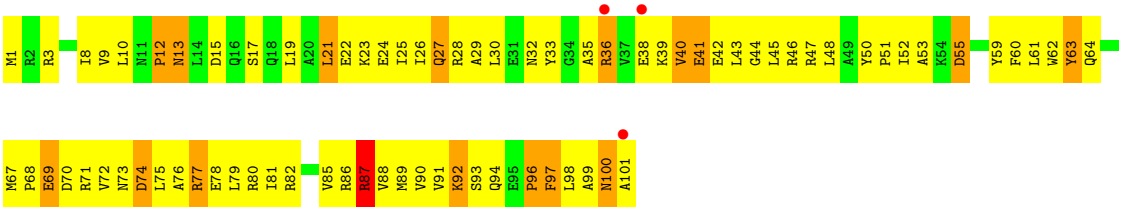




• Molecule 6: 30S ribosomal protein S6

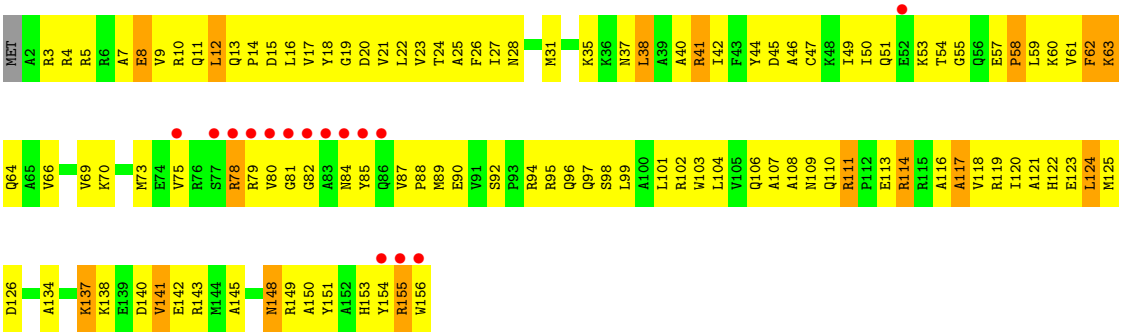
Chain XF:





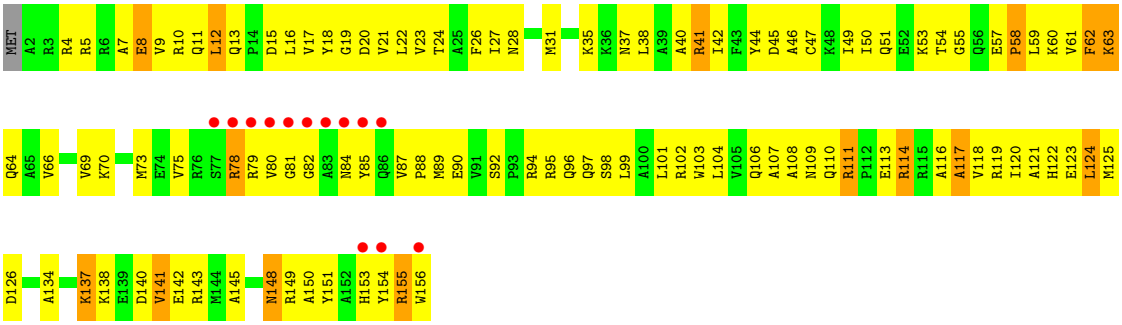
• Molecule 7: 30S ribosomal protein S7

Chain QG:



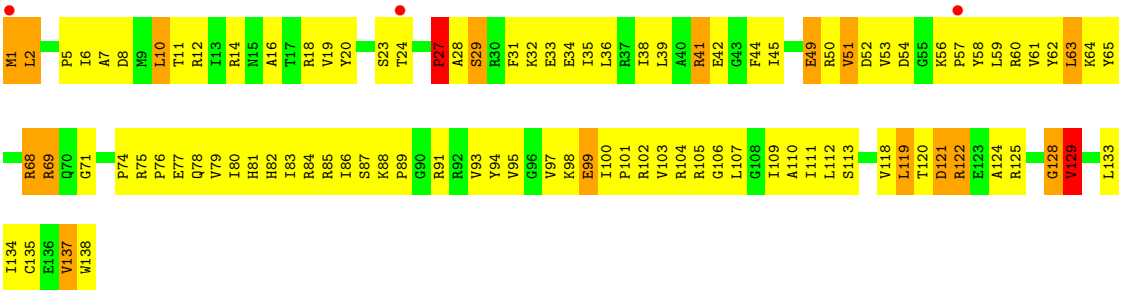
- Molecule 7: 30S ribosomal protein S7

Chain XG:



- Molecule 8: 30S ribosomal protein S8

Chain QH:

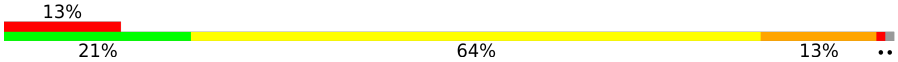


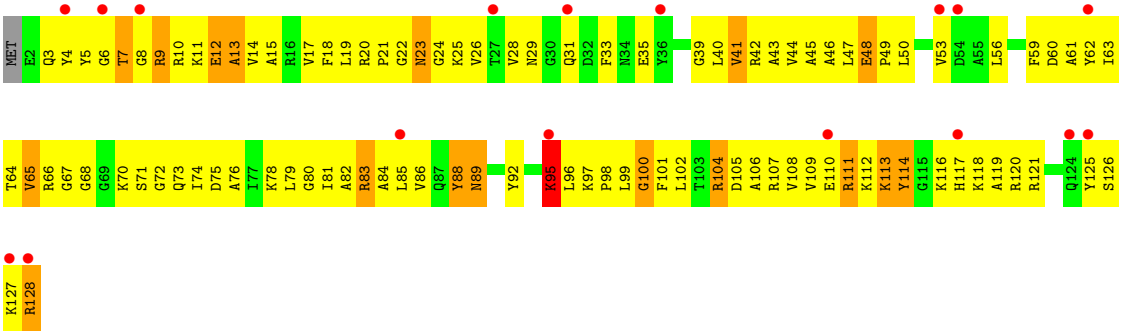
- Molecule 8: 30S ribosomal protein S8

Chain XH:

• Molecule 9: 30S ribosomal protein S9

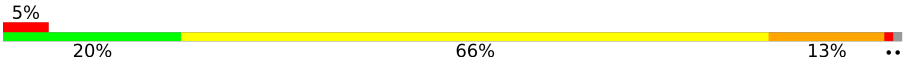
Chain QI:

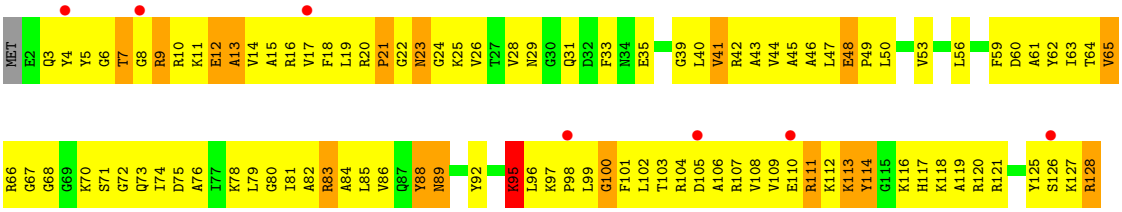




• Molecule 9: 30S ribosomal protein S9

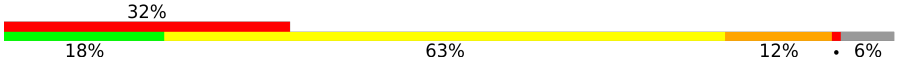
Chain XI:

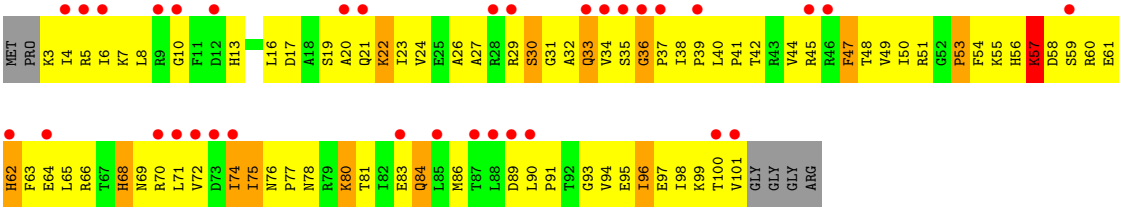




• Molecule 10: 30S ribosomal protein S10

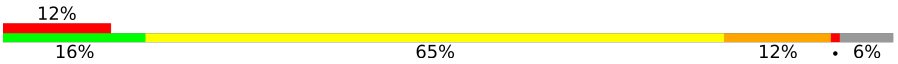
Chain QJ:

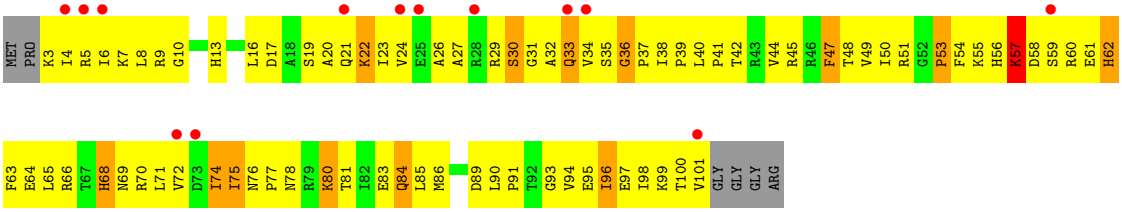




• Molecule 10: 30S ribosomal protein S10

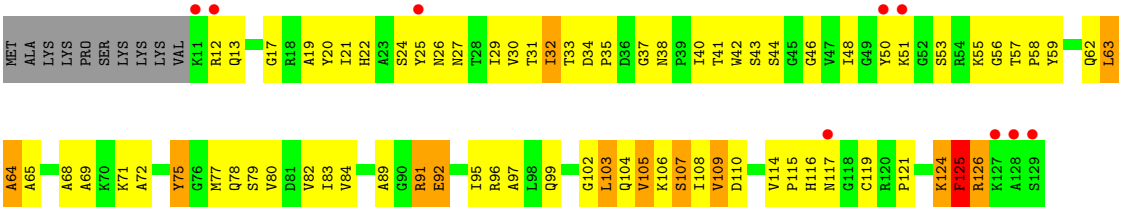
Chain XJ:





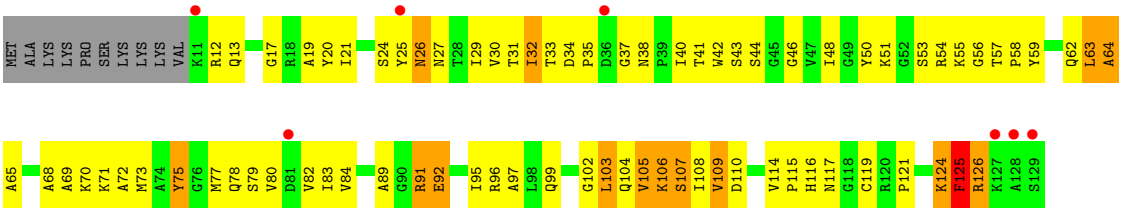
• Molecule 11: 30S ribosomal protein S11

Chain QK:



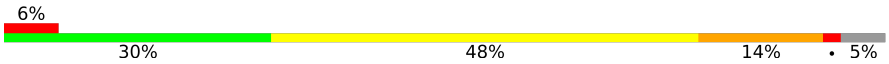
- Molecule 11: 30S ribosomal protein S11

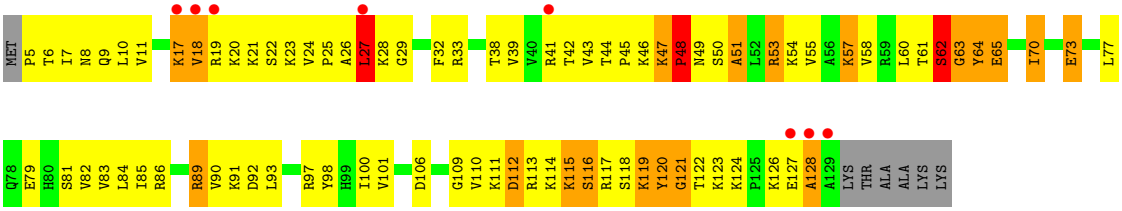
Chain XK:



- Molecule 12: 30S ribosomal protein S12

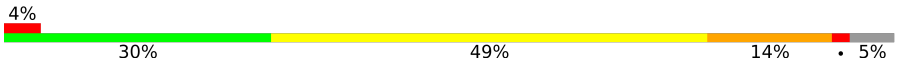
Chain QL:

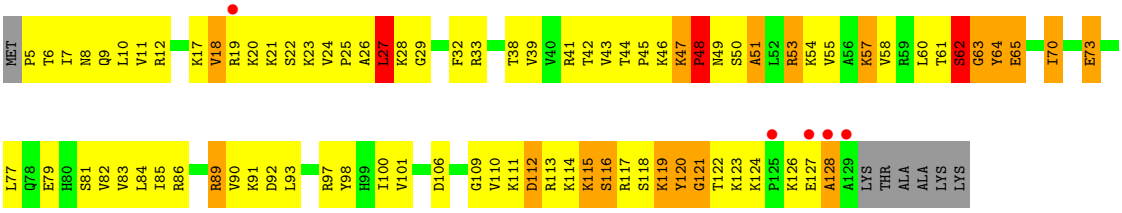




- Molecule 12: 30S ribosomal protein S12

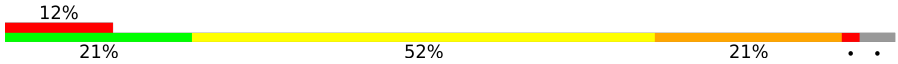
Chain XL:

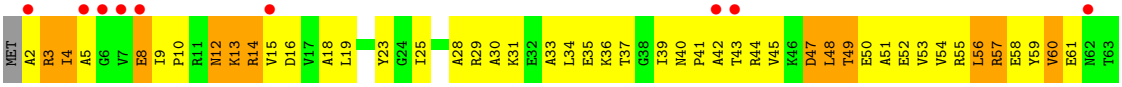


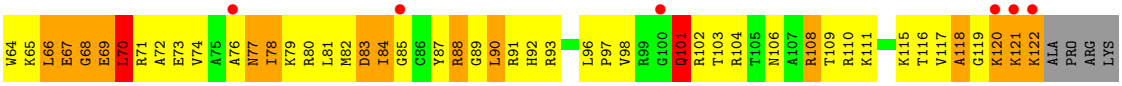


- Molecule 13: 30S ribosomal protein S13

Chain QM:

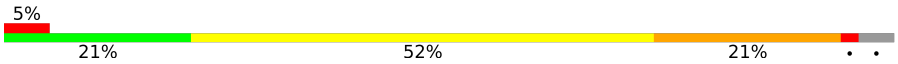


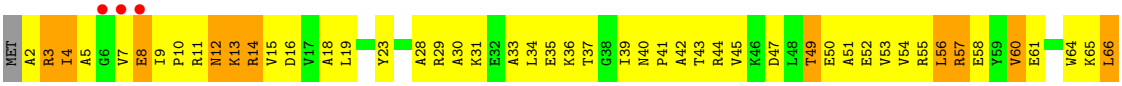


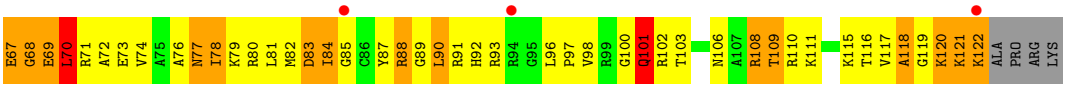


• Molecule 13: 30S ribosomal protein S13

Chain XM:

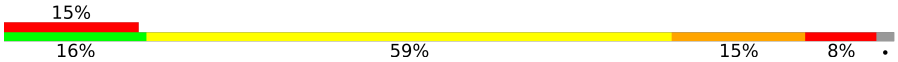


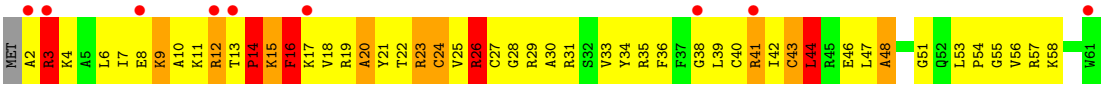




• Molecule 14: 30S ribosomal protein S14

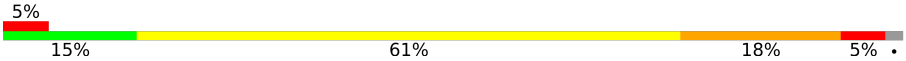
Chain QN:

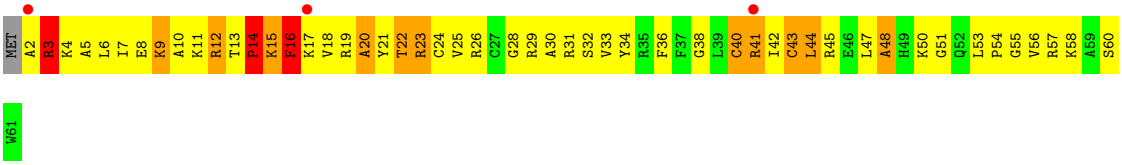




• Molecule 14: 30S ribosomal protein S14

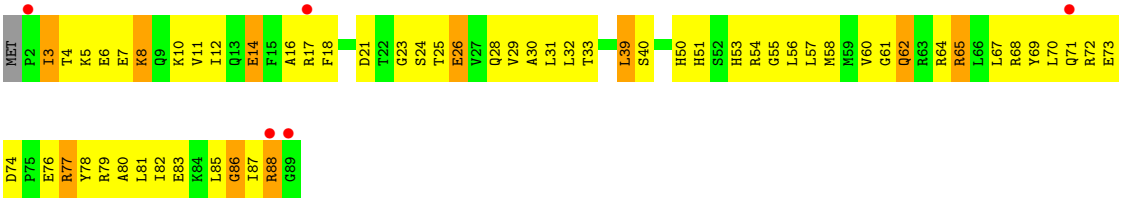
Chain XN:





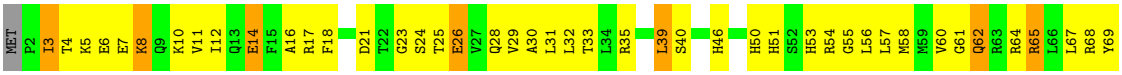
• Molecule 15: 30S ribosomal protein S15

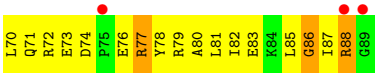
Chain QO:



• Molecule 15: 30S ribosomal protein S15

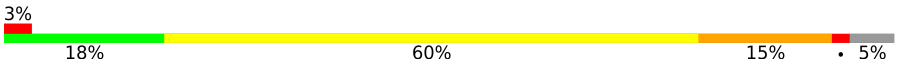
Chain XO:

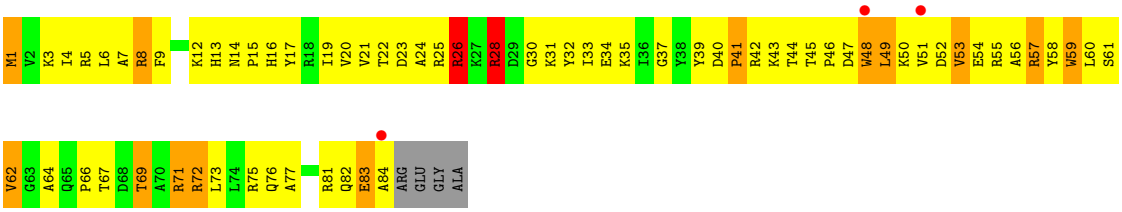




• Molecule 16: 30S ribosomal protein S16

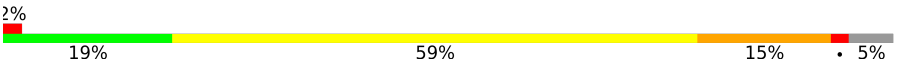
Chain QP:

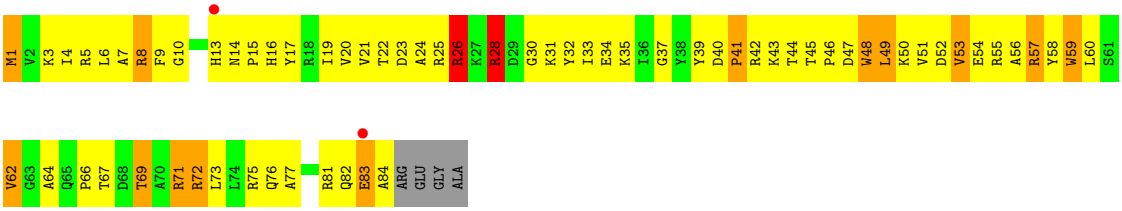




• Molecule 16: 30S ribosomal protein S16

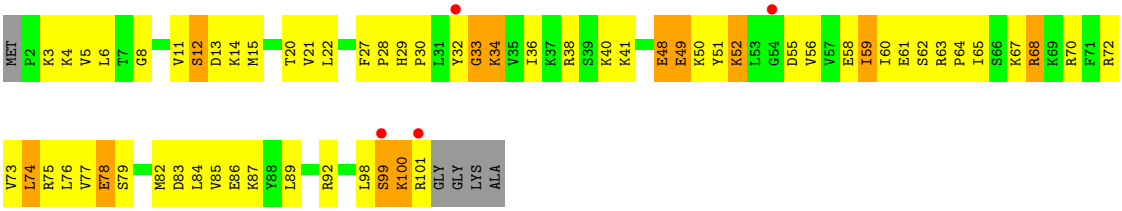
Chain XP:





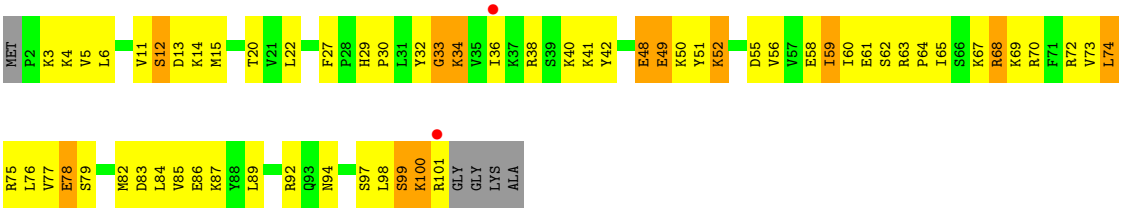
• Molecule 17: 30S ribosomal protein S17

Chain QQ:



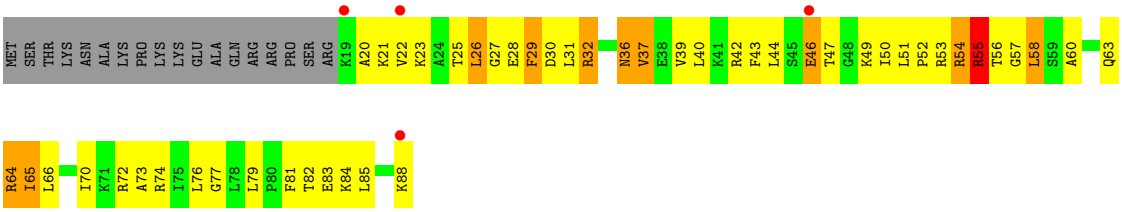
• Molecule 17: 30S ribosomal protein S17

Chain XQ:



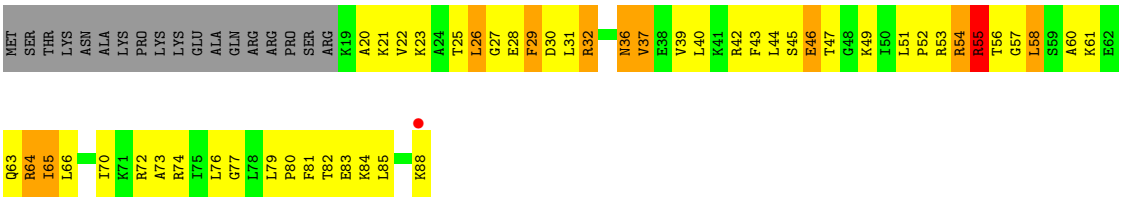
• Molecule 18: 30S ribosomal protein S18

Chain QR: 5% 24% 43% 11% • 20%



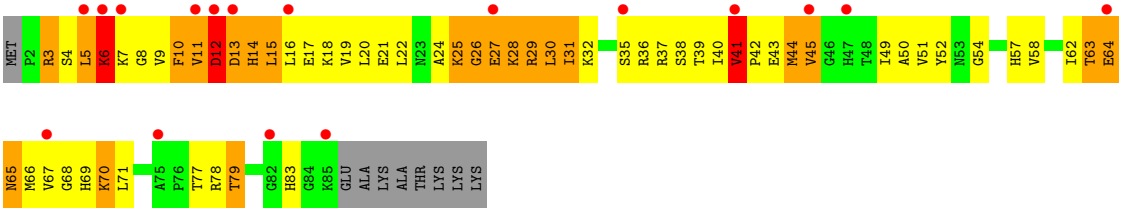
- Molecule 18: 30S ribosomal protein S18

Chain XR: % 22% 45% 11% • 20%



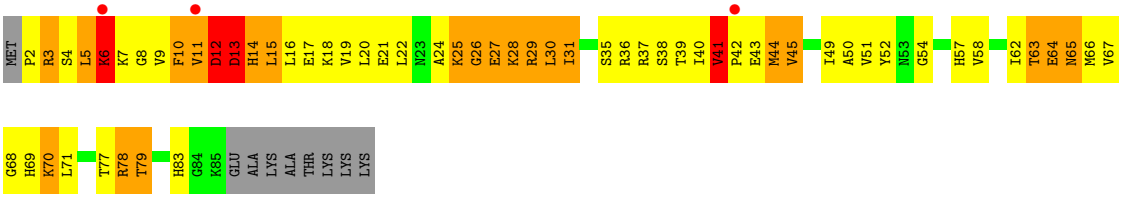
- Molecule 19: 30S ribosomal protein S19

Chain QS: 18% 25% 40% 23% • 10%



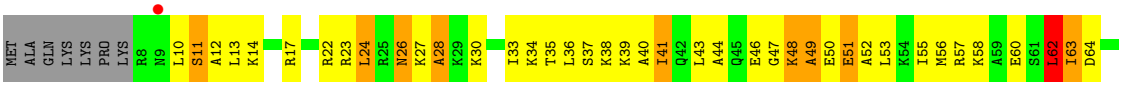
- Molecule 19: 30S ribosomal protein S19

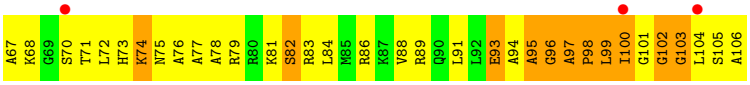
Chain XS: 3% 25% 39% 23% • 10%



- Molecule 20: 30S ribosomal protein S20

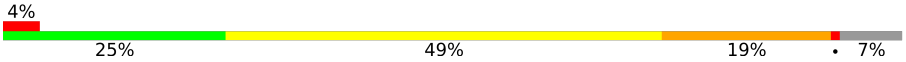
Chain QT: 4% 24% 50% 19% • 7%

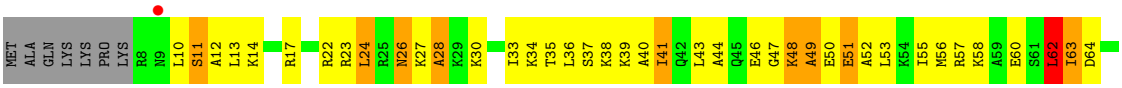




• Molecule 20: 30S ribosomal protein S20

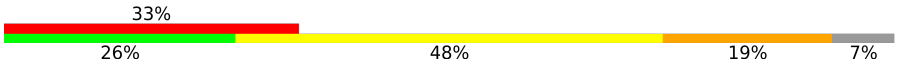
Chain XT:

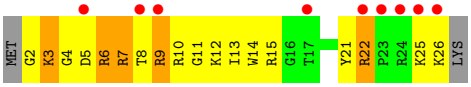




• Molecule 21: 30S ribosomal protein S21

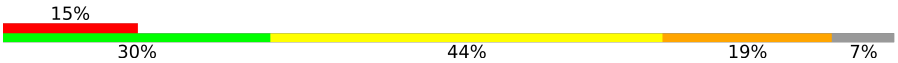
Chain QU:

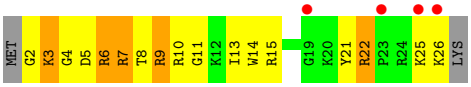




• Molecule 21: 30S ribosomal protein S21

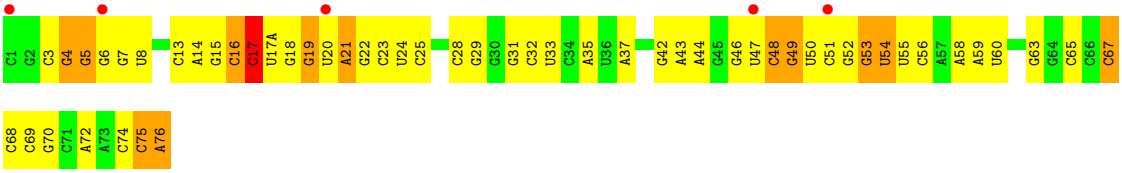
Chain XU:





• Molecule 22: P-site tRNA fMet

Chain QV:



• Molecule 22: P-site tRNA fMet

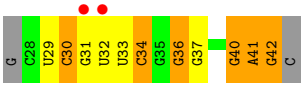
Chain XV:

• Molecule 23: messenger RNA

Chain QY: 12% 24% 41% 24% 12%

• Molecule 23: messenger RNA

Chain XY: 12% 24% 29% 35% 12%



• Molecule 24: A-site ASL SufA6

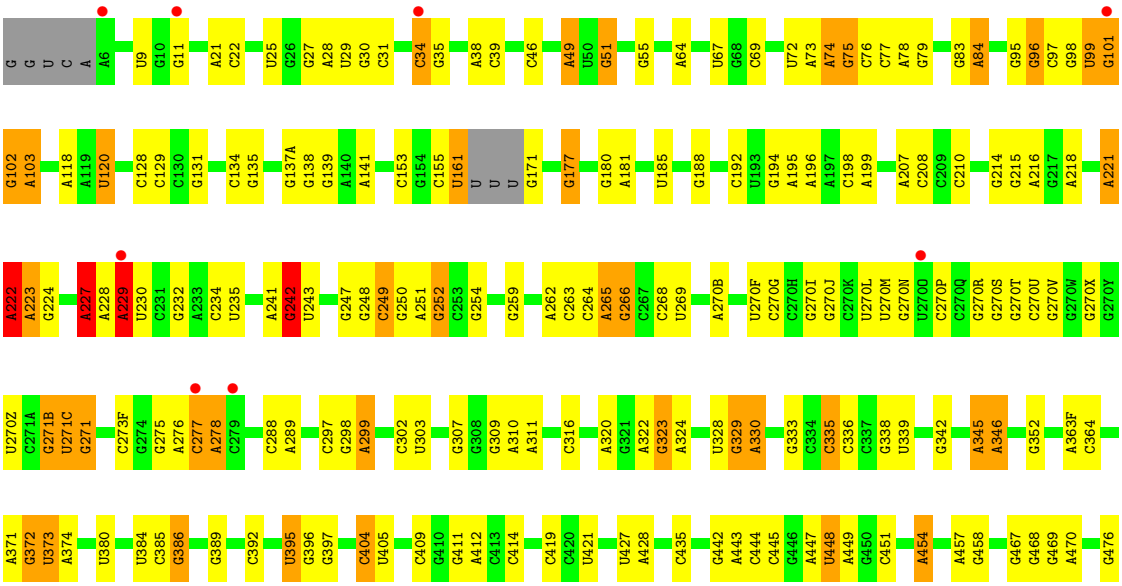
Chain QX: 8% 8% 12% 8% 68%

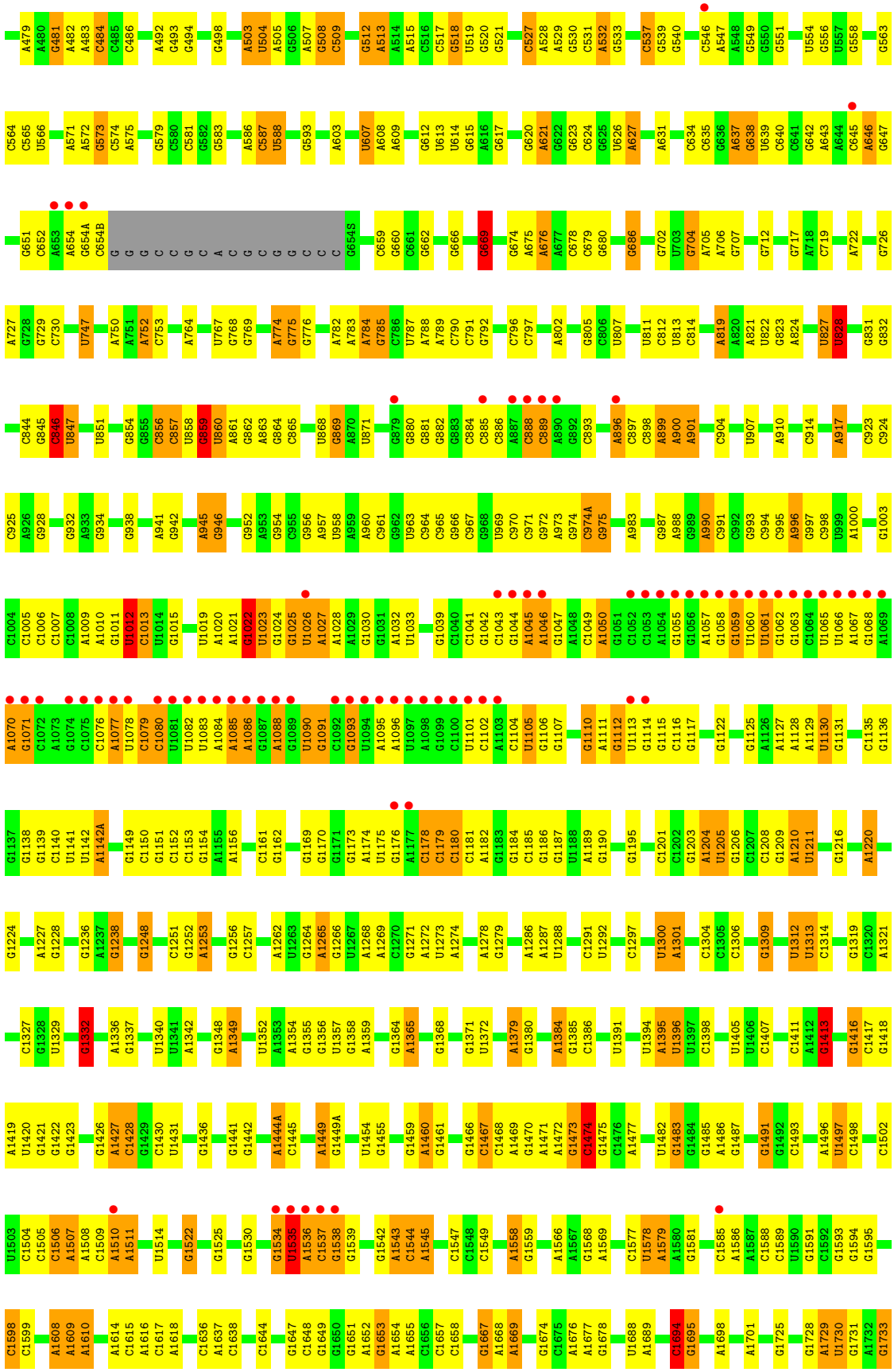
• Molecule 24: A-site ASL SufA6

Chain XX: 8% 8% 12% 8% 68%

• Molecule 25: 23S rRNA

Chain RA: 5% 54% 34% 10%

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C564 C565 U566 A571 A572 G573 C574 A575 G579 C580 C581 G582 G583 A586 C587 U588 G593 A603 U607 A608 A609 G612 U613 U614 G615 A616 G617 G620 A621 G622 G623 G624 G625 U626 A627 A631 C634 C635 G636 A637 G638 U639 C640 C641 G642 A643 A644 C645 A646 G647
G651 C652 A653 A654 G654A C654B G G G C C G C A C G C G G C C C G654S C659 G660 C661 G662 G666 G669 G674 A675 A676 A677 C678 C679 G680 G686 G702 U703 G704 A705 A706 G707 G712 G717 A718 C719 A722 G726
A727 G728 G729 C730 U747 A750 A751 A752 C753 A764 U767 G768 G769 A774 G775 G776 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 C796 C797 A802 G805 C806 U807 U811 C812 U813 C814 A819 A820 A821 U822 G823 A824 U827 U828 G831 G832
C844 G845 C846 U847 U851 G854 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 U868 G869 A870 U871 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 A896 C897 C898 A899 A900 A901 C904 U907 A910 C914 A917 C923 C924
C925 A926 G928 G932 A933 G934 G938 A941 G942 A945 G946 G952 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 C964 C965 G966 C967 G968 U969 C970 C971 G972 A973 G974 C974A G975 A983 G987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 G1003
C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014 G1015 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031 A1032 U1033 G1039 C1040 C1041 C1042 C1043 G1044 A1045 A1046 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069
A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1117 G1122 G1125 A1126 A1127 A1128 A1129 U1130 G1131 C1135 G1136
G1137 G1138 G1139 C1140 U1141 U1142 A1142A G1149 C1150 G1151 C1152 C1153 G1154 A1155 A1156 C1161 G1162 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 C1185 A1186 G1187 U1188 A1189 G1190 G1195 C1201 C1202 G1203 A1204 U1205 G1206 C1207 C1208 G1209 A1210 U1211 G1216 A1220
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A1419 U1420 G1421 G1422 G1423 G1426 A1427 C1428 G1429 C1430 U1431 G1436 G1441 G1442 A1444A C1445 A1449 G1449A U1454 G1455 G1459 A1460 G1461 G1466 C1467 C1468 A1469 G1470 A1471 A1472 G1473 C1474 G1475 C1476 A1477 U1482 G1483 G1484 G1485 A1486 G1487 G1491 G1492 C1493 A1496 U1497 C1498 C1502
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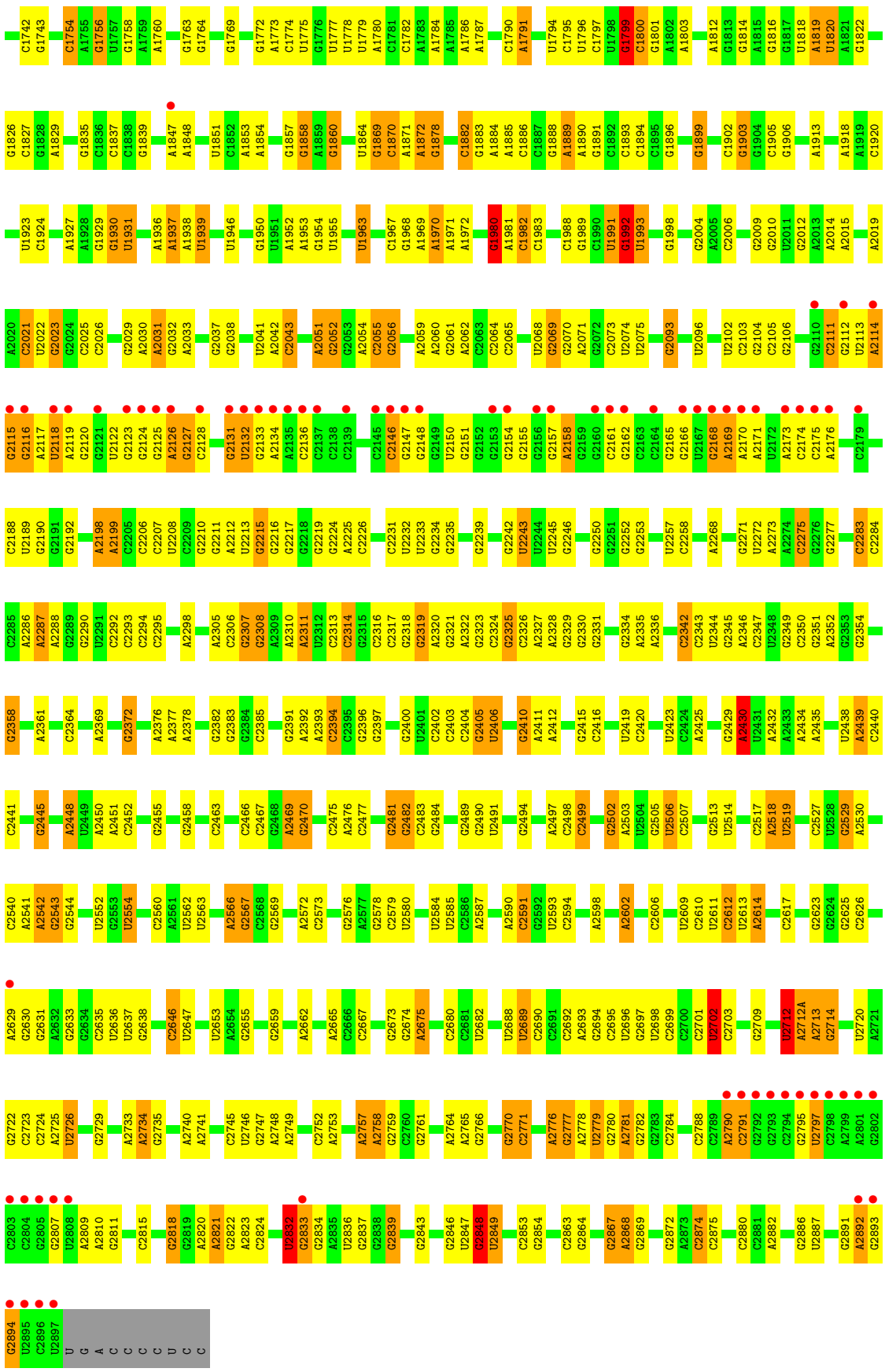
C1598 C1599 A1608 A1609 A1610 A1614 C1615 A1616 C1617 A1618 C1636 A1637 C1638 C1644 G1647 C1648 G1649 G1650 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 G1667 A1668 A1669 G1674 C1675 A1676 A1677 G1678 U1688 A1689 C1694 G1695 A1698 A1701 G1725 G1728 A1729 U1730 G1731 A1732 G1733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G1769
G1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787
C1790 A1791
U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803
A1812 G1813 G1814 A1815 G1816 G1817 U1818 A1819 U1820 A1821 G1822
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G1835 C1836 C1837 C1838 G1839
A1847 A1848
U1851 C1852 A1853 A1854
G1857 G1858 A1859 G1860
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G1899
C1902 G1903 G1904 C1905 G1906
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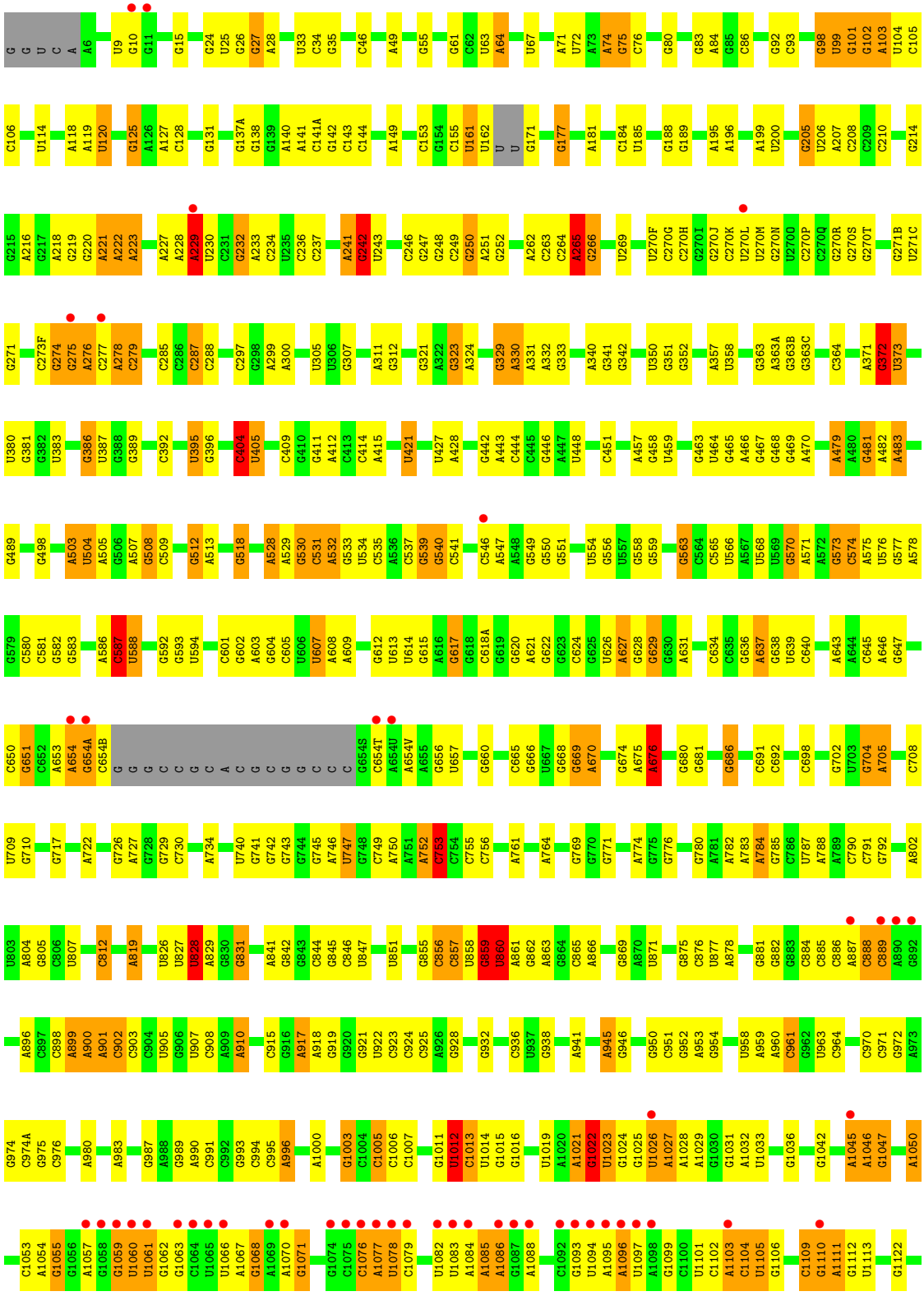
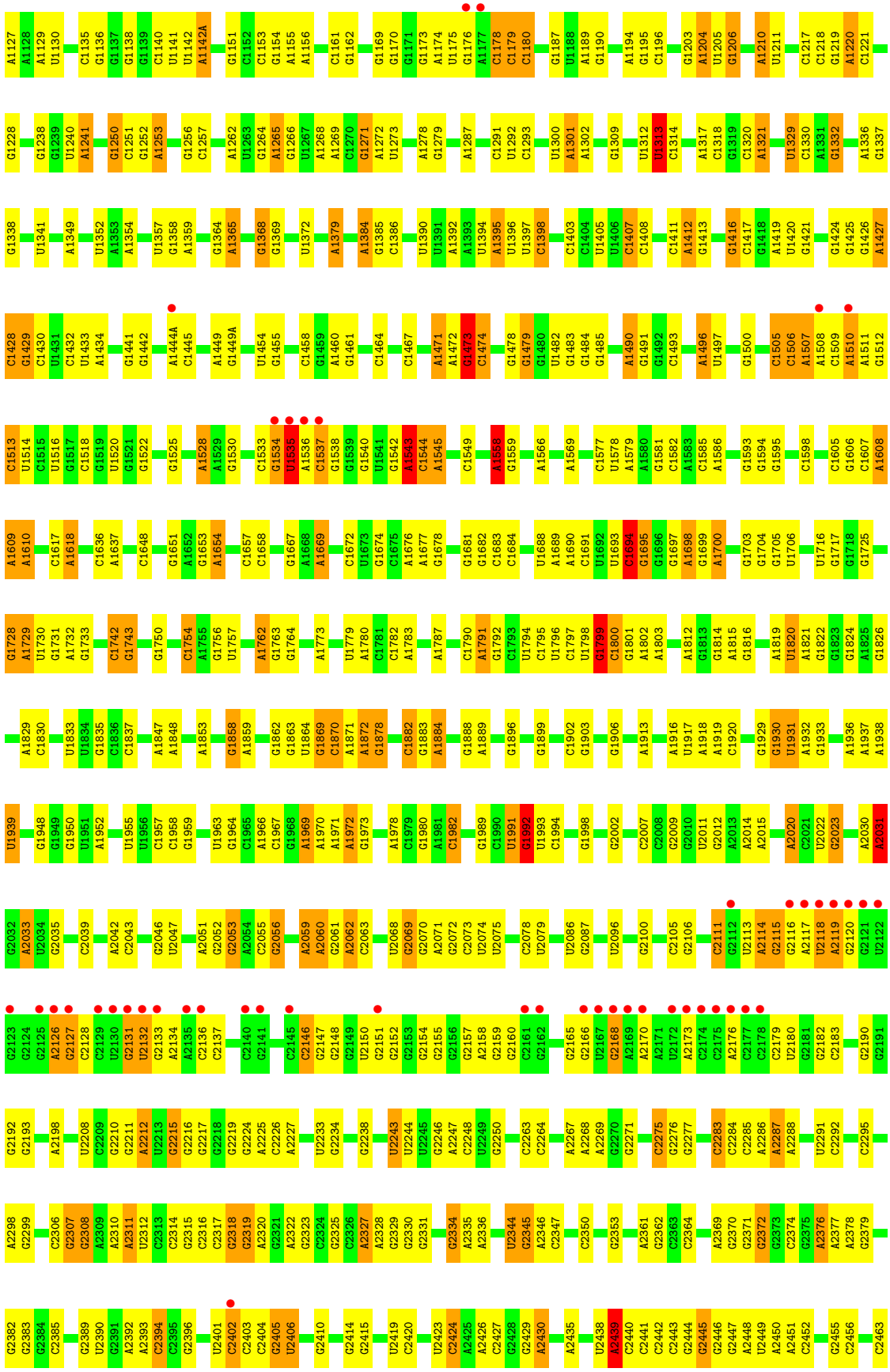
- Molecule 25: 23S rRNA

Chain YA:

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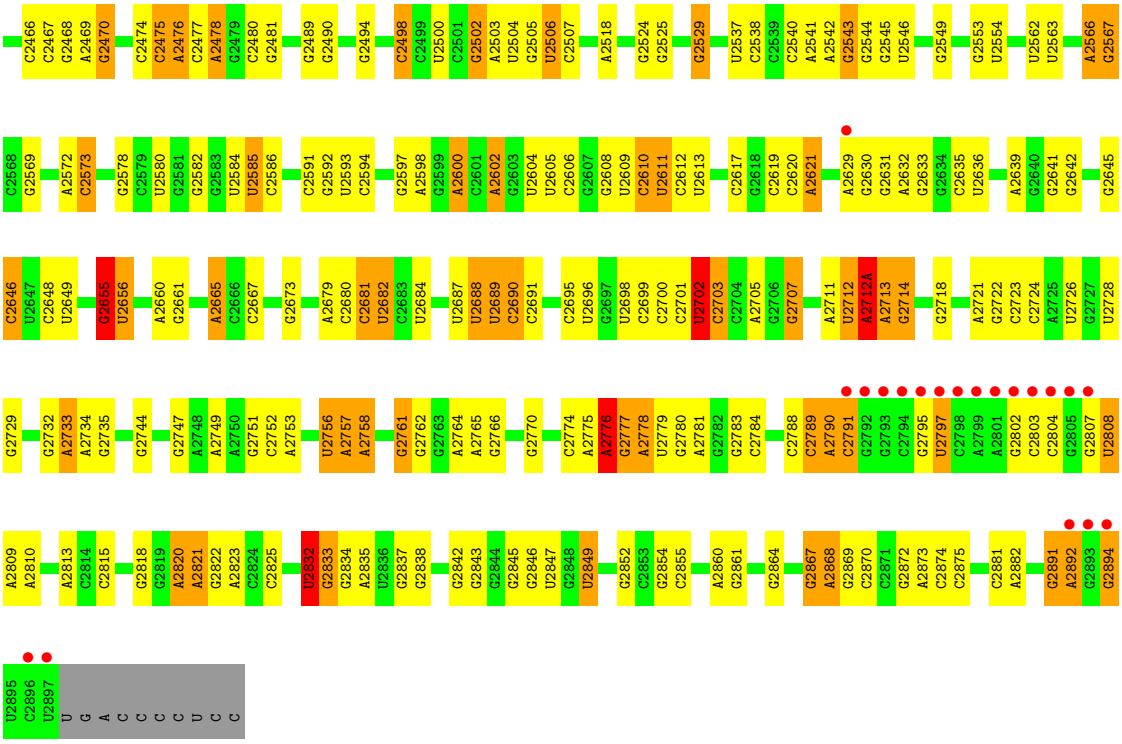
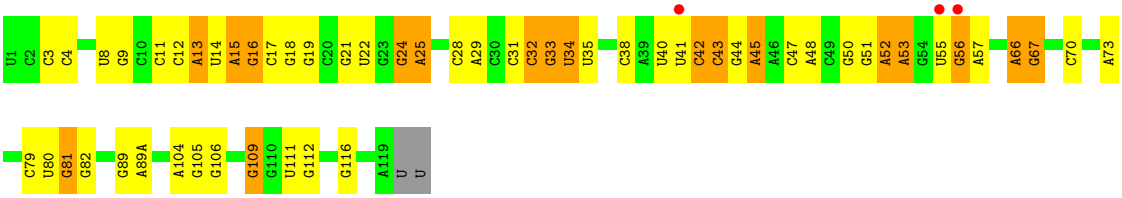


- Molecule 26: 5S rRNA

Chain RB:

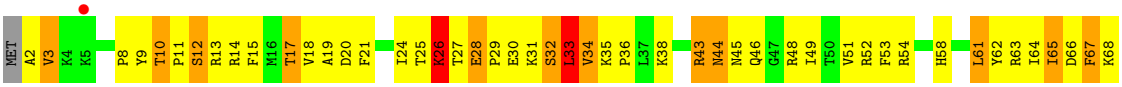


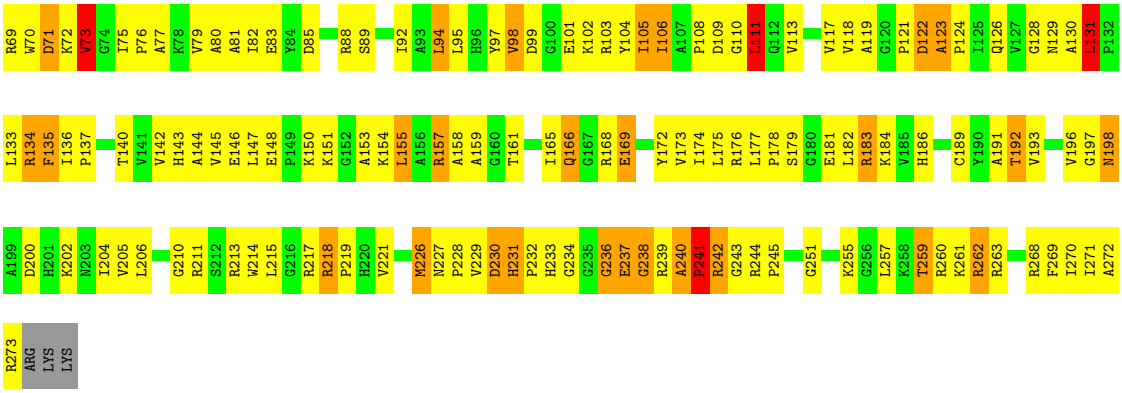
- Molecule 26: 5S rRNA

Chain YB:

- Molecule 27: 50S ribosomal protein L2

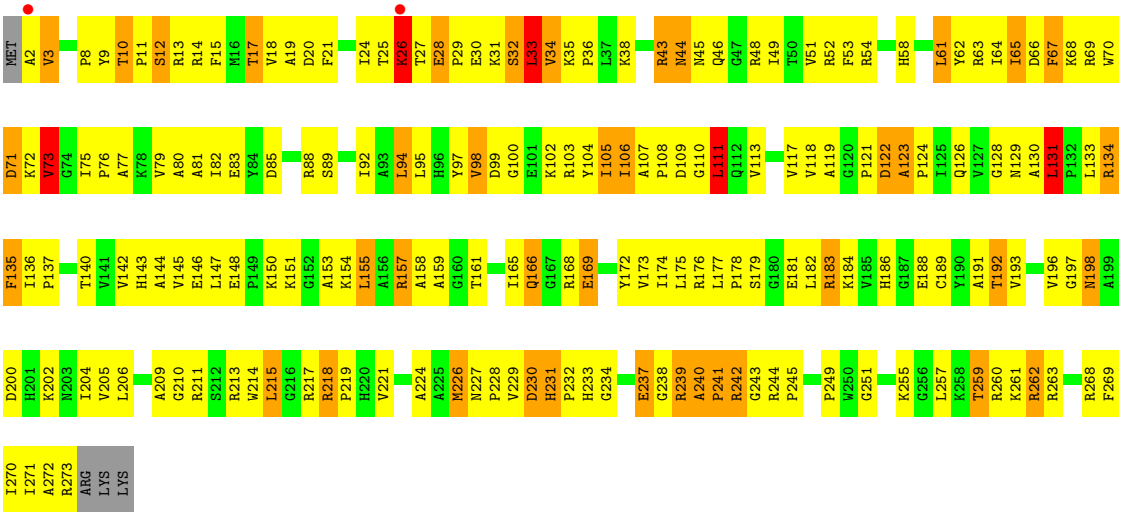
Chain RD:





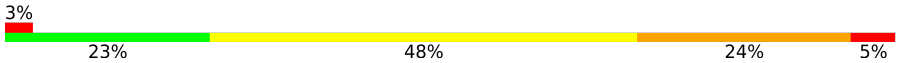
- Molecule 27: 50S ribosomal protein L2

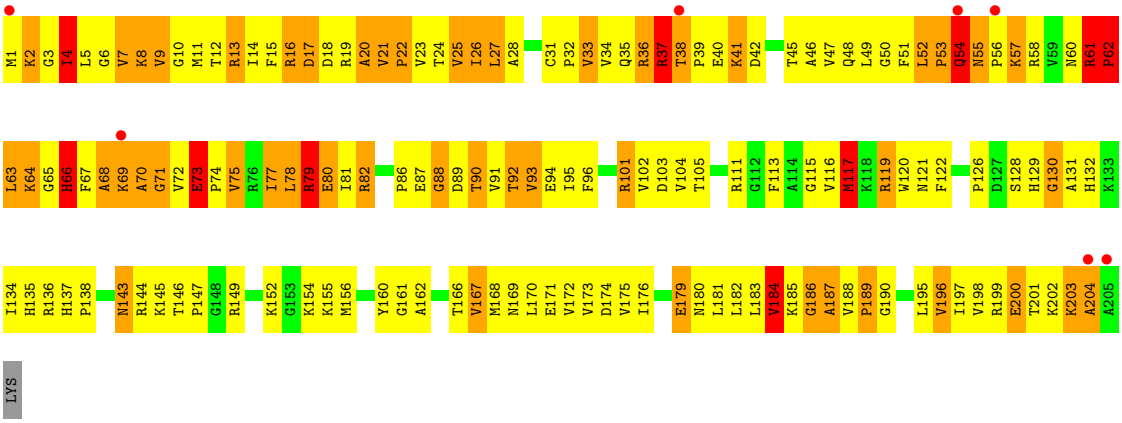
Chain YD:



- Molecule 28: 50S ribosomal protein L3

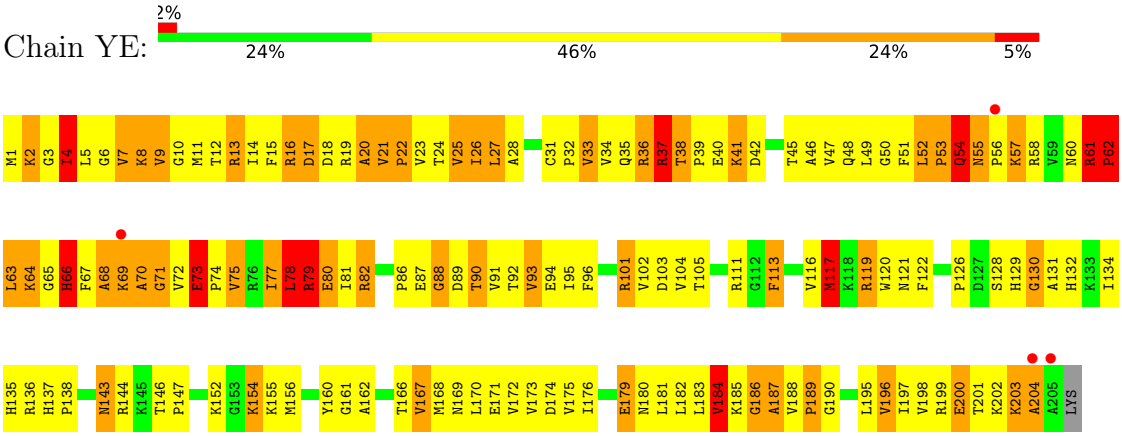
Chain RE:





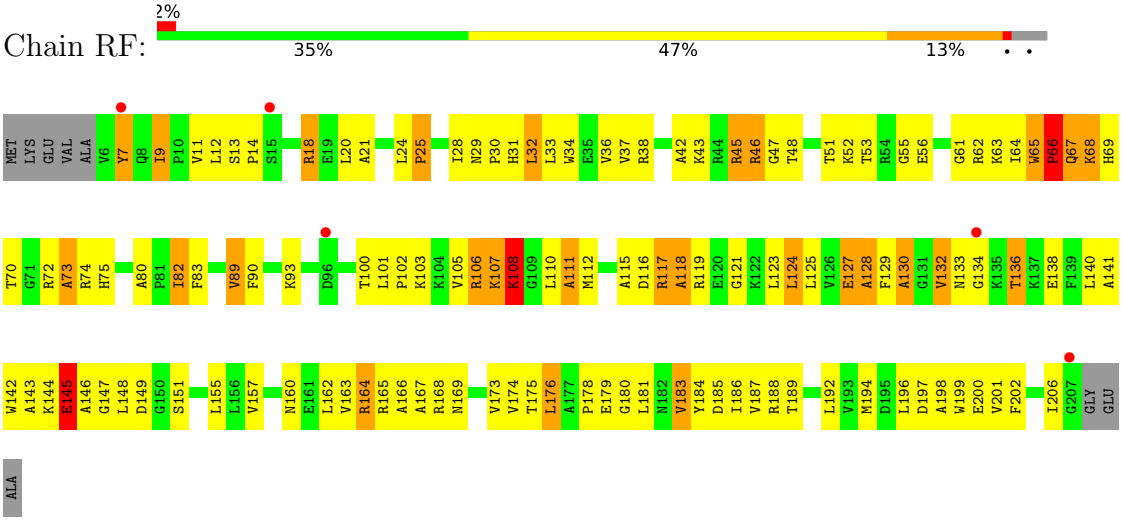
- Molecule 28: 50S ribosomal protein L3

Chain YE:



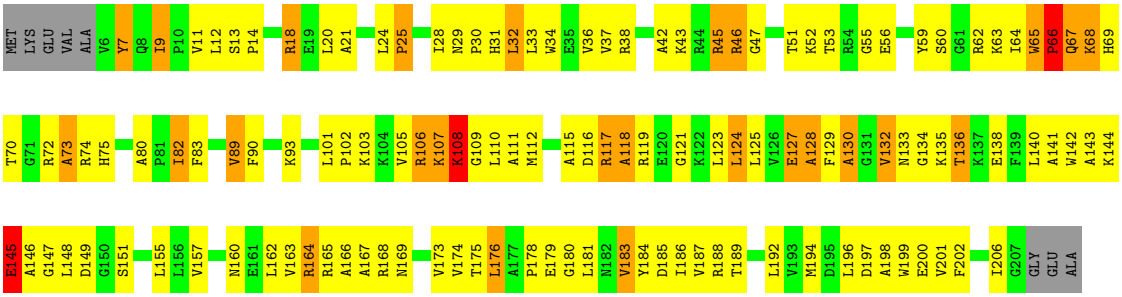
- Molecule 29: 50S ribosomal protein L4

Chain RF:



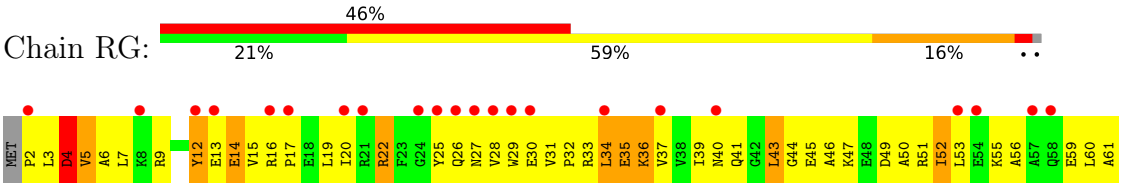
- Molecule 29: 50S ribosomal protein L4

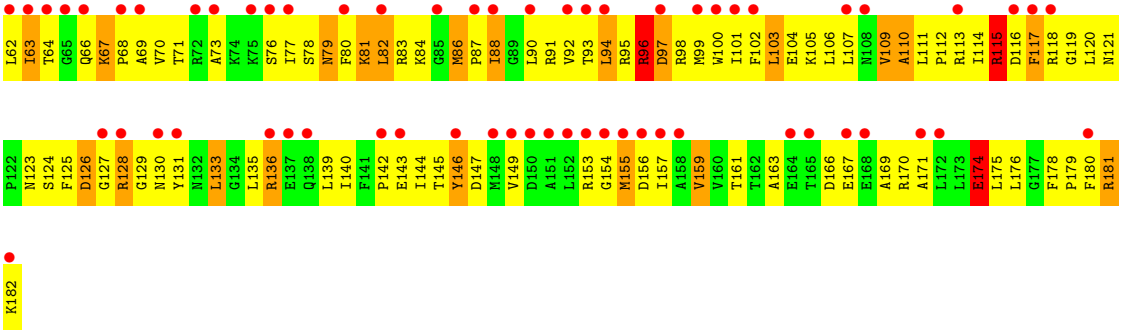
Chain YF:



- Molecule 30: 50S ribosomal protein L5

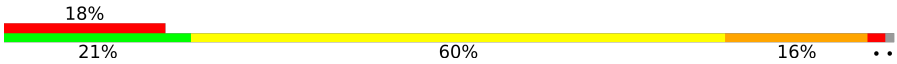
Chain RG:

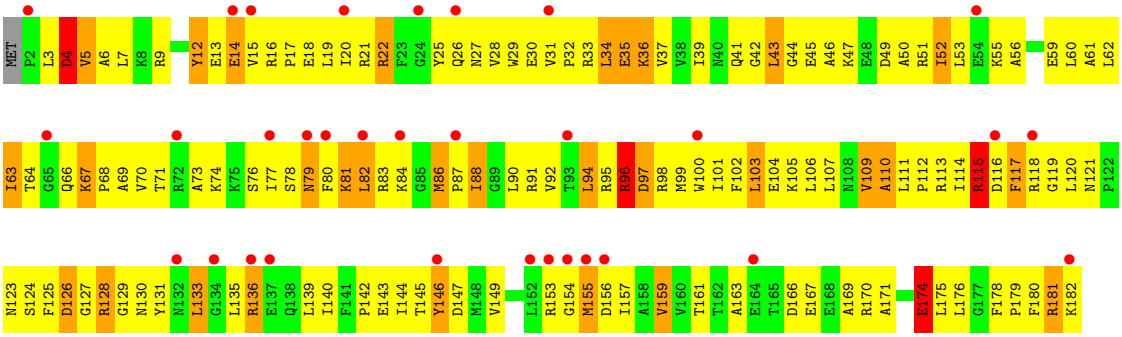




- Molecule 30: 50S ribosomal protein L5

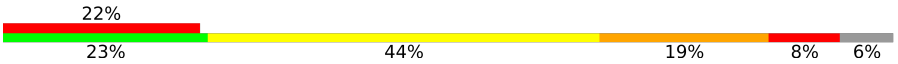
Chain YG:

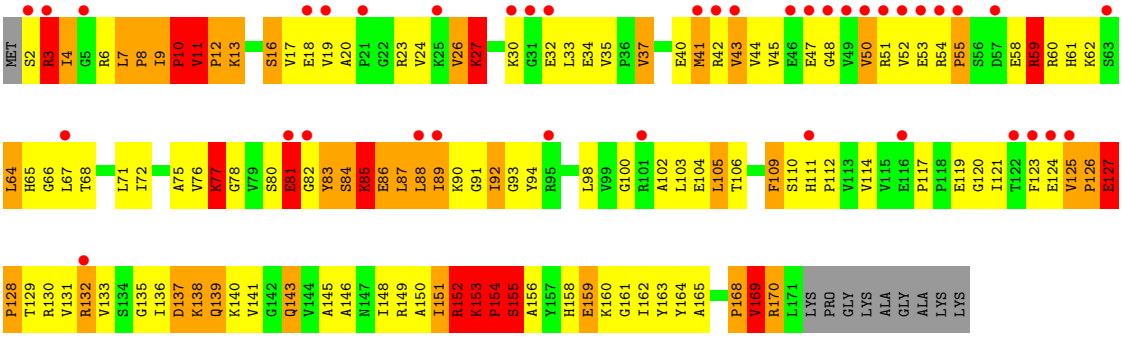




- Molecule 31: 50S ribosomal protein L6

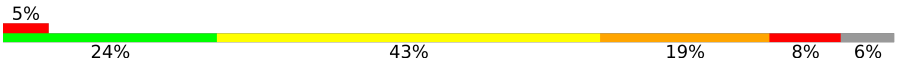
Chain RH:

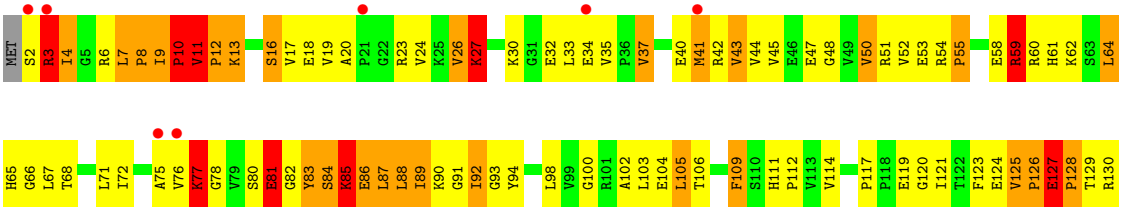




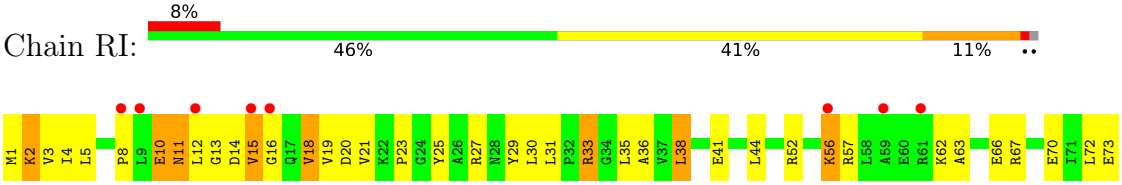
- Molecule 31: 50S ribosomal protein L6

Chain YH:

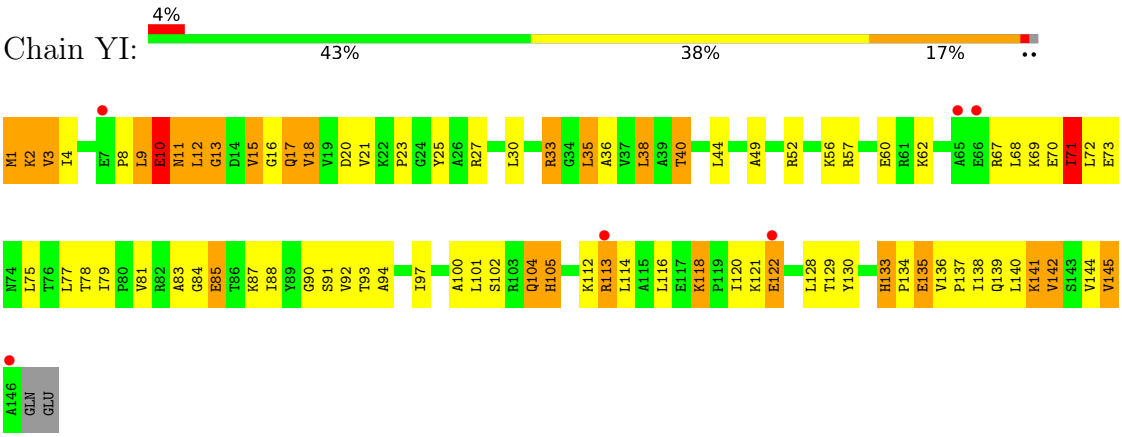




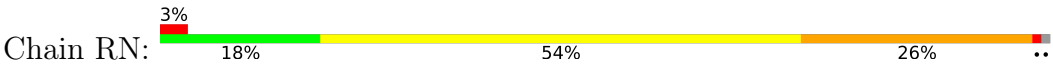
• Molecule 32: 50S ribosomal protein L9

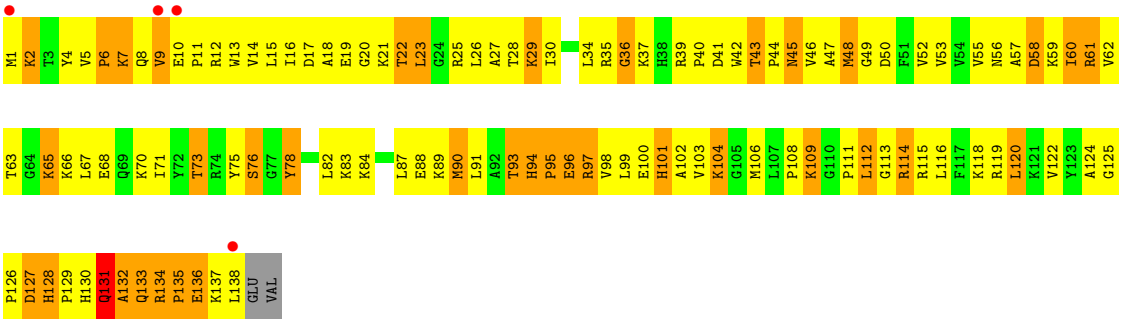


• Molecule 32: 50S ribosomal protein L9

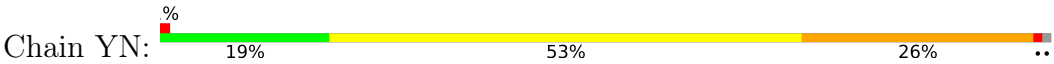


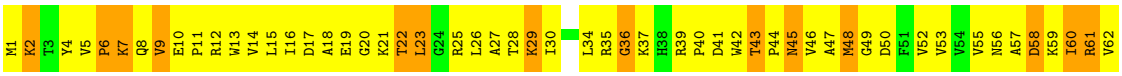
• Molecule 33: 50S ribosomal protein L13

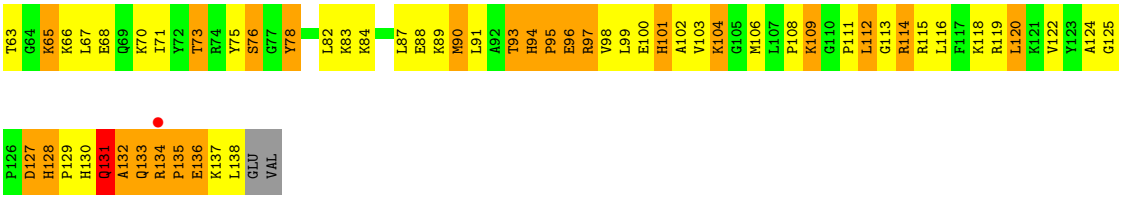




• Molecule 33: 50S ribosomal protein L13

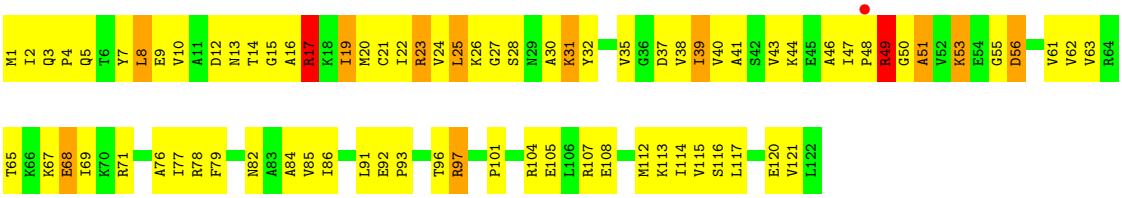






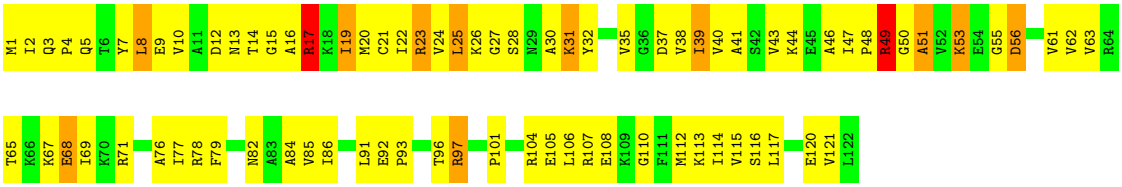
• Molecule 34: 50S ribosomal protein L14

Chain RO:



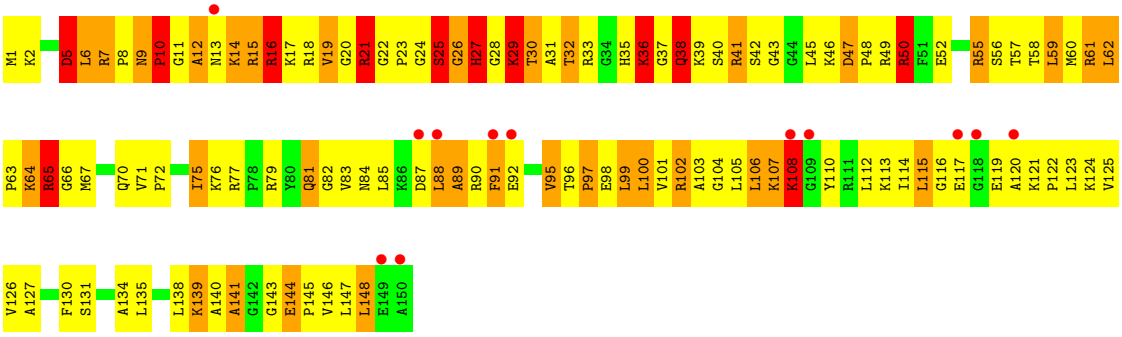
• Molecule 34: 50S ribosomal protein L14

Chain YO:



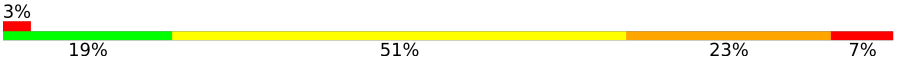
• Molecule 35: 50S ribosomal protein L15

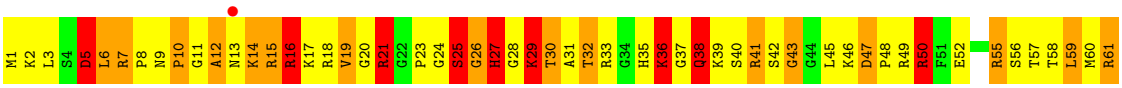
Chain RP:

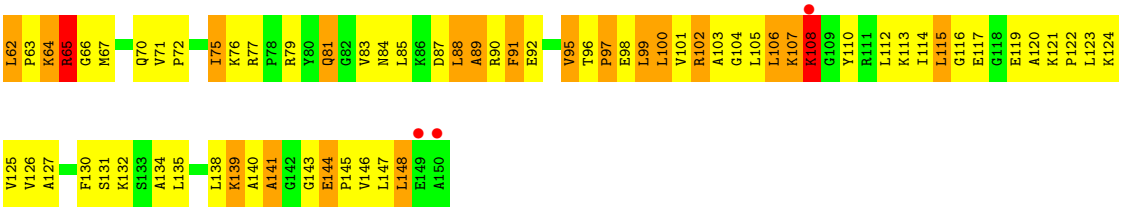


• Molecule 35: 50S ribosomal protein L15

Chain YP:

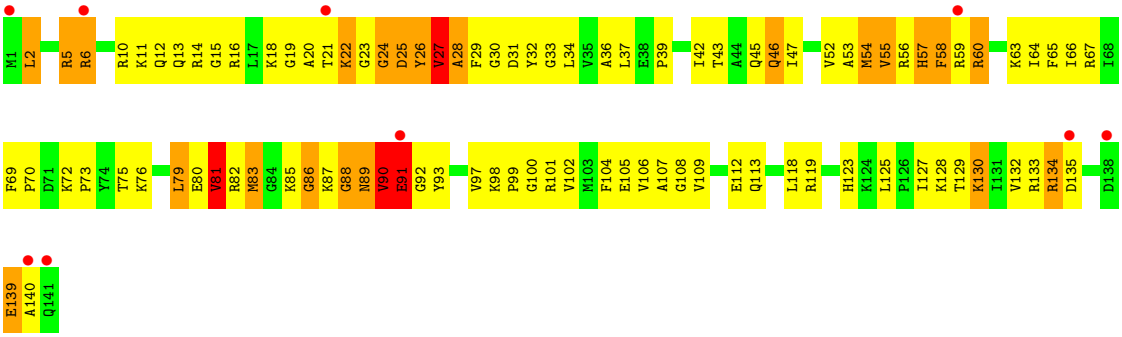






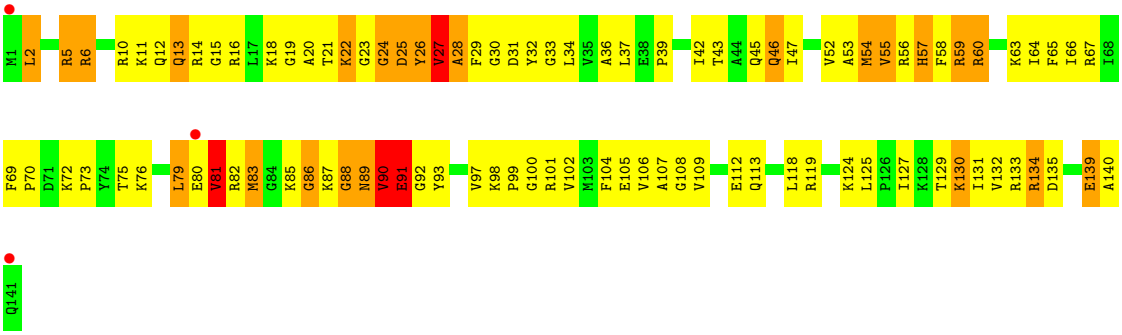
- Molecule 36: 50S ribosomal protein L16

Chain RQ:



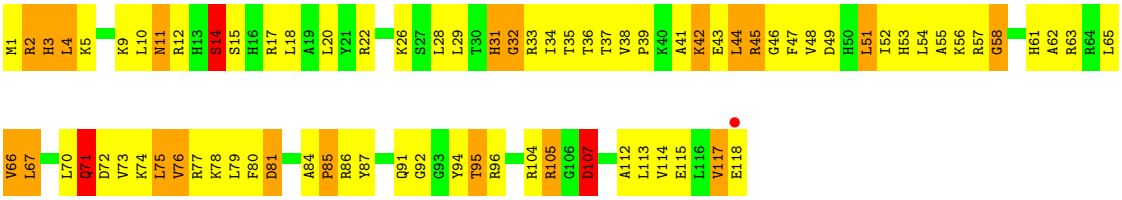
- Molecule 36: 50S ribosomal protein L16

Chain YQ:



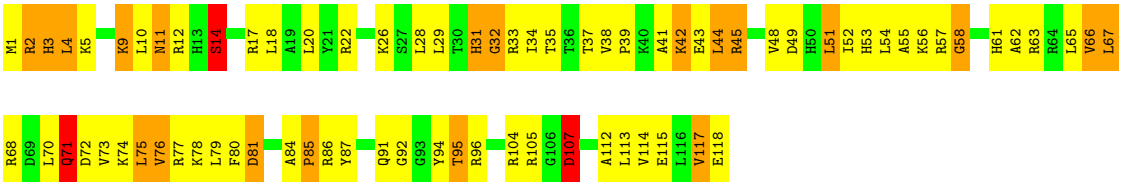
- Molecule 37: 50S ribosomal protein L17

Chain RR:



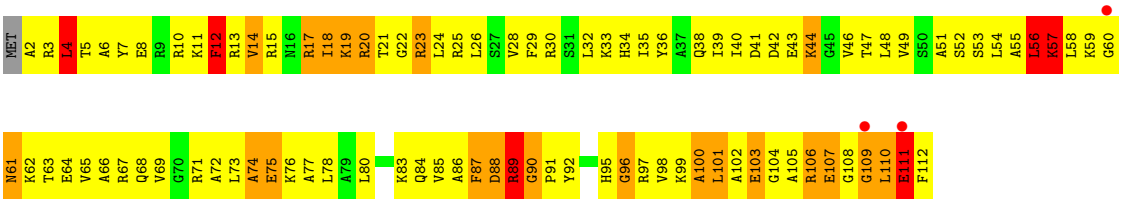
- Molecule 37: 50S ribosomal protein L17

Chain YR:



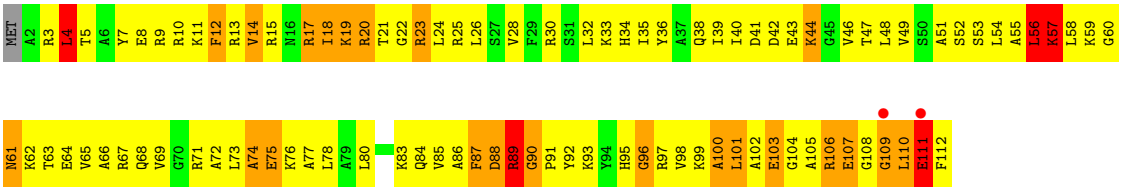
• Molecule 38: 50S ribosomal protein L18

Chain RS:



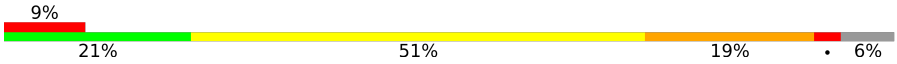
• Molecule 38: 50S ribosomal protein L18

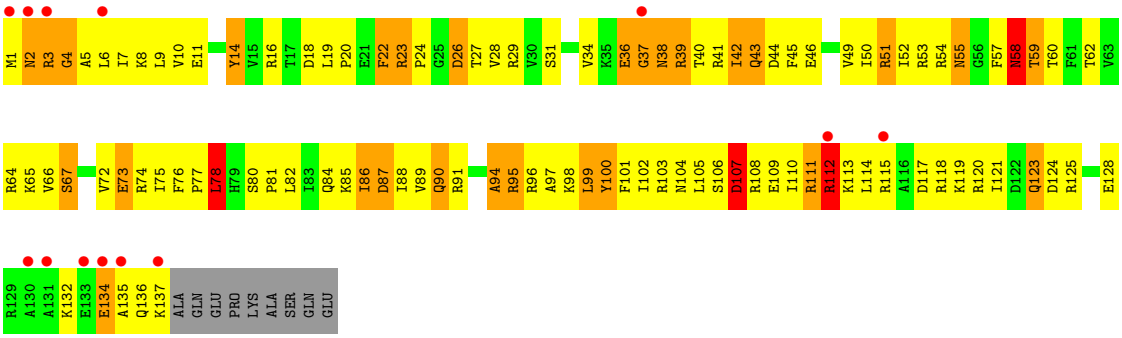
Chain YS:



• Molecule 39: 50S ribosomal protein L19

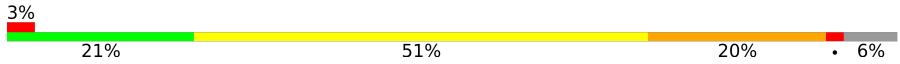
Chain RT:

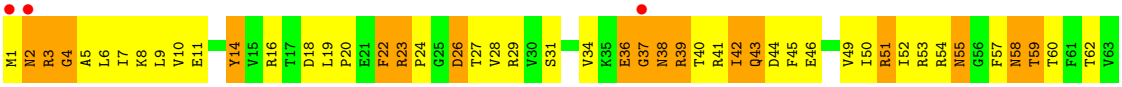


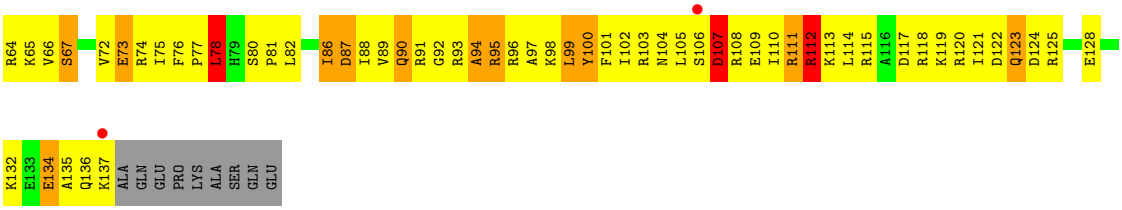


• Molecule 39: 50S ribosomal protein L19

Chain YT:

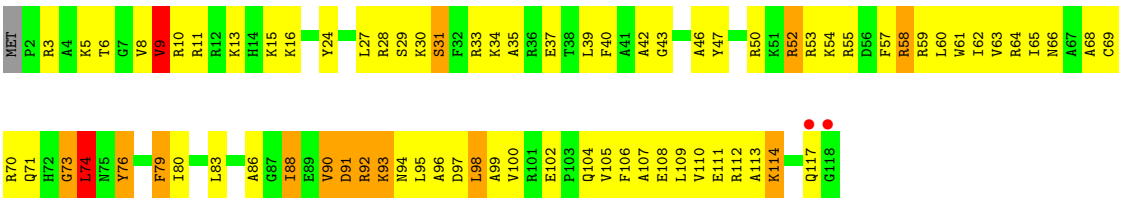






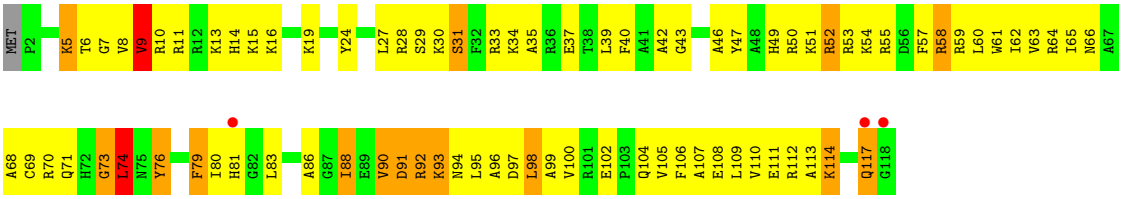
• Molecule 40: 50S ribosomal protein L20

Chain RU:



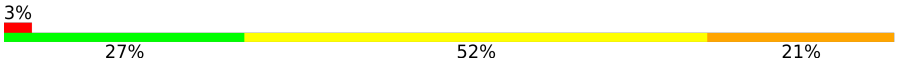
• Molecule 40: 50S ribosomal protein L20

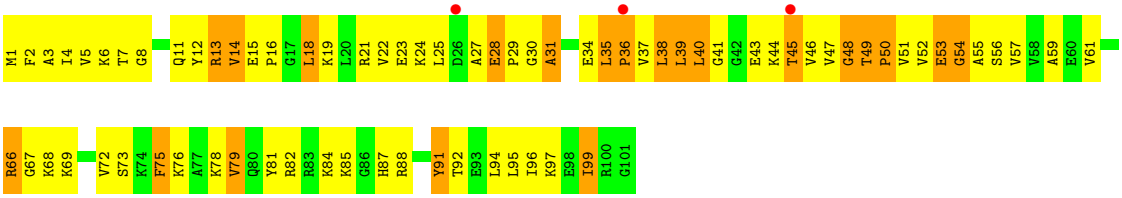
Chain YU:



• Molecule 41: 50S ribosomal protein L21

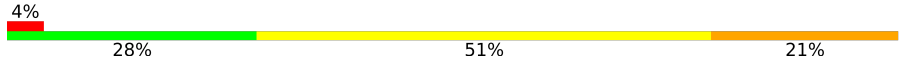
Chain RV:

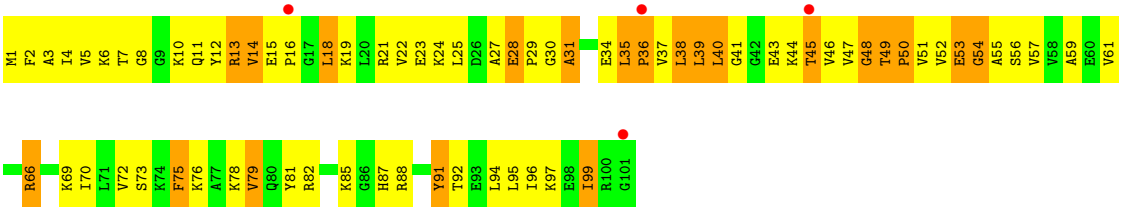




• Molecule 41: 50S ribosomal protein L21

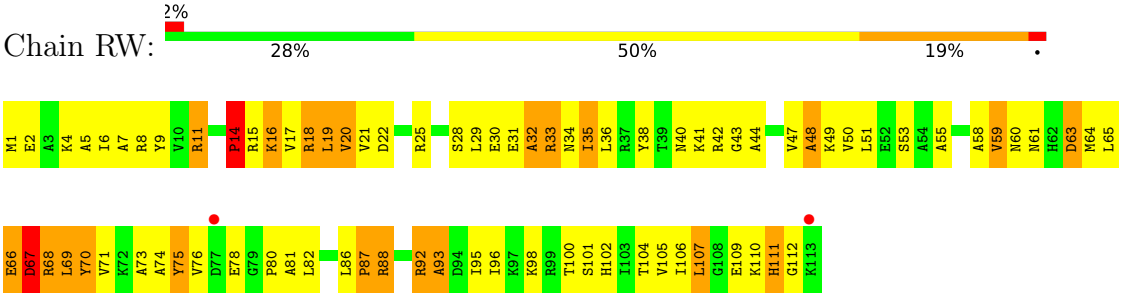
Chain YV:





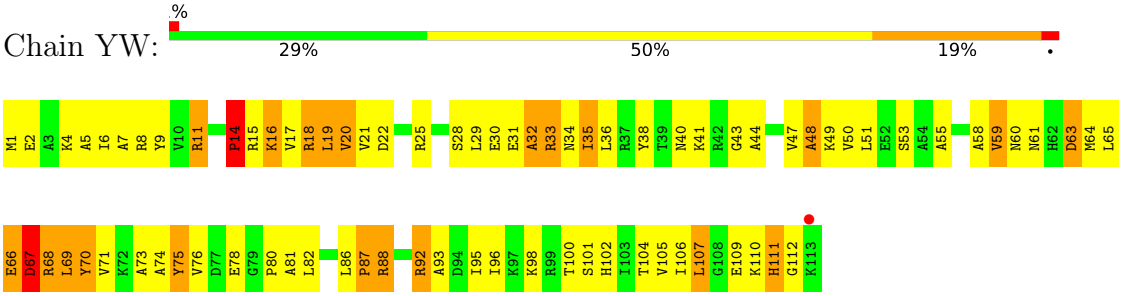
• Molecule 42: 50S ribosomal protein L22

Chain RW:



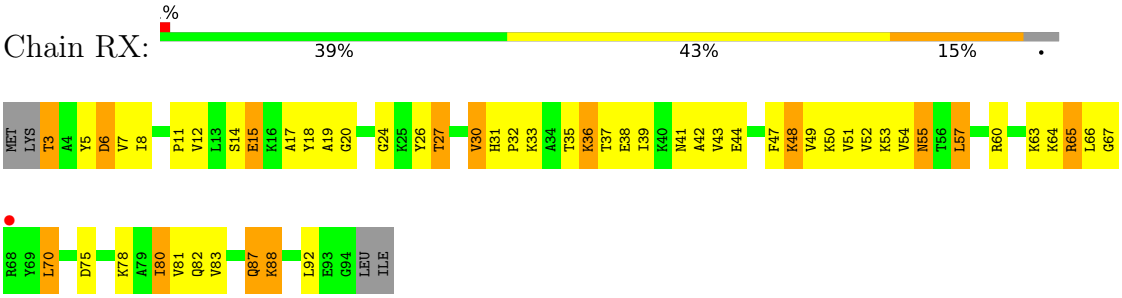
• Molecule 42: 50S ribosomal protein L22

Chain YW:



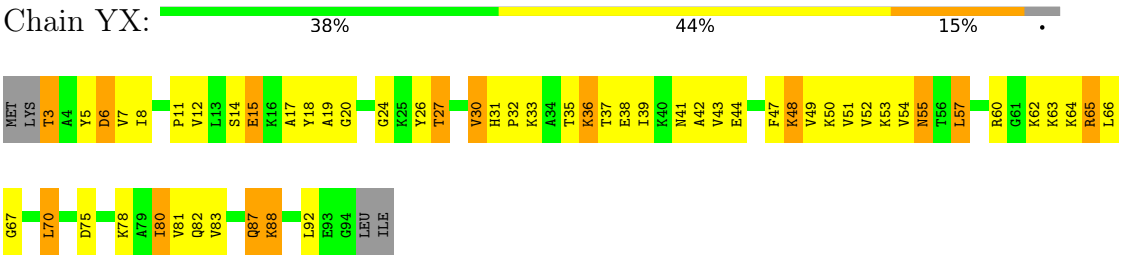
• Molecule 43: 50S ribosomal protein L23

Chain RX:



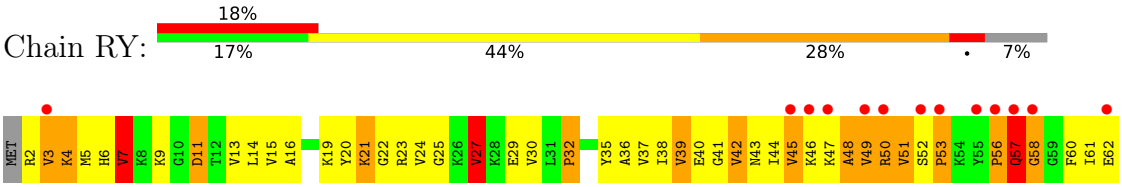
• Molecule 43: 50S ribosomal protein L23

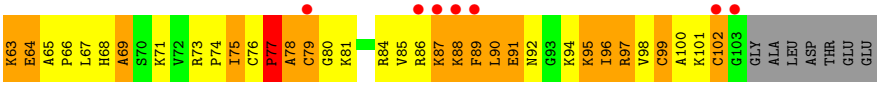
Chain YX:



• Molecule 44: 50S ribosomal protein L24

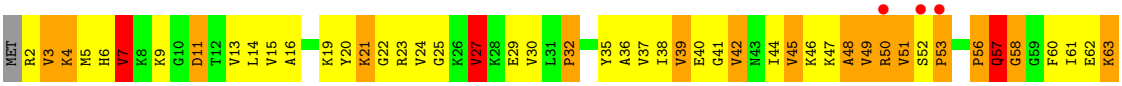
Chain RY:

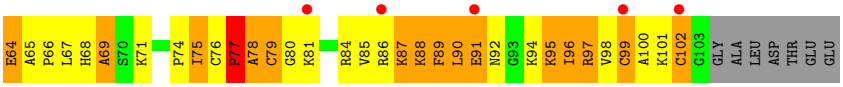




• Molecule 44: 50S ribosomal protein L24

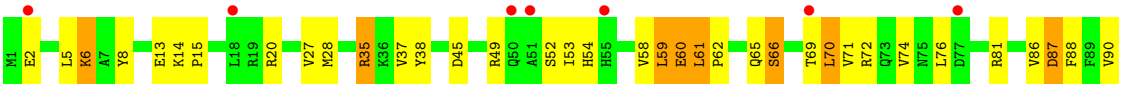
Chain YY:

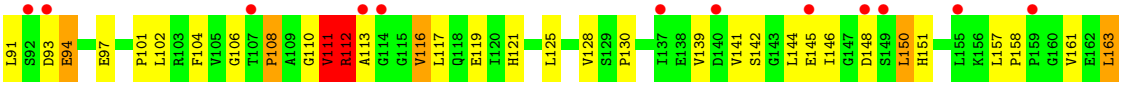


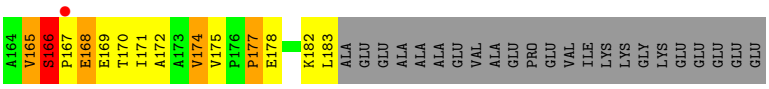


• Molecule 45: 50S ribosomal protein L25

Chain RZ:

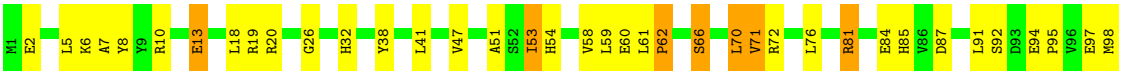


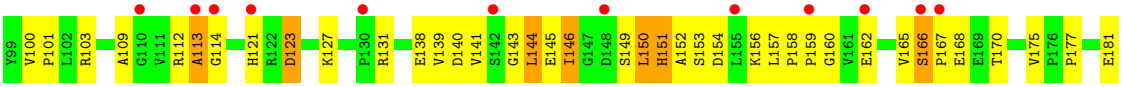


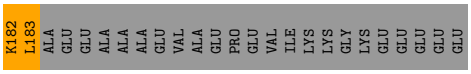


• Molecule 45: 50S ribosomal protein L25

Chain YZ:

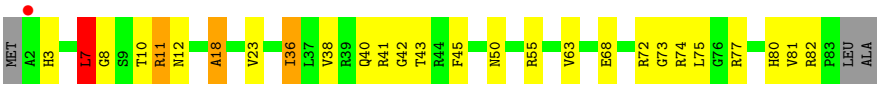






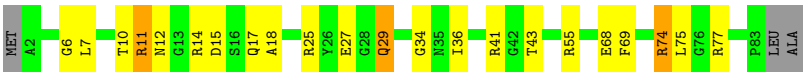
• Molecule 46: 50S ribosomal protein L27

Chain R0:



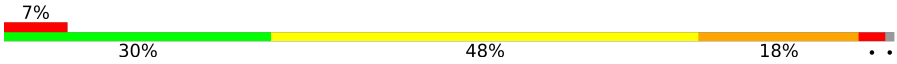
• Molecule 46: 50S ribosomal protein L27

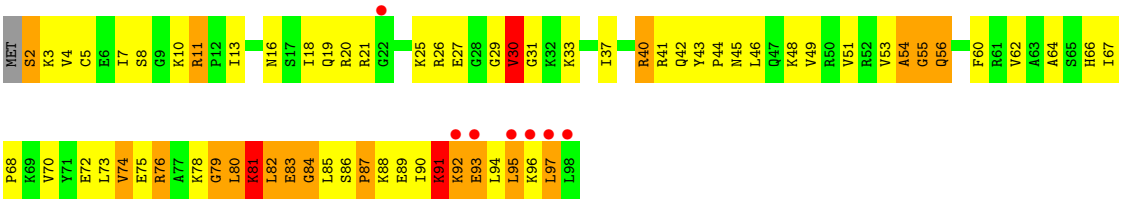
Chain Y0:



- Molecule 47: 50S ribosomal protein L28

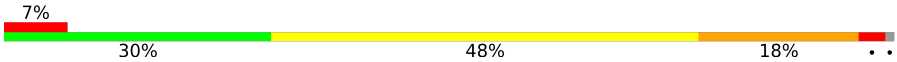
Chain R1:

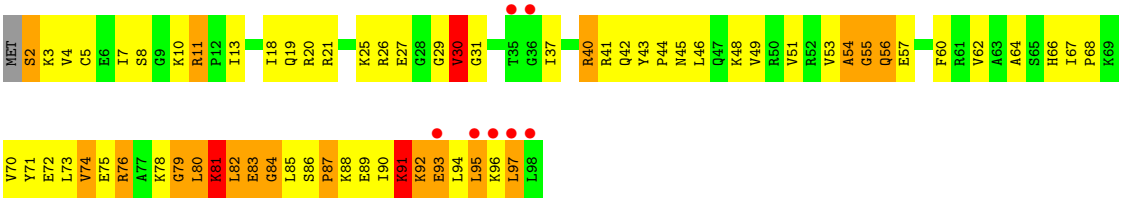




- Molecule 47: 50S ribosomal protein L28

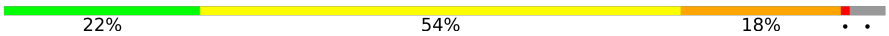
Chain Y1:

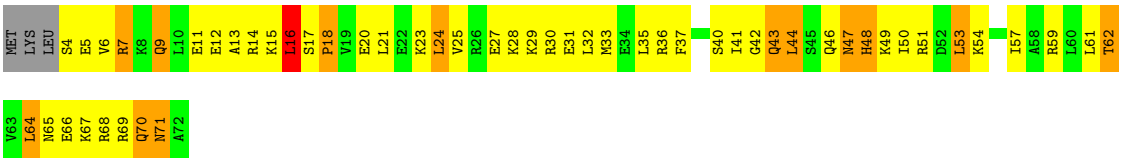




- Molecule 48: 50S ribosomal protein L29

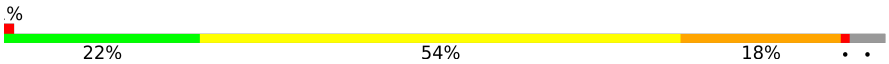
Chain R2:

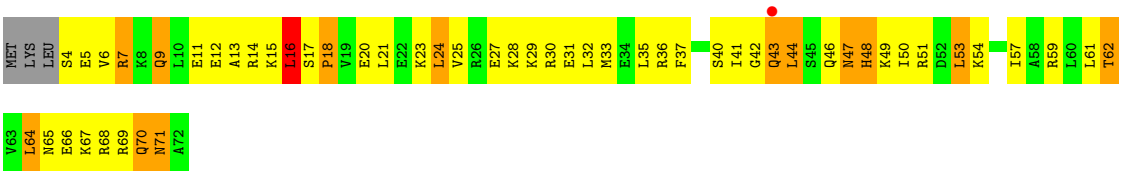




- Molecule 48: 50S ribosomal protein L29

Chain Y2:





- Molecule 49: 50S ribosomal protein L30

Chain R3:

• Molecule 49: 50S ribosomal protein L30

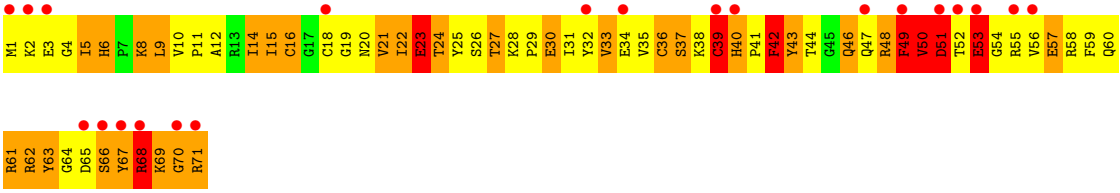
Chain Y3:

• Molecule 50: 50S ribosomal protein L31

Chain R4:

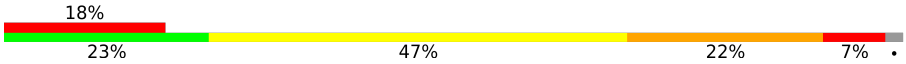
• Molecule 50: 50S ribosomal protein L31

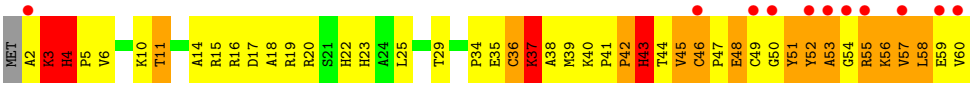
Chain Y4:



• Molecule 51: 50S ribosomal protein L32

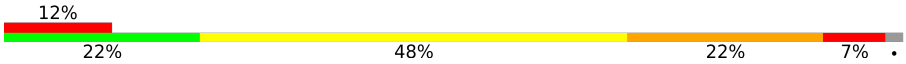
Chain R5:

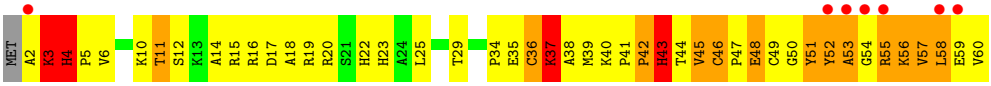




• Molecule 51: 50S ribosomal protein L32

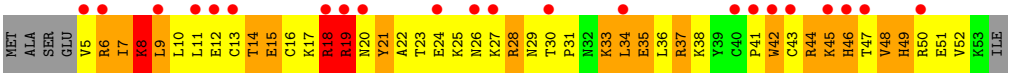
Chain Y5:





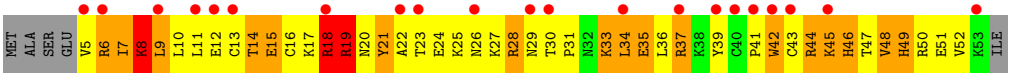
• Molecule 52: 50S ribosomal protein L33

Chain R6:



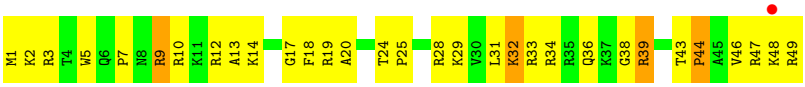
• Molecule 52: 50S ribosomal protein L33

Chain Y6:



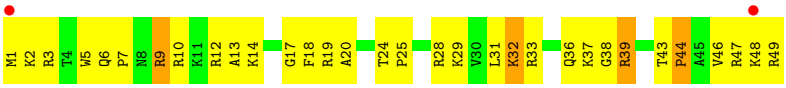
• Molecule 53: 50S ribosomal protein L34

Chain R7:



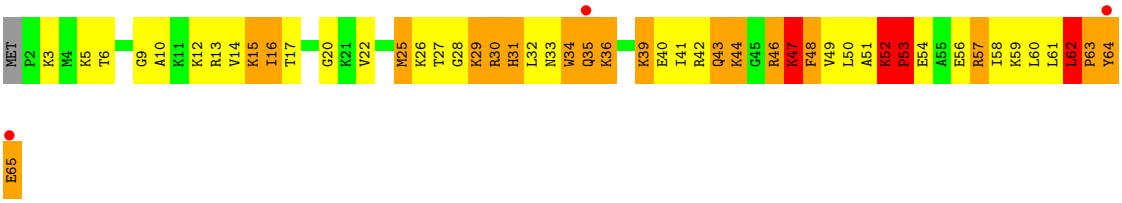
• Molecule 53: 50S ribosomal protein L34

Chain Y7:



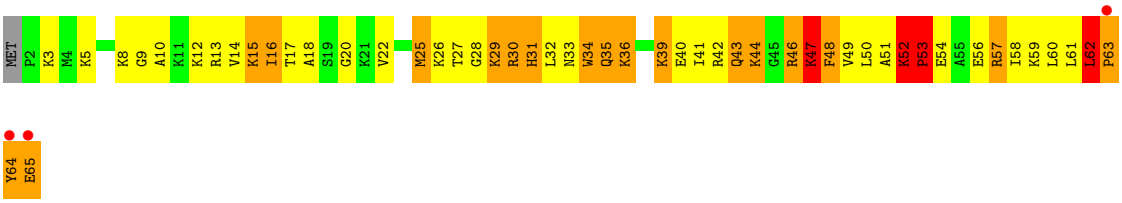
• Molecule 54: 50S ribosomal protein L35

Chain R8:



• Molecule 54: 50S ribosomal protein L35

Chain Y8:

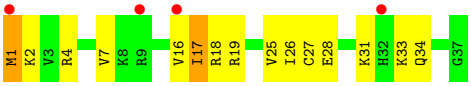


• Molecule 55: 50S ribosomal protein L36

Chain R9:

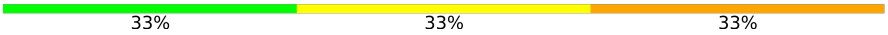
• Molecule 55: 50S ribosomal protein L36

Chain Y9:



• Molecule 56: tRNA acceptor end mimic

Chain Z6:



• Molecule 56: tRNA acceptor end mimic

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	208.25Å 448.40Å 624.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.97 – 3.48 34.97 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (34.97-3.48) 99.2 (34.97-3.30)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.230 , 0.270 0.231 , 0.270	Depositor DCC
R_{free} test set	39762 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 74.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	292002	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: 1MG, MG, PAR, PPU, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	QA	0.31	0/36098	0.83	43/56341 (0.1%)
1	XA	0.35	0/36101	0.86	41/56346 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.36	0/1959	0.65	0/2642
3	QC	0.37	0/1629	0.60	0/2195
3	XC	0.37	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.39	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.60	0/1709
7	XG	0.36	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.36	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.46	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.53	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.39	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.38	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.70	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.38	0/221	0.63	0/288
22	QV	0.53	0/1836	0.99	6/2859 (0.2%)
22	XV	0.52	0/1836	0.99	6/2859 (0.2%)
23	QY	0.28	0/333	1.11	1/517 (0.2%)
23	XY	0.30	0/333	1.11	1/517 (0.2%)
24	QX	0.96	3/193 (1.6%)	1.43	3/299 (1.0%)
24	XX	0.96	3/193 (1.6%)	1.44	3/299 (1.0%)
25	RA	0.38	4/69521 (0.0%)	0.89	62/108529 (0.1%)
25	YA	0.44	4/69543 (0.0%)	0.95	91/108563 (0.1%)
26	RB	0.31	0/2878	0.82	1/4490 (0.0%)
26	YB	0.38	0/2878	0.89	0/4490
27	RD	0.59	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	3/1802 (0.2%)
32	RI	0.32	0/1151	0.58	0/1558
32	YI	0.32	0/1151	0.60	0/1558
33	RN	0.46	0/1131	0.77	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.54	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.95	3/1544 (0.2%)
35	YP	0.50	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.90	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YS	0.45	0/892	0.83	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.47	0/1155	0.73	2/1542 (0.1%)
40	RU	0.48	0/982	0.78	0/1306
40	YU	0.48	0/982	0.78	0/1306
41	RV	0.47	0/790	0.82	0/1057
41	YV	0.47	0/790	0.81	0/1057
42	RW	0.45	0/911	0.75	0/1220
42	YW	0.45	0/911	0.75	0/1220
43	RX	0.56	0/739	0.77	0/993
43	YX	0.56	0/739	0.77	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.29	0/1493	0.53	0/2026
45	YZ	0.33	0/1493	0.56	0/2026
46	R0	0.30	0/657	0.54	1/874 (0.1%)
46	Y0	0.38	0/657	0.54	0/874
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.51	0/583	0.83	1/771 (0.1%)
48	Y2	0.51	0/583	0.84	1/771 (0.1%)
49	R3	0.47	0/474	0.72	0/635
49	Y3	0.43	0/474	0.71	0/635
50	R4	0.38	0/594	0.78	1/795 (0.1%)
50	Y4	0.38	0/594	0.78	1/795 (0.1%)
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.51	0/473	0.74	0/639
52	R6	0.43	0/431	0.76	0/575
52	Y6	0.42	0/431	0.76	0/575
53	R7	0.56	0/438	0.76	0/575
53	Y7	0.56	0/438	0.76	0/575
54	R8	0.62	0/525	0.93	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.35	0/310	0.60	0/407
55	Y9	0.37	0/310	0.61	0/407
56	Z6	0.80	0/40	1.78	1/60 (1.7%)
56	Z8	0.80	0/40	1.80	1/60 (1.7%)
All	All	0.41	16/316383 (0.0%)	0.86	323/473007 (0.1%)

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	RA	1472	A	N9-C8	-11.04	1.28	1.37
27	RD	236	GLY	C-N	8.56	1.53	1.34
25	RA	1472	A	C8-N7	-8.20	1.25	1.31
25	RA	1413	G	N9-C4	-7.25	1.32	1.38
25	YA	1473	G	C8-N7	-6.84	1.26	1.30

The worst 5 of 323 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	QL	47	LYS	C-N-CD	-20.49	75.52	120.60
12	XL	47	LYS	C-N-CD	-20.45	75.61	120.60
23	QY	40	G	P-O3'-C3'	-16.23	100.23	119.70
23	XY	40	G	P-O3'-C3'	-16.18	100.28	119.70
25	RA	1472	A	N7-C8-N9	12.07	119.84	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	536	0
1	XA	32249	0	16279	560	0
2	QB	1924	0	1975	284	0
2	XB	1924	0	1975	290	0
3	QC	1605	0	1668	205	0
3	XC	1605	0	1668	207	0
4	QD	1703	0	1764	254	0
4	XD	1703	0	1765	212	1
5	QE	1155	0	1213	143	0
5	XE	1155	0	1213	136	0
6	QF	843	0	857	93	1
6	XF	843	0	857	98	0
7	QG	1257	0	1296	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1294	143	0
8	QH	1116	0	1175	149	0
8	XH	1116	0	1177	148	0
9	QI	1010	0	1037	146	0
9	XI	1010	0	1037	158	0
10	QJ	801	0	849	150	0
10	XJ	801	0	849	135	0
11	QK	885	0	904	100	0
11	XK	885	0	904	109	0
12	QL	975	0	1062	107	0
12	XL	975	0	1062	103	0
13	QM	964	0	1034	151	0
13	XM	964	0	1034	160	0
14	QN	492	0	529	95	0
14	XN	492	0	529	96	0
15	QO	734	0	771	74	0
15	XO	734	0	771	73	0
16	QP	705	0	725	111	0
16	XP	705	0	725	107	0
17	QQ	834	0	904	81	0
17	XQ	834	0	904	73	0
18	QR	574	0	644	65	0
18	XR	574	0	644	68	0
19	QS	674	0	699	110	0
19	XS	674	0	699	133	0
20	QT	763	0	860	105	0
20	XT	763	0	861	100	0
21	QU	217	0	234	27	0
21	XU	217	0	234	24	0
22	QV	1644	0	836	35	0
22	XV	1644	0	836	35	0
23	QY	323	0	165	4	0
23	XY	323	0	165	7	0
24	QX	173	0	88	7	0
24	XX	173	0	88	6	0
25	RA	62071	0	31288	884	1
25	YA	62091	0	31294	903	1
26	RB	2573	0	1306	66	0
26	YB	2573	0	1306	33	0
27	RD	2115	0	2195	306	0
27	YD	2115	0	2195	331	0
28	RE	1568	0	1634	272	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	263	0
29	RF	1585	0	1632	173	0
29	YF	1585	0	1632	171	0
30	RG	1474	0	1535	207	1
30	YG	1474	0	1535	201	1
31	RH	1307	0	1382	225	0
31	YH	1307	0	1382	226	0
32	RI	1136	0	1223	40	0
32	YI	1136	0	1223	50	0
33	RN	1104	0	1180	197	0
33	YN	1104	0	1180	186	0
34	RO	933	0	996	120	0
34	YO	933	0	996	127	0
35	RP	1145	0	1228	246	0
35	YP	1145	0	1228	239	1
36	RQ	1122	0	1179	153	0
36	YQ	1122	0	1179	150	0
37	RR	968	0	1033	113	0
37	YR	968	0	1033	105	0
38	RS	882	0	943	162	0
38	YS	882	0	943	162	0
39	RT	1141	0	1202	151	0
39	YT	1141	0	1202	154	0
40	RU	964	0	1022	128	0
40	YU	964	0	1022	136	0
41	RV	779	0	852	130	0
41	YV	779	0	852	131	13
42	RW	900	0	964	101	0
42	YW	900	0	964	102	0
43	RX	725	0	778	67	0
43	YX	725	0	778	67	0
44	RY	785	0	878	161	0
44	YY	785	0	878	153	0
45	RZ	1461	0	1493	52	0
45	YZ	1461	0	1493	40	0
46	R0	648	0	672	21	0
46	Y0	648	0	672	23	0
47	R1	763	0	848	143	0
47	Y1	763	0	848	136	0
48	R2	581	0	629	79	0
48	Y2	581	0	629	76	0
49	R3	469	0	518	39	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	42	0
50	R4	581	0	574	148	0
50	Y4	581	0	574	165	0
51	R5	459	0	480	73	0
51	Y5	459	0	480	76	13
52	R6	424	0	450	94	0
52	Y6	424	0	450	92	0
53	R7	430	0	480	39	0
53	Y7	430	0	480	44	0
54	R8	517	0	582	105	0
54	Y8	517	0	582	99	0
55	R9	307	0	335	20	0
55	Y9	307	0	335	18	0
56	Z6	74	0	51	7	0
56	Z8	74	0	51	6	0
57	QA	65	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	RA	241	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RR	2	0	0	0	0
57	XA	74	0	0	0	0
57	Y0	1	0	0	0	0
57	Y5	1	0	0	0	0
57	YA	268	0	0	0	0
57	YB	4	0	0	0	0
57	YE	1	0	0	0	0
57	YP	2	0	0	0	0
58	QA	42	0	45	0	0
58	XA	42	0	45	1	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	R9	1	0	0	0	0
59	XD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	292002	0	198357	14284	17

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 29.

The worst 5 of 14284 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:XN:32:SER:CB	14:XN:41:ARG:HB3	1.23	1.55
14:XN:32:SER:HB3	14:XN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.36	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.35	1.52
4:XD:22:LYS:CG	4:XD:26:CYS:SG	2.01	1.49

The worst 5 of 17 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:50:PRO:C	51:Y5:60:VAL:O[4_445]	1.47	0.73
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.50	0.70
41:YV:51:VAL:N	51:Y5:60:VAL:C[4_445]	1.60	0.60
41:YV:50:PRO:CG	51:Y5:60:VAL:CA[4_445]	1.78	0.42
41:YV:50:PRO:CA	51:Y5:60:VAL:O[4_445]	1.83	0.37

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	3
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	7
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	7
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	0	6
4	XD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	0	5
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	6
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	5
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	7
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	7
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	6
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	7
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	5
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	5
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%)	20 (21%)	9 (9%)	0	7
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	6
11	QK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	11
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	9
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%)	28 (24%)	20 (17%)	0	2
13	XM	119/126 (94%)	71 (60%)	28 (24%)	20 (17%)	0	2
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	1
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	1
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	10
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	10
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	3
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	3
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	8
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	0	4
18	XR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	0	4
19	QS	82/93 (88%)	47 (57%)	17 (21%)	18 (22%)	0	1
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	QT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	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%)	16 (70%)	3 (13%)	4 (17%)	0	1
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	10
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	10
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	6
29	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	0	6
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	4
30	YG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0	4
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	102 (71%)	29 (20%)	13 (9%)	1	7
32	YI	144/148 (97%)	101 (70%)	26 (18%)	17 (12%)	0	4
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	9
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	9
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	6
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	6
37	RR	116/118 (98%)	83 (72%)	19 (16%)	14 (12%)	0	4
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	4
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	86 (75%)	20 (17%)	9 (8%)	1	9
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	9
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	6
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	6
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	15
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	15
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	0
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
45	RZ	181/206 (88%)	126 (70%)	40 (22%)	15 (8%)	1	8
45	YZ	181/206 (88%)	125 (69%)	38 (21%)	18 (10%)	0	6
46	R0	80/85 (94%)	68 (85%)	9 (11%)	3 (4%)	3	24
46	Y0	80/85 (94%)	71 (89%)	9 (11%)	0	100	100
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	4
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	4
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	3
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	3
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	16
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	16
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	13
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100 100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100 100
All	All	11470/12128 (95%)	7650 (67%)	2346 (20%)	1474 (13%)	0 3

5 of 1474 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	QB	205/220 (93%)	181 (88%)	24 (12%)	5 24
2	XB	205/220 (93%)	181 (88%)	24 (12%)	5 24
3	QC	159/188 (85%)	143 (90%)	16 (10%)	7 30
3	XC	159/188 (85%)	143 (90%)	16 (10%)	7 30
4	QD	180/181 (99%)	160 (89%)	20 (11%)	6 26
4	XD	180/181 (99%)	165 (92%)	15 (8%)	11 38
5	QE	116/123 (94%)	108 (93%)	8 (7%)	15 46
5	XE	116/123 (94%)	108 (93%)	8 (7%)	15 46
6	QF	90/90 (100%)	76 (84%)	14 (16%)	2 14
6	XF	90/90 (100%)	76 (84%)	14 (16%)	2 14
7	QG	126/127 (99%)	114 (90%)	12 (10%)	8 32
7	XG	126/127 (99%)	115 (91%)	11 (9%)	10 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	106 (89%)	13 (11%)	6	27
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	27
9	QI	98/99 (99%)	87 (89%)	11 (11%)	6	25
9	XI	98/99 (99%)	87 (89%)	11 (11%)	6	25
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	9	35
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	9	35
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	30
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	30
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	19
12	XL	104/109 (95%)	90 (86%)	14 (14%)	4	19
13	QM	97/101 (96%)	81 (84%)	16 (16%)	2	12
13	XM	97/101 (96%)	81 (84%)	16 (16%)	2	12
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	8
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7	30
15	QO	79/80 (99%)	73 (92%)	6 (8%)	13	42
15	XO	79/80 (99%)	73 (92%)	6 (8%)	13	42
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	21
16	XP	72/74 (97%)	63 (88%)	9 (12%)	4	21
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	18	50
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	50
18	QR	61/77 (79%)	54 (88%)	7 (12%)	5	24
18	XR	61/77 (79%)	54 (88%)	7 (12%)	5	24
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	15
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	15
20	QT	76/82 (93%)	68 (90%)	8 (10%)	7	29
20	XT	76/82 (93%)	68 (90%)	8 (10%)	7	29
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	56
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	56
27	RD	214/218 (98%)	177 (83%)	37 (17%)	2	10
27	YD	214/218 (98%)	177 (83%)	37 (17%)	2	10
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	3
29	RF	161/166 (97%)	140 (87%)	21 (13%)	4	20
29	YF	161/166 (97%)	140 (87%)	21 (13%)	4	20
30	RG	155/156 (99%)	130 (84%)	25 (16%)	2	13
30	YG	155/156 (99%)	130 (84%)	25 (16%)	2	13
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	6
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	6
32	RI	122/124 (98%)	98 (80%)	24 (20%)	1	6
32	YI	122/124 (98%)	98 (80%)	24 (20%)	1	6
33	RN	117/119 (98%)	98 (84%)	19 (16%)	2	12
33	YN	117/119 (98%)	98 (84%)	19 (16%)	2	12
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7	30
34	YO	100/100 (100%)	90 (90%)	10 (10%)	7	30
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	3
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	3
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	12
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	2	12
37	RR	101/101 (100%)	84 (83%)	17 (17%)	2	11
37	YR	101/101 (100%)	84 (83%)	17 (17%)	2	11
38	RS	87/88 (99%)	74 (85%)	13 (15%)	3	15
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	15
39	RT	120/127 (94%)	97 (81%)	23 (19%)	1	6
39	YT	120/127 (94%)	98 (82%)	22 (18%)	1	8
40	RU	93/94 (99%)	80 (86%)	13 (14%)	3	17
40	YU	93/94 (99%)	80 (86%)	13 (14%)	3	17
41	RV	82/82 (100%)	71 (87%)	11 (13%)	4	19
41	YV	82/82 (100%)	71 (87%)	11 (13%)	4	19
42	RW	92/92 (100%)	77 (84%)	15 (16%)	2	12
42	YW	92/92 (100%)	77 (84%)	15 (16%)	2	12
43	RX	74/78 (95%)	63 (85%)	11 (15%)	3	15
43	YX	74/78 (95%)	63 (85%)	11 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RY	85/91 (93%)	70 (82%)	15 (18%)	2	9
44	YY	85/91 (93%)	70 (82%)	15 (18%)	2	9
45	RZ	162/179 (90%)	139 (86%)	23 (14%)	3	17
45	YZ	162/179 (90%)	139 (86%)	23 (14%)	3	17
46	R0	65/67 (97%)	61 (94%)	4 (6%)	18	50
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	9	34
47	R1	82/83 (99%)	67 (82%)	15 (18%)	1	8
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	1	8
48	R2	64/67 (96%)	57 (89%)	7 (11%)	6	27
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	27
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	4
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	4
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	2
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	3
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	3
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	5
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	5
53	R7	42/42 (100%)	39 (93%)	3 (7%)	14	45
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	14	45
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	2
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	2
55	R9	34/34 (100%)	32 (94%)	2 (6%)	19	51
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	51
All	All	9702/10066 (96%)	8296 (86%)	1406 (14%)	3	16

5 of 1406 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	YD	65	ILE
35	YP	144	GLU
27	YD	261	LYS
27	YD	61	LEU
31	YH	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
7	XG	28	ASN
27	YD	166	GLN
7	XG	86	GLN
13	XM	77	ASN
28	YE	135	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	269 (17%)	42 (2%)
1	XA	1499/1522 (98%)	289 (19%)	46 (3%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QY	14/17 (82%)	7 (50%)	1 (7%)
23	XY	14/17 (82%)	7 (50%)	1 (7%)
24	QX	7/25 (28%)	4 (57%)	1 (14%)
24	XX	7/25 (28%)	4 (57%)	1 (14%)
25	RA	2879/2916 (98%)	620 (21%)	66 (2%)
25	YA	2880/2916 (98%)	623 (21%)	60 (2%)
26	RB	119/122 (97%)	24 (20%)	2 (1%)
26	YB	119/122 (97%)	24 (20%)	1 (0%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9190/9364 (98%)	1931 (21%)	223 (2%)

5 of 1931 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C
1	QA	51	A

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	60	A
25	YA	2867	G
1	XA	753	A

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Mol	Chain	Res	Type
25	YA	2776	A
25	YA	1543	A

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	$\#\|Z\| > 2$
56	PPU	Z8	76	57,56	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)
23	1MG	XY	37	23	18,26,27	2.19	2 (11%)	19,39,42	1.55	4 (21%)
56	PPU	Z6	76	56,25	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)
23	1MG	QY	37	23	18,26,27	2.18	2 (11%)	19,39,42	1.56	4 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	Z8	76	57,56	-	2/21/43/44	0/4/4/4
23	1MG	XY	37	23	-	0/3/25/26	0/3/3/3
56	PPU	Z6	76	56,25	-	2/21/43/44	0/4/4/4
23	1MG	QY	37	23	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	O-C	9.30	1.41	1.23
56	Z6	76	PPU	O-C	9.27	1.41	1.23
23	QY	37	1MG	C2-N2	7.38	1.47	1.34
23	XY	37	1MG	C2-N2	7.35	1.47	1.34
56	Z6	76	PPU	C9-N6	-5.95	1.32	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Z8	76	PPU	C3'-N3'-C	-8.60	110.23	123.21
56	Z6	76	PPU	C3'-N3'-C	-8.58	110.27	123.21
56	Z8	76	PPU	N3-C2-N1	-4.71	121.31	128.68
56	Z6	76	PPU	N3-C2-N1	-4.68	121.36	128.68
56	Z6	76	PPU	CA-C-N3'	4.05	121.77	116.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z8	76	PPU	5	0
56	Z6	76	PPU	7	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 680 ligands modelled in this entry, 678 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	PAR	XA	1675	-	45,45,45	1.50	6 (13%)	64,67,67	1.34	5 (7%)
58	PAR	QA	1666	-	45,45,45	1.48	7 (15%)	64,67,67	1.39	9 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	XA	1675	-	-	6/18/94/94	0/4/4/4
58	PAR	QA	1666	-	-	8/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1666	PAR	C64-C54	5.24	1.59	1.52
58	XA	1675	PAR	C64-C54	4.90	1.58	1.52
58	QA	1666	PAR	C52-C42	3.13	1.58	1.52
58	XA	1675	PAR	C52-C42	2.96	1.58	1.52
58	XA	1675	PAR	O54-C14	2.86	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	XA	1675	PAR	O33-C14-C24	4.67	116.27	108.22
58	XA	1675	PAR	C14-O54-C54	4.34	122.20	113.69
58	QA	1666	PAR	O52-C13-C23	3.84	115.91	107.96
58	QA	1666	PAR	C14-O54-C54	3.82	121.18	113.69
58	QA	1666	PAR	O33-C14-C24	3.77	114.70	108.22

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	QA	1666	PAR	C44-C54-C64-N64
58	QA	1666	PAR	O54-C54-C64-N64
58	QA	1666	PAR	O51-C51-C61-O61
58	XA	1675	PAR	O51-C51-C61-O61
58	QA	1666	PAR	C41-C51-C61-O61

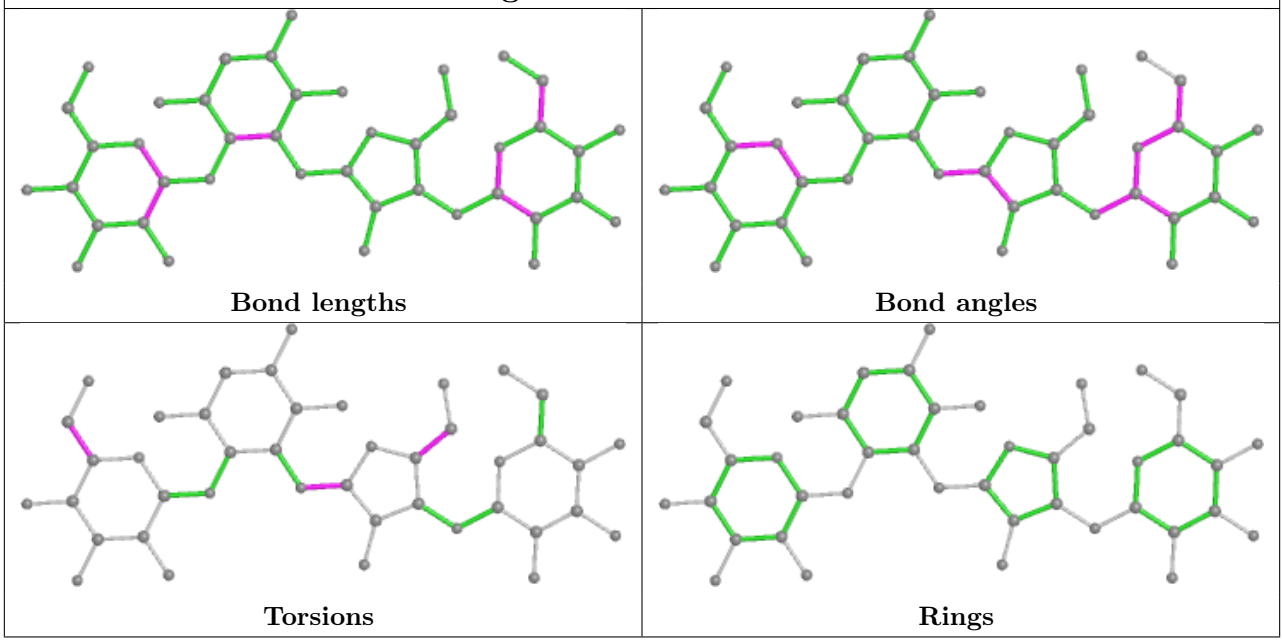
There are no ring outliers.

1 monomer is involved in 1 short contact:

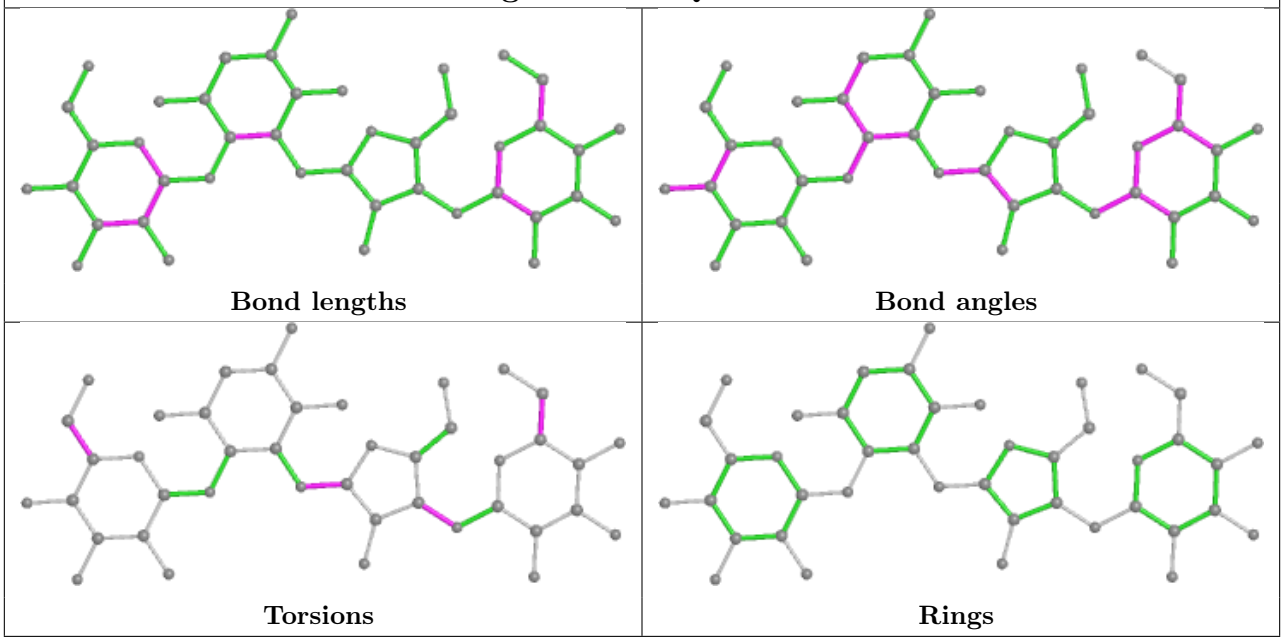
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XA	1675	PAR	1	0

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 XA 1675



Ligand PAR QA 1666



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	QA	1500/1522 (98%)	0.23	45 (3%)	50	47	43, 89, 165, 301	0
1	XA	1500/1522 (98%)	0.12	34 (2%)	60	56	33, 76, 161, 285	0
2	QB	237/256 (92%)	0.60	27 (11%)	5	6	74, 140, 206, 264	0
2	XB	237/256 (92%)	0.50	18 (7%)	13	15	68, 121, 186, 246	0
3	QC	205/239 (85%)	0.57	12 (5%)	22	22	66, 125, 179, 210	0
3	XC	205/239 (85%)	0.20	2 (0%)	82	78	46, 95, 150, 198	0
4	QD	208/209 (99%)	0.24	4 (1%)	66	63	47, 92, 146, 223	0
4	XD	208/209 (99%)	0.34	6 (2%)	51	48	45, 96, 162, 182	0
5	QE	151/162 (93%)	0.39	5 (3%)	46	43	42, 101, 170, 220	0
5	XE	151/162 (93%)	0.23	5 (3%)	46	43	35, 84, 142, 186	0
6	QF	101/101 (100%)	0.34	2 (1%)	65	61	40, 90, 127, 156	0
6	XF	101/101 (100%)	0.35	3 (2%)	50	47	38, 84, 127, 150	0
7	QG	155/156 (99%)	0.62	15 (9%)	7	9	56, 121, 175, 232	0
7	XG	155/156 (99%)	0.47	13 (8%)	11	13	51, 93, 148, 196	0
8	QH	138/138 (100%)	0.27	3 (2%)	62	58	51, 100, 142, 160	0
8	XH	138/138 (100%)	0.14	0	100	100	51, 89, 134, 187	0
9	QI	127/128 (99%)	0.95	17 (13%)	3	4	71, 131, 189, 204	0
9	XI	127/128 (99%)	0.47	7 (5%)	25	24	46, 112, 165, 221	0
10	QJ	99/105 (94%)	1.38	34 (34%)	0	0	80, 153, 212, 237	0
10	XJ	99/105 (94%)	0.95	13 (13%)	3	5	42, 120, 186, 217	0
11	QK	119/129 (92%)	0.75	9 (7%)	13	15	42, 89, 165, 231	0
11	XK	119/129 (92%)	0.37	7 (5%)	22	22	49, 81, 135, 193	0
12	QL	125/132 (94%)	0.53	8 (6%)	19	19	40, 83, 150, 208	0
12	XL	125/132 (94%)	0.24	5 (4%)	38	35	29, 68, 134, 239	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	QM	121/126 (96%)	0.86	15 (12%) 4 5	52, 130, 190, 269	0
13	XM	121/126 (96%)	0.44	6 (4%) 28 27	43, 98, 161, 256	0
14	QN	60/61 (98%)	1.01	9 (15%) 2 3	72, 121, 165, 182	0
14	XN	60/61 (98%)	0.47	3 (5%) 28 27	38, 87, 148, 182	0
15	QO	88/89 (98%)	0.39	5 (5%) 23 22	48, 95, 154, 187	0
15	XO	88/89 (98%)	0.25	3 (3%) 45 42	43, 82, 128, 167	0
16	QP	84/88 (95%)	0.35	3 (3%) 42 40	44, 86, 146, 195	0
16	XP	84/88 (95%)	0.30	2 (2%) 59 55	46, 92, 133, 208	0
17	QQ	100/105 (95%)	0.43	4 (4%) 38 35	63, 94, 151, 215	0
17	XQ	100/105 (95%)	0.30	2 (2%) 65 61	45, 95, 148, 188	0
18	QR	70/88 (79%)	0.35	4 (5%) 23 22	45, 85, 146, 166	0
18	XR	70/88 (79%)	0.24	1 (1%) 75 71	35, 81, 137, 153	0
19	QS	84/93 (90%)	1.10	17 (20%) 1 1	82, 137, 196, 229	0
19	XS	84/93 (90%)	0.39	3 (3%) 42 40	53, 96, 156, 198	0
20	QT	99/106 (93%)	0.50	4 (4%) 38 35	55, 103, 165, 201	0
20	XT	99/106 (93%)	0.41	4 (4%) 38 35	50, 101, 158, 190	0
21	QU	25/27 (92%)	2.09	9 (36%) 0 0	66, 117, 146, 190	0
21	XU	25/27 (92%)	1.46	4 (16%) 1 2	61, 89, 133, 169	0
22	QV	77/77 (100%)	0.47	5 (6%) 18 19	49, 99, 152, 188	0
22	XV	77/77 (100%)	0.46	2 (2%) 56 52	43, 82, 137, 198	0
23	QY	14/17 (82%)	0.79	2 (14%) 2 3	85, 123, 178, 179	0
23	XY	14/17 (82%)	0.92	2 (14%) 2 3	66, 108, 141, 145	0
24	QX	8/25 (32%)	1.59	2 (25%) 0 0	68, 91, 144, 227	0
24	XX	8/25 (32%)	1.16	2 (25%) 0 0	51, 69, 129, 197	0
25	RA	2882/2916 (98%)	0.24	153 (5%) 26 25	32, 68, 203, 342	0
25	YA	2883/2916 (98%)	0.02	116 (4%) 38 35	21, 52, 190, 313	0
26	RB	120/122 (98%)	0.40	3 (2%) 57 53	62, 105, 144, 172	0
26	YB	120/122 (98%)	-0.11	0 100 100	43, 68, 101, 139	0
27	RD	272/276 (98%)	0.02	1 (0%) 92 90	32, 60, 102, 187	0
27	YD	272/276 (98%)	0.09	2 (0%) 87 84	11, 55, 94, 228	0
28	RE	205/206 (99%)	0.24	7 (3%) 45 42	30, 74, 135, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	YE	205/206 (99%)	0.05	4 (1%) 65 61	20, 58, 130, 245	0
29	RF	202/210 (96%)	0.12	5 (2%) 57 53	27, 82, 150, 199	0
29	YF	202/210 (96%)	-0.12	0 100 100	17, 58, 119, 164	0
30	RG	181/182 (99%)	2.10	83 (45%) 0 0	58, 182, 252, 270	0
30	YG	181/182 (99%)	1.24	32 (17%) 1 2	52, 114, 185, 251	0
31	RH	170/180 (94%)	1.20	39 (22%) 0 0	71, 144, 203, 244	0
31	YH	170/180 (94%)	0.42	9 (5%) 26 25	41, 86, 147, 171	0
32	RI	146/148 (98%)	0.45	12 (8%) 11 13	47, 100, 170, 202	0
32	YI	146/148 (98%)	0.22	6 (4%) 37 35	43, 98, 153, 180	0
33	RN	138/140 (98%)	0.22	4 (2%) 51 48	43, 83, 138, 196	0
33	YN	138/140 (98%)	0.02	1 (0%) 87 84	29, 60, 118, 171	0
34	RO	122/122 (100%)	0.19	1 (0%) 86 82	21, 75, 123, 179	0
34	YO	122/122 (100%)	-0.19	0 100 100	18, 59, 94, 134	0
35	RP	150/150 (100%)	0.55	12 (8%) 12 14	21, 86, 180, 219	0
35	YP	150/150 (100%)	0.18	4 (2%) 54 51	14, 67, 136, 235	0
36	RQ	141/141 (100%)	0.40	9 (6%) 19 19	45, 88, 145, 231	0
36	YQ	141/141 (100%)	0.04	3 (2%) 63 60	24, 65, 135, 196	0
37	RR	118/118 (100%)	-0.03	1 (0%) 86 82	38, 69, 130, 147	0
37	YR	118/118 (100%)	-0.19	0 100 100	26, 55, 91, 142	0
38	RS	111/112 (99%)	0.38	3 (2%) 54 51	49, 104, 167, 222	0
38	YS	111/112 (99%)	-0.00	2 (1%) 68 64	39, 71, 123, 181	0
39	RT	137/146 (93%)	0.39	13 (9%) 8 10	42, 86, 185, 226	0
39	YT	137/146 (93%)	0.06	5 (3%) 42 40	25, 70, 160, 220	0
40	RU	117/118 (99%)	0.22	2 (1%) 70 66	31, 69, 130, 222	0
40	YU	117/118 (99%)	0.02	3 (2%) 56 52	21, 50, 107, 201	0
41	RV	101/101 (100%)	0.19	3 (2%) 50 47	44, 92, 155, 249	0
41	YV	101/101 (100%)	0.34	4 (3%) 38 35	26, 71, 136, 264	0
42	RW	113/113 (100%)	0.05	2 (1%) 68 64	31, 63, 128, 188	0
42	YW	113/113 (100%)	-0.08	1 (0%) 84 80	17, 54, 114, 186	0
43	RX	92/96 (95%)	0.15	1 (1%) 80 76	41, 78, 122, 150	0
43	YX	92/96 (95%)	-0.06	0 100 100	28, 56, 92, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	RY	102/110 (92%)	1.04	20 (19%) 1 1	50, 106, 193, 237	0
44	YY	102/110 (92%)	0.43	8 (7%) 13 15	39, 82, 158, 234	0
45	RZ	183/206 (88%)	0.76	20 (10%) 5 7	56, 124, 189, 247	0
45	YZ	183/206 (88%)	0.26	12 (6%) 18 18	41, 86, 169, 257	0
46	R0	82/85 (96%)	-0.03	1 (1%) 79 74	42, 72, 103, 131	0
46	Y0	82/85 (96%)	-0.32	0 100 100	26, 49, 80, 99	0
47	R1	97/98 (98%)	0.74	7 (7%) 15 17	34, 75, 194, 262	0
47	Y1	97/98 (98%)	0.49	7 (7%) 15 17	27, 61, 143, 210	0
48	R2	69/72 (95%)	0.18	0 100 100	48, 94, 168, 184	0
48	Y2	69/72 (95%)	0.06	1 (1%) 75 71	22, 66, 131, 195	0
49	R3	59/60 (98%)	0.73	6 (10%) 6 8	42, 90, 161, 183	0
49	Y3	59/60 (98%)	0.07	2 (3%) 45 42	33, 61, 113, 179	0
50	R4	71/71 (100%)	2.17	30 (42%) 0 0	129, 204, 273, 302	0
50	Y4	71/71 (100%)	1.56	21 (29%) 0 0	84, 166, 258, 313	0
51	R5	59/60 (98%)	0.81	11 (18%) 1 2	25, 73, 191, 257	0
51	Y5	59/60 (98%)	0.56	7 (11%) 4 6	28, 62, 189, 319	0
52	R6	49/54 (90%)	1.94	22 (44%) 0 0	66, 147, 198, 224	0
52	Y6	49/54 (90%)	1.66	21 (42%) 0 0	59, 116, 196, 225	0
53	R7	49/49 (100%)	0.13	1 (2%) 65 61	27, 55, 129, 235	0
53	Y7	49/49 (100%)	-0.10	2 (4%) 37 35	23, 42, 102, 186	0
54	R8	64/65 (98%)	0.45	3 (4%) 31 30	34, 73, 129, 210	0
54	Y8	64/65 (98%)	0.16	3 (4%) 31 30	24, 56, 101, 237	0
55	R9	37/37 (100%)	1.56	8 (21%) 0 1	64, 96, 157, 235	0
55	Y9	37/37 (100%)	1.24	4 (10%) 5 7	48, 83, 136, 176	0
56	Z6	2/3 (66%)	1.63	0 100 100	77, 77, 77, 77	0
56	Z8	2/3 (66%)	1.17	0 100 100	51, 51, 51, 60	0
All	All	20873/21492 (97%)	0.31	1170 (5%) 24 23	11, 79, 179, 342	0

The worst 5 of 1170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	RA	1058	G	15.2
11	QK	129	SER	14.9

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Mol	Chain	Res	Type	RSRZ
28	YE	205	ALA	13.6
40	RU	118	GLY	13.0
25	RA	1060	U	12.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	PPU	Z6	76	37/38	0.83	0.36	73,73,73,73	0
56	PPU	Z8	76	37/38	0.86	0.35	70,70,70,70	0
23	1MG	QY	37	24/25	0.91	0.22	86,86,86,86	0
23	1MG	XY	37	24/25	0.94	0.17	62,62,62,62	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3130	1/1	0.07	0.30	94,94,94,94	0
57	MG	QH	201	1/1	0.28	0.21	74,74,74,74	0
57	MG	RA	3115	1/1	0.41	0.30	47,47,47,47	0
57	MG	QA	1657	1/1	0.43	0.28	108,108,108,108	0
57	MG	QA	1625	1/1	0.43	0.32	94,94,94,94	0
57	MG	RA	3139	1/1	0.44	0.53	51,51,51,51	0
57	MG	YA	3085	1/1	0.45	0.58	65,65,65,65	0
57	MG	YA	3167	1/1	0.47	0.37	42,42,42,42	0
57	MG	QA	1608	1/1	0.50	0.31	68,68,68,68	0
57	MG	RA	3163	1/1	0.50	0.35	79,79,79,79	0
57	MG	XA	1654	1/1	0.52	0.34	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3122	1/1	0.53	0.48	95,95,95,95	0
57	MG	YA	3129	1/1	0.54	0.32	38,38,38,38	0
57	MG	YA	3132	1/1	0.60	0.38	49,49,49,49	0
57	MG	XA	1657	1/1	0.61	0.54	48,48,48,48	0
57	MG	RA	3084	1/1	0.61	0.23	27,27,27,27	0
57	MG	XA	1658	1/1	0.62	0.59	61,61,61,61	0
57	MG	RA	3204	1/1	0.62	0.28	63,63,63,63	0
57	MG	YA	3107	1/1	0.63	0.31	41,41,41,41	0
57	MG	YA	3210	1/1	0.63	0.20	47,47,47,47	0
57	MG	RA	3120	1/1	0.64	0.38	89,89,89,89	0
57	MG	RA	3156	1/1	0.64	0.29	22,22,22,22	0
57	MG	YA	3206	1/1	0.65	0.47	65,65,65,65	0
57	MG	RA	3228	1/1	0.65	0.42	91,91,91,91	0
57	MG	YA	3177	1/1	0.66	0.43	71,71,71,71	0
57	MG	RA	3194	1/1	0.66	0.31	96,96,96,96	0
57	MG	RA	3101	1/1	0.66	0.30	43,43,43,43	0
57	MG	RA	3193	1/1	0.67	0.26	114,114,114,114	0
57	MG	RA	3168	1/1	0.67	0.23	43,43,43,43	0
57	MG	QA	1649	1/1	0.69	0.22	60,60,60,60	0
57	MG	RA	3200	1/1	0.69	0.25	36,36,36,36	0
57	MG	QX	101	1/1	0.69	0.25	67,67,67,67	0
57	MG	QA	1643	1/1	0.69	0.26	61,61,61,61	0
57	MG	RA	3221	1/1	0.70	0.52	55,55,55,55	0
57	MG	QA	1655	1/1	0.70	0.27	48,48,48,48	0
57	MG	YA	3141	1/1	0.71	0.38	79,79,79,79	0
57	MG	YA	3155	1/1	0.71	0.31	48,48,48,48	0
57	MG	XA	1608	1/1	0.72	0.27	60,60,60,60	0
57	MG	QF	201	1/1	0.72	0.48	62,62,62,62	0
57	MG	RA	3218	1/1	0.72	0.14	85,85,85,85	0
57	MG	YA	3166	1/1	0.73	0.64	55,55,55,55	0
57	MG	RA	3223	1/1	0.74	0.49	88,88,88,88	0
57	MG	YA	3106	1/1	0.76	0.18	3,3,3,3	0
57	MG	XA	1664	1/1	0.76	0.36	84,84,84,84	0
57	MG	QA	1628	1/1	0.76	0.25	41,41,41,41	0
57	MG	YB	202	1/1	0.76	0.18	52,52,52,52	0
57	MG	RA	3062	1/1	0.77	0.20	59,59,59,59	0
57	MG	YA	3117	1/1	0.77	0.26	46,46,46,46	0
57	MG	XA	1629	1/1	0.77	0.15	44,44,44,44	0
57	MG	YA	3162	1/1	0.77	0.21	19,19,19,19	0
57	MG	YA	3242	1/1	0.77	0.34	58,58,58,58	0
57	MG	YA	3245	1/1	0.77	0.25	28,28,28,28	0
57	MG	XA	1648	1/1	0.77	0.24	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3118	1/1	0.78	0.28	49,49,49,49	0
57	MG	YA	3151	1/1	0.78	0.21	38,38,38,38	0
57	MG	RA	3091	1/1	0.78	0.42	65,65,65,65	0
57	MG	XA	1673	1/1	0.78	0.49	56,56,56,56	0
57	MG	QA	1654	1/1	0.78	0.21	69,69,69,69	0
57	MG	QA	1637	1/1	0.78	0.30	66,66,66,66	0
59	ZN	XN	101	1/1	0.78	0.22	103,103,103,103	0
57	MG	RA	3177	1/1	0.79	0.25	47,47,47,47	0
57	MG	YA	3191	1/1	0.79	0.21	22,22,22,22	0
57	MG	RA	3209	1/1	0.79	0.14	23,23,23,23	0
57	MG	RA	3138	1/1	0.79	0.27	17,17,17,17	0
57	MG	YA	3016	1/1	0.80	0.21	20,20,20,20	0
57	MG	QA	1661	1/1	0.80	0.12	41,41,41,41	0
57	MG	YA	3153	1/1	0.80	0.38	33,33,33,33	0
57	MG	RA	3188	1/1	0.80	0.20	53,53,53,53	0
57	MG	RA	3199	1/1	0.80	0.43	72,72,72,72	0
57	MG	RA	3157	1/1	0.81	0.24	48,48,48,48	0
57	MG	YA	3185	1/1	0.81	0.25	34,34,34,34	0
57	MG	RA	3210	1/1	0.81	0.14	51,51,51,51	0
57	MG	QA	1617	1/1	0.81	0.62	50,50,50,50	0
57	MG	YA	3118	1/1	0.81	0.33	33,33,33,33	0
57	MG	YA	3218	1/1	0.81	0.20	47,47,47,47	0
57	MG	RA	3233	1/1	0.81	0.34	42,42,42,42	0
57	MG	YA	3072	1/1	0.81	0.32	15,15,15,15	0
57	MG	RA	3241	1/1	0.81	0.23	36,36,36,36	0
57	MG	YA	3175	1/1	0.81	0.13	42,42,42,42	0
57	MG	YA	3262	1/1	0.82	0.37	24,24,24,24	0
57	MG	QA	1618	1/1	0.82	0.30	42,42,42,42	0
59	ZN	R9	101	1/1	0.82	0.09	112,112,112,112	0
57	MG	YA	3250	1/1	0.82	0.27	37,37,37,37	0
57	MG	RA	3179	1/1	0.83	0.28	29,29,29,29	0
57	MG	RA	3180	1/1	0.83	0.29	33,33,33,33	0
57	MG	YA	3230	1/1	0.83	0.14	35,35,35,35	0
57	MG	XA	1620	1/1	0.83	0.21	30,30,30,30	0
57	MG	XA	1668	1/1	0.83	0.19	30,30,30,30	0
57	MG	RA	3135	1/1	0.83	0.28	55,55,55,55	0
57	MG	XA	1638	1/1	0.83	0.37	91,91,91,91	0
57	MG	RA	3171	1/1	0.83	0.18	46,46,46,46	0
57	MG	XA	1649	1/1	0.83	0.35	48,48,48,48	0
57	MG	RA	3122	1/1	0.83	0.28	29,29,29,29	0
57	MG	XA	1662	1/1	0.84	0.10	47,47,47,47	0
57	MG	RA	3133	1/1	0.84	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1624	1/1	0.84	0.27	58,58,58,58	0
57	MG	QA	1664	1/1	0.84	0.26	35,35,35,35	0
57	MG	RA	3103	1/1	0.84	0.17	26,26,26,26	0
57	MG	QM	201	1/1	0.84	0.13	66,66,66,66	0
57	MG	XA	1651	1/1	0.85	0.40	59,59,59,59	0
57	MG	RA	3222	1/1	0.85	0.27	50,50,50,50	0
57	MG	YA	3238	1/1	0.85	0.97	154,154,154,154	0
57	MG	YA	3168	1/1	0.85	0.30	52,52,52,52	0
57	MG	RA	3075	1/1	0.85	0.14	39,39,39,39	0
57	MG	RA	3226	1/1	0.85	0.29	38,38,38,38	0
57	MG	XA	1661	1/1	0.85	0.21	28,28,28,28	0
57	MG	RA	3172	1/1	0.85	0.28	31,31,31,31	0
57	MG	RA	3220	1/1	0.85	0.37	58,58,58,58	0
57	MG	RA	3170	1/1	0.85	0.18	41,41,41,41	0
57	MG	XA	1614	1/1	0.86	0.24	57,57,57,57	0
57	MG	XA	1666	1/1	0.86	0.09	61,61,61,61	0
57	MG	RA	3161	1/1	0.86	0.25	33,33,33,33	0
57	MG	YA	3164	1/1	0.86	0.27	22,22,22,22	0
57	MG	YA	3232	1/1	0.86	0.27	28,28,28,28	0
57	MG	XA	1656	1/1	0.86	0.21	45,45,45,45	0
57	MG	YA	3124	1/1	0.86	0.16	16,16,16,16	0
57	MG	YA	3127	1/1	0.86	0.17	13,13,13,13	0
57	MG	YA	3172	1/1	0.86	0.18	48,48,48,48	0
57	MG	YA	3251	1/1	0.86	0.35	60,60,60,60	0
57	MG	RA	3134	1/1	0.86	0.16	42,42,42,42	0
57	MG	RA	3189	1/1	0.86	0.28	33,33,33,33	0
57	MG	YP	201	1/1	0.86	0.19	153,153,153,153	0
57	MG	QA	1638	1/1	0.86	0.21	54,54,54,54	0
57	MG	RA	3126	1/1	0.86	0.58	39,39,39,39	0
57	MG	YA	3235	1/1	0.87	0.15	37,37,37,37	0
57	MG	XA	1641	1/1	0.87	0.20	17,17,17,17	0
57	MG	RA	3206	1/1	0.87	0.32	26,26,26,26	0
57	MG	XA	1611	1/1	0.87	0.20	8,8,8,8	0
57	MG	RA	3127	1/1	0.87	0.23	36,36,36,36	0
57	MG	YA	3193	1/1	0.87	0.32	35,35,35,35	0
57	MG	RA	3185	1/1	0.87	0.34	45,45,45,45	0
57	MG	YA	3265	1/1	0.87	0.23	36,36,36,36	0
57	MG	YB	201	1/1	0.87	0.21	51,51,51,51	0
57	MG	RA	3159	1/1	0.87	0.25	40,40,40,40	0
57	MG	YA	3146	1/1	0.87	0.25	40,40,40,40	0
57	MG	YP	202	1/1	0.87	0.19	31,31,31,31	0
58	PAR	QA	1666	42/42	0.87	0.30	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	PAR	XA	1675	42/42	0.87	0.33	74,74,74,74	0
57	MG	R0	101	1/1	0.87	0.18	32,32,32,32	0
57	MG	YA	3174	1/1	0.87	0.13	27,27,27,27	0
57	MG	YA	3154	1/1	0.88	0.24	38,38,38,38	0
57	MG	YA	3220	1/1	0.88	0.20	53,53,53,53	0
57	MG	YA	3223	1/1	0.88	0.34	42,42,42,42	0
57	MG	RA	3162	1/1	0.88	0.17	39,39,39,39	0
57	MG	YA	3157	1/1	0.88	0.23	49,49,49,49	0
57	MG	RD	301	1/1	0.88	0.30	38,38,38,38	0
57	MG	RR	202	1/1	0.88	0.18	20,20,20,20	0
57	MG	RA	3142	1/1	0.88	0.17	59,59,59,59	0
57	MG	YA	3243	1/1	0.88	0.27	32,32,32,32	0
57	MG	RA	3195	1/1	0.88	0.36	85,85,85,85	0
57	MG	RA	3008	1/1	0.88	0.24	47,47,47,47	0
57	MG	RA	3026	1/1	0.88	0.11	3,3,3,3	0
57	MG	QA	1650	1/1	0.88	0.12	27,27,27,27	0
57	MG	QA	1601	1/1	0.88	0.32	58,58,58,58	0
57	MG	RA	3207	1/1	0.88	0.36	105,105,105,105	0
57	MG	RA	3229	1/1	0.88	0.28	41,41,41,41	0
57	MG	YA	3012	1/1	0.88	0.36	5,5,5,5	0
57	MG	YA	3150	1/1	0.88	0.14	31,31,31,31	0
57	MG	YA	3195	1/1	0.88	0.24	44,44,44,44	0
57	MG	RA	3191	1/1	0.88	0.25	38,38,38,38	0
57	MG	RA	3235	1/1	0.88	0.35	29,29,29,29	0
57	MG	YA	3213	1/1	0.88	0.09	31,31,31,31	0
57	MG	YA	3226	1/1	0.89	0.17	20,20,20,20	0
57	MG	RA	3009	1/1	0.89	0.16	26,26,26,26	0
57	MG	RA	3131	1/1	0.89	0.27	31,31,31,31	0
57	MG	YA	3234	1/1	0.89	0.17	28,28,28,28	0
57	MG	XA	1628	1/1	0.89	0.10	19,19,19,19	0
57	MG	QA	1636	1/1	0.89	0.10	34,34,34,34	0
57	MG	XA	1665	1/1	0.89	0.32	46,46,46,46	0
57	MG	RA	3217	1/1	0.89	0.12	49,49,49,49	0
57	MG	RA	3183	1/1	0.89	0.38	44,44,44,44	0
57	MG	YA	3248	1/1	0.89	0.13	32,32,32,32	0
57	MG	XA	1670	1/1	0.89	0.22	79,79,79,79	0
57	MG	YA	3143	1/1	0.89	0.29	66,66,66,66	0
57	MG	YA	3253	1/1	0.89	0.34	25,25,25,25	0
57	MG	RA	3184	1/1	0.89	0.28	42,42,42,42	0
57	MG	RF	301	1/1	0.89	0.21	65,65,65,65	0
57	MG	RA	3044	1/1	0.89	0.30	37,37,37,37	0
57	MG	YA	3152	1/1	0.89	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3054	1/1	0.89	0.17	3,3,3,3	0
57	MG	XA	1652	1/1	0.89	0.25	64,64,64,64	0
57	MG	RA	3002	1/1	0.89	0.31	41,41,41,41	0
57	MG	YA	3219	1/1	0.89	0.19	33,33,33,33	0
57	MG	RA	3205	1/1	0.89	0.22	54,54,54,54	0
57	MG	QA	1632	1/1	0.89	0.23	40,40,40,40	0
57	MG	RA	3211	1/1	0.90	0.26	38,38,38,38	0
57	MG	QA	1612	1/1	0.90	0.28	18,18,18,18	0
57	MG	RA	3151	1/1	0.90	0.13	22,22,22,22	0
57	MG	RA	3014	1/1	0.90	0.23	3,3,3,3	0
57	MG	YA	3139	1/1	0.90	0.21	33,33,33,33	0
57	MG	YA	3176	1/1	0.90	0.11	32,32,32,32	0
57	MG	QA	1629	1/1	0.90	0.13	47,47,47,47	0
57	MG	RA	3039	1/1	0.90	0.10	14,14,14,14	0
57	MG	YA	3246	1/1	0.90	0.36	29,29,29,29	0
57	MG	YA	3186	1/1	0.90	0.33	44,44,44,44	0
57	MG	RA	3160	1/1	0.90	0.18	42,42,42,42	0
57	MG	YA	3069	1/1	0.90	0.28	13,13,13,13	0
57	MG	QA	1656	1/1	0.90	0.20	100,100,100,100	0
57	MG	YA	3082	1/1	0.90	1.03	80,80,80,80	0
57	MG	YA	3209	1/1	0.90	0.15	29,29,29,29	0
57	MG	RA	3049	1/1	0.90	0.11	14,14,14,14	0
57	MG	RA	3057	1/1	0.90	0.41	34,34,34,34	0
57	MG	RA	3059	1/1	0.90	0.21	15,15,15,15	0
57	MG	YA	3108	1/1	0.90	0.41	20,20,20,20	0
57	MG	XA	1663	1/1	0.90	0.27	35,35,35,35	0
57	MG	YA	3221	1/1	0.90	1.00	42,42,42,42	0
57	MG	XA	1634	1/1	0.90	0.20	43,43,43,43	0
59	ZN	XD	301	1/1	0.90	0.27	45,45,45,45	0
57	MG	QA	1626	1/1	0.90	0.17	29,29,29,29	0
57	MG	XA	1659	1/1	0.91	0.21	41,41,41,41	0
57	MG	YA	3149	1/1	0.91	0.20	25,25,25,25	0
57	MG	YA	3241	1/1	0.91	0.20	39,39,39,39	0
57	MG	RA	3238	1/1	0.91	0.19	31,31,31,31	0
57	MG	RA	3068	1/1	0.91	0.20	37,37,37,37	0
57	MG	QA	1647	1/1	0.91	0.28	58,58,58,58	0
57	MG	RA	3224	1/1	0.91	0.16	40,40,40,40	0
57	MG	QA	1603	1/1	0.91	0.40	22,22,22,22	0
57	MG	YA	3110	1/1	0.91	0.25	11,11,11,11	0
57	MG	RA	3165	1/1	0.91	0.44	43,43,43,43	0
57	MG	QA	1619	1/1	0.91	0.16	43,43,43,43	0
57	MG	YA	3254	1/1	0.91	0.31	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3163	1/1	0.91	0.21	29,29,29,29	0
57	MG	RA	3182	1/1	0.91	0.31	55,55,55,55	0
57	MG	YA	3266	1/1	0.91	0.22	11,11,11,11	0
57	MG	XA	1672	1/1	0.91	0.10	23,23,23,23	0
57	MG	RA	3143	1/1	0.91	0.18	30,30,30,30	0
57	MG	XA	1618	1/1	0.91	0.28	33,33,33,33	0
57	MG	YA	3224	1/1	0.91	0.10	35,35,35,35	0
57	MG	XA	1619	1/1	0.91	0.25	33,33,33,33	0
57	MG	YA	3229	1/1	0.91	0.18	20,20,20,20	0
57	MG	YA	3038	1/1	0.91	0.25	4,4,4,4	0
57	MG	RA	3236	1/1	0.91	0.25	34,34,34,34	0
57	MG	XA	1621	1/1	0.91	0.35	32,32,32,32	0
57	MG	YA	3217	1/1	0.92	0.24	38,38,38,38	0
57	MG	QA	1644	1/1	0.92	0.14	36,36,36,36	0
57	MG	RA	3145	1/1	0.92	0.27	14,14,14,14	0
57	MG	RA	3148	1/1	0.92	0.23	39,39,39,39	0
57	MG	XA	1627	1/1	0.92	0.10	24,24,24,24	0
57	MG	RA	3104	1/1	0.92	0.11	6,6,6,6	0
57	MG	RA	3227	1/1	0.92	0.12	64,64,64,64	0
57	MG	RA	3174	1/1	0.92	0.15	26,26,26,26	0
57	MG	RA	3010	1/1	0.92	0.15	48,48,48,48	0
57	MG	YA	3158	1/1	0.92	0.18	16,16,16,16	0
57	MG	RA	3178	1/1	0.92	0.16	30,30,30,30	0
57	MG	YA	3075	1/1	0.92	0.13	23,23,23,23	0
57	MG	XA	1642	1/1	0.92	0.18	37,37,37,37	0
57	MG	YA	3236	1/1	0.92	0.21	40,40,40,40	0
57	MG	RA	3116	1/1	0.92	0.21	2,2,2,2	0
57	MG	QA	1662	1/1	0.92	0.11	63,63,63,63	0
57	MG	RA	3055	1/1	0.92	0.22	21,21,21,21	0
57	MG	RA	3239	1/1	0.92	0.38	24,24,24,24	0
57	MG	RA	3121	1/1	0.92	0.27	45,45,45,45	0
57	MG	RB	202	1/1	0.92	0.10	46,46,46,46	0
57	MG	QA	1658	1/1	0.92	0.13	52,52,52,52	0
57	MG	YA	3249	1/1	0.92	0.21	34,34,34,34	0
57	MG	RE	302	1/1	0.92	0.10	11,11,11,11	0
57	MG	YA	3179	1/1	0.92	0.10	40,40,40,40	0
57	MG	YA	3252	1/1	0.92	0.36	41,41,41,41	0
57	MG	YA	3184	1/1	0.92	0.20	35,35,35,35	0
57	MG	RA	3212	1/1	0.92	0.18	37,37,37,37	0
57	MG	RA	3213	1/1	0.92	0.13	44,44,44,44	0
57	MG	YA	3187	1/1	0.92	0.13	19,19,19,19	0
57	MG	RA	3216	1/1	0.92	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1606	1/1	0.92	0.28	29,29,29,29	0
57	MG	YA	3133	1/1	0.92	0.17	12,12,12,12	0
57	MG	YA	3201	1/1	0.92	0.58	23,23,23,23	0
57	MG	YA	3202	1/1	0.92	0.15	33,33,33,33	0
57	MG	RA	3141	1/1	0.92	0.32	34,34,34,34	0
57	MG	RA	3037	1/1	0.92	0.27	26,26,26,26	0
59	ZN	QD	301	1/1	0.92	0.26	53,53,53,53	0
57	MG	RA	3166	1/1	0.92	0.16	53,53,53,53	0
57	MG	YA	3212	1/1	0.92	0.20	67,67,67,67	0
57	MG	RA	3167	1/1	0.92	0.15	56,56,56,56	0
57	MG	YA	3128	1/1	0.93	0.33	34,34,34,34	0
57	MG	QA	1641	1/1	0.93	0.12	22,22,22,22	0
57	MG	YA	3130	1/1	0.93	0.47	52,52,52,52	0
57	MG	RA	3119	1/1	0.93	0.23	28,28,28,28	0
57	MG	XA	1607	1/1	0.93	0.21	25,25,25,25	0
57	MG	YA	3134	1/1	0.93	0.09	37,37,37,37	0
57	MG	YA	3215	1/1	0.93	0.15	24,24,24,24	0
57	MG	RA	3011	1/1	0.93	0.34	48,48,48,48	0
57	MG	QA	1602	1/1	0.93	0.23	24,24,24,24	0
57	MG	XA	1613	1/1	0.93	0.08	14,14,14,14	0
57	MG	YA	3145	1/1	0.93	0.14	23,23,23,23	0
57	MG	QA	1605	1/1	0.93	0.40	15,15,15,15	0
57	MG	YA	3147	1/1	0.93	0.26	28,28,28,28	0
57	MG	RA	3078	1/1	0.93	0.30	34,34,34,34	0
57	MG	YA	3225	1/1	0.93	0.14	21,21,21,21	0
57	MG	RA	3079	1/1	0.93	0.23	32,32,32,32	0
57	MG	YA	3227	1/1	0.93	0.20	26,26,26,26	0
57	MG	XA	1671	1/1	0.93	0.10	43,43,43,43	0
57	MG	RA	3128	1/1	0.93	0.13	55,55,55,55	0
57	MG	RA	3225	1/1	0.93	0.18	51,51,51,51	0
57	MG	QA	1646	1/1	0.93	0.28	46,46,46,46	0
57	MG	QA	1615	1/1	0.93	0.09	66,66,66,66	0
57	MG	RA	3197	1/1	0.93	0.10	42,42,42,42	0
57	MG	YA	3042	1/1	0.93	0.28	11,11,11,11	0
57	MG	RA	3097	1/1	0.93	0.18	7,7,7,7	0
57	MG	YA	3060	1/1	0.93	0.23	24,24,24,24	0
57	MG	RA	3098	1/1	0.93	0.24	11,11,11,11	0
57	MG	RA	3203	1/1	0.93	0.34	61,61,61,61	0
57	MG	YA	3073	1/1	0.93	0.18	7,7,7,7	0
57	MG	RA	3100	1/1	0.93	0.24	43,43,43,43	0
57	MG	YA	3169	1/1	0.93	0.14	30,30,30,30	0
57	MG	YA	3170	1/1	0.93	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1646	1/1	0.93	0.15	24,24,24,24	0
57	MG	YA	3083	1/1	0.93	0.09	0,0,0,0	0
57	MG	RA	3137	1/1	0.93	0.24	36,36,36,36	0
57	MG	YA	3097	1/1	0.93	0.28	30,30,30,30	0
57	MG	YA	3100	1/1	0.93	0.28	7,7,7,7	0
57	MG	RA	3041	1/1	0.93	0.22	20,20,20,20	0
57	MG	YA	3180	1/1	0.93	0.14	31,31,31,31	0
57	MG	XA	1650	1/1	0.93	0.20	31,31,31,31	0
57	MG	RA	3001	1/1	0.93	0.14	2,2,2,2	0
57	MG	QA	1627	1/1	0.93	0.15	92,92,92,92	0
57	MG	XA	1653	1/1	0.93	0.24	62,62,62,62	0
57	MG	RA	3111	1/1	0.93	0.18	20,20,20,20	0
57	MG	QA	1622	1/1	0.93	0.17	33,33,33,33	0
57	MG	QA	1663	1/1	0.93	0.12	85,85,85,85	0
57	MG	YA	3197	1/1	0.93	0.26	16,16,16,16	0
57	MG	YA	3200	1/1	0.93	0.38	39,39,39,39	0
57	MG	RA	3146	1/1	0.93	0.16	37,37,37,37	0
57	MG	RA	3070	1/1	0.94	0.16	11,11,11,11	0
57	MG	RA	3072	1/1	0.94	0.20	16,16,16,16	0
57	MG	YA	3204	1/1	0.94	0.09	32,32,32,32	0
57	MG	XA	1623	1/1	0.94	0.07	27,27,27,27	0
57	MG	RA	3196	1/1	0.94	0.33	46,46,46,46	0
57	MG	YA	3135	1/1	0.94	0.47	40,40,40,40	0
57	MG	RA	3033	1/1	0.94	0.33	11,11,11,11	0
57	MG	YA	3140	1/1	0.94	0.18	3,3,3,3	0
57	MG	YA	3001	1/1	0.94	0.37	7,7,7,7	0
57	MG	YA	3142	1/1	0.94	0.26	14,14,14,14	0
57	MG	YA	3003	1/1	0.94	0.17	9,9,9,9	0
57	MG	RA	3198	1/1	0.94	0.21	22,22,22,22	0
57	MG	XA	1632	1/1	0.94	0.31	27,27,27,27	0
57	MG	YA	3025	1/1	0.94	0.12	4,4,4,4	0
57	MG	YA	3222	1/1	0.94	0.39	40,40,40,40	0
57	MG	YA	3035	1/1	0.94	0.34	12,12,12,12	0
57	MG	QA	1633	1/1	0.94	0.26	20,20,20,20	0
57	MG	XA	1636	1/1	0.94	0.38	23,23,23,23	0
57	MG	YA	3046	1/1	0.94	0.34	11,11,11,11	0
57	MG	QA	1665	1/1	0.94	0.23	29,29,29,29	0
57	MG	XA	1639	1/1	0.94	0.16	59,59,59,59	0
57	MG	RA	3234	1/1	0.94	0.27	44,44,44,44	0
57	MG	YA	3071	1/1	0.94	0.12	18,18,18,18	0
57	MG	YA	3233	1/1	0.94	0.31	32,32,32,32	0
57	MG	RA	3201	1/1	0.94	0.11	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3160	1/1	0.94	0.14	14,14,14,14	0
57	MG	RA	3082	1/1	0.94	0.36	26,26,26,26	0
57	MG	QA	1610	1/1	0.94	0.28	22,22,22,22	0
57	MG	YA	3239	1/1	0.94	0.11	27,27,27,27	0
57	MG	YA	3076	1/1	0.94	0.12	25,25,25,25	0
57	MG	YA	3079	1/1	0.94	0.28	18,18,18,18	0
57	MG	RA	3147	1/1	0.94	0.12	14,14,14,14	0
57	MG	RA	3090	1/1	0.94	0.23	7,7,7,7	0
57	MG	RA	3150	1/1	0.94	0.17	32,32,32,32	0
57	MG	YA	3247	1/1	0.94	0.22	26,26,26,26	0
57	MG	YA	3092	1/1	0.94	0.20	25,25,25,25	0
57	MG	QA	1659	1/1	0.94	0.11	24,24,24,24	0
57	MG	YA	3173	1/1	0.94	0.53	32,32,32,32	0
57	MG	RA	3152	1/1	0.94	0.15	33,33,33,33	0
57	MG	YA	3101	1/1	0.94	0.45	24,24,24,24	0
57	MG	YA	3105	1/1	0.94	0.22	7,7,7,7	0
57	MG	QA	1631	1/1	0.94	0.11	41,41,41,41	0
57	MG	RA	3012	1/1	0.94	0.13	14,14,14,14	0
57	MG	RA	3158	1/1	0.94	0.17	52,52,52,52	0
57	MG	YA	3181	1/1	0.94	0.17	36,36,36,36	0
57	MG	YA	3267	1/1	0.94	0.20	40,40,40,40	0
57	MG	RA	3214	1/1	0.94	0.14	44,44,44,44	0
57	MG	YA	3115	1/1	0.94	0.14	32,32,32,32	0
57	MG	YE	301	1/1	0.94	0.14	8,8,8,8	0
57	MG	QA	1613	1/1	0.94	0.14	22,22,22,22	0
57	MG	RA	3186	1/1	0.94	0.16	52,52,52,52	0
57	MG	RA	3187	1/1	0.94	0.08	25,25,25,25	0
57	MG	YA	3192	1/1	0.94	0.07	19,19,19,19	0
57	MG	RA	3058	1/1	0.94	0.22	27,27,27,27	0
57	MG	RA	3019	1/1	0.94	0.30	21,21,21,21	0
57	MG	QA	1640	1/1	0.94	0.26	37,37,37,37	0
57	MG	RA	3028	1/1	0.94	0.22	37,37,37,37	0
57	MG	YA	3196	1/1	0.95	0.07	11,11,11,11	0
57	MG	YA	3009	1/1	0.95	0.44	16,16,16,16	0
57	MG	YA	3198	1/1	0.95	0.15	21,21,21,21	0
57	MG	RA	3032	1/1	0.95	0.23	44,44,44,44	0
57	MG	RA	3092	1/1	0.95	0.19	35,35,35,35	0
57	MG	RA	3096	1/1	0.95	0.35	22,22,22,22	0
57	MG	YA	3034	1/1	0.95	0.29	7,7,7,7	0
57	MG	RA	3240	1/1	0.95	0.27	23,23,23,23	0
57	MG	YA	3208	1/1	0.95	0.12	30,30,30,30	0
57	MG	RA	3013	1/1	0.95	0.38	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3039	1/1	0.95	0.12	14,14,14,14	0
57	MG	RA	3153	1/1	0.95	0.12	21,21,21,21	0
57	MG	YA	3045	1/1	0.95	0.30	2,2,2,2	0
57	MG	RA	3155	1/1	0.95	0.21	41,41,41,41	0
57	MG	YA	3047	1/1	0.95	0.24	13,13,13,13	0
57	MG	YA	3144	1/1	0.95	0.15	13,13,13,13	0
57	MG	YA	3049	1/1	0.95	0.17	12,12,12,12	0
57	MG	YA	3052	1/1	0.95	0.18	1,1,1,1	0
57	MG	RA	3034	1/1	0.95	0.30	23,23,23,23	0
57	MG	YA	3148	1/1	0.95	0.36	39,39,39,39	0
57	MG	YA	3055	1/1	0.95	0.18	37,37,37,37	0
57	MG	YA	3056	1/1	0.95	0.17	7,7,7,7	0
57	MG	RA	3064	1/1	0.95	0.34	3,3,3,3	0
57	MG	YA	3062	1/1	0.95	0.11	18,18,18,18	0
57	MG	YA	3064	1/1	0.95	0.16	19,19,19,19	0
57	MG	YA	3068	1/1	0.95	0.17	26,26,26,26	0
57	MG	RA	3132	1/1	0.95	0.30	14,14,14,14	0
57	MG	YA	3070	1/1	0.95	0.21	5,5,5,5	0
57	MG	RA	3035	1/1	0.95	0.34	27,27,27,27	0
57	MG	R5	101	1/1	0.95	0.26	51,51,51,51	0
57	MG	YA	3161	1/1	0.95	0.19	29,29,29,29	0
57	MG	QA	1639	1/1	0.95	0.18	45,45,45,45	0
57	MG	YA	3237	1/1	0.95	0.18	9,9,9,9	0
57	MG	RA	3016	1/1	0.95	0.28	4,4,4,4	0
57	MG	RA	3136	1/1	0.95	0.21	26,26,26,26	0
57	MG	YA	3165	1/1	0.95	0.13	21,21,21,21	0
57	MG	XA	1609	1/1	0.95	0.16	28,28,28,28	0
57	MG	RA	3192	1/1	0.95	0.12	19,19,19,19	0
57	MG	XA	1660	1/1	0.95	0.25	54,54,54,54	0
57	MG	RA	3109	1/1	0.95	0.16	21,21,21,21	0
57	MG	QA	1635	1/1	0.95	0.15	49,49,49,49	0
57	MG	YA	3171	1/1	0.95	0.20	22,22,22,22	0
57	MG	YA	3093	1/1	0.95	0.19	18,18,18,18	0
57	MG	RA	3112	1/1	0.95	0.26	14,14,14,14	0
57	MG	RA	3023	1/1	0.95	0.33	8,8,8,8	0
57	MG	RA	3024	1/1	0.95	0.17	17,17,17,17	0
57	MG	RA	3169	1/1	0.95	0.18	44,44,44,44	0
57	MG	XA	1667	1/1	0.95	0.10	55,55,55,55	0
57	MG	YA	3178	1/1	0.95	0.14	10,10,10,10	0
57	MG	RA	3054	1/1	0.95	0.09	14,14,14,14	0
57	MG	XA	1669	1/1	0.95	0.22	17,17,17,17	0
57	MG	YA	3109	1/1	0.95	0.29	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3183	1/1	0.95	0.10	21,21,21,21	0
57	MG	XA	1626	1/1	0.95	0.17	27,27,27,27	0
57	MG	YB	204	1/1	0.95	0.15	45,45,45,45	0
57	MG	QA	1616	1/1	0.95	0.14	18,18,18,18	0
57	MG	RA	3231	1/1	0.95	0.33	14,14,14,14	0
57	MG	RA	3087	1/1	0.95	0.12	27,27,27,27	0
57	MG	YA	3188	1/1	0.95	0.12	18,18,18,18	0
57	MG	RA	3173	1/1	0.95	0.11	90,90,90,90	0
57	MG	QA	1660	1/1	0.95	0.45	35,35,35,35	0
59	ZN	QN	101	1/1	0.95	0.10	87,87,87,87	0
57	MG	YA	3125	1/1	0.95	0.16	65,65,65,65	0
57	MG	YA	3194	1/1	0.95	0.11	34,34,34,34	0
57	MG	YA	3006	1/1	0.95	0.19	1,1,1,1	0
59	ZN	Y9	101	1/1	0.95	0.10	87,87,87,87	0
57	MG	RA	3125	1/1	0.96	0.19	29,29,29,29	0
57	MG	XA	1624	1/1	0.96	0.45	39,39,39,39	0
57	MG	YA	3214	1/1	0.96	0.15	28,28,28,28	0
57	MG	YA	3080	1/1	0.96	0.14	11,11,11,11	0
57	MG	XA	1625	1/1	0.96	0.17	14,14,14,14	0
57	MG	RA	3176	1/1	0.96	0.16	27,27,27,27	0
57	MG	QA	1642	1/1	0.96	0.13	25,25,25,25	0
57	MG	YA	3159	1/1	0.96	0.14	19,19,19,19	0
57	MG	YA	3089	1/1	0.96	0.18	5,5,5,5	0
57	MG	QA	1607	1/1	0.96	0.10	21,21,21,21	0
57	MG	QA	1614	1/1	0.96	0.28	31,31,31,31	0
57	MG	XA	1631	1/1	0.96	0.14	39,39,39,39	0
57	MG	RA	3237	1/1	0.96	0.15	13,13,13,13	0
57	MG	RA	3129	1/1	0.96	0.16	38,38,38,38	0
57	MG	YA	3104	1/1	0.96	0.08	22,22,22,22	0
57	MG	RA	3208	1/1	0.96	0.18	69,69,69,69	0
57	MG	RA	3063	1/1	0.96	0.45	12,12,12,12	0
57	MG	YA	3018	1/1	0.96	0.21	6,6,6,6	0
57	MG	YA	3023	1/1	0.96	0.27	14,14,14,14	0
57	MG	QA	1645	1/1	0.96	0.08	37,37,37,37	0
57	MG	YA	3031	1/1	0.96	0.39	26,26,26,26	0
57	MG	YA	3112	1/1	0.96	0.25	23,23,23,23	0
57	MG	QA	1611	1/1	0.96	0.13	20,20,20,20	0
57	MG	QA	1606	1/1	0.96	0.15	44,44,44,44	0
57	MG	QA	1634	1/1	0.96	0.12	39,39,39,39	0
57	MG	RA	3022	1/1	0.96	0.43	23,23,23,23	0
57	MG	YA	3123	1/1	0.96	0.14	28,28,28,28	0
57	MG	YA	3041	1/1	0.96	0.28	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3244	1/1	0.96	0.27	34,34,34,34	0
57	MG	RA	3110	1/1	0.96	0.09	12,12,12,12	0
57	MG	RA	3077	1/1	0.96	0.27	24,24,24,24	0
57	MG	YA	3182	1/1	0.96	0.50	55,55,55,55	0
57	MG	RA	3190	1/1	0.96	0.15	33,33,33,33	0
57	MG	XA	1603	1/1	0.96	0.20	24,24,24,24	0
57	MG	XA	1605	1/1	0.96	0.17	7,7,7,7	0
57	MG	YA	3131	1/1	0.96	0.17	15,15,15,15	0
57	MG	RA	3219	1/1	0.96	0.18	36,36,36,36	0
57	MG	XA	1655	1/1	0.96	0.30	47,47,47,47	0
57	MG	YA	3189	1/1	0.96	0.08	33,33,33,33	0
57	MG	RA	3164	1/1	0.96	0.09	27,27,27,27	0
57	MG	RA	3045	1/1	0.96	0.27	23,23,23,23	0
57	MG	YA	3136	1/1	0.96	0.09	29,29,29,29	0
57	MG	YA	3057	1/1	0.96	0.12	1,1,1,1	0
57	MG	YA	3059	1/1	0.96	0.24	15,15,15,15	0
57	MG	RA	3113	1/1	0.96	0.14	22,22,22,22	0
57	MG	YB	203	1/1	0.96	0.21	43,43,43,43	0
57	MG	RA	3046	1/1	0.96	0.14	19,19,19,19	0
57	MG	XA	1612	1/1	0.96	0.20	18,18,18,18	0
57	MG	YA	3065	1/1	0.96	0.25	25,25,25,25	0
57	MG	RA	3081	1/1	0.96	0.24	27,27,27,27	0
57	MG	Y5	101	1/1	0.96	0.22	18,18,18,18	0
57	MG	QA	1623	1/1	0.96	0.24	29,29,29,29	0
57	MG	YA	3203	1/1	0.96	0.14	18,18,18,18	0
57	MG	XA	1617	1/1	0.96	0.15	10,10,10,10	0
57	MG	RA	3050	1/1	0.96	0.28	13,13,13,13	0
57	MG	RA	3005	1/1	0.96	0.31	11,11,11,11	0
57	MG	QA	1651	1/1	0.96	0.30	31,31,31,31	0
57	MG	QA	1653	1/1	0.96	0.12	82,82,82,82	0
57	MG	YA	3211	1/1	0.96	0.17	29,29,29,29	0
57	MG	RA	3030	1/1	0.97	0.17	5,5,5,5	0
57	MG	QA	1648	1/1	0.97	0.12	47,47,47,47	0
57	MG	YA	3014	1/1	0.97	0.24	3,3,3,3	0
57	MG	RA	3051	1/1	0.97	0.14	18,18,18,18	0
57	MG	RA	3232	1/1	0.97	0.34	23,23,23,23	0
57	MG	YA	3022	1/1	0.97	0.22	11,11,11,11	0
57	MG	YA	3113	1/1	0.97	0.07	19,19,19,19	0
57	MG	YA	3114	1/1	0.97	0.27	9,9,9,9	0
57	MG	XA	1630	1/1	0.97	0.14	18,18,18,18	0
57	MG	YA	3199	1/1	0.97	0.14	30,30,30,30	0
57	MG	YA	3024	1/1	0.97	0.23	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3053	1/1	0.97	0.17	13,13,13,13	0
57	MG	YA	3120	1/1	0.97	0.17	18,18,18,18	0
57	MG	YA	3026	1/1	0.97	0.29	0,0,0,0	0
57	MG	YA	3028	1/1	0.97	0.10	3,3,3,3	0
57	MG	YA	3205	1/1	0.97	0.12	37,37,37,37	0
57	MG	YA	3029	1/1	0.97	0.14	5,5,5,5	0
57	MG	QV	101	1/1	0.97	0.14	24,24,24,24	0
57	MG	YA	3126	1/1	0.97	0.13	17,17,17,17	0
57	MG	YA	3033	1/1	0.97	0.23	10,10,10,10	0
57	MG	XA	1633	1/1	0.97	0.23	30,30,30,30	0
57	MG	RA	3124	1/1	0.97	0.10	28,28,28,28	0
57	MG	XA	1635	1/1	0.97	0.27	26,26,26,26	0
57	MG	RA	3086	1/1	0.97	0.20	2,2,2,2	0
57	MG	YA	3040	1/1	0.97	0.16	9,9,9,9	0
57	MG	YA	3216	1/1	0.97	0.10	18,18,18,18	0
57	MG	XA	1637	1/1	0.97	0.26	39,39,39,39	0
57	MG	QA	1630	1/1	0.97	0.14	26,26,26,26	0
57	MG	YA	3044	1/1	0.97	0.31	4,4,4,4	0
57	MG	RA	3088	1/1	0.97	0.26	25,25,25,25	0
57	MG	YA	3137	1/1	0.97	0.08	21,21,21,21	0
57	MG	QA	1604	1/1	0.97	0.23	10,10,10,10	0
57	MG	RA	3036	1/1	0.97	0.27	4,4,4,4	0
57	MG	YA	3048	1/1	0.97	0.33	6,6,6,6	0
57	MG	XA	1643	1/1	0.97	0.18	25,25,25,25	0
57	MG	RA	3202	1/1	0.97	0.10	31,31,31,31	0
57	MG	XA	1647	1/1	0.97	0.10	25,25,25,25	0
57	MG	RB	201	1/1	0.97	0.10	54,54,54,54	0
57	MG	QA	1609	1/1	0.97	0.12	14,14,14,14	0
57	MG	RA	3093	1/1	0.97	0.25	10,10,10,10	0
57	MG	RE	301	1/1	0.97	0.21	30,30,30,30	0
57	MG	RA	3060	1/1	0.97	0.19	3,3,3,3	0
57	MG	YA	3061	1/1	0.97	0.19	16,16,16,16	0
57	MG	RA	3061	1/1	0.97	0.23	32,32,32,32	0
57	MG	RR	201	1/1	0.97	0.16	7,7,7,7	0
57	MG	RA	3025	1/1	0.97	0.25	22,22,22,22	0
57	MG	YA	3066	1/1	0.97	0.08	20,20,20,20	0
57	MG	YA	3240	1/1	0.97	0.13	31,31,31,31	0
57	MG	QA	1652	1/1	0.97	0.12	31,31,31,31	0
57	MG	YA	3156	1/1	0.97	0.13	20,20,20,20	0
57	MG	RA	3043	1/1	0.97	0.11	14,14,14,14	0
57	MG	RA	3102	1/1	0.97	0.20	5,5,5,5	0
57	MG	XA	1604	1/1	0.97	0.44	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3066	1/1	0.97	0.24	11,11,11,11	0
57	MG	RA	3175	1/1	0.97	0.10	40,40,40,40	0
57	MG	RA	3027	1/1	0.97	0.26	3,3,3,3	0
57	MG	RA	3107	1/1	0.97	0.12	27,27,27,27	0
57	MG	YA	3077	1/1	0.97	0.28	11,11,11,11	0
57	MG	YA	3078	1/1	0.97	0.17	8,8,8,8	0
57	MG	RA	3215	1/1	0.97	0.19	20,20,20,20	0
57	MG	RA	3108	1/1	0.97	0.28	32,32,32,32	0
57	MG	RA	3069	1/1	0.97	0.06	28,28,28,28	0
57	MG	YA	3256	1/1	0.97	0.13	11,11,11,11	0
57	MG	YA	3259	1/1	0.97	0.30	14,14,14,14	0
57	MG	YA	3261	1/1	0.97	0.29	18,18,18,18	0
57	MG	RA	3144	1/1	0.97	0.20	11,11,11,11	0
57	MG	RA	3006	1/1	0.97	0.19	7,7,7,7	0
57	MG	YA	3087	1/1	0.97	0.32	6,6,6,6	0
57	MG	YA	3088	1/1	0.97	0.29	17,17,17,17	0
57	MG	YA	3268	1/1	0.97	0.30	21,21,21,21	0
57	MG	RA	3029	1/1	0.97	0.22	6,6,6,6	0
57	MG	YA	3090	1/1	0.97	0.28	12,12,12,12	0
57	MG	RA	3073	1/1	0.97	0.21	23,23,23,23	0
57	MG	RA	3074	1/1	0.97	0.12	7,7,7,7	0
57	MG	YA	3094	1/1	0.97	0.11	5,5,5,5	0
57	MG	YA	3095	1/1	0.97	0.33	5,5,5,5	0
57	MG	YA	3096	1/1	0.97	0.37	7,7,7,7	0
57	MG	Y0	101	1/1	0.97	0.22	20,20,20,20	0
57	MG	RA	3114	1/1	0.97	0.14	35,35,35,35	0
57	MG	YA	3098	1/1	0.97	0.15	19,19,19,19	0
57	MG	YA	3099	1/1	0.97	0.17	2,2,2,2	0
57	MG	RA	3047	1/1	0.97	0.33	13,13,13,13	0
57	MG	RA	3048	1/1	0.97	0.38	18,18,18,18	0
57	MG	YA	3102	1/1	0.97	0.44	11,11,11,11	0
57	MG	YA	3103	1/1	0.97	0.31	26,26,26,26	0
57	MG	RA	3117	1/1	0.97	0.11	10,10,10,10	0
57	MG	RA	3154	1/1	0.97	0.10	28,28,28,28	0
57	MG	RA	3080	1/1	0.98	0.29	15,15,15,15	0
57	MG	YA	3019	1/1	0.98	0.25	0,0,0,0	0
57	MG	YA	3086	1/1	0.98	0.27	58,58,58,58	0
57	MG	XA	1644	1/1	0.98	0.12	21,21,21,21	0
57	MG	XA	1645	1/1	0.98	0.28	30,30,30,30	0
57	MG	RA	3007	1/1	0.98	0.26	11,11,11,11	0
57	MG	RA	3003	1/1	0.98	0.39	15,15,15,15	0
57	MG	RA	3004	1/1	0.98	0.26	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3027	1/1	0.98	0.21	9,9,9,9	0
57	MG	RA	3085	1/1	0.98	0.16	11,11,11,11	0
57	MG	RA	3015	1/1	0.98	0.16	19,19,19,19	0
57	MG	YA	3030	1/1	0.98	0.49	19,19,19,19	0
57	MG	RA	3140	1/1	0.98	0.16	27,27,27,27	0
57	MG	YA	3032	1/1	0.98	0.27	3,3,3,3	0
57	MG	RA	3230	1/1	0.98	0.17	15,15,15,15	0
57	MG	YA	3228	1/1	0.98	0.20	4,4,4,4	0
57	MG	RA	3065	1/1	0.98	0.19	23,23,23,23	0
57	MG	XA	1616	1/1	0.98	0.31	14,14,14,14	0
57	MG	YA	3231	1/1	0.98	0.17	23,23,23,23	0
57	MG	YA	3036	1/1	0.98	0.24	9,9,9,9	0
57	MG	QA	1621	1/1	0.98	0.15	35,35,35,35	0
57	MG	RA	3089	1/1	0.98	0.26	6,6,6,6	0
57	MG	RA	3067	1/1	0.98	0.20	12,12,12,12	0
57	MG	RA	3038	1/1	0.98	0.18	8,8,8,8	0
57	MG	RA	3052	1/1	0.98	0.12	9,9,9,9	0
57	MG	YA	3043	1/1	0.98	0.30	12,12,12,12	0
57	MG	XA	1622	1/1	0.98	0.08	33,33,33,33	0
57	MG	RA	3017	1/1	0.98	0.19	7,7,7,7	0
57	MG	YA	3111	1/1	0.98	0.06	5,5,5,5	0
57	MG	RA	3094	1/1	0.98	0.35	23,23,23,23	0
57	MG	RA	3149	1/1	0.98	0.22	28,28,28,28	0
57	MG	RA	3095	1/1	0.98	0.23	6,6,6,6	0
57	MG	RA	3071	1/1	0.98	0.28	18,18,18,18	0
57	MG	YA	3116	1/1	0.98	0.27	12,12,12,12	0
57	MG	YA	3050	1/1	0.98	0.27	6,6,6,6	0
57	MG	RA	3181	1/1	0.98	0.15	43,43,43,43	0
57	MG	YA	3119	1/1	0.98	0.11	22,22,22,22	0
57	MG	RA	3123	1/1	0.98	0.20	19,19,19,19	0
57	MG	YA	3121	1/1	0.98	0.16	31,31,31,31	0
57	MG	RA	3040	1/1	0.98	0.17	3,3,3,3	0
57	MG	RA	3018	1/1	0.98	0.15	9,9,9,9	0
57	MG	RA	3099	1/1	0.98	0.31	19,19,19,19	0
57	MG	YA	3255	1/1	0.98	0.37	0,0,0,0	0
57	MG	RA	3056	1/1	0.98	0.37	12,12,12,12	0
57	MG	YA	3257	1/1	0.98	0.12	12,12,12,12	0
57	MG	YA	3258	1/1	0.98	0.38	9,9,9,9	0
57	MG	RA	3042	1/1	0.98	0.31	18,18,18,18	0
57	MG	YA	3260	1/1	0.98	0.29	11,11,11,11	0
57	MG	YA	3190	1/1	0.98	0.12	13,13,13,13	0
57	MG	QA	1620	1/1	0.98	0.10	29,29,29,29	0

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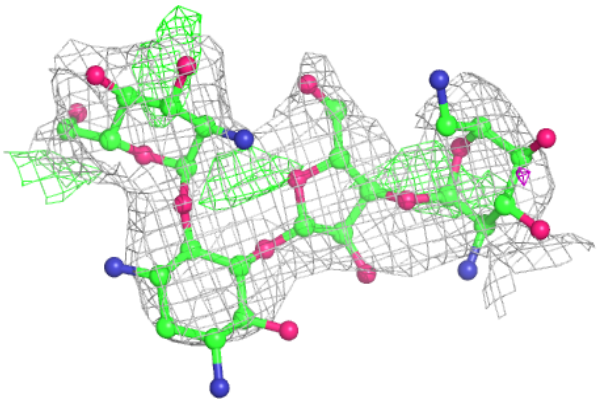
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3263	1/1	0.98	0.10	15,15,15,15	0
57	MG	YA	3264	1/1	0.98	0.20	3,3,3,3	0
57	MG	XA	1674	1/1	0.98	0.13	35,35,35,35	0
57	MG	YA	3063	1/1	0.98	0.21	17,17,17,17	0
57	MG	RA	3020	1/1	0.98	0.17	7,7,7,7	0
57	MG	RA	3021	1/1	0.98	0.37	8,8,8,8	0
57	MG	YA	3004	1/1	0.98	0.13	5,5,5,5	0
57	MG	YA	3067	1/1	0.98	0.31	27,27,27,27	0
57	MG	YA	3005	1/1	0.98	0.09	7,7,7,7	0
57	MG	XA	1601	1/1	0.98	0.26	7,7,7,7	0
57	MG	YA	3007	1/1	0.98	0.14	2,2,2,2	0
57	MG	YA	3008	1/1	0.98	0.23	22,22,22,22	0
57	MG	YA	3138	1/1	0.98	0.12	15,15,15,15	0
57	MG	XA	1602	1/1	0.98	0.16	16,16,16,16	0
57	MG	YA	3010	1/1	0.98	0.20	0,0,0,0	0
57	MG	YA	3011	1/1	0.98	0.28	25,25,25,25	0
57	MG	XA	1640	1/1	0.98	0.10	187,187,187,187	0
57	MG	YA	3207	1/1	0.98	0.30	52,52,52,52	0
57	MG	YA	3013	1/1	0.98	0.35	2,2,2,2	0
57	MG	RA	3105	1/1	0.98	0.13	6,6,6,6	0
57	MG	YA	3015	1/1	0.98	0.43	3,3,3,3	0
57	MG	RA	3106	1/1	0.98	0.24	28,28,28,28	0
57	MG	YA	3017	1/1	0.98	0.21	13,13,13,13	0
57	MG	YA	3053	1/1	0.99	0.17	11,11,11,11	0
57	MG	XA	1610	1/1	0.99	0.20	19,19,19,19	0
57	MG	XA	1615	1/1	0.99	0.27	30,30,30,30	0
57	MG	YA	3081	1/1	0.99	0.23	5,5,5,5	0
57	MG	YA	3020	1/1	0.99	0.46	13,13,13,13	0
57	MG	YA	3037	1/1	0.99	0.11	2,2,2,2	0
57	MG	YA	3084	1/1	0.99	0.38	6,6,6,6	0
57	MG	YA	3058	1/1	0.99	0.34	11,11,11,11	0
57	MG	YA	3021	1/1	0.99	0.30	17,17,17,17	0
57	MG	YA	3002	1/1	0.99	0.29	9,9,9,9	0
57	MG	RA	3031	1/1	0.99	0.24	7,7,7,7	0
57	MG	YA	3074	1/1	0.99	0.32	22,22,22,22	0
57	MG	RA	3076	1/1	0.99	0.12	6,6,6,6	0
57	MG	YA	3091	1/1	0.99	0.32	7,7,7,7	0
57	MG	YA	3051	1/1	0.99	0.20	4,4,4,4	0
57	MG	RA	3083	1/1	0.99	0.26	13,13,13,13	0

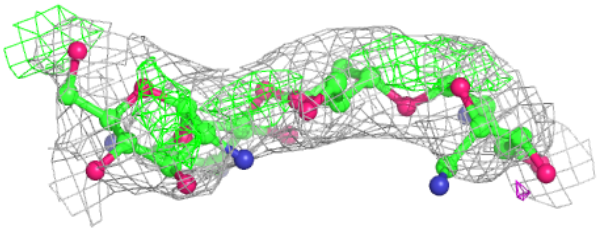
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

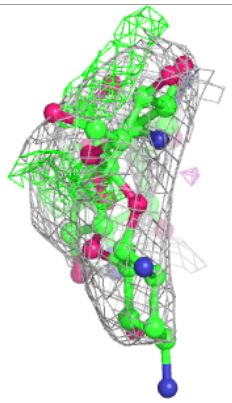
orientation to approximate a three-dimensional view.

Electron density around PAR QA 1666:

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

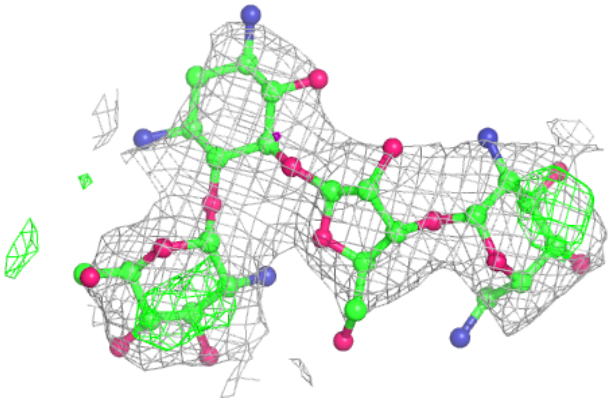


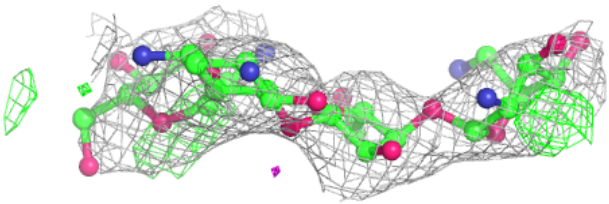


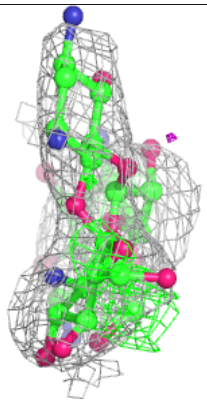


Electron density around PAR XA 1675:

$2mF_o$-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 (i)

There are no such residues in this entry.