wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 09:31 PM EDT

PDB ID	:	6OPE / pdb_00006ope
Title	:	Crystal structure of tRNA^ Ala(GGC) U32-A38 bound to near-cognate 70S A site
Authors	:	Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on	:	2019-04-24
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

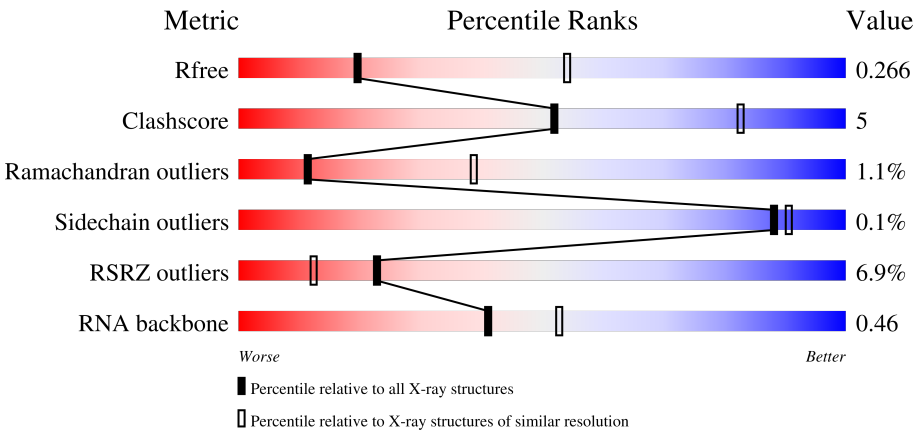
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	2% 66% 28% • •
1	XA	1522	% 68% 27% • •
2	QB	256	8% 71% 20% • 7%
2	XB	256	4% 72% 20% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	QC	239	8% 67% 19% 14%
3	XC	239	5% 71% 15% 14%
4	QD	209	5% 80% 19%
4	XD	209	10% 83% 14% •
5	QE	162	6% 76% 17% • 7%
5	XE	162	4% 84% 9% 7%
6	QF	101	2% 86% 14%
6	XF	101	2% 86% 14%
7	QG	156	7% 85% 14% ••
7	XG	156	4% 89% 10% •
8	QH	138	10% 86% 14%
8	XH	138	4% 75% 24% •
9	QI	128	23% 68% 30% ••
9	XI	128	15% 70% 29% ••
10	QJ	105	28% 65% 30% 6%
10	XJ	105	11% 77% 17% 6%
11	QK	129	6% 72% 19% • 8%
11	XK	129	6% 80% 12% • 8%
12	QL	131	15% 72% 21% •• 5%
12	XL	131	13% 71% 22% • 5%
13	QM	126	17% 64% 30% ••
13	XM	126	14% 75% 21% ••
14	QN	61	31% 75% 23% •
14	XN	61	23% 79% 20% •
15	QO	89	4% 85% 13% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	XO	89	4% 92% 7%
16	QP	88	7% 69% 25% 5%
16	XP	88	5% 78% 16% 5%
17	QQ	105	8% 76% 19% 5%
17	XQ	105	9% 79% 16% 5%
18	QR	88	% 63% 15% 20%
18	XR	88	2% 65% 13% 20%
19	QS	93	20% 62% 25% 10%
19	XS	93	13% 58% 29% 10%
20	QT	106	18% 83% 9% 7%
20	XT	106	25% 74% 17% 7%
21	QU	27	37% 70% 22% 7%
21	XU	27	22% 81% 11% 7%
22	QV	77	4% 73% 27%
22	XV	77	5% 74% 25%
23	QX	19	32% 37% 58% 5%
23	XX	19	42% 42% 47% 5% 5%
24	QY	76	28% 45% 42% 12%
24	XY	76	18% 57% 32% 11%
25	R0	85	11% 79% 15%
25	Y0	85	6% 75% 21%
26	R1	98	10% 80% 17%
26	Y1	98	14% 79% 20%
27	R2	72	7% 65% 28%
27	Y2	72	8% 69% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	R3	60	3% 83% 15%
28	Y3	60	87% 12%
29	R4	71	18% 55% 35% 7%
29	Y4	71	21% 65% 28% 7%
30	R5	60	17% 78% 15% 5%
30	Y5	60	22% 80% 17%
31	R6	54	54% 59% 24% 6% 9%
31	Y6	54	39% 59% 19% 11% 9%
32	R7	49	8% 86% 14%
32	Y7	49	8% 86% 12%
33	R8	65	25% 63% 26% 9%
33	Y8	65	25% 65% 23% 11%
34	R9	37	5% 81% 19%
34	Y9	37	78% 22%
35	RA	2915	3% 67% 28% 5%
35	YA	2915	% 68% 26% 5%
36	RB	122	% 70% 23% 6%
36	YB	122	2% 74% 22%
37	RD	276	9% 75% 20%
37	YD	276	7% 71% 24%
38	RE	206	11% 65% 32%
38	YE	206	10% 73% 24%
39	RF	210	2% 75% 20%
39	YF	210	4% 66% 30%
40	RG	182	8% 79% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	YG	182	3% 80% 19%
41	RH	180	19% 74% 19% 6%
41	YH	180	12% 76% 17% 6%
42	RI	148	5% 73% 21%
42	YI	148	6% 76% 20%
43	RN	140	7% 79% 16%
43	YN	140	4% 84% 13%
44	RO	122	2% 77% 22%
44	YO	122	% 81% 19%
45	RP	150	25% 73% 24%
45	YP	150	15% 73% 24%
46	RQ	141	21% 82% 14%
46	YQ	141	13% 74% 22%
47	RR	118	4% 75% 25%
47	YR	118	4% 77% 21%
48	RS	112	14% 83% 12%
48	YS	112	8% 77% 21%
49	RT	146	9% 66% 25% 6%
49	YT	146	8% 64% 29% 6%
50	RU	118	8% 76% 21%
50	YU	118	3% 81% 14%
51	RV	101	7% 73% 25%
51	YV	101	7% 85% 14%
52	RW	113	5% 81% 19%
52	YW	113	2% 80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	RX	96	8% 78% 16%
53	YX	96	4% 80% 16%
54	RY	110	13% 75% 17% 7%
54	YY	110	2% 78% 14% 7%
55	RZ	206	17% 64% 22% 11%
55	YZ	206	15% 67% 20% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1601	-	-	-	X
56	MG	QA	1612	-	-	-	X
56	MG	QA	1618	-	-	-	X
56	MG	QA	1625	-	-	-	X
56	MG	QA	1628	-	-	-	X
56	MG	QA	1632	-	-	-	X
56	MG	QA	1638	-	-	-	X
56	MG	QA	1643	-	-	-	X
56	MG	QA	1658	-	-	-	X
56	MG	QX	102	-	-	-	X
56	MG	R9	101	-	-	-	X
56	MG	RA	3003	-	-	-	X
56	MG	RA	3011	-	-	-	X
56	MG	RA	3012	-	-	-	X
56	MG	RA	3013	-	-	-	X
56	MG	RA	3035	-	-	-	X
56	MG	RA	3051	-	-	-	X
56	MG	RA	3057	-	-	-	X
56	MG	RA	3067	-	-	-	X
56	MG	RA	3073	-	-	-	X
56	MG	RA	3112	-	-	-	X
56	MG	RA	3118	-	-	-	X
56	MG	RA	3120	-	-	-	X
56	MG	RA	3122	-	-	-	X
56	MG	RA	3126	-	-	-	X
56	MG	RA	3139	-	-	-	X
56	MG	RA	3142	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3146	-	-	-	X
56	MG	RA	3148	-	-	-	X
56	MG	RA	3149	-	-	-	X
56	MG	RA	3151	-	-	-	X
56	MG	RA	3159	-	-	-	X
56	MG	RA	3164	-	-	-	X
56	MG	RA	3166	-	-	-	X
56	MG	RA	3170	-	-	-	X
56	MG	RA	3173	-	-	-	X
56	MG	RA	3178	-	-	-	X
56	MG	RA	3180	-	-	-	X
56	MG	RA	3199	-	-	-	X
56	MG	RA	3202	-	-	-	X
56	MG	RA	3203	-	-	-	X
56	MG	RA	3206	-	-	-	X
56	MG	RA	3215	-	-	-	X
56	MG	RA	3217	-	-	-	X
56	MG	RA	3218	-	-	-	X
56	MG	RA	3223	-	-	-	X
56	MG	RA	3233	-	-	-	X
56	MG	RA	3236	-	-	-	X
56	MG	RA	3244	-	-	-	X
56	MG	RA	3249	-	-	-	X
56	MG	RA	3250	-	-	-	X
56	MG	RA	3252	-	-	-	X
56	MG	RA	3256	-	-	-	X
56	MG	RA	3262	-	-	-	X
56	MG	RA	3266	-	-	-	X
56	MG	RA	3277	-	-	-	X
56	MG	RA	3279	-	-	-	X
56	MG	XA	1607	-	-	-	X
56	MG	XA	1614	-	-	-	X
56	MG	XA	1619	-	-	-	X
56	MG	XA	1632	-	-	-	X
56	MG	XA	1646	-	-	-	X
56	MG	XA	1648	-	-	-	X
56	MG	XA	1654	-	-	-	X
56	MG	XA	1655	-	-	-	X
56	MG	XA	1660	-	-	-	X
56	MG	XA	1662	-	-	-	X
56	MG	XA	1667	-	-	-	X
56	MG	XA	1668	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	XA	1671	-	-	-	X
56	MG	XA	1687	-	-	-	X
56	MG	XA	1691	-	-	-	X
56	MG	XA	1692	-	-	-	X
56	MG	XX	101	-	-	-	X
56	MG	YA	3035	-	-	-	X
56	MG	YA	3106	-	-	-	X
56	MG	YA	3111	-	-	-	X
56	MG	YA	3154	-	-	-	X
56	MG	YA	3155	-	-	-	X
56	MG	YA	3162	-	-	-	X
56	MG	YA	3163	-	-	-	X
56	MG	YA	3168	-	-	-	X
56	MG	YA	3172	-	-	-	X
56	MG	YA	3181	-	-	-	X
56	MG	YA	3182	-	-	-	X
56	MG	YA	3191	-	-	-	X
56	MG	YA	3193	-	-	-	X
56	MG	YA	3197	-	-	-	X
56	MG	YA	3202	-	-	-	X
56	MG	YA	3205	-	-	-	X
56	MG	YA	3206	-	-	-	X
56	MG	YA	3220	-	-	-	X
56	MG	YA	3233	-	-	-	X
56	MG	YA	3239	-	-	-	X
56	MG	YA	3246	-	-	-	X
56	MG	YA	3286	-	-	-	X
56	MG	YA	3288	-	-	-	X
56	MG	YA	3294	-	-	-	X
56	MG	YA	3313	-	-	-	X
56	MG	YA	3321	-	-	-	X
56	MG	YA	3323	-	-	-	X
56	MG	YA	3333	-	-	-	X
56	MG	YA	3337	-	-	-	X
56	MG	YA	3338	-	-	-	X
56	MG	YA	3340	-	-	-	X
56	MG	YA	3346	-	-	-	X
56	MG	YB	201	-	-	-	X
56	MG	YP	201	-	-	-	X
56	MG	YQ	203	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 294981 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	1674	1050	333	284	7	0	0	0
4	XD	208	1674	1050	333	284	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

Continued on next page...

Continued from previous page...

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 type Z.

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 Thx.

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 tRNAfMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	QV	77	1640	732	297	535	76	0	0	0
22	XV	77	1640	732	297	535	76	0	0	0

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	QX	18	396	177	82	119	18	0	0	0
23	XX	18	396	177	82	119	18	0	0	0

- Molecule 24 is a RNA chain called A-site tRNAAla(GGC) U32-A38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	QY	75	1602	714	288	525	75	0	0	0
24	XY	75	1602	714	288	525	75	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L27.

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

- Molecule 26 is a protein called 50S ribosomal protein L28.

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

Continued on next page...

Continued from previous page...

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

- Molecule 27 is a protein called 50S ribosomal protein L29.

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

- Molecule 28 is a protein called 50S ribosomal protein L30.

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

- Molecule 29 is a protein called 50S ribosomal protein L31.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

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

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a RNA chain called 23S rRNA.

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

- Molecule 36 is a RNA chain called 5S rRNA.

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

- Molecule 37 is a protein called 50S ribosomal protein L2.

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

- Molecule 38 is a protein called 50S ribosomal protein L3.

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

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

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

- Molecule 41 is a protein called 50S ribosomal protein L6.

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

- Molecule 42 is a protein called 50S ribosomal protein L9.

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

Continued on next page...

Continued from previous page...

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

- Molecule 43 is a protein called 50S ribosomal protein L13.

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

- Molecule 44 is a protein called 50S ribosomal protein L14.

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

- Molecule 45 is a protein called 50S ribosomal protein L15.

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

- Molecule 46 is a protein called 50S ribosomal protein L16.

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

- Molecule 47 is a protein called 50S ribosomal protein L17.

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

- Molecule 48 is a protein called 50S ribosomal protein L18.

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

- Molecule 49 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L21.

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

- Molecule 52 is a protein called 50S ribosomal protein L22.

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

- Molecule 53 is a protein called 50S ribosomal protein L23.

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

- Molecule 54 is a protein called 50S ribosomal protein L24.

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

- Molecule 55 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	QA	73	73	73	0	0
56	QF	1	1	1	0	0
56	QM	1	1	1	0	0
56	QV	1	1	1	0	0
56	QX	2	2	2	0	0
56	R0	1	1	1	0	0
56	R5	1	1	1	0	0
56	R8	1	1	1	0	0
56	R9	1	1	1	0	0

Continued on next page...

Continued from previous page...

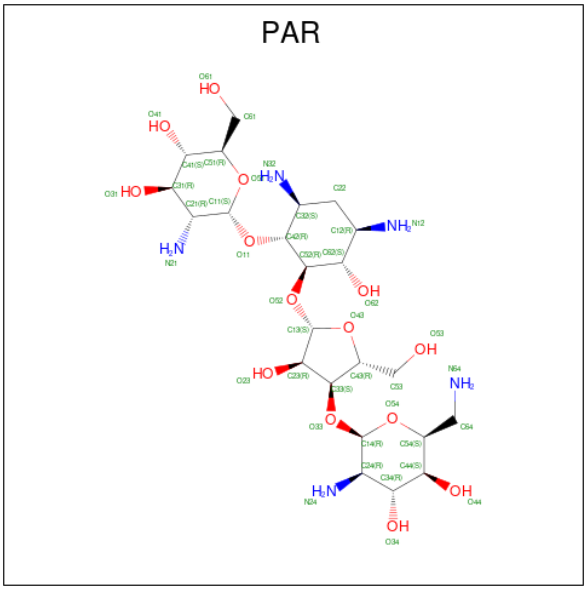
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RA	281	Total 281	Mg 281	0	0
56	RB	4	Total 4	Mg 4	0	0
56	RD	1	Total 1	Mg 1	0	0
56	RE	4	Total 4	Mg 4	0	0
56	RF	1	Total 1	Mg 1	0	0
56	RP	3	Total 3	Mg 3	0	0
56	RR	1	Total 1	Mg 1	0	0
56	RU	1	Total 1	Mg 1	0	0
56	XA	91	Total 91	Mg 91	0	0
56	XF	1	Total 1	Mg 1	0	0
56	XM	1	Total 1	Mg 1	0	0
56	XV	2	Total 2	Mg 2	0	0
56	XX	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	Y1	1	Total 1	Mg 1	0	0
56	Y2	1	Total 1	Mg 1	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	Y6	2	Total 2	Mg 2	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	Y9	1	Total 1	Mg 1	0	0
56	YA	347	Total 347	Mg 347	0	0

Continued on next page...

Continued from previous page...

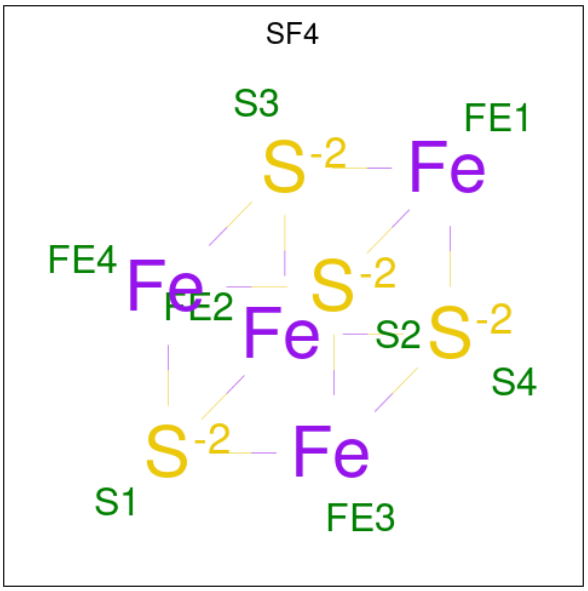
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	YB	6	6	6	0	0
			Total	Mg		
56	YE	3	3	3	0	0
			Total	Mg		
56	YN	1	1	1	0	0
			Total	Mg		
56	YP	3	3	3	0	0
			Total	Mg		
56	YQ	3	3	3	0	0
			Total	Mg		
56	YR	1	1	1	0	0
			Total	Mg		
56	YX	1	1	1	0	0

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



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

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
58	QD	1	8	4	4	0	0
			Total	Fe	S		
58	XD	1	8	4	4	0	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

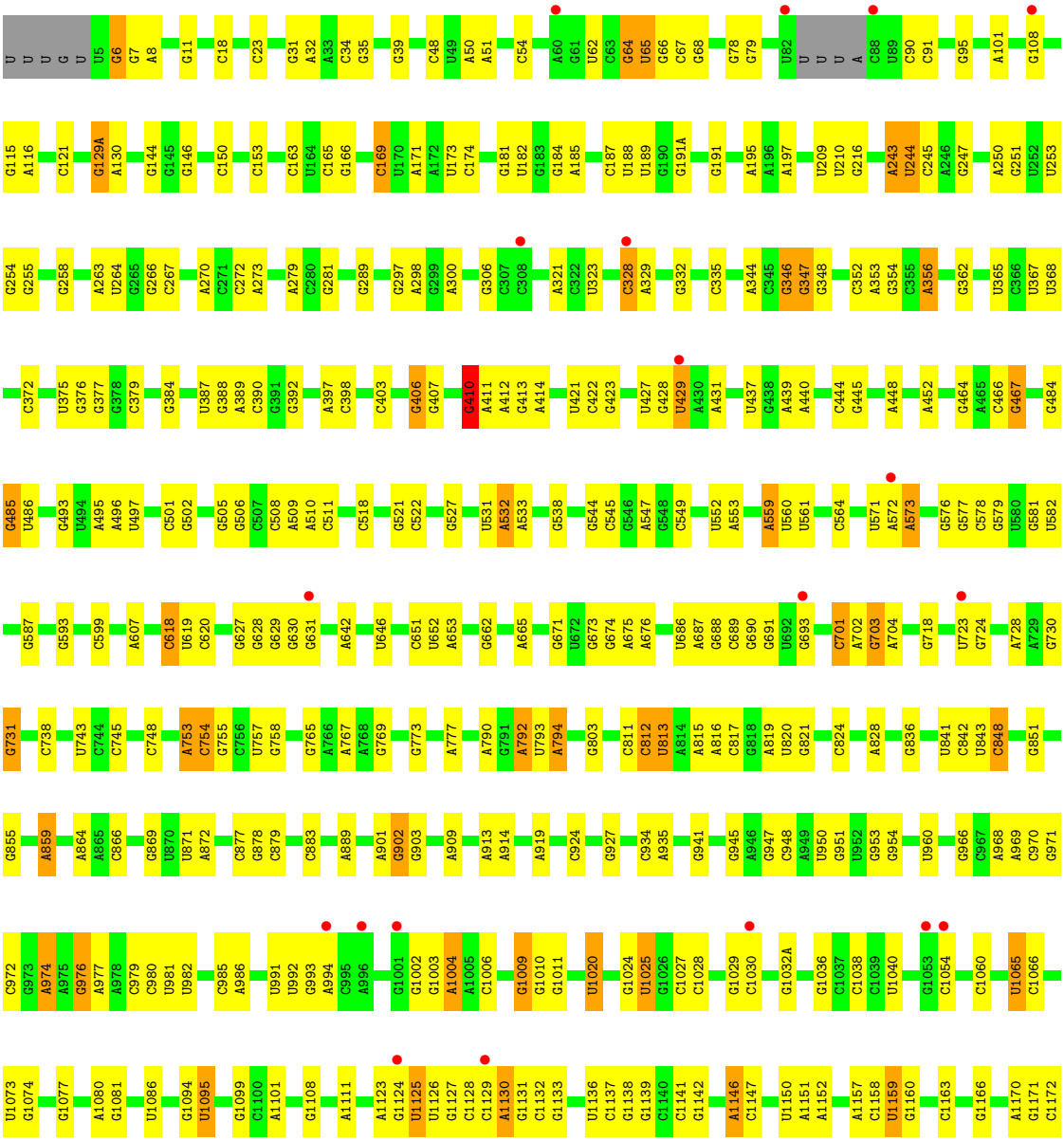
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
59	QN	1	1	1	0	0
			Total	Zn		
59	R9	1	1	1	0	0
			Total	Zn		
59	XN	1	1	1	0	0
			Total	Zn		
59	Y9	1	1	1	0	0

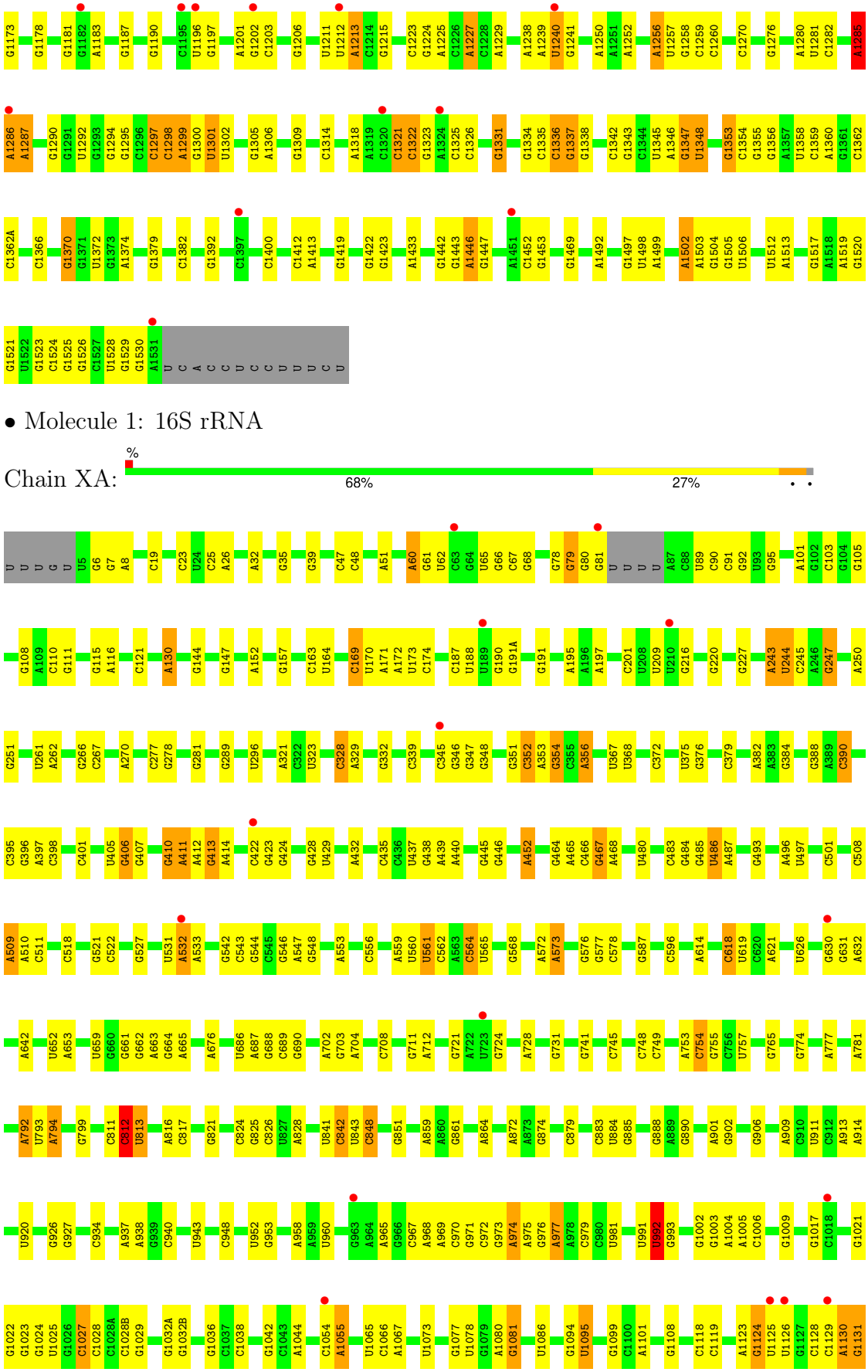
3 Residue-property plots (i)

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

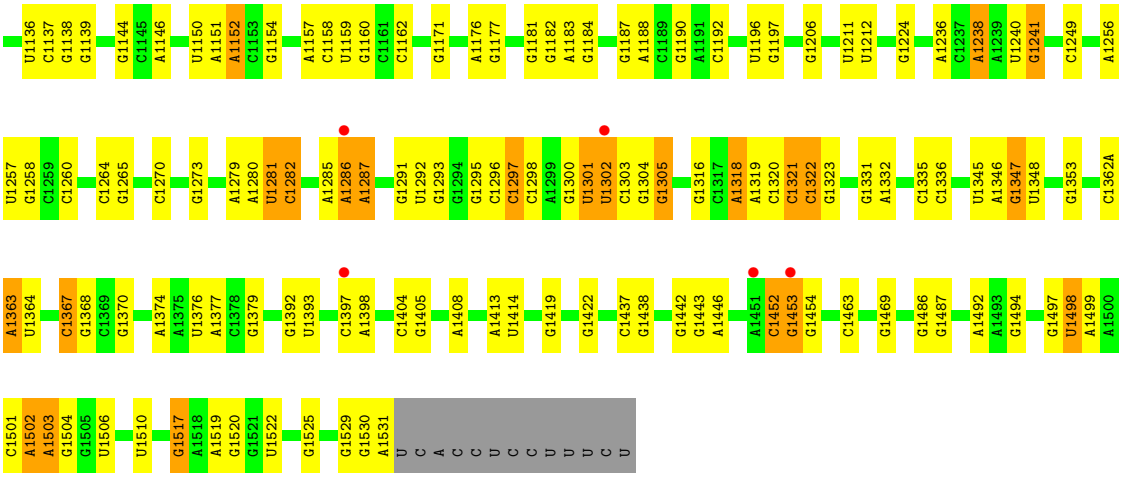
Chain QA:





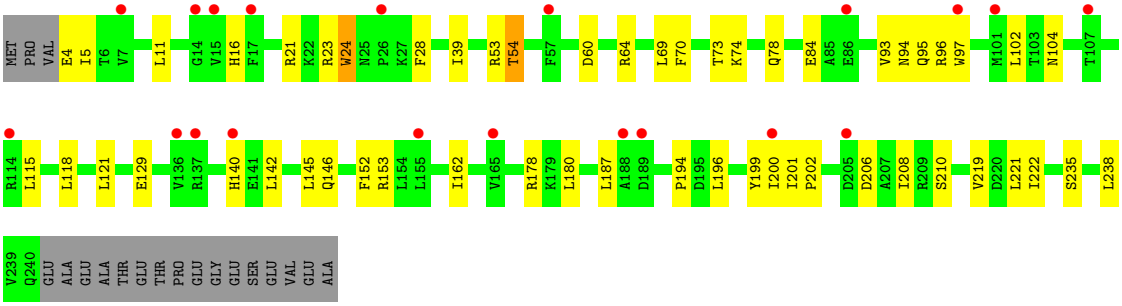
• Molecule 1: 16S rRNA

Chain XA:



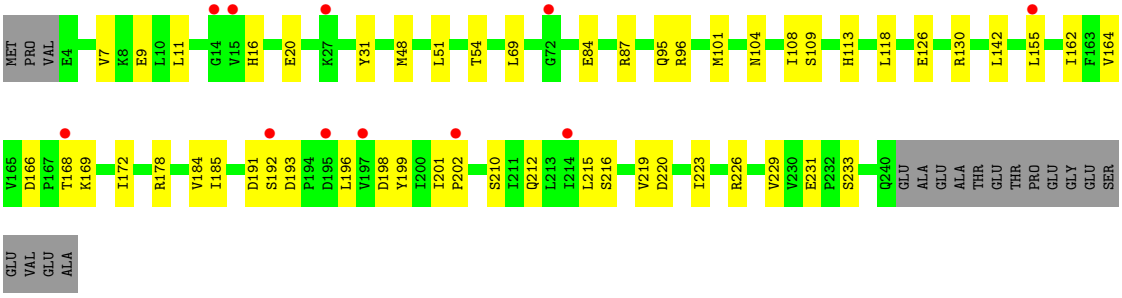
- Molecule 2: 30S ribosomal protein S2

Chain QB:



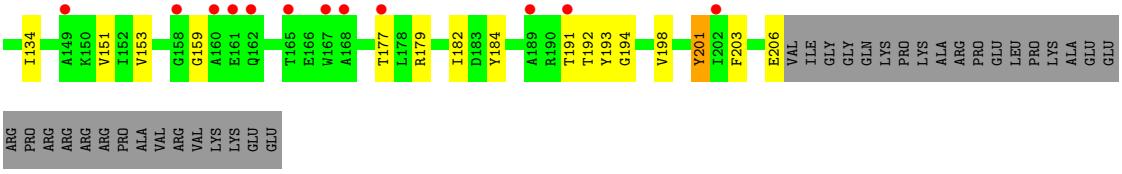
- Molecule 2: 30S ribosomal protein S2

Chain XB:



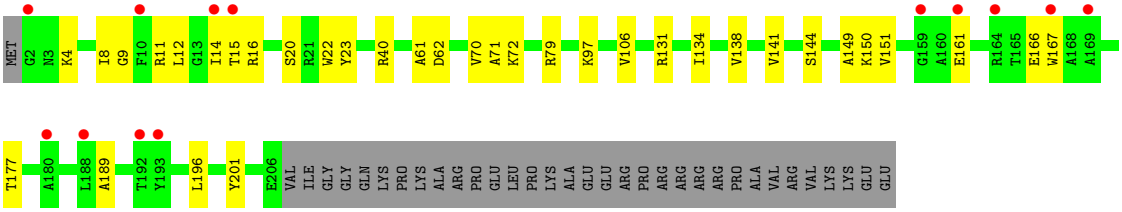
- Molecule 3: 30S ribosomal protein S3

Chain QC:



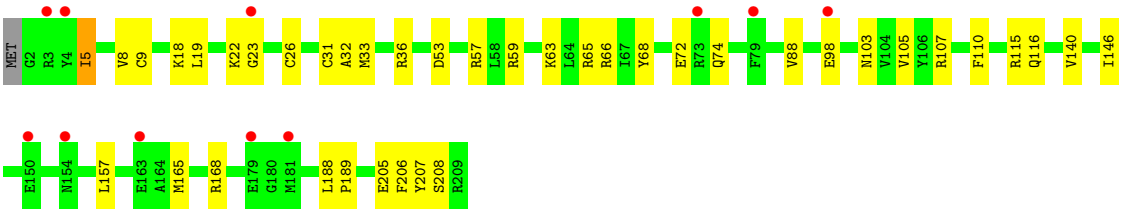
- Molecule 3: 30S ribosomal protein S3

Chain XC:



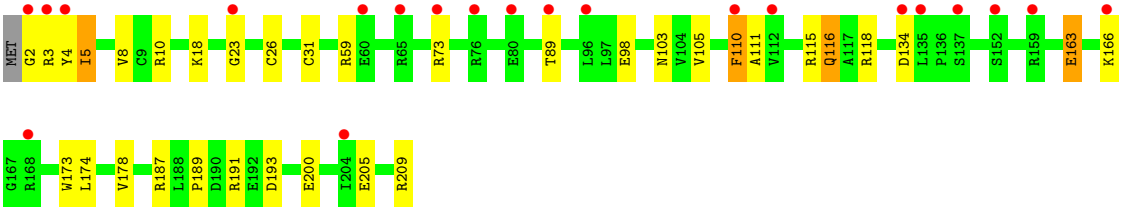
- Molecule 4: 30S ribosomal protein S4

Chain QD:



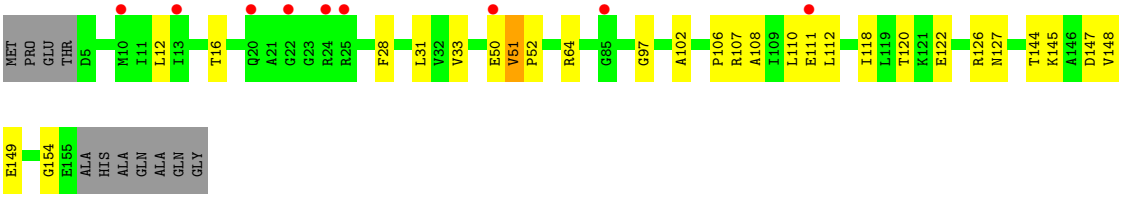
- Molecule 4: 30S ribosomal protein S4

Chain XD:



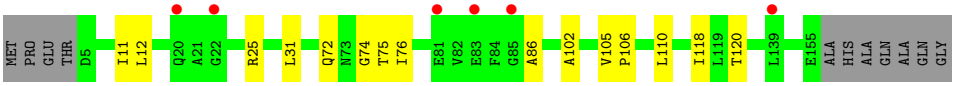
- Molecule 5: 30S ribosomal protein S5

Chain QE:



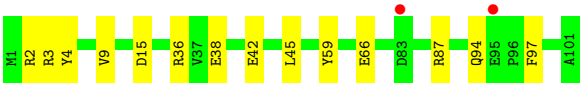
• Molecule 5: 30S ribosomal protein S5

Chain XE:



• Molecule 6: 30S ribosomal protein S6

Chain QF:



• Molecule 6: 30S ribosomal protein S6

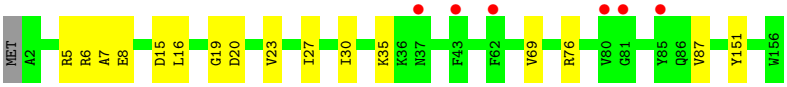
Chain XF:

• Molecule 7: 30S ribosomal protein S7

Chain QG:

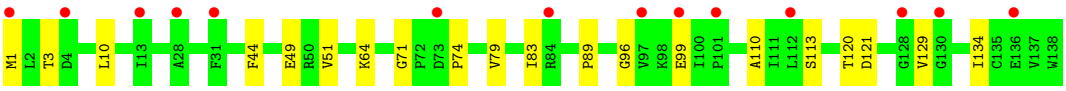
• Molecule 7: 30S ribosomal protein S7

Chain XG:



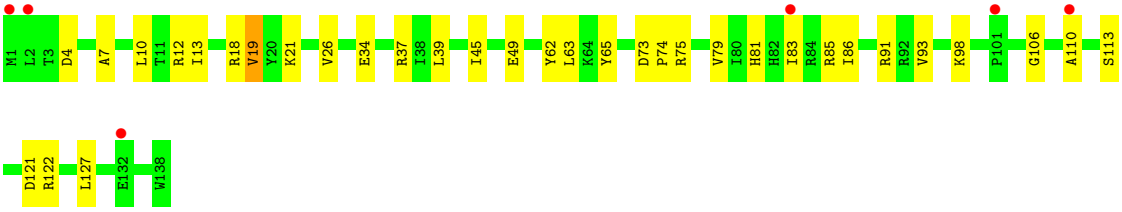
• Molecule 8: 30S ribosomal protein S8

Chain QH:



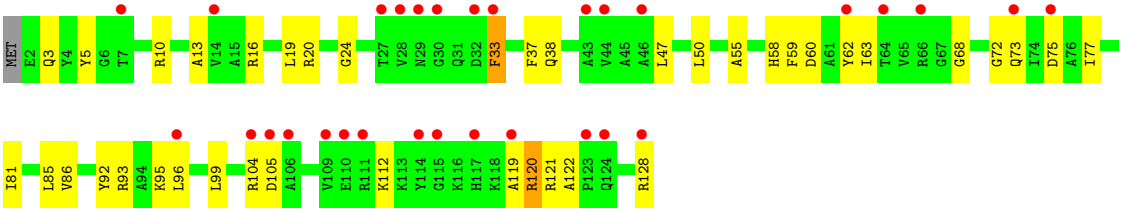
• Molecule 8: 30S ribosomal protein S8

Chain XH:



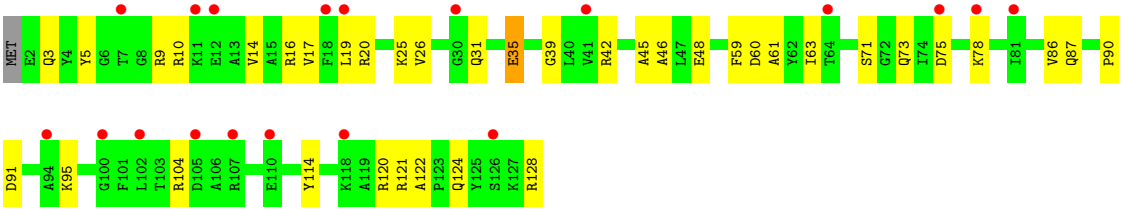
- Molecule 9: 30S ribosomal protein S9

Chain QI:



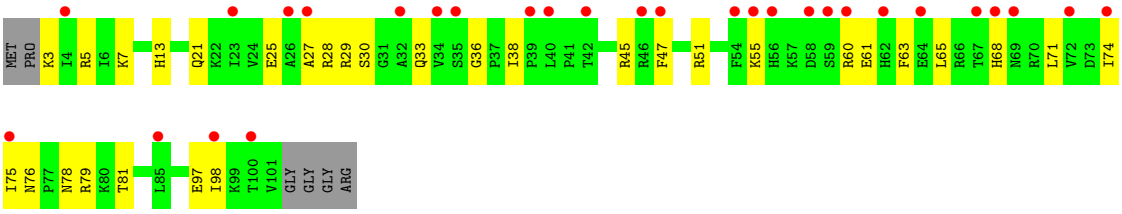
- Molecule 9: 30S ribosomal protein S9

Chain XI:



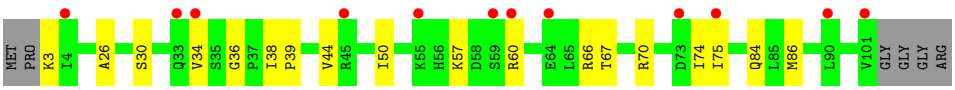
- Molecule 10: 30S ribosomal protein S10

Chain QJ:



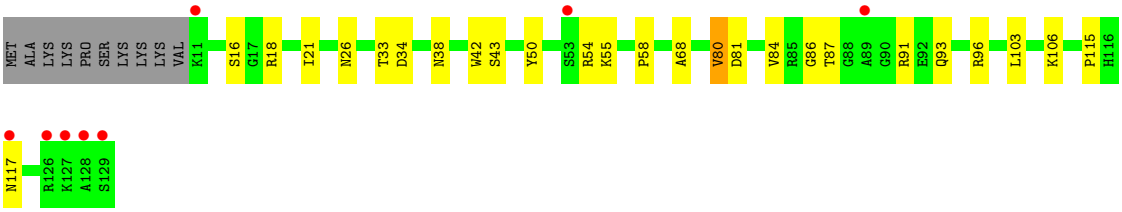
- Molecule 10: 30S ribosomal protein S10

Chain XJ:



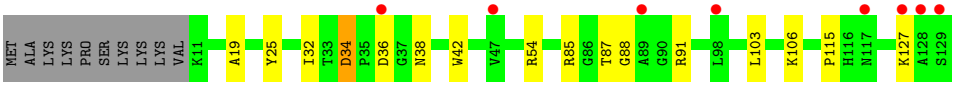
- Molecule 11: 30S ribosomal protein S11

Chain QK:



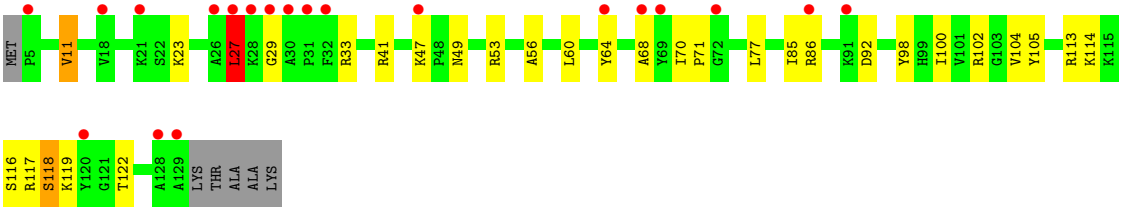
• Molecule 11: 30S ribosomal protein S11

Chain XK:



• Molecule 12: 30S ribosomal protein S12

Chain QL:

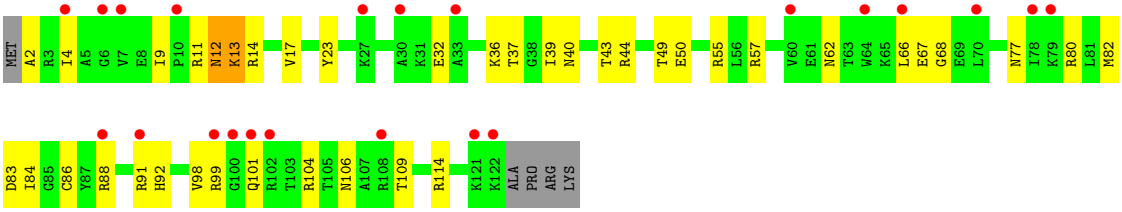


• Molecule 12: 30S ribosomal protein S12

Chain XL:

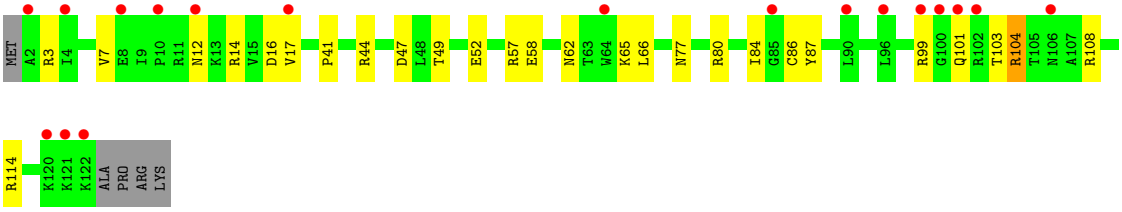
• Molecule 13: 30S ribosomal protein S13

Chain QM:



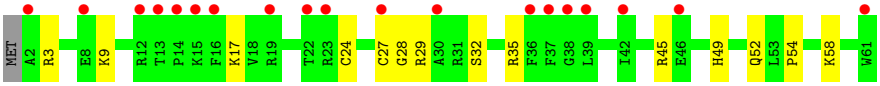
• Molecule 13: 30S ribosomal protein S13

Chain XM:



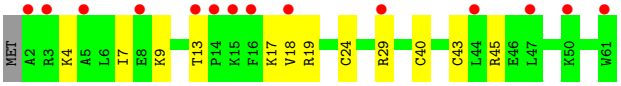
• Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



• Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:

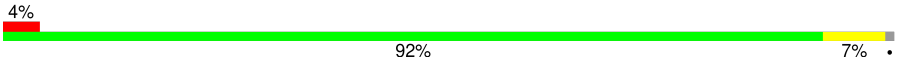


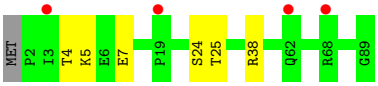
• Molecule 15: 30S ribosomal protein S15

Chain QO:

• Molecule 15: 30S ribosomal protein S15

Chain XO:



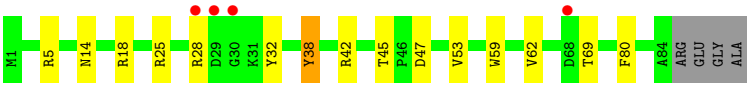


• Molecule 16: 30S ribosomal protein S16

Chain QP:

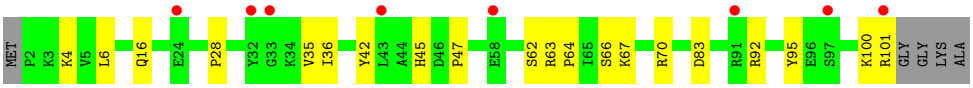
• Molecule 16: 30S ribosomal protein S16

Chain XP:



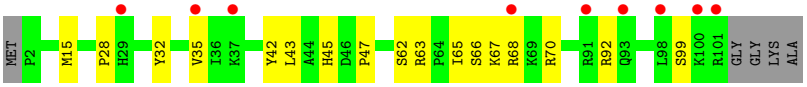
• Molecule 17: 30S ribosomal protein S17

Chain QQ:



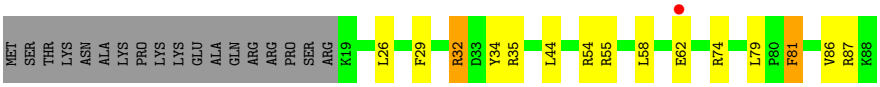
• Molecule 17: 30S ribosomal protein S17

Chain XQ:



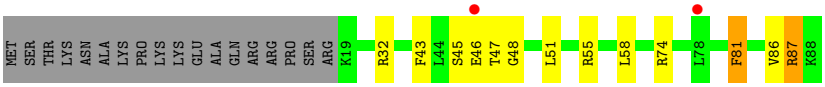
• Molecule 18: 30S ribosomal protein S18

Chain QR:



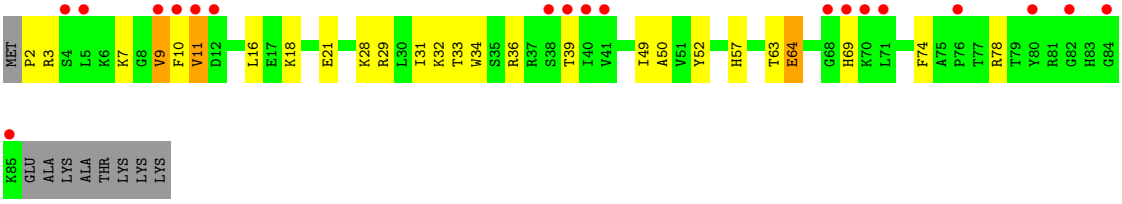
• Molecule 18: 30S ribosomal protein S18

Chain XR:



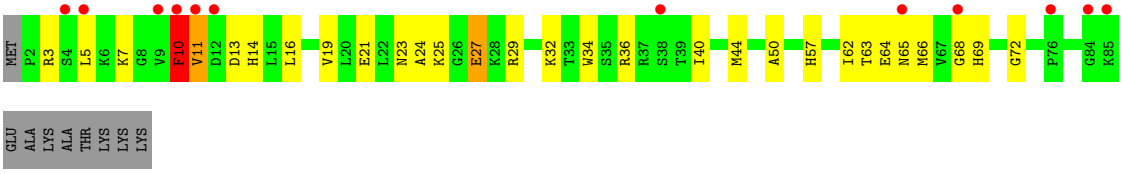
• Molecule 19: 30S ribosomal protein S19

Chain QS:



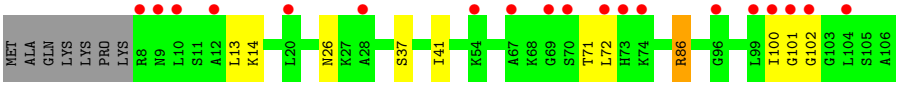
• Molecule 19: 30S ribosomal protein S19

Chain XS:



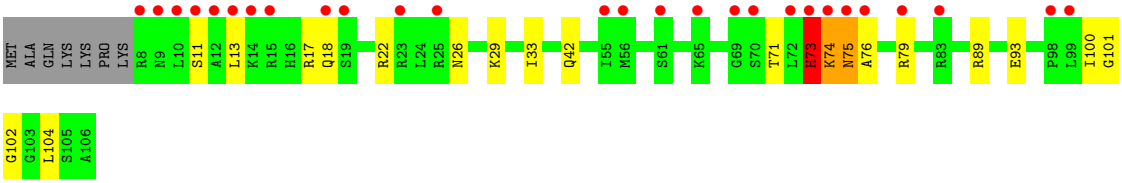
- Molecule 20: 30S ribosomal protein S20

Chain QT:



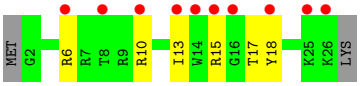
- Molecule 20: 30S ribosomal protein S20

Chain XT:



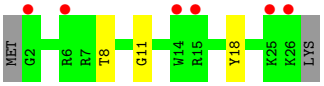
- Molecule 21: 30S ribosomal protein Thx

Chain QU:



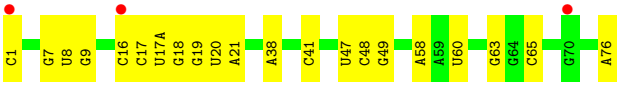
- Molecule 21: 30S ribosomal protein Thx

Chain XU:



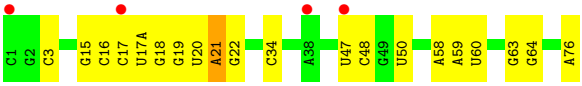
- Molecule 22: P-site tRNAfMet

Chain QV:



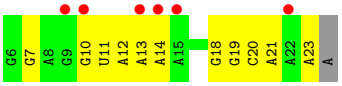
- Molecule 22: P-site tRNAfMet

Chain XV:



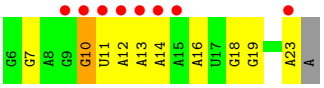
• Molecule 23: mRNA

Chain QX:



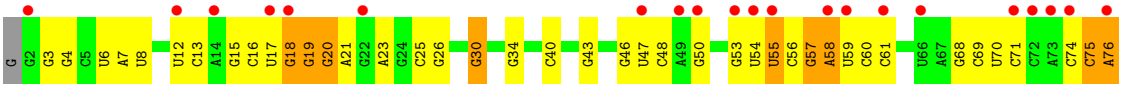
• Molecule 23: mRNA

Chain XX:



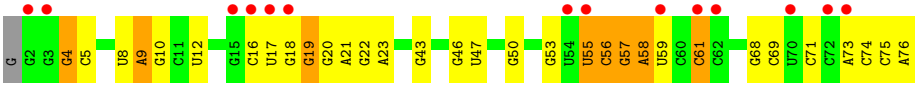
• Molecule 24: A-site tRNAAla(GGC) U32-A38

Chain QY:



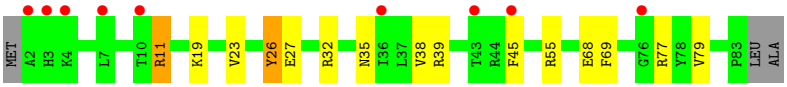
• Molecule 24: A-site tRNAAla(GGC) U32-A38

Chain XY:



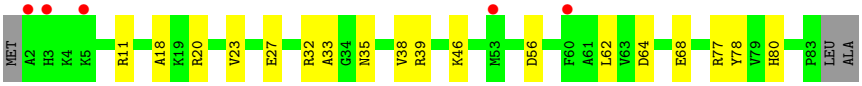
• Molecule 25: 50S ribosomal protein L27

Chain R0:



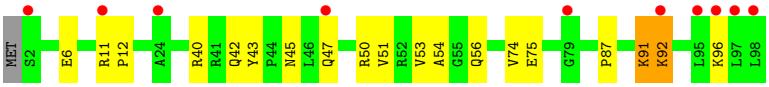
• Molecule 25: 50S ribosomal protein L27

Chain Y0:



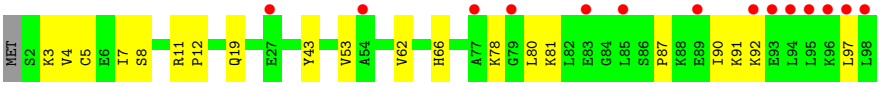
• Molecule 26: 50S ribosomal protein L28

Chain R1:



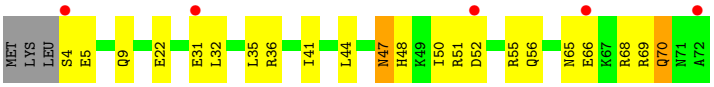
• Molecule 26: 50S ribosomal protein L28

Chain Y1:



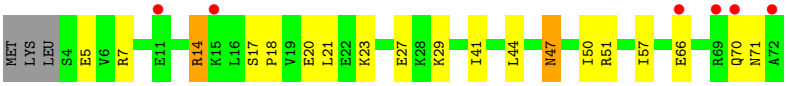
• Molecule 27: 50S ribosomal protein L29

Chain R2:



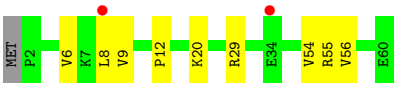
• Molecule 27: 50S ribosomal protein L29

Chain Y2:



• Molecule 28: 50S ribosomal protein L30

Chain R3:

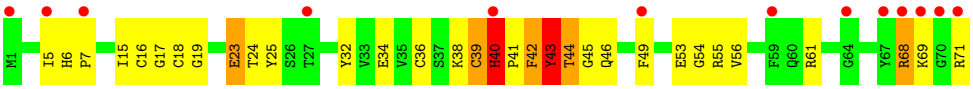


• Molecule 28: 50S ribosomal protein L30

Chain Y3:

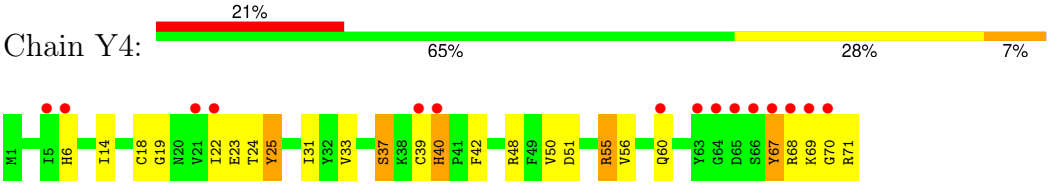
• Molecule 29: 50S ribosomal protein L31

Chain R4:



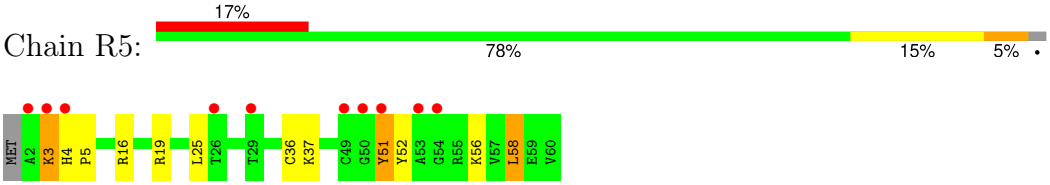
• Molecule 29: 50S ribosomal protein L31

Chain Y4:



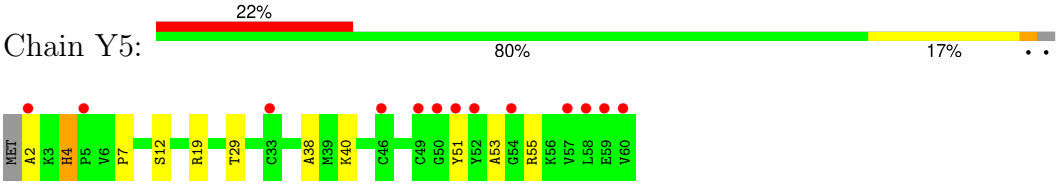
• Molecule 30: 50S ribosomal protein L32

Chain R5:



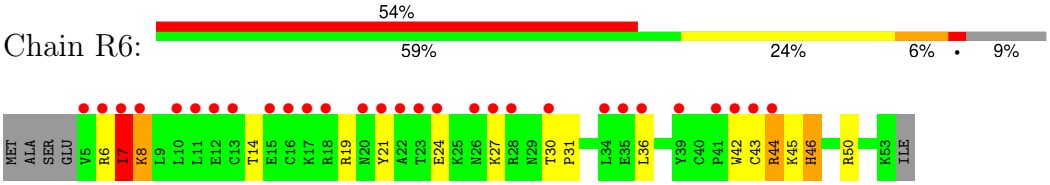
• Molecule 30: 50S ribosomal protein L32

Chain Y5:



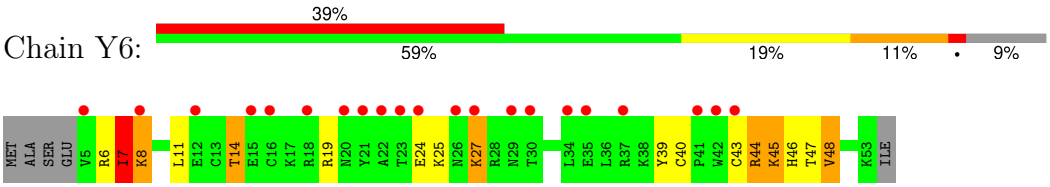
• Molecule 31: 50S ribosomal protein L33

Chain R6:



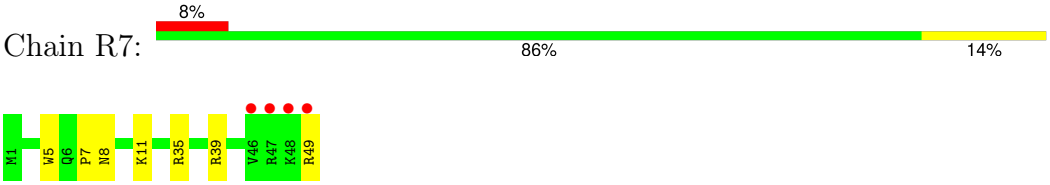
• Molecule 31: 50S ribosomal protein L33

Chain Y6:



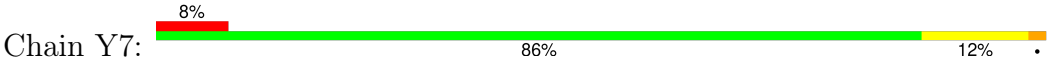
• Molecule 32: 50S ribosomal protein L34

Chain R7:



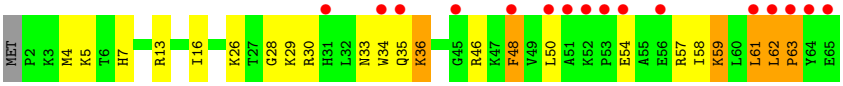
• Molecule 32: 50S ribosomal protein L34

Chain Y7:



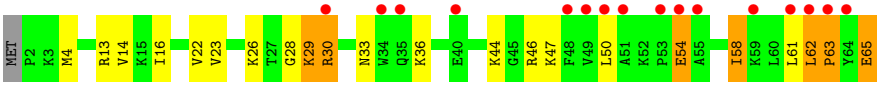
• Molecule 33: 50S ribosomal protein L35

Chain R8:



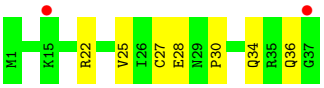
• Molecule 33: 50S ribosomal protein L35

Chain Y8:



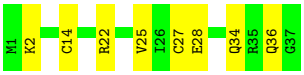
• Molecule 34: 50S ribosomal protein L36

Chain R9:



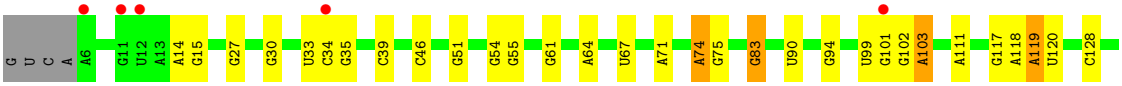
• Molecule 34: 50S ribosomal protein L36

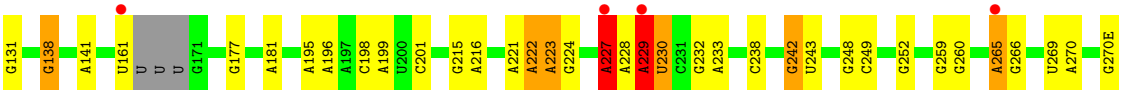
Chain Y9:

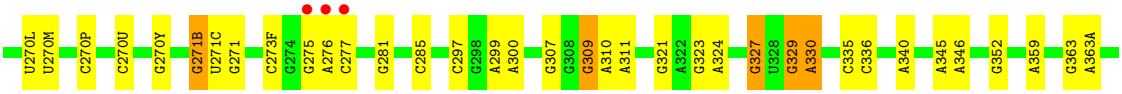


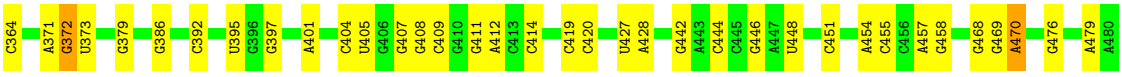
• Molecule 35: 23S rRNA

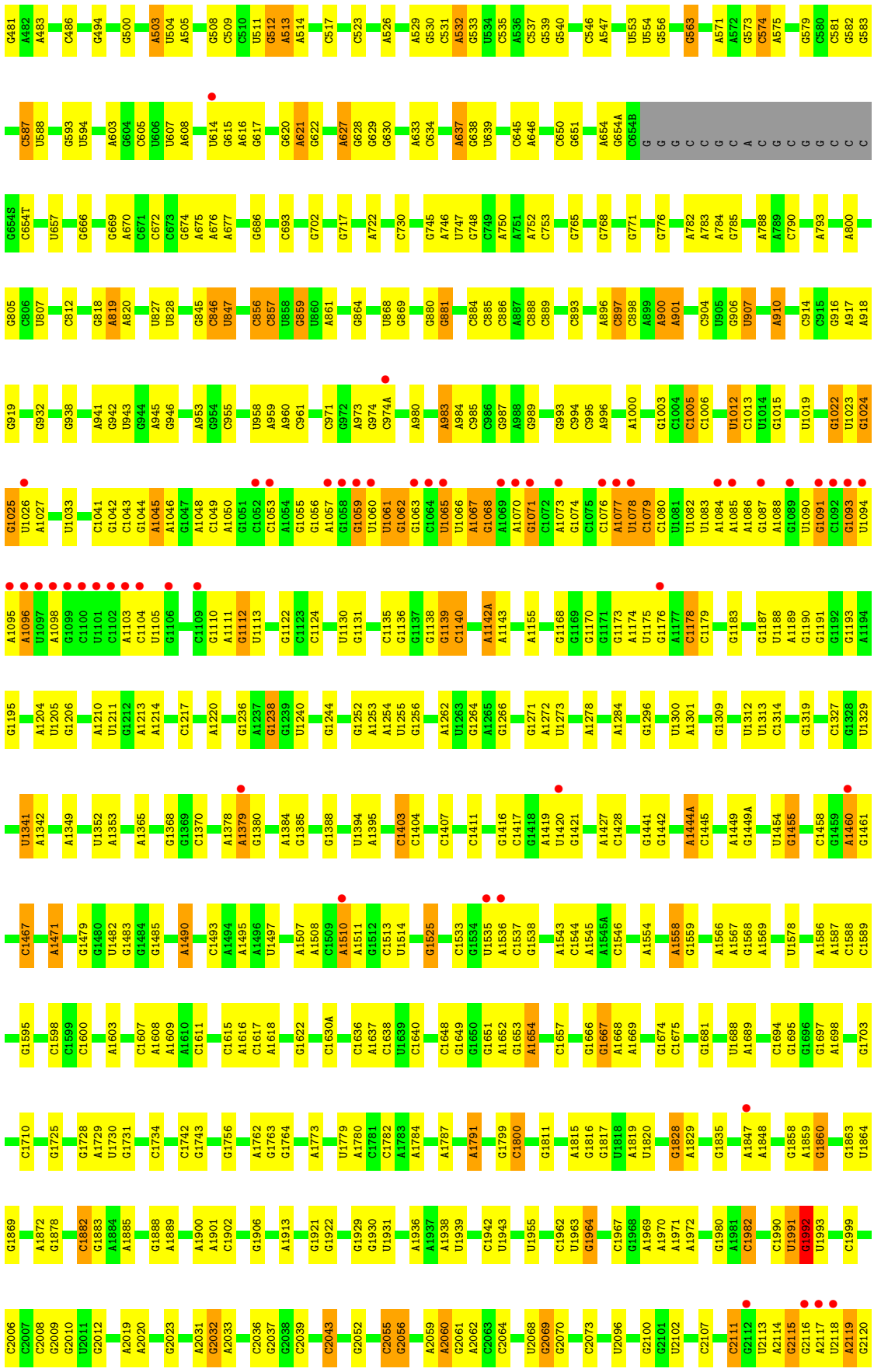
Chain RA:

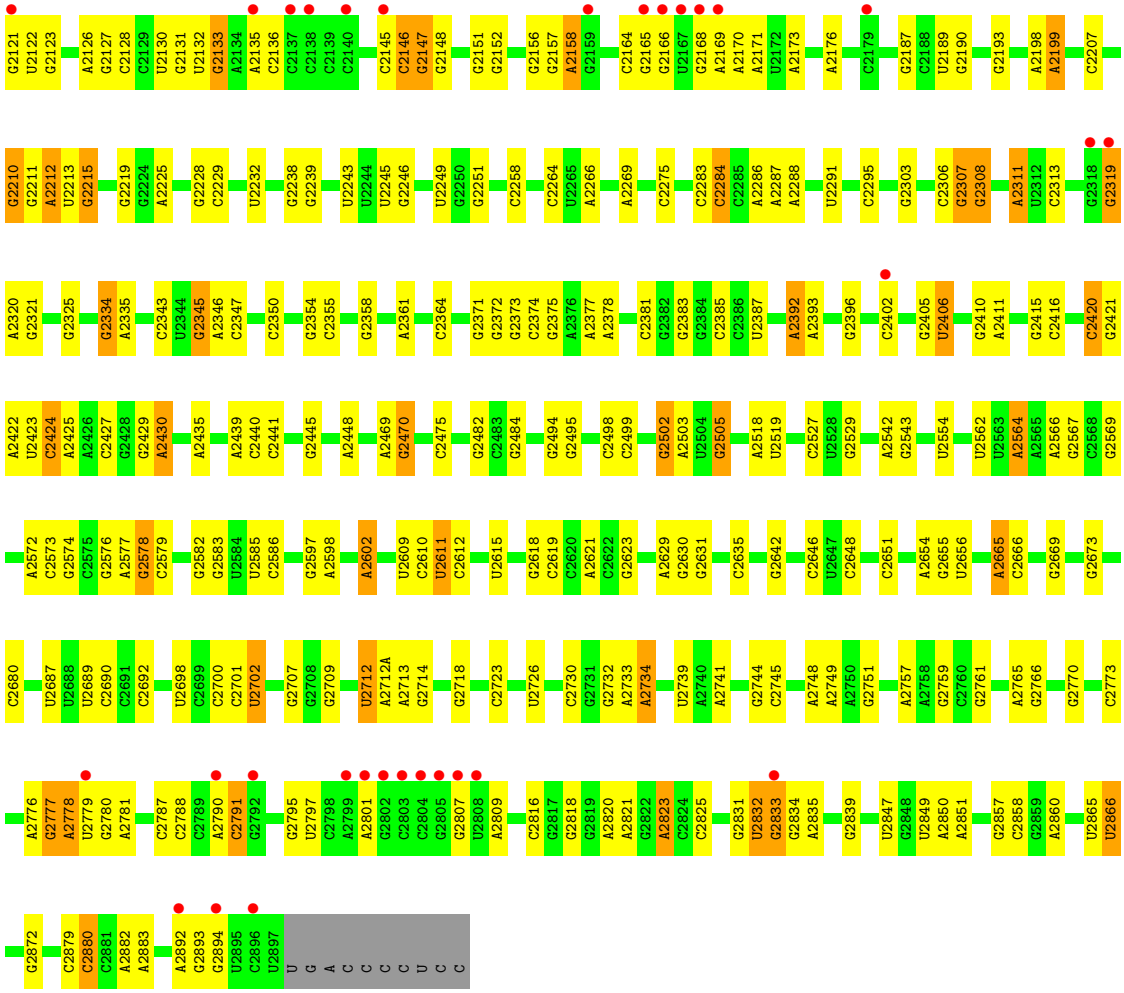






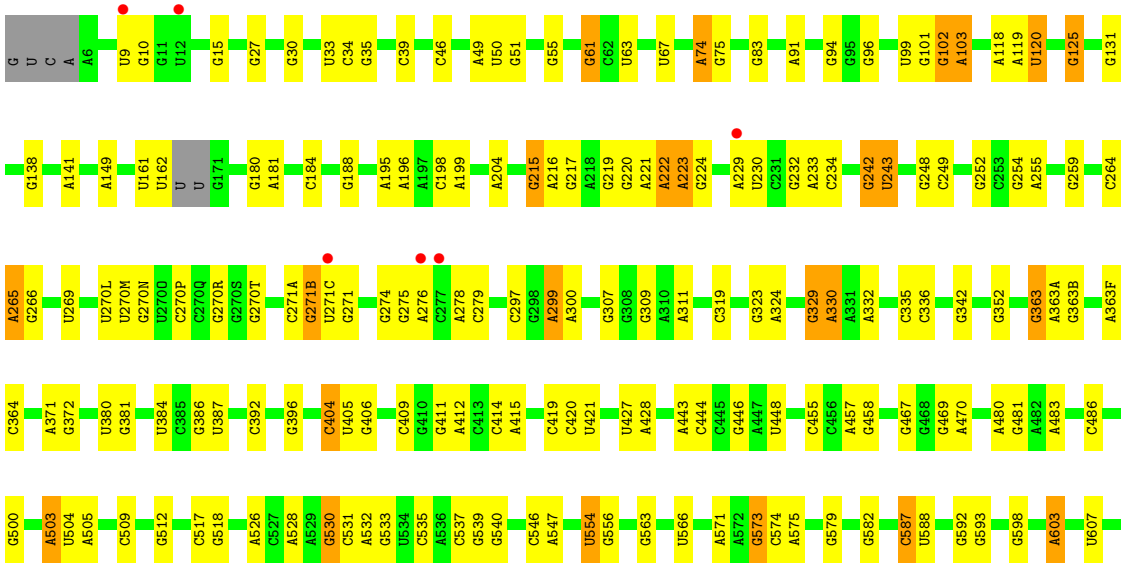


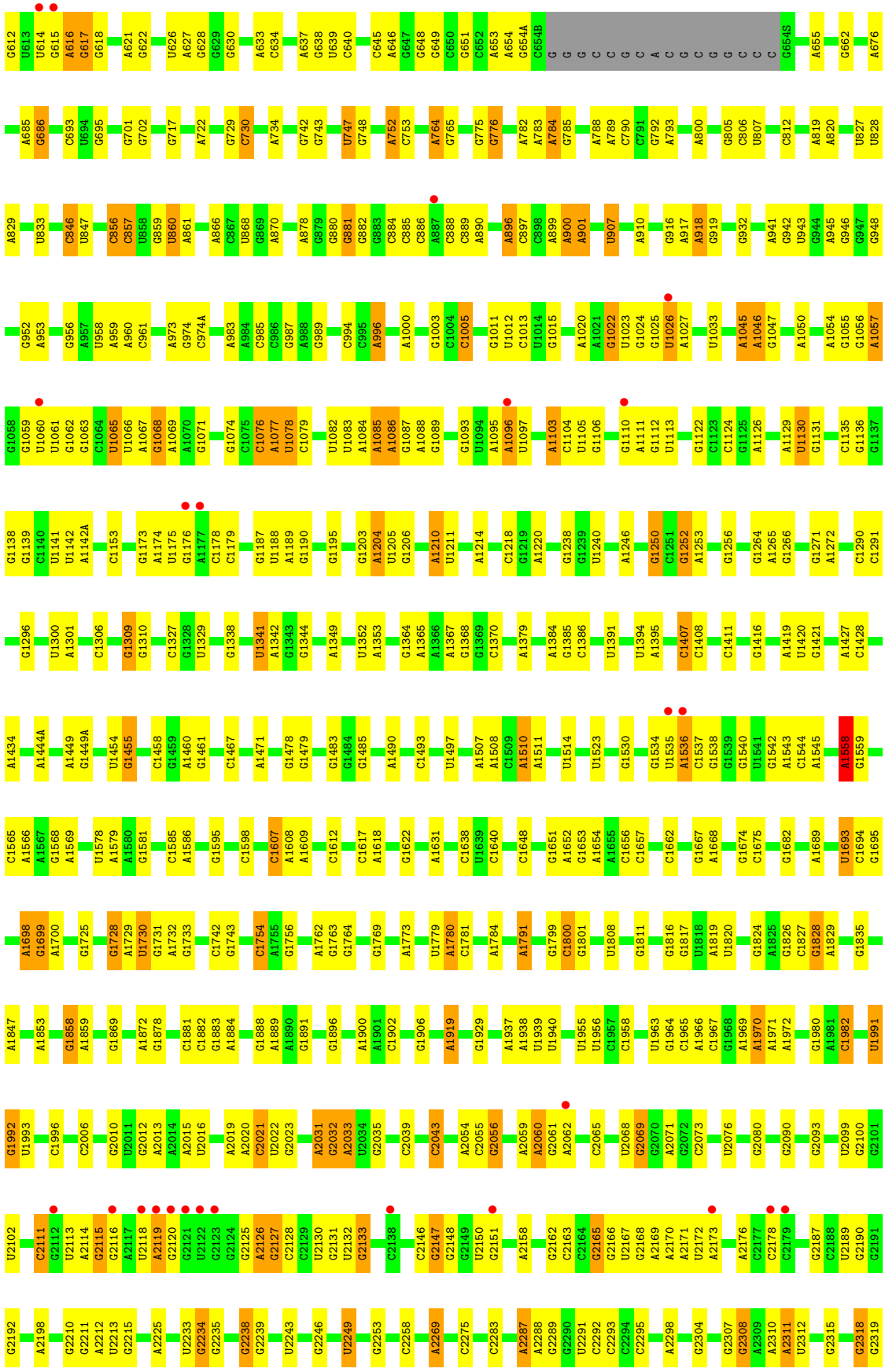

G481 A482 A483 C486 G494 G500 A503 U504 A505 G508 C509 C510 U511 G512 A513 A514 C517 C523 A526 A529 G530 C531 A532 G533 U534 C535 A536 C537 G539 G540 C546 A547 U553 U554 G556 G563 A571 A572 G573 C574 A575 G579 C580 C581 G582 G583
C587 U588 G593 U594 A603 G604 C605 U606 U607 A608 U614 G615 A616 G617 G620 A621 G622 A627 G628 G629 G630 A633 C634 A637 G638 U639 C645 A646 C650 G651 A654 G654A C654B G G G C C G C A C G C G G C C C
G654S C654T U657 G666 G669 A670 C671 C672 C673 G674 A675 A676 A677 G686 C693 G702 G717 A722 C730 G745 A746 U747 G748 C749 A750 A751 A752 C753 G765 G768 G771 G776 A782 A783 A784 G785 A788 A789 C790 A793 A800
G805 C806 U807 C812 G818 A819 A820 U827 U828 G845 C846 U847 C856 C857 U858 G859 U860 A861 G864 U868 G869 G880 G881 C884 C885 C886 A887 C888 C889 C893 A896 C897 C898 A899 A900 A901 C904 U905 G906 U907 A910 C914 C915 G916 A917 A918
G919 G932 G938 A941 G942 U943 G944 A945 G946 A953 C954 C955 U958 A959 A960 C961 C971 G972 A973 G974 C974A A980 A983 A984 C985 C986 G987 A988 G989 G993 C994 C995 A996 A1000 G1003 C1004 C1005 C1006 U1012 C1013 U1014 G1015 U1019 G1022 U1023 G1024
G1025 U1026 A1027 U1033 C1041 G1042 C1043 G1044 A1045 A1046 G1047 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 C1109 G1110 A1111 G1112 U1113 G1122 C1123 C1124 U1130 G1131 C1135 G1136 G1137 G1138 G1139 C1140 A1142A A1143 A1155 G1168 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 G1183 G1187 U1188 A1189 G1190 G1191 G1192 G1193 A1194
G1195 A1204 U1205 G1206 A1210 U1211 G1212 A1213 A1214 C1217 A1220 G1236 A1237 G1238 G1239 U1240 G1244 G1252 A1253 A1254 U1255 G1256 A1262 U1263 G1264 A1265 G1266 G1271 A1272 U1273 A1278 A1284 G1296 U1300 A1301 G1309 U1312 U1313 C1314 G1319 C1327 G1328 U1329
U1341 A1342 A1349 U1352 A1353 A1365 G1368 G1369 C1370 A1378 A1379 G1380 A1384 G1385 G1388 U1394 A1395 C1403 C1404 C1407 C1411 G1416 C1417 G1418 A1419 U1420 G1421 A1427 C1428 G1441 G1442 A1444A C1445 A1449 G1449A U1454 G1455 C1458 G1459 A1460 G1461
C1467 A1471 G1479 G1480 U1482 G1483 G1484 G1485 A1490 C1493 A1494 A1495 A1496 U1497 A1507 A1508 C1509 A1510 A1511 G1512 C1513 U1514 G1525 C1533 G1534 U1535 A1536 C1537 G1538 A1543 C1544 A1545 A1545A C1546 A1554 A1558 G1559 A1566 A1567 G1568 A1569 U1578 A1586 A1587 C1588 C1589
G1595 C1598 C1599 C1600 A1603 C1607 A1608 A1609 A1610 C1611 C1615 A1616 C1617 A1618 G1622 C1630A C1636 A1637 C1638 U1639 C1640 C1648 G1649 G1650 G1651 A1652 G1653 A1654 C1657 G1666 G1667 A1668 A1669 G1674 C1675 G1681 U1688 A1689 C1694 G1695 G1696 G1697 A1698 G1703
C1710 G1725 G1728 A1729 U1730 G1731 C1734 C1742 G1743 G1756 A1762 G1763 G1764 A1773 U1779 A1780 C1781 C1782 A1783 A1784 A1787 A1791 G1799 C1800 G1811 A1815 G1816 G1817 U1818 A1819 U1820 G1828 A1829 G1835 A1847 A1848 G1858 A1859 G1860 G1863 U1864
G1869 A1872 G1878 C1882 G1883 A1884 A1885 G1888 A1889 A1900 A1901 C1902 G1906 A1913 G1921 G1922 G1929 G1930 U1931 A1936 A1937 A1938 U1939 C1942 U1943 U1955 C1962 U1963 G1964 C1967 G1968 A1969 A1970 A1971 A1972 G1980 A1981 C1982 C1990 U1991 G1992 U1993 C1999
C2006 C2007 C2008 G2009 G2010 U2011 G2012 A2019 A2020 G2023 A2031 G2032 A2033 C2036 G2037 G2038 C2039 C2043 G2052 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 U2068 G2069 G2070 C2073 U2096 G2100 G2101 U2102 C2107 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120

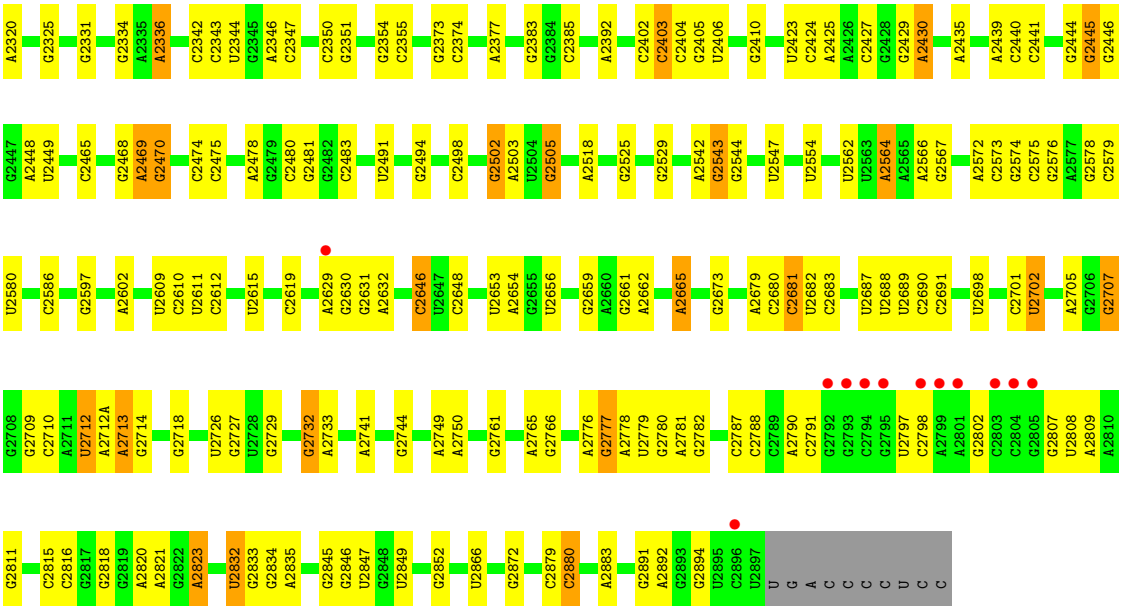


• Molecule 35: 23S rRNA

Chain YA:

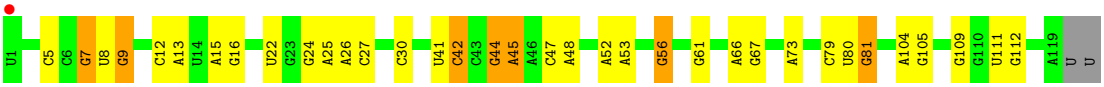



G612 U613 U614 G615 A616 G617 G618 A621 G622 U626 A627 G628 G629 G630 A633 C634 A637 G638 U639 C640 C645 A646 G647 G648 G649 C650 G651 C652 A653 A654 G654A G654B G G G C C G C A C G C G G C C C G654S A655 G662 A676
A685 G686 C693 U694 G695 G701 G702 G717 A722 G729 C730 A734 G742 G743 U747 G748 A752 C753 A764 G765 G775 G776 A782 A783 A784 G785 A788 A789 C790 C791 G792 A793 A800 G805 C806 U807 C812 A819 A820 U827 U828
A829 U833 C846 U847 C856 C857 U858 G859 U860 A861 A866 C867 U868 G869 A870 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 A896 C897 C898 A899 A900 A901 U907 A910 G916 A917 A918 G919 G932 A941 G942 U943 G944 A945 G946 G947 G948
G952 A953 G956 A957 U958 A959 A960 C961 A973 G974 C974A A983 A984 C985 C986 G987 A988 G989 C994 C995 A996 A1000 G1003 C1004 C1005 G1011 U1012 C1013 U1014 G1015 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 U1033 A1045 A1046 G1047 A1050 A1054 G1055 G1056 A1057
G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 G1074 C1075 C1076 A1077 U1078 C1079 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 G1093 U1094 A1095 A1096 U1097 A1103 C1104 U1105 G1106 G1110 A1111 G1112 U1113 G1122 C1123 C1124 G1125 A1126 A1129 U1130 G1131 C1135 G1136 G1137
G1138 G1139 C1140 U1141 U1142 A1142A C1153 G1173 A1174 U1175 G1176 A1177 C1178 C1179 G1187 U1188 A1189 G1190 G1195 G1203 A1204 U1205 G1206 A1210 U1211 A1214 C1218 G1219 A1220 G1238 G1239 U1240 A1246 G1250 C1251 G1252 A1253 G1256 G1264 A1265 G1266 G1271 A1272 C1290 C1291
G1296 U1300 A1301 C1306 G1309 G1310 C1327 G1328 U1329 G1338 U1341 A1342 G1343 G1344 A1349 U1352 A1353 G1364 A1365 A1366 A1367 G1368 G1369 C1370 A1379 A1384 G1385 C1386 U1391 U1394 A1395 C1407 C1408 C1411 G1416 A1419 U1420 G1421 A1427 C1428
A1434 A1444A A1449 G1449A U1454 G1455 C1458 G1459 A1460 G1461 C1467 A1471 G1478 G1479 G1483 G1484 G1485 A1490 C1493 U1497 A1507 A1508 C1509 A1510 A1511 U1514 U1523 G1530 G1534 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 A1545 A1558 G1559
C1565 A1566 A1567 G1568 A1569 U1578 A1579 A1580 G1581 C1585 A1586 G1595 C1598 C1607 A1608 A1609 C1612 C1617 A1618 G1622 A1631 C1638 U1639 C1640 C1648 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1662 G1667 A1668 G1674 C1675 G1682 A1689 U1693 C1694 G1695
A1698 G1699 A1700 G1725 G1728 A1729 U1730 G1731 A1732 G1733 C1742 G1743 C1754 A1755 G1756 A1762 G1763 G1764 G1769 A1773 U1779 A1780 C1781 A1784 A1791 G1799 C1800 G1801 U1808 G1811 G1816 G1817 U1818 A1819 U1820 G1824 A1825 G1826 C1827 G1828 A1829 G1835
A1847 A1853 G1858 A1859 G1869 A1872 G1878 C1881 C1882 G1883 A1884 G1888 A1889 A1890 G1891 G1896 A1900 A1901 C1902 G1906 A1919 G1929 A1937 A1938 U1939 U1940 U1955 U1956 C1957 C1958 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1980 A1981 C1982 U1991
G1992 U1993 C1996 C2006 G2010 U2011 G2012 A2013 A2014 A2015 U2016 A2019 A2020 C2021 U2022 G2023 A2031 G2032 A2033 U2034 G2035 C2039 C2043 A2054 C2055 G2056 A2059 A2060 G2061 A2062 C2065 U2068 G2069 G2070 A2071 G2072 C2073 U2076 G2080 G2090 G2093 U2099 G2100 G2101
U2102 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 C2138 C2146 G2147 G2148 G2149 U2150 G2151 A2158 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 A2176 C2177 C2178 C2179 G2187 C2188 U2189 G2190 G2191
G2192 A2198 G2210 G2211 A2212 U2213 G2215 A2225 U2233 G2234 G2235 G2238 G2239 U2243 G2246 U2249 G2253 C2258 A2269 C2275 C2283 A2287 A2288 G2289 G2290 U2291 C2292 C2293 C2294 C2295 A2298 G2304 G2307 G2308 A2309 A2310 A2311 U2312 G2315 G2318 G2319



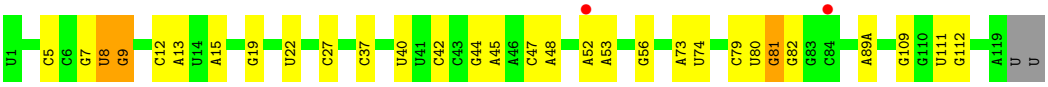
- Molecule 36: 5S rRNA

Chain RB:



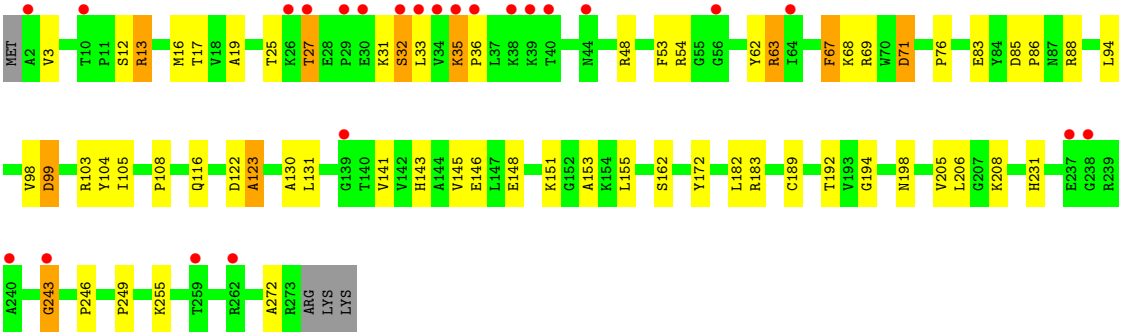
- Molecule 36: 5S rRNA

Chain YB:



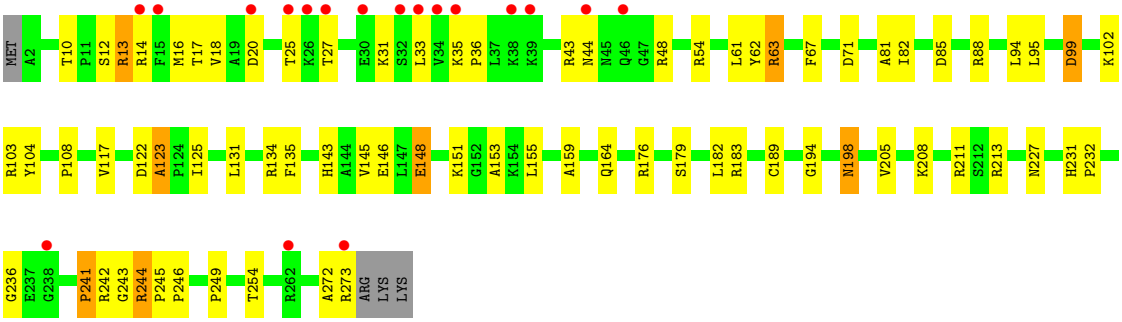
- Molecule 37: 50S ribosomal protein L2

Chain RD:



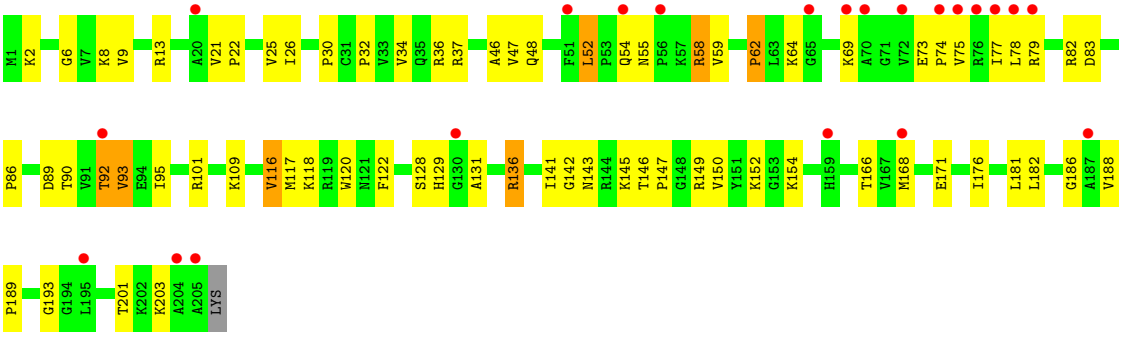
- Molecule 37: 50S ribosomal protein L2

Chain YD:



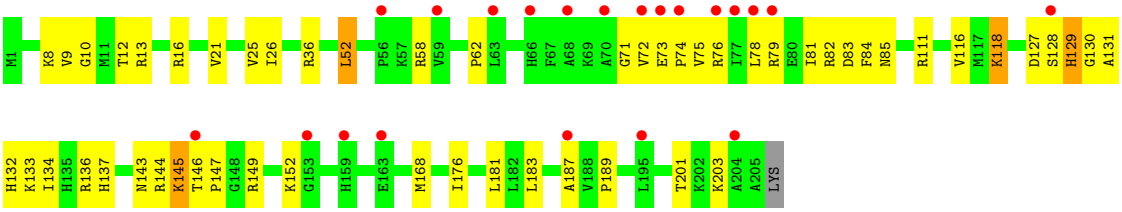
- Molecule 38: 50S ribosomal protein L3

Chain RE:



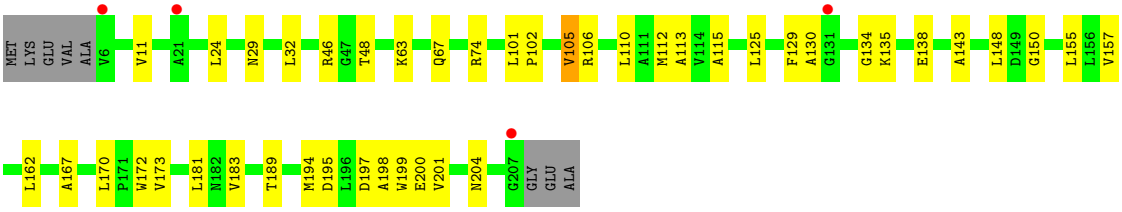
- Molecule 38: 50S ribosomal protein L3

Chain YE:



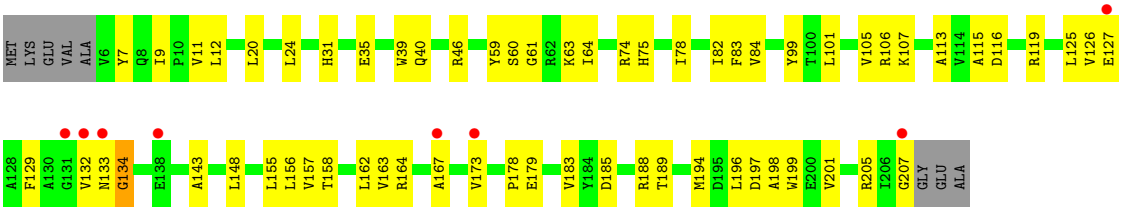
- Molecule 39: 50S ribosomal protein L4

Chain RF:



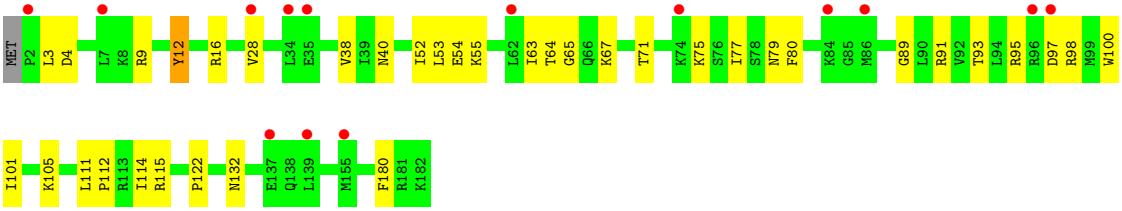
- Molecule 39: 50S ribosomal protein L4

Chain YF:



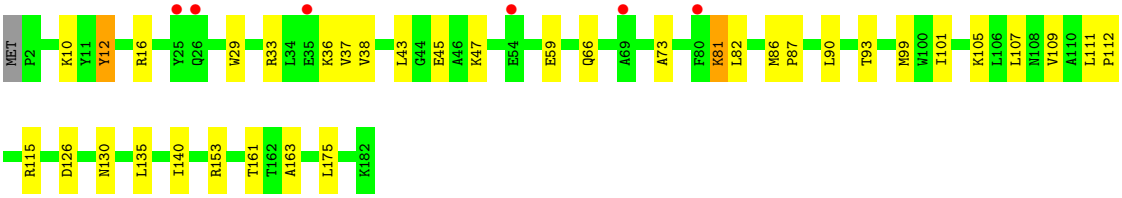
- Molecule 40: 50S ribosomal protein L5

Chain RG:



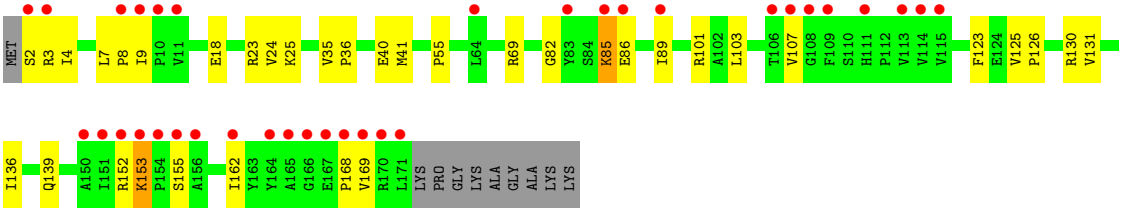
- Molecule 40: 50S ribosomal protein L5

Chain YG:



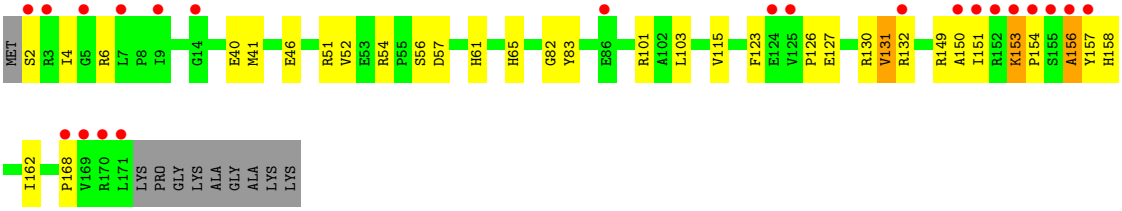
- Molecule 41: 50S ribosomal protein L6

Chain RH:



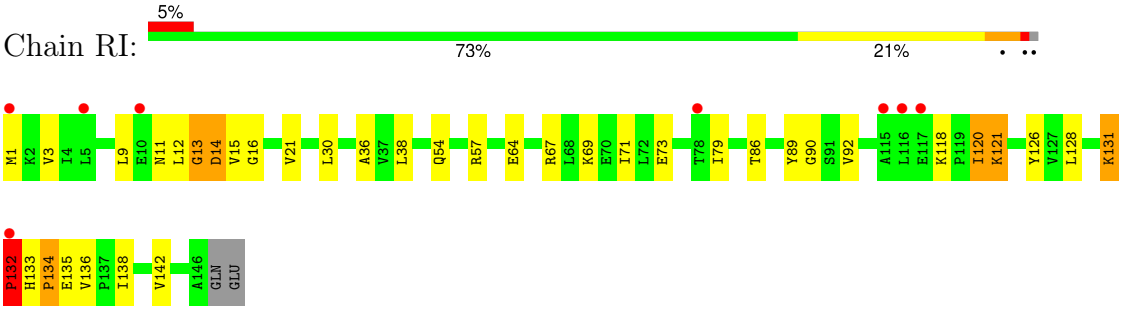
- Molecule 41: 50S ribosomal protein L6

Chain YH:



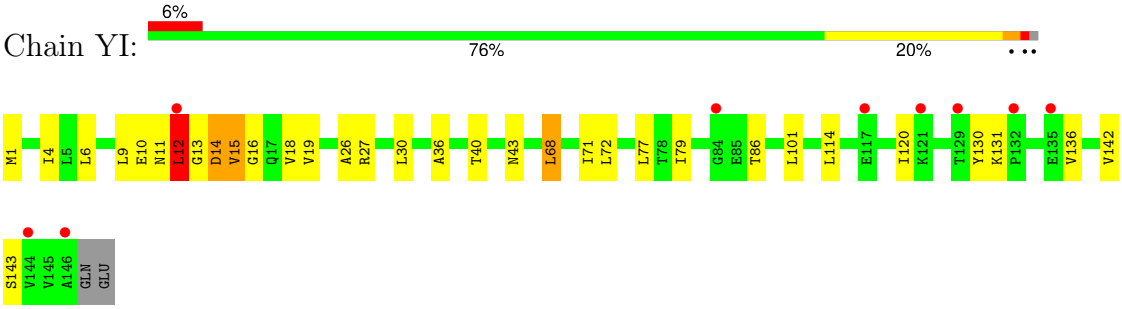
• Molecule 42: 50S ribosomal protein L9

Chain RI:



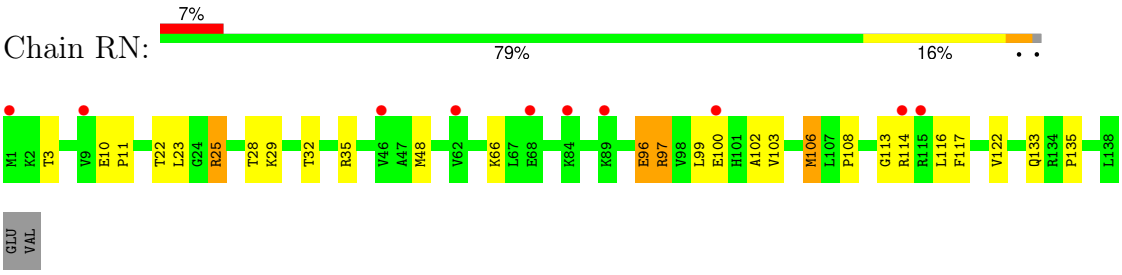
• Molecule 42: 50S ribosomal protein L9

Chain YI:



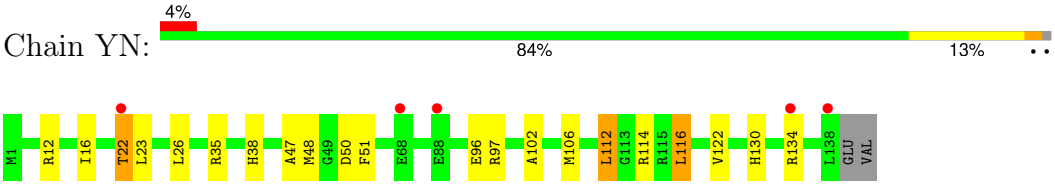
• Molecule 43: 50S ribosomal protein L13

Chain RN:



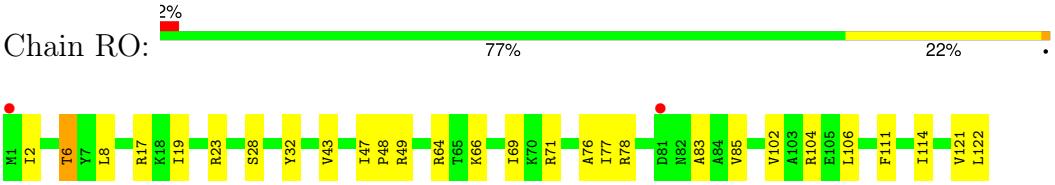
• Molecule 43: 50S ribosomal protein L13

Chain YN:



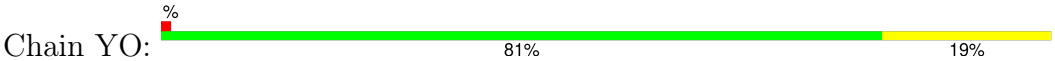
• Molecule 44: 50S ribosomal protein L14

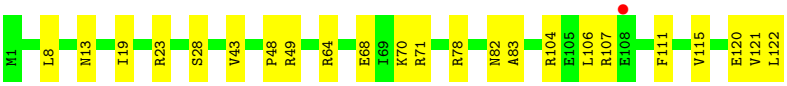
Chain RO:



• Molecule 44: 50S ribosomal protein L14

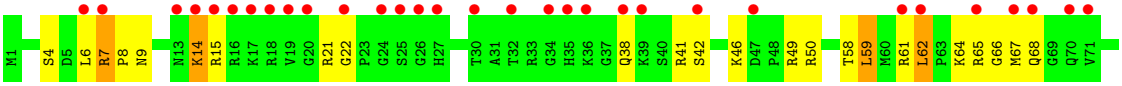
Chain YO:

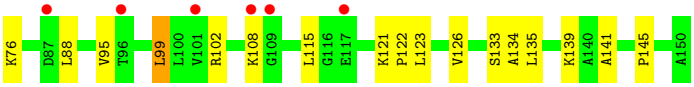




• Molecule 45: 50S ribosomal protein L15

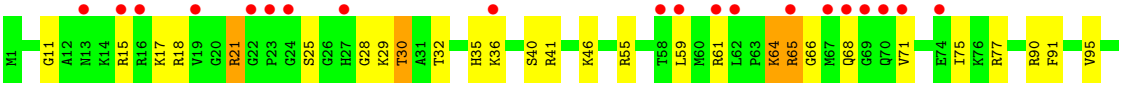
Chain RP:

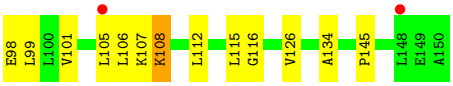




• Molecule 45: 50S ribosomal protein L15

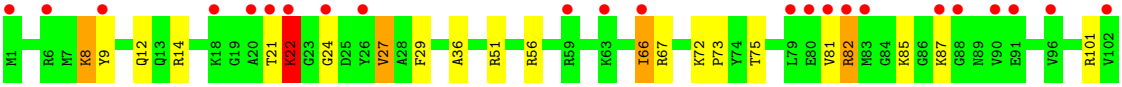
Chain YP:

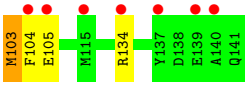




• Molecule 46: 50S ribosomal protein L16

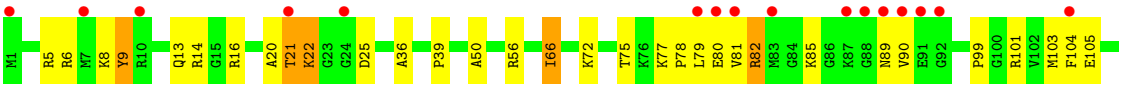
Chain RQ:

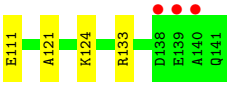




• Molecule 46: 50S ribosomal protein L16

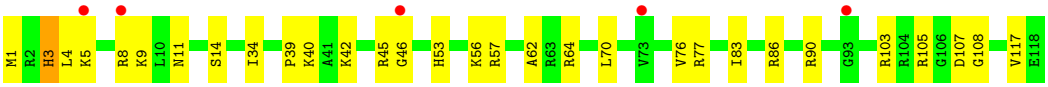
Chain YQ:





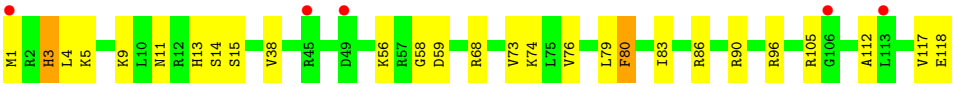
• Molecule 47: 50S ribosomal protein L17

Chain RR:



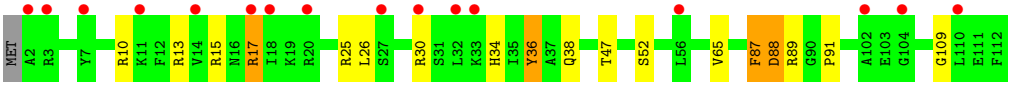
- Molecule 47: 50S ribosomal protein L17

Chain YR:



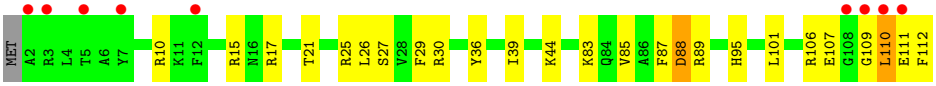
- Molecule 48: 50S ribosomal protein L18

Chain RS:



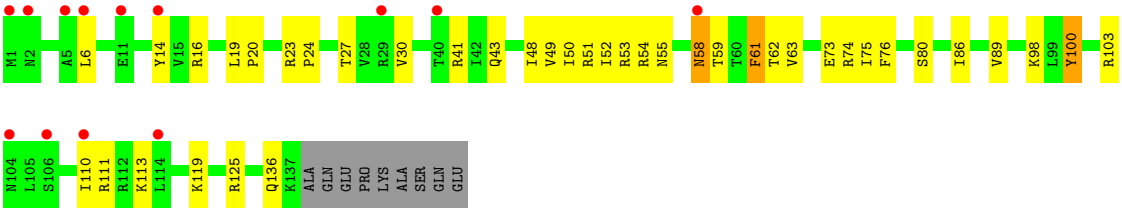
- Molecule 48: 50S ribosomal protein L18

Chain YS:



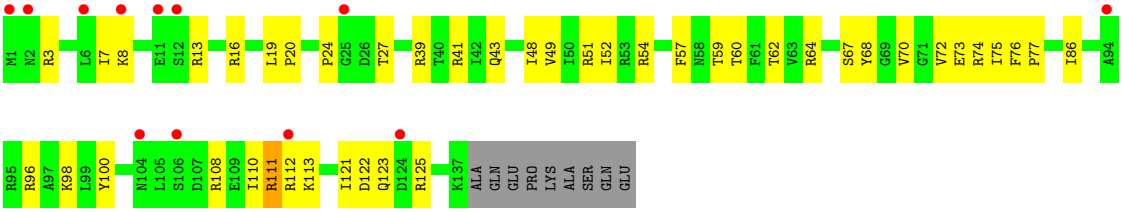
- Molecule 49: 50S ribosomal protein L19

Chain RT:



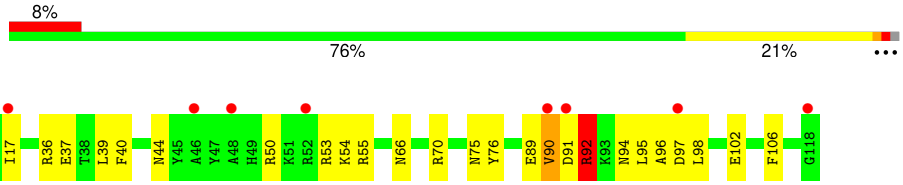
- Molecule 49: 50S ribosomal protein L19

Chain YT:



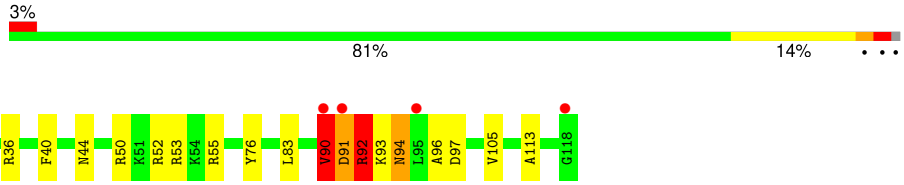
• Molecule 50: 50S ribosomal protein L20

Chain RU:



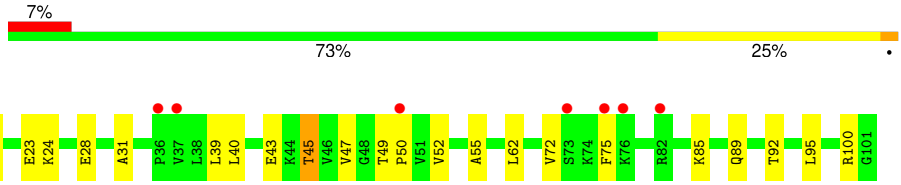
• Molecule 50: 50S ribosomal protein L20

Chain YU:



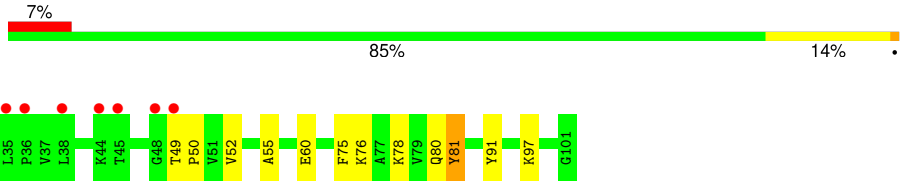
• Molecule 51: 50S ribosomal protein L21

Chain RV:



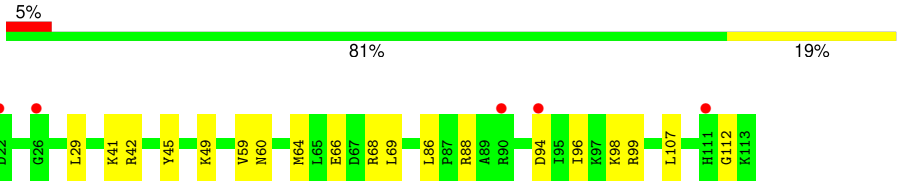
• Molecule 51: 50S ribosomal protein L21

Chain YV:



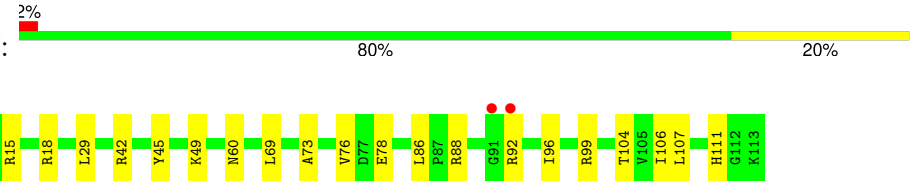
• Molecule 52: 50S ribosomal protein L22

Chain RW:



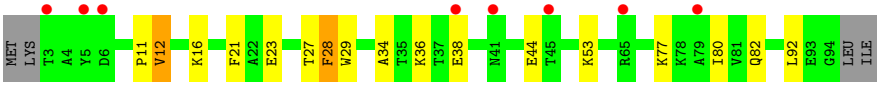
• Molecule 52: 50S ribosomal protein L22

Chain YW:



• Molecule 53: 50S ribosomal protein L23

Chain RX:

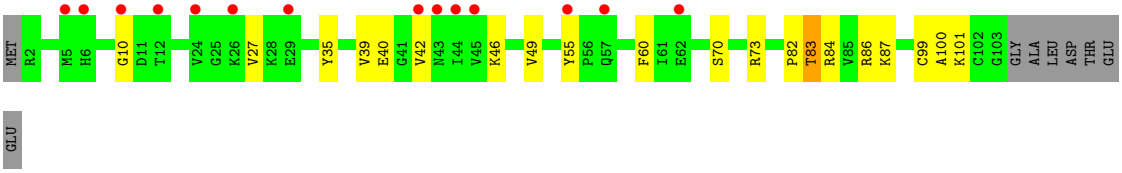


• Molecule 53: 50S ribosomal protein L23

Chain YX:

• Molecule 54: 50S ribosomal protein L24

Chain RY:

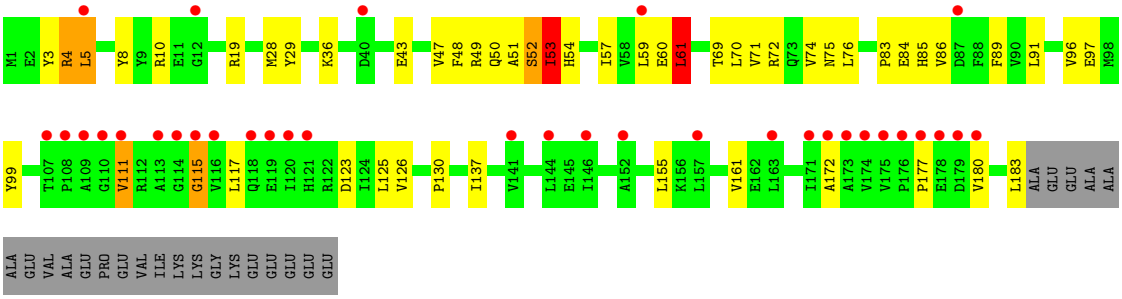


• Molecule 54: 50S ribosomal protein L24

Chain YY:

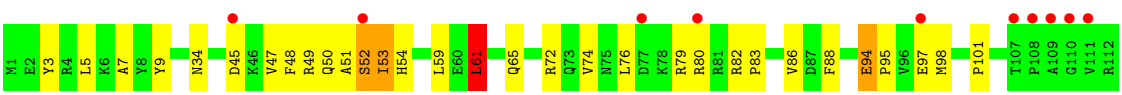
• Molecule 55: 50S ribosomal protein L25

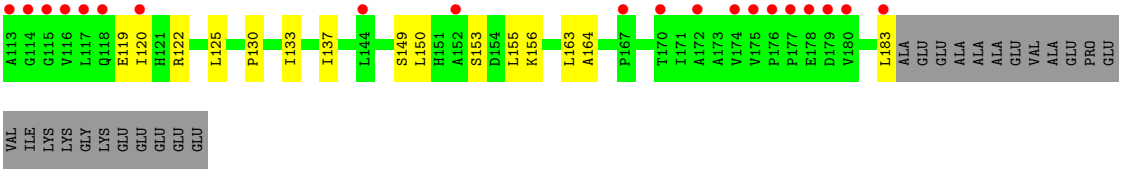
Chain RZ:



• Molecule 55: 50S ribosomal protein L25

Chain YZ:




A113 G114 G115 V116 L117 Q118 E119 I120 H121 R122 L125 P130 I133 I137 L144 S149 L150 H151 A152 S153 D154 L155 K156 L163 A164 P167 T170 I171 A172 A173 V174 V175 P176 P177 E178 D179 V180 L183
ALA GLU GLU ALA ALA ALA GLU VAL ALA GLU PRO GLU
VAL ILE LYS LYS GLY LYS GLU GLU GLU GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.38Å 449.76Å 619.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.10 49.74 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.74-3.10) 97.1 (49.74-3.10)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.225 , 0.266 0.225 , 0.266	Depositor DCC
R_{free} test set	52649 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	294981	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: PAR, ZN, MG, SF4

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	0.53	0/36098	0.49	7/56341 (0.0%)
1	XA	0.57	0/36101	0.50	6/56346 (0.0%)
2	QB	0.44	0/1959	0.96	9/2642 (0.3%)
2	XB	0.49	0/1959	0.94	3/2642 (0.1%)
3	QC	0.45	0/1629	0.89	4/2195 (0.2%)
3	XC	0.48	0/1629	0.83	3/2195 (0.1%)
4	QD	0.54	0/1704	0.87	5/2284 (0.2%)
4	XD	0.55	0/1704	0.90	9/2284 (0.4%)
5	QE	0.50	0/1171	0.91	3/1576 (0.2%)
5	XE	0.52	0/1171	0.84	2/1576 (0.1%)
6	QF	0.53	0/856	0.81	0/1154
6	XF	0.52	0/856	0.83	1/1154 (0.1%)
7	QG	0.45	0/1276	0.96	7/1709 (0.4%)
7	XG	0.47	0/1276	0.93	4/1709 (0.2%)
8	QH	0.46	0/1136	0.89	3/1527 (0.2%)
8	XH	0.53	0/1136	0.86	3/1527 (0.2%)
9	QI	0.50	0/1029	1.14	10/1379 (0.7%)
9	XI	0.49	0/1029	1.03	6/1379 (0.4%)
10	QJ	0.43	0/814	0.98	3/1095 (0.3%)
10	XJ	0.50	0/814	0.87	1/1095 (0.1%)
11	QK	0.51	0/900	0.86	1/1213 (0.1%)
11	XK	0.52	0/900	0.90	4/1213 (0.3%)
12	QL	0.54	0/991	1.05	12/1327 (0.9%)
12	XL	0.59	0/991	1.02	9/1327 (0.7%)
13	QM	0.50	0/974	1.10	6/1303 (0.5%)
13	XM	0.47	0/974	1.07	7/1303 (0.5%)
14	QN	0.49	0/501	0.90	0/664
14	XN	0.55	0/501	1.05	4/664 (0.6%)
15	QO	0.53	0/745	0.81	0/992
15	XO	0.49	0/745	0.81	0/992
16	QP	0.54	0/721	0.95	3/970 (0.3%)
16	XP	0.51	0/721	1.01	2/970 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.53	0/847	0.91	3/1131 (0.3%)
17	XQ	0.51	0/847	0.86	3/1131 (0.3%)
18	QR	0.57	0/579	1.05	2/768 (0.3%)
18	XR	0.56	0/579	0.95	3/768 (0.4%)
19	QS	0.46	0/689	1.06	5/926 (0.5%)
19	XS	0.56	0/689	1.25	12/926 (1.3%)
20	QT	0.52	0/765	0.99	3/1007 (0.3%)
20	XT	0.47	0/765	1.06	4/1007 (0.4%)
21	QU	0.52	0/221	0.82	0/288
21	XU	0.60	0/221	0.93	1/288 (0.3%)
22	QV	0.48	0/1832	0.46	0/2855
22	XV	0.55	0/1832	0.43	0/2855
23	QX	0.41	0/446	0.54	0/695
23	XX	0.45	0/446	0.55	0/695
24	QY	0.38	0/1790	0.47	0/2789
24	XY	0.39	0/1790	0.46	0/2789
25	R0	0.58	0/657	0.89	2/874 (0.2%)
25	Y0	0.64	0/657	0.94	2/874 (0.2%)
26	R1	0.61	0/770	1.06	4/1022 (0.4%)
26	Y1	0.64	0/770	0.98	3/1022 (0.3%)
27	R2	0.56	0/583	0.98	2/771 (0.3%)
27	Y2	0.58	0/583	1.04	4/771 (0.5%)
28	R3	0.45	0/474	0.81	0/635
28	Y3	0.56	0/474	0.82	0/635
29	R4	0.57	0/594	1.44	10/795 (1.3%)
29	Y4	0.50	0/594	1.55	14/795 (1.8%)
30	R5	0.60	0/473	1.25	6/639 (0.9%)
30	Y5	0.68	0/473	1.01	2/639 (0.3%)
31	R6	0.68	0/431	1.60	7/575 (1.2%)
31	Y6	0.67	0/431	1.57	9/575 (1.6%)
32	R7	0.68	0/438	0.86	0/575
32	Y7	0.71	0/438	0.98	3/575 (0.5%)
33	R8	0.66	0/525	1.21	9/691 (1.3%)
33	Y8	0.80	1/525 (0.2%)	1.22	8/691 (1.2%)
34	R9	0.57	0/310	0.71	0/407
34	Y9	0.62	0/310	0.81	0/407
35	RA	0.62	0/69521	0.52	15/108529 (0.0%)
35	YA	0.70	0/69543	0.54	17/108563 (0.0%)
36	RB	0.50	0/2878	0.49	0/4490
36	YB	0.62	0/2878	0.51	0/4490
37	RD	0.67	0/2165	1.03	12/2919 (0.4%)
37	YD	0.74	0/2165	1.03	12/2919 (0.4%)
38	RE	0.62	1/1601 (0.1%)	1.14	16/2160 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YE	0.69	0/1601	1.17	12/2160 (0.6%)
39	RF	0.59	0/1620	0.95	4/2194 (0.2%)
39	YF	0.65	0/1620	0.98	7/2194 (0.3%)
40	RG	0.49	0/1499	1.02	10/2016 (0.5%)
40	YG	0.55	0/1499	0.97	4/2016 (0.2%)
41	RH	0.45	0/1332	1.13	9/1802 (0.5%)
41	YH	0.59	0/1332	1.12	14/1802 (0.8%)
42	RI	0.57	2/1151 (0.2%)	1.32	21/1558 (1.3%)
42	YI	0.50	0/1151	1.16	14/1558 (0.9%)
43	RN	0.57	0/1131	1.05	7/1525 (0.5%)
43	YN	0.62	0/1131	1.02	8/1525 (0.5%)
44	RO	0.60	0/943	0.86	1/1269 (0.1%)
44	YO	0.67	0/943	0.98	1/1269 (0.1%)
45	RP	0.59	0/1162	1.20	7/1544 (0.5%)
45	YP	0.65	0/1162	1.18	12/1544 (0.8%)
46	RQ	0.59	0/1143	1.14	9/1527 (0.6%)
46	YQ	0.65	0/1143	1.18	10/1527 (0.7%)
47	RR	0.63	0/982	0.95	4/1312 (0.3%)
47	YR	0.65	0/982	1.02	5/1312 (0.4%)
48	RS	0.54	0/892	1.21	10/1187 (0.8%)
48	YS	0.58	0/892	1.12	6/1187 (0.5%)
49	RT	0.60	0/1155	1.06	13/1542 (0.8%)
49	YT	0.62	0/1155	1.14	11/1542 (0.7%)
50	RU	0.59	0/982	1.11	10/1306 (0.8%)
50	YU	0.66	0/982	1.05	8/1306 (0.6%)
51	RV	0.54	0/790	1.04	3/1057 (0.3%)
51	YV	0.67	0/790	1.10	4/1057 (0.4%)
52	RW	0.62	0/911	0.92	1/1220 (0.1%)
52	YW	0.63	0/911	0.88	1/1220 (0.1%)
53	RX	0.59	0/739	0.96	4/993 (0.4%)
53	YX	0.65	0/739	0.91	2/993 (0.2%)
54	RY	0.53	0/798	0.97	3/1064 (0.3%)
54	YY	0.63	0/798	1.02	4/1064 (0.4%)
55	RZ	0.46	0/1493	1.07	12/2026 (0.6%)
55	YZ	0.53	0/1493	1.08	8/2026 (0.4%)
All	All	0.61	4/319657 (0.0%)	0.69	589/478147 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
48	RS	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	RI	133	HIS	C-N	5.84	1.47	1.33
38	RE	136	ARG	C-N	-5.40	1.23	1.33
42	RI	134	PRO	N-CD	-5.12	1.40	1.47
33	Y8	23	VAL	CB-CG1	-5.00	1.36	1.52

The worst 5 of 589 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y4	39	CYS	N-CA-C	-12.70	95.90	112.41
13	XM	7	VAL	N-CA-C	-12.60	101.18	113.53
26	R1	75	GLU	N-CA-C	-11.51	100.25	114.75
39	RF	199	TRP	N-CA-C	-11.32	99.96	113.88
35	RA	1992	G	C2'-C3'-O3'	11.15	126.23	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	RS	17	ARG	Sidechain

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	16277	208	0
1	XA	32249	0	16279	180	0
2	QB	1924	0	1975	28	0
2	XB	1924	0	1975	29	0
3	QC	1605	0	1668	37	0
3	XC	1605	0	1668	19	0
4	QD	1674	0	1718	29	0
4	XD	1674	0	1718	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	QE	1155	0	1213	20	0
5	XE	1155	0	1213	8	0
6	QF	843	0	857	11	0
6	XF	843	0	857	8	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	8	0
8	QH	1116	0	1177	13	0
8	XH	1116	0	1177	20	0
9	QI	1010	0	1037	23	0
9	XI	1010	0	1037	24	0
10	QJ	801	0	849	19	0
10	XJ	801	0	849	15	0
11	QK	885	0	904	17	0
11	XK	885	0	904	9	0
12	QL	975	0	1062	17	0
12	XL	975	0	1062	16	0
13	QM	964	0	1034	35	0
13	XM	964	0	1034	16	0
14	QN	492	0	529	14	0
14	XN	492	0	529	5	0
15	QO	734	0	771	7	0
15	XO	734	0	771	4	0
16	QP	705	0	725	14	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	12	0
17	XQ	834	0	904	10	0
18	QR	574	0	644	13	0
18	XR	574	0	644	8	0
19	QS	674	0	699	21	0
19	XS	674	0	699	14	0
20	QT	763	0	860	6	0
20	XT	763	0	861	17	0
21	QU	217	0	234	5	0
21	XU	217	0	234	1	0
22	QV	1640	0	837	5	0
22	XV	1640	0	837	4	0
23	QX	396	0	197	1	0
23	XX	396	0	197	3	0
24	QY	1602	0	811	23	0
24	XY	1602	0	811	10	0
25	R0	648	0	672	15	0
25	Y0	648	0	672	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	R1	763	0	848	12	0
26	Y1	763	0	848	11	0
27	R2	581	0	629	14	0
27	Y2	581	0	629	11	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	4	0
29	R4	581	0	577	17	0
29	Y4	581	0	577	17	0
30	R5	459	0	480	9	0
30	Y5	459	0	480	11	0
31	R6	424	0	450	11	0
31	Y6	424	0	450	9	0
32	R7	430	0	480	7	0
32	Y7	430	0	480	7	0
33	R8	517	0	582	18	0
33	Y8	517	0	582	33	0
34	R9	307	0	335	5	0
34	Y9	307	0	335	6	0
35	RA	62071	0	31280	358	0
35	YA	62091	0	31290	306	0
36	RB	2573	0	1306	16	0
36	YB	2573	0	1306	13	0
37	RD	2115	0	2195	43	0
37	YD	2115	0	2195	53	0
38	RE	1568	0	1634	46	0
38	YE	1568	0	1634	32	0
39	RF	1585	0	1632	24	0
39	YF	1585	0	1632	32	0
40	RG	1474	0	1535	21	0
40	YG	1474	0	1535	19	0
41	RH	1307	0	1382	22	0
41	YH	1307	0	1382	20	0
42	RI	1136	0	1223	12	0
42	YI	1136	0	1223	12	0
43	RN	1104	0	1180	24	0
43	YN	1104	0	1180	9	0
44	RO	933	0	996	23	0
44	YO	933	0	996	19	0
45	RP	1145	0	1227	30	0
45	YP	1145	0	1227	28	0
46	RQ	1122	0	1179	25	0
46	YQ	1122	0	1177	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	RR	968	0	1033	19	0
47	YR	968	0	1033	17	0
48	RS	882	0	943	9	0
48	YS	882	0	943	16	0
49	RT	1141	0	1202	29	0
49	YT	1141	0	1202	24	0
50	RU	964	0	1022	22	0
50	YU	964	0	1022	20	0
51	RV	779	0	852	18	0
51	YV	779	0	852	12	0
52	RW	900	0	964	15	0
52	YW	900	0	964	18	0
53	RX	725	0	778	9	0
53	YX	725	0	778	9	0
54	RY	785	0	878	14	0
54	YY	785	0	878	9	0
55	RZ	1461	0	1493	28	0
55	YZ	1461	0	1493	32	0
56	QA	73	0	0	0	0
56	QF	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	1	0	0	0	0
56	QX	2	0	0	0	0
56	R0	1	0	0	0	0
56	R5	1	0	0	0	0
56	R8	1	0	0	0	0
56	R9	1	0	0	0	0
56	RA	281	0	0	0	0
56	RB	4	0	0	0	0
56	RD	1	0	0	0	0
56	RE	4	0	0	0	0
56	RF	1	0	0	0	0
56	RP	3	0	0	0	0
56	RR	1	0	0	0	0
56	RU	1	0	0	0	0
56	XA	91	0	0	0	0
56	XF	1	0	0	0	0
56	XM	1	0	0	0	0
56	XV	2	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	Y2	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	2	0	0	0	0
56	Y8	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YA	347	0	0	0	0
56	YB	6	0	0	0	0
56	YE	3	0	0	0	0
56	YN	1	0	0	0	0
56	YP	3	0	0	0	0
56	YQ	3	0	0	0	0
56	YR	1	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	0	0
57	XA	42	0	45	4	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	294981	0	199667	2249	0

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 5.

The worst 5 of 2249 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)
55:YZ:94:GLU:CG	55:YZ:95:PRO:HD3	1.74	1.18
35:RA:1138:G:H21	43:RN:106:MET:HE1	1.05	1.09
35:RA:2055:C:H5'	35:RA:2056:G:H5"	1.35	1.07
55:YZ:94:GLU:HB3	55:YZ:95:PRO:CD	1.85	1.07
19:QS:10:PHE:HB2	19:QS:16:LEU:HD11	1.34	1.06

There are no symmetry-related clashes.

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%)	206 (88%)	27 (12%)	2 (1%)	14	44
2	XB	235/256 (92%)	207 (88%)	28 (12%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	QD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24	57
4	XD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24	57
5	QE	149/162 (92%)	138 (93%)	11 (7%)	0	100	100
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	18	49
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	18	49
8	QH	136/138 (99%)	121 (89%)	15 (11%)	0	100	100
8	XH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	QI	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
9	XI	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	47
10	QJ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	XJ	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
12	QL	123/131 (94%)	107 (87%)	15 (12%)	1 (1%)	16	47
12	XL	123/131 (94%)	108 (88%)	10 (8%)	5 (4%)	2	13
13	QM	119/126 (94%)	99 (83%)	19 (16%)	1 (1%)	16	47
13	XM	119/126 (94%)	102 (86%)	17 (14%)	0	100	100
14	QN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	30
15	QO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	XO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	QP	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	8 (10%)	3 (4%)	2	15
20	QT	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	3	18
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
25	R0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
26	R1	95/98 (97%)	80 (84%)	12 (13%)	3 (3%)	3	18
26	Y1	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	5	25
27	R2	67/72 (93%)	59 (88%)	7 (10%)	1 (2%)	8	32
27	Y2	67/72 (93%)	60 (90%)	7 (10%)	0	100	100
28	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	R4	69/71 (97%)	44 (64%)	18 (26%)	7 (10%)	0	3
29	Y4	69/71 (97%)	41 (59%)	26 (38%)	2 (3%)	3	19
30	R5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
30	Y5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
31	R6	47/54 (87%)	31 (66%)	13 (28%)	3 (6%)	1	6
31	Y6	47/54 (87%)	32 (68%)	12 (26%)	3 (6%)	1	6
32	R7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
32	Y7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	R8	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	3	18
33	Y8	62/65 (95%)	51 (82%)	10 (16%)	1 (2%)	7	30
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	35 (100%)	0	0	100	100
37	RD	270/276 (98%)	244 (90%)	21 (8%)	5 (2%)	6	27
37	YD	270/276 (98%)	243 (90%)	26 (10%)	1 (0%)	30	61
38	RE	203/206 (98%)	165 (81%)	35 (17%)	3 (2%)	8	32
38	YE	203/206 (98%)	168 (83%)	30 (15%)	5 (2%)	4	21
39	RF	200/210 (95%)	184 (92%)	13 (6%)	3 (2%)	8	32
39	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	12	41
40	RG	179/182 (98%)	158 (88%)	21 (12%)	0	100	100
40	YG	179/182 (98%)	156 (87%)	22 (12%)	1 (1%)	21	52
41	RH	168/180 (93%)	134 (80%)	30 (18%)	4 (2%)	4	22
41	YH	168/180 (93%)	140 (83%)	26 (16%)	2 (1%)	10	37
42	RI	144/148 (97%)	115 (80%)	21 (15%)	8 (6%)	1	8
42	YI	144/148 (97%)	116 (81%)	22 (15%)	6 (4%)	2	13
43	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	18	49
43	YN	136/140 (97%)	117 (86%)	18 (13%)	1 (1%)	18	49
44	RO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
44	YO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	47
45	RP	148/150 (99%)	117 (79%)	27 (18%)	4 (3%)	4	20
45	YP	148/150 (99%)	118 (80%)	28 (19%)	2 (1%)	9	34
46	RQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	18	49
46	YQ	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	3	19
47	RR	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	7	30
47	YR	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	7	30
48	RS	109/112 (97%)	91 (84%)	15 (14%)	3 (3%)	4	20
48	YS	109/112 (97%)	92 (84%)	16 (15%)	1 (1%)	14	44
49	RT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	YT	135/146 (92%)	117 (87%)	17 (13%)	1 (1%)	18	49
50	RU	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	14	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	YU	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	4	21
51	RV	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	6	25
51	YV	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	12	41
52	RW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
52	YW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
53	RX	90/96 (94%)	81 (90%)	9 (10%)	0	100	100
53	YX	90/96 (94%)	82 (91%)	7 (8%)	1 (1%)	11	39
54	RY	100/110 (91%)	91 (91%)	9 (9%)	0	100	100
54	YY	100/110 (91%)	94 (94%)	6 (6%)	0	100	100
55	RZ	181/206 (88%)	152 (84%)	24 (13%)	5 (3%)	4	20
55	YZ	181/206 (88%)	158 (87%)	19 (10%)	4 (2%)	5	24
All	All	11470/12126 (95%)	10176 (89%)	1168 (10%)	126 (1%)	11	39

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	5	ILE
26	R1	92	LYS
29	R4	24	THR
29	R4	43	TYR
31	R6	8	LYS

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%)	205 (100%)	0	100	100
2	XB	205/220 (93%)	205 (100%)	0	100	100
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	173 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	173/181 (96%)	173 (100%)	0	100	100
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	119/119 (100%)	119 (100%)	0	100	100
8	XH	119/119 (100%)	119 (100%)	0	100	100
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	98/99 (99%)	98 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	89/92 (97%)	89 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	90/99 (91%)	90 (100%)	0	100	100
12	QL	104/108 (96%)	104 (100%)	0	100	100
12	XL	104/108 (96%)	104 (100%)	0	100	100
13	QM	97/101 (96%)	96 (99%)	1 (1%)	68	79
13	XM	97/101 (96%)	97 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	73/80 (91%)	71 (97%)	2 (3%)	39	67
19	XS	73/80 (91%)	73 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
25	R0	65/67 (97%)	65 (100%)	0	100	100
25	Y0	65/67 (97%)	65 (100%)	0	100	100
26	R1	82/83 (99%)	82 (100%)	0	100	100
26	Y1	82/83 (99%)	82 (100%)	0	100	100
27	R2	64/67 (96%)	64 (100%)	0	100	100
27	Y2	64/67 (96%)	64 (100%)	0	100	100
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	51/52 (98%)	51 (100%)	0	100	100
29	R4	63/63 (100%)	63 (100%)	0	100	100
29	Y4	63/63 (100%)	63 (100%)	0	100	100
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	51/52 (98%)	51 (100%)	0	100	100
31	R6	48/52 (92%)	48 (100%)	0	100	100
31	Y6	48/52 (92%)	48 (100%)	0	100	100
32	R7	42/42 (100%)	42 (100%)	0	100	100
32	Y7	42/42 (100%)	42 (100%)	0	100	100
33	R8	54/55 (98%)	54 (100%)	0	100	100
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	30	61
34	R9	34/34 (100%)	34 (100%)	0	100	100
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	214 (100%)	0	100	100
37	YD	214/218 (98%)	214 (100%)	0	100	100
38	RE	165/166 (99%)	165 (100%)	0	100	100
38	YE	165/166 (99%)	165 (100%)	0	100	100
39	RF	161/166 (97%)	161 (100%)	0	100	100
39	YF	161/166 (97%)	161 (100%)	0	100	100
40	RG	155/156 (99%)	155 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	YG	155/156 (99%)	155 (100%)	0	100	100
41	RH	142/148 (96%)	142 (100%)	0	100	100
41	YH	142/148 (96%)	142 (100%)	0	100	100
42	RI	122/124 (98%)	122 (100%)	0	100	100
42	YI	122/124 (98%)	122 (100%)	0	100	100
43	RN	117/119 (98%)	116 (99%)	1 (1%)	70	80
43	YN	117/119 (98%)	117 (100%)	0	100	100
44	RO	100/100 (100%)	99 (99%)	1 (1%)	68	79
44	YO	100/100 (100%)	100 (100%)	0	100	100
45	RP	116/116 (100%)	116 (100%)	0	100	100
45	YP	116/116 (100%)	116 (100%)	0	100	100
46	RQ	111/111 (100%)	111 (100%)	0	100	100
46	YQ	111/111 (100%)	111 (100%)	0	100	100
47	RR	101/101 (100%)	101 (100%)	0	100	100
47	YR	101/101 (100%)	101 (100%)	0	100	100
48	RS	87/88 (99%)	87 (100%)	0	100	100
48	YS	87/88 (99%)	87 (100%)	0	100	100
49	RT	120/127 (94%)	120 (100%)	0	100	100
49	YT	120/127 (94%)	120 (100%)	0	100	100
50	RU	93/94 (99%)	93 (100%)	0	100	100
50	YU	93/94 (99%)	93 (100%)	0	100	100
51	RV	82/82 (100%)	82 (100%)	0	100	100
51	YV	82/82 (100%)	82 (100%)	0	100	100
52	RW	92/92 (100%)	92 (100%)	0	100	100
52	YW	92/92 (100%)	92 (100%)	0	100	100
53	RX	74/78 (95%)	74 (100%)	0	100	100
53	YX	74/78 (95%)	74 (100%)	0	100	100
54	RY	85/91 (93%)	85 (100%)	0	100	100
54	YY	85/91 (93%)	85 (100%)	0	100	100
55	RZ	162/179 (90%)	162 (100%)	0	100	100
55	YZ	162/179 (90%)	162 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9688/10064 (96%)	9681 (100%)	7 (0%)	88 90

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	RN	106	MET
44	RO	6	THR
33	Y8	65	GLU
33	Y8	62	LEU
19	QS	11	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
8	XH	78	GLN
25	Y0	12	ASN
9	XI	31	GLN
13	XM	62	ASN
29	Y4	47	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	271 (18%)	29 (1%)
1	XA	1498/1522 (98%)	282 (18%)	27 (1%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	14 (18%)	0
23	QX	17/19 (89%)	8 (47%)	1 (5%)
23	XX	17/19 (89%)	8 (47%)	1 (5%)
24	QY	74/76 (97%)	28 (37%)	0
24	XY	74/76 (97%)	25 (33%)	0
35	RA	2879/2915 (98%)	591 (20%)	47 (1%)
35	YA	2880/2915 (98%)	589 (20%)	44 (1%)
36	RB	119/122 (97%)	21 (17%)	1 (0%)
36	YB	119/122 (97%)	18 (15%)	0
All	All	9327/9462 (98%)	1870 (20%)	150 (1%)

5 of 1870 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	31	G
1	QA	32	A
1	QA	39	G
1	QA	48	C

5 of 150 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	YA	503	A
35	YA	2566	A
35	YA	752	A
35	YA	1210	A
35	RA	752	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 855 ligands modelled in this entry, 851 are monoatomic - leaving 4 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	SF4	XD	501	4	0,12,12	-	-	-		
58	SF4	QD	501	-	0,12,12	-	-	-		
57	PAR	XA	1670	-	44,45,45	0.86	1 (2%)	63,67,67	1.27	6 (9%)
57	PAR	QA	1663	-	44,45,45	0.81	0	63,67,67	1.26	7 (11%)

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	SF4	XD	501	4	-	-	0/6/5/5
58	SF4	QD	501	-	-	-	0/6/5/5
57	PAR	XA	1670	-	-	4/18/94/94	0/4/4/4
57	PAR	QA	1663	-	-	3/18/94/94	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	XA	1670	PAR	C24-N24	-2.02	1.44	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	QA	1663	PAR	C13-O52-C52	-3.35	110.03	117.98
57	XA	1670	PAR	C13-O52-C52	-3.01	110.85	117.98
57	XA	1670	PAR	O11-C42-C32	-2.97	102.08	109.18
57	QA	1663	PAR	O62-C62-C12	-2.58	105.08	109.90
57	QA	1663	PAR	O33-C33-C23	-2.57	103.05	111.32

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1663	PAR	O54-C54-C64-N64
57	XA	1670	PAR	O54-C14-O33-C33
57	QA	1663	PAR	O51-C51-C61-O61
57	QA	1663	PAR	C23-C33-O33-C14
57	XA	1670	PAR	C43-C33-O33-C14

There are no ring outliers.

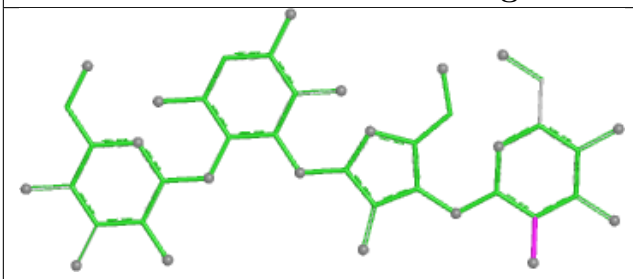
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XA	1670	PAR	4	0

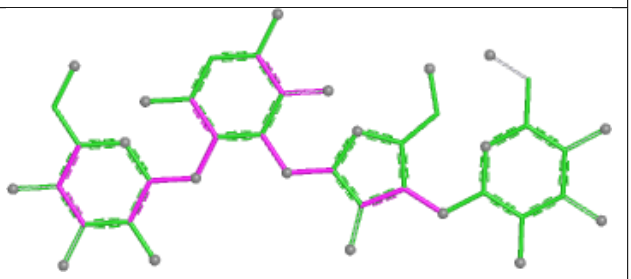
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

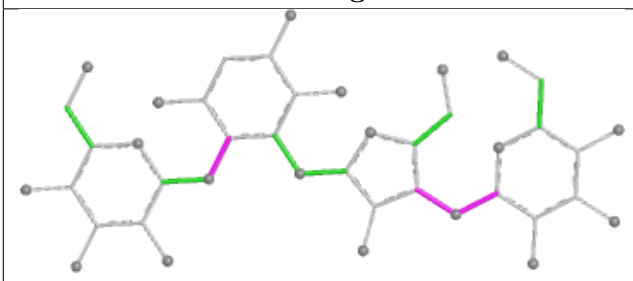
Ligand PAR XA 1670



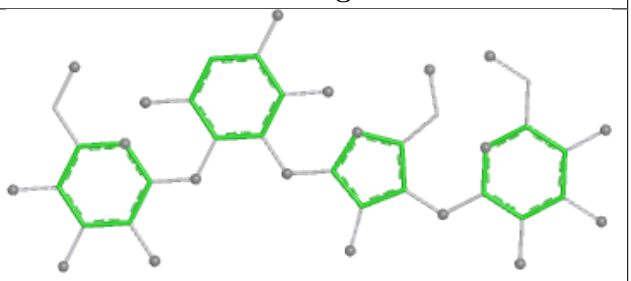
Bond lengths



Bond angles

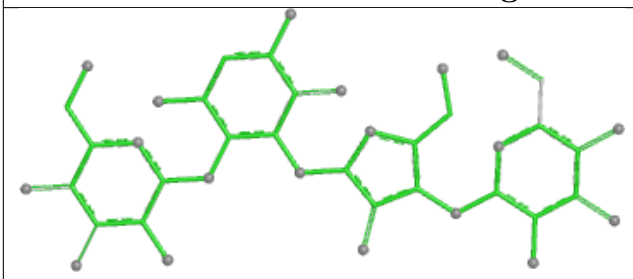


Torsions

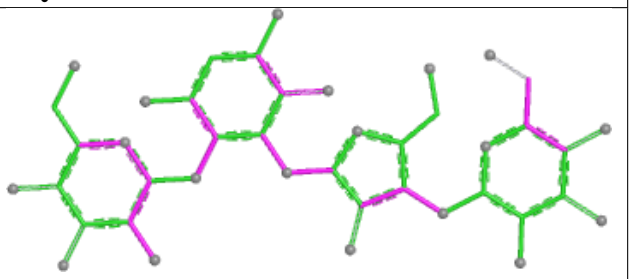


Rings

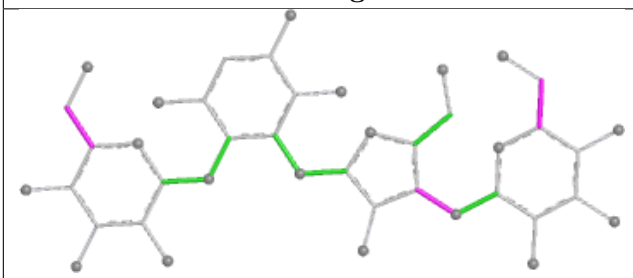
Ligand PAR QA 1663



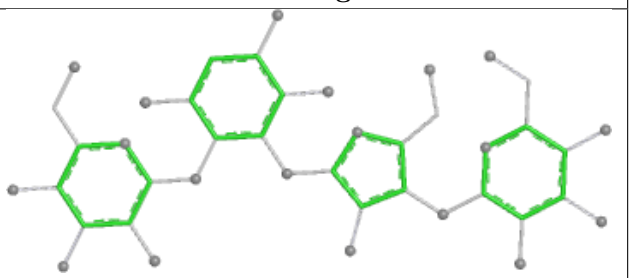
Bond lengths



Bond angles



Torsions



Rings

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%)	0.19	31 (2%)	63	42	53, 93, 175, 270	0
1	XA	1500/1522 (98%)	0.08	20 (1%)	75	56	48, 82, 158, 266	0
2	QB	237/256 (92%)	0.78	20 (8%)	17	9	86, 128, 167, 198	0
2	XB	237/256 (92%)	0.57	11 (4%)	37	20	72, 111, 154, 176	0
3	QC	205/239 (85%)	0.72	18 (8%)	15	9	90, 129, 158, 170	0
3	XC	205/239 (85%)	0.49	13 (6%)	26	14	68, 101, 144, 170	0
4	QD	208/209 (99%)	0.52	11 (5%)	32	17	62, 89, 113, 137	0
4	XD	208/209 (99%)	0.76	21 (10%)	12	6	64, 94, 123, 150	0
5	QE	151/162 (93%)	0.53	9 (5%)	27	15	78, 105, 133, 152	0
5	XE	151/162 (93%)	0.26	6 (3%)	42	23	55, 82, 115, 150	0
6	QF	101/101 (100%)	0.30	2 (1%)	65	44	55, 85, 114, 173	0
6	XF	101/101 (100%)	0.26	2 (1%)	65	44	64, 90, 115, 138	0
7	QG	155/156 (99%)	0.79	11 (7%)	22	12	92, 115, 160, 177	0
7	XG	155/156 (99%)	0.48	6 (3%)	43	24	72, 98, 135, 156	0
8	QH	138/138 (100%)	0.85	14 (10%)	12	6	72, 102, 128, 145	0
8	XH	138/138 (100%)	0.58	6 (4%)	40	22	58, 88, 117, 138	0
9	QI	127/128 (99%)	1.42	30 (23%)	2	1	101, 129, 153, 172	0
9	XI	127/128 (99%)	1.05	19 (14%)	5	3	64, 111, 147, 159	0
10	QJ	99/105 (94%)	1.52	29 (29%)	1	1	111, 138, 174, 179	0
10	XJ	99/105 (94%)	1.12	12 (12%)	8	5	66, 119, 157, 170	0
11	QK	119/129 (92%)	0.81	8 (6%)	24	13	62, 97, 132, 163	0
11	XK	119/129 (92%)	0.75	8 (6%)	24	13	59, 85, 126, 147	0
12	QL	125/131 (95%)	1.15	20 (16%)	5	2	62, 90, 129, 179	0
12	XL	125/131 (95%)	0.79	17 (13%)	7	4	49, 70, 116, 159	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	QM	121/126 (96%)	1.16	22 (18%)	3	1	88, 126, 155, 176	0
13	XM	121/126 (96%)	1.22	18 (14%)	5	3	72, 104, 143, 188	0
14	QN	60/61 (98%)	1.74	19 (31%)	1	1	98, 129, 156, 196	0
14	XN	60/61 (98%)	1.29	14 (23%)	2	1	66, 90, 123, 139	0
15	QO	88/89 (98%)	0.66	4 (4%)	38	20	62, 90, 125, 137	0
15	XO	88/89 (98%)	0.56	4 (4%)	38	20	56, 77, 114, 123	0
16	QP	84/88 (95%)	0.75	6 (7%)	22	12	63, 86, 115, 144	0
16	XP	84/88 (95%)	0.76	4 (4%)	35	19	70, 90, 127, 147	0
17	QQ	100/105 (95%)	0.76	8 (8%)	18	10	66, 91, 123, 149	0
17	XQ	100/105 (95%)	0.67	9 (9%)	15	8	63, 88, 116, 133	0
18	QR	70/88 (79%)	0.41	1 (1%)	73	53	63, 90, 126, 161	0
18	XR	70/88 (79%)	0.43	2 (2%)	53	32	60, 93, 118, 160	0
19	QS	84/93 (90%)	1.38	19 (22%)	2	1	101, 139, 176, 223	0
19	XS	84/93 (90%)	0.79	12 (14%)	6	3	77, 107, 139, 154	0
20	QT	99/106 (93%)	1.20	19 (19%)	3	1	63, 93, 138, 181	0
20	XT	99/106 (93%)	1.38	27 (27%)	1	1	70, 97, 127, 161	0
21	QU	25/27 (92%)	1.89	10 (40%)	1	0	95, 116, 129, 131	0
21	XU	25/27 (92%)	1.49	6 (24%)	2	1	75, 99, 123, 131	0
22	QV	77/77 (100%)	0.48	3 (3%)	43	24	71, 114, 165, 197	0
22	XV	77/77 (100%)	0.37	4 (5%)	33	17	57, 94, 129, 182	0
23	QX	18/19 (94%)	1.55	6 (33%)	1	0	77, 133, 218, 227	0
23	XX	18/19 (94%)	1.71	8 (44%)	0	0	63, 135, 222, 242	0
24	QY	75/76 (98%)	1.52	21 (28%)	1	1	79, 187, 255, 279	0
24	XY	75/76 (98%)	1.06	14 (18%)	3	1	70, 166, 221, 268	0
25	R0	82/85 (96%)	0.93	9 (10%)	10	5	60, 84, 110, 154	0
25	Y0	82/85 (96%)	0.66	5 (6%)	27	15	42, 60, 91, 131	0
26	R1	97/98 (98%)	0.96	10 (10%)	12	6	49, 69, 132, 183	0
26	Y1	97/98 (98%)	0.69	14 (14%)	6	3	34, 58, 127, 176	0
27	R2	69/72 (95%)	0.79	5 (7%)	21	11	59, 90, 130, 181	0
27	Y2	69/72 (95%)	0.71	6 (8%)	16	9	47, 66, 114, 172	0
28	R3	59/60 (98%)	0.71	2 (3%)	48	28	62, 84, 113, 156	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	Y3	59/60 (98%)	0.30	0	100	100	39, 59, 105, 133	0
29	R4	71/71 (100%)	1.31	13 (18%)	3	1	104, 148, 198, 223	0
29	Y4	71/71 (100%)	1.41	15 (21%)	2	1	80, 130, 196, 204	0
30	R5	59/60 (98%)	1.03	10 (16%)	4	2	47, 68, 154, 192	0
30	Y5	59/60 (98%)	1.08	13 (22%)	2	1	32, 60, 158, 166	0
31	R6	49/54 (90%)	2.53	29 (59%)	0	0	54, 98, 149, 190	0
31	Y6	49/54 (90%)	2.08	21 (42%)	0	0	46, 76, 135, 187	0
32	R7	49/49 (100%)	0.70	4 (8%)	17	10	45, 61, 101, 150	0
32	Y7	49/49 (100%)	0.53	4 (8%)	17	10	32, 43, 95, 165	0
33	R8	64/65 (98%)	1.26	16 (25%)	2	1	50, 73, 120, 176	0
33	Y8	64/65 (98%)	1.42	16 (25%)	2	1	41, 57, 93, 204	0
34	R9	37/37 (100%)	0.79	2 (5%)	31	17	68, 89, 125, 166	0
34	Y9	37/37 (100%)	0.28	0	100	100	44, 58, 84, 87	0
35	RA	2882/2915 (98%)	0.05	94 (3%)	49	29	43, 71, 193, 277	0
35	YA	2883/2915 (98%)	-0.11	43 (1%)	72	52	35, 54, 162, 262	0
36	RB	120/122 (98%)	0.22	1 (0%)	82	65	85, 107, 133, 149	0
36	YB	120/122 (98%)	-0.02	2 (1%)	69	48	61, 74, 95, 129	0
37	RD	272/276 (98%)	0.69	24 (8%)	15	9	41, 62, 101, 150	0
37	YD	272/276 (98%)	0.43	18 (6%)	24	13	31, 53, 83, 154	0
38	RE	205/206 (99%)	0.78	22 (10%)	11	6	45, 75, 130, 185	0
38	YE	205/206 (99%)	0.64	21 (10%)	12	6	28, 59, 118, 150	0
39	RF	202/210 (96%)	0.49	4 (1%)	65	44	46, 80, 128, 155	0
39	YF	202/210 (96%)	0.39	8 (3%)	42	23	36, 58, 122, 170	0
40	RG	181/182 (99%)	0.78	14 (7%)	19	10	76, 118, 152, 165	0
40	YG	181/182 (99%)	0.53	6 (3%)	49	29	65, 87, 128, 186	0
41	RH	170/180 (94%)	1.26	35 (20%)	2	1	88, 128, 160, 194	0
41	YH	170/180 (94%)	0.80	22 (12%)	7	4	48, 74, 113, 176	0
42	RI	146/148 (98%)	0.69	8 (5%)	30	16	63, 103, 140, 152	0
42	YI	146/148 (98%)	0.71	9 (6%)	26	14	56, 100, 139, 178	0
43	RN	138/140 (98%)	0.65	10 (7%)	21	11	52, 82, 113, 159	0
43	YN	138/140 (98%)	0.49	5 (3%)	46	26	36, 57, 104, 185	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	RO	122/122 (100%)	0.39	2 (1%) 70 49	45, 71, 97, 116	0
44	YO	122/122 (100%)	0.20	1 (0%) 82 65	34, 57, 82, 100	0
45	RP	150/150 (100%)	1.38	37 (24%) 2 1	53, 93, 141, 205	0
45	YP	150/150 (100%)	0.98	22 (14%) 6 3	29, 70, 117, 168	0
46	RQ	141/141 (100%)	1.31	30 (21%) 2 1	55, 89, 135, 178	0
46	YQ	141/141 (100%)	0.94	19 (13%) 7 4	40, 63, 116, 144	0
47	RR	118/118 (100%)	0.59	5 (4%) 40 22	48, 66, 90, 130	0
47	YR	118/118 (100%)	0.56	5 (4%) 40 22	37, 55, 82, 115	0
48	RS	111/112 (99%)	0.93	16 (14%) 6 3	73, 103, 141, 187	0
48	YS	111/112 (99%)	0.59	9 (8%) 18 10	53, 76, 127, 186	0
49	RT	137/146 (93%)	0.70	13 (9%) 14 7	54, 77, 137, 165	0
49	YT	137/146 (93%)	0.65	12 (8%) 15 9	45, 68, 129, 164	0
50	RU	117/118 (99%)	0.72	9 (7%) 19 10	49, 79, 122, 169	0
50	YU	117/118 (99%)	0.40	4 (3%) 48 28	24, 53, 91, 157	0
51	RV	101/101 (100%)	0.50	7 (6%) 23 12	53, 89, 135, 184	0
51	YV	101/101 (100%)	0.41	7 (6%) 23 12	32, 65, 113, 158	0
52	RW	113/113 (100%)	0.46	6 (5%) 32 17	45, 64, 96, 171	0
52	YW	113/113 (100%)	0.19	2 (1%) 67 47	33, 49, 88, 158	0
53	RX	92/96 (95%)	0.68	8 (8%) 16 9	53, 74, 99, 105	0
53	YX	92/96 (95%)	0.31	4 (4%) 40 22	39, 55, 86, 133	0
54	RY	102/110 (92%)	1.12	14 (13%) 6 4	71, 97, 134, 158	0
54	YY	102/110 (92%)	0.49	2 (1%) 65 44	44, 70, 106, 139	0
55	RZ	183/206 (88%)	1.23	34 (18%) 3 1	93, 135, 195, 224	0
55	YZ	183/206 (88%)	1.07	30 (16%) 4 2	56, 104, 184, 226	0
All	All	21011/21588 (97%)	0.46	1442 (6%) 23 12	24, 81, 157, 279	0

The worst 5 of 1442 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	12.8
11	QK	128	ALA	12.1
11	XK	129	SER	12.1
45	RP	13	ASN	10.6
13	XM	101	GLN	8.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3218	1/1	0.08	1.15	161,161,161,161	0
56	MG	YA	3172	1/1	0.09	0.41	115,115,115,115	0
56	MG	RA	3148	1/1	0.11	0.52	156,156,156,156	0
56	MG	YA	3346	1/1	0.13	0.54	112,112,112,112	0
56	MG	XA	1692	1/1	0.16	0.53	126,126,126,126	0
56	MG	YA	3340	1/1	0.19	0.64	117,117,117,117	0
56	MG	QA	1625	1/1	0.22	0.47	105,105,105,105	0
56	MG	QA	1653	1/1	0.22	0.25	144,144,144,144	0
56	MG	QX	102	1/1	0.23	0.55	137,137,137,137	0
56	MG	XA	1661	1/1	0.24	0.34	139,139,139,139	0
56	MG	RA	3170	1/1	0.24	0.58	159,159,159,159	0
56	MG	QA	1659	1/1	0.24	0.24	154,154,154,154	0
56	MG	RA	3236	1/1	0.24	0.89	182,182,182,182	0
56	MG	RA	3259	1/1	0.24	0.33	105,105,105,105	0
56	MG	RA	3012	1/1	0.25	0.47	120,120,120,120	0
56	MG	RA	3178	1/1	0.25	0.85	102,102,102,102	0
56	MG	RA	3217	1/1	0.26	0.49	74,74,74,74	0
56	MG	YA	3290	1/1	0.26	0.30	73,73,73,73	0
56	MG	RA	3112	1/1	0.29	0.65	131,131,131,131	0
56	MG	XA	1659	1/1	0.29	0.27	112,112,112,112	0
56	MG	YA	3233	1/1	0.32	0.44	90,90,90,90	0
56	MG	YA	3106	1/1	0.32	0.94	126,126,126,126	0
56	MG	RA	3120	1/1	0.33	0.55	106,106,106,106	0
56	MG	RA	3140	1/1	0.33	0.29	89,89,89,89	0
56	MG	RA	3164	1/1	0.34	0.83	121,121,121,121	0
56	MG	QA	1643	1/1	0.34	0.72	140,140,140,140	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1647	1/1	0.34	0.31	129,129,129,129	0
56	MG	RA	3173	1/1	0.34	0.47	109,109,109,109	0
56	MG	RA	3159	1/1	0.35	0.72	104,104,104,104	0
56	MG	YA	3118	1/1	0.37	0.29	52,52,52,52	0
56	MG	XA	1629	1/1	0.37	0.31	82,82,82,82	0
56	MG	QA	1658	1/1	0.37	0.44	108,108,108,108	0
56	MG	RA	3219	1/1	0.38	0.38	126,126,126,126	0
56	MG	RA	3166	1/1	0.38	0.50	126,126,126,126	0
56	MG	RA	3180	1/1	0.38	0.45	80,80,80,80	0
56	MG	QA	1601	1/1	0.38	0.79	134,134,134,134	0
56	MG	RA	3139	1/1	0.38	0.58	133,133,133,133	0
56	MG	YA	3163	1/1	0.39	0.55	137,137,137,137	0
56	MG	RA	3063	1/1	0.40	0.24	111,111,111,111	0
56	MG	YA	3218	1/1	0.41	0.39	99,99,99,99	0
56	MG	XA	1636	1/1	0.42	0.23	75,75,75,75	0
56	MG	XA	1655	1/1	0.42	0.85	127,127,127,127	0
56	MG	QA	1619	1/1	0.43	0.24	79,79,79,79	0
56	MG	XA	1648	1/1	0.44	0.46	101,101,101,101	0
56	MG	RA	3122	1/1	0.44	0.56	124,124,124,124	0
56	MG	YA	3164	1/1	0.44	0.22	57,57,57,57	0
56	MG	XA	1662	1/1	0.45	0.56	105,105,105,105	0
56	MG	RA	3151	1/1	0.45	0.50	95,95,95,95	0
56	MG	XX	101	1/1	0.45	0.45	104,104,104,104	0
56	MG	RA	3206	1/1	0.45	0.47	170,170,170,170	0
56	MG	YA	3202	1/1	0.45	0.55	104,104,104,104	0
56	MG	YA	3220	1/1	0.46	0.49	86,86,86,86	0
56	MG	RA	3130	1/1	0.46	0.26	68,68,68,68	0
56	MG	RA	3215	1/1	0.46	0.48	99,99,99,99	0
56	MG	QA	1656	1/1	0.46	0.23	124,124,124,124	0
56	MG	RA	3195	1/1	0.46	0.35	117,117,117,117	0
56	MG	YA	3246	1/1	0.47	0.65	82,82,82,82	0
56	MG	RA	3013	1/1	0.47	0.64	127,127,127,127	0
56	MG	YA	3155	1/1	0.48	0.54	104,104,104,104	0
56	MG	XA	1619	1/1	0.48	0.45	89,89,89,89	0
56	MG	XA	1654	1/1	0.48	0.72	108,108,108,108	0
56	MG	QA	1618	1/1	0.49	0.62	97,97,97,97	0
56	MG	RA	3102	1/1	0.49	0.23	66,66,66,66	0
56	MG	YA	3168	1/1	0.49	0.49	102,102,102,102	0
56	MG	RA	3126	1/1	0.50	0.47	77,77,77,77	0
56	MG	RA	3249	1/1	0.51	0.91	117,117,117,117	0
56	MG	RA	3057	1/1	0.51	0.57	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1607	1/1	0.51	0.40	93,93,93,93	0
56	MG	RA	3118	1/1	0.51	0.48	153,153,153,153	0
56	MG	QA	1620	1/1	0.51	0.22	113,113,113,113	0
56	MG	YA	3342	1/1	0.51	0.27	97,97,97,97	0
56	MG	RA	3051	1/1	0.51	0.52	88,88,88,88	0
56	MG	QA	1655	1/1	0.52	0.33	125,125,125,125	0
56	MG	XA	1667	1/1	0.52	0.44	107,107,107,107	0
56	MG	R9	101	1/1	0.53	0.67	140,140,140,140	0
56	MG	XA	1608	1/1	0.54	0.15	147,147,147,147	0
56	MG	RA	3202	1/1	0.54	0.44	196,196,196,196	0
56	MG	XA	1657	1/1	0.54	0.27	96,96,96,96	0
56	MG	YA	3288	1/1	0.54	0.50	106,106,106,106	0
56	MG	YA	3321	1/1	0.55	0.54	90,90,90,90	0
56	MG	QA	1637	1/1	0.55	0.29	74,74,74,74	0
56	MG	RA	3192	1/1	0.55	0.39	101,101,101,101	0
56	MG	YA	3206	1/1	0.55	0.61	103,103,103,103	0
56	MG	YQ	203	1/1	0.55	0.49	104,104,104,104	0
56	MG	RA	3245	1/1	0.56	0.36	79,79,79,79	0
56	MG	RA	3207	1/1	0.56	0.30	77,77,77,77	0
56	MG	XA	1614	1/1	0.56	0.43	114,114,114,114	0
56	MG	XA	1658	1/1	0.56	0.26	88,88,88,88	0
56	MG	QA	1644	1/1	0.56	0.14	142,142,142,142	0
56	MG	XA	1602	1/1	0.57	0.30	85,85,85,85	0
56	MG	RA	3003	1/1	0.57	0.57	172,172,172,172	0
56	MG	RA	3220	1/1	0.57	0.20	102,102,102,102	0
56	MG	YP	201	1/1	0.58	0.55	102,102,102,102	0
56	MG	QA	1612	1/1	0.58	0.62	85,85,85,85	0
56	MG	RA	3221	1/1	0.59	0.27	90,90,90,90	0
56	MG	YA	3286	1/1	0.59	0.41	83,83,83,83	0
56	MG	QA	1635	1/1	0.59	0.35	103,103,103,103	0
56	MG	RA	3191	1/1	0.59	0.19	102,102,102,102	0
56	MG	QA	1617	1/1	0.59	0.36	62,62,62,62	0
56	MG	XA	1689	1/1	0.60	0.23	65,65,65,65	0
56	MG	YA	3238	1/1	0.60	0.18	67,67,67,67	0
56	MG	YB	201	1/1	0.60	0.48	97,97,97,97	0
56	MG	XA	1690	1/1	0.60	0.20	49,49,49,49	0
56	MG	RA	3153	1/1	0.60	0.28	116,116,116,116	0
56	MG	QA	1657	1/1	0.61	0.28	102,102,102,102	0
56	MG	RA	3210	1/1	0.61	0.36	103,103,103,103	0
56	MG	RA	3263	1/1	0.61	0.34	75,75,75,75	0
56	MG	RA	3201	1/1	0.61	0.37	92,92,92,92	0
56	MG	QA	1647	1/1	0.61	0.28	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3143	1/1	0.61	0.35	102,102,102,102	0
56	MG	RA	3045	1/1	0.62	0.38	105,105,105,105	0
56	MG	QA	1642	1/1	0.62	0.20	96,96,96,96	0
56	MG	QA	1626	1/1	0.62	0.13	71,71,71,71	0
56	MG	QA	1632	1/1	0.62	0.76	113,113,113,113	0
56	MG	XA	1620	1/1	0.62	0.22	83,83,83,83	0
56	MG	RA	3223	1/1	0.63	0.58	120,120,120,120	0
56	MG	RA	3133	1/1	0.63	0.35	113,113,113,113	0
56	MG	RA	3113	1/1	0.63	0.34	72,72,72,72	0
56	MG	QA	1672	1/1	0.63	0.36	82,82,82,82	0
56	MG	QA	1614	1/1	0.63	0.35	67,67,67,67	0
56	MG	YA	3234	1/1	0.63	0.35	129,129,129,129	0
56	MG	RA	3073	1/1	0.64	0.52	92,92,92,92	0
56	MG	YA	3326	1/1	0.64	0.33	78,78,78,78	0
56	MG	RA	3121	1/1	0.64	0.35	89,89,89,89	0
56	MG	YA	3241	1/1	0.64	0.34	128,128,128,128	0
56	MG	RA	3155	1/1	0.64	0.19	69,69,69,69	0
56	MG	XA	1611	1/1	0.64	0.30	73,73,73,73	0
56	MG	YA	3222	1/1	0.64	0.28	64,64,64,64	0
56	MG	RA	3264	1/1	0.64	0.18	66,66,66,66	0
56	MG	XA	1663	1/1	0.65	0.27	109,109,109,109	0
56	MG	YA	3333	1/1	0.65	0.45	74,74,74,74	0
56	MG	XA	1646	1/1	0.65	0.41	122,122,122,122	0
56	MG	RA	3181	1/1	0.65	0.32	78,78,78,78	0
56	MG	XA	1634	1/1	0.66	0.21	72,72,72,72	0
56	MG	RA	3044	1/1	0.66	0.36	78,78,78,78	0
56	MG	YA	3205	1/1	0.66	0.40	66,66,66,66	0
56	MG	QA	1638	1/1	0.66	0.41	97,97,97,97	0
56	MG	YA	3217	1/1	0.66	0.29	126,126,126,126	0
56	MG	YA	3252	1/1	0.66	0.20	37,37,37,37	0
56	MG	RA	3277	1/1	0.66	0.44	71,71,71,71	0
56	MG	YB	203	1/1	0.66	0.23	77,77,77,77	0
56	MG	RA	3279	1/1	0.66	0.86	105,105,105,105	0
56	MG	XA	1632	1/1	0.66	0.49	92,92,92,92	0
56	MG	RA	3150	1/1	0.67	0.19	86,86,86,86	0
56	MG	XA	1633	1/1	0.67	0.36	95,95,95,95	0
56	MG	RA	3271	1/1	0.67	0.29	86,86,86,86	0
56	MG	XA	1691	1/1	0.67	0.57	98,98,98,98	0
56	MG	XA	1650	1/1	0.67	0.11	106,106,106,106	0
56	MG	RA	3011	1/1	0.67	0.54	108,108,108,108	0
56	MG	YA	3187	1/1	0.67	0.12	57,57,57,57	0
56	MG	XA	1644	1/1	0.67	0.22	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3323	1/1	0.67	0.48	77,77,77,77	0
56	MG	RP	203	1/1	0.68	0.30	79,79,79,79	0
56	MG	RA	3001	1/1	0.68	0.23	64,64,64,64	0
56	MG	RA	3209	1/1	0.68	0.36	130,130,130,130	0
56	MG	RA	3142	1/1	0.68	0.42	176,176,176,176	0
56	MG	YA	3300	1/1	0.68	0.35	78,78,78,78	0
56	MG	YA	3239	1/1	0.68	0.44	133,133,133,133	0
56	MG	RA	3212	1/1	0.68	0.28	71,71,71,71	0
56	MG	YA	3193	1/1	0.68	0.67	108,108,108,108	0
56	MG	XM	201	1/1	0.69	0.16	111,111,111,111	0
56	MG	RA	3067	1/1	0.69	0.51	55,55,55,55	0
56	MG	RA	3135	1/1	0.69	0.27	52,52,52,52	0
56	MG	RA	3161	1/1	0.69	0.33	85,85,85,85	0
56	MG	YA	3182	1/1	0.69	0.49	91,91,91,91	0
56	MG	XA	1668	1/1	0.69	0.60	92,92,92,92	0
56	MG	RA	3199	1/1	0.70	0.58	93,93,93,93	0
56	MG	RA	3035	1/1	0.70	0.61	78,78,78,78	0
56	MG	YA	3337	1/1	0.70	0.58	88,88,88,88	0
56	MG	RA	3177	1/1	0.70	0.30	95,95,95,95	0
56	MG	QA	1607	1/1	0.70	0.18	76,76,76,76	0
56	MG	YA	3103	1/1	0.70	0.17	61,61,61,61	0
56	MG	RB	203	1/1	0.70	0.34	64,64,64,64	0
56	MG	RA	3262	1/1	0.70	0.45	86,86,86,86	0
56	MG	YA	3154	1/1	0.70	0.42	81,81,81,81	0
56	MG	YP	203	1/1	0.70	0.32	47,47,47,47	0
56	MG	QA	1648	1/1	0.70	0.37	97,97,97,97	0
56	MG	YA	3198	1/1	0.71	0.31	67,67,67,67	0
56	MG	YA	3162	1/1	0.71	0.42	72,72,72,72	0
56	MG	YA	3294	1/1	0.71	0.55	98,98,98,98	0
56	MG	YA	3298	1/1	0.71	0.23	89,89,89,89	0
56	MG	YA	3191	1/1	0.71	0.43	80,80,80,80	0
56	MG	RA	3247	1/1	0.71	0.21	66,66,66,66	0
56	MG	QA	1661	1/1	0.72	0.10	137,137,137,137	0
56	MG	RA	3196	1/1	0.72	0.29	90,90,90,90	0
56	MG	QA	1621	1/1	0.72	0.38	118,118,118,118	0
56	MG	YA	3061	1/1	0.72	0.25	44,44,44,44	0
56	MG	QA	1645	1/1	0.72	0.34	74,74,74,74	0
56	MG	YA	3165	1/1	0.72	0.21	77,77,77,77	0
56	MG	YA	3308	1/1	0.72	0.29	83,83,83,83	0
56	MG	QA	1649	1/1	0.72	0.38	79,79,79,79	0
56	MG	RA	3123	1/1	0.72	0.40	72,72,72,72	0
56	MG	YA	3122	1/1	0.72	0.27	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1642	1/1	0.73	0.20	81,81,81,81	0
56	MG	RA	3146	1/1	0.73	0.51	92,92,92,92	0
56	MG	YA	3329	1/1	0.73	0.23	66,66,66,66	0
56	MG	RA	3273	1/1	0.73	0.34	55,55,55,55	0
56	MG	RA	3152	1/1	0.73	0.21	48,48,48,48	0
56	MG	RA	3127	1/1	0.73	0.17	39,39,39,39	0
56	MG	XA	1664	1/1	0.73	0.36	87,87,87,87	0
56	MG	RA	3246	1/1	0.73	0.28	108,108,108,108	0
56	MG	YA	3114	1/1	0.73	0.23	43,43,43,43	0
56	MG	YA	3225	1/1	0.73	0.17	36,36,36,36	0
56	MG	QA	1602	1/1	0.73	0.26	43,43,43,43	0
56	MG	XA	1637	1/1	0.73	0.15	63,63,63,63	0
56	MG	XA	1638	1/1	0.73	0.17	66,66,66,66	0
56	MG	YA	3131	1/1	0.74	0.17	50,50,50,50	0
56	MG	RA	3275	1/1	0.74	0.36	92,92,92,92	0
56	MG	RA	3214	1/1	0.74	0.23	74,74,74,74	0
56	MG	RA	3266	1/1	0.74	0.49	80,80,80,80	0
56	MG	YQ	202	1/1	0.74	0.32	80,80,80,80	0
56	MG	XA	1680	1/1	0.74	0.36	56,56,56,56	0
56	MG	YA	3111	1/1	0.75	0.43	102,102,102,102	0
56	MG	YA	3262	1/1	0.75	0.24	70,70,70,70	0
56	MG	YA	3181	1/1	0.75	0.49	65,65,65,65	0
56	MG	RA	3083	1/1	0.75	0.25	64,64,64,64	0
56	MG	RA	3225	1/1	0.75	0.26	68,68,68,68	0
56	MG	XA	1613	1/1	0.75	0.13	52,52,52,52	0
56	MG	RA	3278	1/1	0.75	0.34	75,75,75,75	0
56	MG	RA	3233	1/1	0.75	0.48	91,91,91,91	0
56	MG	QA	1631	1/1	0.76	0.12	68,68,68,68	0
56	MG	YA	3167	1/1	0.76	0.20	35,35,35,35	0
56	MG	RA	3256	1/1	0.76	0.51	74,74,74,74	0
56	MG	RD	301	1/1	0.76	0.28	57,57,57,57	0
56	MG	QA	1670	1/1	0.76	0.32	77,77,77,77	0
56	MG	RA	3186	1/1	0.76	0.13	57,57,57,57	0
56	MG	RA	3080	1/1	0.76	0.24	49,49,49,49	0
56	MG	RA	3231	1/1	0.76	0.14	50,50,50,50	0
56	MG	XA	1684	1/1	0.77	0.30	61,61,61,61	0
56	MG	YA	3035	1/1	0.77	0.45	61,61,61,61	0
56	MG	YA	3199	1/1	0.77	0.20	53,53,53,53	0
56	MG	YA	3240	1/1	0.77	0.30	95,95,95,95	0
56	MG	RA	3244	1/1	0.77	0.44	56,56,56,56	0
56	MG	YA	3203	1/1	0.77	0.28	88,88,88,88	0
56	MG	RA	3252	1/1	0.77	0.47	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	QA	1628	1/1	0.77	0.72	96,96,96,96	0
56	MG	YA	3211	1/1	0.77	0.20	62,62,62,62	0
56	MG	YA	3179	1/1	0.77	0.26	71,71,71,71	0
56	MG	YA	3156	1/1	0.77	0.38	75,75,75,75	0
56	MG	YA	3158	1/1	0.77	0.19	43,43,43,43	0
56	MG	QA	1623	1/1	0.77	0.40	92,92,92,92	0
56	MG	YA	3190	1/1	0.77	0.21	64,64,64,64	0
56	MG	RA	3046	1/1	0.77	0.31	47,47,47,47	0
56	MG	YA	3197	1/1	0.78	0.72	82,82,82,82	0
56	MG	YA	3313	1/1	0.78	0.53	87,87,87,87	0
56	MG	RA	3099	1/1	0.78	0.40	42,42,42,42	0
56	MG	QA	1654	1/1	0.78	0.31	77,77,77,77	0
56	MG	RA	3042	1/1	0.78	0.30	46,46,46,46	0
56	MG	RB	202	1/1	0.78	0.14	75,75,75,75	0
56	MG	XA	1671	1/1	0.78	0.52	62,62,62,62	0
56	MG	YA	3144	1/1	0.78	0.10	35,35,35,35	0
56	MG	XA	1678	1/1	0.78	0.28	55,55,55,55	0
56	MG	YA	3039	1/1	0.78	0.30	44,44,44,44	0
56	MG	RA	3203	1/1	0.78	0.62	101,101,101,101	0
56	MG	YA	3189	1/1	0.78	0.28	67,67,67,67	0
56	MG	YA	3291	1/1	0.78	0.34	90,90,90,90	0
56	MG	YA	3076	1/1	0.78	0.39	54,54,54,54	0
56	MG	RA	3162	1/1	0.78	0.19	58,58,58,58	0
56	MG	RA	3183	1/1	0.78	0.22	49,49,49,49	0
56	MG	YA	3301	1/1	0.78	0.13	28,28,28,28	0
56	MG	QA	1608	1/1	0.79	0.17	79,79,79,79	0
56	MG	QA	1646	1/1	0.79	0.23	97,97,97,97	0
56	MG	YA	3338	1/1	0.79	0.74	94,94,94,94	0
56	MG	RA	3149	1/1	0.79	0.48	89,89,89,89	0
56	MG	XA	1666	1/1	0.79	0.13	145,145,145,145	0
56	MG	RA	3250	1/1	0.79	0.50	63,63,63,63	0
56	MG	YA	3145	1/1	0.79	0.23	49,49,49,49	0
56	MG	YA	3151	1/1	0.79	0.15	38,38,38,38	0
56	MG	XA	1625	1/1	0.79	0.10	45,45,45,45	0
56	MG	XA	1669	1/1	0.79	0.11	43,43,43,43	0
56	MG	YA	3228	1/1	0.79	0.23	60,60,60,60	0
56	MG	R0	101	1/1	0.79	0.26	57,57,57,57	0
56	MG	YA	3285	1/1	0.80	0.23	57,57,57,57	0
56	MG	RA	3222	1/1	0.80	0.21	86,86,86,86	0
56	MG	YA	3088	1/1	0.80	0.39	45,45,45,45	0
56	MG	RA	3235	1/1	0.80	0.35	51,51,51,51	0
56	MG	QA	1630	1/1	0.80	0.12	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3293	1/1	0.80	0.38	73,73,73,73	0
56	MG	XA	1660	1/1	0.80	0.44	72,72,72,72	0
56	MG	RA	3224	1/1	0.80	0.20	63,63,63,63	0
56	MG	QA	1660	1/1	0.80	0.09	87,87,87,87	0
56	MG	QA	1639	1/1	0.80	0.26	81,81,81,81	0
56	MG	YA	3125	1/1	0.80	0.39	51,51,51,51	0
56	MG	XA	1631	1/1	0.80	0.24	71,71,71,71	0
56	MG	XA	1687	1/1	0.80	0.50	85,85,85,85	0
56	MG	YA	3282	1/1	0.80	0.20	40,40,40,40	0
56	MG	QA	1650	1/1	0.81	0.22	68,68,68,68	0
56	MG	RA	3276	1/1	0.81	0.35	84,84,84,84	0
56	MG	RA	3132	1/1	0.81	0.31	65,65,65,65	0
56	MG	RA	3055	1/1	0.81	0.12	33,33,33,33	0
56	MG	RA	3092	1/1	0.81	0.16	57,57,57,57	0
56	MG	XA	1618	1/1	0.81	0.32	43,43,43,43	0
56	MG	YA	3046	1/1	0.81	0.24	24,24,24,24	0
56	MG	YA	3344	1/1	0.81	0.12	44,44,44,44	0
56	MG	YA	3169	1/1	0.81	0.21	58,58,58,58	0
56	MG	QF	201	1/1	0.81	0.18	87,87,87,87	0
56	MG	QA	1651	1/1	0.81	0.17	88,88,88,88	0
56	MG	RA	3125	1/1	0.81	0.21	71,71,71,71	0
56	MG	QA	1603	1/1	0.81	0.54	93,93,93,93	0
56	MG	QA	1641	1/1	0.81	0.29	72,72,72,72	0
56	MG	YA	3188	1/1	0.81	0.15	72,72,72,72	0
56	MG	YA	3157	1/1	0.82	0.10	16,16,16,16	0
56	MG	YA	3091	1/1	0.82	0.32	64,64,64,64	0
56	MG	YA	3316	1/1	0.82	0.26	47,47,47,47	0
56	MG	RA	3010	1/1	0.82	0.27	35,35,35,35	0
56	MG	RA	3198	1/1	0.82	0.10	64,64,64,64	0
56	MG	RA	3138	1/1	0.82	0.37	47,47,47,47	0
56	MG	RA	3184	1/1	0.82	0.41	140,140,140,140	0
56	MG	Y6	102	1/1	0.82	0.10	9,9,9,9	0
56	MG	Y9	101	1/1	0.82	0.40	82,82,82,82	0
56	MG	YA	3033	1/1	0.82	0.24	43,43,43,43	0
56	MG	YA	3127	1/1	0.82	0.10	34,34,34,34	0
56	MG	YA	3215	1/1	0.82	0.13	36,36,36,36	0
56	MG	RA	3009	1/1	0.82	0.26	36,36,36,36	0
56	MG	XA	1681	1/1	0.82	0.32	58,58,58,58	0
56	MG	RA	3016	1/1	0.82	0.53	82,82,82,82	0
56	MG	YA	3060	1/1	0.82	0.21	39,39,39,39	0
56	MG	RA	3248	1/1	0.82	0.24	71,71,71,71	0
56	MG	YA	3226	1/1	0.82	0.10	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3114	1/1	0.82	0.16	48,48,48,48	0
56	MG	RA	3101	1/1	0.82	0.11	32,32,32,32	0
56	MG	YA	3025	1/1	0.83	0.34	26,26,26,26	0
56	MG	RA	3238	1/1	0.83	0.28	46,46,46,46	0
56	MG	XA	1649	1/1	0.83	0.30	81,81,81,81	0
56	MG	YA	3330	1/1	0.83	0.20	84,84,84,84	0
56	MG	YA	3096	1/1	0.83	0.23	39,39,39,39	0
56	MG	YA	3140	1/1	0.83	0.27	49,49,49,49	0
56	MG	YA	3141	1/1	0.83	0.26	38,38,38,38	0
56	MG	YA	3102	1/1	0.83	0.29	48,48,48,48	0
56	MG	XA	1685	1/1	0.83	0.43	58,58,58,58	0
56	MG	YA	3147	1/1	0.83	0.30	58,58,58,58	0
56	MG	YA	3171	1/1	0.83	0.21	73,73,73,73	0
56	MG	YA	3148	1/1	0.83	0.14	36,36,36,36	0
56	MG	YA	3306	1/1	0.83	0.40	90,90,90,90	0
56	MG	YA	3045	1/1	0.83	0.17	31,31,31,31	0
56	MG	RA	3111	1/1	0.83	0.41	69,69,69,69	0
56	MG	RA	3060	1/1	0.83	0.10	26,26,26,26	0
56	MG	RA	3104	1/1	0.83	0.20	57,57,57,57	0
56	MG	YX	101	1/1	0.83	0.23	101,101,101,101	0
56	MG	YA	3263	1/1	0.84	0.68	70,70,70,70	0
56	MG	QA	1636	1/1	0.84	0.21	52,52,52,52	0
56	MG	XV	101	1/1	0.84	0.20	77,77,77,77	0
56	MG	RP	202	1/1	0.84	0.36	95,95,95,95	0
56	MG	YA	3166	1/1	0.84	0.12	27,27,27,27	0
56	MG	RA	3097	1/1	0.84	0.51	87,87,87,87	0
56	MG	YA	3071	1/1	0.84	0.18	27,27,27,27	0
56	MG	RA	3269	1/1	0.84	0.40	60,60,60,60	0
56	MG	YA	3170	1/1	0.84	0.19	79,79,79,79	0
56	MG	YA	3297	1/1	0.84	0.16	56,56,56,56	0
56	MG	QA	1652	1/1	0.84	0.13	142,142,142,142	0
56	MG	RA	3048	1/1	0.84	0.33	38,38,38,38	0
56	MG	YA	3129	1/1	0.84	0.26	45,45,45,45	0
56	MG	YA	3302	1/1	0.84	0.41	85,85,85,85	0
56	MG	RA	3160	1/1	0.84	0.27	74,74,74,74	0
56	MG	YA	3132	1/1	0.84	0.15	40,40,40,40	0
56	MG	YA	3183	1/1	0.84	0.12	48,48,48,48	0
56	MG	XA	1639	1/1	0.84	0.62	79,79,79,79	0
56	MG	YA	3317	1/1	0.84	0.20	50,50,50,50	0
56	MG	YA	3261	1/1	0.85	0.60	71,71,71,71	0
56	MG	RA	3119	1/1	0.85	0.20	98,98,98,98	0
56	MG	RA	3211	1/1	0.85	0.09	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1673	1/1	0.85	0.39	62,62,62,62	0
56	MG	RA	3145	1/1	0.85	0.23	43,43,43,43	0
56	MG	YA	3055	1/1	0.85	0.48	91,91,91,91	0
56	MG	R5	101	1/1	0.85	0.14	31,31,31,31	0
56	MG	RA	3077	1/1	0.85	0.27	41,41,41,41	0
56	MG	YA	3150	1/1	0.85	0.27	78,78,78,78	0
56	MG	XA	1621	1/1	0.85	0.29	41,41,41,41	0
56	MG	QA	1662	1/1	0.85	0.23	63,63,63,63	0
56	MG	YA	3085	1/1	0.85	0.11	23,23,23,23	0
56	MG	YA	3128	1/1	0.85	0.31	39,39,39,39	0
56	MG	RB	201	1/1	0.85	0.14	72,72,72,72	0
56	MG	YA	3242	1/1	0.85	0.27	63,63,63,63	0
56	MG	YA	3243	1/1	0.85	0.34	53,53,53,53	0
56	MG	RA	3189	1/1	0.85	0.32	69,69,69,69	0
56	MG	YA	3159	1/1	0.85	0.21	30,30,30,30	0
56	MG	YA	3259	1/1	0.85	0.33	46,46,46,46	0
56	MG	YA	3260	1/1	0.85	0.38	56,56,56,56	0
56	MG	RA	3176	1/1	0.86	0.12	51,51,51,51	0
56	MG	QA	1634	1/1	0.86	0.18	59,59,59,59	0
56	MG	YA	3196	1/1	0.86	0.29	99,99,99,99	0
56	MG	RE	301	1/1	0.86	0.24	34,34,34,34	0
56	MG	RA	3193	1/1	0.86	0.16	121,121,121,121	0
56	MG	XA	1652	1/1	0.86	0.15	46,46,46,46	0
56	MG	YA	3248	1/1	0.86	0.20	36,36,36,36	0
56	MG	RA	3134	1/1	0.86	0.31	66,66,66,66	0
56	MG	RA	3062	1/1	0.86	0.23	29,29,29,29	0
56	MG	RA	3197	1/1	0.86	0.17	75,75,75,75	0
56	MG	QA	1615	1/1	0.86	0.12	92,92,92,92	0
56	MG	XA	1683	1/1	0.86	0.50	66,66,66,66	0
56	MG	YA	3213	1/1	0.86	0.33	57,57,57,57	0
56	MG	YA	3271	1/1	0.86	0.16	60,60,60,60	0
56	MG	YA	3273	1/1	0.86	0.17	37,37,37,37	0
56	MG	YA	3175	1/1	0.86	0.08	35,35,35,35	0
56	MG	YA	3176	1/1	0.86	0.29	61,61,61,61	0
56	MG	YA	3178	1/1	0.86	0.28	44,44,44,44	0
56	MG	YA	3153	1/1	0.86	0.09	27,27,27,27	0
56	MG	YA	3347	1/1	0.86	0.40	74,74,74,74	0
56	MG	RA	3251	1/1	0.86	0.47	78,78,78,78	0
56	MG	RA	3154	1/1	0.86	0.20	57,57,57,57	0
56	MG	RA	3065	1/1	0.86	0.29	25,25,25,25	0
56	MG	QA	1668	1/1	0.86	0.53	90,90,90,90	0
56	MG	YQ	201	1/1	0.86	0.33	105,105,105,105	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3261	1/1	0.86	0.16	38,38,38,38	0
56	MG	RA	3174	1/1	0.86	0.08	52,52,52,52	0
56	MG	YA	3130	1/1	0.86	0.40	69,69,69,69	0
56	MG	RA	3074	1/1	0.87	0.20	53,53,53,53	0
56	MG	YA	3001	1/1	0.87	0.40	128,128,128,128	0
56	MG	YA	3146	1/1	0.87	0.17	48,48,48,48	0
56	MG	XA	1643	1/1	0.87	0.24	63,63,63,63	0
56	MG	YA	3257	1/1	0.87	0.23	32,32,32,32	0
56	MG	YA	3319	1/1	0.87	0.10	41,41,41,41	0
56	MG	XA	1630	1/1	0.87	0.33	68,68,68,68	0
56	MG	RA	3274	1/1	0.87	0.25	59,59,59,59	0
56	MG	QA	1610	1/1	0.87	0.17	24,24,24,24	0
56	MG	RA	3089	1/1	0.87	0.41	60,60,60,60	0
56	MG	RA	3090	1/1	0.87	0.26	51,51,51,51	0
56	MG	YA	3265	1/1	0.87	0.66	72,72,72,72	0
56	MG	YA	3334	1/1	0.87	0.74	98,98,98,98	0
56	MG	YA	3180	1/1	0.87	0.39	70,70,70,70	0
56	MG	YA	3047	1/1	0.87	0.16	19,19,19,19	0
56	MG	XA	1635	1/1	0.87	0.36	62,62,62,62	0
56	MG	XA	1651	1/1	0.87	0.28	68,68,68,68	0
56	MG	RA	3136	1/1	0.87	0.15	71,71,71,71	0
56	MG	RU	201	1/1	0.87	0.24	104,104,104,104	0
56	MG	YA	3229	1/1	0.87	0.10	38,38,38,38	0
56	MG	YA	3161	1/1	0.87	0.17	46,46,46,46	0
56	MG	RA	3165	1/1	0.87	0.20	73,73,73,73	0
56	MG	YA	3235	1/1	0.87	0.31	66,66,66,66	0
56	MG	YP	202	1/1	0.87	0.12	76,76,76,76	0
56	MG	XA	1656	1/1	0.87	0.35	60,60,60,60	0
56	MG	YA	3135	1/1	0.87	0.16	42,42,42,42	0
56	MG	YA	3136	1/1	0.87	0.10	34,34,34,34	0
56	MG	Y6	101	1/1	0.87	0.09	25,25,25,25	0
56	MG	RA	3156	1/1	0.87	0.13	46,46,46,46	0
56	MG	YA	3117	1/1	0.88	0.56	68,68,68,68	0
56	MG	RA	3006	1/1	0.88	0.42	65,65,65,65	0
56	MG	YA	3212	1/1	0.88	0.16	43,43,43,43	0
56	MG	RA	3226	1/1	0.88	0.28	80,80,80,80	0
56	MG	RA	3179	1/1	0.88	0.09	15,15,15,15	0
56	MG	YA	3216	1/1	0.88	0.12	51,51,51,51	0
56	MG	YA	3324	1/1	0.88	0.18	29,29,29,29	0
56	MG	YA	3048	1/1	0.88	0.24	26,26,26,26	0
56	MG	RA	3124	1/1	0.88	0.33	61,61,61,61	0
56	MG	YA	3219	1/1	0.88	0.18	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3015	1/1	0.88	0.16	40,40,40,40	0
56	MG	RA	3100	1/1	0.88	0.33	52,52,52,52	0
56	MG	XA	1626	1/1	0.88	0.29	71,71,71,71	0
56	MG	RA	3041	1/1	0.88	0.15	26,26,26,26	0
56	MG	RA	3258	1/1	0.88	0.31	61,61,61,61	0
56	MG	XA	1682	1/1	0.88	0.21	48,48,48,48	0
56	MG	YA	3232	1/1	0.88	0.15	65,65,65,65	0
56	MG	YA	3090	1/1	0.88	0.21	33,33,33,33	0
56	MG	RA	3239	1/1	0.88	0.44	73,73,73,73	0
56	MG	YA	3012	1/1	0.88	0.28	36,36,36,36	0
56	MG	YA	3237	1/1	0.88	0.18	58,58,58,58	0
56	MG	YB	204	1/1	0.88	0.39	58,58,58,58	0
56	MG	RA	3185	1/1	0.88	0.11	59,59,59,59	0
56	MG	YA	3029	1/1	0.88	0.15	28,28,28,28	0
56	MG	RA	3094	1/1	0.88	0.36	60,60,60,60	0
56	MG	RA	3147	1/1	0.88	0.20	67,67,67,67	0
56	MG	XA	1688	1/1	0.88	0.45	80,80,80,80	0
56	MG	YA	3173	1/1	0.88	0.38	72,72,72,72	0
56	MG	YA	3245	1/1	0.88	0.36	47,47,47,47	0
56	MG	YA	3315	1/1	0.89	0.09	30,30,30,30	0
56	MG	QA	1640	1/1	0.89	0.15	52,52,52,52	0
56	MG	RA	3232	1/1	0.89	0.45	81,81,81,81	0
56	MG	RA	3253	1/1	0.89	0.19	37,37,37,37	0
56	MG	YA	3041	1/1	0.89	0.11	9,9,9,9	0
56	MG	YA	3044	1/1	0.89	0.31	34,34,34,34	0
56	MG	QA	1629	1/1	0.89	0.15	52,52,52,52	0
56	MG	RA	3216	1/1	0.89	0.14	47,47,47,47	0
56	MG	YA	3269	1/1	0.89	0.14	14,14,14,14	0
56	MG	RA	3200	1/1	0.89	0.08	22,22,22,22	0
56	MG	YA	3331	1/1	0.89	0.21	53,53,53,53	0
56	MG	RA	3260	1/1	0.89	0.30	57,57,57,57	0
56	MG	YA	3230	1/1	0.89	0.27	60,60,60,60	0
56	MG	YA	3284	1/1	0.89	0.13	16,16,16,16	0
56	MG	RA	3076	1/1	0.89	0.14	52,52,52,52	0
56	MG	RA	3023	1/1	0.89	0.27	37,37,37,37	0
56	MG	RA	3079	1/1	0.89	0.22	33,33,33,33	0
56	MG	YA	3065	1/1	0.89	0.12	45,45,45,45	0
56	MG	RA	3024	1/1	0.89	0.18	36,36,36,36	0
56	MG	YA	3075	1/1	0.89	0.08	33,33,33,33	0
56	MG	RA	3082	1/1	0.89	0.16	39,39,39,39	0
56	MG	YA	3079	1/1	0.89	0.21	26,26,26,26	0
56	MG	YA	3081	1/1	0.89	0.21	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YE	301	1/1	0.89	0.17	17,17,17,17	0
56	MG	YA	3299	1/1	0.89	0.20	36,36,36,36	0
56	MG	XA	1675	1/1	0.89	0.27	36,36,36,36	0
56	MG	RA	3267	1/1	0.89	0.28	29,29,29,29	0
56	MG	RA	3028	1/1	0.89	0.17	47,47,47,47	0
56	MG	RA	3034	1/1	0.89	0.27	48,48,48,48	0
56	MG	RA	3163	1/1	0.89	0.17	53,53,53,53	0
56	MG	QA	1633	1/1	0.89	0.19	84,84,84,84	0
56	MG	RA	3237	1/1	0.90	0.28	50,50,50,50	0
56	MG	RA	3110	1/1	0.90	0.09	47,47,47,47	0
56	MG	RA	3020	1/1	0.90	0.20	52,52,52,52	0
56	MG	QA	1613	1/1	0.90	0.16	47,47,47,47	0
56	MG	QA	1669	1/1	0.90	0.15	49,49,49,49	0
56	MG	YA	3126	1/1	0.90	0.09	31,31,31,31	0
56	MG	RA	3182	1/1	0.90	0.15	58,58,58,58	0
56	MG	QA	1616	1/1	0.90	0.30	70,70,70,70	0
56	MG	YA	3320	1/1	0.90	0.37	67,67,67,67	0
56	MG	YA	3255	1/1	0.90	0.32	23,23,23,23	0
56	MG	YA	3207	1/1	0.90	0.06	25,25,25,25	0
56	MG	RA	3032	1/1	0.90	0.24	34,34,34,34	0
56	MG	RA	3168	1/1	0.90	0.18	45,45,45,45	0
56	MG	YA	3328	1/1	0.90	0.10	40,40,40,40	0
56	MG	QA	1604	1/1	0.90	0.22	32,32,32,32	0
56	MG	RA	3187	1/1	0.90	0.25	60,60,60,60	0
56	MG	RA	3188	1/1	0.90	0.22	92,92,92,92	0
56	MG	YA	3264	1/1	0.90	0.27	48,48,48,48	0
56	MG	RA	3172	1/1	0.90	0.10	37,37,37,37	0
56	MG	YA	3336	1/1	0.90	0.20	61,61,61,61	0
56	MG	RA	3254	1/1	0.90	0.28	63,63,63,63	0
56	MG	QA	1674	1/1	0.90	0.08	140,140,140,140	0
56	MG	YA	3143	1/1	0.90	0.09	27,27,27,27	0
56	MG	YA	3341	1/1	0.90	0.19	48,48,48,48	0
56	MG	RA	3158	1/1	0.90	0.38	76,76,76,76	0
56	MG	YA	3283	1/1	0.90	0.15	28,28,28,28	0
56	MG	XA	1674	1/1	0.90	0.12	52,52,52,52	0
56	MG	YA	3087	1/1	0.90	0.26	32,32,32,32	0
56	MG	YA	3010	1/1	0.90	0.28	36,36,36,36	0
56	MG	RA	3088	1/1	0.90	0.14	39,39,39,39	0
56	MG	YA	3013	1/1	0.90	0.16	9,9,9,9	0
56	MG	YB	206	1/1	0.90	0.13	56,56,56,56	0
56	MG	YA	3185	1/1	0.90	0.07	34,34,34,34	0
56	MG	XA	1627	1/1	0.90	0.17	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1679	1/1	0.90	0.08	50,50,50,50	0
56	MG	YA	3031	1/1	0.90	0.26	36,36,36,36	0
56	MG	YA	3236	1/1	0.90	0.26	54,54,54,54	0
56	MG	RA	3053	1/1	0.90	0.29	39,39,39,39	0
56	MG	RB	204	1/1	0.90	0.34	57,57,57,57	0
56	MG	YA	3113	1/1	0.90	0.13	41,41,41,41	0
57	PAR	XA	1670	42/42	0.90	0.13	59,64,86,122	0
56	MG	RA	3131	1/1	0.91	0.25	56,56,56,56	0
56	MG	QV	101	1/1	0.91	0.18	47,47,47,47	0
56	MG	Y0	101	1/1	0.91	0.18	33,33,33,33	0
56	MG	RA	3029	1/1	0.91	0.17	12,12,12,12	0
56	MG	YA	3089	1/1	0.91	0.16	18,18,18,18	0
56	MG	RA	3171	1/1	0.91	0.15	35,35,35,35	0
56	MG	Y8	101	1/1	0.91	0.17	31,31,31,31	0
56	MG	RF	301	1/1	0.91	0.08	59,59,59,59	0
56	MG	YA	3098	1/1	0.91	0.18	30,30,30,30	0
56	MG	YA	3303	1/1	0.91	0.14	43,43,43,43	0
56	MG	RP	201	1/1	0.91	0.49	207,207,207,207	0
56	MG	YA	3307	1/1	0.91	0.25	147,147,147,147	0
56	MG	YA	3007	1/1	0.91	0.21	26,26,26,26	0
56	MG	YA	3310	1/1	0.91	0.11	31,31,31,31	0
56	MG	RA	3190	1/1	0.91	0.07	42,42,42,42	0
56	MG	YA	3107	1/1	0.91	0.17	38,38,38,38	0
56	MG	YA	3231	1/1	0.91	0.11	49,49,49,49	0
56	MG	RA	3072	1/1	0.91	0.30	53,53,53,53	0
56	MG	RA	3093	1/1	0.91	0.14	23,23,23,23	0
56	MG	XA	1601	1/1	0.91	0.19	24,24,24,24	0
56	MG	QA	1624	1/1	0.91	0.33	79,79,79,79	0
56	MG	YA	3030	1/1	0.91	0.16	16,16,16,16	0
56	MG	YA	3120	1/1	0.91	0.31	78,78,78,78	0
56	MG	YA	3325	1/1	0.91	0.07	31,31,31,31	0
56	MG	XA	1606	1/1	0.91	0.41	57,57,57,57	0
56	MG	XA	1677	1/1	0.91	0.15	49,49,49,49	0
56	MG	RA	3194	1/1	0.91	0.12	75,75,75,75	0
56	MG	RA	3268	1/1	0.91	0.09	9,9,9,9	0
56	MG	XA	1610	1/1	0.91	0.15	37,37,37,37	0
56	MG	YA	3043	1/1	0.91	0.27	38,38,38,38	0
56	MG	QA	1671	1/1	0.91	0.13	54,54,54,54	0
56	MG	YA	3186	1/1	0.91	0.18	45,45,45,45	0
56	MG	RA	3054	1/1	0.91	0.30	29,29,29,29	0
56	MG	QA	1605	1/1	0.91	0.53	62,62,62,62	0
56	MG	RA	3141	1/1	0.91	0.20	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3022	1/1	0.91	0.17	40,40,40,40	0
56	MG	YA	3050	1/1	0.91	0.21	21,21,21,21	0
56	MG	YA	3192	1/1	0.91	0.09	45,45,45,45	0
56	MG	YA	3052	1/1	0.91	0.26	37,37,37,37	0
56	MG	YA	3195	1/1	0.91	0.23	70,70,70,70	0
56	MG	RA	3058	1/1	0.91	0.17	32,32,32,32	0
56	MG	RA	3103	1/1	0.91	0.19	35,35,35,35	0
56	MG	QA	1606	1/1	0.91	0.10	49,49,49,49	0
56	MG	YB	205	1/1	0.91	0.47	77,77,77,77	0
56	MG	QA	1609	1/1	0.91	0.13	57,57,57,57	0
56	MG	YA	3200	1/1	0.91	0.06	41,41,41,41	0
56	MG	YA	3069	1/1	0.91	0.30	42,42,42,42	0
56	MG	YA	3070	1/1	0.91	0.11	16,16,16,16	0
56	MG	YA	3204	1/1	0.91	0.09	30,30,30,30	0
56	MG	RA	3025	1/1	0.91	0.30	29,29,29,29	0
56	MG	YA	3072	1/1	0.91	0.10	41,41,41,41	0
56	MG	XA	1628	1/1	0.91	0.07	38,38,38,38	0
56	MG	XF	201	1/1	0.91	0.21	65,65,65,65	0
56	MG	RA	3257	1/1	0.91	0.22	46,46,46,46	0
56	MG	YA	3063	1/1	0.92	0.18	23,23,23,23	0
56	MG	XA	1676	1/1	0.92	0.20	60,60,60,60	0
56	MG	YA	3109	1/1	0.92	0.26	29,29,29,29	0
56	MG	RA	3265	1/1	0.92	0.25	38,38,38,38	0
56	MG	RA	3228	1/1	0.92	0.23	45,45,45,45	0
56	MG	YA	3177	1/1	0.92	0.22	53,53,53,53	0
56	MG	YA	3296	1/1	0.92	0.61	84,84,84,84	0
56	MG	YA	3335	1/1	0.92	0.29	53,53,53,53	0
56	MG	R8	101	1/1	0.92	0.11	47,47,47,47	0
56	MG	YA	3116	1/1	0.92	0.12	24,24,24,24	0
56	MG	RA	3087	1/1	0.92	0.21	28,28,28,28	0
56	MG	YA	3339	1/1	0.92	0.13	40,40,40,40	0
56	MG	YA	3073	1/1	0.92	0.27	58,58,58,58	0
56	MG	YA	3036	1/1	0.92	0.24	25,25,25,25	0
56	MG	RA	3116	1/1	0.92	0.12	24,24,24,24	0
56	MG	XA	1665	1/1	0.92	0.24	57,57,57,57	0
56	MG	YA	3305	1/1	0.92	0.22	47,47,47,47	0
56	MG	QA	1665	1/1	0.92	0.19	58,58,58,58	0
56	MG	RA	3204	1/1	0.92	0.19	72,72,72,72	0
56	MG	YB	202	1/1	0.92	0.17	34,34,34,34	0
56	MG	RA	3007	1/1	0.92	0.32	71,71,71,71	0
56	MG	YA	3160	1/1	0.92	0.15	43,43,43,43	0
56	MG	YA	3311	1/1	0.92	0.17	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	XA	1686	1/1	0.92	0.14	61,61,61,61	0
56	MG	XA	1640	1/1	0.92	0.26	45,45,45,45	0
56	MG	XA	1641	1/1	0.92	0.16	36,36,36,36	0
56	MG	QA	1611	1/1	0.92	0.19	35,35,35,35	0
56	MG	RA	3040	1/1	0.92	0.11	19,19,19,19	0
56	MG	YA	3019	1/1	0.92	0.21	18,18,18,18	0
56	MG	YA	3138	1/1	0.92	0.08	30,30,30,30	0
56	MG	YA	3139	1/1	0.92	0.20	34,34,34,34	0
56	MG	RA	3242	1/1	0.92	0.10	28,28,28,28	0
57	PAR	QA	1663	42/42	0.92	0.11	59,59,76,103	0
56	MG	YA	3026	1/1	0.92	0.15	26,26,26,26	0
56	MG	YA	3201	1/1	0.93	0.09	71,71,71,71	0
56	MG	YA	3123	1/1	0.93	0.07	16,16,16,16	0
56	MG	XA	1623	1/1	0.93	0.06	32,32,32,32	0
56	MG	XA	1624	1/1	0.93	0.20	34,34,34,34	0
56	MG	YA	3318	1/1	0.93	0.27	49,49,49,49	0
56	MG	RA	3084	1/1	0.93	0.06	15,15,15,15	0
56	MG	RA	3213	1/1	0.93	0.15	33,33,33,33	0
56	MG	YA	3016	1/1	0.93	0.28	28,28,28,28	0
56	MG	YA	3209	1/1	0.93	0.25	52,52,52,52	0
56	MG	XA	1653	1/1	0.93	0.27	70,70,70,70	0
56	MG	RA	3085	1/1	0.93	0.07	14,14,14,14	0
56	MG	RA	3070	1/1	0.93	0.14	32,32,32,32	0
56	MG	YA	3327	1/1	0.93	0.42	59,59,59,59	0
56	MG	YA	3214	1/1	0.93	0.17	47,47,47,47	0
56	MG	YA	3268	1/1	0.93	0.13	23,23,23,23	0
56	MG	YA	3133	1/1	0.93	0.15	46,46,46,46	0
56	MG	RA	3021	1/1	0.93	0.10	33,33,33,33	0
56	MG	RA	3107	1/1	0.93	0.06	35,35,35,35	0
56	MG	YA	3276	1/1	0.93	0.08	22,22,22,22	0
56	MG	YA	3278	1/1	0.93	0.12	18,18,18,18	0
56	MG	YA	3279	1/1	0.93	0.29	164,164,164,164	0
56	MG	RA	3109	1/1	0.93	0.10	43,43,43,43	0
56	MG	YA	3032	1/1	0.93	0.17	9,9,9,9	0
56	MG	RR	201	1/1	0.93	0.17	41,41,41,41	0
56	MG	RA	3031	1/1	0.93	0.17	22,22,22,22	0
56	MG	RA	3129	1/1	0.93	0.12	59,59,59,59	0
56	MG	YA	3037	1/1	0.93	0.20	39,39,39,39	0
56	MG	YA	3343	1/1	0.93	0.29	57,57,57,57	0
56	MG	YA	3227	1/1	0.93	0.07	36,36,36,36	0
56	MG	YA	3038	1/1	0.93	0.19	22,22,22,22	0
56	MG	RA	3002	1/1	0.93	0.27	118,118,118,118	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	QA	1666	1/1	0.93	0.20	29,29,29,29	0
56	MG	RA	3061	1/1	0.93	0.09	9,9,9,9	0
56	MG	RA	3169	1/1	0.93	0.22	35,35,35,35	0
56	MG	QA	1667	1/1	0.93	0.18	33,33,33,33	0
56	MG	YA	3152	1/1	0.93	0.22	63,63,63,63	0
56	MG	RA	3095	1/1	0.93	0.14	22,22,22,22	0
56	MG	RA	3227	1/1	0.93	0.14	90,90,90,90	0
56	MG	RA	3208	1/1	0.93	0.36	69,69,69,69	0
56	MG	XA	1617	1/1	0.93	0.19	46,46,46,46	0
56	MG	YA	3051	1/1	0.93	0.25	36,36,36,36	0
56	MG	RA	3229	1/1	0.93	0.11	17,17,17,17	0
56	MG	RA	3036	1/1	0.93	0.28	44,44,44,44	0
56	MG	YA	3057	1/1	0.93	0.10	9,9,9,9	0
56	MG	RA	3018	1/1	0.93	0.13	24,24,24,24	0
56	MG	QX	101	1/1	0.93	0.28	76,76,76,76	0
56	MG	YA	3312	1/1	0.93	0.23	44,44,44,44	0
56	MG	YA	3015	1/1	0.94	0.20	31,31,31,31	0
56	MG	YA	3184	1/1	0.94	0.09	36,36,36,36	0
56	MG	YA	3101	1/1	0.94	0.10	10,10,10,10	0
56	MG	YA	3067	1/1	0.94	0.20	23,23,23,23	0
56	MG	YA	3289	1/1	0.94	0.23	39,39,39,39	0
56	MG	RA	3205	1/1	0.94	0.23	53,53,53,53	0
56	MG	YA	3018	1/1	0.94	0.14	21,21,21,21	0
56	MG	YA	3332	1/1	0.94	0.10	42,42,42,42	0
56	MG	YA	3247	1/1	0.94	0.18	30,30,30,30	0
56	MG	XA	1615	1/1	0.94	0.29	36,36,36,36	0
56	MG	YA	3249	1/1	0.94	0.12	46,46,46,46	0
56	MG	YA	3251	1/1	0.94	0.26	18,18,18,18	0
56	MG	RA	3078	1/1	0.94	0.17	47,47,47,47	0
56	MG	YA	3110	1/1	0.94	0.11	29,29,29,29	0
56	MG	YA	3256	1/1	0.94	0.50	48,48,48,48	0
56	MG	RA	3069	1/1	0.94	0.15	37,37,37,37	0
56	MG	RA	3086	1/1	0.94	0.19	21,21,21,21	0
56	MG	RA	3234	1/1	0.94	0.46	65,65,65,65	0
56	MG	YA	3304	1/1	0.94	0.23	37,37,37,37	0
56	MG	RE	303	1/1	0.94	0.12	29,29,29,29	0
56	MG	YA	3002	1/1	0.94	0.17	20,20,20,20	0
56	MG	YA	3084	1/1	0.94	0.10	9,9,9,9	0
56	MG	YA	3004	1/1	0.94	0.09	9,9,9,9	0
56	MG	YA	3309	1/1	0.94	0.23	43,43,43,43	0
56	MG	YA	3121	1/1	0.94	0.07	11,11,11,11	0
56	MG	YA	3034	1/1	0.94	0.27	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	QA	1627	1/1	0.94	0.05	34,34,34,34	0
56	MG	YA	3270	1/1	0.94	0.13	22,22,22,22	0
56	MG	YA	3124	1/1	0.94	0.24	50,50,50,50	0
56	MG	RA	3071	1/1	0.94	0.20	37,37,37,37	0
56	MG	YA	3275	1/1	0.94	0.32	49,49,49,49	0
56	MG	RA	3167	1/1	0.94	0.20	62,62,62,62	0
56	MG	YA	3277	1/1	0.94	0.26	31,31,31,31	0
56	MG	YA	3062	1/1	0.94	0.18	28,28,28,28	0
56	MG	YA	3092	1/1	0.94	0.07	23,23,23,23	0
56	MG	YR	201	1/1	0.94	0.11	28,28,28,28	0
56	MG	YA	3322	1/1	0.94	0.14	35,35,35,35	0
56	MG	YA	3208	1/1	0.94	0.13	48,48,48,48	0
56	MG	RA	3068	1/1	0.94	0.17	40,40,40,40	0
56	MG	YA	3287	1/1	0.95	0.04	9,9,9,9	0
56	MG	RA	3030	1/1	0.95	0.16	30,30,30,30	0
56	MG	RA	3014	1/1	0.95	0.44	63,63,63,63	0
56	MG	RE	302	1/1	0.95	0.18	37,37,37,37	0
56	MG	RA	3056	1/1	0.95	0.08	32,32,32,32	0
56	MG	YA	3149	1/1	0.95	0.14	36,36,36,36	0
56	MG	YA	3017	1/1	0.95	0.08	16,16,16,16	0
56	MG	RA	3091	1/1	0.95	0.15	27,27,27,27	0
56	MG	YA	3253	1/1	0.95	0.12	9,9,9,9	0
56	MG	YA	3119	1/1	0.95	0.24	33,33,33,33	0
56	MG	YA	3078	1/1	0.95	0.22	31,31,31,31	0
56	MG	Y2	101	1/1	0.95	0.16	57,57,57,57	0
56	MG	YA	3020	1/1	0.95	0.14	12,12,12,12	0
56	MG	YA	3221	1/1	0.95	0.13	33,33,33,33	0
56	MG	YA	3021	1/1	0.95	0.14	11,11,11,11	0
56	MG	YA	3023	1/1	0.95	0.15	26,26,26,26	0
56	MG	Y5	101	1/1	0.95	0.09	36,36,36,36	0
56	MG	RA	3115	1/1	0.95	0.07	21,21,21,21	0
56	MG	RA	3241	1/1	0.95	0.07	33,33,33,33	0
56	MG	YA	3056	1/1	0.95	0.07	10,10,10,10	0
56	MG	RA	3108	1/1	0.95	0.13	47,47,47,47	0
56	MG	XA	1616	1/1	0.95	0.22	34,34,34,34	0
56	MG	YA	3093	1/1	0.95	0.10	13,13,13,13	0
56	MG	YA	3272	1/1	0.95	0.15	26,26,26,26	0
56	MG	RA	3117	1/1	0.95	0.05	20,20,20,20	0
56	MG	YA	3274	1/1	0.95	0.06	24,24,24,24	0
56	MG	XA	1645	1/1	0.95	0.11	37,37,37,37	0
56	MG	RA	3081	1/1	0.95	0.25	34,34,34,34	0
56	MG	YA	3064	1/1	0.95	0.17	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3137	1/1	0.95	0.09	31,31,31,31	0
56	MG	RA	3128	1/1	0.95	0.09	38,38,38,38	0
56	MG	YA	3280	1/1	0.95	0.19	31,31,31,31	0
56	MG	YA	3104	1/1	0.95	0.17	18,18,18,18	0
56	MG	YA	3066	1/1	0.95	0.07	26,26,26,26	0
56	MG	YA	3008	1/1	0.95	0.14	11,11,11,11	0
56	MG	YA	3068	1/1	0.95	0.07	22,22,22,22	0
56	MG	QA	1673	1/1	0.95	0.32	62,62,62,62	0
56	MG	XA	1603	1/1	0.96	0.25	41,41,41,41	0
56	MG	RA	3255	1/1	0.96	0.10	48,48,48,48	0
56	MG	YA	3244	1/1	0.96	0.17	56,56,56,56	0
56	MG	RA	3005	1/1	0.96	0.31	60,60,60,60	0
56	MG	YA	3077	1/1	0.96	0.18	12,12,12,12	0
56	MG	YA	3054	1/1	0.96	0.09	9,9,9,9	0
56	MG	YA	3009	1/1	0.96	0.11	21,21,21,21	0
56	MG	YA	3080	1/1	0.96	0.11	17,17,17,17	0
56	MG	RA	3064	1/1	0.96	0.29	17,17,17,17	0
56	MG	YA	3083	1/1	0.96	0.14	19,19,19,19	0
56	MG	QA	1664	1/1	0.96	0.12	43,43,43,43	0
56	MG	RA	3272	1/1	0.96	0.06	48,48,48,48	0
56	MG	YA	3086	1/1	0.96	0.17	30,30,30,30	0
56	MG	RA	3105	1/1	0.96	0.12	22,22,22,22	0
56	MG	RA	3106	1/1	0.96	0.11	22,22,22,22	0
56	MG	YA	3174	1/1	0.96	0.11	16,16,16,16	0
56	MG	RA	3026	1/1	0.96	0.14	42,42,42,42	0
56	MG	YA	3292	1/1	0.96	0.21	40,40,40,40	0
56	MG	RA	3033	1/1	0.96	0.14	28,28,28,28	0
56	MG	YE	303	1/1	0.96	0.08	15,15,15,15	0
56	MG	YN	201	1/1	0.96	0.15	32,32,32,32	0
56	MG	RA	3004	1/1	0.96	0.11	34,34,34,34	0
56	MG	RA	3157	1/1	0.96	0.17	38,38,38,38	0
56	MG	RA	3019	1/1	0.96	0.12	29,29,29,29	0
56	MG	YA	3266	1/1	0.96	0.12	26,26,26,26	0
56	MG	RA	3280	1/1	0.96	0.07	35,35,35,35	0
56	MG	YA	3024	1/1	0.96	0.12	14,14,14,14	0
56	MG	YA	3100	1/1	0.96	0.13	9,9,9,9	0
56	MG	RA	3281	1/1	0.96	0.29	146,146,146,146	0
56	MG	RA	3230	1/1	0.96	0.17	9,9,9,9	0
56	MG	YA	3049	1/1	0.96	0.14	15,15,15,15	0
59	ZN	QN	101	1/1	0.96	0.10	182,182,182,182	0
56	MG	YA	3005	1/1	0.97	0.07	9,9,9,9	0
56	MG	YA	3006	1/1	0.97	0.08	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	RA	3008	1/1	0.97	0.21	31,31,31,31	0
56	MG	YA	3250	1/1	0.97	0.26	28,28,28,28	0
56	MG	XA	1672	1/1	0.97	0.21	39,39,39,39	0
56	MG	RA	3096	1/1	0.97	0.19	23,23,23,23	0
56	MG	XA	1604	1/1	0.97	0.29	31,31,31,31	0
56	MG	YA	3254	1/1	0.97	0.14	17,17,17,17	0
56	MG	XA	1622	1/1	0.97	0.06	34,34,34,34	0
56	MG	YA	3295	1/1	0.97	0.23	31,31,31,31	0
56	MG	YA	3097	1/1	0.97	0.12	34,34,34,34	0
56	MG	RA	3047	1/1	0.97	0.11	24,24,24,24	0
56	MG	YA	3258	1/1	0.97	0.10	20,20,20,20	0
56	MG	YA	3099	1/1	0.97	0.13	11,11,11,11	0
56	MG	YA	3223	1/1	0.97	0.04	9,9,9,9	0
56	MG	YA	3224	1/1	0.97	0.07	9,9,9,9	0
56	MG	YA	3014	1/1	0.97	0.20	9,9,9,9	0
56	MG	YA	3042	1/1	0.97	0.13	9,9,9,9	0
56	MG	YA	3345	1/1	0.97	0.29	47,47,47,47	0
56	MG	RA	3098	1/1	0.97	0.07	16,16,16,16	0
56	MG	YA	3194	1/1	0.97	0.13	39,39,39,39	0
56	MG	YA	3134	1/1	0.97	0.10	10,10,10,10	0
56	MG	YA	3267	1/1	0.97	0.11	9,9,9,9	0
56	MG	RA	3017	1/1	0.97	0.11	17,17,17,17	0
56	MG	XA	1609	1/1	0.97	0.21	30,30,30,30	0
56	MG	Y1	101	1/1	0.97	0.09	49,49,49,49	0
56	MG	RA	3049	1/1	0.97	0.06	9,9,9,9	0
56	MG	YA	3108	1/1	0.97	0.06	9,9,9,9	0
56	MG	YE	302	1/1	0.97	0.10	9,9,9,9	0
56	MG	RA	3075	1/1	0.97	0.10	24,24,24,24	0
56	MG	XA	1612	1/1	0.97	0.08	20,20,20,20	0
56	MG	YA	3142	1/1	0.97	0.09	18,18,18,18	0
56	MG	RA	3027	1/1	0.97	0.12	21,21,21,21	0
56	MG	RA	3175	1/1	0.97	0.08	26,26,26,26	0
56	MG	RA	3243	1/1	0.97	0.04	31,31,31,31	0
56	MG	QA	1622	1/1	0.97	0.11	41,41,41,41	0
56	MG	YA	3028	1/1	0.97	0.05	9,9,9,9	0
56	MG	YA	3281	1/1	0.97	0.17	27,27,27,27	0
56	MG	RA	3039	1/1	0.97	0.05	9,9,9,9	0
56	MG	YA	3210	1/1	0.97	0.06	51,51,51,51	0
56	MG	YA	3003	1/1	0.97	0.10	9,9,9,9	0
58	SF4	QD	501	8/8	0.97	0.07	67,82,98,141	0
56	MG	RA	3270	1/1	0.97	0.10	25,25,25,25	0
59	ZN	Y9	102	1/1	0.97	0.04	59,59,59,59	0

Continued on next page...

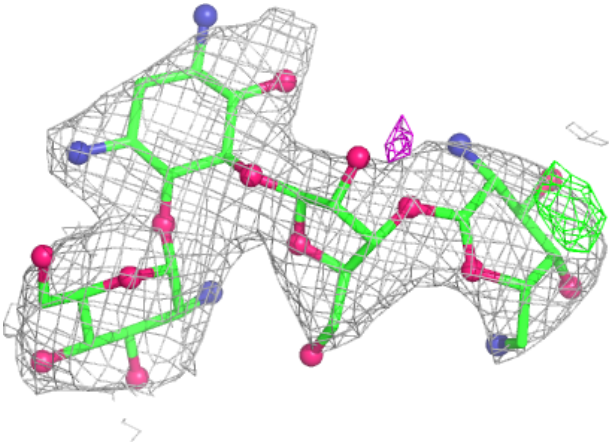
Continued from previous page...

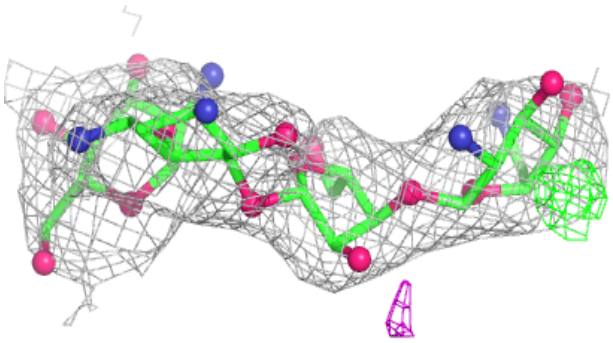
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	YA	3314	1/1	0.98	0.26	51,51,51,51	0
56	MG	RA	3052	1/1	0.98	0.04	15,15,15,15	0
56	MG	RA	3059	1/1	0.98	0.04	22,22,22,22	0
56	MG	RA	3137	1/1	0.98	0.15	13,13,13,13	0
56	MG	YA	3082	1/1	0.98	0.12	12,12,12,12	0
56	MG	YA	3040	1/1	0.98	0.06	9,9,9,9	0
56	MG	YA	3053	1/1	0.98	0.05	9,9,9,9	0
56	MG	RA	3038	1/1	0.98	0.08	15,15,15,15	0
56	MG	RA	3240	1/1	0.98	0.10	23,23,23,23	0
56	MG	RE	304	1/1	0.98	0.20	37,37,37,37	0
56	MG	YA	3105	1/1	0.98	0.04	9,9,9,9	0
56	MG	RA	3144	1/1	0.98	0.18	16,16,16,16	0
56	MG	YA	3058	1/1	0.98	0.35	38,38,38,38	0
56	MG	QM	201	1/1	0.98	0.04	61,61,61,61	0
56	MG	YA	3022	1/1	0.98	0.11	9,9,9,9	0
56	MG	XV	102	1/1	0.98	0.11	24,24,24,24	0
56	MG	XA	1605	1/1	0.98	0.29	39,39,39,39	0
58	SF4	XD	501	8/8	0.98	0.06	59,74,81,83	0
56	MG	YA	3094	1/1	0.98	0.08	9,9,9,9	0
59	ZN	R9	102	1/1	0.98	0.04	97,97,97,97	0
59	ZN	XN	101	1/1	0.98	0.07	97,97,97,97	0
56	MG	YA	3095	1/1	0.98	0.07	11,11,11,11	0
56	MG	YA	3059	1/1	0.99	0.05	9,9,9,9	0
56	MG	YA	3115	1/1	0.99	0.07	9,9,9,9	0
56	MG	YA	3074	1/1	0.99	0.16	16,16,16,16	0
56	MG	RA	3043	1/1	0.99	0.06	11,11,11,11	0
56	MG	RA	3050	1/1	0.99	0.04	14,14,14,14	0
56	MG	RA	3066	1/1	0.99	0.04	9,9,9,9	0
56	MG	YA	3011	1/1	0.99	0.05	9,9,9,9	0
56	MG	YA	3027	1/1	0.99	0.23	9,9,9,9	0
56	MG	YA	3112	1/1	0.99	0.03	11,11,11,11	0
56	MG	RA	3037	1/1	0.99	0.04	9,9,9,9	0

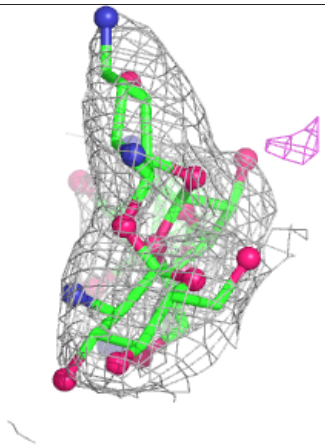
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR XA 1670:

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

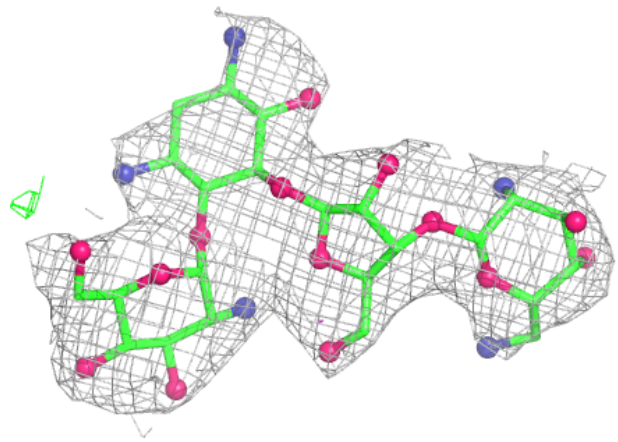


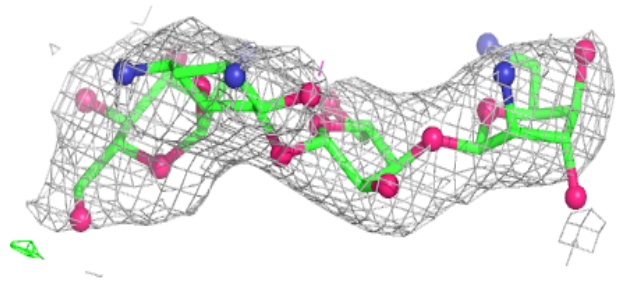


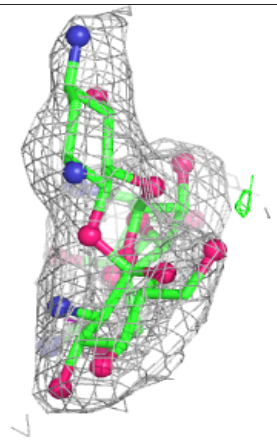


Electron density around PAR QA 1663:

$2mF_o$-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.